Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Position	Bit Substructure
P30939	662	O-C-C-O-C
P30939	864	CC1C(Cl)CCC1
P30939	474	S:C:C:N
P30939	427	C(#C)(-C)
P30939	27	>= 2 Na
P30939	343	C(~C)(~Cl)(~H)
P30939	616	C:C:N:N:C
P30939	651	O-C:C:C-C
P30939	176	>= 5 unsaturated non-aromatic nitrogen-containing ring s
P30939	266	Li-C
P30939	159	>= 3 saturated or aromatic nitrogen-containing ring size :
P30939	371	C(~H)(:C)(:C)
P30939	744	Oc1cc(Br)ccc1
P30939	456	P(-O)(=O)
P30939	575	O-C-C:C-O
P30939	829	SC1C(S)CCCC1
P30939	666	C=C-C-O-C
P30939	657	C-N-C:C-C
P30939	17	>= 8 N
P30939	204	>= 4 unsaturated non-aromatic nitrogen-containing ring s
P30939	844	CC1CC(Br)CC1
P30939	411	P(~O)(~O)
P30939	195	>= 3 saturated or aromatic heteroatom-containing ring si
P30939	777	CC1CCC(O)CC1
P30939	429	C(#N)(-C)
P30939	36	>= 8 S
P30939	678	C-C-C=C-C
P30939	871	SC1C(S)CCC1
P30939	8	>= 4 B
P30939	313	O-Si
P30939	211	>= 5 unsaturated non-aromatic nitrogen-containing ring s
P30939	60	>= 1 Ni
P30939	80	>= 1 Sn
P30939	851	SC1CC(N)CC1
P30939	136	>= 2 any ring size 4
P30939	359	C(~C)(:N)(:N)
P30939	123	>= 2 saturated or aromatic carbon-only ring size 3
P30939	661	O-C-O-C-C
P30939	612	N-C-O-C-C
P30939	336	C(~C)(~C)(~C)(~N)
P30939	153	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	563	O-C-O-C
P30939	811	SC1CC(Br)CCC1
P30939	319	Al-Cl
P30939	628	C-N-C-C:C
P30939	168	>= 4 unsaturated non-aromatic carbon-only ring size 5

P30939	436	C(-C)(-H)(=O)
P30939	132	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	495	C-N-C:C
P30939	111	>= 1 Tm
P30939	139	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	326	As-As
P30939	53	>= 1 Sc
P30939	750	Nc1cc(Cl)ccc1
P30939	700	O-C-C-C-C-C-O-C
P30939	90	>= 1 Re
P30939	818	CC1C(C)CCCC1
P30939	215	>= 1 saturated or aromatic nitrogen-containing ring size
P30939	803	OC1CC(O)CCC1
P30939	296	C-Se
P30939	793	NC1CCC(Br)CC1
P30939	764	Oc1c(Cl)cccc1
P30939	440	C(-C)(-O)(=O)
P30939	528	[#1]-N-C-[#1]
P30939	784	OC1CCC(N)CC1
P30939	238	>= 2 unsaturated non-aromatic carbon-only ring size 8
P30939	378	C(~N)(:C)(:N)
P30939	602	O=C-C-N-C
P30939	396	N(~C)(:C)
P30939	579	O=C-C-C-C
P30939	484	N-C:N:C
P30939	425	P=O
P30939	29	>= 2 Si
P30939	165	>= 4 saturated or aromatic carbon-only ring size 5
P30939	230	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	272	B-H
P30939	81	>= 1 Sb
P30939	87	>= 1 Hf
P30939	574	O-C-C:C-C
P30939	185	>= 2 any ring size 6
P30939	620	C:C-O-C-C
P30939	854	NC1CC(N)CC1
P30939	835	NC1C(Br)CCCC1
P30939	638	O-C-C-C-N
P30939	39	>= 4 Cl
P30939	507	C-C-S-C
P30939	18	>= 1 O
P30939	591	Cl-C-C-C-C
P30939	395	N(~C)(~O)
P30939	626	C-O-C:C-C
P30939	302	N-F
P30939	688	C-C-C-C-C-C-C
P30939	102	>= 1 Nd
P30939	441	C(-C)(=C)

P30939	351	C(~C)(~N)
P30939	724	Sc1ccc(S)cc1
P30939	845	OC1CC(O)CC1
P30939	214	>= 1 saturated or aromatic carbon-only ring size 7
P30939	647	O=C-N-C-N
P30939	621	N-C:C:C:N
P30939	870	OC1C(Br)CCC1
P30939	856	NC1CC(Br)CC1
P30939	611	N-C-C-N-C
P30939	737	Cc1cc(N)ccc1
P30939	79	>= 1 In
P30939	812	NC1CC(N)CCC1
P30939	606	O-C:C-C-C
P30939	779	CC1CCC(N)CC1
P30939	673	O=C-C=C-N
P30939	389	C(:N)(:N)
P30939	263	Li-H
P30939	571	[#1]-C-O-[#1]
P30939	780	CC1CCC(Cl)CC1
P30939	791	NC1CCC(N)CC1
P30939	428	C(#C)(-H)
P30939	220	>= 2 any ring size 7
P30939	437	C(-C)(-N)(=C)
P30939	399	N(~H)(:C)
P30939	852	SC1CC(Cl)CC1
P30939	19	>= 2 O
P30939	357	C(~C)(:C)(:N)
P30939	801	CC1CC(Cl)CCC1
P30939	822	CC1C(Cl)CCCC1
P30939	6	>= 1 B
P30939	367	C(~H)(~O)(~O)
P30939	828	OC1C(Br)CCCC1
P30939	316	F-P
P30939	530	N:C-C:C
P30939	623	O=C-C:C-C
P30939	540	C-N-C-[#1]
P30939	813	NC1CC(Cl)CCC1
P30939	82	>= 1 Te
P30939	682	O-C-C-C-C-N
P30939	549	N-C-C:C
P30939	289	C-Mg
P30939	97	>= 1 Pb
P30939	807	OC1CC(Br)CCC1
P30939	449	C(-N)(=C)
P30939	329	C(~Br)(~H)
P30939	144	>= 1 saturated or aromatic carbon-only ring size 5
P30939	201	>= 4 saturated or aromatic nitrogen-containing ring size 6
P30939	500	C-S-C:C

P30939	705	O=C-C-C-C-C(O)-C
P30939	409	O(:C)(:C)
P30939	600	N-C:C:C-C
P30939	344	C(~C)(~H)
P30939	878	ClC1C(Cl)CCC1
P30939	583	Cl-C:C-O-C
P30939	635	N-N-C-N-[#1]
P30939	821	CC1C(N)CCCC1
P30939	38	>= 2 Cl
P30939	546	N-C:C-[#1]
P30939	120	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	235	>= 2 saturated or aromatic carbon-only ring size 8
P30939	770	Nc1c(N)cccc1
P30939	347	C(~C)(~H)(~O)(~O)
P30939	5	>= 2 Li
P30939	321	Si-Si
P30939	368	C(~H)(~S)
P30939	181	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	381	C(~O)(:C)
P30939	695	O=C-C-C-C-C-N
P30939	679	C-C-C-C-C-C
P30939	417	C#C
P30939	406	O(~C)(~H)
P30939	125	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	309	O-O
P30939	716	Cc1ccc(N)cc1
P30939	806	OC1CC(Cl)CCC1
P30939	305	N-S
P30939	273	B-B
P30939	696	C-C-C-C-C-C-C-C
P30939	375	C(~N)(~N)
P30939	58	>= 1 Fe
P30939	645	O=C-N-C-C
P30939	267	Li-O
P30939	366	C(~H)(~O)
P30939	862	CC1C(S)CCC1
P30939	814	NC1CC(Br)CCC1
P30939	174	>= 5 saturated or aromatic heteroatom-containing ring si
P30939	383	C(~S)(:C)
P30939	391	N(~C)(~C)(~C)
P30939	782	OC1CCC(O)CC1
P30939	138	>= 2 saturated or aromatic nitrogen-containing ring size 4
P30939	880	BrC1C(Br)CCC1
P30939	354	C(~C)(~Si)
P30939	625	O=C-C:C-O
P30939	101	>= 1 Pr
P30939	393	N(~C)(~H)
P30939	550	Cl-C-C-C

P30939	34	>= 2 S
P30939	772	Nc1c(Br)cccc1
P30939	632	C-C-O-C:C
P30939	216	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	689	O-C-C-C-C-C-C
P30939	861	CC1C(O)CCC1
P30939	739	Cc1cc(Br)ccc1
P30939	124	>= 2 saturated or aromatic nitrogen-containing ring size
P30939	432	C(-C)(-C)(=O)
P30939	481	O-S-C:C
P30939	580	O=C-C-C-N
P30939	472	C:N:C-C
P30939	465	O=S-C-C
P30939	213	>= 1 any ring size 7
P30939	509	Br-C:C-C
P30939	526	Cl-C:C-Cl
P30939	325	As-H
P30939	37	>= 1 Cl
P30939	387	C(:C)(:N)
P30939	112	>= 1 Yb
P30939	374	C(~H)(~H)(~H)
P30939	278	B-Si
P30939	295	C-As
P30939	826	OC1C(N)CCCC1
P30939	769	Sc1c(Br)cccc1
P30939	455	N(-O)(=O)
P30939	233	>= 1 unsaturated non-aromatic heteroatom-containing ri
P30939	592	N-C-C-C-C
P30939	512	C-[As]-O-[#1]
P30939	189	>= 2 unsaturated non-aromatic carbon-only ring size 6
P30939	400	N(~H)(:C)(:C)
P30939	340	C(~C)(~C)(~N)
P30939	262	>= 4 hetero-aromatic rings
P30939	364	C(~F)(:C)
P30939	560	N-C-N-C
P30939	337	C(~C)(~C)(~C)(~O)
P30939	790	SC1CCC(Br)CC1
P30939	719	Oc1ccc(O)cc1
P30939	431	C(-C)(-C)(=N)
P30939	397	N(~C)(:C)(:C)
P30939	352	C(~C)(~O)
P30939	369	C(~H)(~Si)
P30939	728	Nc1ccc(N)cc1
P30939	714	Cc1ccc(O)cc1
P30939	461	O-C-C=N
P30939	831	SC1C(Cl)CCCC1
P30939	339	C(~C)(~C)(~H)(~O)
P30939	353	C(~C)(~S)

P30939	182	>= 1 unsaturated non-aromatic carbon-only ring size 6
P30939	167	>= 4 saturated or aromatic heteroatom-containing ring si
P30939	576	N=C-C:C-[#1]
P30939	173	>= 5 saturated or aromatic nitrogen-containing ring size :
P30939	487	N-C=N-C
P30939	485	N:C:C:N
P30939	223	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	617	C-C-C-O-[#1]
P30939	521	C:N-C-[#1]
P30939	732	Clc1ccc(Br)cc1
P30939	738	Cc1cc(Cl)ccc1
P30939	736	Cc1cc(S)ccc1
P30939	523	N:C:C-C
P30939	468	O=S-C-N
P30939	188	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	570	C:C-C-C
P30939	636	C-N-C-N-C
P30939	710	C-C-C(C)-C-C
P30939	503	Cl-C:C-[#1]
P30939	690	O-C-C-C-C-C-O
P30939	511	S=C-N-[#1]
P30939	253	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	83	>= 1 Xe
P30939	147	>= 1 unsaturated non-aromatic carbon-only ring size 5
P30939	722	Oc1ccc(Cl)cc1
P30939	105	>= 1 Eu
P30939	754	Brc1cc(Br)ccc1
P30939	701	O-C-C-C-C-C(O)-C
P30939	249	>= 1 saturated or aromatic carbon-only ring size 10
P30939	63	>= 1 Ga
P30939	246	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	797	CC1CC(C)CCC1
P30939	388	C(:C)(:N)(:N)
P30939	49	>= 1 Be
P30939	231	>= 1 unsaturated non-aromatic carbon-only ring size 8
P30939	650	O=C-N-C=O
P30939	108	>= 1 Dy
P30939	1	>= 8 H
P30939	561	Cl-C-C=O
P30939	119	>= 1 unsaturated non-aromatic carbon-only ring size 3
P30939	275	B-N
P30939	11	>= 8 C
P30939	778	CC1CCC(S)CC1
P30939	843	CC1CC(Cl)CC1
P30939	875	NC1C(N)CCC1
P30939	304	N-P
P30939	476	C-O-C=C
P30939	283	C-H

P30939	324	P-P
P30939	77	>= 1 Ag
P30939	35	>= 4 S
P30939	179	>= 1 saturated or aromatic carbon-only ring size 6
P30939	810	SC1CC(Cl)CCC1
P30939	197	>= 3 unsaturated non-aromatic nitrogen-containing ring s
P30939	506	C-C:N:C
P30939	205	>= 4 unsaturated non-aromatic heteroatom-containing rir
P30939	76	>= 1 Pd
P30939	876	NC1C(Cl)CC1
P30939	131	>= 1 saturated or aromatic nitrogen-containing ring size 4
P30939	7	>= 2 B
P30939	192	>= 3 any ring size 6
P30939	21	>= 8 O
P30939	518	O=C-N-N
P30939	362	C(~Cl)(:C)
P30939	143	>= 1 any ring size 5
P30939	28	>= 1 Si
P30939	660	C-C=C-C-C
P30939	505	Cl-C:C-O
P30939	285	C-N
P30939	355	C(~C)(:C)
P30939	52	>= 1 Ca
P30939	720	Oc1ccc(S)cc1
P30939	479	S-C-S-C
P30939	50	>= 1 Mg
P30939	386	C(:C)(:C)(:N)
P30939	88	>= 1 Ta
P30939	572	N:C:N:C
P30939	815	ClC1CC(Cl)CCC1
P30939	805	OC1CC(N)CCC1
P30939	473	S-C:N:C
P30939	164	>= 4 any ring size 5
P30939	452	C(-O)(=O)
P30939	687	O=C-C-C-C=O
P30939	588	O=C-C-C=O
P30939	464	N-C-C=C
P30939	717	Cc1ccc(Cl)cc1
P30939	763	Oc1c(N)cccc1
P30939	327	C(~Br)(~C)
P30939	186	>= 2 saturated or aromatic carbon-only ring size 6
P30939	729	Nc1ccc(Cl)cc1
P30939	306	N-Cl
P30939	516	[#1]-C=C-[#1]
P30939	67	>= 1 Kr
P30939	281	B-Cl
P30939	749	Nc1cc(N)ccc1
P30939	482	C:N-C:C

P30939	488	N-C=N-[#1]
P30939	55	>= 1 V
P30939	491	C-N:C-[#1]
P30939	543	O-C:C-N
P30939	554	Br-C-C-C
P30939	788	SC1CCC(N)CC1
P30939	847	OC1CC(N)CC1
P30939	46	>= 1 I
P30939	430	C(-C)(-C)(=C)
P30939	639	O-C-C-C-O
P30939	358	C(~C)(:N)
P30939	837	ClC1C(Br)CCCC1
P30939	311	O-Na
P30939	103	>= 1 Pm
P30939	293	C-S
P30939	527	C:C:N-[#1]
P30939	163	>= 3 unsaturated non-aromatic heteroatom-containing rir
P30939	499	N-C:C:N
P30939	301	N-O
P30939	796	BrC1CCC(Br)CC1
P30939	496	N:N-C-[#1]
P30939	874	SC1C(Br)CCC1
P30939	48	>= 4 I
P30939	735	Cc1cc(O)ccc1
P30939	564	C=C-C=C
P30939	691	O-C-C-C-C-C-N
P30939	740	Oc1cc(O)ccc1
P30939	531	S-C:C-C
P30939	356	C(~C)(:C)(:C)
P30939	338	C(~C)(~C)(~H)(~N)
P30939	15	>= 2 N
P30939	69	>= 1 Sr
P30939	577	C:C-N-C:C
P30939	817	BrC1CC(Br)CCC1
P30939	601	N-C:C:C-N
P30939	284	C-C
P30939	24	>= 2 F
P30939	727	Sc1ccc(Br)cc1
P30939	298	C-I
P30939	675	Br-C-C-C:C
P30939	134	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	715	Cc1ccc(S)cc1
P30939	264	Li-Li
P30939	61	>= 1 Cu
P30939	424	N=P
P30939	680	O-C-C-C-C-C
P30939	659	O-C-C-N-C
P30939	493	O=C-C:C

P30939	450	C(-N)(=N)
P30939	85	>= 1 Ba
P30939	492	N-C:O:C
P30939	30	>= 1 P
P30939	25	>= 4 F
P30939	562	Br-C-C=O
P30939	566	O-C-C-N
P30939	422	N=N
P30939	286	C-O
P30939	255	>= 1 aromatic ring
P30939	879	ClC1C(Br)CCC1
P30939	95	>= 1 Hg
P30939	398	N(~H)(~N)
P30939	314	O-P
P30939	454	N(-C)(=O)
P30939	109	>= 1 Ho
P30939	401	N(~O)(~O)
P30939	839	CC1CC(C)CC1
P30939	68	>= 1 Rb
P30939	459	S(=O)(=O)
P30939	471	S:C:C:C
P30939	229	>= 1 saturated or aromatic nitrogen-containing ring size 8
P30939	137	>= 2 saturated or aromatic carbon-only ring size 4
P30939	548	O-C-C:C
P30939	226	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	379	C(~N)(:N)
P30939	702	O-C-C-C-C-C-N-C
P30939	129	>= 1 any ring size 4
P30939	649	O=N-C:C-O
P30939	460	C-C-C#C
P30939	846	OC1CC(S)CC1
P30939	457	S(-C)(=O)
P30939	515	N-N-C-C
P30939	261	>= 4 aromatic rings
P30939	501	Cl-C:C-C
P30939	860	CC1C(C)CCC1
P30939	288	C-Na
P30939	290	C-Al
P30939	270	Li-S
P30939	170	>= 4 unsaturated non-aromatic heteroatom-containing rir
P30939	157	>= 3 any ring size 5
P30939	218	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	221	>= 2 saturated or aromatic carbon-only ring size 7
P30939	130	>= 1 saturated or aromatic carbon-only ring size 4
P30939	158	>= 3 saturated or aromatic carbon-only ring size 5
P30939	741	Oc1cc(S)ccc1
P30939	534	S-C:C-O
P30939	470	C:C-C=C

P30939	135	>= 1 unsaturated non-aromatic heteroatom-containing rir
P30939	93	>= 1 Pt
P30939	610	C-O-C-O-C
P30939	31	>= 2 P
P30939	292	C-P
P30939	57	>= 1 Mn
P30939	104	>= 1 Sm
P30939	162	>= 3 unsaturated non-aromatic nitrogen-containing ring s
P30939	207	>= 5 saturated or aromatic carbon-only ring size 6
P30939	161	>= 3 unsaturated non-aromatic carbon-only ring size 5
P30939	276	B-O
P30939	279	B-P
P30939	242	>= 1 saturated or aromatic carbon-only ring size 9
P30939	228	>= 1 saturated or aromatic carbon-only ring size 8
P30939	240	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	827	OC1C(Cl)CCCC1
P30939	234	>= 2 any ring size 8
P30939	751	Nc1cc(Br)ccc1
P30939	469	S-S-C:C
P30939	41	>= 1 K
P30939	303	N-Si
P30939	868	OC1C(N)CCC1
P30939	663	O-C-C-O-[#1]
P30939	98	>= 1 Bi
P30939	730	Nc1ccc(Br)cc1
P30939	489	N-C-S-C
P30939	300	N-N
P30939	384	C(:C)(:C)
P30939	212	>= 5 unsaturated non-aromatic heteroatom-containing rir
P30939	415	Si(~C)(~C)
P30939	258	>= 2 hetero-aromatic rings
P30939	443	C(-C)(=O)
P30939	9	>= 2 C
P30939	257	>= 2 aromatic rings
P30939	307	N-Br
P30939	54	>= 1 Ti
P30939	613	C-N-C-C-C
P30939	245	>= 1 unsaturated non-aromatic carbon-only ring size 9
P30939	86	>= 1 Lu
P30939	156	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	486	N-C:N:N
P30939	256	>= 1 hetero-aromatic ring
P30939	322	Si-Cl
P30939	693	O=C-C-C-C-C-O
P30939	603	C-C:C:C-C
P30939	51	>= 1 Al
P30939	44	>= 2 Br
P30939	629	S-C:C:C-N

P30939	418	C=N
P30939	590	C-C:C-O-[#1]
P30939	674	N-C-N-C:C
P30939	804	OC1CC(S)CCC1
P30939	420	C=O
P30939	840	CC1CC(O)CC1
P30939	699	O-C-C-C-C-C(C)-C
P30939	553	O=C-C=C
P30939	435	C(-C)(-H)(=N)
P30939	148	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	522	C-N-N-[#1]
P30939	118	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	403	N(:C)(:C)
P30939	260	>= 3 hetero-aromatic rings
P30939	713	Cc1ccc(C)cc1
P30939	121	>= 1 unsaturated non-aromatic heteroatom-containing rir
P30939	849	OC1CC(Br)CC1
P30939	373	C(~H)(:N)
P30939	96	>= 1 Tl
P30939	219	>= 1 unsaturated non-aromatic heteroatom-containing rir
P30939	328	C(~Br)(~C)(~C)
P30939	154	>= 2 unsaturated non-aromatic carbon-only ring size 5
P30939	330	C(~Br)(:C)
P30939	490	C-C-C=C
P30939	151	>= 2 saturated or aromatic carbon-only ring size 5
P30939	834	NC1C(Cl)CCCC1
P30939	335	C(~C)(~C)(~C)(~H)
P30939	40	>= 8 Cl
P30939	544	O-C:C-O
P30939	775	Brc1c(Br)cccc1
P30939	377	C(~N)(:C)(:C)
P30939	568	N#C-C-C
P30939	711	C-C(C)(C)-C-C
P30939	513	S:C:C-[#1]
P30939	198	>= 3 unsaturated non-aromatic heteroatom-containing rir
P30939	107	>= 1 Tb
P30939	694	O=C-C-C-C-C=O
P30939	646	O=C-N-C-[#1]
P30939	533	S-C:C-N
P30939	608	C-C-C-C:C
P30939	832	SC1C(Br)CCCC1
P30939	405	O(~C)(~C)
P30939	480	C:S:C-C
P30939	113	>= 1 Tc
P30939	631	O-C:C-O-[#1]
P30939	413	S(~C)(~H)
P30939	539	N=C-C-[#1]
P30939	545	N-C:C-C

P30939	259	>= 3 aromatic rings
P30939	282	B-Br
P30939	798	CC1CC(O)CCC1
P30939	578	C-C:C-C:C
P30939	475	S-C=N-C
P30939	376	C(~N)(:C)
P30939	2	>= 16 H
P30939	820	CC1C(S)CCCC1
P30939	586	C-S-C-C-C
P30939	745	Sc1cc(S)ccc1
P30939	637	O-C-C-C-C
P30939	858	ClC1CC(Br)CC1
P30939	184	>= 1 unsaturated non-aromatic heteroatom-containing rir
P30939	573	O-C-C=C
P30939	742	Oc1cc(N)ccc1
P30939	463	N:C-S-[#1]
P30939	345	C(~C)(~H)(~N)
P30939	825	OC1C(S)CCCC1
P30939	785	OC1CCC(Cl)CC1
P30939	416	C=C
P30939	753	Clc1cc(Br)ccc1
P30939	833	NC1C(N)CCCC1
P30939	426	P=P
P30939	4	>= 1 Li
P30939	323	P-H
P30939	524	C-C=C-C
P30939	333	C(~C)(~C)(~C)
P30939	676	N#C-C-C-C
P30939	236	>= 2 saturated or aromatic nitrogen-containing ring size 8
P30939	116	>= 1 saturated or aromatic carbon-only ring size 3
P30939	84	>= 1 Cs
P30939	597	O=C-C-C:C
P30939	412	S(~C)(~C)
P30939	708	C-C(C)-C-C
P30939	792	NC1CCC(Cl)CC1
P30939	145	>= 1 saturated or aromatic nitrogen-containing ring size 3
P30939	664	C-C=C-C=C
P30939	175	>= 5 unsaturated non-aromatic carbon-only ring size 5
P30939	442	C(-C)(=N)
P30939	799	CC1CC(S)CCC1
P30939	10	>= 4 C
P30939	762	Oc1c(S)cccc1
P30939	532	S-C:C-[#1]
P30939	757	Cc1c(S)cccc1
P30939	502	N-C=C-[#1]
P30939	494	O=C-C:N
P30939	477	N-N-C:C
P30939	160	>= 3 saturated or aromatic heteroatom-containing ring si

P30939	334	C(~C)(~C)(~C)(~C)
P30939	640	C=C-C-C-C
P30939	686	O=C-C-C-C-O
P30939	447	C(-H)(=N)
P30939	199	>= 4 any ring size 6
P30939	172	>= 5 saturated or aromatic carbon-only ring size 5
P30939	193	>= 3 saturated or aromatic carbon-only ring size 6
P30939	142	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	684	O=C-C-C-C-C
P30939	243	>= 1 saturated or aromatic nitrogen-containing ring size 9
P30939	478	S-C=N-[#1]
P30939	106	>= 1 Gd
P30939	766	Sc1c(S)cccc1
P30939	71	>= 1 Zr
P30939	248	>= 1 any ring size 10
P30939	274	B-C
P30939	582	C-C-C-C-C
P30939	504	N:C:N-C
P30939	842	CC1CC(N)CC1
P30939	100	>= 1 Ce
P30939	146	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	171	>= 5 any ring size 5
P30939	194	>= 3 saturated or aromatic nitrogen-containing ring size 6
P30939	65	>= 1 As
P30939	331	C(~Br)(:N)
P30939	32	>= 4 P
P30939	794	ClC1CCC(Cl)CC1
P30939	407	O(~C)(~P)
P30939	203	>= 4 unsaturated non-aromatic carbon-only ring size 6
P30939	756	Cc1c(O)cccc1
P30939	767	Sc1c(N)cccc1
P30939	122	>= 2 any ring size 3
P30939	783	OC1CCC(S)CC1
P30939	747	Sc1cc(Cl)ccc1
P30939	451	C(-N)(=O)
P30939	349	C(~C)(~H)(~S)
P30939	62	>= 1 Zn
P30939	72	>= 1 Nb
P30939	648	O=N-C:C-N
P30939	133	>= 1 unsaturated non-aromatic carbon-only ring size 4
P30939	408	O(~H)(~S)
P30939	177	>= 5 unsaturated non-aromatic heteroatom-containing rir
P30939	795	ClC1CCC(Br)CC1
P30939	644	C-C=N-N-C
P30939	166	>= 4 saturated or aromatic nitrogen-containing ring size 3
P30939	557	N:C-O-[#1]
P30939	877	NC1C(Br)CCC1
P30939	317	F-S

P30939	853	SC1CC(Br)CC1
P30939	867	OC1C(S)CCC1
P30939	823	CC1C(Br)CCCC1
P30939	372	C(~H)(:C)(:N)
P30939	508	S=C-N-C
P30939	619	O-C-C=C-C
P30939	141	>= 2 unsaturated non-aromatic nitrogen-containing ring s
P30939	446	C(-H)(=C)
P30939	567	O-C-C-O
P30939	584	C:C-C=C-C
P30939	14	>= 1 N
P30939	152	>= 2 saturated or aromatic nitrogen-containing ring size :
P30939	618	C:C-C-C:C
P30939	733	Brc1ccc(Br)cc1
P30939	382	C(~O)(:C)(:C)
P30939	525	[As]-C:C-[#1]
P30939	605	O=C-C-O-C
P30939	115	>= 1 any ring size 3
P30939	819	CC1C(O)CCCC1
P30939	830	SC1C(N)CCCC1
P30939	42	>= 2 K
P30939	299	N-H
P30939	200	>= 4 saturated or aromatic carbon-only ring size 6
P30939	698	O-C-C-C-C-C-C-C
P30939	596	N=C-N-C-C
P30939	692	O=C-C-C-C-C-C
P30939	529	Cl-C-C-Cl
P30939	538	N=C-C-C
P30939	627	O=[As]-C:C:C
P30939	704	O=C-C-C-C-C-C-C
P30939	535	O=C-C-C
P30939	191	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	731	Clc1ccc(Cl)cc1
P30939	547	N-C:C-N
P30939	630	O-C:C-O-C
P30939	91	>= 1 Os
P30939	598	Cl-C:C:C-C
P30939	672	O=C-C=C-[#1]
P30939	587	N-C:C-O-[#1]
P30939	615	N-C-C-O-C
P30939	761	Oc1c(O)cccc1
P30939	20	>= 4 O
P30939	280	B-S
P30939	332	C(~C)(~C)
P30939	677	C-C=C-C:C
P30939	318	Al-H
P30939	556	C=C-C-C
P30939	149	>= 1 unsaturated non-aromatic heteroatom-containing rir

P30939	771	Nc1c(Cl)cccc1
P30939	537	O=C-C-O
P30939	269	Li-P
P30939	438	C(-C)(-N)(=N)
P30939	190	>= 2 unsaturated non-aromatic nitrogen-containing ring s
P30939	458	S(-O)(=O)
P30939	12	>= 16 C
P30939	402	N(~O)(:O)
P30939	726	Sc1ccc(Cl)cc1
P30939	685	O=C-C-C-C-N
P30939	671	O=C-C=C-C
P30939	655	O-C-C-C:C
P30939	251	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	150	>= 2 any ring size 5
P30939	78	>= 1 Cd
P30939	110	>= 1 Er
P30939	517	N-N-C-N
P30939	0	>= 4 H
P30939	56	>= 1 Cr
P30939	114	>= 1 U
P30939	609	Cl-C-C-N-C
P30939	836	ClC1C(Cl)CCCC1
P30939	809	SC1CC(N)CCC1
P30939	776	CC1CCC(C)CC1
P30939	209	>= 5 saturated or aromatic heteroatom-containing ring si
P30939	225	>= 2 unsaturated non-aromatic nitrogen-containing ring s
P30939	869	OC1C(Cl)CCC1
P30939	390	N(~C)(~C)
P30939	350	C(~C)(~I)
P30939	542	O-C:C-[#1]
P30939	593	N-C-C-C-N
P30939	187	>= 2 saturated or aromatic nitrogen-containing ring size (
P30939	394	N(~C)(~H)(~N)
P30939	848	OC1CC(Cl)CC1
P30939	703	O-C-C-C-C-C(N)-C
P30939	277	B-F
P30939	748	Sc1cc(Br)ccc1
P30939	363	C(~F)(~F)
P30939	26	>= 1 Na
P30939	419	C#N
P30939	773	Clc1c(Cl)cccc1
P30939	342	C(~C)(~Cl)
P30939	183	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	599	[#1]-C-C=C-[#1]
P30939	652	O-C:C:C-N
P30939	787	SC1CCC(S)CC1
P30939	287	C-F
P30939	155	>= 2 unsaturated non-aromatic nitrogen-containing ring s

P30939	73	>= 1 Mo
P30939	404	N(:C)(:C)(:C)
P30939	643	[#1]-C-C-N-[#1]
P30939	222	>= 2 saturated or aromatic nitrogen-containing ring size
P30939	348	C(~C)(~H)(~P)
P30939	196	>= 3 unsaturated non-aromatic carbon-only ring size 6
P30939	669	Cl-C:C-C=O
P30939	634	C-C-C:C-C
P30939	392	N(~C)(~C)(~H)
P30939	467	C=N-N-C
P30939	217	>= 1 unsaturated non-aromatic carbon-only ring size 7
P30939	127	>= 2 unsaturated non-aromatic nitrogen-containing ring s
P30939	768	Sc1c(Cl)cccc1
P30939	385	C(:C)(:C)(:C)
P30939	800	CC1CC(N)CCC1
P30939	667	C=C-C-O-[#1]
P30939	232	>= 1 unsaturated non-aromatic nitrogen-containing ring s
P30939	734	Cc1cc(C)ccc1
P30939	559	O-C-N-[#1]
P30939	94	>= 1 Au
P30939	725	Sc1ccc(N)cc1
P30939	294	C-Cl
P30939	180	>= 1 saturated or aromatic nitrogen-containing ring size
P30939	23	>= 1 F
P30939	789	SC1CCC(Cl)CC1
P30939	510	[#1]-N-N-[#1]
P30939	380	C(~O)(~O)
P30939	681	O-C-C-C-C-O
P30939	43	>= 1 Br
P30939	712	C-C(C)-C(C)-C
P30939	315	O-K
P30939	483	N-S-C:C
P30939	760	Cc1c(Br)cccc1
P30939	462	O-C-C=O
P30939	541	O-C:C-C
P30939	421	C=S
P30939	758	Cc1c(N)cccc1
P30939	746	Sc1cc(N)ccc1
P30939	551	Cl-C-C-O
P30939	16	>= 4 N
P30939	668	C-C:C-C-C
P30939	297	C-Br
P30939	565	C:C-O-C
P30939	140	>= 2 unsaturated non-aromatic carbon-only ring size 4
P30939	448	C(-H)(=O)
P30939	70	>= 1 Y
P30939	607	N-C-C-C:C
P30939	202	>= 4 saturated or aromatic heteroatom-containing ring si

P30939	92	>= 1 Ir
P30939	581	O=C-C-C-O
P30939	697	C-C-C-C-C-C(C)-C
P30939	423	N=O
P30939	589	C-C:C-O-C
P30939	265	Li-B
P30939	658	C-C-S-C-C
P30939	857	ClC1CC(Cl)CC1
P30939	850	SC1CC(S)CC1
P30939	365	C(~H)(~N)
P30939	126	>= 2 unsaturated non-aromatic carbon-only ring size 3
P30939	558	O=N-C:C
P30939	227	>= 1 any ring size 8
P30939	445	C(-H)(-N)(=C)
P30939	665	N-C:C-C-C
P30939	64	>= 1 Ge
P30939	653	O-C:C:C-O
P30939	752	Clc1cc(Cl)ccc1
P30939	66	>= 1 Se
P30939	755	Cc1c(C)cccc1
P30939	341	C(~C)(~C)(~O)
P30939	624	O=C-C:C-N
P30939	210	>= 5 unsaturated non-aromatic carbon-only ring size 6
P30939	595	C:C-C-C-C
P30939	519	N=C-N-C
P30939	743	Oc1cc(Cl)ccc1
P30939	802	CC1CC(Br)CCC1
P30939	444	C(-Cl)(=O)
P30939	13	>= 32 C
P30939	781	CC1CCC(Br)CC1
P30939	498	O-C=C-C
P30939	250	>= 1 saturated or aromatic nitrogen-containing ring size
P30939	604	C-O-C-C:C
P30939	721	Oc1ccc(N)cc1
P30939	718	Cc1ccc(Br)cc1
P30939	361	C(~Cl)(~H)
P30939	552	C:C-C:C
P30939	310	O-Mg
P30939	555	N=C-C=C
P30939	838	BrC1C(Br)CCCC1
P30939	536	O=C-C-N
P30939	117	>= 1 saturated or aromatic nitrogen-containing ring size
P30939	514	O-N-C-C
P30939	670	Br-C:C:C-C
P30939	268	Li-F
P30939	642	O-C-C-C=O
P30939	308	O-H
P30939	614	C-C-O-C-C

P30939	520	C=C-C:C
P30939	252	>= 1 unsaturated non-aromatic carbon-only ring size 10
P30939	656	C-C-N-C-C
P30939	466	N#C-C=C
P30939	312	O-Al
P30939	497	O-C:C:N
P30939	33	>= 1 S
P30939	414	S(~C)(~O)
P30939	128	>= 2 unsaturated non-aromatic heteroatom-containing rir
P30939	841	CC1CC(S)CC1
P30939	271	Li-Cl
P30939	855	NC1CC(Cl)CC1
P30939	178	>= 1 any ring size 6
P30939	759	Cc1c(Cl)cccc1
P30939	434	C(-C)(-H)(=C)
P30939	433	C(-C)(-Cl)(=O)
P30939	47	>= 2 I
P30939	244	>= 1 saturated or aromatic heteroatom-containing ring si
P30939	99	>= 1 La
P30939	206	>= 5 any ring size 6
P30939	706	O=C-C-C-C-C(=O)-C
P30939	816	ClC1CC(Br)CCC1
P30939	633	N-C-C:C-C
P30939	654	N-C-N-C-C
P30939	569	N-C-C-N
P30939	320	Si-H
P30939	439	C(-C)(-N)(=O)
P30939	370	C(~H)(:C)
P30939	410	P(~C)(~C)
P30939	89	>= 1 W
P30939	59	>= 1 Co
P30939	360	C(~Cl)(~Cl)
P30939	453	N(-C)(=C)
P30939	723	Oc1ccc(Br)cc1
P30939	859	BrC1CC(Br)CC1
P30939	237	>= 2 saturated or aromatic heteroatom-containing ring si
P30939	873	SC1C(Cl)CCC1
P30939	3	>= 32 H
P30939	346	C(~C)(~H)(~O)
P30939	808	SC1CC(S)CCC1
P30939	169	>= 4 unsaturated non-aromatic nitrogen-containing ring s
P30939	641	O-C-C-C=C
P30939	786	OC1CCC(Br)CC1
P30939	239	>= 2 unsaturated non-aromatic nitrogen-containing ring s
P30939	75	>= 1 Rh
P30939	865	CC1C(Br)CCC1
P30939	707	O=C-C-C-C-C(N)-C
P30939	247	>= 1 unsaturated non-aromatic heteroatom-containing rir

P30939	22	>= 16 O
P30939	872	SC1C(N)CCC1
P30939	45	>= 4 Br
P30939	224	>= 2 unsaturated non-aromatic carbon-only ring size 7
P30939	291	C-Si
P30939	622	O=C-O-C:C
P30939	863	CC1C(N)CCC1
P30939	774	Clc1c(Br)cccc1
P30939	709	C-C(C)-C-C-C
P30939	254	>= 1 unsaturated non-aromatic heteroatom-containing rir
P30939	208	>= 5 saturated or aromatic nitrogen-containing ring size (
P30939	585	C-C:C-N-C
P30939	74	>= 1 Ru
P30939	765	Oc1c(Br)cccc1
P30939	824	OC1C(O)CCCC1
P30939	683	N-C-C-C-C-C
P30939	866	OC1C(O)CCC1
P30939	594	C-O-C-C=C
P30939	241	>= 1 any ring size 9

Fingerprints（continued)

W	P	Q
2.4839171	2.483548147	0.000369
2.4056075	2.405607951	-4.07E-07
2.1695516	2.172356688	-0.002805
2.1637016	2.162950563	0.0007511
1.9997677	1.999768381	-7.29E-07
1.8516059	1.851605697	2.48E-07
1.7491585	1.749499747	-0.000341
1.7438973	1.743236969	0.0006603
1.6325208	1.632520723	8.32E-08
1.6235771	1.623576628	4.63E-07
1.590105	1.590105167	-1.76E-07
1.5617502	1.562337911	-0.000588
1.5496695	1.549691727	-2.22E-05
1.5120808	1.512424954	-0.000344
1.4872464	1.489331715	-0.002085
1.4471433	1.447143515	-2.12E-07
1.4063036	1.407036693	-0.000733
1.3738287	1.373298503	0.0005302
1.3412738	1.342650197	-0.001376
1.3330135	1.333013717	-1.89E-07
1.3252924	1.325292871	-4.31E-07
1.3071207	1.307465321	-0.000345
1.3024379	1.301037191	0.0014007
1.265729	1.264606474	0.0011225
1.2621227	1.261723683	0.000399
1.2462846	1.246284923	-3.31E-07
1.2426774	1.242917889	-0.00024
1.2397677	1.23976787	-2.19E-07
1.2123454	1.212344903	5.13E-07
1.2103864	1.210386403	3.49E-08
1.1976593	1.19765896	3.52E-07
1.1833537	1.18335397	-2.35E-07
1.1833336	1.183333805	-1.66E-07
1.1383426	1.138342845	-2.36E-07
1.1142285	1.115036995	-0.000808
1.1136938	1.112728961	0.0009649
1.1092363	1.109236344	1.07E-09
1.1077811	1.106936715	0.0008444
1.1056754	1.102765874	0.0029095
1.0936514	1.096091627	-0.00244
1.0885111	1.088769055	-0.000258
1.063245	1.062400575	0.0008445
1.060417	1.06087507	-0.000458
1.050275	1.050275578	-5.68E-07
1.025226	1.024822768	0.0004032
1.0235509	1.023551195	-2.50E-07

0.988824	0.988337476	0.0004865
0.9748937	0.974698711	0.0001949
0.9558786	0.95580798	7.06E-05
0.9375699	0.937569896	4.62E-08
0.937258	0.937258057	-7.76E-08
0.9133706	0.913370764	-1.80E-07
0.9101871	0.910186922	1.78E-07
0.908146	0.908982095	-0.000836
0.9028574	0.903703968	-0.000847
0.8904701	0.89046997	1.77E-07
0.8774105	0.874867926	0.0025426
0.861161	0.862169346	-0.001008
0.8446632	0.845946419	-0.001283
0.8420243	0.842024079	2.67E-07
0.8377204	0.838794559	-0.001074
0.8330961	0.833155114	-5.90E-05
0.8166903	0.818662962	-0.001973
0.8052711	0.805940748	-0.00067
0.8050807	0.805416771	-0.000336
0.801256	0.801255672	3.11E-07
0.7900812	0.791236813	-0.001156
0.773655	0.770689923	0.0029651
0.7706401	0.770316131	0.000324
0.770291	0.769414408	0.0008766
0.7667397	0.764483134	0.0022566
0.7615622	0.76170397	-0.000142
0.742406	0.742814582	-0.000409
0.7308442	0.730832851	1.14E-05
0.7244769	0.724476712	2.15E-07
0.7218857	0.721885513	1.39E-07
0.7168074	0.716807195	2.00E-07
0.7115475	0.711547642	-1.00E-07
0.7104517	0.71135842	-0.000907
0.6976532	0.697668629	-1.55E-05
0.6896602	0.688792009	0.0008682
0.6852075	0.685207721	-2.06E-07
0.6846613	0.684506046	0.0001552
0.6770232	0.677654631	-0.000631
0.6763221	0.676845509	-0.000523
0.6745885	0.676701767	-0.002113
0.6734117	0.6738343	-0.000423
0.6716687	0.671344045	0.0003247
0.6696932	0.671038377	-0.001345
0.6669139	0.667623005	-0.000709
0.6660907	0.666090923	-1.80E-07
0.6614025	0.661735494	-0.000333
0.6601205	0.660120062	4.16E-07
0.6583158	0.658880011	-0.000564

0.62605	0.627659665	-0.00161
0.5972217	0.595118959	0.0021027
0.588137	0.588173762	-3.67E-05
0.5836021	0.584682996	-0.001081
0.5778877	0.577528937	0.0003587
0.5756441	0.575947806	-0.000304
0.5683022	0.56830211	1.09E-07
0.5560759	0.556075616	2.46E-07
0.5544954	0.553417615	0.0010778
0.5465229	0.546269347	0.0002535
0.5422428	0.542242706	1.18E-07
0.5411631	0.541001688	0.0001615
0.5345824	0.533607073	0.0009753
0.5308362	0.52774607	0.0030901
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-0.018488	-0.017820246	-0.000668
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-0.019096	-0.019409932	0.0003138
-0.019105	-0.019186545	8.12E-05
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-0.021678	-0.021678204	-1.48E-07
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-0.021809	-0.021809404	5.90E-08
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-0.628136	-0.627284361	-0.000852
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-0.779774	-0.779774085	3.68E-07
-0.780709	-0.782808157	0.0020994
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-0.807729	-0.808744799	0.0010156
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-0.820557	-0.820556238	-3.32E-07
-0.821008	-0.821009234	8.75E-07
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-1.027239	-1.027923337	0.000684
-1.037143	-1.037142723	-7.47E-08
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-1.040708	-1.040317144	-0.00039
-1.043445	-1.043445054	2.43E-07
-1.049138	-1.049137819	-1.34E-07
-1.053705	-1.053705166	2.47E-07
-1.061455	-1.061454678	1.58E-07
-1.076656	-1.078701643	0.0020456
-1.111368	-1.112569569	0.0012012
-1.1212	-1.121199664	-1.03E-07
-1.134058	-1.134057528	-1.00E-07
-1.150547	-1.150547203	-2.21E-07
-1.151555	-1.151555304	-9.07E-08
-1.15418	-1.156807549	0.0026271
-1.157867	-1.157948219	8.10E-05
-1.168605	-1.168605456	6.44E-08
-1.169207	-1.168554599	-0.000652
-1.189424	-1.190625481	0.0012013
-1.192242	-1.192242222	-9.02E-08
-1.194801	-1.194800829	-4.38E-08
-1.201777	-1.201777223	7.42E-08
-1.232444	-1.233119635	0.0006755
-1.240636	-1.240636692	1.98E-07

-1.254278	-1.254278409	4.14E-07
-1.273658	-1.273658127	8.90E-08
-1.300449	-1.300448935	2.51E-08
-1.311177	-1.311177374	2.65E-07
-1.317922	-1.317512784	-0.000409
-1.323727	-1.324736815	0.0010097
-1.364879	-1.364736582	-0.000143
-1.392859	-1.392859075	-1.13E-08
-1.39399	-1.392257414	-0.001733
-1.458355	-1.458355691	1.99E-07
-1.50739	-1.50738957	-1.10E-07
-1.526547	-1.52707669	0.0005301
-1.544823	-1.544823883	3.87E-07
-1.563488	-1.564854762	0.001367
-1.687203	-1.687128135	-7.46E-05
-1.722209	-1.724740557	0.0025312
-1.747407	-1.747407434	2.57E-07
-1.778353	-1.777619626	-0.000733
-1.922732	-1.922732406	4.80E-07

Data S1. Ranking of importance of substructure features from Pubchem Fing

GPCR ID	Bit Position	Bit Substructure
P28566	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8
P28566	571	[#1]-C-O-[#1]
P28566	243	>= 1 saturated or aromatic nitrogen-containing ring size 9
P28566	529	Cl-C-C-Cl
P28566	38	>= 2 Cl
P28566	310	O-Mg
P28566	696	C-C-C-C-C-C-C-C
P28566	763	Oc1c(N)cccc1
P28566	745	Sc1cc(S)ccc1
P28566	737	Cc1cc(N)ccc1
P28566	698	O-C-C-C-C-C-C-C
P28566	682	O-C-C-C-C-N
P28566	620	C:C-O-C-C
P28566	727	Sc1ccc(Br)cc1
P28566	146	>= 1 saturated or aromatic heteroatom-containing ring size 5
P28566	179	>= 1 saturated or aromatic carbon-only ring size 6
P28566	558	O=N-C:C
P28566	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5
P28566	784	OC1CCC(N)CC1
P28566	498	O-C=C-C
P28566	330	C(~Br)(:C)
P28566	607	N-C-C-C:C
P28566	757	Cc1c(S)cccc1
P28566	443	C(-C)(=O)
P28566	519	N=C-N-C
P28566	583	Cl-C:C-O-C
P28566	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10
P28566	474	S:C:C:N
P28566	485	N:C:C:N
P28566	750	Nc1cc(Cl)ccc1
P28566	500	C-S-C:C
P28566	804	OC1CC(S)CCC1
P28566	562	Br-C-C=O
P28566	215	>= 1 saturated or aromatic nitrogen-containing ring size 7
P28566	23	>= 1 F
P28566	819	CC1C(O)CCCC1
P28566	816	ClC1CC(Br)CCC1
P28566	391	N(~C)(~C)(~C)
P28566	145	>= 1 saturated or aromatic nitrogen-containing ring size 5
P28566	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6
P28566	105	>= 1 Eu
P28566	408	O(~H)(~S)
P28566	210	>= 5 unsaturated non-aromatic carbon-only ring size 6
P28566	26	>= 1 Na
P28566	854	NC1CC(N)CC1
P28566	104	>= 1 Sm

P28566	242	>= 1 saturated or aromatic carbon-only ring size 9
P28566	347	C(~C)(~H)(~O)(~O)
P28566	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9
P28566	872	SC1C(N)CCC1
P28566	593	N-C-C-C-N
P28566	207	>= 5 saturated or aromatic carbon-only ring size 6
P28566	326	As-As
P28566	172	>= 5 saturated or aromatic carbon-only ring size 5
P28566	252	>= 1 unsaturated non-aromatic carbon-only ring size 10
P28566	93	>= 1 Pt
P28566	563	O-C-O-C
P28566	115	>= 1 any ring size 3
P28566	165	>= 4 saturated or aromatic carbon-only ring size 5
P28566	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8
P28566	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5
P28566	360	C(~Cl)(~Cl)
P28566	159	>= 3 saturated or aromatic nitrogen-containing ring size 5
P28566	1	>= 8 H
P28566	821	CC1C(N)CCCC1
P28566	487	N-C=N-C
P28566	731	Clc1ccc(Cl)cc1
P28566	393	N(~C)(~H)
P28566	512	C-[As]-O-[#1]
P28566	320	Si-H
P28566	728	Nc1ccc(N)cc1
P28566	459	S(=O)(=O)
P28566	494	O=C-C:N
P28566	465	O=S-C-C
P28566	877	NC1C(Br)CCC1
P28566	66	>= 1 Se
P28566	76	>= 1 Pd
P28566	578	C-C:C-C:C
P28566	766	Sc1c(S)cccc1
P28566	538	N=C-C-C
P28566	137	>= 2 saturated or aromatic carbon-only ring size 4
P28566	316	F-P
P28566	319	Al-Cl
P28566	77	>= 1 Ag
P28566	8	>= 4 B
P28566	48	>= 4 I
P28566	6	>= 1 B
P28566	250	>= 1 saturated or aromatic nitrogen-containing ring size 10
P28566	552	C:C-C:C
P28566	424	N=P
P28566	671	O=C-C=C-C
P28566	321	Si-Si
P28566	313	O-Si
P28566	333	C(~C)(~C)(~C)

P28566	528	[#1]-N-C-[#1]
P28566	261	>= 4 aromatic rings
P28566	532	S-C:C-[#1]
P28566	813	NC1CC(Cl)CCC1
P28566	245	>= 1 unsaturated non-aromatic carbon-only ring size 9
P28566	615	N-C-C-O-C
P28566	388	C(:C)(:N)(:N)
P28566	335	C(~C)(~C)(~C)(~H)
P28566	342	C(~C)(~Cl)
P28566	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4
P28566	293	C-S
P28566	434	C(-C)(-H)(=C)
P28566	244	>= 1 saturated or aromatic heteroatom-containing ring size 9
P28566	224	>= 2 unsaturated non-aromatic carbon-only ring size 7
P28566	29	>= 2 Si
P28566	770	Nc1c(N)cccc1
P28566	384	C(:C)(:C)
P28566	28	>= 1 Si
P28566	110	>= 1 Er
P28566	522	C-N-N-[#1]
P28566	553	O=C-C=C
P28566	508	S=C-N-C
P28566	442	C(-C)(=N)
P28566	209	>= 5 saturated or aromatic heteroatom-containing ring size 6
P28566	640	C=C-C-C-C
P28566	610	C-O-C-O-C
P28566	491	C-N:C-[#1]
P28566	779	CC1CCC(N)CC1
P28566	59	>= 1 Co
P28566	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7
P28566	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7
P28566	49	>= 1 Be
P28566	797	CC1CC(C)CCC1
P28566	517	N-N-C-N
P28566	132	>= 1 saturated or aromatic heteroatom-containing ring size 4
P28566	697	C-C-C-C-C-C(C)-C
P28566	445	C(-H)(-N)(=C)
P28566	268	Li-F
P28566	263	Li-H
P28566	354	C(~C)(~Si)
P28566	373	C(~H)(:N)
P28566	69	>= 1 Sr
P28566	712	C-C(C)-C(C)-C
P28566	638	O-C-C-C-N
P28566	691	O-C-C-C-C-C-N
P28566	656	C-C-N-C-C
P28566	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5
P28566	590	C-C:C-O-[#1]

P28566	641	O-C-C-C=C
P28566	181	>= 1 saturated or aromatic heteroatom-containing ring size 6
P28566	131	>= 1 saturated or aromatic nitrogen-containing ring size 4
P28566	734	Cc1cc(C)ccc1
P28566	374	C(~H)(~H)(~H)
P28566	716	Cc1ccc(N)cc1
P28566	581	O=C-C-C-O
P28566	685	O=C-C-C-C-N
P28566	637	O-C-C-C-C
P28566	125	>= 2 saturated or aromatic heteroatom-containing ring size 3
P28566	659	O-C-C-N-C
P28566	589	C-C:C-O-C
P28566	787	SC1CCC(S)CC1
P28566	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6
P28566	271	Li-Cl
P28566	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6
P28566	790	SC1CCC(Br)CC1
P28566	523	N:C:C-C
P28566	775	Brc1c(Br)cccc1
P28566	34	>= 2 S
P28566	585	C-C:C-N-C
P28566	555	N=C-C=C
P28566	592	N-C-C-C-C
P28566	743	Oc1cc(Cl)ccc1
P28566	801	CC1CC(Cl)CCC1
P28566	706	O=C-C-C-C-C(=O)-C
P28566	0	>= 4 H
P28566	52	>= 1 Ca
P28566	295	C-As
P28566	343	C(~C)(~Cl)(~H)
P28566	201	>= 4 saturated or aromatic nitrogen-containing ring size 6
P28566	468	O=S-C-N
P28566	405	O(~C)(~C)
P28566	623	O=C-C:C-C
P28566	280	B-S
P28566	724	Sc1ccc(S)cc1
P28566	168	>= 4 unsaturated non-aromatic carbon-only ring size 5
P28566	5	>= 2 Li
P28566	456	P(-O)(=O)
P28566	20	>= 4 O
P28566	86	>= 1 Lu
P28566	531	S-C:C-C
P28566	850	SC1CC(S)CC1
P28566	144	>= 1 saturated or aromatic carbon-only ring size 5
P28566	780	CC1CCC(Cl)CC1
P28566	868	OC1C(N)CCC1
P28566	160	>= 3 saturated or aromatic heteroatom-containing ring size 5
P28566	415	Si(~C)(~C)

P28566	231	>= 1 unsaturated non-aromatic carbon-only ring size 8
P28566	467	C=N-N-C
P28566	550	Cl-C-C-C
P28566	658	C-C-S-C-C
P28566	213	>= 1 any ring size 7
P28566	789	SC1CCC(Cl)CC1
P28566	769	Sc1c(Br)cccc1
P28566	267	Li-O
P28566	481	O-S-C:C
P28566	223	>= 2 saturated or aromatic heteroatom-containing ring size 7
P28566	24	>= 2 F
P28566	662	O-C-C-O-C
P28566	828	OC1C(Br)CCCC1
P28566	704	O=C-C-C-C-C-C-C
P28566	648	O=N-C:C-N
P28566	548	O-C-C:C
P28566	289	C-Mg
P28566	603	C-C:C:C-C
P28566	644	C-C=N-N-C
P28566	455	N(-O)(=O)
P28566	122	>= 2 any ring size 3
P28566	721	Oc1ccc(N)cc1
P28566	878	ClC1C(Cl)CCC1
P28566	431	C(-C)(-C)(=N)
P28566	772	Nc1c(Br)cccc1
P28566	470	C:C-C=C
P28566	596	N=C-N-C-C
P28566	157	>= 3 any ring size 5
P28566	758	Cc1c(N)cccc1
P28566	686	O=C-C-C-C-O
P28566	742	Oc1cc(N)ccc1
P28566	672	O=C-C=C-[#1]
P28566	606	O-C:C-C-C
P28566	180	>= 1 saturated or aromatic nitrogen-containing ring size 6
P28566	621	N-C:C:C:N
P28566	194	>= 3 saturated or aromatic nitrogen-containing ring size 6
P28566	58	>= 1 Fe
P28566	435	C(-C)(-H)(=N)
P28566	409	O(:C)(:C)
P28566	9	>= 2 C
P28566	700	O-C-C-C-C-C-C-O-C
P28566	438	C(-C)(-N)(=N)
P28566	302	N-F
P28566	164	>= 4 any ring size 5
P28566	539	N=C-C-[#1]
P28566	861	CC1C(O)CCC1
P28566	681	O-C-C-C-C-C-O
P28566	151	>= 2 saturated or aromatic carbon-only ring size 5

P28566	195	>= 3 saturated or aromatic heteroatom-containing ring size 6
P28566	437	C(-C)(-N)(=C)
P28566	793	NC1CCC(Br)CC1
P28566	352	C(~C)(~O)
P28566	599	[#1]-C-C=C-[#1]
P28566	87	>= 1 Hf
P28566	516	[#1]-C=C-[#1]
P28566	726	Sc1ccc(Cl)cc1
P28566	406	O(~C)(~H)
P28566	653	O-C:C:C-O
P28566	629	S-C:C:C-N
P28566	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6
P28566	323	P-H
P28566	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3
P28566	830	SC1C(N)CCCC1
P28566	16	>= 4 N
P28566	13	>= 32 C
P28566	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6
P28566	652	O-C:C:C-N
P28566	785	OC1CCC(Cl)CC1
P28566	262	>= 4 hetero-aromatic rings
P28566	200	>= 4 saturated or aromatic carbon-only ring size 6
P28566	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5
P28566	597	O=C-C-C:C
P28566	452	C(-O)(=O)
P28566	113	>= 1 Tc
P28566	174	>= 5 saturated or aromatic heteroatom-containing ring size 5
P28566	853	SC1CC(Br)CC1
P28566	730	Nc1ccc(Br)cc1
P28566	312	O-Al
P28566	824	OC1C(O)CCCC1
P28566	161	>= 3 unsaturated non-aromatic carbon-only ring size 5
P28566	423	N=O
P28566	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4
P28566	839	CC1CC(C)CC1
P28566	612	N-C-O-C-C
P28566	627	O=[As]-C:C:C
P28566	594	C-O-C-C=C
P28566	826	OC1C(N)CCCC1
P28566	738	Cc1cc(Cl)ccc1
P28566	732	Clc1ccc(Br)cc1
P28566	513	S:C:C-[#1]
P28566	811	SC1CC(Br)CCC1
P28566	554	Br-C-C-C
P28566	413	S(~C)(~H)
P28566	559	O-C-N-[#1]
P28566	206	>= 5 any ring size 6
P28566	298	C-I

P28566	385	C(:C)(:C)(:C)
P28566	540	C-N-C-[#1]
P28566	380	C(~O)(~O)
P28566	422	N=N
P28566	835	NC1C(Br)CCCC1
P28566	407	O(~C)(~P)
P28566	108	>= 1 Dy
P28566	117	>= 1 saturated or aromatic nitrogen-containing ring size 3
P28566	17	>= 8 N
P28566	444	C(-Cl)(=O)
P28566	196	>= 3 unsaturated non-aromatic carbon-only ring size 6
P28566	673	O=C-C=C-N
P28566	92	>= 1 Ir
P28566	777	CC1CCC(O)CC1
P28566	674	N-C-N-C:C
P28566	688	C-C-C-C-C-C-C
P28566	515	N-N-C-C
P28566	419	C#N
P28566	625	O=C-C:C-O
P28566	560	N-C-N-C
P28566	60	>= 1 Ni
P28566	792	NC1CCC(Cl)CC1
P28566	404	N(:C)(:C)(:C)
P28566	432	C(-C)(-C)(=O)
P28566	80	>= 1 Sn
P28566	227	>= 1 any ring size 8
P28566	524	C-C=C-C
P28566	546	N-C:C-[#1]
P28566	806	OC1CC(Cl)CCC1
P28566	717	Cc1ccc(Cl)cc1
P28566	364	C(~F)(:C)
P28566	102	>= 1 Nd
P28566	833	NC1C(N)CCCC1
P28566	574	O-C-C:C-C
P28566	44	>= 2 Br
P28566	411	P(~O)(~O)
P28566	614	C-C-O-C-C
P28566	568	N#C-C-C
P28566	880	BrC1C(Br)CCC1
P28566	649	O=N-C:C-O
P28566	739	Cc1cc(Br)ccc1
P28566	414	S(~C)(~O)
P28566	818	CC1C(C)CCCC1
P28566	383	C(~S)(:C)
P28566	832	SC1C(Br)CCCC1
P28566	234	>= 2 any ring size 8
P28566	748	Sc1cc(Br)ccc1
P28566	711	C-C(C)(C)-C-C

P28566	363	C(~F)(~F)
P28566	428	C(#C)(-H)
P28566	755	Cc1c(C)cccc1
P28566	657	C-N-C:C-C
P28566	83	>= 1 Xe
P28566	57	>= 1 Mn
P28566	520	C=C-C:C
P28566	341	C(~C)(~C)(~O)
P28566	359	C(~C)(:N)(:N)
P28566	100	>= 1 Ce
P28566	236	>= 2 saturated or aromatic nitrogen-containing ring size 8
P28566	740	Oc1cc(O)ccc1
P28566	863	CC1C(N)CCC1
P28566	842	CC1CC(N)CC1
P28566	773	Clc1c(Cl)cccc1
P28566	645	O=C-N-C-C
P28566	214	>= 1 saturated or aromatic carbon-only ring size 7
P28566	457	S(-C)(=O)
P28566	707	O=C-C-C-C-C(N)-C
P28566	502	N-C=C-[#1]
P28566	521	C:N-C-[#1]
P28566	651	O-C:C:C-C
P28566	173	>= 5 saturated or aromatic nitrogen-containing ring size 5
P28566	7	>= 2 B
P28566	794	ClC1CCC(Cl)CC1
P28566	744	Oc1cc(Br)ccc1
P28566	266	Li-C
P28566	505	Cl-C:C-O
P28566	140	>= 2 unsaturated non-aromatic carbon-only ring size 4
P28566	634	C-C-C:C-C
P28566	237	>= 2 saturated or aromatic heteroatom-containing ring size 8
P28566	114	>= 1 U
P28566	192	>= 3 any ring size 6
P28566	21	>= 8 O
P28566	353	C(~C)(~S)
P28566	617	C-C-C-O-[#1]
P28566	377	C(~N)(:C)(:C)
P28566	264	Li-Li
P28566	89	>= 1 W
P28566	689	O-C-C-C-C-C-C
P28566	749	Nc1cc(N)ccc1
P28566	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6
P28566	265	Li-B
P28566	873	SC1C(Cl)CCC1
P28566	530	N:C-C:C
P28566	448	C(-H)(=O)
P28566	279	B-P
P28566	741	Oc1cc(S)ccc1

P28566	760	Cc1c(Br)cccc1
P28566	836	ClC1C(Cl)CCCC1
P28566	856	NC1CC(Br)CC1
P28566	871	SC1C(S)CCC1
P28566	329	C(~Br)(~H)
P28566	55	>= 1 V
P28566	729	Nc1ccc(Cl)cc1
P28566	527	C:C:N-[#1]
P28566	584	C:C-C=C-C
P28566	510	[#1]-N-N-[#1]
P28566	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5
P28566	504	N:C:N-C
P28566	153	>= 2 saturated or aromatic heteroatom-containing ring size 5
P28566	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5
P28566	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9
P28566	65	>= 1 As
P28566	643	[#1]-C-C-N-[#1]
P28566	123	>= 2 saturated or aromatic carbon-only ring size 3
P28566	40	>= 8 Cl
P28566	290	C-Al
P28566	827	OC1C(Cl)CCCC1
P28566	807	OC1CC(Br)CCC1
P28566	97	>= 1 Pb
P28566	825	OC1C(S)CCCC1
P28566	45	>= 4 Br
P28566	626	C-O-C:C-C
P28566	31	>= 2 P
P28566	542	O-C:C-[#1]
P28566	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3
P28566	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8
P28566	855	NC1CC(Cl)CC1
P28566	875	NC1C(N)CCC1
P28566	492	N-C:O:C
P28566	619	O-C-C=C-C
P28566	774	Clc1c(Br)cccc1
P28566	761	Oc1c(O)cccc1
P28566	852	SC1CC(Cl)CC1
P28566	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3
P28566	72	>= 1 Nb
P28566	74	>= 1 Ru
P28566	221	>= 2 saturated or aromatic carbon-only ring size 7
P28566	348	C(~C)(~H)(~P)
P28566	94	>= 1 Au
P28566	869	OC1C(Cl)CCC1
P28566	303	N-Si
P28566	306	N-Cl
P28566	256	>= 1 hetero-aromatic ring
P28566	867	OC1C(S)CCC1

P28566	61	>= 1 Cu
P28566	119	>= 1 unsaturated non-aromatic carbon-only ring size 3
P28566	63	>= 1 Ga
P28566	32	>= 4 P
P28566	3	>= 32 H
P28566	22	>= 16 O
P28566	257	>= 2 aromatic rings
P28566	99	>= 1 La
P28566	47	>= 2 I
P28566	322	Si-Cl
P28566	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4
P28566	862	CC1C(S)CCC1
P28566	220	>= 2 any ring size 7
P28566	42	>= 2 K
P28566	282	B-Br
P28566	471	S:C:C:C
P28566	864	CC1C(Cl)CCC1
P28566	51	>= 1 Al
P28566	324	P-P
P28566	556	C=C-C-C
P28566	725	Sc1ccc(N)cc1
P28566	85	>= 1 Ba
P28566	370	C(~H)(:C)
P28566	429	C(#N)(-C)
P28566	561	Cl-C-C=O
P28566	238	>= 2 unsaturated non-aromatic carbon-only ring size 8
P28566	315	O-K
P28566	570	C:C-C-C
P28566	545	N-C:C-C
P28566	273	B-B
P28566	402	N(~O)(:O)
P28566	251	>= 1 saturated or aromatic heteroatom-containing ring size 10
P28566	551	Cl-C-C-O
P28566	601	N-C:C:C-N
P28566	430	C(-C)(-C)(=C)
P28566	107	>= 1 Tb
P28566	602	O=C-C-N-C
P28566	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7
P28566	336	C(~C)(~C)(~C)(~N)
P28566	270	Li-S
P28566	276	B-O
P28566	300	N-N
P28566	654	N-C-N-C-C
P28566	675	Br-C-C-C:C
P28566	718	Cc1ccc(Br)cc1
P28566	392	N(~C)(~C)(~H)
P28566	781	CC1CCC(Br)CC1
P28566	591	Cl-C-C-C-C

P28566	713	Cc1ccc(C)cc1
P28566	357	C(~C)(:C)(:N)
P28566	525	[As]-C:C-[#1]
P28566	564	C=C-C=C
P28566	722	Oc1ccc(Cl)cc1
P28566	400	N(~H)(:C)(:C)
P28566	719	Oc1ccc(O)cc1
P28566	788	SC1CCC(N)CC1
P28566	387	C(:C)(:N)
P28566	514	O-N-C-C
P28566	715	Cc1ccc(S)cc1
P28566	68	>= 1 Rb
P28566	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6
P28566	203	>= 4 unsaturated non-aromatic carbon-only ring size 6
P28566	318	Al-H
P28566	786	OC1CCC(Br)CC1
P28566	79	>= 1 In
P28566	345	C(~C)(~H)(~N)
P28566	778	CC1CCC(S)CC1
P28566	199	>= 4 any ring size 6
P28566	694	O=C-C-C-C-C=O
P28566	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3
P28566	598	Cl-C:C:C-C
P28566	497	O-C:C:N
P28566	478	S-C=N-[#1]
P28566	314	O-P
P28566	480	C:S:C-C
P28566	37	>= 1 Cl
P28566	646	O=C-N-C-[#1]
P28566	378	C(~N)(:C)(:N)
P28566	368	C(~H)(~S)
P28566	451	C(-N)(=O)
P28566	860	CC1C(C)CCC1
P28566	518	O=C-N-N
P28566	808	SC1CC(S)CCC1
P28566	78	>= 1 Cd
P28566	608	C-C-C-C:C
P28566	260	>= 3 hetero-aromatic rings
P28566	143	>= 1 any ring size 5
P28566	628	C-N-C-C:C
P28566	693	O=C-C-C-C-C-O
P28566	334	C(~C)(~C)(~C)(~C)
P28566	25	>= 4 F
P28566	133	>= 1 unsaturated non-aromatic carbon-only ring size 4
P28566	870	OC1C(Br)CCC1
P28566	577	C:C-N-C:C
P28566	720	Oc1ccc(S)cc1
P28566	376	C(~N)(:C)

P28566	690	O-C-C-C-C-C-O
P28566	783	OC1CCC(S)CC1
P28566	64	>= 1 Ge
P28566	228	>= 1 saturated or aromatic carbon-only ring size 8
P28566	138	>= 2 saturated or aromatic nitrogen-containing ring size 4
P28566	188	>= 2 saturated or aromatic heteroatom-containing ring size 6
P28566	647	O=C-N-C-N
P28566	417	C#C
P28566	118	>= 1 saturated or aromatic heteroatom-containing ring size 3
P28566	427	C(#C)(-C)
P28566	475	S-C=N-C
P28566	814	NC1CC(Br)CCC1
P28566	325	As-H
P28566	309	O-O
P28566	611	N-C-C-N-C
P28566	36	>= 8 S
P28566	394	N(~C)(~H)(~N)
P28566	630	O-C:C-O-C
P28566	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6
P28566	483	N-S-C:C
P28566	327	C(~Br)(~C)
P28566	803	OC1CC(O)CCC1
P28566	106	>= 1 Gd
P28566	791	NC1CCC(N)CC1
P28566	187	>= 2 saturated or aromatic nitrogen-containing ring size 6
P28566	43	>= 1 Br
P28566	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10
P28566	847	OC1CC(N)CC1
P28566	736	Cc1cc(S)ccc1
P28566	484	N-C:N:C
P28566	339	C(~C)(~C)(~H)(~O)
P28566	572	N:C:N:C
P28566	795	ClC1CCC(Br)CC1
P28566	389	C(:N)(:N)
P28566	752	Clc1cc(Cl)ccc1
P28566	576	N=C-C:C-[#1]
P28566	692	O=C-C-C-C-C-C
P28566	139	>= 2 saturated or aromatic heteroatom-containing ring size 4
P28566	410	P(~C)(~C)
P28566	450	C(-N)(=N)
P28566	91	>= 1 Os
P28566	495	C-N-C:C
P28566	501	Cl-C:C-C
P28566	398	N(~H)(~N)
P28566	759	Cc1c(Cl)cccc1
P28566	840	CC1CC(O)CC1
P28566	843	CC1CC(Cl)CC1
P28566	831	SC1C(Cl)CCCC1

P28566	609	Cl-C-C-N-C
P28566	678	C-C-C=C-C
P28566	665	N-C:C-C-C
P28566	397	N(~C)(:C)(:C)
P28566	386	C(:C)(:C)(:N)
P28566	499	N-C:C:N
P28566	30	>= 1 P
P28566	851	SC1CC(N)CC1
P28566	479	S-C-S-C
P28566	185	>= 2 any ring size 6
P28566	566	O-C-C-N
P28566	129	>= 1 any ring size 4
P28566	362	C(~Cl)(:C)
P28566	258	>= 2 hetero-aromatic rings
P28566	235	>= 2 saturated or aromatic carbon-only ring size 8
P28566	822	CC1C(Cl)CCCC1
P28566	371	C(~H)(:C)(:C)
P28566	381	C(~O)(:C)
P28566	189	>= 2 unsaturated non-aromatic carbon-only ring size 6
P28566	765	Oc1c(Br)cccc1
P28566	288	C-Na
P28566	809	SC1CC(N)CCC1
P28566	296	C-Se
P28566	328	C(~Br)(~C)(~C)
P28566	11	>= 8 C
P28566	255	>= 1 aromatic ring
P28566	767	Sc1c(N)cccc1
P28566	396	N(~C)(:C)
P28566	667	C=C-C-O-[#1]
P28566	331	C(~Br)(:N)
P28566	820	CC1C(S)CCCC1
P28566	624	O=C-C:C-N
P28566	469	S-S-C:C
P28566	544	O-C:C-O
P28566	838	BrC1C(Br)CCCC1
P28566	291	C-Si
P28566	534	S-C:C-O
P28566	14	>= 1 N
P28566	857	ClC1CC(Cl)CC1
P28566	600	N-C:C:C-C
P28566	588	O=C-C-C=O
P28566	453	N(-C)(=C)
P28566	186	>= 2 saturated or aromatic carbon-only ring size 6
P28566	147	>= 1 unsaturated non-aromatic carbon-only ring size 5
P28566	365	C(~H)(~N)
P28566	46	>= 1 I
P28566	403	N(:C)(:C)
P28566	709	C-C(C)-C-C-C

P28566	311	O-Na
P28566	412	S(~C)(~C)
P28566	98	>= 1 Bi
P28566	669	Cl-C:C-C=O
P28566	2	>= 16 H
P28566	278	B-Si
P28566	241	>= 1 any ring size 9
P28566	482	C:N-C:C
P28566	150	>= 2 any ring size 5
P28566	533	S-C:C-N
P28566	62	>= 1 Zn
P28566	269	Li-P
P28566	616	C:C:N:N:C
P28566	462	O-C-C=O
P28566	88	>= 1 Ta
P28566	703	O-C-C-C-C-C(N)-C
P28566	297	C-Br
P28566	536	O=C-C-N
P28566	699	O-C-C-C-C-C(C)-C
P28566	496	N:N-C-[#1]
P28566	440	C(-C)(-O)(=O)
P28566	874	SC1C(Br)CCC1
P28566	567	O-C-C-O
P28566	604	C-O-C-C:C
P28566	124	>= 2 saturated or aromatic nitrogen-containing ring size 3
P28566	676	N#C-C-C-C
P28566	660	C-C=C-C-C
P28566	461	O-C-C=N
P28566	216	>= 1 saturated or aromatic heteroatom-containing ring size 7
P28566	580	O=C-C-C-N
P28566	829	SC1C(S)CCCC1
P28566	805	OC1CC(N)CCC1
P28566	735	Cc1cc(O)ccc1
P28566	472	C:N:C-C
P28566	369	C(~H)(~Si)
P28566	178	>= 1 any ring size 6
P28566	337	C(~C)(~C)(~C)(~O)
P28566	15	>= 2 N
P28566	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5
P28566	401	N(~O)(~O)
P28566	622	O=C-O-C:C
P28566	10	>= 4 C
P28566	358	C(~C)(:N)
P28566	679	C-C-C-C-C-C
P28566	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5
P28566	802	CC1CC(Br)CCC1
P28566	372	C(~H)(:C)(:N)
P28566	733	Brc1ccc(Br)cc1

P28566	464	N-C-C=C
P28566	751	Nc1cc(Br)ccc1
P28566	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5
P28566	351	C(~C)(~N)
P28566	834	NC1C(Cl)CCCC1
P28566	565	C:C-O-C
P28566	618	C:C-C-C:C
P28566	449	C(-N)(=C)
P28566	650	O=C-N-C=O
P28566	90	>= 1 Re
P28566	308	O-H
P28566	171	>= 5 any ring size 5
P28566	54	>= 1 Ti
P28566	283	C-H
P28566	53	>= 1 Sc
P28566	841	CC1CC(S)CC1
P28566	33	>= 1 S
P28566	547	N-C:C-N
P28566	230	>= 1 saturated or aromatic heteroatom-containing ring size 8
P28566	463	N:C-S-[#1]
P28566	67	>= 1 Kr
P28566	426	P=P
P28566	815	ClC1CC(Cl)CCC1
P28566	844	CC1CC(Br)CC1
P28566	356	C(~C)(:C)(:C)
P28566	361	C(~Cl)(~H)
P28566	771	Nc1c(Cl)cccc1
P28566	41	>= 1 K
P28566	666	C=C-C-O-C
P28566	208	>= 5 saturated or aromatic nitrogen-containing ring size 6
P28566	154	>= 2 unsaturated non-aromatic carbon-only ring size 5
P28566	632	C-C-O-C:C
P28566	753	Clc1cc(Br)ccc1
P28566	642	O-C-C-C=O
P28566	281	B-Cl
P28566	259	>= 3 aromatic rings
P28566	776	CC1CCC(C)CC1
P28566	84	>= 1 Cs
P28566	433	C(-C)(-Cl)(=O)
P28566	466	N#C-C=C
P28566	859	BrC1CC(Br)CC1
P28566	277	B-F
P28566	317	F-S
P28566	349	C(~C)(~H)(~S)
P28566	489	N-C-S-C
P28566	635	N-N-C-N-[#1]
P28566	50	>= 1 Mg
P28566	756	Cc1c(O)cccc1

P28566	849	OC1CC(Br)CC1
P28566	746	Sc1cc(N)ccc1
P28566	285	C-N
P28566	344	C(~C)(~H)
P28566	488	N-C=N-[#1]
P28566	152	>= 2 saturated or aromatic nitrogen-containing ring size 5
P28566	390	N(~C)(~C)
P28566	633	N-C-C:C-C
P28566	12	>= 16 C
P28566	664	C-C=C-C=C
P28566	399	N(~H)(:C)
P28566	639	O-C-C-C-O
P28566	286	C-O
P28566	858	ClC1CC(Br)CC1
P28566	421	C=S
P28566	876	NC1C(Cl)CC1
P28566	702	O-C-C-C-C-C-C-N-C
P28566	798	CC1CC(O)CCC1
P28566	4	>= 1 Li
P28566	670	Br-C:C:C-C
P28566	418	C=N
P28566	684	O=C-C-C-C-C
P28566	768	Sc1c(Cl)cccc1
P28566	535	O=C-C-C
P28566	355	C(~C)(:C)
P28566	367	C(~H)(~O)(~O)
P28566	490	C-C-C=C
P28566	701	O-C-C-C-C-C(O)-C
P28566	507	C-C-S-C
P28566	541	O-C:C-C
P28566	764	Oc1c(Cl)cccc1
P28566	130	>= 1 saturated or aromatic carbon-only ring size 4
P28566	292	C-P
P28566	166	>= 4 saturated or aromatic nitrogen-containing ring size 5
P28566	812	NC1CC(N)CCC1
P28566	249	>= 1 saturated or aromatic carbon-only ring size 10
P28566	714	Cc1ccc(O)cc1
P28566	294	C-Cl
P28566	687	O=C-C-C-C=O
P28566	782	OC1CCC(O)CC1
P28566	476	C-O-C=C
P28566	575	O-C-C:C-O
P28566	710	C-C-C(C)-C-C
P28566	509	Br-C:C-C
P28566	723	Oc1ccc(Br)cc1
P28566	56	>= 1 Cr
P28566	95	>= 1 Hg
P28566	447	C(-H)(=N)

P28566	73	>= 1 Mo
P28566	436	C(-C)(-H)(=O)
P28566	663	O-C-C-O-[#1]
P28566	799	CC1CC(S)CCC1
P28566	503	Cl-C:C-[#1]
P28566	846	OC1CC(S)CC1
P28566	350	C(~C)(~I)
P28566	866	OC1C(O)CCC1
P28566	493	O=C-C:C
P28566	683	N-C-C-C-C-C
P28566	705	O=C-C-C-C-C(O)-C
P28566	395	N(~C)(~O)
P28566	810	SC1CC(Cl)CCC1
P28566	668	C-C:C-C-C
P28566	126	>= 2 unsaturated non-aromatic carbon-only ring size 3
P28566	605	O=C-C-O-C
P28566	19	>= 2 O
P28566	486	N-C:N:N
P28566	458	S(-O)(=O)
P28566	116	>= 1 saturated or aromatic carbon-only ring size 3
P28566	103	>= 1 Pm
P28566	382	C(~O)(:C)(:C)
P28566	586	C-S-C-C-C
P28566	71	>= 1 Zr
P28566	680	O-C-C-C-C-C
P28566	661	O-C-O-C-C
P28566	549	N-C-C:C
P28566	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4
P28566	340	C(~C)(~C)(~N)
P28566	754	Brc1cc(Br)ccc1
P28566	506	C-C:N:C
P28566	837	ClC1C(Br)CCCC1
P28566	287	C-F
P28566	800	CC1CC(N)CCC1
P28566	817	BrC1CC(Br)CCC1
P28566	82	>= 1 Te
P28566	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6
P28566	573	O-C-C=C
P28566	543	O-C:C-N
P28566	346	C(~C)(~H)(~O)
P28566	307	N-Br
P28566	823	CC1C(Br)CCCC1
P28566	75	>= 1 Rh
P28566	275	B-N
P28566	477	N-N-C:C
P28566	379	C(~N)(:N)
P28566	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5
P28566	111	>= 1 Tm

P28566	762	Oc1c(S)cccc1
P28566	167	>= 4 saturated or aromatic heteroatom-containing ring size 5
P28566	796	BrC1CCC(Br)CC1
P28566	35	>= 4 S
P28566	101	>= 1 Pr
P28566	193	>= 3 saturated or aromatic carbon-only ring size 6
P28566	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8
P28566	420	C=O
P28566	557	N:C-O-[#1]
P28566	217	>= 1 unsaturated non-aromatic carbon-only ring size 7
P28566	299	N-H
P28566	865	CC1C(Br)CCC1
P28566	109	>= 1 Ho
P28566	158	>= 3 saturated or aromatic carbon-only ring size 5
P28566	537	O=C-C-O
P28566	27	>= 2 Na
P28566	274	B-C
P28566	96	>= 1 Tl
P28566	879	ClC1C(Br)CCC1
P28566	677	C-C=C-C:C
P28566	579	O=C-C-C-C
P28566	454	N(-C)(=O)
P28566	136	>= 2 any ring size 4
P28566	569	N-C-C-N
P28566	595	C:C-C-C-C
P28566	70	>= 1 Y
P28566	366	C(~H)(~O)
P28566	441	C(-C)(=C)
P28566	582	C-C-C-C-C
P28566	301	N-O
P28566	446	C(-H)(=C)
P28566	439	C(-C)(-N)(=O)
P28566	708	C-C(C)-C-C
P28566	375	C(~N)(~N)
P28566	587	N-C:C-O-[#1]
P28566	182	>= 1 unsaturated non-aromatic carbon-only ring size 6
P28566	848	OC1CC(Cl)CC1
P28566	747	Sc1cc(Cl)ccc1
P28566	338	C(~C)(~C)(~H)(~N)
P28566	112	>= 1 Yb
P28566	473	S-C:N:C
P28566	304	N-P
P28566	81	>= 1 Sb
P28566	332	C(~C)(~C)
P28566	425	P=O
P28566	18	>= 1 O
P28566	511	S=C-N-[#1]
P28566	655	O-C-C-C:C

P28566	284	C-C
P28566	222	>= 2 saturated or aromatic nitrogen-containing ring size 7
P28566	636	C-N-C-N-C
P28566	272	B-H
P28566	631	O-C:C-O-[#1]
P28566	526	Cl-C:C-Cl
P28566	613	C-N-C-C-C
P28566	416	C=C
P28566	248	>= 1 any ring size 10
P28566	229	>= 1 saturated or aromatic nitrogen-containing ring size 8
P28566	695	O=C-C-C-C-C-N
P28566	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7
P28566	39	>= 4 Cl
P28566	175	>= 5 unsaturated non-aromatic carbon-only ring size 5
P28566	845	OC1CC(O)CC1
P28566	202	>= 4 saturated or aromatic heteroatom-containing ring size 6
P28566	305	N-S
P28566	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6
P28566	460	C-C-C#C

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Data S1. Ranking of importance of substructure features from Pubchem Fingerp

GPCR ID	Bit Position	Bit Substructure	W
P47898	306	N-Cl	2.5081126
P47898	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	2.0222894
P47898	582	C-C-C-C-C	1.9552281
P47898	662	O-C-C-O-C	1.9063671
P47898	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	1.7997715
P47898	875	NC1C(N)CCC1	1.7818123
P47898	403	N(:C)(:C)	1.7184526
P47898	825	OC1C(S)CCCC1	1.6365843
P47898	407	O(~C)(~P)	1.62995
P47898	878	ClC1C(Cl)CCC1	1.5980651
P47898	93	>= 1 Pt	1.5891932
P47898	48	>= 4 I	1.5251895
P47898	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	1.4751824
P47898	628	C-N-C-C:C	1.4504459
P47898	303	N-Si	1.4331569
P47898	548	O-C-C:C	1.4268479
P47898	283	C-H	1.4190877
P47898	751	Nc1cc(Br)ccc1	1.4068938
P47898	275	B-N	1.3567984
P47898	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	1.3558861
P47898	310	O-Mg	1.3550453
P47898	56	>= 1 Cr	1.241704
P47898	564	C=C-C=C	1.227565
P47898	733	Brc1ccc(Br)cc1	1.2264255
P47898	214	>= 1 saturated or aromatic carbon-only ring size 7	1.2246288
P47898	524	C-C=C-C	1.2086343
P47898	511	S=C-N-[#1]	1.206717
P47898	465	O=S-C-C	1.2051642
P47898	268	Li-F	1.2025606
P47898	353	C(~C)(~S)	1.1771985
P47898	420	C=O	1.1580103
P47898	356	C(~C)(:C)(:C)	1.1570753
P47898	433	C(-C)(-Cl)(=O)	1.1490072
P47898	373	C(~H)(:N)	1.1480721
P47898	760	Cc1c(Br)cccc1	1.1322026
P47898	164	>= 4 any ring size 5	1.1313668
P47898	324	P-P	1.1238577
P47898	477	N-N-C:C	1.0894728
P47898	658	C-C-S-C-C	1.0595182
P47898	644	C-C=N-N-C	1.0591204
P47898	635	N-N-C-N-[#1]	1.0585513
P47898	220	>= 2 any ring size 7	1.0575056
P47898	565	C:C-O-C	1.034157
P47898	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	1.0292698
P47898	358	C(~C)(:N)	1.0259607
P47898	827	OC1C(Cl)CCCC1	1.0245995

P47898	872	SC1C(N)CCC1	1.0163907
P47898	600	N-C:C:C-C	1.0126778
P47898	580	O=C-C-C-N	0.9888332
P47898	382	C(~O)(:C)(:C)	0.9608768
P47898	623	O=C-C:C-C	0.9527836
P47898	96	>= 1 Tl	0.9477322
P47898	664	C-C=C-C=C	0.9410669
P47898	42	>= 2 K	0.9392952
P47898	586	C-S-C-C-C	0.9268806
P47898	82	>= 1 Te	0.9168986
P47898	450	C(-N)(=N)	0.9152593
P47898	369	C(~H)(~Si)	0.883416
P47898	526	Cl-C:C-Cl	0.8796149
P47898	307	N-Br	0.8779535
P47898	311	O-Na	0.8705467
P47898	267	Li-O	0.8622802
P47898	463	N:C-S-[#1]	0.8577671
P47898	837	ClC1C(Br)CCCC1	0.8277299
P47898	791	NC1CCC(N)CC1	0.826933
P47898	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.8139199
P47898	70	>= 1 Y	0.8069517
P47898	359	C(~C)(:N)(:N)	0.8053454
P47898	562	Br-C-C=O	0.7957203
P47898	301	N-O	0.7928107
P47898	13	>= 32 C	0.7926652
P47898	706	O=C-C-C-C-C(=O)-C	0.7751242
P47898	730	Nc1ccc(Br)cc1	0.7739262
P47898	495	C-N-C:C	0.7697495
P47898	772	Nc1c(Br)cccc1	0.7695014
P47898	55	>= 1 V	0.763957
P47898	274	B-C	0.7451909
P47898	476	C-O-C=C	0.7381128
P47898	360	C(~Cl)(~Cl)	0.7365074
P47898	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.7335123
P47898	289	C-Mg	0.7274248
P47898	102	>= 1 Nd	0.7256801
P47898	810	SC1CC(Cl)CCC1	0.7242422
P47898	804	OC1CC(S)CCC1	0.7126024
P47898	15	>= 2 N	0.7083207
P47898	434	C(-C)(-H)(=C)	0.7005204
P47898	521	C:N-C-[#1]	0.6987719
P47898	815	ClC1CC(Cl)CCC1	0.680691
P47898	608	C-C-C-C:C	0.6787607
P47898	458	S(-O)(=O)	0.6776275
P47898	617	C-C-C-O-[#1]	0.6756379
P47898	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.6721232
P47898	508	S=C-N-C	0.6720406
P47898	789	SC1CCC(Cl)CC1	0.665962

P47898	115	>= 1 any ring size 3	0.6607142
P47898	383	C(~S)(:C)	0.6569185
P47898	316	F-P	0.6452707
P47898	276	B-O	0.6383727
P47898	753	Clc1cc(Br)ccc1	0.631492
P47898	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.630275
P47898	739	Cc1cc(Br)ccc1	0.6177476
P47898	486	N-C:N:N	0.6121666
P47898	501	Cl-C:C-C	0.6034309
P47898	696	C-C-C-C-C-C-C-C	0.601819
P47898	674	N-C-N-C:C	0.5992454
P47898	335	C(~C)(~C)(~C)(~H)	0.5887698
P47898	436	C(-C)(-H)(=O)	0.5881788
P47898	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.5812607
P47898	874	SC1C(Br)CCC1	0.5753498
P47898	661	O-C-O-C-C	0.5737398
P47898	286	C-O	0.5737373
P47898	514	O-N-C-C	0.5711401
P47898	618	C:C-C-C:C	0.565447
P47898	266	Li-C	0.5612466
P47898	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.5436357
P47898	632	C-C-O-C:C	0.5291634
P47898	112	>= 1 Yb	0.5255871
P47898	747	Sc1cc(Cl)ccc1	0.5192842
P47898	568	N#C-C-C	0.5116671
P47898	30	>= 1 P	0.5011332
P47898	314	O-P	4.99E-01
P47898	473	S-C:N:C	0.4783302
P47898	323	P-H	0.474227
P47898	700	O-C-C-C-C-C-O-C	0.4727998
P47898	297	C-Br	0.4683257
P47898	574	O-C-C:C-C	0.4591586
P47898	592	N-C-C-C-C	0.4506651
P47898	522	C-N-N-[#1]	0.4482059
P47898	467	C=N-N-C	0.4445772
P47898	717	Cc1ccc(Cl)cc1	0.4381349
P47898	499	N-C:C:N	0.435763
P47898	65	>= 1 As	0.4348581
P47898	338	C(~C)(~C)(~H)(~N)	0.4274609
P47898	421	C=S	0.4267015
P47898	227	>= 1 any ring size 8	0.4245633
P47898	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.4230477
P47898	317	F-S	4.15E-01
P47898	468	O=S-C-N	0.4142907
P47898	264	Li-Li	0.4134189
P47898	516	[#1]-C=C-[#1]	0.4076477
P47898	3	>= 32 H	0.4034703
P47898	802	CC1CC(Br)CCC1	0.4032581

P47898	873	SC1C(Cl)CCC1	0.3992055
P47898	551	Cl-C-C-O	0.3945364
P47898	682	O-C-C-C-C-N	0.3939485
P47898	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.3938321
P47898	539	N=C-C-[#1]	0.3869167
P47898	18	>= 1 O	0.38642
P47898	372	C(~H)(:C)(:N)	0.3788509
P47898	667	C=C-C-O-[#1]	0.3753782
P47898	94	>= 1 Au	0.3693782
P47898	794	ClC1CCC(Cl)CC1	0.3683713
P47898	466	N#C-C=C	0.3652483
P47898	36	>= 8 S	0.3596035
P47898	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.3560683
P47898	731	Clc1ccc(Cl)cc1	0.3512635
P47898	464	N-C-C=C	0.3497708
P47898	33	>= 1 S	0.3495355
P47898	172	>= 5 saturated or aromatic carbon-only ring size 5	0.3491503
P47898	782	OC1CCC(O)CC1	0.3472598
P47898	695	O=C-C-C-C-C-N	0.3385718
P47898	638	O-C-C-C-N	0.3348114
P47898	785	OC1CCC(Cl)CC1	0.3343555
P47898	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.326742
P47898	350	C(~C)(~I)	0.3260258
P47898	642	O-C-C-C=O	0.3249441
P47898	337	C(~C)(~C)(~C)(~O)	0.3194735
P47898	348	C(~C)(~H)(~P)	0.3186568
P47898	752	Clc1cc(Cl)ccc1	0.3172365
P47898	298	C-I	0.3110186
P47898	44	>= 2 Br	0.3109504
P47898	671	O=C-C=C-C	0.3101877
P47898	39	>= 4 Cl	0.3029025
P47898	37	>= 1 Cl	0.3027468
P47898	630	O-C:C-O-C	0.3013872
P47898	643	[#1]-C-C-N-[#1]	0.2866136
P47898	7	>= 2 B	0.2839023
P47898	702	O-C-C-C-C-C-N-C	0.2810089
P47898	455	N(-O)(=O)	0.2764102
P47898	451	C(-N)(=O)	0.2747281
P47898	295	C-As	0.2668287
P47898	260	>= 3 hetero-aromatic rings	0.249044
P47898	392	N(~C)(~C)(~H)	0.2481571
P47898	25	>= 4 F	0.245581
P47898	339	C(~C)(~C)(~H)(~O)	0.2433858
P47898	192	>= 3 any ring size 6	0.2394053
P47898	774	Clc1c(Br)cccc1	0.2375495
P47898	529	Cl-C-C-Cl	0.2373225
P47898	621	N-C:C:C:N	0.2347177
P47898	768	Sc1c(Cl)cccc1	0.2346761

P47898	397	N(~C)(:C)(:C)	0.2308163
P47898	90	>= 1 Re	0.225634
P47898	380	C(~O)(~O)	0.2228018
P47898	797	CC1CC(C)CCC1	0.2218078
P47898	16	>= 4 N	0.2216254
P47898	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.2194628
P47898	8	>= 4 B	0.2135965
P47898	296	C-Se	0.2085248
P47898	441	C(-C)(=C)	0.2058139
P47898	680	O-C-C-C-C-C	0.2051394
P47898	583	Cl-C:C-O-C	0.2010376
P47898	272	B-H	2.00E-01
P47898	707	O=C-C-C-C-C(N)-C	0.1986146
P47898	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.1977848
P47898	684	O=C-C-C-C-C	0.1952062
P47898	758	Cc1c(N)cccc1	0.1937027
P47898	554	Br-C-C-C	0.1936242
P47898	525	[As]-C:C-[#1]	0.187735
P47898	305	N-S	0.1855238
P47898	213	>= 1 any ring size 7	0.1839688
P47898	750	Nc1cc(Cl)ccc1	0.1830963
P47898	29	>= 2 Si	0.1818683
P47898	418	C=N	0.1813834
P47898	726	Sc1ccc(Cl)cc1	0.1786935
P47898	482	C:N-C:C	0.1768807
P47898	440	C(-C)(-O)(=O)	0.1740592
P47898	681	O-C-C-C-C-O	0.1644293
P47898	52	>= 1 Ca	0.1599735
P47898	452	C(-O)(=O)	0.1584318
P47898	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.1572325
P47898	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.154594
P47898	496	N:N-C-[#1]	0.1499667
P47898	299	N-H	0.148627
P47898	615	N-C-C-O-C	0.1485499
P47898	699	O-C-C-C-C-C(C)-C	0.1484895
P47898	734	Cc1cc(C)ccc1	0.1476029
P47898	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.1474124
P47898	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.1465194
P47898	399	N(~H)(:C)	0.144877
P47898	714	Cc1ccc(O)cc1	0.1441548
P47898	821	CC1C(N)CCCC1	0.1410639
P47898	757	Cc1c(S)cccc1	0.1395052
P47898	755	Cc1c(C)cccc1	0.1380635
P47898	567	O-C-C-O	0.1347074
P47898	110	>= 1 Er	0.1328981
P47898	715	Cc1ccc(S)cc1	0.1325558
P47898	740	Oc1cc(O)ccc1	0.1325014
P47898	479	S-C-S-C	0.1302159

P47898	234	>= 2 any ring size 8	0.1235
P47898	398	N(~H)(~N)	0.1232576
P47898	781	CC1CCC(Br)CC1	0.1224284
P47898	593	N-C-C-C-N	0.1203551
P47898	12	>= 16 C	0.1134241
P47898	259	>= 3 aromatic rings	0.1129076
P47898	111	>= 1 Tm	0.1107555
P47898	334	C(~C)(~C)(~C)(~C)	0.1087527
P47898	558	O=N-C:C	0.1086459
P47898	470	C:C-C=C	0.1008016
P47898	1	>= 8 H	0.0996131
P47898	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.0970976
P47898	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0951669
P47898	737	Cc1cc(N)ccc1	0.0929333
P47898	669	Cl-C:C-C=O	0.0870831
P47898	355	C(~C)(:C)	0.0863826
P47898	678	C-C-C=C-C	0.0824167
P47898	78	>= 1 Cd	8.11E-02
P47898	494	O=C-C:N	0.078139
P47898	498	O-C=C-C	0.0781125
P47898	542	O-C:C-[#1]	0.0738097
P47898	777	CC1CCC(O)CC1	0.0733438
P47898	354	C(~C)(~Si)	0.0723308
P47898	294	C-Cl	0.0706186
P47898	735	Cc1cc(O)ccc1	0.0702534
P47898	544	O-C:C-O	0.0680714
P47898	288	C-Na	0.0670113
P47898	99	>= 1 La	0.0667052
P47898	113	>= 1 Tc	0.0666613
P47898	689	O-C-C-C-C-C-C	0.066187
P47898	53	>= 1 Sc	0.0653447
P47898	38	>= 2 Cl	0.0651792
P47898	308	O-H	0.0645355
P47898	410	P(~C)(~C)	0.0637028
P47898	77	>= 1 Ag	0.0633569
P47898	814	NC1CC(Br)CCC1	0.0630069
P47898	24	>= 2 F	0.0600288
P47898	320	Si-H	0.0596091
P47898	762	Oc1c(S)cccc1	0.0589192
P47898	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0589137
P47898	277	B-F	0.0580607
P47898	720	Oc1ccc(S)cc1	0.0575791
P47898	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0568722
P47898	185	>= 2 any ring size 6	0.0548859
P47898	76	>= 1 Pd	0.0542993
P47898	614	C-C-O-C-C	0.0539237
P47898	611	N-C-C-N-C	0.0524908
P47898	716	Cc1ccc(N)cc1	0.0516632

P47898	487	N-C=N-C	0.051337
P47898	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0506289
P47898	143	>= 1 any ring size 5	0.0490563
P47898	282	B-Br	0.0482128
P47898	319	Al-Cl	0.0456231
P47898	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.045203
P47898	129	>= 1 any ring size 4	0.0447316
P47898	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0429332
P47898	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.0425743
P47898	818	CC1C(C)CCCC1	0.0421092
P47898	541	O-C:C-C	0.0409636
P47898	532	S-C:C-[#1]	0.0404378
P47898	579	O=C-C-C-C	0.0400251
P47898	431	C(-C)(-C)(=N)	0.0398711
P47898	607	N-C-C-C:C	0.0396474
P47898	686	O=C-C-C-C-O	0.0390538
P47898	171	>= 5 any ring size 5	0.038521
P47898	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	3.78E-02
P47898	21	>= 8 O	0.0377597
P47898	513	S:C:C-[#1]	0.0374917
P47898	438	C(-C)(-N)(=N)	0.0374612
P47898	694	O=C-C-C-C-C=O	0.0348915
P47898	446	C(-H)(=C)	0.034874
P47898	775	Brc1c(Br)cccc1	0.0344518
P47898	395	N(~C)(~O)	0.0330603
P47898	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0329113
P47898	591	Cl-C-C-C-C	0.0322145
P47898	533	S-C:C-N	0.0316434
P47898	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0310494
P47898	738	Cc1cc(Cl)ccc1	0.029337
P47898	504	N:C:N-C	0.0285776
P47898	331	C(~Br)(:N)	0.0272829
P47898	379	C(~N)(:N)	0.0264436
P47898	2	>= 16 H	0.0249069
P47898	675	Br-C-C-C:C	0.0236359
P47898	799	CC1CC(S)CCC1	0.0230606
P47898	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.022393
P47898	770	Nc1c(N)cccc1	0.0220085
P47898	851	SC1CC(N)CC1	0.021843
P47898	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.0212356
P47898	114	>= 1 U	0.0211767
P47898	5	>= 2 Li	0.0204178
P47898	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0202495
P47898	850	SC1CC(S)CC1	0.0200877
P47898	461	O-C-C=N	0.0195735
P47898	786	OC1CCC(Br)CC1	0.0193603
P47898	206	>= 5 any ring size 6	0.0188484
P47898	59	>= 1 Co	0.018616

P47898	561	Cl-C-C=O	0.0183675
P47898	605	O=C-C-O-C	0.0171534
P47898	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0170065
P47898	847	OC1CC(N)CC1	0.0169344
P47898	784	OC1CCC(N)CC1	0.0168558
P47898	292	C-P	0.0166932
P47898	877	NC1C(Br)CCC1	0.0166161
P47898	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0163707
P47898	325	As-H	0.0162762
P47898	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.0161224
P47898	575	O-C-C:C-O	0.0160976
P47898	545	N-C:C-C	0.0159638
P47898	852	SC1CC(Cl)CC1	0.0151069
P47898	425	P=O	0.0150955
P47898	86	>= 1 Lu	0.0150754
P47898	46	>= 1 I	0.0149448
P47898	550	Cl-C-C-C	0.0147173
P47898	569	N-C-C-N	0.0134742
P47898	828	OC1C(Br)CCCC1	0.0129454
P47898	653	O-C:C:C-O	0.0122386
P47898	493	O=C-C:C	0.0110483
P47898	6	>= 1 B	0.0103253
P47898	813	NC1CC(Cl)CCC1	0.0102325
P47898	665	N-C:C-C-C	0.0102219
P47898	688	C-C-C-C-C-C-C	0.009972
P47898	83	>= 1 Xe	0.0085605
P47898	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.0084835
P47898	879	ClC1C(Br)CCC1	0.0084578
P47898	817	BrC1CC(Br)CCC1	0.0084053
P47898	816	ClC1CC(Br)CCC1	0.008314
P47898	43	>= 1 Br	0.0078756
P47898	273	B-B	0.0073974
P47898	746	Sc1cc(N)ccc1	0.0071891
P47898	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0070434
P47898	489	N-C-S-C	0.0069639
P47898	826	OC1C(N)CCCC1	0.0064388
P47898	710	C-C-C(C)-C-C	0.006135
P47898	336	C(~C)(~C)(~C)(~N)	0.0059356
P47898	868	OC1C(N)CCC1	0.005913
P47898	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.0056901
P47898	49	>= 1 Be	0.0055963
P47898	507	C-C-S-C	0.0055508
P47898	285	C-N	0.0054098
P47898	792	NC1CCC(Cl)CC1	0.0052319
P47898	32	>= 4 P	0.0048405
P47898	349	C(~C)(~H)(~S)	0.0037295
P47898	741	Oc1cc(S)ccc1	0.0035175
P47898	84	>= 1 Cs	0.0034766

P47898	719	Oc1ccc(O)cc1	0.0033256
P47898	69	>= 1 Sr	0.0033125
P47898	365	C(~H)(~N)	0.00321
P47898	387	C(:C)(:N)	0.0023258
P47898	459	S(=O)(=O)	0.0020512
P47898	820	CC1C(S)CCCC1	0.0020343
P47898	756	Cc1c(O)cccc1	0.0019324
P47898	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0018058
P47898	627	O=[As]-C:C:C	0.0017411
P47898	570	C:C-C-C	0.0015573
P47898	766	Sc1c(S)cccc1	0.0015279
P47898	773	Clc1c(Cl)cccc1	0.001318
P47898	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.0012828
P47898	849	OC1CC(Br)CC1	0.0010993
P47898	60	>= 1 Ni	0.0009711
P47898	413	S(~C)(~H)	0.0006335
P47898	445	C(-H)(-N)(=C)	0.0006062
P47898	389	C(:N)(:N)	0.0006005
P47898	478	S-C=N-[#1]	0.0004984
P47898	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0002772
P47898	732	Clc1ccc(Br)cc1	5.31E-05
P47898	361	C(~Cl)(~H)	2.66E-05
P47898	228	>= 1 saturated or aromatic carbon-only ring size 8	5.69E-06
P47898	871	SC1C(S)CCC1	3.75E-09
P47898	85	>= 1 Ba	5.82E-10
P47898	57	>= 1 Mn	-3.51E-10
P47898	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	-4.87E-10
P47898	0	>= 4 H	-5.04E-10
P47898	256	>= 1 hetero-aromatic ring	-1.02E-09
P47898	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	-1.32E-09
P47898	61	>= 1 Cu	-1.43E-09
P47898	40	>= 8 Cl	-1.65E-09
P47898	864	CC1C(Cl)CCC1	-2.28E-09
P47898	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	-3.53E-09
P47898	248	>= 1 any ring size 10	-3.66E-09
P47898	97	>= 1 Pb	-5.09E-09
P47898	552	C:C-C:C	-0.000389
P47898	362	C(~Cl)(:C)	-0.000562
P47898	619	O-C-C=C-C	-0.000577
P47898	622	O=C-O-C:C	-0.000593
P47898	47	>= 2 I	-0.000675
P47898	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.000782
P47898	754	Brc1cc(Br)ccc1	-0.000842
P47898	388	C(:C)(:N)(:N)	-0.000965
P47898	483	N-S-C:C	-0.001238
P47898	848	OC1CC(Cl)CC1	-0.001279
P47898	584	C:C-C=C-C	-0.001305
P47898	659	O-C-C-N-C	-0.001325

P47898	333	C(~C)(~C)(~C)	-0.001339
P47898	322	Si-Cl	-0.001748
P47898	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.001767
P47898	318	Al-H	-2.02E-03
P47898	95	>= 1 Hg	-0.002086
P47898	578	C-C:C-C:C	-0.002105
P47898	585	C-C:C-N-C	-0.002458
P47898	543	O-C:C-N	-0.002753
P47898	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	-0.003009
P47898	385	C(:C)(:C)(:C)	-0.003219
P47898	371	C(~H)(:C)(:C)	-0.00324
P47898	801	CC1CC(Cl)CCC1	-0.003255
P47898	63	>= 1 Ga	-0.003271
P47898	290	C-Al	-0.003681
P47898	503	Cl-C:C-[#1]	-0.003732
P47898	402	N(~O)(:O)	-0.00391
P47898	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	-0.004239
P47898	502	N-C=C-[#1]	-0.004394
P47898	144	>= 1 saturated or aromatic carbon-only ring size 5	-0.004535
P47898	101	>= 1 Pr	-0.004987
P47898	807	OC1CC(Br)CCC1	-0.005118
P47898	713	Cc1ccc(C)cc1	-0.005291
P47898	271	Li-Cl	-0.005625
P47898	108	>= 1 Dy	-0.005665
P47898	723	Oc1ccc(Br)cc1	-0.006362
P47898	594	C-O-C-C=C	-0.006656
P47898	280	B-S	-0.007178
P47898	604	C-O-C-C:C	-0.007378
P47898	523	N:C:C-C	-0.007391
P47898	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	-0.007528
P47898	693	O=C-C-C-C-C-O	-0.008097
P47898	744	Oc1cc(Br)ccc1	-0.008532
P47898	800	CC1CC(N)CCC1	-0.00865
P47898	81	>= 1 Sb	-0.00872
P47898	556	C=C-C-C	-0.009095
P47898	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	-0.009411
P47898	846	OC1CC(S)CC1	-0.009595
P47898	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	-0.010317
P47898	822	CC1C(Cl)CCCC1	-0.010328
P47898	709	C-C(C)-C-C-C	-0.010409
P47898	92	>= 1 Ir	-0.010766
P47898	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	-0.010888
P47898	235	>= 2 saturated or aromatic carbon-only ring size 8	-0.010908
P47898	601	N-C:C:C-N	-0.011046
P47898	537	O=C-C-O	-0.012119
P47898	340	C(~C)(~C)(~N)	-0.01228
P47898	553	O=C-C=C	-0.012545
P47898	411	P(~O)(~O)	-0.012888

P47898	759	Cc1c(Cl)cccc1	−0.012957
P47898	384	C(:C)(:C)	−0.013401
P47898	843	CC1CC(Cl)CC1	−0.015806
P47898	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.016123
P47898	22	>= 16 O	−0.016391
P47898	287	C-F	−0.01685
P47898	867	OC1C(S)CCC1	−0.017643
P47898	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.018785
P47898	291	C-Si	−0.018942
P47898	518	O=C-N-N	−0.019423
P47898	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.019707
P47898	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.020833
P47898	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.020949
P47898	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.02121
P47898	527	C:C:N-[#1]	−0.021218
P47898	302	N-F	−0.021704
P47898	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.022356
P47898	535	O=C-C-C	−0.022718
P47898	510	[#1]-N-N-[#1]	−0.023182
P47898	546	N-C:C-[#1]	−0.023377
P47898	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.025431
P47898	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.025663
P47898	519	N=C-N-C	−0.025718
P47898	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.02779
P47898	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.028873
P47898	269	Li-P	−0.029479
P47898	423	N=O	−0.029912
P47898	390	N(~C)(~C)	−0.03001
P47898	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.031262
P47898	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.032042
P47898	72	>= 1 Nb	−0.033081
P47898	860	CC1C(C)CCC1	−0.033736
P47898	670	Br-C:C:C-C	−0.034106
P47898	610	C-O-C-O-C	−0.035184
P47898	327	C(~Br)(~C)	−0.03522
P47898	396	N(~C)(:C)	−0.036822
P47898	697	C-C-C-C-C-C(C)-C	−0.037257
P47898	363	C(~F)(~F)	−0.037316
P47898	429	C(#N)(-C)	−0.037851
P47898	491	C-N:C-[#1]	−0.038119
P47898	861	CC1C(O)CCC1	−0.038572
P47898	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.038847
P47898	654	N-C-N-C-C	−0.039362
P47898	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.040605
P47898	415	Si(~C)(~C)	−0.04092
P47898	530	N:C-C:C	−0.041081
P47898	745	Sc1cc(S)ccc1	−0.041556
P47898	549	N-C-C:C	−0.042037

P47898	104	>= 1 Sm	−0.042073
P47898	17	>= 8 N	−0.042225
P47898	798	CC1CC(O)CCC1	−0.042796
P47898	625	O=C-C:C-O	−0.042807
P47898	321	Si-Si	−0.043203
P47898	460	C-C-C#C	−0.043295
P47898	261	>= 4 aromatic rings	−0.043631
P47898	572	N:C:N:C	−0.044997
P47898	28	>= 1 Si	−0.04545
P47898	469	S-S-C:C	−0.046395
P47898	705	O=C-C-C-C-C(O)-C	−0.0465
P47898	855	NC1CC(Cl)CC1	−0.047739
P47898	626	C-O-C:C-C	−0.049203
P47898	859	BrC1CC(Br)CC1	−0.049498
P47898	109	>= 1 Ho	−0.049604
P47898	475	S-C=N-C	−0.052889
P47898	595	C:C-C-C-C	−0.053156
P47898	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.053392
P47898	540	C-N-C-[#1]	−0.053719
P47898	87	>= 1 Hf	−0.054378
P47898	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.054758
P47898	35	>= 4 S	−0.054857
P47898	265	Li-B	−0.054986
P47898	80	>= 1 Sn	−0.055104
P47898	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.055813
P47898	71	>= 1 Zr	−0.056781
P47898	736	Cc1cc(S)ccc1	−0.058034
P47898	9	>= 2 C	−0.059254
P47898	853	SC1CC(Br)CC1	−0.059417
P47898	34	>= 2 S	−0.059631
P47898	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.060234
P47898	481	O-S-C:C	−0.060294
P47898	790	SC1CCC(Br)CC1	−0.060799
P47898	374	C(~H)(~H)(~H)	−0.060888
P47898	606	O-C:C-C-C	−0.061946
P47898	765	Oc1c(Br)cccc1	−0.062934
P47898	858	ClC1CC(Br)CC1	−0.064601
P47898	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.064831
P47898	862	CC1C(S)CCC1	−0.065066
P47898	629	S-C:C:C-N	−0.065166
P47898	401	N(~O)(~O)	−0.065212
P47898	566	O-C-C-N	−0.065277
P47898	89	>= 1 W	−0.065295
P47898	748	Sc1cc(Br)ccc1	−0.065712
P47898	428	C(#C)(-H)	−0.06575
P47898	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.066262
P47898	796	BrC1CCC(Br)CC1	−0.06643
P47898	270	Li-S	−0.066646

P47898	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.066829
P47898	528	[#1]-N-C-[#1]	−0.066963
P47898	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.066994
P47898	698	O-C-C-C-C-C-C-C	−0.067522
P47898	417	C#C	−0.067949
P47898	505	Cl-C:C-O	−0.070943
P47898	805	OC1CC(N)CCC1	−0.071399
P47898	357	C(~C)(:C)(:N)	−0.071708
P47898	776	CC1CCC(C)CC1	−0.072412
P47898	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.073162
P47898	788	SC1CCC(N)CC1	−0.074117
P47898	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.077065
P47898	581	O=C-C-C-O	−0.077096
P47898	573	O-C-C=C	−0.078553
P47898	783	OC1CCC(S)CC1	−0.07973
P47898	136	>= 2 any ring size 4	−0.07988
P47898	685	O=C-C-C-C-N	−0.08034
P47898	377	C(~N)(:C)(:C)	−0.080589
P47898	342	C(~C)(~Cl)	−0.081586
P47898	150	>= 2 any ring size 5	−0.082301
P47898	409	O(:C)(:C)	−0.083976
P47898	480	C:S:C-C	−0.084128
P47898	835	NC1C(Br)CCCC1	−0.084156
P47898	809	SC1CC(N)CCC1	−0.085355
P47898	701	O-C-C-C-C-C(O)-C	−0.085641
P47898	812	NC1CC(N)CCC1	−0.086578
P47898	834	NC1C(Cl)CCCC1	−0.088352
P47898	538	N=C-C-C	−0.088881
P47898	437	C(-C)(-N)(=C)	−0.089487
P47898	344	C(~C)(~H)	−0.089728
P47898	351	C(~C)(~N)	−0.092401
P47898	679	C-C-C-C-C-C	−0.092638
P47898	691	O-C-C-C-C-C-N	−0.093507
P47898	23	>= 1 F	−0.093732
P47898	547	N-C:C-N	−0.094374
P47898	703	O-C-C-C-C-C(N)-C	−0.094386
P47898	577	C:C-N-C:C	−0.094943
P47898	599	[#1]-C-C=C-[#1]	−0.096329
P47898	341	C(~C)(~C)(~O)	−0.096406
P47898	408	O(~H)(~S)	−0.098677
P47898	326	As-As	−0.100905
P47898	315	O-K	−0.103489
P47898	515	N-N-C-C	−0.104341
P47898	690	O-C-C-C-C-C-O	−0.107012
P47898	646	O=C-N-C-[#1]	−0.107686
P47898	312	O-Al	−0.108834
P47898	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.111219
P47898	609	Cl-C-C-N-C	−0.112487

P47898	14	>= 1 N	−0.114125
P47898	258	>= 2 hetero-aromatic rings	−0.118236
P47898	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.121254
P47898	668	C-C:C-C-C	−0.124742
P47898	41	>= 1 K	−0.128508
P47898	430	C(-C)(-C)(=C)	−0.129734
P47898	819	CC1C(O)CCCC1	−0.129758
P47898	857	ClC1CC(Cl)CC1	−0.134354
P47898	557	N:C-O-[#1]	−0.139416
P47898	68	>= 1 Rb	−0.146261
P47898	443	C(-C)(=O)	−0.148224
P47898	456	P(-O)(=O)	−0.148701
P47898	806	OC1CC(Cl)CCC1	−0.14948
P47898	536	O=C-C-N	−0.151948
P47898	588	O=C-C-C=O	−0.152019
P47898	457	S(-C)(=O)	−0.152148
P47898	660	C-C=C-C-C	−0.152895
P47898	763	Oc1c(N)cccc1	−0.15604
P47898	613	C-N-C-C-C	−0.156495
P47898	651	O-C:C:C-C	−0.157655
P47898	743	Oc1cc(Cl)ccc1	−0.160716
P47898	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.162982
P47898	416	C=C	−0.166052
P47898	840	CC1CC(O)CC1	−0.170647
P47898	345	C(~C)(~H)(~N)	−0.174684
P47898	375	C(~N)(~N)	−0.178554
P47898	838	BrC1C(Br)CCCC1	−0.179601
P47898	602	O=C-C-N-C	−0.180776
P47898	386	C(:C)(:C)(:N)	−0.181817
P47898	764	Oc1c(Cl)cccc1	−0.184016
P47898	711	C-C(C)(C)-C-C	−0.188548
P47898	367	C(~H)(~O)(~O)	−0.192043
P47898	856	NC1CC(Br)CC1	−0.195765
P47898	512	C-[As]-O-[#1]	−0.200049
P47898	650	O=C-N-C=O	−0.202835
P47898	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.206811
P47898	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.213133
P47898	576	N=C-C:C-[#1]	−0.220049
P47898	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.220166
P47898	492	N-C:O:C	−0.220452
P47898	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.221416
P47898	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.222321
P47898	462	O-C-C=O	−0.229162
P47898	484	N-C:N:C	−0.232805
P47898	830	SC1C(N)CCCC1	−0.234693
P47898	563	O-C-O-C	−0.236414
P47898	870	OC1C(Br)CCC1	−0.236421
P47898	439	C(-C)(-N)(=O)	−0.242441

P47898	346	C(~C)(~H)(~O)	−0.258363
P47898	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.26175
P47898	391	N(~C)(~C)(~C)	−0.267931
P47898	405	O(~C)(~C)	−0.273907
P47898	624	O=C-C:C-N	−0.27607
P47898	263	Li-H	−0.276979
P47898	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.278062
P47898	419	C#N	−0.280483
P47898	471	S:C:C:C	−0.281879
P47898	728	Nc1ccc(N)cc1	−0.287142
P47898	364	C(~F)(:C)	−0.28803
P47898	555	N=C-C=C	−0.290072
P47898	488	N-C=N-[#1]	−0.291236
P47898	655	O-C-C-C:C	−0.292015
P47898	559	O-C-N-[#1]	−0.295316
P47898	771	Nc1c(Cl)cccc1	−0.301858
P47898	866	OC1C(O)CCC1	−0.305314
P47898	66	>= 1 Se	−0.307905
P47898	404	N(:C)(:C)(:C)	−0.31047
P47898	729	Nc1ccc(Cl)cc1	−0.3136
P47898	103	>= 1 Pm	−0.314295
P47898	649	O=N-C:C-O	−0.317392
P47898	506	C-C:N:C	−0.325016
P47898	672	O=C-C=C-[#1]	−0.328446
P47898	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.329705
P47898	304	N-P	−0.338752
P47898	122	>= 2 any ring size 3	−0.338773
P47898	426	P=P	−0.340625
P47898	400	N(~H)(:C)(:C)	−0.348791
P47898	490	C-C-C=C	−0.349544
P47898	742	Oc1cc(N)ccc1	−0.350541
P47898	845	OC1CC(O)CC1	−0.353379
P47898	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.355217
P47898	779	CC1CCC(N)CC1	−0.35712
P47898	449	C(-N)(=C)	−0.358463
P47898	378	C(~N)(:C)(:N)	−0.35961
P47898	712	C-C(C)-C(C)-C	−0.360887
P47898	676	N#C-C-C-C	−0.365936
P47898	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.366697
P47898	587	N-C:C-O-[#1]	−0.372336
P47898	412	S(~C)(~C)	−0.376562
P47898	597	O=C-C-C:C	−0.378462
P47898	278	B-Si	−0.384977
P47898	560	N-C-N-C	−0.386676
P47898	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.389918
P47898	107	>= 1 Tb	−0.392567
P47898	636	C-N-C-N-C	−0.395035
P47898	100	>= 1 Ce	−0.397349

P47898	832	SC1C(Br)CCCC1	−0.400464
P47898	442	C(-C)(=N)	−0.404149
P47898	257	>= 2 aromatic rings	−0.404189
P47898	683	N-C-C-C-C-C	−0.404363
P47898	647	O=C-N-C-N	−0.410849
P47898	596	N=C-N-C-C	−0.41544
P47898	612	N-C-O-C-C	−0.416642
P47898	20	>= 4 O	−0.423999
P47898	865	CC1C(Br)CCC1	−0.424129
P47898	4	>= 1 Li	−0.424179
P47898	54	>= 1 Ti	−0.427068
P47898	534	S-C:C-O	−0.429319
P47898	19	>= 2 O	−0.437573
P47898	718	Cc1ccc(Br)cc1	−0.442504
P47898	876	NC1C(Cl)CC1	−0.442853
P47898	376	C(~N)(:C)	−0.442995
P47898	656	C-C-N-C-C	−0.450883
P47898	368	C(~H)(~S)	−0.452712
P47898	352	C(~C)(~O)	−0.454245
P47898	279	B-P	−0.460072
P47898	831	SC1C(Cl)CCCC1	−0.462059
P47898	366	C(~H)(~O)	−0.463002
P47898	58	>= 1 Fe	−0.464624
P47898	422	N=N	−0.464637
P47898	571	[#1]-C-O-[#1]	−0.467601
P47898	724	Sc1ccc(S)cc1	−0.470907
P47898	453	N(-C)(=C)	−0.47267
P47898	704	O=C-C-C-C-C-C-C	−0.48521
P47898	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.48645
P47898	836	ClC1C(Cl)CCCC1	−0.488163
P47898	854	NC1CC(N)CC1	−0.488383
P47898	520	C=C-C:C	−0.488799
P47898	74	>= 1 Ru	−0.491179
P47898	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.493527
P47898	255	>= 1 aromatic ring	−0.497492
P47898	474	S:C:C:N	−0.500231
P47898	839	CC1CC(C)CC1	−0.504183
P47898	106	>= 1 Gd	−0.506347
P47898	844	CC1CC(Br)CC1	−0.506708
P47898	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.508636
P47898	509	Br-C:C-C	−0.508758
P47898	435	C(-C)(-H)(=N)	−0.509757
P47898	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.51192
P47898	31	>= 2 P	−0.512689
P47898	880	BrC1C(Br)CCC1	−0.516974
P47898	620	C:C-O-C-C	−0.520637
P47898	497	O-C:C:N	−0.521127
P47898	793	NC1CCC(Br)CC1	−0.523345

P47898	841	CC1CC(S)CC1	−0.525553
P47898	157	>= 3 any ring size 5	−0.527726
P47898	687	O=C-C-C-C=O	−0.528735
P47898	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.537172
P47898	869	OC1C(Cl)CCC1	−0.537882
P47898	778	CC1CCC(S)CC1	−0.542726
P47898	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.543485
P47898	64	>= 1 Ge	−0.554497
P47898	749	Nc1cc(N)ccc1	−0.556615
P47898	88	>= 1 Ta	−0.562306
P47898	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.562366
P47898	692	O=C-C-C-C-C-C	−0.565522
P47898	808	SC1CC(S)CCC1	−0.570991
P47898	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.574098
P47898	393	N(~C)(~H)	−0.578646
P47898	645	O=C-N-C-C	−0.585608
P47898	769	Sc1c(Br)cccc1	−0.586361
P47898	500	C-S-C:C	−0.59021
P47898	394	N(~C)(~H)(~N)	−0.597106
P47898	370	C(~H)(:C)	−0.600207
P47898	300	N-N	−0.607946
P47898	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.610193
P47898	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.622998
P47898	641	O-C-C-C=C	−0.62405
P47898	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.625281
P47898	309	O-O	−0.627705
P47898	313	O-Si	−0.630113
P47898	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.632867
P47898	281	B-Cl	−0.635746
P47898	427	C(#C)(-C)	−0.651355
P47898	824	OC1C(O)CCCC1	−0.653602
P47898	79	>= 1 In	−0.6651
P47898	45	>= 4 Br	−0.670374
P47898	598	Cl-C:C:C-C	−0.680678
P47898	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.682942
P47898	199	>= 4 any ring size 6	−0.690287
P47898	633	N-C-C:C-C	−0.696766
P47898	414	S(~C)(~O)	−0.697562
P47898	381	C(~O)(:C)	−0.702465
P47898	767	Sc1c(N)cccc1	−0.702827
P47898	406	O(~C)(~H)	−0.709144
P47898	637	O-C-C-C-C	−0.713746
P47898	727	Sc1ccc(Br)cc1	−0.726597
P47898	330	C(~Br)(:C)	−0.763032
P47898	98	>= 1 Bi	−0.778635
P47898	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.782679
P47898	590	C-C:C-O-[#1]	−0.78465
P47898	432	C(-C)(-C)(=O)	−0.797158

P47898	178	>= 1 any ring size 6	−0.799872
P47898	842	CC1CC(N)CC1	−0.800058
P47898	725	Sc1ccc(N)cc1	−0.800229
P47898	603	C-C:C:C-C	−0.802828
P47898	328	C(~Br)(~C)(~C)	−0.805551
P47898	51	>= 1 Al	−0.807876
P47898	517	N-N-C-N	−0.826786
P47898	666	C=C-C-O-C	−0.849605
P47898	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.850263
P47898	780	CC1CCC(Cl)CC1	−0.858222
P47898	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.861434
P47898	284	C-C	−0.861656
P47898	589	C-C:C-O-C	−0.862922
P47898	293	C-S	−0.874911
P47898	631	O-C:C-O-[#1]	−0.887938
P47898	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.903792
P47898	833	NC1C(N)CCCC1	−0.906813
P47898	27	>= 2 Na	−0.907612
P47898	787	SC1CCC(S)CC1	−0.907778
P47898	863	CC1C(N)CCC1	−0.941389
P47898	663	O-C-C-O-[#1]	−0.952205
P47898	332	C(~C)(~C)	−0.985768
P47898	11	>= 8 C	−0.990646
P47898	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−1.000977
P47898	721	Oc1ccc(N)cc1	−1.010012
P47898	485	N:C:C:N	−1.010618
P47898	105	>= 1 Eu	−1.01368
P47898	329	C(~Br)(~H)	−1.015812
P47898	10	>= 4 C	−1.020293
P47898	73	>= 1 Mo	−1.025962
P47898	448	C(-H)(=O)	−1.034971
P47898	67	>= 1 Kr	−1.039854
P47898	200	>= 4 saturated or aromatic carbon-only ring size 6	−1.087751
P47898	472	C:N:C-C	−1.093465
P47898	803	OC1CC(O)CCC1	−1.097207
P47898	652	O-C:C:C-N	−1.098461
P47898	829	SC1C(S)CCCC1	−1.108547
P47898	62	>= 1 Zn	−1.124357
P47898	347	C(~C)(~H)(~O)(~O)	−1.149931
P47898	75	>= 1 Rh	−1.155962
P47898	343	C(~C)(~Cl)(~H)	−1.179451
P47898	673	O=C-C=C-N	−1.181554
P47898	262	>= 4 hetero-aromatic rings	−1.189579
P47898	26	>= 1 Na	−1.216189
P47898	91	>= 1 Os	−1.225389
P47898	531	S-C:C-C	−1.225746
P47898	708	C-C(C)-C-C	−1.26E+00
P47898	454	N(-C)(=O)	−1.312002

P47898	795	ClC1CCC(Br)CC1	−1.341152
P47898	722	Oc1ccc(Cl)cc1	−1.372753
P47898	811	SC1CC(Br)CCC1	−1.380191
P47898	447	C(-H)(=N)	−1.398909
P47898	444	C(-Cl)(=O)	−1.449195
P47898	823	CC1C(Br)CCCC1	−1.477514
P47898	639	O-C-C-C-O	−1.512557
P47898	634	C-C-C:C-C	−1.526909
P47898	424	N=P	−1.61964
P47898	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.64131
P47898	657	C-N-C:C-C	−1.64429
P47898	648	O=N-C:C-N	−1.763812
P47898	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−1.777431
P47898	677	C-C=C-C:C	−1.820967
P47898	761	Oc1c(O)cccc1	−1.832759
P47898	241	>= 1 any ring size 9	−1.88087
P47898	616	C:C:N:N:C	−1.919717
P47898	640	C=C-C-C-C	−1.929268
P47898	50	>= 1 Mg	−2.052485

rints（continued)

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-1.880870237	1.51E-09
-1.92025302	0.0005362
-1.928974132	-0.000294
-2.052484863	5.17E-09

Data S1. Ranking of importance of substructure features from Pubchem Fingerpı

GPCR ID	Bit Posit	Bit Substructure	W	P
O95136	572	N:C:N:C	2.485139	2.4887807
O95136	329	C(~Br)(~H)	2.179172	2.1791744
O95136	76	>= 1 Pd	2.049658	2.0496532
O95136	764	Oc1c(Cl)cccc1	1.884299	1.8839381
O95136	80	>= 1 Sn	1.834559	1.8345615
O95136	810	SC1CC(Cl)CCC1	1.823803	1.8239401
O95136	107	>= 1 Tb	1.799479	1.7994849
O95136	618	C:C-C-C:C	1.727467	1.7279859
O95136	68	>= 1 Rb	1.665378	1.6653761
O95136	471	S:C:C:C	1.511099	1.5147466
O95136	575	O-C-C:C-O	1.457064	1.4611617
O95136	490	C-C-C=C	1.405181	1.4061609
O95136	766	Sc1c(S)cccc1	1.380214	1.3789943
O95136	803	OC1CC(O)CCC1	1.370562	1.3675989
O95136	434	C(-C)(-H)(=C)	1.341976	1.341685
O95136	91	>= 1 Os	1.340381	1.340386
O95136	545	N-C:C-C	1.322617	1.3269022
O95136	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.310434	1.3104371
O95136	3	>= 32 H	1.24667	1.2466717
O95136	314	O-P	1.244482	1.2447525
O95136	69	>= 1 Sr	1.216174	1.2161727
O95136	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	1.214839	1.2148374
O95136	470	C:C-C=C	1.213631	1.2129421
O95136	860	CC1C(C)CCC1	1.188006	1.1946732
O95136	668	C-C:C-C-C	1.179104	1.1727613
O95136	496	N:N-C-[#1]	1.12821	1.1317817
O95136	683	N-C-C-C-C-C	1.11842	1.1178155
O95136	213	>= 1 any ring size 7	1.115178	1.121419
O95136	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	1.102257	1.1022599
O95136	856	NC1CC(Br)CC1	1.094403	1.0944061
O95136	822	CC1C(Cl)CCCC1	1.052627	1.0556565
O95136	171	>= 5 any ring size 5	1.042422	1.0424257
O95136	671	O=C-C=C-C	1.019725	1.0173651
O95136	88	>= 1 Ta	1.015359	1.0153542
O95136	405	O(~C)(~C)	1.012612	1.010442
O95136	75	>= 1 Rh	1.010597	1.0105995
O95136	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.99966	0.9999013
O95136	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.995564	0.9964104
O95136	751	Nc1cc(Br)ccc1	0.986727	0.9864418
O95136	690	O-C-C-C-C-C-O	0.964023	0.96029
O95136	831	SC1C(Cl)CCCC1	0.958303	0.9577316
O95136	753	Clc1cc(Br)ccc1	0.954123	0.9537873
O95136	74	>= 1 Ru	0.948212	0.9482132
O95136	746	Sc1cc(N)ccc1	0.925372	0.9207226
O95136	61	>= 1 Cu	0.918699	0.918705
O95136	677	C-C=C-C:C	0.909906	0.9090545

O95136	115	>= 1 any ring size 3	0.870179	0.8734744
O95136	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.86496	0.8649561
O95136	33	>= 1 S	0.860118	0.8647465
O95136	472	C:N:C-C	0.857358	0.8616615
O95136	734	Cc1cc(C)ccc1	0.85299	0.8525406
O95136	867	OC1C(S)CCC1	0.843867	0.8438703
O95136	651	O-C:C:C-C	0.838785	0.841348
O95136	774	Clc1c(Br)cccc1	0.836052	0.8360518
O95136	77	>= 1 Ag	0.828827	0.8288243
O95136	561	Cl-C-C=O	0.805873	0.8032087
O95136	73	>= 1 Mo	0.797742	0.7977435
O95136	714	Cc1ccc(O)cc1	0.787623	0.7913835
O95136	7	>= 2 B	0.78737	0.7873676
O95136	296	C-Se	0.784417	0.7844199
O95136	475	S-C=N-C	0.784218	0.7868509
O95136	97	>= 1 Pb	0.775691	0.7756914
O95136	313	O-Si	0.772443	0.7724449
O95136	71	>= 1 Zr	0.771635	0.771637
O95136	482	C:N-C:C	0.769559	0.7755573
O95136	89	>= 1 W	0.735195	0.7351998
O95136	297	C-Br	0.734439	0.7331079
O95136	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.733606	0.7336018
O95136	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.72547	0.7254698
O95136	739	Cc1cc(Br)ccc1	0.706572	0.7090184
O95136	172	>= 5 saturated or aromatic carbon-only ring size 5	0.703947	0.7039379
O95136	113	>= 1 Tc	0.697781	0.6977772
O95136	374	C(~H)(~H)(~H)	0.6832	0.684338
O95136	92	>= 1 Ir	0.678781	0.6787773
O95136	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.676661	0.6766616
O95136	158	>= 3 saturated or aromatic carbon-only ring size 5	0.674166	0.6741693
O95136	693	O=C-C-C-C-C-O	0.672619	0.6773563
O95136	847	OC1CC(N)CC1	0.672202	0.6722053
O95136	112	>= 1 Yb	0.67111	0.6711028
O95136	645	O=C-N-C-C	0.664748	0.6654091
O95136	150	>= 2 any ring size 5	0.664191	0.6634221
O95136	532	S-C:C-[#1]	0.657741	0.6603384
O95136	878	ClC1C(Cl)CCC1	0.656022	0.6560209
O95136	748	Sc1cc(Br)ccc1	0.652703	0.6511239
O95136	830	SC1C(N)CCCC1	0.644504	0.6470031
O95136	381	C(~O)(:C)	0.632134	0.6249803
O95136	28	>= 1 Si	0.620972	0.6209741
O95136	515	N-N-C-C	0.614816	0.6137384
O95136	32	>= 4 P	0.609348	0.609354
O95136	70	>= 1 Y	0.600828	0.6008332
O95136	652	O-C:C:C-N	0.595303	0.594281
O95136	661	O-C-O-C-C	0.580767	0.5795783
O95136	429	C(#N)(-C)	0.578352	0.5826574
O95136	687	O=C-C-C-C=O	0.577568	0.5758927

O95136	854	NC1CC(N)CC1	0.575131	0.575133
O95136	100	>= 1 Ce	0.574283	0.5742747
O95136	388	C(:C)(:N)(:N)	0.571965	0.5706012
O95136	858	ClC1CC(Br)CC1	0.566094	0.5660911
O95136	122	>= 2 any ring size 3	0.565378	0.5653781
O95136	414	S(~C)(~O)	0.564223	0.5640213
O95136	571	[#1]-C-O-[#1]	0.532134	0.5352227
O95136	463	N:C-S-[#1]	0.53032	0.5303142
O95136	640	C=C-C-C-C	0.524503	0.5280395
O95136	757	Cc1c(S)cccc1	0.514017	0.5116406
O95136	877	NC1C(Br)CCC1	0.506651	0.5066495
O95136	285	C-N	0.50484	0.508115
O95136	387	C(:C)(:N)	0.500621	0.5017514
O95136	266	Li-C	0.498783	0.4987838
O95136	639	O-C-C-C-O	0.494447	0.5021923
O95136	823	CC1C(Br)CCCC1	0.4897	0.4931291
O95136	819	CC1C(O)CCCC1	0.46846	0.4627563
O95136	529	Cl-C-C-Cl	0.464303	0.4645512
O95136	666	C=C-C-O-C	0.462968	0.4688312
O95136	382	C(~O)(:C)(:C)	0.460848	0.4571598
O95136	93	>= 1 Pt	0.452161	0.4521622
O95136	483	N-S-C:C	0.444838	0.444815
O95136	466	N#C-C=C	0.444544	0.4467452
O95136	42	>= 2 K	0.441544	0.4415399
O95136	763	Oc1c(N)cccc1	0.436624	0.4331023
O95136	643	[#1]-C-C-N-[#1]	0.434594	0.4398889
O95136	827	OC1C(Cl)CCCC1	0.434393	0.4340176
O95136	812	NC1CC(N)CCC1	0.433967	0.429949
O95136	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.433142	0.4331773
O95136	838	BrC1C(Br)CCCC1	0.430594	0.4305972
O95136	502	N-C=C-[#1]	0.43046	0.43231
O95136	39	>= 4 Cl	0.429432	0.4301121
O95136	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.418994	0.4189944
O95136	345	C(~C)(~H)(~N)	0.417466	0.4128587
O95136	362	C(~Cl)(:C)	0.41303	0.4130716
O95136	717	Cc1ccc(Cl)cc1	0.411821	0.4117726
O95136	771	Nc1c(Cl)cccc1	0.40855	0.4016342
O95136	843	CC1CC(Cl)CC1	0.405324	0.4053249
O95136	325	As-H	0.399819	0.3998271
O95136	443	C(-C)(=O)	0.399809	0.4046873
O95136	800	CC1CC(N)CCC1	0.396619	0.4026558
O95136	675	Br-C-C-C:C	0.394508	0.3950809
O95136	657	C-N-C:C-C	0.391601	0.390677
O95136	511	S=C-N-[#1]	0.391595	0.3952113
O95136	307	N-Br	0.383776	0.3837767
O95136	629	S-C:C:C-N	0.371668	0.3749678
O95136	461	O-C-C=N	0.366889	0.3668279
O95136	724	Sc1ccc(S)cc1	0.362544	0.3622351

O95136	818	CC1C(C)CCCC1	0.36193	0.356842
O95136	614	C-C-O-C-C	0.357888	0.3558414
O95136	676	N#C-C-C-C	0.354725	0.348903
O95136	808	SC1CC(S)CCC1	0.351595	0.3516002
O95136	698	O-C-C-C-C-C-C-C	0.345217	0.3419413
O95136	616	C:C:N:N:C	0.341585	0.3394492
O95136	448	C(-H)(=O)	0.338098	0.3359389
O95136	65	>= 1 As	0.335488	0.3354939
O95136	796	BrC1CCC(Br)CC1	0.327279	0.3272762
O95136	104	>= 1 Sm	0.322794	0.3227922
O95136	509	Br-C:C-C	0.32074	0.3198678
O95136	358	C(~C)(:N)	0.320396	0.3163822
O95136	773	Clc1c(Cl)cccc1	0.316399	0.3175603
O95136	349	C(~C)(~H)(~S)	0.314587	0.3170044
O95136	428	C(#C)(-H)	0.312904	0.3105764
O95136	523	N:C:C-C	0.309799	0.3105755
O95136	696	C-C-C-C-C-C-C-C	0.306102	0.3035219
O95136	335	C(~C)(~C)(~C)(~H)	0.304903	0.3098257
O95136	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.299438	0.2994364
O95136	334	C(~C)(~C)(~C)(~C)	0.298157	0.3049795
O95136	17	>= 8 N	0.296016	0.2974545
O95136	310	O-Mg	0.294064	0.2940619
O95136	720	Oc1ccc(S)cc1	0.285507	0.2836105
O95136	123	>= 2 saturated or aromatic carbon-only ring size 3	0.27909	0.279092
O95136	596	N=C-N-C-C	0.277751	0.2740528
O95136	460	C-C-C#C	0.276929	0.2767954
O95136	547	N-C:C-N	0.275451	0.2776627
O95136	798	CC1CC(O)CCC1	0.272445	0.2683272
O95136	143	>= 1 any ring size 5	0.263163	0.2650174
O95136	841	CC1CC(S)CC1	0.262136	0.2621417
O95136	824	OC1C(O)CCCC1	0.261248	0.2596977
O95136	23	>= 1 F	0.253797	0.2496502
O95136	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.251702	0.2494924
O95136	697	C-C-C-C-C-C(C)-C	0.251673	0.2471588
O95136	832	SC1C(Br)CCCC1	0.250142	0.2501436
O95136	813	NC1CC(Cl)CCC1	0.249574	0.2507684
O95136	637	O-C-C-C-C	0.246866	0.2449284
O95136	607	N-C-C-C:C	0.246023	0.2422188
O95136	617	C-C-C-O-[#1]	0.245361	0.2430092
O95136	84	>= 1 Cs	0.244746	0.2447463
O95136	48	>= 4 I	0.242121	0.2421229
O95136	13	>= 32 C	0.239708	0.2367607
O95136	809	SC1CC(N)CCC1	0.235849	0.2311984
O95136	864	CC1C(Cl)CCC1	0.234622	0.2346264
O95136	834	NC1C(Cl)CCCC1	0.232127	0.2252085
O95136	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.22462	0.2243503
O95136	655	O-C-C-C:C	0.224375	0.2259137
O95136	728	Nc1ccc(N)cc1	0.224053	0.226309

O95136	442	C(-C)(=N)	0.210065	0.2118088
O95136	712	C-C(C)-C(C)-C	0.20697	0.2071667
O95136	27	>= 2 Na	0.202641	0.202642
O95136	862	CC1C(S)CCC1	0.199255	0.1998885
O95136	294	C-Cl	0.19869	0.2003352
O95136	418	C=N	0.198349	0.2009158
O95136	735	Cc1cc(O)ccc1	0.198307	0.1963791
O95136	682	O-C-C-C-C-N	0.186786	0.1841482
O95136	86	>= 1 Lu	0.183364	0.1833646
O95136	389	C(:N)(:N)	0.181331	0.1844912
O95136	784	OC1CCC(N)CC1	0.178652	0.1772995
O95136	129	>= 1 any ring size 4	0.178372	0.184113
O95136	792	NC1CCC(Cl)CC1	0.175071	0.1737925
O95136	37	>= 1 Cl	0.173353	0.1690143
O95136	518	O=C-N-N	0.168319	0.1681612
O95136	369	C(~H)(~Si)	0.165528	0.1655305
O95136	286	C-O	0.159833	0.1533318
O95136	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.159599	0.1616081
O95136	353	C(~C)(~S)	0.157768	0.147761
O95136	363	C(~F)(~F)	0.155511	0.1577891
O95136	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.153411	0.1523517
O95136	658	C-C-S-C-C	0.150387	0.1511616
O95136	821	CC1C(N)CCCC1	0.149712	0.1440271
O95136	192	>= 3 any ring size 6	0.143127	0.1378976
O95136	440	C(-C)(-O)(=O)	0.138257	0.1396124
O95136	473	S-C:N:C	0.135802	0.128517
O95136	249	>= 1 saturated or aromatic carbon-only ring size 10	0.135657	0.1356598
O95136	308	O-H	0.133457	0.1306752
O95136	654	N-C-N-C-C	0.131887	0.1332466
O95136	305	N-S	0.129576	0.1314589
O95136	538	N=C-C-C	0.129085	0.1310794
O95136	590	C-C:C-O-[#1]	0.1282	0.1230922
O95136	392	N(~C)(~C)(~H)	0.122129	0.1237024
O95136	612	N-C-O-C-C	0.120866	0.1251791
O95136	437	C(-C)(-N)(=C)	0.11748	0.1241324
O95136	2	>= 16 H	0.115609	0.1156076
O95136	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.114544	0.1165615
O95136	820	CC1C(S)CCCC1	0.111709	0.1128331
O95136	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.108655	0.1125753
O95136	207	>= 5 saturated or aromatic carbon-only ring size 6	0.107045	0.1068768
O95136	62	>= 1 Zn	0.107004	0.1070046
O95136	524	C-C=C-C	0.105363	0.1057011
O95136	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.105108	0.105159
O95136	519	N=C-N-C	0.103237	0.1013854
O95136	528	[#1]-N-C-[#1]	0.100436	0.1023439
O95136	425	P=O	0.095953	0.0963517
O95136	765	Oc1c(Br)cccc1	0.094932	0.0921546
O95136	102	>= 1 Nd	0.094627	0.0946292

O95136	756	Cc1c(O)cccc1	0.091431	0.0887635
O95136	750	Nc1cc(Cl)ccc1	0.089352	0.0905472
O95136	794	ClC1CCC(Cl)CC1	0.088001	0.0803888
O95136	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.086541	0.0865352
O95136	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.086048	0.0844579
O95136	299	N-H	0.084176	0.0818026
O95136	606	O-C:C-C-C	0.081876	0.0822527
O95136	613	C-N-C-C-C	0.080503	0.0796751
O95136	711	C-C(C)(C)-C-C	0.080223	0.0833736
O95136	817	BrC1CC(Br)CCC1	0.078645	0.0797998
O95136	636	C-N-C-N-C	0.078269	0.0733756
O95136	50	>= 1 Mg	0.076512	0.0765129
O95136	394	N(~C)(~H)(~N)	0.076471	0.0737379
O95136	407	O(~C)(~P)	0.071232	0.0681153
O95136	566	O-C-C-N	0.070431	0.0700114
O95136	568	N#C-C-C	0.070314	0.0726429
O95136	713	Cc1ccc(C)cc1	0.070154	0.0650629
O95136	674	N-C-N-C:C	0.068523	0.074814
O95136	18	>= 1 O	0.067835	0.0773768
O95136	875	NC1C(N)CCC1	0.06669	0.0666908
O95136	303	N-Si	0.066491	0.0664873
O95136	289	C-Mg	0.066452	0.0664548
O95136	589	C-C:C-O-C	0.065924	0.0639066
O95136	512	C-[As]-O-[#1]	0.065613	0.0656102
O95136	772	Nc1c(Br)cccc1	0.065441	0.0654419
O95136	859	BrC1CC(Br)CC1	0.064219	0.0642153
O95136	55	>= 1 V	0.064135	0.0641423
O95136	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.063922	0.0639364
O95136	791	NC1CCC(N)CC1	0.063197	0.0644262
O95136	295	C-As	0.062024	0.062018
O95136	786	OC1CCC(Br)CC1	0.061493	0.0602439
O95136	848	OC1CC(Cl)CC1	0.061298	0.0612975
O95136	438	C(-C)(-N)(=N)	0.061261	0.0551664
O95136	846	OC1CC(S)CC1	0.060891	0.060891
O95136	730	Nc1ccc(Br)cc1	0.060659	0.0632737
O95136	373	C(~H)(:N)	0.060587	0.0648414
O95136	795	ClC1CCC(Br)CC1	0.060399	0.0604027
O95136	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.059899	0.0598994
O95136	539	N=C-C-[#1]	0.058405	0.0561956
O95136	60	>= 1 Ni	0.058001	0.058
O95136	390	N(~C)(~C)	0.057242	0.057645
O95136	880	BrC1C(Br)CCC1	0.056245	0.0562405
O95136	550	Cl-C-C-C	0.055696	0.0570202
O95136	577	C:C-N-C:C	0.055365	0.0539034
O95136	356	C(~C)(:C)(:C)	0.053845	0.0517319
O95136	630	O-C:C-O-C	0.052744	0.0512553
O95136	99	>= 1 La	0.051736	0.0517365
O95136	411	P(~O)(~O)	0.051603	0.0532651

O95136	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.051509	0.0515095
O95136	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.051501	0.0523355
O95136	130	>= 1 saturated or aromatic carbon-only ring size 4	0.050817	0.0458467
O95136	43	>= 1 Br	0.050728	0.0493396
O95136	599	[#1]-C-C=C-[#1]	0.05004	0.0487791
O95136	52	>= 1 Ca	0.049118	0.0491187
O95136	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.048312	0.0483098
O95136	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.047297	0.0483799
O95136	729	Nc1ccc(Cl)cc1	0.046391	0.0451181
O95136	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.04629	0.0489246
O95136	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.045025	0.0520902
O95136	476	C-O-C=C	0.044414	0.043674
O95136	417	C#C	0.043576	0.0411125
O95136	456	P(-O)(=O)	0.043291	0.0436885
O95136	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.042228	0.0422321
O95136	301	N-O	0.04144	0.0393526
O95136	622	O=C-O-C:C	0.041036	0.041331
O95136	79	>= 1 In	0.03999	0.0399936
O95136	605	O=C-C-O-C	0.039887	0.0335079
O95136	776	CC1CCC(C)CC1	0.039756	0.0392936
O95136	554	Br-C-C-C	0.039506	0.0386393
O95136	602	O=C-C-N-C	0.039349	0.034215
O95136	833	NC1C(N)CCCC1	0.039115	0.0380211
O95136	530	N:C-C:C	0.039018	0.0400366
O95136	319	Al-Cl	0.03853	0.0385286
O95136	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.038112	0.0381138
O95136	638	O-C-C-C-N	0.037959	0.0281161
O95136	836	ClC1C(Cl)CCCC1	0.037872	0.0390314
O95136	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.037003	0.0378479
O95136	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.036525	0.0365253
O95136	445	C(-H)(-N)(=C)	0.036162	0.0323997
O95136	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.035942	0.0359365
O95136	31	>= 2 P	0.035899	0.0313999
O95136	241	>= 1 any ring size 9	0.03447	0.0344735
O95136	828	OC1C(Br)CCCC1	0.032473	0.0297017
O95136	26	>= 1 Na	0.031988	0.0321785
O95136	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.031877	0.0311962
O95136	63	>= 1 Ga	0.030643	0.030639
O95136	587	N-C:C-O-[#1]	0.029694	0.0273497
O95136	670	Br-C:C:C-C	0.029668	0.0302479
O95136	267	Li-O	0.028648	0.02865
O95136	281	B-Cl	0.027896	0.0278988
O95136	598	Cl-C:C:C-C	0.027521	0.0248839
O95136	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.025946	0.0210958
O95136	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.025809	0.0174047
O95136	553	O=C-C=C	0.025756	0.0235166
O95136	433	C(-C)(-Cl)(=O)	0.024442	0.0244466
O95136	692	O=C-C-C-C-C-C	0.024219	0.0232827

O95136	277	B-F	0.023807	0.0238098
O95136	337	C(~C)(~C)(~C)(~O)	0.023222	0.02071
O95136	491	C-N:C-[#1]	0.023157	0.0282734
O95136	400	N(~H)(:C)(:C)	0.022366	0.0219606
O95136	845	OC1CC(O)CC1	0.022103	0.0220951
O95136	558	O=N-C:C	0.02201	0.0227686
O95136	788	SC1CCC(N)CC1	0.021248	0.0220308
O95136	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.021044	0.0216328
O95136	567	O-C-C-O	0.020957	0.0188948
O95136	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.020933	0.0209414
O95136	499	N-C:C:N	0.020923	0.0245043
O95136	287	C-F	0.020611	0.0164656
O95136	874	SC1C(Br)CCC1	0.020479	0.0204763
O95136	506	C-C:N:C	0.020384	0.0246845
O95136	716	Cc1ccc(N)cc1	0.020288	0.025899
O95136	424	N=P	0.02025	0.0202492
O95136	265	Li-B	0.019045	0.0190446
O95136	447	C(-H)(=N)	0.01901	0.0213617
O95136	842	CC1CC(N)CC1	0.018072	0.0164865
O95136	199	>= 4 any ring size 6	0.017275	0.0115863
O95136	361	C(~Cl)(~H)	0.017229	0.0194157
O95136	352	C(~C)(~O)	0.017222	0.0094842
O95136	357	C(~C)(:C)(:N)	0.016962	0.0227322
O95136	94	>= 1 Au	0.016955	0.0169513
O95136	214	>= 1 saturated or aromatic carbon-only ring size 7	0.015301	0.0209225
O95136	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.015195	0.0151928
O95136	16	>= 4 N	0.014979	0.0184401
O95136	552	C:C-C:C	0.014139	0.0134478
O95136	57	>= 1 Mn	0.01401	0.0140093
O95136	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.013962	0.0139632
O95136	825	OC1C(S)CCCC1	0.01377	0.0148976
O95136	40	>= 8 Cl	0.013684	0.013672
O95136	743	Oc1cc(Cl)ccc1	0.013042	0.0158927
O95136	346	C(~C)(~H)(~O)	0.012665	0.0130765
O95136	342	C(~C)(~Cl)	0.012266	0.0139134
O95136	646	O=C-N-C-[#1]	0.012091	0.0137172
O95136	501	Cl-C:C-C	0.011829	0.0092164
O95136	623	O=C-C:C-C	0.01147	0.013658
O95136	588	O=C-C-C=O	0.010833	0.009157
O95136	368	C(~H)(~S)	0.010811	0.0120397
O95136	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.010531	0.010534
O95136	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.010195	0.0101935
O95136	635	N-N-C-N-[#1]	0.010149	0.0125335
O95136	544	O-C:C-O	0.009875	0.0083928
O95136	49	>= 1 Be	0.009446	0.0094408
O95136	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.009401	0.0093976
O95136	260	>= 3 hetero-aromatic rings	0.008934	0.0089286
O95136	703	O-C-C-C-C-C(N)-C	0.008785	0.009131

O95136	793	NC1CCC(Br)CC1	0.007711	0.010324
O95136	402	N(~O)(:O)	0.007184	0.0061527
O95136	777	CC1CCC(O)CC1	0.007031	0.0100718
O95136	200	>= 4 saturated or aromatic carbon-only ring size 6	0.006858	0.006683
O95136	449	C(-N)(=C)	0.006656	0.0095775
O95136	344	C(~C)(~H)	0.006489	0.0067261
O95136	278	B-Si	0.006482	0.0064845
O95136	255	>= 1 aromatic ring	0.006192	0.006185
O95136	323	P-H	0.006138	0.0061356
O95136	54	>= 1 Ti	0.006092	0.0060895
O95136	259	>= 3 aromatic rings	0.006037	0.006033
O95136	15	>= 2 N	0.005865	0.0024859
O95136	581	O=C-C-C-O	0.005672	−0.000214
O95136	336	C(~C)(~C)(~C)(~N)	0.005134	0.0050467
O95136	455	N(-O)(=O)	0.004808	0.0023143
O95136	4	>= 1 Li	0.004675	0.004678
O95136	457	S(-C)(=O)	0.004518	0.0043203
O95136	85	>= 1 Ba	0.004054	0.0040481
O95136	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.00385	0.0038497
O95136	403	N(:C)(:C)	0.003791	0.0057947
O95136	264	Li-Li	0.003725	0.0037258
O95136	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.00358	0.0035821
O95136	221	>= 2 saturated or aromatic carbon-only ring size 7	0.003398	0.0034018
O95136	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.003205	0.0032058
O95136	108	>= 1 Dy	0.002995	0.0029926
O95136	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.00259	0.0021832
O95136	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.002329	0.0023263
O95136	354	C(~C)(~Si)	0.00213	0.0021155
O95136	404	N(:C)(:C)(:C)	0.002108	0.000433
O95136	624	O=C-C:C-N	0.002043	−0.003521
O95136	787	SC1CCC(S)CC1	0.001787	0.001481
O95136	811	SC1CC(Br)CCC1	0.001782	0.0001986
O95136	22	>= 16 O	0.001767	0.0017668
O95136	741	Oc1cc(S)ccc1	0.001728	0.0020264
O95136	678	C-C-C=C-C	0.001666	−0.00025
O95136	565	C:C-O-C	0.001644	0.0009088
O95136	242	>= 1 saturated or aromatic carbon-only ring size 9	0.00158	0.0015769
O95136	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.001546	0.0015471
O95136	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.001458	0.0014503
O95136	271	Li-Cl	0.001429	0.0014296
O95136	732	Clc1ccc(Br)cc1	0.001398	0.0013993
O95136	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.000863	0.0008601
O95136	835	NC1C(Br)CCCC1	0.000859	0.000858
O95136	775	Brc1c(Br)cccc1	0.000673	0.0006759
O95136	680	O-C-C-C-C-C	0.000632	−0.005192
O95136	686	O=C-C-C-C-O	0.000607	0.0039609
O95136	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.000551	0.000549
O95136	193	>= 3 saturated or aromatic carbon-only ring size 6	0.000479	0.0003138

O95136	562	Br-C-C=O	0.000351	-0.006622
O95136	413	S(~C)(~H)	0.000311	0.0003356
O95136	762	Oc1c(S)cccc1	9.65E-05	0.0012234
O95136	549	N-C-C:C	3.12E-05	0.0020321
O95136	51	>= 1 Al	7.27E-06	0
O95136	109	>= 1 Ho	3.48E-06	0
O95136	279	B-P	3.47E-06	0
O95136	272	B-H	2.93E-06	0
O95136	525	[As]-C:C-[#1]	2.03E-06	0
O95136	53	>= 1 Sc	1.59E-07	0
O95136	857	ClC1CC(Cl)CC1	-2.83E-07	0
O95136	164	>= 4 any ring size 5	-4.98E-07	0
O95136	262	>= 4 hetero-aromatic rings	-9.32E-07	0
O95136	41	>= 1 K	-2.27E-06	0
O95136	872	SC1C(N)CCC1	-2.51E-06	0
O95136	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	-3.81E-06	0
O95136	426	P=P	-8.76E-06	0
O95136	111	>= 1 Tm	-1.07E-05	-1.69E-05
O95136	257	>= 2 aromatic rings	-7.17E-05	-7.08E-05
O95136	274	B-C	-0.0001	0
O95136	10	>= 4 C	-0.00011	0.0017773
O95136	105	>= 1 Eu	-0.00037	-0.000363
O95136	591	Cl-C-C-C-C	-0.00042	-0.002084
O95136	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	-0.00053	-0.000531
O95136	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	-0.00054	0.0039313
O95136	585	C-C:C-N-C	-0.00055	-0.001469
O95136	450	C(-N)(=N)	-0.00077	-0.000524
O95136	789	SC1CCC(Cl)CC1	-0.00101	-0.000484
O95136	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	-0.00112	-0.001117
O95136	768	Sc1c(Cl)cccc1	-0.00114	-0.001717
O95136	534	S-C:C-O	-0.00115	-0.000176
O95136	45	>= 4 Br	-0.00146	-0.001468
O95136	21	>= 8 O	-0.00155	-0.0057
O95136	0	>= 4 H	-0.00159	-0.001588
O95136	662	O-C-C-O-C	-0.0016	0.0064816
O95136	537	O=C-C-O	-0.00161	0.0002094
O95136	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	-0.0018	-0.001792
O95136	480	C:S:C-C	-0.00196	0.0025579
O95136	557	N:C-O-[#1]	-0.00234	-0.004131
O95136	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	-0.00272	-0.000633
O95136	441	C(-C)(=C)	-0.00305	-0.000618
O95136	338	C(~C)(~C)(~H)(~N)	-0.00311	-0.001047
O95136	409	O(:C)(:C)	-0.00315	-0.001693
O95136	95	>= 1 Hg	-0.00317	-0.003179
O95136	551	Cl-C-C-O	-0.00375	0.0014805
O95136	1	>= 8 H	-0.00376	-0.00375
O95136	715	Cc1ccc(S)cc1	-0.00377	-0.006125
O95136	427	C(#C)(-C)	-0.00381	-0.006271

O95136	477	N-N-C:C	−0.00402	9.11E−05
O95136	273	B-B	−0.00407	−0.00407
O95136	865	CC1C(Br)CCC1	−0.0041	−0.004103
O95136	30	>= 1 P	−0.00421	−0.003951
O95136	508	S=C-N-C	−0.00443	−0.000117
O95136	309	O-O	−0.00481	−0.004816
O95136	87	>= 1 Hf	−0.006	−0.006008
O95136	632	C-C-O-C:C	−0.00646	−0.007151
O95136	667	C=C-C-O-[#1]	−0.00664	−0.004357
O95136	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.00705	−0.007057
O95136	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.00711	−0.007115
O95136	804	OC1CC(S)CCC1	−0.00783	−0.007519
O95136	526	Cl-C:C-Cl	−0.00799	−0.007751
O95136	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.00827	−0.008273
O95136	839	CC1CC(C)CC1	−0.00832	0
O95136	66	>= 1 Se	−0.00833	−0.008329
O95136	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.00839	−0.00839
O95136	514	O-N-C-C	−0.00851	−0.009655
O95136	781	CC1CCC(Br)CC1	−0.00855	−0.007351
O95136	723	Oc1ccc(Br)cc1	−0.00896	−0.010217
O95136	805	OC1CC(N)CCC1	−0.00926	−0.010749
O95136	331	C(~Br)(:N)	−0.00935	−0.009109
O95136	731	Clc1ccc(Cl)cc1	−0.00951	−0.017122
O95136	837	ClC1C(Br)CCCC1	−0.00962	−0.009629
O95136	681	O-C-C-C-C-O	−0.01029	−0.015454
O95136	101	>= 1 Pr	−0.01047	−0.010459
O95136	601	N-C:C:C-N	−0.01093	−0.011542
O95136	350	C(~C)(~I)	−0.01123	−0.013982
O95136	758	Cc1c(N)cccc1	−0.01156	−0.013522
O95136	641	O-C-C-C=C	−0.01166	−0.009668
O95136	695	O=C-C-C-C-C-N	−0.01183	−0.016783
O95136	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.01219	−0.012187
O95136	227	>= 1 any ring size 8	−0.01286	−0.01286
O95136	421	C=S	−0.01299	−0.006697
O95136	343	C(~C)(~Cl)(~H)	−0.01313	−0.010951
O95136	597	O=C-C-C:C	−0.01345	−0.02092
O95136	372	C(~H)(:C)(:N)	−0.0137	−0.013818
O95136	767	Sc1c(N)cccc1	−0.01416	−0.008751
O95136	422	N=N	−0.01422	−0.009783
O95136	375	C(~N)(~N)	−0.01428	−0.010866
O95136	269	Li-P	−0.0144	−0.014402
O95136	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.01499	−0.01499
O95136	326	As-As	−0.01532	−0.015331
O95136	341	C(~C)(~C)(~O)	−0.01591	−0.011791
O95136	563	O-C-O-C	−0.01765	−0.018822
O95136	383	C(~S)(:C)	−0.01791	−0.019653
O95136	560	N-C-N-C	−0.01823	−0.01774
O95136	44	>= 2 Br	−0.01833	−0.017009

O95136	505	Cl-C:C-O	−0.01851 −0.013261
O95136	495	C-N-C:C	−0.01858 −0.020163
O95136	29	>= 2 Si	−0.01879 −0.01879
O95136	304	N-P	−0.01884 −0.020244
O95136	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.01891 −0.018909
O95136	536	O=C-C-N	−0.01982 −0.013501
O95136	866	OC1C(O)CCC1	−0.01993 −0.019917
O95136	465	O=S-C-C	−0.01996 −0.017418
O95136	114	>= 1 U	−0.02007 −0.020074
O95136	500	C-S-C:C	−0.0206 −0.021371
O95136	647	O=C-N-C-N	−0.02117 −0.019308
O95136	36	>= 8 S	−0.0217 −0.021699
O95136	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.02235 −0.022343
O95136	578	C-C:C-C:C	−0.02295 −0.023795
O95136	410	P(~C)(~C)	−0.02296 −0.037256
O95136	592	N-C-C-C-C	−0.02343 −0.027394
O95136	384	C(:C)(:C)	−0.02356 −0.025934
O95136	737	Cc1cc(N)ccc1	−0.02427 −0.017111
O95136	332	C(~C)(~C)	−0.02443 −0.022554
O95136	685	O=C-C-C-C-N	−0.02624 −0.028052
O95136	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.0272 −0.035306
O95136	749	Nc1cc(N)ccc1	−0.02732 −0.030298
O95136	14	>= 1 N	−0.02915 −0.025872
O95136	365	C(~H)(~N)	−0.03029 −0.035502
O95136	510	[#1]-N-N-[#1]	−0.03155 −0.031632
O95136	298	C-I	−0.03212 −0.034864
O95136	625	O=C-C:C-O	−0.03242 −0.029751
O95136	275	B-N	−0.03243 −0.032432
O95136	355	C(~C)(:C)	−0.03247 −0.031545
O95136	726	Sc1ccc(Cl)cc1	−0.03296 −0.032435
O95136	556	C=C-C-C	−0.03509 −0.034111
O95136	412	S(~C)(~C)	−0.03527 −0.037652
O95136	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.03614 −0.035763
O95136	633	N-C-C:C-C	−0.03685 −0.04013
O95136	46	>= 1 I	−0.03756 −0.038146
O95136	489	N-C-S-C	−0.03986 −0.042982
O95136	487	N-C=N-C	−0.04012 −0.038306
O95136	282	B-Br	−0.04236 −0.042349
O95136	380	C(~O)(~O)	−0.04281 −0.046606
O95136	760	Cc1c(Br)cccc1	−0.04361 −0.040189
O95136	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.04406 −0.043686
O95136	220	>= 2 any ring size 7	−0.0441 −0.04409
O95136	322	Si-Cl	−0.04643 −0.046429
O95136	507	C-C-S-C	−0.04787 −0.051289
O95136	579	O=C-C-C-C	−0.04787 −0.046991
O95136	34	>= 2 S	−0.04971 −0.050412
O95136	583	Cl-C:C-O-C	−0.05073 −0.04548
O95136	371	C(~H)(:C)(:C)	−0.05181 −0.055708

O95136	719	Oc1ccc(O)cc1	−0.05187	−0.048441
O95136	694	O=C-C-C-C-C=O	−0.05276	−0.059423
O95136	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.05342	−0.053421
O95136	6	>= 1 B	−0.05466	−0.05455
O95136	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.05524	−0.055234
O95136	621	N-C:C:C:N	−0.0561	−0.056633
O95136	802	CC1CC(Br)CCC1	−0.05697	−0.05452
O95136	454	N(-C)(=O)	−0.05789	−0.057964
O95136	595	C:C-C-C-C	−0.05844	−0.059343
O95136	5	>= 2 Li	−0.05959	−0.059585
O95136	98	>= 1 Bi	−0.06058	−0.060576
O95136	649	O=N-C:C-O	−0.06128	−0.063714
O95136	377	C(~N)(:C)(:C)	−0.06134	−0.066465
O95136	704	O=C-C-C-C-C-C-C	−0.06138	−0.065076
O95136	376	C(~N)(:C)	−0.06143	−0.058397
O95136	478	S-C=N-[#1]	−0.06158	−0.064647
O95136	432	C(-C)(-C)(=O)	−0.06166	−0.061195
O95136	370	C(~H)(:C)	−0.06249	−0.063243
O95136	660	C-C=C-C-C	−0.06347	−0.065374
O95136	790	SC1CCC(Br)CC1	−0.06371	−0.06371
O95136	291	C-Si	−0.06376	−0.063758
O95136	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.06395	−0.063946
O95136	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.06558	−0.065575
O95136	481	O-S-C:C	−0.06562	−0.067093
O95136	59	>= 1 Co	−0.06563	−0.065628
O95136	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.0657	−0.065698
O95136	814	NC1CC(Br)CCC1	−0.06594	−0.066225
O95136	330	C(~Br)(:C)	−0.06624	−0.068435
O95136	58	>= 1 Fe	−0.06641	−0.066398
O95136	669	Cl-C:C-C=O	−0.06868	−0.06785
O95136	642	O-C-C-C=O	−0.07041	−0.076293
O95136	516	[#1]-C=C-[#1]	−0.07269	−0.072308
O95136	474	S:C:C:N	−0.0769	−0.072484
O95136	367	C(~H)(~O)(~O)	−0.07834	−0.077654
O95136	659	O-C-C-N-C	−0.0792	−0.086002
O95136	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.08018	−0.080291
O95136	430	C(-C)(-C)(=C)	−0.08061	−0.081025
O95136	736	Cc1cc(S)ccc1	−0.08069	−0.07897
O95136	20	>= 4 O	−0.0821	−0.079929
O95136	157	>= 3 any ring size 5	−0.0838	−0.08808
O95136	709	C-C(C)-C-C-C	−0.08402	−0.086771
O95136	844	CC1CC(Br)CC1	−0.08513	−0.085126
O95136	351	C(~C)(~N)	−0.09109	−0.089602
O95136	24	>= 2 F	−0.09314	−0.092337
O95136	574	O-C-C:C-C	−0.09368	−0.095253
O95136	650	O=C-N-C=O	−0.09628	−0.098771
O95136	206	>= 5 any ring size 6	−0.0963	−0.092274
O95136	710	C-C-C(C)-C-C	−0.09641	−0.096396

O95136	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−0.0975	−0.097462
O95136	38	>= 2 Cl	−0.10067	−0.099281
O95136	815	ClC1CC(Cl)CCC1	−0.10111	−0.099729
O95136	628	C-N-C-C:C	−0.1036	−0.107217
O95136	631	O-C:C-O-[#1]	−0.10368	−0.103565
O95136	19	>= 2 O	−0.10476	−0.098509
O95136	420	C=O	−0.10602	−0.10037
O95136	185	>= 2 any ring size 6	−0.10666	−0.101175
O95136	603	C-C:C:C-C	−0.10884	−0.114087
O95136	386	C(:C)(:C)(:N)	−0.11194	−0.112529
O95136	270	Li-S	−0.11326	−0.113256
O95136	423	N=O	−0.11378	−0.113869
O95136	620	C:C-O-C-C	−0.11634	−0.117028
O95136	35	>= 4 S	−0.11946	−0.119462
O95136	178	>= 1 any ring size 6	−0.12152	−0.112114
O95136	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.12281	−0.125074
O95136	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.12652	−0.126528
O95136	348	C(~C)(~H)(~P)	−0.12883	−0.139459
O95136	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.13046	−0.13046
O95136	290	C-Al	−0.1309	−0.130901
O95136	707	O=C-C-C-C-C(N)-C	−0.13097	−0.131702
O95136	706	O=C-C-C-C-C(=O)-C	−0.13399	−0.137221
O95136	406	O(~C)(~H)	−0.13479	−0.138335
O95136	705	O=C-C-C-C-C(O)-C	−0.13523	−0.136788
O95136	807	OC1CC(Br)CCC1	−0.13665	−0.136507
O95136	431	C(-C)(-C)(=N)	−0.13717	−0.142655
O95136	691	O-C-C-C-C-C-N	−0.13971	−0.149139
O95136	738	Cc1cc(Cl)ccc1	−0.14062	−0.144229
O95136	778	CC1CCC(S)CC1	−0.14066	−0.142514
O95136	300	N-N	−0.1415	−0.148367
O95136	569	N-C-C-N	−0.15014	−0.15171
O95136	468	O=S-C-N	−0.15202	−0.148373
O95136	759	Cc1c(Cl)cccc1	−0.15359	−0.150558
O95136	600	N-C:C:C-C	−0.15699	−0.154407
O95136	663	O-C-C-O-[#1]	−0.1583	−0.164408
O95136	333	C(~C)(~C)(~C)	−0.16033	−0.16064
O95136	540	C-N-C-[#1]	−0.16781	−0.171265
O95136	593	N-C-C-C-N	−0.17029	−0.170751
O95136	699	O-C-C-C-C-C(C)-C	−0.17045	−0.166923
O95136	136	>= 2 any ring size 4	−0.18176	−0.185409
O95136	873	SC1C(Cl)CCC1	−0.18339	−0.183393
O95136	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.18428	−0.184279
O95136	850	SC1CC(S)CC1	−0.1869	−0.186899
O95136	328	C(~Br)(~C)(~C)	−0.1944	−0.19531
O95136	467	C=N-N-C	−0.19486	−0.200566
O95136	317	F-S	−0.19781	−0.197808
O95136	780	CC1CCC(Cl)CC1	−0.20182	−0.201861
O95136	459	S(=O)(=O)	−0.20415	−0.202335

O95136	535	O=C-C-C	−0.20967	−0.211875
O95136	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.21425	−0.214248
O95136	479	S-C-S-C	−0.21496	−0.212568
O95136	582	C-C-C-C-C	−0.21522	−0.214275
O95136	785	OC1CCC(Cl)CC1	−0.21637	−0.212522
O95136	576	N=C-C:C-[#1]	−0.21797	−0.216235
O95136	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.21929	−0.219286
O95136	684	O=C-C-C-C-C	−0.2193	−0.224872
O95136	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.22219	−0.222184
O95136	488	N-C=N-[#1]	−0.22244	−0.221571
O95136	64	>= 1 Ge	−0.22417	−0.22417
O95136	634	C-C-C:C-C	−0.22599	−0.232335
O95136	653	O-C:C:C-O	−0.22641	−0.228559
O95136	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.22825	−0.22825
O95136	604	C-O-C-C:C	−0.23005	−0.228661
O95136	379	C(~N)(:N)	−0.23153	−0.229593
O95136	256	>= 1 hetero-aromatic ring	−0.23304	−0.233044
O95136	548	O-C-C:C	−0.23592	−0.236661
O95136	318	Al-H	−0.23638	−0.236379
O95136	543	O-C:C-N	−0.23846	−0.238152
O95136	397	N(~C)(:C)(:C)	−0.24125	−0.240448
O95136	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.2422	−0.244133
O95136	770	Nc1c(N)cccc1	−0.24417	−0.244225
O95136	542	O-C:C-[#1]	−0.24559	−0.240876
O95136	531	S-C:C-C	−0.25323	−0.253734
O95136	339	C(~C)(~C)(~H)(~O)	−0.25352	−0.248969
O95136	755	Cc1c(C)cccc1	−0.2614	−0.265252
O95136	311	O-Na	−0.26651	−0.26651
O95136	391	N(~C)(~C)(~C)	−0.26709	−0.260743
O95136	744	Oc1cc(Br)ccc1	−0.26739	−0.267238
O95136	664	C-C=C-C=C	−0.26959	−0.270693
O95136	779	CC1CCC(N)CC1	−0.26965	−0.264954
O95136	83	>= 1 Xe	−0.27446	−0.274466
O95136	619	O-C-C=C-C	−0.2761	−0.278222
O95136	840	CC1CC(O)CC1	−0.28233	−0.282326
O95136	408	O(~H)(~S)	−0.28333	−0.284011
O95136	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.28349	−0.281305
O95136	610	C-O-C-O-C	−0.28375	−0.284917
O95136	464	N-C-C=C	−0.28426	−0.28254
O95136	745	Sc1cc(S)ccc1	−0.28948	−0.28948
O95136	439	C(-C)(-N)(=O)	−0.29189	−0.287004
O95136	364	C(~F)(:C)	−0.29274	−0.281234
O95136	67	>= 1 Kr	−0.29285	−0.292853
O95136	806	OC1CC(Cl)CCC1	−0.29702	−0.294168
O95136	12	>= 16 C	−0.29875	−0.298506
O95136	366	C(~H)(~O)	−0.30506	−0.305084
O95136	863	CC1C(N)CCC1	−0.30689	−0.307152
O95136	752	Clc1cc(Cl)ccc1	−0.30803	−0.306651

O95136	868	OC1C(N)CCC1	−0.31081	−0.310801
O95136	485	N:C:C:N	−0.31244	−0.314153
O95136	280	B-S	−0.31281	−0.312811
O95136	401	N(~O)(~O)	−0.31353	−0.316022
O95136	321	Si-Si	−0.32031	−0.320305
O95136	725	Sc1ccc(N)cc1	−0.32255	−0.321776
O95136	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.32422	−0.318004
O95136	497	O-C:C:N	−0.32458	−0.322137
O95136	801	CC1CC(Cl)CCC1	−0.33346	−0.337067
O95136	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.34104	−0.339741
O95136	615	N-C-C-O-C	−0.34709	−0.346878
O95136	626	C-O-C:C-C	−0.35301	−0.355034
O95136	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.35436	−0.353513
O95136	689	O-C-C-C-C-C-C	−0.35723	−0.35366
O95136	718	Cc1ccc(Br)cc1	−0.35864	−0.357432
O95136	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.3605	−0.353438
O95136	462	O-C-C=O	−0.36143	−0.359603
O95136	586	C-S-C-C-C	−0.37111	−0.374375
O95136	656	C-C-N-C-C	−0.3727	−0.371326
O95136	248	>= 1 any ring size 10	−0.37432	−0.374322
O95136	722	Oc1ccc(Cl)cc1	−0.37909	−0.37525
O95136	292	C-P	−0.38142	−0.379535
O95136	399	N(~H)(:C)	−0.39164	−0.392292
O95136	493	O=C-C:C	−0.39526	−0.389333
O95136	855	NC1CC(Cl)CC1	−0.39714	−0.397138
O95136	451	C(-N)(=O)	−0.39937	−0.396976
O95136	452	C(-O)(=O)	−0.40117	−0.401231
O95136	302	N-F	−0.40353	−0.403535
O95136	378	C(~N)(:C)(:N)	−0.40804	−0.406882
O95136	359	C(~C)(:N)(:N)	−0.40902	−0.417437
O95136	517	N-N-C-N	−0.41005	−0.404936
O95136	580	O=C-C-C-N	−0.4197	−0.410709
O95136	870	OC1C(Br)CCC1	−0.42103	−0.421034
O95136	533	S-C:C-N	−0.43117	−0.427794
O95136	522	C-N-N-[#1]	−0.43217	−0.42916
O95136	665	N-C:C-C-C	−0.433	−0.435404
O95136	702	O-C-C-C-C-C-N-C	−0.44225	−0.440914
O95136	594	C-O-C-C=C	−0.44241	−0.436555
O95136	446	C(-H)(=C)	−0.44437	−0.441784
O95136	444	C(-Cl)(=O)	−0.45437	−0.45437
O95136	306	N-Cl	−0.45941	−0.459406
O95136	648	O=N-C:C-N	−0.46602	−0.464214
O95136	769	Sc1c(Br)cccc1	−0.4731	−0.473092
O95136	754	Brc1cc(Br)ccc1	−0.47531	−0.474162
O95136	385	C(:C)(:C)(:C)	−0.47708	−0.475872
O95136	608	C-C-C-C:C	−0.48697	−0.487871
O95136	672	O=C-C=C-[#1]	−0.48819	−0.493484
O95136	234	>= 2 any ring size 8	−0.49023	−0.490231

O95136	340	C(~C)(~C)(~N)	−0.49121	−0.486384
O95136	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.4921	−0.492106
O95136	708	C-C(C)-C-C	−0.49644	−0.490448
O95136	395	N(~C)(~O)	−0.50493	−0.507018
O95136	871	SC1C(S)CCC1	−0.50837	−0.508367
O95136	644	C-C=N-N-C	−0.51612	−0.513595
O95136	740	Oc1cc(O)ccc1	−0.5192	−0.522164
O95136	573	O-C-C=C	−0.5199	−0.519298
O95136	611	N-C-C-N-C	−0.53147	−0.524141
O95136	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.53396	−0.533959
O95136	673	O=C-C=C-N	−0.53517	−0.538097
O95136	527	C:C:N-[#1]	−0.53819	−0.541471
O95136	782	OC1CCC(O)CC1	−0.53836	−0.534925
O95136	284	C-C	−0.54195	−0.540073
O95136	679	C-C-C-C-C-C	−0.54831	−0.551358
O95136	816	ClC1CC(Br)CCC1	−0.5535	−0.553829
O95136	721	Oc1ccc(N)cc1	−0.55539	−0.556744
O95136	276	B-O	−0.56257	−0.562572
O95136	312	O-Al	−0.56362	−0.563619
O95136	469	S-S-C:C	−0.56483	−0.56483
O95136	829	SC1C(S)CCCC1	−0.58867	−0.589892
O95136	876	NC1C(Cl)CC1	−0.59454	−0.594541
O95136	283	C-H	−0.60223	−0.600348
O95136	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.605	−0.604998
O95136	324	P-P	−0.60669	−0.60669
O95136	96	>= 1 Tl	−0.60721	−0.607204
O95136	11	>= 8 C	−0.60923	−0.609045
O95136	783	OC1CCC(S)CC1	−0.61455	−0.616447
O95136	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.62826	−0.628703
O95136	78	>= 1 Cd	−0.63134	−0.63134
O95136	416	C=C	−0.63883	−0.63639
O95136	498	O-C=C-C	−0.65753	−0.654672
O95136	56	>= 1 Cr	−0.66045	−0.660449
O95136	453	N(-C)(=C)	−0.66874	−0.664998
O95136	82	>= 1 Te	−0.67082	−0.670824
O95136	8	>= 4 B	−0.67681	−0.676821
O95136	347	C(~C)(~H)(~O)(~O)	−0.67825	−0.680621
O95136	393	N(~C)(~H)	−0.67925	−0.68224
O95136	861	CC1C(O)CCC1	−0.6861	−0.686107
O95136	494	O=C-C:N	−0.68748	−0.688901
O95136	258	>= 2 hetero-aromatic rings	−0.68756	−0.687557
O95136	396	N(~C)(:C)	−0.6899	−0.688767
O95136	555	N=C-C=C	−0.69064	−0.694648
O95136	869	OC1C(Cl)CCC1	−0.69154	−0.691548
O95136	797	CC1CC(C)CCC1	−0.69387	−0.692832
O95136	521	C:N-C-[#1]	−0.69527	−0.693074
O95136	727	Sc1ccc(Br)cc1	−0.70302	−0.703013
O95136	851	SC1CC(N)CC1	−0.71332	−0.71332

O95136	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.71884	−0.718843
O95136	261	>= 4 aromatic rings	−0.72155	−0.721554
O95136	360	C(~Cl)(~Cl)	−0.72416	−0.724155
O95136	761	Oc1c(O)cccc1	−0.7316	−0.733156
O95136	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.73596	−0.733925
O95136	546	N-C:C-[#1]	−0.74276	−0.738446
O95136	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.75261	−0.753671
O95136	458	S(-O)(=O)	−0.76141	−0.765255
O95136	327	C(~Br)(~C)	−0.76875	−0.770088
O95136	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.77666	−0.776661
O95136	799	CC1CC(S)CCC1	−0.78049	−0.779472
O95136	47	>= 2 I	−0.78542	−0.785416
O95136	415	Si(~C)(~C)	−0.79223	−0.792227
O95136	541	O-C:C-C	−0.79573	−0.792873
O95136	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.79932	−0.799318
O95136	609	Cl-C-C-N-C	−0.80046	−0.807212
O95136	25	>= 4 F	−0.80448	−0.811384
O95136	826	OC1C(N)CCCC1	−0.80538	−0.808901
O95136	486	N-C:N:N	−0.80726	−0.805843
O95136	110	>= 1 Er	−0.81164	−0.811646
O95136	733	Brc1ccc(Br)cc1	−0.82508	−0.825075
O95136	288	C-Na	−0.82559	−0.82559
O95136	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.83304	−0.842721
O95136	584	C:C-C=C-C	−0.84064	−0.84149
O95136	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.85113	−0.847705
O95136	700	O-C-C-C-C-C-O-C	−0.85943	−0.863163
O95136	435	C(-C)(-H)(=N)	−0.86153	−0.862271
O95136	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.86318	−0.85989
O95136	852	SC1CC(Cl)CC1	−0.86487	−0.864862
O95136	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.87914	−0.87914
O95136	564	C=C-C=C	−0.88429	−0.888415
O95136	504	N:C:N-C	−0.8961	−0.895453
O95136	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.90197	−0.901965
O95136	90	>= 1 Re	−0.90539	−0.905386
O95136	503	Cl-C:C-[#1]	−0.91858	−0.911523
O95136	316	F-P	−0.94349	−0.943489
O95136	320	Si-H	−0.96201	−0.962015
O95136	742	Oc1cc(N)ccc1	−0.9664	−0.967899
O95136	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.99262	−0.990584
O95136	103	>= 1 Pm	−1.00548	−1.005475
O95136	293	C-S	−1.01545	−1.019555
O95136	398	N(~H)(~N)	−1.03201	−1.034603
O95136	849	OC1CC(Br)CC1	−1.05773	−1.057729
O95136	853	SC1CC(Br)CC1	−1.07151	−1.071508
O95136	559	O-C-N-[#1]	−1.12825	−1.131397
O95136	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−1.13516	−1.135157
O95136	627	O=[As]-C:C:C	−1.15297	−1.152972
O95136	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−1.18616	−1.186163

O95136	436	C(-C)(-H)(=O)	-1.21597 -1.216424
O95136	492	N-C:O:C	-1.21971 -1.22132
O95136	484	N-C:N:C	-1.23561 -1.233689
O95136	747	Sc1cc(Cl)ccc1	-1.23733 -1.237198
O95136	263	Li-H	-1.23804 -1.238042
O95136	570	C:C-C-C	-1.247 -1.250465
O95136	106	>= 1 Gd	-1.35036 -1.35036
O95136	315	O-K	-1.40003 -1.400032
O95136	688	C-C-C-C-C-C-C	-1.41434 -1.413136
O95136	268	Li-F	-1.43194 -1.431951
O95136	72	>= 1 Nb	-1.50403 -1.504034
O95136	419	C#N	-1.55101 -1.551976
O95136	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	-1.56924 -1.569243
O95136	879	ClC1C(Br)CCC1	-1.67144 -1.671437
O95136	701	O-C-C-C-C-C(O)-C	-1.6741 -1.680279
O95136	9	>= 2 C	-1.69326 -1.691383
O95136	520	C=C-C:C	-1.71905 -1.719741
O95136	513	S:C:C-[#1]	-1.78025 -1.775241
O95136	81	>= 1 Sb	-1.94344 -1.943442

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q9H228	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	2.1550091
Q9H228	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	2.1092753
Q9H228	820	CC1C(S)CCCC1	2.0592762
Q9H228	272	B-H	2.028134
Q9H228	676	N#C-C-C-C	2.0202661
Q9H228	512	C-[As]-O-[#1]	1.9159144
Q9H228	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	1.9060201
Q9H228	792	NC1CCC(Cl)CC1	1.8954195
Q9H228	497	O-C:C:N	1.8557237
Q9H228	851	SC1CC(N)CC1	1.8129888
Q9H228	872	SC1C(N)CCC1	1.8120969
Q9H228	877	NC1C(Br)CCC1	1.7873988
Q9H228	275	B-N	1.7454933
Q9H228	868	OC1C(N)CCC1	1.7213761
Q9H228	785	OC1CCC(Cl)CC1	1.7025259
Q9H228	61	>= 1 Cu	1.688376
Q9H228	516	[#1]-C=C-[#1]	1.620227
Q9H228	677	C-C=C-C:C	1.611942
Q9H228	320	Si-H	1.6013422
Q9H228	474	S:C:C:N	1.5135958
Q9H228	780	CC1CCC(Cl)CC1	1.5110493
Q9H228	450	C(-N)(=N)	1.4924752
Q9H228	655	O-C-C-C:C	1.4801329
Q9H228	788	SC1CCC(N)CC1	1.4510122
Q9H228	620	C:C-O-C-C	1.4507932
Q9H228	35	>= 4 S	1.4451428
Q9H228	618	C:C-C-C:C	1.4392917
Q9H228	705	O=C-C-C-C-C(O)-C	1.4378673
Q9H228	296	C-Se	1.4341031
Q9H228	82	>= 1 Te	1.375706
Q9H228	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	1.2905163
Q9H228	509	Br-C:C-C	1.2850978
Q9H228	880	BrC1C(Br)CCC1	1.2816648
Q9H228	595	C:C-C-C-C	1.2482397
Q9H228	31	>= 2 P	1.2409285
Q9H228	14	>= 1 N	1.2387246
Q9H228	52	>= 1 Ca	1.2050077
Q9H228	113	>= 1 Tc	1.2006439
Q9H228	522	C-N-N-[#1]	1.1981405
Q9H228	759	Cc1c(Cl)cccc1	1.1979838
Q9H228	448	C(-H)(=O)	1.1847911
Q9H228	193	>= 3 saturated or aromatic carbon-only ring size 6	1.1616375
Q9H228	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	1.1523142
Q9H228	407	O(~C)(~P)	1.1473362
Q9H228	827	OC1C(Cl)CCCC1	1.1461122
Q9H228	446	C(-H)(=C)	1.1368803

Q9H228	666	C=C-C-O-C	1.1320955
Q9H228	783	OC1CCC(S)CC1	1.1181091
Q9H228	627	O=[As]-C:C:C	1.1097018
Q9H228	714	Cc1ccc(O)cc1	1.1078076
Q9H228	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	1.1067378
Q9H228	818	CC1C(C)CCCC1	1.1027256
Q9H228	2	>= 16 H	1.0930844
Q9H228	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	1.0909807
Q9H228	518	O=C-N-N	1.0732772
Q9H228	425	P=O	1.0638067
Q9H228	718	Cc1ccc(Br)cc1	1.0580285
Q9H228	107	>= 1 Tb	1.0365594
Q9H228	298	C-I	1.0347498
Q9H228	491	C-N:C-[#1]	1.0273718
Q9H228	411	P(~O)(~O)	1.0241733
Q9H228	493	O=C-C:C	1.0192187
Q9H228	363	C(~F)(~F)	1.0187267
Q9H228	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	1.0016987
Q9H228	386	C(:C)(:C)(:N)	1.0009661
Q9H228	565	C:C-O-C	0.9969485
Q9H228	488	N-C=N-[#1]	0.996182
Q9H228	305	N-S	0.9882134
Q9H228	767	Sc1c(N)cccc1	0.9860034
Q9H228	692	O=C-C-C-C-C-C	0.982894
Q9H228	802	CC1CC(Br)CCC1	0.9819854
Q9H228	498	O-C=C-C	0.973699
Q9H228	85	>= 1 Ba	0.9709114
Q9H228	430	C(-C)(-C)(=C)	0.9690089
Q9H228	507	C-C-S-C	0.9635731
Q9H228	576	N=C-C:C-[#1]	0.953839
Q9H228	22	>= 16 O	0.9486035
Q9H228	106	>= 1 Gd	0.9463643
Q9H228	100	>= 1 Ce	0.9446799
Q9H228	271	Li-Cl	0.9395337
Q9H228	848	OC1CC(Cl)CC1	0.9367834
Q9H228	552	C:C-C:C	0.9348955
Q9H228	879	ClC1C(Br)CCC1	0.9326788
Q9H228	744	Oc1cc(Br)ccc1	0.9233549
Q9H228	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.92213
Q9H228	392	N(~C)(~C)(~H)	0.9214983
Q9H228	343	C(~C)(~Cl)(~H)	0.9190891
Q9H228	707	O=C-C-C-C-C(N)-C	0.9158147
Q9H228	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.9136245
Q9H228	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.903999
Q9H228	795	ClC1CCC(Br)CC1	0.9034767
Q9H228	5	>= 2 Li	0.9022023
Q9H228	303	N-Si	0.9018096
Q9H228	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.8984889

Q9H228	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.8935423
Q9H228	3	>= 32 H	0.8898951
Q9H228	550	Cl-C-C-C	0.8870397
Q9H228	137	>= 2 saturated or aromatic carbon-only ring size 4	0.8848161
Q9H228	649	O=N-C:C-O	0.8810088
Q9H228	789	SC1CCC(Cl)CC1	0.8748269
Q9H228	643	[#1]-C-C-N-[#1]	0.8704786
Q9H228	457	S(-C)(=O)	0.8551673
Q9H228	44	>= 2 Br	0.8537887
Q9H228	836	ClC1C(Cl)CCCC1	0.8529217
Q9H228	19	>= 2 O	0.8393445
Q9H228	869	OC1C(Cl)CCC1	0.8249373
Q9H228	301	N-O	0.822465
Q9H228	381	C(~O)(:C)	0.8163632
Q9H228	264	Li-Li	0.8142707
Q9H228	73	>= 1 Mo	0.8106983
Q9H228	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.8049032
Q9H228	622	O=C-O-C:C	0.8040104
Q9H228	633	N-C-C:C-C	0.8022773
Q9H228	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.7910105
Q9H228	504	N:C:N-C	0.7892004
Q9H228	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.7887099
Q9H228	678	C-C-C=C-C	0.7769652
Q9H228	735	Cc1cc(O)ccc1	0.7620666
Q9H228	781	CC1CCC(Br)CC1	0.7586924
Q9H228	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.7572625
Q9H228	92	>= 1 Ir	0.7528337
Q9H228	111	>= 1 Tm	0.7518231
Q9H228	839	CC1CC(C)CC1	0.7489163
Q9H228	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.7475481
Q9H228	273	B-B	0.7425209
Q9H228	426	P=P	0.7387876
Q9H228	297	C-Br	0.738399
Q9H228	537	O=C-C-O	0.7328713
Q9H228	213	>= 1 any ring size 7	0.7310635
Q9H228	280	B-S	0.7243307
Q9H228	83	>= 1 Xe	0.7057874
Q9H228	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.7009573
Q9H228	90	>= 1 Re	0.7001671
Q9H228	763	Oc1c(N)cccc1	0.6942695
Q9H228	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.6824007
Q9H228	598	Cl-C:C:C-C	0.6693882
Q9H228	715	Cc1ccc(S)cc1	0.6622834
Q9H228	234	>= 2 any ring size 8	0.6612657
Q9H228	602	O=C-C-N-C	0.6563476
Q9H228	102	>= 1 Nd	0.65445
Q9H228	56	>= 1 Cr	0.64694
Q9H228	431	C(-C)(-C)(=N)	0.6462403

Q9H228	544	O-C:C-O	0.6437971
Q9H228	811	SC1CC(Br)CCC1	0.6406132
Q9H228	103	>= 1 Pm	0.6294677
Q9H228	533	S-C:C-N	0.62557
Q9H228	650	O=C-N-C=O	0.6210444
Q9H228	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.6136365
Q9H228	330	C(~Br)(:C)	0.6071118
Q9H228	312	O-Al	0.6063611
Q9H228	527	C:C:N-[#1]	0.6062734
Q9H228	867	OC1C(S)CCC1	0.6016403
Q9H228	626	C-O-C:C-C	0.5943253
Q9H228	665	N-C:C-C-C	0.5905899
Q9H228	661	O-C-O-C-C	0.5821648
Q9H228	365	C(~H)(~N)	0.5776016
Q9H228	480	C:S:C-C	0.5728501
Q9H228	267	Li-O	0.5707947
Q9H228	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.5697213
Q9H228	796	BrC1CCC(Br)CC1	0.5662772
Q9H228	308	O-H	0.5634491
Q9H228	317	F-S	0.5609685
Q9H228	96	>= 1 Tl	0.5595241
Q9H228	702	O-C-C-C-C-C-N-C	0.5534449
Q9H228	571	[#1]-C-O-[#1]	0.5514916
Q9H228	130	>= 1 saturated or aromatic carbon-only ring size 4	0.5494503
Q9H228	105	>= 1 Eu	0.5448097
Q9H228	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.5423526
Q9H228	464	N-C-C=C	0.5368473
Q9H228	579	O=C-C-C-C	0.5345531
Q9H228	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.5317149
Q9H228	875	NC1C(N)CCC1	0.5313136
Q9H228	761	Oc1c(O)cccc1	0.5236186
Q9H228	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.5203246
Q9H228	821	CC1C(N)CCCC1	0.5191151
Q9H228	601	N-C:C:C-N	0.5152869
Q9H228	438	C(-C)(-N)(=N)	0.5152506
Q9H228	207	>= 5 saturated or aromatic carbon-only ring size 6	0.5105114
Q9H228	349	C(~C)(~H)(~S)	0.5057515
Q9H228	803	OC1CC(O)CCC1	0.5057104
Q9H228	840	CC1CC(O)CC1	0.5046067
Q9H228	751	Nc1cc(Br)ccc1	0.4998174
Q9H228	641	O-C-C-C=C	0.4995442
Q9H228	645	O=C-N-C-C	0.4963926
Q9H228	575	O-C-C:C-O	0.4953195
Q9H228	621	N-C:C:C:N	0.4949289
Q9H228	682	O-C-C-C-C-N	0.492913
Q9H228	494	O=C-C:N	0.4913765
Q9H228	81	>= 1 Sb	0.4843998
Q9H228	700	O-C-C-C-C-C-O-C	0.4762613

Q9H228	26	>= 1 Na	0.4745479
Q9H228	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.4668909
Q9H228	489	N-C-S-C	0.4659019
Q9H228	292	C-P	0.4655548
Q9H228	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.4638301
Q9H228	637	O-C-C-C-C	0.4636234
Q9H228	697	C-C-C-C-C-C(C)-C	0.4595497
Q9H228	690	O-C-C-C-C-C-O	0.4500542
Q9H228	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.4492602
Q9H228	260	>= 3 hetero-aromatic rings	0.4476347
Q9H228	342	C(~C)(~Cl)	0.4382067
Q9H228	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.4354395
Q9H228	461	O-C-C=N	0.4280011
Q9H228	728	Nc1ccc(N)cc1	0.4275546
Q9H228	179	>= 1 saturated or aromatic carbon-only ring size 6	0.4268102
Q9H228	268	Li-F	0.4264255
Q9H228	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.4178445
Q9H228	25	>= 4 F	0.4165868
Q9H228	553	O=C-C=C	0.4067321
Q9H228	762	Oc1c(S)cccc1	0.4060433
Q9H228	681	O-C-C-C-C-O	0.4020915
Q9H228	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.4013479
Q9H228	640	C=C-C-C-C	0.3989378
Q9H228	302	N-F	0.3987366
Q9H228	864	CC1C(Cl)CCC1	0.3969521
Q9H228	583	Cl-C:C-O-C	0.3945344
Q9H228	67	>= 1 Kr	0.3942024
Q9H228	367	C(~H)(~O)(~O)	0.3933154
Q9H228	172	>= 5 saturated or aromatic carbon-only ring size 5	0.3927842
Q9H228	286	C-O	0.3913565
Q9H228	756	Cc1c(O)cccc1	0.3838012
Q9H228	186	>= 2 saturated or aromatic carbon-only ring size 6	0.3784703
Q9H228	600	N-C:C:C-C	0.3778624
Q9H228	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.3755125
Q9H228	672	O=C-C=C-[#1]	0.3715773
Q9H228	638	O-C-C-C-N	0.3660249
Q9H228	739	Cc1cc(Br)ccc1	0.3509614
Q9H228	235	>= 2 saturated or aromatic carbon-only ring size 8	0.3507504
Q9H228	866	OC1C(O)CCC1	0.3458016
Q9H228	696	C-C-C-C-C-C-C-C	0.3418237
Q9H228	625	O=C-C:C-O	0.3402057
Q9H228	64	>= 1 Ge	0.3398002
Q9H228	688	C-C-C-C-C-C-C	0.3326034
Q9H228	376	C(~N)(:C)	0.3314237
Q9H228	281	B-Cl	0.32268
Q9H228	144	>= 1 saturated or aromatic carbon-only ring size 5	0.3205181
Q9H228	358	C(~C)(:N)	0.317864
Q9H228	441	C(-C)(=C)	0.306161

Q9H228	361	C(~Cl)(~H)	0.304265
Q9H228	101	>= 1 Pr	0.2983112
Q9H228	559	O-C-N-[#1]	0.2961022
Q9H228	652	O-C:C:C-N	0.2945216
Q9H228	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.2932884
Q9H228	65	>= 1 As	0.2912813
Q9H228	794	ClC1CCC(Cl)CC1	0.2901366
Q9H228	416	C=C	0.2886691
Q9H228	39	>= 4 Cl	0.2868043
Q9H228	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.2752681
Q9H228	710	C-C-C(C)-C-C	0.2749273
Q9H228	658	C-C-S-C-C	0.2699797
Q9H228	604	C-O-C-C:C	0.2683828
Q9H228	355	C(~C)(:C)	0.2677305
Q9H228	572	N:C:N:C	0.2635044
Q9H228	506	C-C:N:C	0.2625277
Q9H228	536	O=C-C-N	0.2589609
Q9H228	357	C(~C)(:C)(:N)	0.258345
Q9H228	870	OC1C(Br)CCC1	0.2576667
Q9H228	521	C:N-C-[#1]	0.2520376
Q9H228	806	OC1CC(Cl)CCC1	0.2507589
Q9H228	609	Cl-C-C-N-C	0.2490275
Q9H228	227	>= 1 any ring size 8	0.2490161
Q9H228	59	>= 1 Co	0.2375012
Q9H228	449	C(-N)(=C)	0.2370676
Q9H228	54	>= 1 Ti	0.2345226
Q9H228	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.2302049
Q9H228	784	OC1CCC(N)CC1	0.2275138
Q9H228	295	C-As	0.2220806
Q9H228	501	Cl-C:C-C	0.215557
Q9H228	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.2121877
Q9H228	547	N-C:C-N	0.2079078
Q9H228	809	SC1CC(N)CCC1	0.2077414
Q9H228	548	O-C-C:C	0.2062619
Q9H228	68	>= 1 Rb	0.2053557
Q9H228	16	>= 4 N	0.1988797
Q9H228	772	Nc1c(Br)cccc1	0.1953364
Q9H228	299	N-H	0.1948055
Q9H228	769	Sc1c(Br)cccc1	0.1847309
Q9H228	377	C(~N)(:C)(:C)	0.1795995
Q9H228	94	>= 1 Au	0.1785994
Q9H228	437	C(-C)(-N)(=C)	0.1774081
Q9H228	800	CC1CC(N)CCC1	0.1763612
Q9H228	551	Cl-C-C-O	0.1738566
Q9H228	745	Sc1cc(S)ccc1	0.1692351
Q9H228	351	C(~C)(~N)	0.1683283
Q9H228	817	BrC1CC(Br)CCC1	0.1673529
Q9H228	382	C(~O)(:C)(:C)	0.1622875

Q9H228	680	O-C-C-C-C-C	0.1620409
Q9H228	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.1615704
Q9H228	543	O-C:C-N	0.1601131
Q9H228	596	N=C-N-C-C	0.1598406
Q9H228	699	O-C-C-C-C-C(C)-C	0.1596666
Q9H228	561	Cl-C-C=O	0.1554057
Q9H228	593	N-C-C-C-N	0.1535516
Q9H228	558	O=N-C:C	0.1520211
Q9H228	443	C(-C)(=O)	0.1463327
Q9H228	53	>= 1 Sc	0.1461841
Q9H228	206	>= 5 any ring size 6	0.1456983
Q9H228	276	B-O	0.1416005
Q9H228	586	C-S-C-C-C	0.1328955
Q9H228	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.1305768
Q9H228	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.1265046
Q9H228	617	C-C-C-O-[#1]	0.1227797
Q9H228	115	>= 1 any ring size 3	0.1215406
Q9H228	826	OC1C(N)CCCC1	0.1206797
Q9H228	860	CC1C(C)CCC1	0.1206705
Q9H228	644	C-C=N-N-C	0.1198859
Q9H228	287	C-F	0.1196351
Q9H228	136	>= 2 any ring size 4	0.1159172
Q9H228	412	S(~C)(~C)	0.1141095
Q9H228	546	N-C:C-[#1]	0.1115796
Q9H228	466	N#C-C=C	0.1096292
Q9H228	150	>= 2 any ring size 5	0.1081125
Q9H228	300	N-N	0.1069559
Q9H228	754	Brc1cc(Br)ccc1	0.102894
Q9H228	487	N-C=N-C	0.1025942
Q9H228	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.1004893
Q9H228	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.0937796
Q9H228	49	>= 1 Be	0.0865828
Q9H228	549	N-C-C:C	0.084917
Q9H228	683	N-C-C-C-C-C	0.0803973
Q9H228	517	N-N-C-N	0.0772554
Q9H228	335	C(~C)(~C)(~C)(~H)	0.0762026
Q9H228	689	O-C-C-C-C-C-C	0.0761889
Q9H228	15	>= 2 N	0.0735656
Q9H228	452	C(-O)(=O)	0.0728135
Q9H228	545	N-C:C-C	0.0715282
Q9H228	57	>= 1 Mn	0.0707547
Q9H228	378	C(~N)(:C)(:N)	0.0694586
Q9H228	334	C(~C)(~C)(~C)(~C)	0.0681712
Q9H228	447	C(-H)(=N)	0.0650799
Q9H228	556	C=C-C-C	0.0649329
Q9H228	396	N(~C)(:C)	0.0631805
Q9H228	599	[#1]-C-C=C-[#1]	0.0622249
Q9H228	353	C(~C)(~S)	0.0598419

Q9H228	77	>= 1 Ag	0.0572957
Q9H228	384	C(:C)(:C)	0.0568117
Q9H228	459	S(=O)(=O)	0.0551867
Q9H228	568	N#C-C-C	0.0531629
Q9H228	508	S=C-N-C	0.0522017
Q9H228	591	Cl-C-C-C-C	0.0497117
Q9H228	541	O-C:C-C	0.0472906
Q9H228	32	>= 4 P	0.043925
Q9H228	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0410302
Q9H228	366	C(~H)(~O)	0.0410125
Q9H228	362	C(~Cl)(:C)	0.0345027
Q9H228	122	>= 2 any ring size 3	0.0335081
Q9H228	48	>= 4 I	0.0330628
Q9H228	422	N=N	0.0328063
Q9H228	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.032773
Q9H228	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.0327074
Q9H228	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0326077
Q9H228	723	Oc1ccc(Br)cc1	0.0319671
Q9H228	511	S=C-N-[#1]	0.0317645
Q9H228	850	SC1CC(S)CC1	0.0315526
Q9H228	256	>= 1 hetero-aromatic ring	0.031248
Q9H228	258	>= 2 hetero-aromatic rings	0.0311933
Q9H228	108	>= 1 Dy	0.0311119
Q9H228	819	CC1C(O)CCCC1	0.0296273
Q9H228	324	P-P	0.0292485
Q9H228	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.02923
Q9H228	293	C-S	0.0287908
Q9H228	41	>= 1 K	0.026924
Q9H228	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.0263216
Q9H228	660	C-C=C-C-C	0.0262238
Q9H228	453	N(-C)(=C)	0.0261469
Q9H228	468	O=S-C-N	0.0260933
Q9H228	257	>= 2 aromatic rings	0.0237072
Q9H228	289	C-Mg	0.0228132
Q9H228	581	O=C-C-C-O	0.0218827
Q9H228	524	C-C=C-C	0.0208169
Q9H228	143	>= 1 any ring size 5	0.0199688
Q9H228	525	[As]-C:C-[#1]	0.0199524
Q9H228	380	C(~O)(~O)	0.0198836
Q9H228	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0193131
Q9H228	413	S(~C)(~H)	0.0188018
Q9H228	616	C:C:N:N:C	0.0185854
Q9H228	738	Cc1cc(Cl)ccc1	0.0185581
Q9H228	557	N:C-O-[#1]	0.0182116
Q9H228	331	C(~Br)(:N)	0.018028
Q9H228	485	N:C:C:N	0.0178361
Q9H228	771	Nc1c(Cl)cccc1	0.0155996
Q9H228	519	N=C-N-C	0.0147003

Q9H228	314	O-P	0.0144283
Q9H228	484	N-C:N:C	0.0142107
Q9H228	404	N(:C)(:C)(:C)	0.0128723
Q9H228	332	C(~C)(~C)	0.0128071
Q9H228	360	C(~Cl)(~Cl)	0.010853
Q9H228	88	>= 1 Ta	0.0101249
Q9H228	337	C(~C)(~C)(~C)(~O)	0.0100897
Q9H228	726	Sc1ccc(Cl)cc1	0.0096686
Q9H228	387	C(:C)(:N)	0.0095484
Q9H228	304	N-P	0.0092063
Q9H228	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0082018
Q9H228	71	>= 1 Zr	0.0075262
Q9H228	782	OC1CCC(O)CC1	0.0071874
Q9H228	624	O=C-C:C-N	0.0069082
Q9H228	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0068687
Q9H228	554	Br-C-C-C	0.0066001
Q9H228	78	>= 1 Cd	0.0065808
Q9H228	164	>= 4 any ring size 5	0.0065283
Q9H228	862	CC1C(S)CCC1	0.0056431
Q9H228	402	N(~O)(:O)	0.0052608
Q9H228	290	C-Al	0.0051576
Q9H228	791	NC1CCC(N)CC1	0.0044484
Q9H228	478	S-C=N-[#1]	0.0037173
Q9H228	470	C:C-C=C	0.0035967
Q9H228	766	Sc1c(S)cccc1	0.003437
Q9H228	277	B-F	0.0032448
Q9H228	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.0030611
Q9H228	496	N:N-C-[#1]	0.0027649
Q9H228	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.0024493
Q9H228	629	S-C:C:C-N	0.0022905
Q9H228	47	>= 2 I	0.0021687
Q9H228	424	N=P	0.0020449
Q9H228	730	Nc1ccc(Br)cc1	0.0018426
Q9H228	255	>= 1 aromatic ring	0.001781
Q9H228	816	ClC1CC(Br)CCC1	0.0016246
Q9H228	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.0013503
Q9H228	874	SC1C(Br)CCC1	0.0012874
Q9H228	375	C(~N)(~N)	0.0009917
Q9H228	444	C(-Cl)(=O)	0.0008496
Q9H228	741	Oc1cc(S)ccc1	0.0004741
Q9H228	13	>= 32 C	0.0004458
Q9H228	713	Cc1ccc(C)cc1	0.0003397
Q9H228	45	>= 4 Br	0.0002533
Q9H228	787	SC1CCC(S)CC1	0.0001353
Q9H228	89	>= 1 W	0.0001076
Q9H228	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	6.43E-05
Q9H228	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	1.43E-05
Q9H228	259	>= 3 aromatic rings	6.08E-07

Q9H228	315	O-K	2.01E-07
Q9H228	326	As-As	1.06E-07
Q9H228	733	Brc1ccc(Br)cc1	-1.52E-07
Q9H228	835	NC1C(Br)CCCC1	-2.07E-07
Q9H228	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	-2.24E-07
Q9H228	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	-0.000351
Q9H228	853	SC1CC(Br)CC1	-0.00041
Q9H228	112	>= 1 Yb	-0.000455
Q9H228	729	Nc1ccc(Cl)cc1	-0.000557
Q9H228	323	P-H	-0.000789
Q9H228	74	>= 1 Ru	-0.000848
Q9H228	648	O=N-C:C-N	-0.001289
Q9H228	265	Li-B	-0.001366
Q9H228	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	-0.001455
Q9H228	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	-0.002348
Q9H228	610	C-O-C-O-C	-0.00298
Q9H228	592	N-C-C-C-C	-0.003356
Q9H228	249	>= 1 saturated or aromatic carbon-only ring size 10	-0.003449
Q9H228	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	-0.004119
Q9H228	282	B-Br	-0.004479
Q9H228	454	N(-C)(=O)	-0.00477
Q9H228	523	N:C:C-C	-0.005329
Q9H228	418	C=N	-0.005733
Q9H228	241	>= 1 any ring size 9	-0.007045
Q9H228	490	C-C-C=C	-0.007294
Q9H228	97	>= 1 Pb	-0.007349
Q9H228	371	C(~H)(:C)(:C)	-0.008127
Q9H228	659	O-C-C-N-C	-0.008383
Q9H228	29	>= 2 Si	-0.008897
Q9H228	27	>= 2 Na	-0.00914
Q9H228	63	>= 1 Ga	-0.010532
Q9H228	775	Brc1c(Br)cccc1	-0.010583
Q9H228	114	>= 1 U	-0.010705
Q9H228	110	>= 1 Er	-0.010884
Q9H228	540	C-N-C-[#1]	-0.014837
Q9H228	116	>= 1 saturated or aromatic carbon-only ring size 3	-0.015735
Q9H228	813	NC1CC(Cl)CCC1	-0.017255
Q9H228	395	N(~C)(~O)	-0.017262
Q9H228	401	N(~O)(~O)	-0.017818
Q9H228	716	Cc1ccc(N)cc1	-0.018165
Q9H228	165	>= 4 saturated or aromatic carbon-only ring size 5	-0.01982
Q9H228	4	>= 1 Li	-0.02008
Q9H228	417	C#C	-0.020828
Q9H228	847	OC1CC(N)CC1	-0.022426
Q9H228	805	OC1CC(N)CCC1	-0.022555
Q9H228	72	>= 1 Nb	-0.022751
Q9H228	673	O=C-C=C-N	-0.022818
Q9H228	46	>= 1 I	-0.024922

Q9H228	30	>= 1 P	−0.025073
Q9H228	642	O-C-C-C=O	−0.02562
Q9H228	311	O-Na	−0.025826
Q9H228	288	C-Na	−0.026248
Q9H228	582	C-C-C-C-C	−0.026376
Q9H228	91	>= 1 Os	−0.027846
Q9H228	263	Li-H	−0.027991
Q9H228	590	C-C:C-O-[#1]	−0.028194
Q9H228	844	CC1CC(Br)CC1	−0.028763
Q9H228	569	N-C-C-N	−0.028994
Q9H228	801	CC1CC(Cl)CCC1	−0.029038
Q9H228	50	>= 1 Mg	−0.029939
Q9H228	564	C=C-C=C	−0.030048
Q9H228	845	OC1CC(O)CC1	−0.030671
Q9H228	854	NC1CC(N)CC1	−0.031246
Q9H228	859	BrC1CC(Br)CC1	−0.033565
Q9H228	440	C(-C)(-O)(=O)	−0.03392
Q9H228	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.035179
Q9H228	394	N(~C)(~H)(~N)	−0.035586
Q9H228	570	C:C-C-C	−0.036333
Q9H228	605	O=C-C-O-C	−0.036786
Q9H228	104	>= 1 Sm	−0.039106
Q9H228	653	O-C:C:C-O	−0.039509
Q9H228	793	NC1CCC(Br)CC1	−0.04145
Q9H228	613	C-N-C-C-C	−0.041567
Q9H228	285	C-N	−0.042091
Q9H228	442	C(-C)(=N)	−0.042128
Q9H228	364	C(~F)(:C)	−0.044393
Q9H228	465	O=S-C-C	−0.044452
Q9H228	725	Sc1ccc(N)cc1	−0.045309
Q9H228	748	Sc1cc(Br)ccc1	−0.047704
Q9H228	462	O-C-C=O	−0.04887
Q9H228	60	>= 1 Ni	−0.050213
Q9H228	76	>= 1 Pd	−0.050263
Q9H228	669	Cl-C:C-C=O	−0.051986
Q9H228	23	>= 1 F	−0.052584
Q9H228	711	C-C(C)(C)-C-C	−0.053044
Q9H228	17	>= 8 N	−0.054867
Q9H228	352	C(~C)(~O)	−0.055713
Q9H228	687	O=C-C-C-C=O	−0.056337
Q9H228	51	>= 1 Al	−0.059294
Q9H228	535	O=C-C-C	−0.060045
Q9H228	345	C(~C)(~H)(~N)	−0.060642
Q9H228	671	O=C-C=C-C	−0.063816
Q9H228	1	>= 8 H	−0.064248
Q9H228	11	>= 8 C	−0.067106
Q9H228	266	Li-C	−0.067645
Q9H228	157	>= 3 any ring size 5	−0.070231

Q9H228	270	Li-S	−0.07077
Q9H228	327	C(~Br)(~C)	−0.071373
Q9H228	639	O-C-C-C-O	−0.071379
Q9H228	405	O(~C)(~C)	−0.071402
Q9H228	779	CC1CCC(N)CC1	−0.071493
Q9H228	28	>= 1 Si	−0.071772
Q9H228	632	C-C-O-C:C	−0.073049
Q9H228	529	Cl-C-C-Cl	−0.075581
Q9H228	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.075719
Q9H228	283	C-H	−0.076197
Q9H228	472	C:N:C-C	−0.076753
Q9H228	858	ClC1CC(Br)CC1	−0.078448
Q9H228	309	O-O	−0.079521
Q9H228	347	C(~C)(~H)(~O)(~O)	−0.079946
Q9H228	359	C(~C)(:N)(:N)	−0.080377
Q9H228	291	C-Si	−0.080485
Q9H228	374	C(~H)(~H)(~H)	−0.081181
Q9H228	668	C-C:C-C-C	−0.081699
Q9H228	338	C(~C)(~C)(~H)(~N)	−0.08624
Q9H228	436	C(-C)(-H)(=O)	−0.08779
Q9H228	837	ClC1C(Br)CCCC1	−0.088788
Q9H228	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.089555
Q9H228	842	CC1CC(N)CC1	−0.090877
Q9H228	703	O-C-C-C-C-C(N)-C	−0.091114
Q9H228	220	>= 2 any ring size 7	−0.091569
Q9H228	354	C(~C)(~Si)	−0.095109
Q9H228	538	N=C-C-C	−0.095313
Q9H228	636	C-N-C-N-C	−0.095828
Q9H228	12	>= 16 C	−0.098131
Q9H228	467	C=N-N-C	−0.099322
Q9H228	530	N:C-C:C	−0.102483
Q9H228	36	>= 8 S	−0.103183
Q9H228	580	O=C-C-C-N	−0.105466
Q9H228	654	N-C-N-C-C	−0.109162
Q9H228	87	>= 1 Hf	−0.109701
Q9H228	356	C(~C)(:C)(:C)	−0.11194
Q9H228	482	C:N-C:C	−0.115624
Q9H228	499	N-C:C:N	−0.119319
Q9H228	329	C(~Br)(~H)	−0.120067
Q9H228	752	Clc1cc(Cl)ccc1	−0.121537
Q9H228	532	S-C:C-[#1]	−0.12251
Q9H228	797	CC1CC(C)CCC1	−0.128494
Q9H228	20	>= 4 O	−0.129969
Q9H228	451	C(-N)(=O)	−0.130233
Q9H228	397	N(~C)(:C)(:C)	−0.130832
Q9H228	350	C(~C)(~I)	−0.1332
Q9H228	712	C-C(C)-C(C)-C	−0.135094
Q9H228	423	N=O	−0.13651

Q9H228	647	O=C-N-C-N	−0.144401
Q9H228	731	Clc1ccc(Cl)cc1	−0.147328
Q9H228	185	>= 2 any ring size 6	−0.151985
Q9H228	615	N-C-C-O-C	−0.153381
Q9H228	34	>= 2 S	−0.153765
Q9H228	435	C(-C)(-H)(=N)	−0.154633
Q9H228	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.157326
Q9H228	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.158382
Q9H228	607	N-C-C-C:C	−0.160021
Q9H228	445	C(-H)(-N)(=C)	−0.161877
Q9H228	830	SC1C(N)CCCC1	−0.165147
Q9H228	734	Cc1cc(C)ccc1	−0.166214
Q9H228	383	C(~S)(:C)	−0.167471
Q9H228	483	N-S-C:C	−0.167691
Q9H228	812	NC1CC(N)CCC1	−0.172069
Q9H228	863	CC1C(N)CCC1	−0.173262
Q9H228	399	N(~H)(:C)	−0.176415
Q9H228	814	NC1CC(Br)CCC1	−0.178077
Q9H228	80	>= 1 Sn	−0.179429
Q9H228	471	S:C:C:C	−0.184584
Q9H228	38	>= 2 Cl	−0.186779
Q9H228	567	O-C-C-O	−0.18838
Q9H228	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.188835
Q9H228	348	C(~C)(~H)(~P)	−0.190951
Q9H228	513	S:C:C-[#1]	−0.193882
Q9H228	667	C=C-C-O-[#1]	−0.195853
Q9H228	855	NC1CC(Cl)CC1	−0.196841
Q9H228	321	Si-Si	−0.197971
Q9H228	732	Clc1ccc(Br)cc1	−0.198754
Q9H228	33	>= 1 S	−0.200014
Q9H228	368	C(~H)(~S)	−0.208056
Q9H228	685	O=C-C-C-C-N	−0.209149
Q9H228	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.213588
Q9H228	6	>= 1 B	−0.216157
Q9H228	336	C(~C)(~C)(~C)(~N)	−0.216264
Q9H228	346	C(~C)(~H)(~O)	−0.226567
Q9H228	261	>= 4 aromatic rings	−0.227148
Q9H228	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.227292
Q9H228	171	>= 5 any ring size 5	−0.228054
Q9H228	790	SC1CCC(Br)CC1	−0.228477
Q9H228	93	>= 1 Pt	−0.229165
Q9H228	749	Nc1cc(N)ccc1	−0.231931
Q9H228	773	Clc1c(Cl)cccc1	−0.233782
Q9H228	674	N-C-N-C:C	−0.235557
Q9H228	663	O-C-C-O-[#1]	−0.241009
Q9H228	736	Cc1cc(S)ccc1	−0.244758
Q9H228	398	N(~H)(~N)	−0.246016
Q9H228	341	C(~C)(~C)(~O)	−0.246594

Q9H228	878	ClC1C(Cl)CCC1	−0.248752
Q9H228	307	N-Br	−0.249243
Q9H228	455	N(-O)(=O)	−0.250561
Q9H228	708	C-C(C)-C-C	−0.25461
Q9H228	841	CC1CC(S)CC1	−0.256484
Q9H228	679	C-C-C-C-C-C	−0.261854
Q9H228	339	C(~C)(~C)(~H)(~O)	−0.264095
Q9H228	578	C-C:C-C:C	−0.264367
Q9H228	542	O-C:C-[#1]	−0.266644
Q9H228	479	S-C-S-C	−0.266989
Q9H228	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.268112
Q9H228	757	Cc1c(S)cccc1	−0.268329
Q9H228	675	Br-C-C-C:C	−0.271715
Q9H228	495	C-N-C:C	−0.274222
Q9H228	385	C(:C)(:C)(:C)	−0.287085
Q9H228	319	Al-Cl	−0.287493
Q9H228	765	Oc1c(Br)cccc1	−0.290139
Q9H228	619	O-C-C=C-C	−0.291945
Q9H228	743	Oc1cc(Cl)ccc1	−0.292662
Q9H228	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.297445
Q9H228	698	O-C-C-C-C-C-C-C	−0.299056
Q9H228	486	N-C:N:N	−0.300057
Q9H228	62	>= 1 Zn	−0.304804
Q9H228	476	C-O-C=C	−0.309874
Q9H228	370	C(~H)(:C)	−0.310216
Q9H228	129	>= 1 any ring size 4	−0.313082
Q9H228	109	>= 1 Ho	−0.319688
Q9H228	843	CC1CC(Cl)CC1	−0.326866
Q9H228	400	N(~H)(:C)(:C)	−0.331948
Q9H228	871	SC1C(S)CCC1	−0.334944
Q9H228	824	OC1C(O)CCCC1	−0.340659
Q9H228	614	C-C-O-C-C	−0.342522
Q9H228	656	C-C-N-C-C	−0.343504
Q9H228	833	NC1C(N)CCCC1	−0.34375
Q9H228	432	C(-C)(-C)(=O)	−0.34433
Q9H228	313	O-Si	−0.345855
Q9H228	589	C-C:C-O-C	−0.349435
Q9H228	340	C(~C)(~C)(~N)	−0.355463
Q9H228	75	>= 1 Rh	−0.355549
Q9H228	831	SC1C(Cl)CCCC1	−0.357823
Q9H228	294	C-Cl	−0.358116
Q9H228	55	>= 1 V	−0.360976
Q9H228	279	B-P	−0.366913
Q9H228	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.367278
Q9H228	372	C(~H)(:C)(:N)	−0.367998
Q9H228	646	O=C-N-C-[#1]	−0.370332
Q9H228	500	C-S-C:C	−0.372121
Q9H228	463	N:C-S-[#1]	−0.37586

Q9H228	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.37966
Q9H228	808	SC1CC(S)CCC1	−0.381029
Q9H228	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.381168
Q9H228	369	C(~H)(~Si)	−0.388119
Q9H228	37	>= 1 Cl	−0.390234
Q9H228	325	As-H	−0.390927
Q9H228	403	N(:C)(:C)	−0.393838
Q9H228	670	Br-C:C:C-C	−0.401534
Q9H228	528	[#1]-N-C-[#1]	−0.402966
Q9H228	815	ClC1CC(Cl)CCC1	−0.40542
Q9H228	588	O=C-C-C=O	−0.40899
Q9H228	192	>= 3 any ring size 6	−0.424504
Q9H228	834	NC1C(Cl)CCCC1	−0.425251
Q9H228	724	Sc1ccc(S)cc1	−0.434207
Q9H228	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.435466
Q9H228	662	O-C-C-O-C	−0.439555
Q9H228	721	Oc1ccc(N)cc1	−0.441618
Q9H228	717	Cc1ccc(Cl)cc1	−0.449728
Q9H228	753	Clc1cc(Br)ccc1	−0.460418
Q9H228	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.461478
Q9H228	657	C-N-C:C-C	−0.467043
Q9H228	597	O=C-C-C:C	−0.470085
Q9H228	807	OC1CC(Br)CCC1	−0.47162
Q9H228	563	O-C-O-C	−0.473242
Q9H228	856	NC1CC(Br)CC1	−0.473824
Q9H228	758	Cc1c(N)cccc1	−0.476351
Q9H228	603	C-C:C:C-C	−0.478915
Q9H228	406	O(~C)(~H)	−0.481315
Q9H228	776	CC1CCC(C)CC1	−0.482127
Q9H228	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.485071
Q9H228	832	SC1C(Br)CCCC1	−0.485846
Q9H228	473	S-C:N:C	−0.488929
Q9H228	823	CC1C(Br)CCCC1	−0.50375
Q9H228	691	O-C-C-C-C-C-N	−0.516682
Q9H228	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.522094
Q9H228	24	>= 2 F	−0.528054
Q9H228	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.529326
Q9H228	750	Nc1cc(Cl)ccc1	−0.536196
Q9H228	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.538058
Q9H228	664	C-C=C-C=C	−0.540088
Q9H228	429	C(#N)(-C)	−0.55812
Q9H228	539	N=C-C-[#1]	−0.558932
Q9H228	623	O=C-C:C-C	−0.562148
Q9H228	40	>= 8 Cl	−0.564844
Q9H228	420	C=O	−0.572432
Q9H228	684	O=C-C-C-C-C	−0.573209
Q9H228	778	CC1CCC(S)CC1	−0.575185
Q9H228	18	>= 1 O	−0.575768

Q9H228	686	O=C-C-C-C-O	−0.57849
Q9H228	760	Cc1c(Br)cccc1	−0.59024
Q9H228	531	S-C:C-C	−0.597528
Q9H228	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.599957
Q9H228	829	SC1C(S)CCCC1	−0.600498
Q9H228	306	N-Cl	−0.611447
Q9H228	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.611714
Q9H228	410	P(~C)(~C)	−0.614589
Q9H228	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.615071
Q9H228	634	C-C-C:C-C	−0.620353
Q9H228	0	>= 4 H	−0.626366
Q9H228	693	O=C-C-C-C-C-O	−0.634118
Q9H228	43	>= 1 Br	−0.637493
Q9H228	764	Oc1c(Cl)cccc1	−0.642947
Q9H228	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.643747
Q9H228	21	>= 8 O	−0.65859
Q9H228	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.670254
Q9H228	630	O-C:C-O-C	−0.672668
Q9H228	631	O-C:C-O-[#1]	−0.674227
Q9H228	86	>= 1 Lu	−0.674929
Q9H228	408	O(~H)(~S)	−0.684003
Q9H228	510	[#1]-N-N-[#1]	−0.68853
Q9H228	709	C-C(C)-C-C-C	−0.689618
Q9H228	84	>= 1 Cs	−0.697181
Q9H228	428	C(#C)(-H)	−0.702226
Q9H228	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.707069
Q9H228	439	C(-C)(-N)(=O)	−0.708701
Q9H228	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.709888
Q9H228	755	Cc1c(C)cccc1	−0.71641
Q9H228	278	B-Si	−0.718321
Q9H228	577	C:C-N-C:C	−0.720266
Q9H228	585	C-C:C-N-C	−0.721315
Q9H228	526	Cl-C:C-Cl	−0.722206
Q9H228	876	NC1C(Cl)CC1	−0.727107
Q9H228	704	O=C-C-C-C-C-C-C	−0.735946
Q9H228	390	N(~C)(~C)	−0.736541
Q9H228	274	B-C	−0.744751
Q9H228	505	Cl-C:C-O	−0.748352
Q9H228	379	C(~N)(:N)	−0.754929
Q9H228	322	Si-Cl	−0.755754
Q9H228	747	Sc1cc(Cl)ccc1	−0.758114
Q9H228	560	N-C-N-C	−0.759992
Q9H228	706	O=C-C-C-C-C(=O)-C	−0.764293
Q9H228	701	O-C-C-C-C-C(O)-C	−0.764494
Q9H228	427	C(#C)(-C)	−0.77358
Q9H228	9	>= 2 C	−0.774711
Q9H228	310	O-Mg	−0.77789
Q9H228	520	C=C-C:C	−0.789138

Q9H228	594	C-O-C-C=C	−0.795082
Q9H228	822	CC1C(Cl)CCCC1	−0.795462
Q9H228	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.804329
Q9H228	8	>= 4 B	−0.805015
Q9H228	391	N(~C)(~C)(~C)	−0.807624
Q9H228	695	O=C-C-C-C-C-N	−0.808607
Q9H228	456	P(-O)(=O)	−0.812838
Q9H228	475	S-C=N-C	−0.81461
Q9H228	694	O=C-C-C-C-C=O	−0.825582
Q9H228	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.830794
Q9H228	409	O(:C)(:C)	−0.832624
Q9H228	388	C(:C)(:N)(:N)	−0.844647
Q9H228	737	Cc1cc(N)ccc1	−0.848252
Q9H228	10	>= 4 C	−0.859451
Q9H228	611	N-C-C-N-C	−0.862238
Q9H228	608	C-C-C-C:C	−0.87287
Q9H228	515	N-N-C-C	−0.873861
Q9H228	651	O-C:C:C-C	−0.879375
Q9H228	774	Clc1c(Br)cccc1	−0.884839
Q9H228	492	N-C:O:C	−0.889895
Q9H228	628	C-N-C-C:C	−0.895519
Q9H228	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.901057
Q9H228	562	Br-C-C=O	−0.903978
Q9H228	414	S(~C)(~O)	−0.907409
Q9H228	573	O-C-C=C	−0.908957
Q9H228	199	>= 4 any ring size 6	−0.928588
Q9H228	720	Oc1ccc(S)cc1	−0.929171
Q9H228	42	>= 2 K	−0.934316
Q9H228	99	>= 1 La	−0.93963
Q9H228	248	>= 1 any ring size 10	−0.9429
Q9H228	852	SC1CC(Cl)CC1	−0.94832
Q9H228	786	OC1CCC(Br)CC1	−0.948753
Q9H228	566	O-C-C-N	−0.952626
Q9H228	828	OC1C(Br)CCCC1	−0.954544
Q9H228	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.961343
Q9H228	555	N=C-C=C	−0.985815
Q9H228	865	CC1C(Br)CCC1	−0.987588
Q9H228	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.991556
Q9H228	849	OC1CC(Br)CC1	−1.005826
Q9H228	98	>= 1 Bi	−1.007241
Q9H228	328	C(~Br)(~C)(~C)	−1.009111
Q9H228	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−1.015904
Q9H228	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−1.023382
Q9H228	719	Oc1ccc(O)cc1	−1.031276
Q9H228	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−1.039257
Q9H228	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−1.05208
Q9H228	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−1.057292
Q9H228	481	O-S-C:C	−1.060177

Q9H228	770	Nc1c(N)cccc1	−1.062102
Q9H228	66	>= 1 Se	−1.065565
Q9H228	810	SC1CC(Cl)CCC1	−1.066758
Q9H228	502	N-C=C-[#1]	−1.070435
Q9H228	742	Oc1cc(N)ccc1	−1.075811
Q9H228	316	F-P	−1.07659
Q9H228	798	CC1CC(O)CCC1	−1.078878
Q9H228	95	>= 1 Hg	−1.082392
Q9H228	612	N-C-O-C-C	−1.085261
Q9H228	846	OC1CC(S)CC1	−1.092143
Q9H228	123	>= 2 saturated or aromatic carbon-only ring size 3	−1.093538
Q9H228	373	C(~H)(:N)	−1.094654
Q9H228	433	C(-C)(-Cl)(=O)	−1.096365
Q9H228	584	C:C-C=C-C	−1.101788
Q9H228	69	>= 1 Sr	−1.127227
Q9H228	574	O-C-C:C-C	−1.136593
Q9H228	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−1.139764
Q9H228	221	>= 2 saturated or aromatic carbon-only ring size 7	−1.14414
Q9H228	178	>= 1 any ring size 6	−1.144232
Q9H228	70	>= 1 Y	−1.145464
Q9H228	746	Sc1cc(N)ccc1	−1.147031
Q9H228	587	N-C:C-O-[#1]	−1.162168
Q9H228	214	>= 1 saturated or aromatic carbon-only ring size 7	−1.176695
Q9H228	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−1.191142
Q9H228	799	CC1CC(S)CCC1	−1.196109
Q9H228	838	BrC1C(Br)CCCC1	−1.209056
Q9H228	460	C-C-C#C	−1.210753
Q9H228	419	C#N	−1.2435
Q9H228	514	O-N-C-C	−1.247952
Q9H228	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−1.25943
Q9H228	873	SC1C(Cl)CCC1	−1.277737
Q9H228	333	C(~C)(~C)(~C)	−1.294854
Q9H228	344	C(~C)(~H)	−1.314868
Q9H228	825	OC1C(S)CCCC1	−1.357852
Q9H228	534	S-C:C-O	−1.37367
Q9H228	79	>= 1 In	−1.381362
Q9H228	857	ClC1CC(Cl)CC1	−1.394576
Q9H228	768	Sc1c(Cl)cccc1	−1.397633
Q9H228	318	Al-H	−1.436299
Q9H228	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−1.437043
Q9H228	284	C-C	−1.451558
Q9H228	804	OC1CC(S)CCC1	−1.456193
Q9H228	477	N-N-C:C	−1.458505
Q9H228	389	C(:N)(:N)	−1.474299
Q9H228	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−1.501028
Q9H228	393	N(~C)(~H)	−1.512788
Q9H228	458	S(-O)(=O)	−1.518435
Q9H228	503	Cl-C:C-[#1]	−1.520116

Q9H228	269	Li-P	−1.551607
Q9H228	262	>= 4 hetero-aromatic rings	−1.585679
Q9H228	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−1.593337
Q9H228	861	CC1C(O)CCC1	−1.594159
Q9H228	727	Sc1ccc(Br)cc1	−1.597996
Q9H228	7	>= 2 B	−1.605082
Q9H228	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−1.611823
Q9H228	421	C=S	−1.664883
Q9H228	722	Oc1ccc(Cl)cc1	−1.680109
Q9H228	469	S-S-C:C	−1.705718
Q9H228	58	>= 1 Fe	−1.720557
Q9H228	635	N-N-C-N-[#1]	−1.983941
Q9H228	740	Oc1cc(O)ccc1	−1.989171
Q9H228	606	O-C:C-C-C	−2.006399
Q9H228	415	Si(~C)(~C)	−2.009327
Q9H228	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−2.117281
Q9H228	777	CC1CCC(O)CC1	−2.202362
Q9H228	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−2.224888
Q9H228	434	C(-C)(-H)(=C)	−2.254836

Fingerprints（continued)

P	Q
2.159735984	-0.004727
2.10927552	-2.20E-07
2.06113468	-0.001859
2.028133924	6.72E-08
2.021587734	-0.001322
1.915914029	3.29E-07
1.905386905	0.0006332
1.895976638	-0.000557
1.856402429	-0.000679
1.812989592	-7.62E-07
1.812096889	4.54E-08
1.787398428	3.45E-07
1.745492412	8.42E-07
1.721376549	-4.00E-07
1.702897229	-0.000371
1.688375826	2.16E-07
1.618254689	0.0019723
1.611051542	0.0008905
1.601342147	7.06E-09
1.51202199	0.0015738
1.512528003	-0.001479
1.493063581	-0.000588
1.478199671	0.0019332
1.450508728	0.0005035
1.450030708	0.0007625
1.445142481	2.85E-07
1.442390308	-0.003099
1.438420484	-0.000553
1.434103305	-2.00E-07
1.375705662	3.19E-07
1.291161654	-0.000645
1.284010245	0.0010875
1.28166459	2.23E-07
1.249529897	-0.00129
1.237695653	0.0032328
1.239767678	-0.001043
1.205007572	1.56E-07
1.200643184	7.56E-07
1.200811986	-0.002672
1.19890775	-0.000924
1.184077726	0.0007134
1.161241708	0.0003958
1.152313405	7.56E-07
1.146750484	0.0005857
1.147143687	-0.001032
1.135636766	0.0012436

1.13353591	-0.00144
1.119309803	-0.001201
1.109701493	3.54E-07
1.108739021	-0.000931
1.10673678	1.05E-06
1.100917101	0.0018085
1.093084709	-3.03E-07
1.090980408	2.42E-07
1.073427993	-0.000151
1.061971223	0.0018355
1.058684069	-0.000656
1.036559712	-2.77E-07
1.034838221	-8.85E-05
1.029277158	-0.001905
1.025075674	-0.000902
1.019614132	-0.000395
1.016275134	0.0024515
1.001698645	7.75E-08
1.000583206	0.0003829
0.996718105	0.0002304
0.994795906	0.0013861
0.990623526	-0.00241
0.987114773	-0.001111
0.982607911	0.0002861
0.981591741	0.0003937
0.974816635	-0.001118
0.970911642	-2.34E-07
0.972438618	-0.00343
0.961178364	0.0023947
0.954599316	-0.00076
0.948603454	4.04E-08
0.946363771	4.79E-07
0.944679954	-8.09E-09
0.939533957	-2.77E-07
0.936783247	1.06E-07
0.932254571	0.0026409
0.932678439	3.98E-07
0.922893321	0.0004616
0.922130586	-5.61E-07
0.920539524	0.0009588
0.919462556	-0.000373
0.916662212	-0.000847
0.911582102	0.0020424
0.903998565	4.81E-07
0.903476618	6.06E-08
0.902202147	1.88E-07
0.901809081	4.81E-07
0.896341998	0.0021469

0.893543638	-1.37E-06
0.889894893	1.99E-07
0.887884704	-0.000845
0.884815164	9.13E-07
0.879528415	0.0014804
0.874047081	0.0007798
0.872539966	-0.002061
0.857434658	-0.002267
0.851511402	0.0022773
0.852677528	0.0002442
0.840262666	-0.000918
0.824937283	4.58E-08
0.824062201	-0.001597
0.816504404	-0.000141
0.814270593	7.90E-08
0.810698404	-8.35E-08
0.80465404	0.0002491
0.803538882	0.0004715
0.800660173	0.0016171
0.791010993	-5.27E-07
0.795641876	-0.006441
0.78870974	2.10E-07
0.777050178	-8.50E-05
0.76362415	-0.001558
0.759348432	-0.000656
0.757262257	2.60E-07
0.752833702	-1.10E-08
0.751823462	-3.46E-07
0.748904268	1.20E-05
0.747547523	5.84E-07
0.742521184	-2.66E-07
0.738787503	6.98E-08
0.740469868	-0.002071
0.732892468	-2.12E-05
0.730276345	0.0007872
0.724330655	4.34E-08
0.705787097	3.52E-07
0.702551759	-0.001594
0.700168112	-1.05E-06
0.697031515	-0.002762
0.682401224	-4.87E-07
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0.663432909	-0.00115
0.661265961	-2.88E-07
0.656915893	-0.000568
0.654450802	-7.59E-07
0.646940376	-3.63E-07
0.641936351	0.004304

0.643925892	-0.000129
0.639946878	0.0006663
0.629468091	-4.16E-07
0.628496966	-0.002927
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0.613925036	-0.000289
0.605808407	0.0013034
0.606360059	1.03E-06
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0.601640448	-1.85E-07
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0.582655482	-0.000491
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0.570795024	-3.61E-07
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0.566277523	-2.85E-07
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0.560968359	1.60E-07
0.559523873	2.12E-07
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0.554397225	-0.002906
0.548974799	0.0004755
0.544809403	3.15E-07
0.542352374	1.90E-07
0.538845567	-0.001998
0.532844686	0.0017084
0.530049772	0.0016652
0.53131329	3.32E-07
0.524628995	-0.00101
0.520324209	3.48E-07
0.523377477	-0.004262
0.516297797	-0.001011
0.514123451	0.0011271
0.510586633	-7.52E-05
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0.506547224	-0.000837
0.504606882	-1.75E-07
0.49927657	0.0005408
0.504062029	-0.004518
0.492548628	0.0038439
0.498642485	-0.003323
0.492611796	0.0023171
0.491757855	0.0011552
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0.466890791	6.44E-08
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0.466369452	-0.002539
0.46654944	-0.002926
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0.426039337	0.0015153
0.426698818	0.0001113
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0.41784441	9.42E-08
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0.409456805	-0.002725
0.406480602	-0.000437
0.403234103	-0.001143
0.401348015	-8.77E-08
0.399216348	-0.000279
0.398735736	8.57E-07
0.396951703	3.65E-07
0.394146593	0.0003878
0.394202328	5.55E-08
0.39294716	0.0003682
0.392785156	-9.74E-07
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0.384387631	-0.000586
0.377634133	0.0008362
0.377314983	0.0005474
0.375876686	-0.000364
0.370787469	0.0007898
0.365792704	0.0002322
0.350565947	0.0003954
0.350751047	-6.00E-07
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0.293209343	0.0013122
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0.275268064	4.63E-10
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0.274202354	-0.004223
0.27053734	-0.002155
0.268367316	-0.000637
0.263327634	0.0001768
0.262652078	-0.000124
0.259426865	-0.000466
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0.24907133	0.0016875
0.250102797	-0.001075
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0.222080314	2.64E-07
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0.206846564	0.0010613
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0.168215147	-0.000862
0.161132952	0.0011545

0.16357048	-0.00153
0.161891697	-0.000321
0.160508864	-0.000396
0.161127449	-0.001287
0.159645481	2.12E-05
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0.152512996	0.0010386
0.150297864	0.0017232
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0.146184769	-6.52E-07
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0.141600703	-2.44E-07
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0.130576978	-1.71E-07
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0.120718824	0.0020609
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0.120322544	0.0003479
0.115155053	0.0047309
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0.117119877	-0.001203
0.11930507	-0.005196
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0.048407634	-0.001117
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0.026308112	-8.43E-05
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0.019952869	-4.78E-07
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0.022156371	-0.003571
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0.014372331	-0.000162
0.012551928	0.0003204
0.014913386	-0.002106
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0.010125444	-5.17E-07
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0.00888891	0.0007797
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0.006579757	1.01E-06
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0.0051584	-7.51E-07
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0.00408379	-0.000367
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0.005075147	-0.001638
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0.001350494	-2.21E-07
0.001287856	-5.06E-07
-0.004579294	0.005571
0.000849836	-2.25E-07
0.001783589	-0.001309
0	0.0004458
-0.0003616	0.0007013
0.000253856	-5.26E-07
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0.000108027	-4.69E-07
6.51E-05	-7.75E-07
1.44E-05	-1.35E-07
0	6.08E-07

0	2.01E-07
0	1.06E-07
0	-1.52E-07
0	-2.07E-07
0	-2.24E-07
-0.000351112	2.29E-07
-0.000409383	-2.92E-07
-0.000455421	1.31E-07
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-0.000788213	-9.26E-07
-0.000847561	-3.64E-07
-0.001172755	-0.000116
-0.001365396	-6.99E-07
-0.004606867	0.0031517
-0.004390402	0.0020422
-0.002962343	-1.81E-05
-0.001426487	-0.001929
-0.003449154	2.66E-07
-0.004118991	2.21E-07
-0.004478975	2.25E-07
-0.006424509	0.0016544
-0.003423366	-0.001906
-0.002600919	-0.003132
-0.007045207	-1.54E-07
-0.008602545	0.001309
-0.007349325	6.52E-08
-0.00836996	0.0002426
-0.007121983	-0.001261
-0.008896936	1.41E-07
-0.009138627	-1.13E-06
-0.010532002	2.45E-07
-0.010583478	9.58E-07
-0.010705896	8.80E-07
-0.010882873	-6.42E-07
-0.014378163	-0.000458
-0.015746321	1.12E-05
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-0.015665221	-0.001597
-0.016021375	-0.001797
-0.018656024	0.0004912
-0.019820143	-1.73E-07
-0.020080393	1.29E-07
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-0.022425703	1.41E-07
-0.021971892	-0.000584
-0.022751097	3.07E-07
-0.022220305	-0.000598
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-0.027991077	2.94E-07
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-0.028763053	2.72E-07
-0.027956667	-0.001038
-0.029288472	0.0002506
-0.029938725	1.35E-08
-0.027875025	-0.002173
-0.030669938	-8.19E-07
-0.031245077	-8.14E-07
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-0.037089971	0.0003035
-0.039106206	3.40E-07
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-0.040844131	-0.000723
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-0.046511727	0.0020602
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-0.050263593	1.13E-07
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-0.052905329	-0.000138
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-0.059744151	-0.000301
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-0.063063094	-0.000753
-0.064248603	5.26E-07
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-0.067645101	1.10E-08
-0.070228783	-1.79E-06

-0.070770437	4.74E-07
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-0.071110091	-0.000383
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-0.077767839	0.0021871
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-0.074091294	-0.002106
-0.076628018	-0.000125
-0.07844757	-7.89E-07
-0.0795209	1.65E-07
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-0.080484951	-2.02E-07
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-2.254683968	-0.000152

Data S1. Ranking of importance of substructure features from Pubchem Fi

GPCR ID	Bit Posit	Bit Substructure	W
Q15391	670	Br-C:C:C-C	2.5975999
Q15391	875	NC1C(N)CCC1	2.5255066
Q15391	729	Nc1ccc(Cl)cc1	2.4578197
Q15391	97	>= 1 Pb	2.4546691
Q15391	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	2.4324138
Q15391	43	>= 1 Br	2.3521165
Q15391	498	O-C=C-C	2.2360375
Q15391	876	NC1C(Cl)CC1	2.2190153
Q15391	587	N-C:C-O-[#1]	2.1977019
Q15391	532	S-C:C-[#1]	2.170212
Q15391	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	2.1437301
Q15391	445	C(-H)(-N)(=C)	2.083371
Q15391	358	C(~C)(:N)	2.0596453
Q15391	650	O=C-N-C=O	1.999107
Q15391	300	N-N	1.9471408
Q15391	669	Cl-C:C-C=O	1.94E+00
Q15391	4	>= 1 Li	1.9229372
Q15391	41	>= 1 K	1.9173884
Q15391	734	Cc1cc(C)ccc1	1.9150624
Q15391	834	NC1C(Cl)CCCC1	1.8915916
Q15391	694	O=C-C-C-C-C=O	1.8635806
Q15391	264	Li-Li	1.8603987
Q15391	720	Oc1ccc(S)cc1	1.8359543
Q15391	387	C(:C)(:N)	1.8052458
Q15391	324	P-P	1.8021161
Q15391	443	C(-C)(=O)	1.7402853
Q15391	523	N:C:C-C	1.6930487
Q15391	104	>= 1 Sm	1.6875858
Q15391	279	B-P	1.6759423
Q15391	111	>= 1 Tm	1.6720842
Q15391	767	Sc1c(N)cccc1	1.6719441
Q15391	717	Cc1ccc(Cl)cc1	1.6608749
Q15391	874	SC1C(Br)CCC1	1.6534243
Q15391	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	1.6308769
Q15391	397	N(~C)(:C)(:C)	1.6197776
Q15391	594	C-O-C-C=C	1.6129335
Q15391	508	S=C-N-C	1.5958531
Q15391	24	>= 2 F	1.5538084
Q15391	456	P(-O)(=O)	1.5510049
Q15391	872	SC1C(N)CCC1	1.5035644
Q15391	378	C(~N)(:C)(:N)	1.460195
Q15391	592	N-C-C-C-C	1.4068719
Q15391	474	S:C:C:N	1.4062546
Q15391	281	B-Cl	1.3945986
Q15391	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	1.3743292
Q15391	29	>= 2 Si	1.371849

Q15391	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	1.3665299
Q15391	486	N-C:N:N	1.3197656
Q15391	662	O-C-C-O-C	1.306428
Q15391	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	1.303019
Q15391	854	NC1CC(N)CC1	1.299001
Q15391	278	B-Si	1.2935692
Q15391	61	>= 1 Cu	1.2770563
Q15391	392	N(~C)(~C)(~H)	1.273354
Q15391	52	>= 1 Ca	1.240905
Q15391	801	CC1CC(Cl)CCC1	1.2404056
Q15391	765	Oc1c(Br)cccc1	1.2301217
Q15391	492	N-C:O:C	1.2253605
Q15391	74	>= 1 Ru	1.1900107
Q15391	837	ClC1C(Br)CCCC1	1.17E+00
Q15391	440	C(-C)(-O)(=O)	1.1644036
Q15391	87	>= 1 Hf	1.1475958
Q15391	354	C(~C)(~Si)	1.146738
Q15391	405	O(~C)(~C)	1.1448923
Q15391	92	>= 1 Ir	1.1437034
Q15391	668	C-C:C-C-C	1.1328497
Q15391	607	N-C-C-C:C	1.1310066
Q15391	491	C-N:C-[#1]	1.1305282
Q15391	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	1.1263779
Q15391	679	C-C-C-C-C-C	1.1201677
Q15391	496	N:N-C-[#1]	1.1116595
Q15391	449	C(-N)(=C)	1.1084771
Q15391	844	CC1CC(Br)CC1	1.1036675
Q15391	641	O-C-C-C=C	1.09E+00
Q15391	438	C(-C)(-N)(=N)	1.0832802
Q15391	46	>= 1 I	1.0802353
Q15391	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.0740522
Q15391	363	C(~F)(~F)	1.0657911
Q15391	315	O-K	1.047418
Q15391	683	N-C-C-C-C-C	1.0394371
Q15391	795	ClC1CCC(Br)CC1	1.0357369
Q15391	590	C-C:C-O-[#1]	1.0350521
Q15391	242	>= 1 saturated or aromatic carbon-only ring size 9	1.0219207
Q15391	72	>= 1 Nb	1.0201216
Q15391	658	C-C-S-C-C	1.0199725
Q15391	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	1.0154728
Q15391	746	Sc1cc(N)ccc1	1.0100911
Q15391	543	O-C:C-N	1.0077877
Q15391	290	C-Al	1.0049009
Q15391	352	C(~C)(~O)	0.9968726
Q15391	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.9904932
Q15391	677	C-C=C-C:C	0.9903997
Q15391	861	CC1C(O)CCC1	0.9897741
Q15391	630	O-C:C-O-C	0.971607

Q15391	115	>= 1 any ring size 3	0.9699555
Q15391	817	BrC1CC(Br)CCC1	0.9519357
Q15391	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.9489517
Q15391	772	Nc1c(Br)cccc1	9.47E-01
Q15391	516	[#1]-C=C-[#1]	0.9451671
Q15391	692	O=C-C-C-C-C-C	0.9428691
Q15391	330	C(~Br)(:C)	0.9410738
Q15391	777	CC1CCC(O)CC1	0.9390357
Q15391	518	O=C-N-N	0.9319698
Q15391	347	C(~C)(~H)(~O)(~O)	0.9287712
Q15391	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.9262551
Q15391	618	C:C-C-C:C	0.9228661
Q15391	294	C-Cl	0.9129525
Q15391	379	C(~N)(:N)	0.9127397
Q15391	381	C(~O)(:C)	0.9122573
Q15391	368	C(~H)(~S)	0.9088547
Q15391	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.8998501
Q15391	272	B-H	0.8989197
Q15391	5	>= 2 Li	0.8974869
Q15391	673	O=C-C=C-N	0.8908536
Q15391	207	>= 5 saturated or aromatic carbon-only ring size 6	0.8875922
Q15391	709	C-C(C)-C-C-C	0.8863246
Q15391	877	NC1C(Br)CCC1	0.8858396
Q15391	85	>= 1 Ba	0.8853189
Q15391	727	Sc1ccc(Br)cc1	0.8847497
Q15391	589	C-C:C-O-C	0.8839494
Q15391	357	C(~C)(:C)(:N)	0.8815828
Q15391	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.8769869
Q15391	850	SC1CC(S)CC1	0.8670148
Q15391	289	C-Mg	0.8641262
Q15391	284	C-C	0.8608377
Q15391	450	C(-N)(=N)	0.8550801
Q15391	865	CC1C(Br)CCC1	0.8525101
Q15391	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.850008
Q15391	805	OC1CC(N)CCC1	0.84546
Q15391	598	Cl-C:C:C-C	0.8415197
Q15391	775	Brc1c(Br)cccc1	0.8393265
Q15391	700	O-C-C-C-C-C-O-C	0.836634
Q15391	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.8268116
Q15391	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.824534
Q15391	691	O-C-C-C-C-C-N	0.8245031
Q15391	25	>= 4 F	0.8238345
Q15391	465	O=S-C-C	0.8120347
Q15391	632	C-C-O-C:C	0.8111862
Q15391	466	N#C-C=C	0.8106041
Q15391	510	[#1]-N-N-[#1]	0.806418
Q15391	707	O=C-C-C-C-C(N)-C	0.8048635
Q15391	416	C=C	0.8021282

Q15391	353	C(~C)(~S)	0.7950793
Q15391	667	C=C-C-O-[#1]	0.7934541
Q15391	760	Cc1c(Br)cccc1	0.7839465
Q15391	538	N=C-C-C	0.7820338
Q15391	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.7776568
Q15391	851	SC1CC(N)CC1	0.7768761
Q15391	697	C-C-C-C-C-C(C)-C	0.7745691
Q15391	652	O-C:C:C-N	0.7739922
Q15391	276	B-O	0.7673178
Q15391	441	C(-C)(=C)	0.7652501
Q15391	597	O=C-C-C:C	0.7586931
Q15391	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.7516246
Q15391	653	O-C:C:C-O	0.7492959
Q15391	779	CC1CCC(N)CC1	0.7475007
Q15391	312	O-Al	0.7469724
Q15391	9	>= 2 C	0.7452269
Q15391	578	C-C:C-C:C	0.7421449
Q15391	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.7412056
Q15391	582	C-C-C-C-C	0.7404818
Q15391	108	>= 1 Dy	0.7397098
Q15391	785	OC1CCC(Cl)CC1	0.734078
Q15391	503	Cl-C:C-[#1]	0.7323414
Q15391	288	C-Na	0.7282476
Q15391	331	C(~Br)(:N)	0.7275539
Q15391	840	CC1CC(O)CC1	0.7261851
Q15391	380	C(~O)(~O)	0.7228877
Q15391	341	C(~C)(~C)(~O)	0.712899
Q15391	428	C(#C)(-H)	0.7108922
Q15391	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.7090466
Q15391	536	O=C-C-N	0.7044357
Q15391	782	OC1CCC(O)CC1	0.7035814
Q15391	605	O=C-C-O-C	0.7002354
Q15391	383	C(~S)(:C)	0.6986947
Q15391	497	O-C:C:N	0.69576
Q15391	659	O-C-C-N-C	0.6844711
Q15391	568	N#C-C-C	0.6809692
Q15391	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.6717825
Q15391	859	BrC1CC(Br)CC1	0.6709389
Q15391	95	>= 1 Hg	0.6705275
Q15391	130	>= 1 saturated or aromatic carbon-only ring size 4	0.6685731
Q15391	820	CC1C(S)CCCC1	0.668066
Q15391	90	>= 1 Re	6.64E-01
Q15391	39	>= 4 Cl	0.6628742
Q15391	561	Cl-C-C=O	0.6625986
Q15391	509	Br-C:C-C	0.6608037
Q15391	647	O=C-N-C-N	0.6574478
Q15391	280	B-S	0.6500415
Q15391	462	O-C-C=O	0.6385854

Q15391	269	Li-P	0.6370411
Q15391	846	OC1CC(S)CC1	0.6246242
Q15391	350	C(~C)(~I)	0.6245354
Q15391	33	>= 1 S	0.6241774
Q15391	586	C-S-C-C-C	0.6218983
Q15391	333	C(~C)(~C)(~C)	0.6209771
Q15391	643	[#1]-C-C-N-[#1]	0.6202277
Q15391	388	C(:C)(:N)(:N)	0.6184903
Q15391	742	Oc1cc(N)ccc1	0.6162922
Q15391	45	>= 4 Br	0.6097506
Q15391	348	C(~C)(~H)(~P)	0.5998684
Q15391	292	C-P	0.5904692
Q15391	285	C-N	0.5843233
Q15391	638	O-C-C-C-N	0.5797571
Q15391	476	C-O-C=C	0.5780966
Q15391	106	>= 1 Gd	0.5731996
Q15391	585	C-C:C-N-C	0.5716304
Q15391	214	>= 1 saturated or aromatic carbon-only ring size 7	0.5659368
Q15391	57	>= 1 Mn	0.5628184
Q15391	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.5526207
Q15391	542	O-C:C-[#1]	0.5502126
Q15391	265	Li-B	0.5414348
Q15391	221	>= 2 saturated or aromatic carbon-only ring size 7	0.5374427
Q15391	743	Oc1cc(Cl)ccc1	0.5360505
Q15391	485	N:C:C:N	0.5357447
Q15391	848	OC1CC(Cl)CC1	0.5246344
Q15391	803	OC1CC(O)CCC1	0.5228312
Q15391	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.5218827
Q15391	640	C=C-C-C-C	0.5074628
Q15391	857	ClC1CC(Cl)CC1	0.4981957
Q15391	672	O=C-C=C-[#1]	0.4961914
Q15391	325	As-H	0.495914
Q15391	366	C(~H)(~O)	0.4924369
Q15391	731	Clc1ccc(Cl)cc1	0.4921513
Q15391	427	C(#C)(-C)	0.4909584
Q15391	712	C-C(C)-C(C)-C	0.4905605
Q15391	69	>= 1 Sr	0.4836437
Q15391	602	O=C-C-N-C	0.4829063
Q15391	533	S-C:C-N	0.4824712
Q15391	577	C:C-N-C:C	0.4800601
Q15391	17	>= 8 N	0.4793586
Q15391	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.4748131
Q15391	351	C(~C)(~N)	0.4612834
Q15391	552	C:C-C:C	0.4605735
Q15391	75	>= 1 Rh	0.4601797
Q15391	390	N(~C)(~C)	0.4587407
Q15391	103	>= 1 Pm	0.4587323
Q15391	627	O=[As]-C:C:C	0.456587

Q15391	514	O-N-C-C	0.4550139
Q15391	414	S(~C)(~O)	0.4486556
Q15391	763	Oc1c(N)cccc1	0.4409089
Q15391	110	>= 1 Er	0.4396659
Q15391	680	O-C-C-C-C-C	0.4380555
Q15391	21	>= 8 O	0.4379191
Q15391	344	C(~C)(~H)	0.4375729
Q15391	256	>= 1 hetero-aromatic ring	0.436868
Q15391	511	S=C-N-[#1]	0.4292235
Q15391	684	O=C-C-C-C-C	0.4287532
Q15391	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.4270239
Q15391	490	C-C-C=C	0.4269443
Q15391	554	Br-C-C-C	0.4259568
Q15391	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.4229942
Q15391	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.4218595
Q15391	112	>= 1 Yb	0.4189006
Q15391	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.4128606
Q15391	389	C(:N)(:N)	0.4088118
Q15391	713	Cc1ccc(C)cc1	0.4078752
Q15391	863	CC1C(N)CCC1	0.4075551
Q15391	18	>= 1 O	0.4053381
Q15391	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.4006976
Q15391	576	N=C-C:C-[#1]	0.3937859
Q15391	784	OC1CCC(N)CC1	0.3937076
Q15391	838	BrC1C(Br)CCCC1	0.3921932
Q15391	480	C:S:C-C	0.389472
Q15391	257	>= 2 aromatic rings	0.3875718
Q15391	461	O-C-C=N	0.3870728
Q15391	12	>= 16 C	0.3851372
Q15391	479	S-C-S-C	0.3784711
Q15391	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.3751789
Q15391	40	>= 8 Cl	0.3746553
Q15391	355	C(~C)(:C)	0.3739185
Q15391	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.3727182
Q15391	531	S-C:C-C	0.3690899
Q15391	811	SC1CC(Br)CCC1	0.365204
Q15391	631	O-C:C-O-[#1]	0.3554284
Q15391	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.355352
Q15391	31	>= 2 P	0.3552323
Q15391	714	Cc1ccc(O)cc1	0.3543752
Q15391	80	>= 1 Sn	0.3441818
Q15391	55	>= 1 V	0.3414046
Q15391	296	C-Se	0.3406461
Q15391	1	>= 8 H	0.3399267
Q15391	769	Sc1c(Br)cccc1	3.39E-01
Q15391	164	>= 4 any ring size 5	0.3368743
Q15391	526	Cl-C:C-Cl	0.3344533
Q15391	297	C-Br	0.3306444

Q15391	51	>= 1 Al	0.3295792
Q15391	404	N(:C)(:C)(:C)	0.3273764
Q15391	267	Li-O	0.3246531
Q15391	678	C-C-C=C-C	0.3241759
Q15391	144	>= 1 saturated or aromatic carbon-only ring size 5	0.3229113
Q15391	291	C-Si	0.3190007
Q15391	0	>= 4 H	0.3188614
Q15391	453	N(-C)(=C)	0.3188397
Q15391	6	>= 1 B	0.3138351
Q15391	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.3112381
Q15391	633	N-C-C:C-C	0.3076713
Q15391	100	>= 1 Ce	0.303546
Q15391	362	C(~Cl)(:C)	0.3034895
Q15391	642	O-C-C-C=O	0.2970928
Q15391	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.2961796
Q15391	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.2952131
Q15391	687	O=C-C-C-C=O	0.2914061
Q15391	448	C(-H)(=O)	0.2896025
Q15391	563	O-C-O-C	0.2886131
Q15391	101	>= 1 Pr	0.2823178
Q15391	193	>= 3 saturated or aromatic carbon-only ring size 6	0.2790498
Q15391	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.2711651
Q15391	62	>= 1 Zn	0.2707518
Q15391	753	Clc1cc(Br)ccc1	0.2699058
Q15391	556	C=C-C-C	0.2688851
Q15391	56	>= 1 Cr	0.2666789
Q15391	790	SC1CCC(Br)CC1	0.2626046
Q15391	873	SC1C(Cl)CCC1	0.2614534
Q15391	13	>= 32 C	0.2613643
Q15391	715	Cc1ccc(S)cc1	0.2602328
Q15391	192	>= 3 any ring size 6	0.2590307
Q15391	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.2569123
Q15391	754	Brc1cc(Br)ccc1	0.2499309
Q15391	334	C(~C)(~C)(~C)(~C)	0.24871
Q15391	548	O-C-C:C	0.2446658
Q15391	395	N(~C)(~O)	0.2392072
Q15391	30	>= 1 P	0.2294923
Q15391	606	O-C:C-C-C	0.2287811
Q15391	660	C-C=C-C-C	0.2230025
Q15391	273	B-B	0.2212974
Q15391	494	O=C-C:N	0.2197243
Q15391	340	C(~C)(~C)(~N)	0.214089
Q15391	158	>= 3 saturated or aromatic carbon-only ring size 5	0.2135307
Q15391	481	O-S-C:C	0.2129199
Q15391	572	N:C:N:C	0.2124967
Q15391	49	>= 1 Be	0.2088881
Q15391	728	Nc1ccc(N)cc1	0.2026064
Q15391	704	O=C-C-C-C-C-C-C	0.2021266

Q15391	58	>= 1 Fe	0.1940396
Q15391	855	NC1CC(Cl)CC1	0.1839298
Q15391	382	C(~O)(:C)(:C)	0.1831398
Q15391	655	O-C-C-C:C	0.1823193
Q15391	853	SC1CC(Br)CC1	0.1789072
Q15391	463	N:C-S-[#1]	1.77E-01
Q15391	318	Al-H	0.1675129
Q15391	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.1672426
Q15391	136	>= 2 any ring size 4	0.163728
Q15391	824	OC1C(O)CCCC1	0.1633018
Q15391	868	OC1C(N)CCC1	0.1624105
Q15391	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.16207
Q15391	495	C-N-C:C	0.1584104
Q15391	277	B-F	0.1583958
Q15391	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.1496414
Q15391	723	Oc1ccc(Br)cc1	0.1487692
Q15391	505	Cl-C:C-O	0.1460036
Q15391	816	ClC1CC(Br)CCC1	0.1457499
Q15391	260	>= 3 hetero-aromatic rings	0.1454979
Q15391	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.1360401
Q15391	399	N(~H)(:C)	0.1356394
Q15391	818	CC1C(C)CCCC1	0.1304388
Q15391	612	N-C-O-C-C	0.1284458
Q15391	259	>= 3 aromatic rings	0.1280591
Q15391	338	C(~C)(~C)(~H)(~N)	0.1235838
Q15391	27	>= 2 Na	0.122734
Q15391	421	C=S	0.1222946
Q15391	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.121304
Q15391	530	N:C-C:C	0.1203602
Q15391	102	>= 1 Nd	0.1203395
Q15391	76	>= 1 Pd	0.1132311
Q15391	539	N=C-C-[#1]	0.1126352
Q15391	417	C#C	0.1098036
Q15391	274	B-C	0.1015544
Q15391	423	N=O	0.1007805
Q15391	738	Cc1cc(Cl)ccc1	0.0980731
Q15391	364	C(~F)(:C)	0.0960637
Q15391	93	>= 1 Pt	0.0892898
Q15391	36	>= 8 S	0.0885746
Q15391	50	>= 1 Mg	0.0815179
Q15391	63	>= 1 Ga	0.0802619
Q15391	319	Al-Cl	0.0793209
Q15391	545	N-C:C-C	0.0724108
Q15391	10	>= 4 C	0.0677874
Q15391	609	Cl-C-C-N-C	0.0670183
Q15391	524	C-C=C-C	0.0669879
Q15391	151	>= 2 saturated or aromatic carbon-only ring size 5	0.0638701
Q15391	745	Sc1cc(S)ccc1	0.0628775

Q15391	384	C(:C)(:C)	0.0577341
Q15391	507	C-C-S-C	0.0565606
Q15391	520	C=C-C:C	0.0517629
Q15391	301	N-O	0.0512237
Q15391	635	N-N-C-N-[#1]	0.048154
Q15391	299	N-H	0.0474518
Q15391	396	N(~C)(:C)	0.0440648
Q15391	493	O=C-C:C	0.0382898
Q15391	780	CC1CCC(Cl)CC1	0.037771
Q15391	468	O=S-C-N	0.0322326
Q15391	810	SC1CC(Cl)CCC1	0.0317621
Q15391	122	>= 2 any ring size 3	0.0316728
Q15391	67	>= 1 Kr	2.93E-02
Q15391	682	O-C-C-C-C-N	0.0274904
Q15391	615	N-C-C-O-C	0.0269056
Q15391	819	CC1C(O)CCCC1	0.0265049
Q15391	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.0257067
Q15391	430	C(-C)(-C)(=C)	0.0224041
Q15391	434	C(-C)(-H)(=C)	0.0218915
Q15391	701	O-C-C-C-C-C(O)-C	0.0214918
Q15391	186	>= 2 saturated or aromatic carbon-only ring size 6	0.0206276
Q15391	553	O=C-C=C	0.0182216
Q15391	550	Cl-C-C-C	0.0158419
Q15391	628	C-N-C-C:C	0.0154899
Q15391	19	>= 2 O	0.0144006
Q15391	557	N:C-O-[#1]	0.0133608
Q15391	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0133367
Q15391	843	CC1CC(Cl)CC1	0.0132723
Q15391	773	Clc1c(Cl)cccc1	0.0128433
Q15391	261	>= 4 aromatic rings	0.0123404
Q15391	178	>= 1 any ring size 6	0.012057
Q15391	37	>= 1 Cl	0.0119331
Q15391	776	CC1CCC(C)CC1	0.0110409
Q15391	459	S(=O)(=O)	0.0095151
Q15391	749	Nc1cc(N)ccc1	0.0093557
Q15391	864	CC1C(Cl)CCC1	0.0092619
Q15391	78	>= 1 Cd	0.0092204
Q15391	502	N-C=C-[#1]	0.0080834
Q15391	458	S(-O)(=O)	0.007915
Q15391	770	Nc1c(N)cccc1	0.00737
Q15391	879	ClC1C(Br)CCC1	0.0069241
Q15391	157	>= 3 any ring size 5	0.0064886
Q15391	337	C(~C)(~C)(~C)(~O)	0.0061606
Q15391	306	N-Cl	0.0060021
Q15391	758	Cc1c(N)cccc1	0.0059872
Q15391	275	B-N	0.0058562
Q15391	271	Li-Cl	0.0055095
Q15391	675	Br-C-C-C:C	0.0049581

Q15391	455	N(-O)(=O)	0.0044179
Q15391	424	N=P	0.0042263
Q15391	446	C(-H)(=C)	0.0039718
Q15391	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.0038738
Q15391	411	P(~O)(~O)	0.0028662
Q15391	706	O=C-C-C-C-C(=O)-C	0.0025506
Q15391	601	N-C:C:C-N	0.0022957
Q15391	266	Li-C	0.0022915
Q15391	730	Nc1ccc(Br)cc1	0.0015604
Q15391	454	N(-C)(=O)	0.0015063
Q15391	200	>= 4 saturated or aromatic carbon-only ring size 6	0.0014881
Q15391	361	C(~Cl)(~H)	0.0010678
Q15391	475	S-C=N-C	0.0010396
Q15391	702	O-C-C-C-C-C-N-C	0.0006443
Q15391	835	NC1C(Br)CCCC1	0.0006005
Q15391	622	O=C-O-C:C	0.0005897
Q15391	2	>= 16 H	0.0004285
Q15391	471	S:C:C:C	0.000406
Q15391	105	>= 1 Eu	0.0001424
Q15391	529	Cl-C-C-Cl	9.80E-05
Q15391	483	N-S-C:C	7.46E-05
Q15391	109	>= 1 Ho	-5.96E-05
Q15391	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.000141
Q15391	751	Nc1cc(Br)ccc1	-0.000774
Q15391	588	O=C-C-C=O	-0.001076
Q15391	22	>= 16 O	-0.001212
Q15391	860	CC1C(C)CCC1	-0.001504
Q15391	81	>= 1 Sb	-0.00155
Q15391	42	>= 2 K	-0.001994
Q15391	303	N-Si	-0.002331
Q15391	470	C:C-C=C	-0.002798
Q15391	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	-0.003057
Q15391	747	Sc1cc(Cl)ccc1	-0.003098
Q15391	457	S(-C)(=O)	-0.004151
Q15391	464	N-C-C=C	-0.005021
Q15391	774	Clc1c(Br)cccc1	-0.005699
Q15391	248	>= 1 any ring size 10	-6.19E-03
Q15391	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	-0.006422
Q15391	26	>= 1 Na	-0.006927
Q15391	637	O-C-C-C-C	-0.007302
Q15391	736	Cc1cc(S)ccc1	-0.00732
Q15391	639	O-C-C-C-O	-0.007484
Q15391	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	-0.010124
Q15391	79	>= 1 In	-0.010797
Q15391	228	>= 1 saturated or aromatic carbon-only ring size 8	-0.010824
Q15391	412	S(~C)(~C)	-0.010841
Q15391	64	>= 1 Ge	-0.01101
Q15391	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	-1.19E-02

Q15391	227	>= 1 any ring size 8	−0.012011
Q15391	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.012356
Q15391	54	>= 1 Ti	−0.012633
Q15391	329	C(~Br)(~H)	−0.012656
Q15391	619	O-C-C=C-C	−0.014573
Q15391	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.015805
Q15391	220	>= 2 any ring size 7	−0.016638
Q15391	636	C-N-C-N-C	−0.019574
Q15391	708	C-C(C)-C-C	−0.021006
Q15391	469	S-S-C:C	−0.021779
Q15391	566	O-C-C-N	−0.026235
Q15391	199	>= 4 any ring size 6	−0.026851
Q15391	370	C(~H)(:C)	−0.02857
Q15391	722	Oc1ccc(Cl)cc1	−0.030556
Q15391	422	N=N	−0.031235
Q15391	307	N-Br	−0.032533
Q15391	579	O=C-C-C-C	−0.033011
Q15391	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.034098
Q15391	519	N=C-N-C	−0.037734
Q15391	705	O=C-C-C-C-C(O)-C	−0.037914
Q15391	600	N-C:C:C-C	−0.039234
Q15391	663	O-C-C-O-[#1]	−0.039376
Q15391	596	N=C-N-C-C	−3.95E−02
Q15391	371	C(~H)(:C)(:C)	−0.040485
Q15391	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.045697
Q15391	262	>= 4 hetero-aromatic rings	−0.047479
Q15391	858	ClC1CC(Br)CC1	−0.049424
Q15391	698	O-C-C-C-C-C-C-C	−0.049749
Q15391	150	>= 2 any ring size 5	−0.051811
Q15391	528	[#1]-N-C-[#1]	−0.055191
Q15391	65	>= 1 As	−0.067096
Q15391	477	N-N-C:C	−0.06879
Q15391	442	C(-C)(=N)	−0.071865
Q15391	574	O-C-C:C-C	−0.076686
Q15391	761	Oc1c(O)cccc1	−0.08149
Q15391	825	OC1C(S)CCCC1	−0.085628
Q15391	400	N(~H)(:C)(:C)	−0.086878
Q15391	66	>= 1 Se	−0.088591
Q15391	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.091531
Q15391	308	O-H	−0.09655
Q15391	527	C:C:N-[#1]	−0.098986
Q15391	44	>= 2 Br	−0.101858
Q15391	676	N#C-C-C-C	−0.103093
Q15391	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.10985
Q15391	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.116353
Q15391	500	C-S-C:C	−0.11948
Q15391	86	>= 1 Lu	−0.125097
Q15391	800	CC1CC(N)CCC1	−0.127773

Q15391	99	>= 1 La	-0.128313
Q15391	725	Sc1ccc(N)cc1	-1.29E-01
Q15391	504	N:C:N-C	-0.13084
Q15391	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	-0.131671
Q15391	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	-0.136331
Q15391	836	ClC1C(Cl)CCCC1	-0.136658
Q15391	77	>= 1 Ag	-0.141674
Q15391	293	C-S	-0.142877
Q15391	20	>= 4 O	-0.144934
Q15391	282	B-Br	-0.149307
Q15391	778	CC1CCC(S)CC1	-0.150196
Q15391	571	[#1]-C-O-[#1]	-0.151284
Q15391	107	>= 1 Tb	-0.154396
Q15391	813	NC1CC(Cl)CCC1	-0.156638
Q15391	540	C-N-C-[#1]	-0.162137
Q15391	328	C(~Br)(~C)(~C)	-0.162141
Q15391	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	-0.164818
Q15391	849	OC1CC(Br)CC1	-0.165888
Q15391	791	NC1CCC(N)CC1	-0.168157
Q15391	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-1.70E-01
Q15391	611	N-C-C-N-C	-0.170881
Q15391	447	C(-H)(=N)	-0.172056
Q15391	821	CC1C(N)CCCC1	-0.174512
Q15391	437	C(-C)(-N)(=C)	-0.17545
Q15391	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-0.179454
Q15391	551	Cl-C-C-O	-0.183515
Q15391	832	SC1C(Br)CCCC1	-0.184487
Q15391	762	Oc1c(S)cccc1	-0.186168
Q15391	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	-0.187805
Q15391	748	Sc1cc(Br)ccc1	-0.193827
Q15391	613	C-N-C-C-C	-0.194002
Q15391	847	OC1CC(N)CC1	-0.194376
Q15391	537	O=C-C-O	-0.196333
Q15391	696	C-C-C-C-C-C-C-C	-0.198093
Q15391	744	Oc1cc(Br)ccc1	-0.199367
Q15391	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.20244
Q15391	268	Li-F	-0.20291
Q15391	771	Nc1c(Cl)cccc1	-0.206105
Q15391	316	F-P	-0.207
Q15391	343	C(~C)(~Cl)(~H)	-0.208521
Q15391	814	NC1CC(Br)CCC1	-0.20931
Q15391	645	O=C-N-C-C	-0.213818
Q15391	608	C-C-C-C:C	-0.215708
Q15391	88	>= 1 Ta	-0.218773
Q15391	129	>= 1 any ring size 4	-0.221218
Q15391	436	C(-C)(-H)(=O)	-0.222239
Q15391	558	O=N-C:C	-0.222276
Q15391	623	O=C-C:C-C	-0.239673

Q15391	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.240273
Q15391	804	OC1CC(S)CCC1	−0.243656
Q15391	721	Oc1ccc(N)cc1	−0.24523
Q15391	686	O=C-C-C-C-O	−0.246092
Q15391	699	O-C-C-C-C-C(C)-C	−0.251215
Q15391	688	C-C-C-C-C-C-C	−0.255317
Q15391	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.256548
Q15391	34	>= 2 S	−0.26052
Q15391	429	C(#N)(-C)	−0.262285
Q15391	501	Cl-C:C-C	−0.262492
Q15391	317	F-S	−0.262542
Q15391	741	Oc1cc(S)ccc1	−0.265405
Q15391	376	C(~N)(:C)	−0.270406
Q15391	735	Cc1cc(O)ccc1	−0.27055
Q15391	346	C(~C)(~H)(~O)	−0.272648
Q15391	391	N(~C)(~C)(~C)	−0.276389
Q15391	415	Si(~C)(~C)	−0.276531
Q15391	750	Nc1cc(Cl)ccc1	−0.278379
Q15391	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.27955
Q15391	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.289903
Q15391	681	O-C-C-C-C-O	−0.296885
Q15391	648	O=N-C:C-N	−0.304139
Q15391	737	Cc1cc(N)ccc1	−0.305393
Q15391	740	Oc1cc(O)ccc1	−0.307997
Q15391	314	O-P	−0.309472
Q15391	71	>= 1 Zr	−0.315061
Q15391	311	O-Na	−0.315567
Q15391	661	O-C-O-C-C	−0.317888
Q15391	867	OC1C(S)CCC1	−0.32025
Q15391	570	C:C-C-C	−0.322064
Q15391	512	C-[As]-O-[#1]	−0.328547
Q15391	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.331882
Q15391	16	>= 4 N	−0.332802
Q15391	792	NC1CCC(Cl)CC1	−0.334238
Q15391	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.334753
Q15391	213	>= 1 any ring size 7	−0.334933
Q15391	365	C(~H)(~N)	−0.337407
Q15391	624	O=C-C:C-N	−0.342277
Q15391	143	>= 1 any ring size 5	−0.34672
Q15391	809	SC1CC(N)CCC1	−0.356846
Q15391	426	P=P	−0.357615
Q15391	593	N-C-C-C-N	−0.358176
Q15391	866	OC1C(O)CCC1	−0.359887
Q15391	241	>= 1 any ring size 9	−0.362474
Q15391	467	C=N-N-C	−0.363322
Q15391	599	[#1]-C-C=C-[#1]	−0.364134
Q15391	335	C(~C)(~C)(~C)(~H)	−0.373335
Q15391	829	SC1C(S)CCCC1	−0.381242

Q15391	796	BrC1CCC(Br)CC1	−0.383749
Q15391	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.399918
Q15391	420	C=O	−0.406704
Q15391	489	N-C-S-C	−0.406821
Q15391	559	O-C-N-[#1]	−0.419069
Q15391	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.421102
Q15391	7	>= 2 B	−0.421534
Q15391	752	Clc1cc(Cl)ccc1	−0.425935
Q15391	38	>= 2 Cl	−0.429374
Q15391	565	C:C-O-C	−0.439068
Q15391	807	OC1CC(Br)CCC1	−0.442779
Q15391	654	N-C-N-C-C	−0.449491
Q15391	549	N-C-C:C	−0.45029
Q15391	309	O-O	−0.452694
Q15391	703	O-C-C-C-C-C(N)-C	−0.452978
Q15391	562	Br-C-C=O	−0.453345
Q15391	797	CC1CC(C)CCC1	−0.45367
Q15391	841	CC1CC(S)CC1	−0.454509
Q15391	604	C-O-C-C:C	−0.454541
Q15391	845	OC1CC(O)CC1	−0.455954
Q15391	610	C-O-C-O-C	−0.463893
Q15391	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.468364
Q15391	91	>= 1 Os	−0.470622
Q15391	711	C-C(C)(C)-C-C	−0.472662
Q15391	842	CC1CC(N)CC1	−0.477469
Q15391	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.4789
Q15391	616	C:C:N:N:C	−0.479877
Q15391	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.480633
Q15391	473	S-C:N:C	−0.485444
Q15391	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.486796
Q15391	625	O=C-C:C-O	−0.487659
Q15391	478	S-C=N-[#1]	−0.488316
Q15391	185	>= 2 any ring size 6	−0.490672
Q15391	569	N-C-C-N	−0.496566
Q15391	59	>= 1 Co	−0.503981
Q15391	581	O=C-C-C-O	−0.506467
Q15391	304	N-P	−0.50819
Q15391	313	O-Si	−0.508572
Q15391	833	NC1C(N)CCCC1	−0.508583
Q15391	406	O(~C)(~H)	−0.510935
Q15391	15	>= 2 N	−0.519776
Q15391	827	OC1C(Cl)CCCC1	−0.523707
Q15391	806	OC1CC(Cl)CCC1	−0.524563
Q15391	345	C(~C)(~H)(~N)	−0.527988
Q15391	826	OC1C(N)CCCC1	−0.528712
Q15391	766	Sc1c(S)cccc1	−0.529705
Q15391	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.53245
Q15391	823	CC1C(Br)CCCC1	−0.539397

Q15391	789	SC1CCC(Cl)CC1	−0.539558
Q15391	719	Oc1ccc(O)cc1	−0.547503
Q15391	68	>= 1 Rb	−0.548705
Q15391	451	C(-N)(=O)	−0.55174
Q15391	444	C(-Cl)(=O)	−0.551809
Q15391	584	C:C-C=C-C	−0.558988
Q15391	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.562536
Q15391	878	ClC1C(Cl)CCC1	−0.565883
Q15391	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.566791
Q15391	418	C=N	−0.569576
Q15391	402	N(~O)(:O)	−0.579871
Q15391	336	C(~C)(~C)(~C)(~N)	−0.583279
Q15391	617	C-C-C-O-[#1]	−0.585146
Q15391	432	C(-C)(-C)(=O)	−0.58763
Q15391	403	N(:C)(:C)	−0.587888
Q15391	674	N-C-N-C:C	−0.588455
Q15391	393	N(~C)(~H)	−0.597464
Q15391	372	C(~H)(:C)(:N)	−0.599597
Q15391	726	Sc1ccc(Cl)cc1	−0.601345
Q15391	83	>= 1 Xe	−0.602782
Q15391	323	P-H	−0.603071
Q15391	394	N(~C)(~H)(~N)	−0.608747
Q15391	525	[As]-C:C-[#1]	−0.608956
Q15391	764	Oc1c(Cl)cccc1	−0.609879
Q15391	53	>= 1 Sc	−0.612424
Q15391	439	C(-C)(-N)(=O)	−0.614478
Q15391	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.616014
Q15391	802	CC1CC(Br)CCC1	−0.633702
Q15391	377	C(~N)(:C)(:C)	−0.636725
Q15391	626	C-O-C:C-C	−0.646933
Q15391	716	Cc1ccc(N)cc1	−0.64726
Q15391	283	C-H	−0.651972
Q15391	547	N-C:C-N	−0.655239
Q15391	856	NC1CC(Br)CC1	−0.661934
Q15391	634	C-C-C:C-C	−0.662279
Q15391	409	O(:C)(:C)	−0.663433
Q15391	327	C(~Br)(~C)	−0.667128
Q15391	320	Si-H	−0.670124
Q15391	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.672105
Q15391	815	ClC1CC(Cl)CCC1	−0.679979
Q15391	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.685935
Q15391	8	>= 4 B	−0.693891
Q15391	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.697577
Q15391	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.697766
Q15391	84	>= 1 Cs	−0.697957
Q15391	305	N-S	−0.701627
Q15391	852	SC1CC(Cl)CC1	−0.70496
Q15391	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.718071

Q15391	116	>= 1 saturated or aromatic carbon-only ring size 3	-0.72066
Q15391	342	C(~C)(~Cl)	-0.722791
Q15391	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	-0.725842
Q15391	724	Sc1ccc(S)cc1	-0.732204
Q15391	690	O-C-C-C-C-C-O	-0.732269
Q15391	555	N=C-C=C	-0.733241
Q15391	401	N(~O)(~O)	-0.735349
Q15391	374	C(~H)(~H)(~H)	-0.736432
Q15391	60	>= 1 Ni	-7.48E-01
Q15391	786	OC1CCC(Br)CC1	-0.757248
Q15391	408	O(~H)(~S)	-0.759554
Q15391	73	>= 1 Mo	-0.759936
Q15391	544	O-C:C-O	-0.767295
Q15391	718	Cc1ccc(Br)cc1	-0.771301
Q15391	580	O=C-C-C-N	-0.777702
Q15391	756	Cc1c(O)cccc1	-0.791341
Q15391	822	CC1C(Cl)CCCC1	-0.793377
Q15391	646	O=C-N-C-[#1]	-0.798738
Q15391	534	S-C:C-O	-0.80545
Q15391	367	C(~H)(~O)(~O)	-0.814522
Q15391	522	C-N-N-[#1]	-0.816756
Q15391	595	C:C-C-C-C	-0.817571
Q15391	385	C(:C)(:C)(:C)	-0.819665
Q15391	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	-0.820237
Q15391	739	Cc1cc(Br)ccc1	-0.828995
Q15391	794	ClC1CCC(Cl)CC1	-0.854393
Q15391	484	N-C:N:C	-0.855382
Q15391	89	>= 1 W	-0.856767
Q15391	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-0.864493
Q15391	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	-0.866061
Q15391	710	C-C-C(C)-C-C	-0.86978
Q15391	322	Si-Cl	-0.871535
Q15391	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	-0.876949
Q15391	98	>= 1 Bi	-0.879812
Q15391	788	SC1CCC(N)CC1	-0.886339
Q15391	567	O-C-C-O	-0.896033
Q15391	621	N-C:C:C:N	-0.90816
Q15391	499	N-C:C:N	-0.914029
Q15391	869	OC1C(Cl)CCC1	-0.918959
Q15391	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	-0.922261
Q15391	871	SC1C(S)CCC1	-0.928565
Q15391	799	CC1CC(S)CCC1	-0.930222
Q15391	114	>= 1 U	-0.945976
Q15391	732	Clc1ccc(Br)cc1	-0.950303
Q15391	310	O-Mg	-0.953822
Q15391	546	N-C:C-[#1]	-0.955283
Q15391	839	CC1CC(C)CC1	-0.968578
Q15391	23	>= 1 F	-0.96937

Q15391	433	C(-C)(-Cl)(=O)	−0.971532
Q15391	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.972083
Q15391	369	C(~H)(~Si)	−0.981479
Q15391	657	C-N-C:C-C	−0.982433
Q15391	82	>= 1 Te	−0.984129
Q15391	564	C=C-C=C	−0.99347
Q15391	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−1.004162
Q15391	781	CC1CCC(Br)CC1	−1.022214
Q15391	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−1.023379
Q15391	35	>= 4 S	−1.023977
Q15391	535	O=C-C-C	−1.024055
Q15391	573	O-C-C=C	−1.031634
Q15391	614	C-C-O-C-C	−1.035083
Q15391	32	>= 4 P	−1.036217
Q15391	298	C-I	−1.038084
Q15391	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−1.042971
Q15391	413	S(~C)(~H)	−1.046351
Q15391	302	N-F	−1.048203
Q15391	560	N-C-N-C	−1.054435
Q15391	644	C-C=N-N-C	−1.083994
Q15391	339	C(~C)(~C)(~H)(~O)	−1.094209
Q15391	488	N-C=N-[#1]	−1.098568
Q15391	487	N-C=N-C	−1.107689
Q15391	575	O-C-C:C-O	−1.110489
Q15391	665	N-C:C-C-C	−1.111302
Q15391	70	>= 1 Y	−1.116035
Q15391	603	C-C:C:C-C	−1.118578
Q15391	171	>= 5 any ring size 5	−1.118977
Q15391	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−1.119869
Q15391	482	C:N-C:C	−1.120202
Q15391	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−1.124206
Q15391	435	C(-C)(-H)(=N)	−1.141303
Q15391	517	N-N-C-N	−1.143739
Q15391	386	C(:C)(:C)(:N)	−1.145467
Q15391	113	>= 1 Tc	−1.150648
Q15391	431	C(-C)(-C)(=N)	−1.152311
Q15391	664	C-C=C-C=C	−1.154736
Q15391	94	>= 1 Au	−1.169961
Q15391	649	O=N-C:C-O	−1.17701
Q15391	96	>= 1 Tl	−1.178993
Q15391	513	S:C:C-[#1]	−1.180032
Q15391	695	O=C-C-C-C-C-N	−1.181731
Q15391	651	O-C:C:C-C	−1.195427
Q15391	693	O=C-C-C-C-C-O	−1.198453
Q15391	258	>= 2 hetero-aromatic rings	−1.204012
Q15391	3	>= 32 H	−1.212482
Q15391	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−1.21952
Q15391	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−1.229067

Q15391	460	C-C-C#C	−1.230665
Q15391	759	Cc1c(Cl)cccc1	−1.238443
Q15391	671	O=C-C=C-C	−1.240167
Q15391	689	O-C-C-C-C-C-C	−1.268448
Q15391	326	As-As	−1.270592
Q15391	831	SC1C(Cl)CCCC1	−1.275135
Q15391	521	C:N-C-[#1]	−1.276793
Q15391	808	SC1CC(S)CCC1	−1.284401
Q15391	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−1.290409
Q15391	28	>= 1 Si	−1.293808
Q15391	359	C(~C)(:N)(:N)	−1.302959
Q15391	620	C:C-O-C-C	−1.319218
Q15391	407	O(~C)(~P)	−1.32391
Q15391	862	CC1C(S)CCC1	−1.336474
Q15391	332	C(~C)(~C)	−1.356913
Q15391	356	C(~C)(:C)(:C)	−1.366907
Q15391	419	C#N	−1.372531
Q15391	398	N(~H)(~N)	−1.384445
Q15391	656	C-C-N-C-C	−1.386551
Q15391	666	C=C-C-O-C	−1.421637
Q15391	179	>= 1 saturated or aromatic carbon-only ring size 6	−1.423349
Q15391	425	P=O	−1.428663
Q15391	812	NC1CC(N)CCC1	−1.460247
Q15391	360	C(~Cl)(~Cl)	−1.501232
Q15391	47	>= 2 I	−1.507615
Q15391	206	>= 5 any ring size 6	−1.509968
Q15391	515	N-N-C-C	−1.512946
Q15391	541	O-C:C-C	−1.51479
Q15391	793	NC1CCC(Br)CC1	−1.517941
Q15391	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−1.52E+00
Q15391	286	C-O	−1.534127
Q15391	506	C-C:N:C	−1.536132
Q15391	270	Li-S	−1.541043
Q15391	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−1.549468
Q15391	783	OC1CCC(S)CC1	−1.555264
Q15391	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−1.573872
Q15391	287	C-F	−1.577456
Q15391	880	BrC1C(Br)CCC1	−1.580754
Q15391	349	C(~C)(~H)(~S)	−1.584522
Q15391	472	C:N:C-C	−1.585647
Q15391	629	S-C:C:C-N	−1.587216
Q15391	14	>= 1 N	−1.593789
Q15391	321	Si-Si	−1.604915
Q15391	757	Cc1c(S)cccc1	−1.607029
Q15391	787	SC1CCC(S)CC1	−1.646097
Q15391	234	>= 2 any ring size 8	−1.673582
Q15391	685	O=C-C-C-C-N	−1.70E+00
Q15391	295	C-As	−1.754935

Q15391	255	>= 1 aromatic ring	−1.860646
Q15391	410	P(~C)(~C)	−1.899567
Q15391	235	>= 2 saturated or aromatic carbon-only ring size 8	−1.944518
Q15391	733	Brc1ccc(Br)cc1	−1.961565
Q15391	11	>= 8 C	−1.972406
Q15391	755	Cc1c(C)cccc1	−1.993257
Q15391	263	Li-H	−2.058922
Q15391	828	OC1C(Br)CCCC1	−2.063029
Q15391	798	CC1CC(O)CCC1	−2.06E+00
Q15391	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−2.108014
Q15391	48	>= 4 I	−2.149107
Q15391	583	Cl-C:C-O-C	−2.184581
Q15391	830	SC1C(N)CCCC1	−2.190133
Q15391	591	Cl-C-C-C-C	−2.212474
Q15391	373	C(~H)(:N)	−2.433516
Q15391	452	C(-O)(=O)	−2.52142
Q15391	768	Sc1c(Cl)cccc1	−2.566509
Q15391	375	C(~N)(~N)	−2.576592
Q15391	870	OC1C(Br)CCC1	−2.61475

ingerprints（continued)

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-0.557561 -0.0014268
-0.562536 -4.66E-08
-0.565883 -3.26E-08
-0.566791 -4.85E-09
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-0.583511 -0.0016346
-0.587668   3.73E-05
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-0.593274 -0.0041892
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-1.212482 -4.00E-08
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-1.227487 -0.0015797

-1.227035 -0.0036301
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-1.261273 -0.0071753
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-1.373673 0.00114276
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-1.518872 0.00408159
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-1.533607 -0.0005206
-1.536299 0.00016663
-1.541043 -2.01E-08
-1.549468   4.15E-08
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-1.575721 0.00184957
-1.570932 -0.0065236
-1.580754   8.47E-08
-1.579746 -0.0047757
-1.585814 0.00016656
-1.583623 -0.0035923
-1.593939 0.00015047
-1.604915 -3.75E-08
-1.604634 -0.0023943
-1.646097 -6.41E-08
-1.673582   1.08E-08
  -1.6992 -0.0029134
-1.754935   9.37E-09

-1.860646	6.63E-09
-1.899567	5.57E-08
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-1.961565	5.56E-09
-1.972519	0.00011264
-1.992641	-0.0006163
-2.058922	-3.64E-09
-2.063029	4.49E-08
-2.068472	0.00465625
-2.108014	5.45E-08
-2.149107	1.11E-08
-2.184581	-2.26E-08
-2.18974	-0.000393
-2.213324	0.00084967
-2.432715	-0.0008007
-2.519807	-1.61E-03
-2.566768	0.00025916
-2.576436	-0.0001561
-2.61475	-1.39E-08

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P51582	837	ClC1C(Br)CCCC1	2.5816457
P51582	20	>= 4 O	1.8426125
P51582	480	C:S:C-C	1.7588988
P51582	278	B-Si	1.6674489
P51582	607	N-C-C-C:C	1.6218197
P51582	651	O-C:C:C-C	1.6108728
P51582	608	C-C-C-C:C	1.6002737
P51582	731	Clc1ccc(Cl)cc1	1.5306922
P51582	565	C:C-O-C	1.506286
P51582	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	1.4924647
P51582	345	C(~C)(~H)(~N)	1.4879878
P51582	765	Oc1c(Br)cccc1	1.4856919
P51582	818	CC1C(C)CCCC1	1.483431
P51582	490	C-C-C=C	1.4820861
P51582	288	C-Na	1.4803546
P51582	780	CC1CCC(Cl)CC1	1.4738757
P51582	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	1.4565858
P51582	214	>= 1 saturated or aromatic carbon-only ring size 7	1.4470789
P51582	329	C(~Br)(~H)	1.3765618
P51582	615	N-C-C-O-C	1.3608938
P51582	510	[#1]-N-N-[#1]	1.3604546
P51582	704	O=C-C-C-C-C-C-C	1.3520723
P51582	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	1.3483101
P51582	771	Nc1c(Cl)cccc1	1.3467726
P51582	0	>= 4 H	1.3374816
P51582	440	C(-C)(-O)(=O)	1.3243494
P51582	368	C(~H)(~S)	1.3085165
P51582	25	>= 4 F	1.2701691
P51582	512	C-[As]-O-[#1]	1.2690493
P51582	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	1.2628381
P51582	705	O=C-C-C-C-C(O)-C	1.2569713
P51582	84	>= 1 Cs	1.2297733
P51582	496	N:N-C-[#1]	1.2018289
P51582	249	>= 1 saturated or aromatic carbon-only ring size 10	1.1942717
P51582	574	O-C-C:C-C	1.1818046
P51582	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	1.1787591
P51582	661	O-C-O-C-C	1.1772524
P51582	151	>= 2 saturated or aromatic carbon-only ring size 5	1.1701703
P51582	825	OC1C(S)CCCC1	1.1542603
P51582	561	Cl-C-C=O	1.1266766
P51582	850	SC1CC(S)CC1	1.1128827
P51582	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	1.0880356
P51582	82	>= 1 Te	1.0854336
P51582	777	CC1CCC(O)CC1	1.0787994
P51582	371	C(~H)(:C)(:C)	1.0754106
P51582	819	CC1C(O)CCCC1	1.0735132

P51582	375	C(~N)(~N)	1.0732035
P51582	530	N:C-C:C	1.0649038
P51582	318	Al-H	1.0568561
P51582	431	C(-C)(-C)(=N)	1.0480834
P51582	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	1.0377265
P51582	531	S-C:C-C	1.0354477
P51582	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	1.0250033
P51582	873	SC1C(Cl)CCC1	0.9950999
P51582	784	OC1CCC(N)CC1	0.9922508
P51582	583	Cl-C:C-O-C	0.9846839
P51582	567	O-C-C-O	0.9659544
P51582	722	Oc1ccc(Cl)cc1	0.9611263
P51582	783	OC1CCC(S)CC1	0.9522572
P51582	81	>= 1 Sb	0.9325869
P51582	259	>= 3 aromatic rings	0.8961539
P51582	301	N-O	0.8847772
P51582	136	>= 2 any ring size 4	0.8810429
P51582	864	CC1C(Cl)CCC1	0.8804022
P51582	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.8773533
P51582	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.8742716
P51582	447	C(-H)(=N)	0.8595446
P51582	621	N-C:C:C:N	0.8473108
P51582	94	>= 1 Au	0.8466282
P51582	270	Li-S	0.8452198
P51582	263	Li-H	0.8302857
P51582	673	O=C-C=C-N	0.8229399
P51582	576	N=C-C:C-[#1]	0.8114469
P51582	122	>= 2 any ring size 3	0.8108577
P51582	44	>= 2 Br	0.7923332
P51582	40	>= 8 Cl	0.7914708
P51582	6	>= 1 B	0.7892614
P51582	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.7744409
P51582	706	O=C-C-C-C-C(=O)-C	0.7726913
P51582	847	OC1CC(N)CC1	0.7708666
P51582	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.7705502
P51582	334	C(~C)(~C)(~C)(~C)	0.7567538
P51582	549	N-C-C:C	0.7482832
P51582	752	Clc1cc(Cl)ccc1	0.7474575
P51582	260	>= 3 hetero-aromatic rings	0.745817
P51582	350	C(~C)(~I)	0.7436619
P51582	841	CC1CC(S)CC1	0.7354852
P51582	59	>= 1 Co	0.7304093
P51582	417	C#C	0.7294783
P51582	104	>= 1 Sm	0.7199514
P51582	860	CC1C(C)CCC1	0.7137278
P51582	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.7106833
P51582	829	SC1C(S)CCCC1	0.7091413
P51582	290	C-Al	0.7078124

P51582	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.7071631
P51582	73	>= 1 Mo	0.7062044
P51582	430	C(-C)(-C)(=C)	0.6946039
P51582	666	C=C-C-O-C	0.6750703
P51582	602	O=C-C-N-C	0.6686695
P51582	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.6669226
P51582	690	O-C-C-C-C-C-O	0.6668263
P51582	643	[#1]-C-C-N-[#1]	0.6551353
P51582	91	>= 1 Os	0.6454969
P51582	98	>= 1 Bi	0.6432483
P51582	287	C-F	0.6311901
P51582	743	Oc1cc(Cl)ccc1	0.6166917
P51582	617	C-C-C-O-[#1]	0.6148205
P51582	687	O=C-C-C-C=O	0.6028681
P51582	309	O-O	0.6009686
P51582	632	C-C-O-C:C	0.5949822
P51582	420	C=O	0.5934736
P51582	413	S(~C)(~H)	0.5922
P51582	692	O=C-C-C-C-C-C	0.5904201
P51582	505	Cl-C:C-O	0.5784833
P51582	809	SC1CC(N)CCC1	0.5763895
P51582	256	>= 1 hetero-aromatic ring	0.5755413
P51582	400	N(~H)(:C)(:C)	0.5722824
P51582	851	SC1CC(N)CC1	0.5705342
P51582	737	Cc1cc(N)ccc1	0.5649257
P51582	681	O-C-C-C-C-O	0.5646199
P51582	710	C-C-C(C)-C-C	0.5404758
P51582	446	C(-H)(=C)	0.5393727
P51582	416	C=C	0.5380252
P51582	330	C(~Br)(:C)	0.536246
P51582	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.5348107
P51582	48	>= 4 I	0.5282897
P51582	150	>= 2 any ring size 5	0.5260472
P51582	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.524546
P51582	700	O-C-C-C-C-C-O-C	0.507708
P51582	445	C(-H)(-N)(=C)	0.4885213
P51582	723	Oc1ccc(Br)cc1	0.4876465
P51582	509	Br-C:C-C	0.4819324
P51582	697	C-C-C-C-C-C(C)-C	0.4816191
P51582	500	C-S-C:C	0.4697676
P51582	366	C(~H)(~O)	0.4543299
P51582	207	>= 5 saturated or aromatic carbon-only ring size 6	0.4532284
P51582	695	O=C-C-C-C-C-N	0.4511559
P51582	444	C(-Cl)(=O)	0.4500919
P51582	874	SC1C(Br)CCC1	0.4497164
P51582	280	B-S	0.4481863
P51582	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.4445315
P51582	683	N-C-C-C-C-C	0.4373155

P51582	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.4316073
P51582	614	C-C-O-C-C	0.4248863
P51582	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.4215079
P51582	702	O-C-C-C-C-C-N-C	0.4187049
P51582	107	>= 1 Tb	0.4157751
P51582	312	O-Al	0.4156879
P51582	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.4120618
P51582	511	S=C-N-[#1]	0.4111703
P51582	5	>= 2 Li	0.4097045
P51582	179	>= 1 saturated or aromatic carbon-only ring size 6	0.4092237
P51582	670	Br-C:C-C-C	0.3934993
P51582	680	O-C-C-C-C-C	0.3924966
P51582	437	C(-C)(-N)(=C)	0.3863122
P51582	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.3768746
P51582	719	Oc1ccc(O)cc1	0.3628901
P51582	527	C:C:N-[#1]	0.36288
P51582	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.3612659
P51582	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.3605374
P51582	436	C(-C)(-H)(=O)	0.3491466
P51582	649	O=N-C:C-O	0.3416654
P51582	630	O-C:C-O-C	0.3343321
P51582	741	Oc1cc(S)ccc1	0.3303968
P51582	41	>= 1 K	0.328277
P51582	426	P=P	0.3202287
P51582	337	C(~C)(~C)(~C)(~O)	0.3170326
P51582	646	O=C-N-C-[#1]	0.3140257
P51582	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.3130408
P51582	804	OC1CC(S)CCC1	0.3120875
P51582	66	>= 1 Se	0.2957924
P51582	433	C(-C)(-Cl)(=O)	0.2913088
P51582	728	Nc1ccc(N)cc1	0.2912139
P51582	484	N-C:N:C	0.2841836
P51582	185	>= 2 any ring size 6	0.2757866
P51582	397	N(~C)(:C)(:C)	0.270296
P51582	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.2698809
P51582	844	CC1CC(Br)CC1	0.2650946
P51582	464	N-C-C=C	0.2643213
P51582	815	ClC1CC(Cl)CCC1	0.2581498
P51582	387	C(:C)(:N)	0.2577633
P51582	689	O-C-C-C-C-C-C	0.2574945
P51582	709	C-C(C)-C-C-C	0.2551469
P51582	868	OC1C(N)CCC1	0.2482017
P51582	367	C(~H)(~O)(~O)	0.2473279
P51582	691	O-C-C-C-C-C-N	0.2463102
P51582	854	NC1CC(N)CC1	0.2410321
P51582	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.2385226
P51582	638	O-C-C-C-N	0.2328795
P51582	33	>= 1 S	0.229949

P51582	502	N-C=C-[#1]	0.2271315
P51582	591	Cl-C-C-C-C	0.2231471
P51582	678	C-C-C=C-C	0.2194239
P51582	679	C-C-C-C-C-C	0.2189559
P51582	546	N-C:C-[#1]	0.2189411
P51582	74	>= 1 Ru	0.2186518
P51582	609	Cl-C-C-N-C	0.2185974
P51582	568	N#C-C-C	0.2172843
P51582	258	>= 2 hetero-aromatic rings	0.2120314
P51582	778	CC1CCC(S)CC1	0.2119679
P51582	362	C(~Cl)(:C)	0.2105582
P51582	37	>= 1 Cl	0.2100002
P51582	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.2071557
P51582	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.206696
P51582	406	O(~C)(~H)	0.2065545
P51582	763	Oc1c(N)cccc1	0.2054293
P51582	283	C-H	0.1991781
P51582	833	NC1C(N)CCCC1	0.1939685
P51582	639	O-C-C-C-O	0.1858613
P51582	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.1832518
P51582	696	C-C-C-C-C-C-C-C	0.1802865
P51582	624	O=C-C:C-N	0.1766833
P51582	199	>= 4 any ring size 6	0.176661
P51582	38	>= 2 Cl	0.1741171
P51582	86	>= 1 Lu	0.168905
P51582	759	Cc1c(Cl)cccc1	0.1676097
P51582	653	O-C:C:C-O	0.167434
P51582	533	S-C:C-N	0.166732
P51582	483	N-S-C:C	0.1608321
P51582	677	C-C=C-C:C	0.1578802
P51582	28	>= 1 Si	0.1455678
P51582	352	C(~C)(~O)	0.1446106
P51582	642	O-C-C-C=O	0.1421329
P51582	360	C(~Cl)(~Cl)	0.139174
P51582	137	>= 2 saturated or aromatic carbon-only ring size 4	0.1348776
P51582	650	O=C-N-C=O	0.1304497
P51582	328	C(~Br)(~C)(~C)	0.1283497
P51582	491	C-N:C-[#1]	0.1266532
P51582	749	Nc1cc(N)ccc1	0.1203542
P51582	27	>= 2 Na	0.1160633
P51582	293	C-S	0.1136281
P51582	95	>= 1 Hg	0.1114871
P51582	544	O-C:C-O	0.110245
P51582	542	O-C:C-[#1]	0.1101131
P51582	257	>= 2 aromatic rings	0.1100363
P51582	601	N-C:C:C-N	0.1046383
P51582	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.101985
P51582	560	N-C-N-C	0.0967398

P51582	359	C(~C)(:N)(:N)	0.0950893
P51582	314	O-P	0.0939482
P51582	742	Oc1cc(N)ccc1	0.0918651
P51582	698	O-C-C-C-C-C-C-C	0.0886451
P51582	412	S(~C)(~C)	0.0881037
P51582	438	C(-C)(-N)(=N)	0.0877715
P51582	736	Cc1cc(S)ccc1	0.0858242
P51582	807	OC1CC(Br)CCC1	0.080919
P51582	708	C-C(C)-C-C	0.0808943
P51582	404	N(:C)(:C)(:C)	0.0780487
P51582	43	>= 1 Br	0.0752268
P51582	206	>= 5 any ring size 6	0.0743486
P51582	192	>= 3 any ring size 6	0.0713641
P51582	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.0689412
P51582	813	NC1CC(Cl)CCC1	0.0685946
P51582	657	C-N-C:C-C	0.0675736
P51582	598	Cl-C:C:C-C	0.0663375
P51582	747	Sc1cc(Cl)ccc1	0.0659984
P51582	557	N:C-O-[#1]	0.0656598
P51582	365	C(~H)(~N)	0.0655706
P51582	463	N:C-S-[#1]	0.065283
P51582	869	OC1C(Cl)CCC1	0.0652401
P51582	699	O-C-C-C-C-C(C)-C	0.0650423
P51582	518	O=C-N-N	0.0644244
P51582	648	O=N-C:C-N	0.0635345
P51582	589	C-C:C-O-C	0.0626872
P51582	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.0626266
P51582	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0619057
P51582	75	>= 1 Rh	0.0611346
P51582	612	N-C-O-C-C	0.0611345
P51582	794	ClC1CCC(Cl)CC1	0.060817
P51582	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.06054
P51582	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0602799
P51582	625	O=C-C:C-O	0.0600975
P51582	373	C(~H)(:N)	0.059934
P51582	526	Cl-C:C-Cl	0.059709
P51582	622	O=C-O-C:C	0.0596868
P51582	467	C=N-N-C	0.0581359
P51582	35	>= 4 S	0.0577324
P51582	228	>= 1 saturated or aromatic carbon-only ring size 8	0.0564287
P51582	770	Nc1c(N)cccc1	0.0552822
P51582	297	C-Br	0.0542825
P51582	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0535639
P51582	418	C=N	0.0535444
P51582	56	>= 1 Cr	0.0530592
P51582	592	N-C-C-C-C	0.050653
P51582	795	ClC1CCC(Br)CC1	0.0503811
P51582	348	C(~C)(~H)(~P)	0.0493343

P51582	559	O-C-N-[#1]	0.0488013
P51582	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.0456613
P51582	403	N(:C)(:C)	0.0450934
P51582	513	S:C:C-[#1]	0.0446995
P51582	498	O-C=C-C	0.0446938
P51582	402	N(~O)(:O)	0.0446849
P51582	308	O-H	0.0444487
P51582	164	>= 4 any ring size 5	0.0429774
P51582	479	S-C-S-C	0.0423314
P51582	285	C-N	0.042203
P51582	802	CC1CC(Br)CCC1	0.0393645
P51582	88	>= 1 Ta	0.0386766
P51582	71	>= 1 Zr	0.0351889
P51582	112	>= 1 Yb	0.0350659
P51582	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.0344774
P51582	322	Si-Cl	0.0343102
P51582	248	>= 1 any ring size 10	0.0342676
P51582	424	N=P	0.0338615
P51582	395	N(~C)(~O)	0.0337107
P51582	374	C(~H)(~H)(~H)	0.0336298
P51582	676	N#C-C-C-C	0.0320811
P51582	220	>= 2 any ring size 7	0.0311942
P51582	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.0311667
P51582	388	C(:C)(:N)(:N)	0.0309861
P51582	378	C(~N)(:C)(:N)	0.0309254
P51582	279	B-P	0.0307685
P51582	472	C:N:C-C	0.030045
P51582	85	>= 1 Ba	0.0297937
P51582	810	SC1CC(Cl)CCC1	0.0294917
P51582	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0292751
P51582	714	Cc1ccc(O)cc1	0.0290522
P51582	29	>= 2 Si	0.0283004
P51582	32	>= 4 P	0.0279289
P51582	693	O=C-C-C-C-C-O	0.0270253
P51582	623	O=C-C:C-C	0.0262047
P51582	640	C=C-C-C-C	0.0255101
P51582	347	C(~C)(~H)(~O)(~O)	0.0242434
P51582	394	N(~C)(~H)(~N)	0.0239139
P51582	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.022319
P51582	853	SC1CC(Br)CC1	0.021779
P51582	39	>= 4 Cl	0.0217591
P51582	423	N=O	0.0216392
P51582	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.021217
P51582	291	C-Si	0.0210168
P51582	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.020957
P51582	96	>= 1 Tl	0.020938
P51582	261	>= 4 aromatic rings	0.020141
P51582	688	C-C-C-C-C-C-C	0.0198234

P51582	767	Sc1c(N)cccc1	0.0197689
P51582	674	N-C-N-C:C	0.019544
P51582	452	C(-O)(=O)	0.0186561
P51582	70	>= 1 Y	0.0185294
P51582	1	>= 8 H	0.0182397
P51582	750	Nc1cc(Cl)ccc1	0.018182
P51582	143	>= 1 any ring size 5	0.0179634
P51582	281	B-Cl	0.0166806
P51582	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0166733
P51582	87	>= 1 Hf	0.0165282
P51582	799	CC1CC(S)CCC1	0.0164011
P51582	434	C(-C)(-H)(=C)	0.0163939
P51582	838	BrC1C(Br)CCCC1	0.0160689
P51582	272	B-H	0.0154461
P51582	327	C(~Br)(~C)	0.0149901
P51582	803	OC1CC(O)CCC1	0.0147594
P51582	450	C(-N)(=N)	0.0146398
P51582	488	N-C=N-[#1]	0.0140969
P51582	572	N:C:N:C	0.0139452
P51582	515	N-N-C-C	0.0127504
P51582	389	C(:N)(:N)	0.0125955
P51582	593	N-C-C-C-N	0.0125879
P51582	848	OC1CC(Cl)CC1	0.0121844
P51582	596	N=C-N-C-C	0.0121365
P51582	21	>= 8 O	0.0118264
P51582	89	>= 1 W	0.0115559
P51582	67	>= 1 Kr	0.0112454
P51582	828	OC1C(Br)CCCC1	0.010569
P51582	751	Nc1cc(Br)ccc1	0.0105331
P51582	789	SC1CCC(Cl)CC1	0.0104483
P51582	830	SC1C(N)CCCC1	0.0101001
P51582	541	O-C:C-C	0.0100534
P51582	51	>= 1 Al	0.0093481
P51582	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0092477
P51582	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0088058
P51582	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.0080764
P51582	738	Cc1cc(Cl)ccc1	0.0079713
P51582	553	O=C-C=C	0.0076109
P51582	213	>= 1 any ring size 7	0.007458
P51582	786	OC1CCC(Br)CC1	0.0074129
P51582	805	OC1CC(N)CCC1	0.0071952
P51582	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0070704
P51582	111	>= 1 Tm	0.0062159
P51582	19	>= 2 O	0.0057121
P51582	106	>= 1 Gd	0.0053971
P51582	779	CC1CCC(N)CC1	0.0051456
P51582	720	Oc1ccc(S)cc1	0.0047083
P51582	49	>= 1 Be	0.0046226

P51582	102	>= 1 Nd	0.0042856
P51582	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.0038694
P51582	636	C-N-C-N-C	0.0036138
P51582	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0034369
P51582	31	>= 2 P	0.0033566
P51582	379	C(~N)(:N)	0.0033267
P51582	654	N-C-N-C-C	0.0030555
P51582	820	CC1C(S)CCCC1	0.003052
P51582	806	OC1CC(Cl)CCC1	0.0027363
P51582	604	C-O-C-C:C	0.0023137
P51582	757	Cc1c(S)cccc1	0.0022717
P51582	788	SC1CCC(N)CC1	0.0019872
P51582	460	C-C-C#C	0.0016345
P51582	386	C(:C)(:C)(:N)	0.0015993
P51582	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0015282
P51582	863	CC1C(N)CCC1	0.0014233
P51582	808	SC1CC(S)CCC1	0.0012852
P51582	766	Sc1c(S)cccc1	0.0008071
P51582	494	O=C-C:N	0.0007954
P51582	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0007311
P51582	644	C-C=N-N-C	0.000682
P51582	4	>= 1 Li	0.0005314
P51582	47	>= 2 I	0.00046
P51582	313	O-Si	0.0004501
P51582	123	>= 2 saturated or aromatic carbon-only ring size 3	0.000393
P51582	36	>= 8 S	0.0003143
P51582	53	>= 1 Sc	0.0003125
P51582	506	C-C:N:C	0.0002656
P51582	110	>= 1 Er	0.0001793
P51582	522	C-N-N-[#1]	0.0001018
P51582	369	C(~H)(~Si)	5.04E-05
P51582	80	>= 1 Sn	7.35E-07
P51582	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	4.89E-07
P51582	769	Sc1c(Br)cccc1	1.08E-07
P51582	862	CC1C(S)CCC1	1.66E-08
P51582	525	[As]-C:C-[#1]	-2.51E-08
P51582	8	>= 4 B	-5.71E-08
P51582	478	S-C=N-[#1]	-1.30E-07
P51582	64	>= 1 Ge	-3.22E-07
P51582	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	-9.50E-07
P51582	734	Cc1cc(C)ccc1	-0.000137
P51582	631	O-C:C-O-[#1]	-0.000152
P51582	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-0.000208
P51582	827	OC1C(Cl)CCCC1	-0.000333
P51582	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	-0.000396
P51582	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	-0.000719
P51582	341	C(~C)(~C)(~O)	-0.000754
P51582	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	-0.000783

P51582	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.000875
P51582	255	>= 1 aromatic ring	−0.000954
P51582	481	O-S-C:C	−0.001016
P51582	656	C-C-N-C-C	−0.001199
P51582	730	Nc1ccc(Br)cc1	−0.001278
P51582	662	O-C-C-O-C	−0.001317
P51582	764	Oc1c(Cl)cccc1	−0.001319
P51582	103	>= 1 Pm	−0.001402
P51582	729	Nc1ccc(Cl)cc1	−0.001486
P51582	321	Si-Si	−0.001666
P51582	774	Clc1c(Br)cccc1	−0.00186
P51582	178	>= 1 any ring size 6	−0.001895
P51582	339	C(~C)(~C)(~H)(~O)	−0.001925
P51582	745	Sc1cc(S)ccc1	−0.002007
P51582	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.002043
P51582	660	C-C=C-C-C	−0.00234
P51582	669	Cl-C:C-C=O	−0.002491
P51582	620	C:C-O-C-C	−0.002508
P51582	11	>= 8 C	−0.002536
P51582	227	>= 1 any ring size 8	−0.002579
P51582	453	N(-C)(=C)	−0.002973
P51582	800	CC1CC(N)CCC1	−0.003423
P51582	68	>= 1 Rb	−0.003589
P51582	587	N-C:C-O-[#1]	−0.003683
P51582	273	B-B	−0.003714
P51582	458	S(-O)(=O)	−0.00403
P51582	616	C:C:N:N:C	−0.004036
P51582	685	O=C-C-C-C-N	−0.004108
P51582	443	C(-C)(=O)	−0.004168
P51582	486	N-C:N:N	−0.004302
P51582	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.004971
P51582	842	CC1CC(N)CC1	−0.004985
P51582	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.005145
P51582	129	>= 1 any ring size 4	−0.005203
P51582	83	>= 1 Xe	−0.005336
P51582	551	Cl-C-C-O	−0.00564
P51582	857	ClC1CC(Cl)CC1	−0.005651
P51582	45	>= 4 Br	−0.005946
P51582	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.005981
P51582	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.006007
P51582	694	O=C-C-C-C-C=O	−0.006027
P51582	595	C:C-C-C-C	−0.006192
P51582	876	NC1C(Cl)CC1	−0.006465
P51582	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.006677
P51582	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.007132
P51582	319	Al-Cl	−0.007382
P51582	547	N-C:C-N	−0.007483
P51582	355	C(~C)(:C)	−0.007539

P51582	550	Cl-C-C-C	−0.007804
P51582	634	C-C-C:C-C	−0.007853
P51582	414	S(~C)(~O)	−0.00793
P51582	267	Li-O	−0.008019
P51582	269	Li-P	−0.008421
P51582	469	S-S-C:C	−0.008629
P51582	716	Cc1ccc(N)cc1	−0.008663
P51582	62	>= 1 Zn	−0.008691
P51582	377	C(~N)(:C)(:C)	−0.008715
P51582	840	CC1CC(O)CC1	−0.009063
P51582	315	O-K	−0.009399
P51582	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.009554
P51582	762	Oc1c(S)cccc1	−0.009592
P51582	295	C-As	−0.009839
P51582	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.010052
P51582	14	>= 1 N	−0.010776
P51582	793	NC1CCC(Br)CC1	−0.010904
P51582	432	C(-C)(-C)(=O)	−0.011103
P51582	3	>= 32 H	−0.011454
P51582	442	C(-C)(=N)	−0.011812
P51582	299	N-H	−0.012203
P51582	652	O-C:C:C-N	−0.012235
P51582	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.012244
P51582	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.012843
P51582	845	OC1CC(O)CC1	−0.013013
P51582	18	>= 1 O	−0.013269
P51582	590	C-C:C-O-[#1]	−0.013373
P51582	792	NC1CCC(Cl)CC1	−0.01616
P51582	97	>= 1 Pb	−0.016227
P51582	503	Cl-C:C-[#1]	−0.016269
P51582	756	Cc1c(O)cccc1	−0.016609
P51582	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.01665
P51582	115	>= 1 any ring size 3	−0.016816
P51582	555	N=C-C=C	−0.017328
P51582	578	C-C:C-C:C	−0.017631
P51582	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.017795
P51582	305	N-S	−0.018359
P51582	773	Clc1c(Cl)cccc1	−0.018719
P51582	569	N-C-C-N	−0.019286
P51582	858	ClC1CC(Br)CC1	−0.01991
P51582	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.019959
P51582	396	N(~C)(:C)	−0.020073
P51582	90	>= 1 Re	−0.020317
P51582	524	C-C=C-C	−0.021051
P51582	865	CC1C(Br)CCC1	−0.02164
P51582	627	O=[As]-C:C:C	−0.021686
P51582	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.021743
P51582	303	N-Si	−0.021991

P51582	618	C:C-C-C:C	−0.022033
P51582	419	C#N	−0.022504
P51582	46	>= 1 I	−0.02338
P51582	556	C=C-C-C	−0.023714
P51582	489	N-C-S-C	−0.024469
P51582	449	C(-N)(=C)	−0.025773
P51582	628	C-N-C-C:C	−0.026355
P51582	686	O=C-C-C-C-O	−0.026864
P51582	713	Cc1ccc(C)cc1	−0.027296
P51582	521	C:N-C-[#1]	−0.027345
P51582	543	O-C:C-N	−0.027483
P51582	839	CC1CC(C)CC1	−0.027522
P51582	501	Cl-C:C-C	−0.028059
P51582	358	C(~C)(:N)	−0.029122
P51582	324	P-P	−0.029702
P51582	459	S(=O)(=O)	−0.030172
P51582	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.031091
P51582	361	C(~Cl)(~H)	−0.03115
P51582	356	C(~C)(:C)(:C)	−0.031894
P51582	877	NC1C(Br)CCC1	−0.033454
P51582	725	Sc1ccc(N)cc1	−0.033647
P51582	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.034311
P51582	109	>= 1 Ho	−0.034322
P51582	335	C(~C)(~C)(~C)(~H)	−0.034786
P51582	760	Cc1c(Br)cccc1	−0.034927
P51582	349	C(~C)(~H)(~S)	−0.035056
P51582	558	O=N-C:C	−0.0358
P51582	16	>= 4 N	−0.036115
P51582	428	C(#C)(-H)	−0.03692
P51582	831	SC1C(Cl)CCCC1	−0.037191
P51582	306	N-Cl	−0.03727
P51582	26	>= 1 Na	−0.037282
P51582	22	>= 16 O	−0.037305
P51582	540	C-N-C-[#1]	−0.040554
P51582	58	>= 1 Fe	−0.041222
P51582	495	C-N-C:C	−0.041599
P51582	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.041718
P51582	61	>= 1 Cu	−0.042826
P51582	822	CC1C(Cl)CCCC1	−0.043354
P51582	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.045116
P51582	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.045964
P51582	879	ClC1C(Br)CCC1	−0.046133
P51582	268	Li-F	−0.048415
P51582	775	Brc1c(Br)cccc1	−0.048944
P51582	398	N(~H)(~N)	−0.049496
P51582	732	Clc1ccc(Br)cc1	−0.049577
P51582	664	C-C=C-C=C	−0.050186
P51582	42	>= 2 K	−0.051095

P51582	271	Li-Cl	−0.052976
P51582	72	>= 1 Nb	−0.053285
P51582	811	SC1CC(Br)CCC1	−0.056018
P51582	78	>= 1 Cd	−0.056657
P51582	835	NC1C(Br)CCCC1	−0.057022
P51582	466	N#C-C=C	−0.057228
P51582	55	>= 1 V	−0.057564
P51582	529	Cl-C-C-Cl	−0.058371
P51582	7	>= 2 B	−0.063127
P51582	724	Sc1ccc(S)cc1	−0.063653
P51582	266	Li-C	−0.064191
P51582	304	N-P	−0.064543
P51582	824	OC1C(O)CCCC1	−0.064875
P51582	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.065053
P51582	782	OC1CCC(O)CC1	−0.065422
P51582	310	O-Mg	−0.066244
P51582	867	OC1C(S)CCC1	−0.066883
P51582	856	NC1CC(Br)CC1	−0.066999
P51582	100	>= 1 Ce	−0.067011
P51582	619	O-C-C=C-C	−0.068106
P51582	791	NC1CCC(N)CC1	−0.068373
P51582	781	CC1CCC(Br)CC1	−0.068876
P51582	861	CC1C(O)CCC1	−0.070427
P51582	320	Si-H	−0.071737
P51582	392	N(~C)(~C)(~H)	−0.073159
P51582	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.075035
P51582	611	N-C-C-N-C	−0.075339
P51582	30	>= 1 P	−0.075987
P51582	425	P=O	−0.078684
P51582	603	C-C:C:C-C	−0.079611
P51582	234	>= 2 any ring size 8	−0.079958
P51582	755	Cc1c(C)cccc1	−0.080049
P51582	284	C-C	−0.080345
P51582	577	C:C-N-C:C	−0.082085
P51582	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.083338
P51582	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.085104
P51582	566	O-C-C-N	−0.086492
P51582	12	>= 16 C	−0.08669
P51582	552	C:C-C:C	−0.086912
P51582	451	C(-N)(=O)	−0.08752
P51582	776	CC1CCC(C)CC1	−0.089208
P51582	17	>= 8 N	−0.089336
P51582	580	O=C-C-C-N	−0.094048
P51582	435	C(-C)(-H)(=N)	−0.095867
P51582	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.095974
P51582	641	O-C-C-C=C	−0.100699
P51582	157	>= 3 any ring size 5	−0.101756
P51582	672	O=C-C=C-[#1]	−0.10687

P51582	357	C(~C)(:C)(:N)	-0.111379
P51582	586	C-S-C-C-C	-0.114549
P51582	579	O=C-C-C-C	-0.119213
P51582	171	>= 5 any ring size 5	-0.121221
P51582	878	ClC1C(Cl)CCC1	-0.121419
P51582	113	>= 1 Tc	-0.122271
P51582	645	O=C-N-C-C	-0.122574
P51582	535	O=C-C-C	-0.123405
P51582	462	O-C-C=O	-0.123924
P51582	665	N-C:C-C-C	-0.124946
P51582	422	N=N	-0.125089
P51582	532	S-C:C-[#1]	-0.127111
P51582	733	Brc1ccc(Br)cc1	-0.128129
P51582	703	O-C-C-C-C-C(N)-C	-0.128443
P51582	455	N(-O)(=O)	-0.12944
P51582	382	C(~O)(:C)(:C)	-0.130333
P51582	340	C(~C)(~C)(~N)	-0.13363
P51582	370	C(~H)(:C)	-0.137442
P51582	748	Sc1cc(Br)ccc1	-0.137508
P51582	364	C(~F)(:C)	-0.138406
P51582	584	C:C-C=C-C	-0.140838
P51582	727	Sc1ccc(Br)cc1	-0.141306
P51582	497	O-C:C:N	-0.14255
P51582	326	As-As	-0.14332
P51582	390	N(~C)(~C)	-0.143681
P51582	823	CC1C(Br)CCCC1	-0.143978
P51582	475	S-C=N-C	-0.148243
P51582	523	N:C:C-C	-0.151779
P51582	817	BrC1CC(Br)CCC1	-0.152394
P51582	302	N-F	-0.162514
P51582	108	>= 1 Dy	-0.166674
P51582	474	S:C:C:N	-0.167386
P51582	826	OC1C(N)CCCC1	-0.175694
P51582	880	BrC1C(Br)CCC1	-0.176926
P51582	711	C-C(C)(C)-C-C	-0.178867
P51582	508	S=C-N-C	-0.179724
P51582	721	Oc1ccc(N)cc1	-0.186238
P51582	383	C(~S)(:C)	-0.186428
P51582	323	P-H	-0.186947
P51582	282	B-Br	-0.191809
P51582	105	>= 1 Eu	-0.194705
P51582	77	>= 1 Ag	-0.195857
P51582	610	C-O-C-O-C	-0.199572
P51582	812	NC1CC(N)CCC1	-0.201978
P51582	343	C(~C)(~Cl)(~H)	-0.202312
P51582	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	-0.208612
P51582	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	-0.208972
P51582	855	NC1CC(Cl)CC1	-0.219398

P51582	536	O=C-C-N	−0.22087
P51582	613	C-N-C-C-C	−0.221136
P51582	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.222332
P51582	787	SC1CCC(S)CC1	−0.233954
P51582	520	C=C-C:C	−0.234705
P51582	439	C(-C)(-N)(=O)	−0.235801
P51582	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.244169
P51582	300	N-N	−0.250356
P51582	482	C:N-C:C	−0.253903
P51582	353	C(~C)(~S)	−0.25668
P51582	344	C(~C)(~H)	−0.260395
P51582	629	S-C:C:C-N	−0.26052
P51582	241	>= 1 any ring size 9	−0.260849
P51582	457	S(-C)(=O)	−0.264648
P51582	52	>= 1 Ca	−0.266177
P51582	866	OC1C(O)CCC1	−0.267741
P51582	801	CC1CC(Cl)CCC1	−0.270085
P51582	772	Nc1c(Br)cccc1	−0.270327
P51582	658	C-C-S-C-C	−0.27245
P51582	647	O=C-N-C-N	−0.277525
P51582	538	N=C-C-C	−0.277587
P51582	663	O-C-C-O-[#1]	−0.278209
P51582	10	>= 4 C	−0.281618
P51582	2	>= 16 H	−0.282849
P51582	600	N-C:C:C-C	−0.290976
P51582	814	NC1CC(Br)CCC1	−0.295951
P51582	545	N-C:C-C	−0.296388
P51582	667	C=C-C-O-[#1]	−0.299207
P51582	336	C(~C)(~C)(~C)(~N)	−0.301961
P51582	408	O(~H)(~S)	−0.302892
P51582	581	O=C-C-C-O	−0.31372
P51582	93	>= 1 Pt	−0.313959
P51582	626	C-O-C:C-C	−0.320253
P51582	507	C-C-S-C	−0.320259
P51582	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.321239
P51582	407	O(~C)(~P)	−0.325404
P51582	410	P(~C)(~C)	−0.329583
P51582	34	>= 2 S	−0.330396
P51582	23	>= 1 F	−0.331048
P51582	758	Cc1c(N)cccc1	−0.339424
P51582	57	>= 1 Mn	−0.343825
P51582	718	Cc1ccc(Br)cc1	−0.353633
P51582	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.357979
P51582	363	C(~F)(~F)	−0.360193
P51582	429	C(#N)(-C)	−0.367089
P51582	726	Sc1ccc(Cl)cc1	−0.367463
P51582	554	Br-C-C-C	−0.369769
P51582	385	C(:C)(:C)(:C)	−0.370022

P51582	331	C(~Br)(:N)	−0.37156
P51582	746	Sc1cc(N)ccc1	−0.376929
P51582	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.380245
P51582	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.38472
P51582	65	>= 1 As	−0.385311
P51582	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.389
P51582	534	S-C:C-O	−0.390842
P51582	468	O=S-C-N	−0.395886
P51582	836	ClC1C(Cl)CCCC1	−0.396989
P51582	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.397462
P51582	846	OC1CC(S)CC1	−0.401392
P51582	528	[#1]-N-C-[#1]	−0.405152
P51582	99	>= 1 La	−0.405254
P51582	401	N(~O)(~O)	−0.406891
P51582	421	C=S	−0.410977
P51582	753	Clc1cc(Br)ccc1	−0.417912
P51582	821	CC1C(N)CCCC1	−0.422835
P51582	573	O-C-C=C	−0.42945
P51582	487	N-C=N-C	−0.431844
P51582	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.433224
P51582	637	O-C-C-C-C	−0.435093
P51582	380	C(~O)(~O)	−0.437806
P51582	69	>= 1 Sr	−0.449174
P51582	264	Li-Li	−0.461497
P51582	393	N(~C)(~H)	−0.462875
P51582	832	SC1C(Br)CCCC1	−0.463127
P51582	785	OC1CCC(Cl)CC1	−0.467671
P51582	548	O-C-C:C	−0.468232
P51582	477	N-N-C:C	−0.477754
P51582	24	>= 2 F	−0.478162
P51582	381	C(~O)(:C)	−0.479415
P51582	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.483542
P51582	682	O-C-C-C-C-N	−0.483676
P51582	294	C-Cl	−0.486634
P51582	354	C(~C)(~Si)	−0.490516
P51582	798	CC1CC(O)CCC1	−0.490675
P51582	384	C(:C)(:C)	−0.495015
P51582	859	BrC1CC(Br)CC1	−0.496954
P51582	485	N:C:C:N	−0.501062
P51582	570	C:C-C-C	−0.502932
P51582	605	O=C-C-O-C	−0.508261
P51582	79	>= 1 In	−0.521092
P51582	399	N(~H)(:C)	−0.525528
P51582	585	C-C:C-N-C	−0.525695
P51582	849	OC1CC(Br)CC1	−0.526157
P51582	317	F-S	−0.526326
P51582	276	B-O	−0.529142
P51582	289	C-Mg	−0.530324

P51582	456	P(-O)(=O)	−0.532184
P51582	701	O-C-C-C-C-C(O)-C	−0.532374
P51582	707	O=C-C-C-C-C(N)-C	−0.535853
P51582	633	N-C-C:C-C	−0.538777
P51582	599	[#1]-C-C=C-[#1]	−0.53931
P51582	441	C(-C)(=C)	−0.542451
P51582	376	C(~N)(:C)	−0.559861
P51582	454	N(-C)(=O)	−0.562589
P51582	415	Si(~C)(~C)	−0.567359
P51582	517	N-N-C-N	−0.568573
P51582	15	>= 2 N	−0.591021
P51582	872	SC1C(N)CCC1	−0.592206
P51582	744	Oc1cc(Br)ccc1	−0.59413
P51582	564	C=C-C=C	−0.59564
P51582	50	>= 1 Mg	−0.596558
P51582	659	O-C-C-N-C	−0.601011
P51582	575	O-C-C:C-O	−0.602558
P51582	277	B-F	−0.602733
P51582	712	C-C(C)-C(C)-C	−0.610542
P51582	311	O-Na	−0.619351
P51582	114	>= 1 U	−0.627934
P51582	797	CC1CC(C)CCC1	−0.629898
P51582	875	NC1C(N)CCC1	−0.630415
P51582	571	[#1]-C-O-[#1]	−0.634107
P51582	492	N-C:O:C	−0.648654
P51582	63	>= 1 Ga	−0.65359
P51582	60	>= 1 Ni	−0.655043
P51582	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.664882
P51582	739	Cc1cc(Br)ccc1	−0.666301
P51582	342	C(~C)(~Cl)	−0.66904
P51582	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.677438
P51582	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.690708
P51582	635	N-N-C-N-[#1]	−0.700007
P51582	740	Oc1cc(O)ccc1	−0.704163
P51582	834	NC1C(Cl)CCCC1	−0.704666
P51582	54	>= 1 Ti	−0.711292
P51582	470	C:C-C=C	−0.719529
P51582	325	As-H	−0.727416
P51582	372	C(~H)(:C)(:N)	−0.732138
P51582	471	S:C:C:C	−0.732262
P51582	790	SC1CCC(Br)CC1	−0.732733
P51582	338	C(~C)(~C)(~H)(~N)	−0.736145
P51582	768	Sc1c(Cl)cccc1	−0.742026
P51582	655	O-C-C-C:C	−0.74272
P51582	870	OC1C(Br)CCC1	−0.743507
P51582	298	C-I	−0.746605
P51582	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.746928
P51582	519	N=C-N-C	−0.748832

P51582	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.763739
P51582	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.772666
P51582	409	O(:C)(:C)	−0.773612
P51582	852	SC1CC(Cl)CC1	−0.774558
P51582	715	Cc1ccc(S)cc1	−0.780572
P51582	761	Oc1c(O)cccc1	−0.782285
P51582	465	O=S-C-C	−0.788309
P51582	606	O-C:C-C-C	−0.788701
P51582	537	O=C-C-O	−0.792369
P51582	427	C(#C)(-C)	−0.792954
P51582	262	>= 4 hetero-aromatic rings	−0.809309
P51582	13	>= 32 C	−0.815355
P51582	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.818926
P51582	514	O-N-C-C	−0.819606
P51582	411	P(~O)(~O)	−0.838042
P51582	588	O=C-C-C=O	−0.84044
P51582	684	O=C-C-C-C-C	−0.845049
P51582	516	[#1]-C=C-[#1]	−0.855175
P51582	292	C-P	−0.856842
P51582	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.859769
P51582	493	O=C-C:C	−0.863001
P51582	582	C-C-C-C-C	−0.867346
P51582	448	C(-H)(=O)	−0.882562
P51582	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.886955
P51582	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.890379
P51582	296	C-Se	−0.894853
P51582	717	Cc1ccc(Cl)cc1	−0.939165
P51582	275	B-N	−0.947376
P51582	333	C(~C)(~C)(~C)	−0.956369
P51582	461	O-C-C=N	−0.963783
P51582	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.972409
P51582	351	C(~C)(~N)	−0.983768
P51582	594	C-O-C-C=C	−1.011331
P51582	843	CC1CC(Cl)CC1	−1.021928
P51582	193	>= 3 saturated or aromatic carbon-only ring size 6	−1.048822
P51582	274	B-C	−1.118952
P51582	473	S-C:N:C	−1.126196
P51582	391	N(~C)(~C)(~C)	−1.127391
P51582	200	>= 4 saturated or aromatic carbon-only ring size 6	−1.139925
P51582	499	N-C:C:N	−1.146628
P51582	563	O-C-O-C	−1.152269
P51582	871	SC1C(S)CCC1	−1.173868
P51582	754	Brc1cc(Br)ccc1	−1.175386
P51582	562	Br-C-C=O	−1.189213
P51582	332	C(~C)(~C)	−1.196317
P51582	158	>= 3 saturated or aromatic carbon-only ring size 5	−1.215776
P51582	9	>= 2 C	−1.221154
P51582	307	N-Br	−1.225858

P51582	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−1.236597
P51582	405	O(~C)(~C)	−1.239223
P51582	476	C-O-C=C	−1.240407
P51582	286	C-O	−1.3096
P51582	597	O=C-C-C:C	−1.332722
P51582	539	N=C-C-[#1]	−1.334742
P51582	504	N:C:N-C	−1.337851
P51582	101	>= 1 Pr	−1.340913
P51582	76	>= 1 Pd	−1.342954
P51582	675	Br-C-C-C:C	−1.482507
P51582	671	O=C-C=C-C	−1.538184
P51582	346	C(~C)(~H)(~O)	−1.563168
P51582	796	BrC1CCC(Br)CC1	−1.676464
P51582	316	F-P	−1.779937
P51582	668	C-C:C-C-C	−1.780113
P51582	735	Cc1cc(O)ccc1	−1.848681
P51582	816	ClC1CC(Br)CCC1	−1.867196
P51582	265	Li-B	−1.953216
P51582	92	>= 1 Ir	−2.031319

Fingerprints（continued)

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1.4856923	-3.57E-07
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1.4734249	0.0004507
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1.1266765	1.22E-07
1.1128835	-8.09E-07
1.0880354	2.15E-07
1.0854341	-4.65E-07
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1.0767848	-0.003272

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0.9956019 -0.003351
0.9846833 5.75E-07
0.9683729 -0.002418
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0.9522477 9.46E-06
0.9325877 -7.37E-07
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0.7304087 6.54E-07
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0.719952 -5.81E-07
0.7167524 -0.003025
0.7096582 0.0010252
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-0.475718 -0.002036
-0.463517 -0.014645
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-0.479154 -0.004388
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-0.490968 0.0043341
-0.490567 5.04E-05
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-0.494078 -0.000937
-0.496955 7.47E-07
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-0.509485 0.0012237
-0.521092 -3.25E-07
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-0.526327 3.81E-07
-0.529141 -2.42E-07
-0.530325 8.81E-07

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-0.630416 2.85E-07
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-0.65359 2.07E-07
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-0.669438 0.0003983
-0.677438 -5.33E-07
-0.690708 2.85E-07
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-0.704153 -9.30E-06
-0.704635 -3.08E-05
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-0.734805 -0.00134
-0.741653 -0.000373
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-0.743507 -3.73E-07
-0.742857 -0.003748
-0.746928 -3.87E-07
-0.750309 0.001477

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-0.776951 0.0033396
-0.774557 -6.50E-07
-0.775331 -0.005241
-0.782287 1.07E-06
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-0.857064 0.0018884
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-0.959819 0.0034498
-0.963073 -0.00071
-0.973191 0.0007827
-0.98298 -0.000788
-1.013963 0.0026322
-1.021928 -4.06E-08
-1.048373 -0.000449
-1.118952 2.69E-07
-1.126791 0.0005947
-1.123842 -0.003549
-1.139925 3.14E-07
-1.142727 -0.003901
-1.154694 0.0024247
-1.173868 1.44E-07
-1.175387 4.49E-07
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-1.194673 -0.001644
-1.215777 1.08E-06
-1.219509 -0.001644
-1.225858 1.88E-07

-1.236598 9.36E-07
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-1.308908 -0.000692
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-1.536041 -0.002143
-1.568416 0.0052484
-1.676465 4.24E-07
-1.779937 -3.23E-07
-1.780382 0.0002686
-1.846021 -0.00266
-1.867195 -1.75E-07
-1.953215 -9.92E-07
-2.031319 -4.88E-07

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q15077	758	Cc1c(N)cccc1	2.4150731
Q15077	593	N-C-C-C-N	2.1104478
Q15077	746	Sc1cc(N)ccc1	2.0966193
Q15077	554	Br-C-C-C	1.9238394
Q15077	315	O-K	1.8822949
Q15077	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	1.8730511
Q15077	794	ClC1CCC(Cl)CC1	1.7769827
Q15077	9	>= 2 C	1.7633817
Q15077	496	N:N-C-[#1]	1.7494914
Q15077	532	S-C:C-[#1]	1.6798655
Q15077	831	SC1C(Cl)CCCC1	1.5861856
Q15077	419	C#N	1.5650405
Q15077	763	Oc1c(N)cccc1	1.5616972
Q15077	722	Oc1ccc(Cl)cc1	1.545077
Q15077	860	CC1C(C)CCC1	1.5292455
Q15077	603	C-C:C:C-C	1.5118612
Q15077	257	>= 2 aromatic rings	1.5118302
Q15077	768	Sc1c(Cl)cccc1	1.5067507
Q15077	481	O-S-C:C	1.5017225
Q15077	622	O=C-O-C:C	1.4992585
Q15077	466	N#C-C=C	1.4795952
Q15077	53	>= 1 Sc	1.47621
Q15077	796	BrC1CCC(Br)CC1	1.4617741
Q15077	651	O-C:C:C-C	1.4008217
Q15077	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	1.3837821
Q15077	580	O=C-C-C-N	1.381722
Q15077	248	>= 1 any ring size 10	1.3257052
Q15077	261	>= 4 aromatic rings	1.2943426
Q15077	297	C-Br	1.2905903
Q15077	87	>= 1 Hf	1.2775129
Q15077	641	O-C-C-C=C	1.2656545
Q15077	734	Cc1cc(C)ccc1	1.2609966
Q15077	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	1.259818
Q15077	1	>= 8 H	1.2593336
Q15077	692	O=C-C-C-C-C-C	1.2449803
Q15077	857	ClC1CC(Cl)CC1	1.2208489
Q15077	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	1.2056315
Q15077	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	1.1773615
Q15077	806	OC1CC(Cl)CCC1	1.1727814
Q15077	380	C(~O)(~O)	1.1680204
Q15077	690	O-C-C-C-C-C-O	1.145218
Q15077	760	Cc1c(Br)cccc1	1.1104144
Q15077	684	O=C-C-C-C-C	1.1102329
Q15077	424	N=P	1.1027034
Q15077	801	CC1CC(Cl)CCC1	1.1019326
Q15077	595	C:C-C-C-C	1.1016694

Q15077	446	C(-H)(=C)	1.0955096
Q15077	653	O-C:C:C-O	1.0939389
Q15077	283	C-H	1.0753986
Q15077	718	Cc1ccc(Br)cc1	1.0622681
Q15077	703	O-C-C-C-C-C(N)-C	1.0583131
Q15077	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	1.0549605
Q15077	819	CC1C(O)CCCC1	1.0508194
Q15077	846	OC1CC(S)CC1	1.0497557
Q15077	636	C-N-C-N-C	1.0407528
Q15077	565	C:C-O-C	1.030316
Q15077	29	>= 2 Si	1.0138674
Q15077	517	N-N-C-N	1.0072448
Q15077	855	NC1CC(Cl)CC1	1.0053606
Q15077	405	O(~C)(~C)	1.0016139
Q15077	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.9785746
Q15077	524	C-C=C-C	0.9699963
Q15077	469	S-S-C:C	0.9667967
Q15077	15	>= 2 N	0.9657502
Q15077	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.9657069
Q15077	715	Cc1ccc(S)cc1	0.9566838
Q15077	442	C(-C)(=N)	0.9509172
Q15077	587	N-C:C-O-[#1]	0.9394766
Q15077	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.9378532
Q15077	863	CC1C(N)CCC1	0.9276329
Q15077	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.9247379
Q15077	825	OC1C(S)CCCC1	0.9172228
Q15077	331	C(~Br)(:N)	0.911405
Q15077	249	>= 1 saturated or aromatic carbon-only ring size 10	0.9095912
Q15077	136	>= 2 any ring size 4	0.8985701
Q15077	7	>= 2 B	0.8903314
Q15077	626	C-O-C:C-C	0.8817508
Q15077	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.8807489
Q15077	75	>= 1 Rh	0.879058
Q15077	779	CC1CCC(N)CC1	0.8735368
Q15077	795	ClC1CCC(Br)CC1	0.8726008
Q15077	519	N=C-N-C	0.8612386
Q15077	460	C-C-C#C	0.8477745
Q15077	536	O=C-C-N	0.8325095
Q15077	435	C(-C)(-H)(=N)	0.810564
Q15077	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.7764931
Q15077	408	O(~H)(~S)	0.7752071
Q15077	50	>= 1 Mg	0.7661466
Q15077	712	C-C(C)-C(C)-C	0.7388866
Q15077	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.7207281
Q15077	395	N(~C)(~O)	0.7176498
Q15077	598	Cl-C:C:C-C	0.706006
Q15077	555	N=C-C=C	0.701244
Q15077	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.6983828

Q15077	262	>= 4 hetero-aromatic rings	0.686089
Q15077	642	O-C-C-C=O	0.6842405
Q15077	783	OC1CCC(S)CC1	0.6719144
Q15077	546	N-C:C-[#1]	0.6705931
Q15077	751	Nc1cc(Br)ccc1	0.66898
Q15077	724	Sc1ccc(S)cc1	0.6530096
Q15077	328	C(~Br)(~C)(~C)	0.6527007
Q15077	313	O-Si	0.6512327
Q15077	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.639897
Q15077	815	ClC1CC(Cl)CCC1	0.636194
Q15077	844	CC1CC(Br)CC1	0.6316439
Q15077	220	>= 2 any ring size 7	0.6262302
Q15077	764	Oc1c(Cl)cccc1	0.622245
Q15077	37	>= 1 Cl	0.6191924
Q15077	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.6169747
Q15077	841	CC1CC(S)CC1	0.6161496
Q15077	566	O-C-C-N	0.6142266
Q15077	639	O-C-C-C-O	0.6034175
Q15077	668	C-C:C-C-C	0.5970033
Q15077	356	C(~C)(:C)(:C)	0.5816554
Q15077	818	CC1C(C)CCCC1	0.5794736
Q15077	123	>= 2 saturated or aromatic carbon-only ring size 3	0.5734825
Q15077	584	C:C-C=C-C	0.5706833
Q15077	326	As-As	0.5694257
Q15077	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.5678281
Q15077	870	OC1C(Br)CCC1	0.56637
Q15077	301	N-O	0.5660527
Q15077	707	O=C-C-C-C-C(N)-C	0.5536857
Q15077	33	>= 1 S	0.5536358
Q15077	400	N(~H)(:C)(:C)	0.5535762
Q15077	5	>= 2 Li	0.5390466
Q15077	744	Oc1cc(Br)ccc1	0.5235673
Q15077	754	Brc1cc(Br)ccc1	0.5215653
Q15077	852	SC1CC(Cl)CC1	0.5198608
Q15077	320	Si-H	0.511764
Q15077	772	Nc1c(Br)cccc1	0.5070774
Q15077	63	>= 1 Ga	0.5056016
Q15077	737	Cc1cc(N)ccc1	0.5031017
Q15077	463	N:C-S-[#1]	0.4986058
Q15077	701	O-C-C-C-C-C(O)-C	0.4948472
Q15077	325	As-H	0.4846868
Q15077	58	>= 1 Fe	0.4826379
Q15077	784	OC1CCC(N)CC1	0.4794682
Q15077	572	N:C:N:C	0.4786511
Q15077	811	SC1CC(Br)CCC1	0.4761309
Q15077	425	P=O	0.4723949
Q15077	360	C(~Cl)(~Cl)	0.4723423
Q15077	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.4518175

Q15077	130	>= 1 saturated or aromatic carbon-only ring size 4	0.449322
Q15077	165	>= 4 saturated or aromatic carbon-only ring size 5	0.4447469
Q15077	723	Oc1ccc(Br)cc1	0.4408818
Q15077	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.4332751
Q15077	865	CC1C(Br)CCC1	0.4311434
Q15077	369	C(~H)(~Si)	0.4103251
Q15077	514	O-N-C-C	0.4099437
Q15077	107	>= 1 Tb	0.4093915
Q15077	716	Cc1ccc(N)cc1	0.4013081
Q15077	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.3936365
Q15077	84	>= 1 Cs	0.3916962
Q15077	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.3886399
Q15077	808	SC1CC(S)CCC1	0.388061
Q15077	30	>= 1 P	0.3698085
Q15077	635	N-N-C-N-[#1]	0.3665093
Q15077	824	OC1C(O)CCCC1	0.3470008
Q15077	727	Sc1ccc(Br)cc1	0.3469387
Q15077	54	>= 1 Ti	0.3448362
Q15077	577	C:C-N-C:C	0.3430734
Q15077	354	C(~C)(~Si)	0.3365872
Q15077	185	>= 2 any ring size 6	0.3346041
Q15077	443	C(-C)(=O)	0.3307318
Q15077	850	SC1CC(S)CC1	0.3275832
Q15077	562	Br-C-C=O	0.327081
Q15077	3	>= 32 H	0.3253279
Q15077	705	O=C-C-C-C-C(O)-C	0.3239326
Q15077	228	>= 1 saturated or aromatic carbon-only ring size 8	0.3205927
Q15077	406	O(~C)(~H)	0.3171209
Q15077	822	CC1C(Cl)CCCC1	0.3142793
Q15077	46	>= 1 I	0.3134226
Q15077	319	Al-Cl	0.2923037
Q15077	436	C(-C)(-H)(=O)	0.2916454
Q15077	880	BrC1C(Br)CCC1	0.2867201
Q15077	298	C-I	0.2805364
Q15077	500	C-S-C:C	0.2794446
Q15077	368	C(~H)(~S)	0.2733486
Q15077	551	Cl-C-C-O	0.2707069
Q15077	790	SC1CCC(Br)CC1	0.2662449
Q15077	19	>= 2 O	0.2620667
Q15077	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.2596261
Q15077	832	SC1C(Br)CCCC1	0.2572983
Q15077	537	O=C-C-O	0.2541011
Q15077	403	N(:C)(:C)	0.2510854
Q15077	601	N-C:C:C-N	0.2496054
Q15077	349	C(~C)(~H)(~S)	0.2452057
Q15077	327	C(~Br)(~C)	0.2331983
Q15077	41	>= 1 K	0.2299115
Q15077	392	N(~C)(~C)(~H)	0.2275643

Q15077	438	C(-C)(-N)(=N)	0.218153
Q15077	98	>= 1 Bi	0.2141184
Q15077	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.2139511
Q15077	658	C-C-S-C-C	0.2102969
Q15077	60	>= 1 Ni	0.2100127
Q15077	508	S=C-N-C	0.2031852
Q15077	93	>= 1 Pt	0.1978569
Q15077	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.1945234
Q15077	413	S(~C)(~H)	0.1917156
Q15077	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.1813777
Q15077	265	Li-B	0.1809771
Q15077	775	Brc1c(Br)cccc1	0.1777332
Q15077	814	NC1CC(Br)CCC1	0.1743254
Q15077	610	C-O-C-O-C	0.1730532
Q15077	340	C(~C)(~C)(~N)	0.166927
Q15077	643	[#1]-C-C-N-[#1]	0.1655706
Q15077	91	>= 1 Os	0.1636796
Q15077	122	>= 2 any ring size 3	0.1630134
Q15077	277	B-F	0.1562739
Q15077	632	C-C-O-C:C	0.1527688
Q15077	56	>= 1 Cr	0.1491936
Q15077	504	N:C:N-C	0.1481949
Q15077	31	>= 2 P	0.1471432
Q15077	430	C(-C)(-C)(=C)	0.1459059
Q15077	512	C-[As]-O-[#1]	0.1408802
Q15077	34	>= 2 S	0.1385946
Q15077	473	S-C:N:C	0.133713
Q15077	531	S-C:C-C	0.1323459
Q15077	873	SC1C(Cl)CCC1	0.1268885
Q15077	535	O=C-C-C	0.1246017
Q15077	92	>= 1 Ir	0.1224901
Q15077	47	>= 2 I	0.1167607
Q15077	330	C(~Br)(:C)	0.1150882
Q15077	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.1129821
Q15077	278	B-Si	0.1129667
Q15077	686	O=C-C-C-C-O	0.1125413
Q15077	650	O=C-N-C=O	0.1104145
Q15077	807	OC1CC(Br)CCC1	0.1022741
Q15077	527	C:C:N-[#1]	0.0992719
Q15077	788	SC1CCC(N)CC1	0.0983275
Q15077	698	O-C-C-C-C-C-C-C	0.0976368
Q15077	688	C-C-C-C-C-C-C	0.0957592
Q15077	708	C-C(C)-C-C	0.0949841
Q15077	696	C-C-C-C-C-C-C-C	0.0944323
Q15077	732	Clc1ccc(Br)cc1	0.0935564
Q15077	526	Cl-C:C-Cl	0.0934281
Q15077	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0855973
Q15077	805	OC1CC(N)CCC1	0.084557

Q15077	725	Sc1ccc(N)cc1	0.0843661
Q15077	809	SC1CC(N)CCC1	0.0838223
Q15077	617	C-C-C-O-[#1]	0.0815491
Q15077	666	C=C-C-O-C	0.0815401
Q15077	488	N-C=N-[#1]	0.0812795
Q15077	847	OC1CC(N)CC1	0.0744447
Q15077	164	>= 4 any ring size 5	0.0744395
Q15077	18	>= 1 O	0.0742448
Q15077	594	C-O-C-C=C	0.0738315
Q15077	502	N-C=C-[#1]	0.0734742
Q15077	476	C-O-C=C	0.0696506
Q15077	539	N=C-C-[#1]	0.0695085
Q15077	310	O-Mg	0.0669066
Q15077	82	>= 1 Te	0.0667325
Q15077	649	O=N-C:C-O	0.0667009
Q15077	468	O=S-C-N	0.0666841
Q15077	268	Li-F	0.0664676
Q15077	296	C-Se	0.0662443
Q15077	289	C-Mg	0.0643929
Q15077	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.0642928
Q15077	569	N-C-C-N	0.064262
Q15077	398	N(~H)(~N)	0.0641979
Q15077	399	N(~H)(:C)	0.063572
Q15077	318	Al-H	0.0626062
Q15077	853	SC1CC(Br)CC1	0.0624615
Q15077	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0620926
Q15077	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.0620255
Q15077	827	OC1C(Cl)CCCC1	0.061688
Q15077	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0589646
Q15077	541	O-C:C-C	0.0588455
Q15077	874	SC1C(Br)CCC1	0.0587408
Q15077	321	Si-Si	0.057888
Q15077	699	O-C-C-C-C-C(C)-C	0.0562191
Q15077	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.0561827
Q15077	599	[#1]-C-C=C-[#1]	0.0552882
Q15077	70	>= 1 Y	0.0548602
Q15077	843	CC1CC(Cl)CC1	0.0539633
Q15077	655	O-C-C-C:C	0.0535174
Q15077	770	Nc1c(N)cccc1	0.0527036
Q15077	422	N=N	0.0523019
Q15077	295	C-As	0.0516998
Q15077	415	Si(~C)(~C)	0.0506652
Q15077	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0493479
Q15077	570	C:C-C-C	0.0485538
Q15077	335	C(~C)(~C)(~C)(~H)	0.0476597
Q15077	352	C(~C)(~O)	0.0475376
Q15077	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0464643
Q15077	371	C(~H)(:C)(:C)	0.0452505

Q15077	538	N=C-C-C	0.0451901
Q15077	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0442818
Q15077	304	N-P	0.0437523
Q15077	543	O-C:C-N	0.0436892
Q15077	280	B-S	0.0434114
Q15077	267	Li-O	0.043284
Q15077	394	N(~C)(~H)(~N)	0.0409706
Q15077	613	C-N-C-C-C	0.0408856
Q15077	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0408566
Q15077	282	B-Br	0.0404021
Q15077	450	C(-N)(=N)	0.0399946
Q15077	745	Sc1cc(S)ccc1	0.0397208
Q15077	407	O(~C)(~P)	0.0383356
Q15077	462	O-C-C=O	0.0368724
Q15077	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0368556
Q15077	614	C-C-O-C-C	0.0359849
Q15077	375	C(~N)(~N)	0.0359632
Q15077	654	N-C-N-C-C	0.0351463
Q15077	305	N-S	0.0351231
Q15077	578	C-C:C-C:C	0.0350719
Q15077	157	>= 3 any ring size 5	0.0348269
Q15077	475	S-C=N-C	0.0346487
Q15077	431	C(-C)(-C)(=N)	0.033656
Q15077	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0334596
Q15077	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0329937
Q15077	17	>= 8 N	0.0327937
Q15077	348	C(~C)(~H)(~P)	0.0327771
Q15077	426	P=P	0.0323714
Q15077	640	C=C-C-C-C	0.0322566
Q15077	386	C(:C)(:C)(:N)	0.0319715
Q15077	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0316504
Q15077	370	C(~H)(:C)	0.0286308
Q15077	11	>= 8 C	0.0282092
Q15077	339	C(~C)(~C)(~H)(~O)	0.0278331
Q15077	358	C(~C)(:N)	0.0261278
Q15077	567	O-C-C-O	0.0232243
Q15077	609	Cl-C-C-N-C	0.0231933
Q15077	679	C-C-C-C-C-C	0.0225813
Q15077	272	B-H	0.0223809
Q15077	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.0218964
Q15077	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0218353
Q15077	624	O=C-C:C-N	0.0211794
Q15077	474	S:C:C:N	0.0207312
Q15077	789	SC1CCC(Cl)CC1	0.0202164
Q15077	659	O-C-C-N-C	0.0198919
Q15077	771	Nc1c(Cl)cccc1	0.0196121
Q15077	101	>= 1 Pr	0.0192688
Q15077	774	Clc1c(Br)cccc1	0.0190909

Q15077	207	>= 5 saturated or aromatic carbon-only ring size 6	0.0186203
Q15077	665	N-C:C-C-C	0.0183212
Q15077	115	>= 1 any ring size 3	0.017997
Q15077	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.0179864
Q15077	582	C-C-C-C-C	0.0179034
Q15077	311	O-Na	0.0175944
Q15077	276	B-O	0.0172813
Q15077	820	CC1C(S)CCCC1	0.0163894
Q15077	859	BrC1CC(Br)CC1	0.0160689
Q15077	89	>= 1 W	0.0158888
Q15077	501	Cl-C:C-C	0.0153881
Q15077	389	C(:N)(:N)	0.0153439
Q15077	345	C(~C)(~H)(~N)	0.0151332
Q15077	590	C-C:C-O-[#1]	0.0133569
Q15077	388	C(:C)(:N)(:N)	0.0132145
Q15077	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.0127533
Q15077	21	>= 8 O	0.0126133
Q15077	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0123685
Q15077	336	C(~C)(~C)(~C)(~N)	0.0123161
Q15077	802	CC1CC(Br)CCC1	0.0120749
Q15077	559	O-C-N-[#1]	0.0118744
Q15077	680	O-C-C-C-C-C	0.0116708
Q15077	585	C-C:C-N-C	0.0112695
Q15077	638	O-C-C-C-N	0.0112595
Q15077	260	>= 3 hetero-aromatic rings	0.010684
Q15077	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.0102906
Q15077	494	O=C-C:N	0.0102402
Q15077	568	N#C-C-C	0.0102223
Q15077	663	O-C-C-O-[#1]	0.0101753
Q15077	529	Cl-C-C-Cl	0.0097334
Q15077	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0092468
Q15077	738	Cc1cc(Cl)ccc1	0.0089755
Q15077	672	O=C-C=C-[#1]	0.0089608
Q15077	817	BrC1CC(Br)CCC1	0.0088498
Q15077	804	OC1CC(S)CCC1	0.0082194
Q15077	621	N-C:C:C:N	0.0073325
Q15077	787	SC1CCC(S)CC1	0.0071368
Q15077	284	C-C	0.0071124
Q15077	479	S-C-S-C	0.0066216
Q15077	477	N-N-C:C	0.0061417
Q15077	710	C-C-C(C)-C-C	0.0059736
Q15077	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0056464
Q15077	835	NC1C(Br)CCCC1	0.0056393
Q15077	378	C(~N)(:C)(:N)	0.0052688
Q15077	38	>= 2 Cl	0.0051305
Q15077	836	ClC1C(Cl)CCCC1	0.0049442
Q15077	200	>= 4 saturated or aromatic carbon-only ring size 6	0.0037977
Q15077	838	BrC1C(Br)CCCC1	0.0035669

Q15077	840	CC1CC(O)CC1	0.0035652
Q15077	72	>= 1 Nb	0.0033797
Q15077	417	C#C	0.0033432
Q15077	39	>= 4 Cl	0.0029657
Q15077	605	O=C-C-O-C	0.0029055
Q15077	361	C(~Cl)(~H)	0.0028192
Q15077	602	O=C-C-N-C	0.0027352
Q15077	773	Clc1c(Cl)cccc1	0.002341
Q15077	837	ClC1C(Br)CCCC1	0.0019241
Q15077	830	SC1C(N)CCCC1	0.0017167
Q15077	628	C-N-C-C:C	0.0013666
Q15077	752	Clc1cc(Cl)ccc1	0.0013343
Q15077	112	>= 1 Yb	0.0013129
Q15077	877	NC1C(Br)CCC1	0.0010387
Q15077	571	[#1]-C-O-[#1]	0.0006885
Q15077	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.0006669
Q15077	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.0005831
Q15077	411	P(~O)(~O)	0.0003942
Q15077	854	NC1CC(N)CC1	0.0002395
Q15077	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0002217
Q15077	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.0001972
Q15077	76	>= 1 Pd	6.86E-06
Q15077	49	>= 1 Be	4.88E-06
Q15077	544	O-C:C-O	3.97E-06
Q15077	102	>= 1 Nd	1.31E-06
Q15077	99	>= 1 La	1.00E-06
Q15077	858	ClC1CC(Br)CC1	-1.29E-07
Q15077	303	N-Si	-1.27E-06
Q15077	848	OC1CC(Cl)CC1	-1.53E-06
Q15077	444	C(-Cl)(=O)	-2.28E-06
Q15077	733	Brc1ccc(Br)cc1	-6.54E-05
Q15077	786	OC1CCC(Br)CC1	-0.000307
Q15077	45	>= 4 Br	-0.000492
Q15077	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	-0.00051
Q15077	77	>= 1 Ag	-0.000546
Q15077	59	>= 1 Co	-0.000611
Q15077	359	C(~C)(:N)(:N)	-0.00067
Q15077	625	O=C-C:C-O	-0.001197
Q15077	866	OC1C(O)CCC1	-0.001245
Q15077	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.001292
Q15077	16	>= 4 N	-0.001572
Q15077	151	>= 2 saturated or aromatic carbon-only ring size 5	-0.001589
Q15077	74	>= 1 Ru	-0.001634
Q15077	700	O-C-C-C-C-C-O-C	-0.001768
Q15077	57	>= 1 Mn	-0.001886
Q15077	186	>= 2 saturated or aromatic carbon-only ring size 6	-0.002031
Q15077	396	N(~C)(:C)	-0.002154
Q15077	750	Nc1cc(Cl)ccc1	-0.002225

Q15077	782	OC1CCC(O)CC1	−0.002319
Q15077	291	C-Si	−0.002568
Q15077	459	S(=O)(=O)	−0.002753
Q15077	412	S(~C)(~C)	−0.002777
Q15077	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.002976
Q15077	409	O(:C)(:C)	−0.00308
Q15077	23	>= 1 F	−0.003797
Q15077	470	C:C-C=C	−0.003925
Q15077	81	>= 1 Sb	−0.003987
Q15077	227	>= 1 any ring size 8	−0.004199
Q15077	495	C-N-C:C	−0.004405
Q15077	377	C(~N)(:C)(:C)	−0.005389
Q15077	597	O=C-C-C:C	−0.005488
Q15077	334	C(~C)(~C)(~C)(~C)	−0.005506
Q15077	687	O=C-C-C-C=O	−0.005594
Q15077	875	NC1C(N)CCC1	−0.005771
Q15077	433	C(-C)(-Cl)(=O)	−0.005976
Q15077	306	N-Cl	−0.006168
Q15077	673	O=C-C=C-N	−0.006255
Q15077	740	Oc1cc(O)ccc1	−0.006262
Q15077	515	N-N-C-C	−0.006338
Q15077	498	O-C=C-C	−0.006416
Q15077	307	N-Br	−0.006423
Q15077	2	>= 16 H	−0.006875
Q15077	540	C-N-C-[#1]	−0.007022
Q15077	600	N-C:C:C-C	−0.007073
Q15077	739	Cc1cc(Br)ccc1	−0.007088
Q15077	522	C-N-N-[#1]	−0.007348
Q15077	61	>= 1 Cu	−0.007553
Q15077	85	>= 1 Ba	−0.009008
Q15077	685	O=C-C-C-C-N	−0.009033
Q15077	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.009153
Q15077	756	Cc1c(O)cccc1	−0.009168
Q15077	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.009239
Q15077	591	Cl-C-C-C-C	−0.009365
Q15077	418	C=N	−0.009546
Q15077	871	SC1C(S)CCC1	−0.009653
Q15077	113	>= 1 Tc	−0.00972
Q15077	691	O-C-C-C-C-C-N	−0.009801
Q15077	678	C-C-C=C-C	−0.010004
Q15077	367	C(~H)(~O)(~O)	−0.010033
Q15077	828	OC1C(Br)CCCC1	−0.01028
Q15077	316	F-P	−0.010474
Q15077	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.010967
Q15077	548	O-C-C:C	−0.011471
Q15077	719	Oc1ccc(O)cc1	−0.011739
Q15077	111	>= 1 Tm	−0.011802
Q15077	363	C(~F)(~F)	−0.012311

Q15077	637	O-C-C-C-C	−0.012364
Q15077	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.01311
Q15077	799	CC1CC(S)CCC1	−0.013113
Q15077	451	C(-N)(=O)	−0.013441
Q15077	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.013775
Q15077	682	O-C-C-C-C-N	−0.013869
Q15077	344	C(~C)(~H)	−0.0139
Q15077	14	>= 1 N	−0.013999
Q15077	503	Cl-C:C-[#1]	−0.014075
Q15077	357	C(~C)(:C)(:N)	−0.014282
Q15077	762	Oc1c(S)cccc1	−0.015352
Q15077	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.015733
Q15077	669	Cl-C:C-C=O	−0.015889
Q15077	849	OC1CC(Br)CC1	−0.016095
Q15077	178	>= 1 any ring size 6	−0.016391
Q15077	748	Sc1cc(Br)ccc1	−0.016542
Q15077	287	C-F	−0.016565
Q15077	292	C-P	−0.01704
Q15077	104	>= 1 Sm	−0.017407
Q15077	441	C(-C)(=C)	−0.018649
Q15077	523	N:C:C-C	−0.018675
Q15077	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.018981
Q15077	62	>= 1 Zn	−0.019117
Q15077	410	P(~C)(~C)	−0.019629
Q15077	670	Br-C:C:C-C	−0.019758
Q15077	96	>= 1 Tl	−0.020284
Q15077	414	S(~C)(~O)	−0.020537
Q15077	785	OC1CCC(Cl)CC1	−0.020581
Q15077	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.02096
Q15077	878	ClC1C(Cl)CCC1	−0.021006
Q15077	97	>= 1 Pb	−0.021037
Q15077	109	>= 1 Ho	−0.021048
Q15077	851	SC1CC(N)CC1	−0.021355
Q15077	343	C(~C)(~Cl)(~H)	−0.021414
Q15077	432	C(-C)(-C)(=O)	−0.021749
Q15077	350	C(~C)(~I)	−0.022172
Q15077	645	O=C-N-C-C	−0.023167
Q15077	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.023354
Q15077	274	B-C	−0.023381
Q15077	563	O-C-O-C	−0.023895
Q15077	213	>= 1 any ring size 7	−0.024138
Q15077	36	>= 8 S	−0.02457
Q15077	308	O-H	−0.024622
Q15077	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.025168
Q15077	510	[#1]-N-N-[#1]	−0.026251
Q15077	387	C(:C)(:N)	−0.026806
Q15077	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.026874
Q15077	437	C(-C)(-N)(=C)	−0.026932

Q15077	423	N=O	−0.027961
Q15077	455	N(-O)(=O)	−0.028395
Q15077	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.028475
Q15077	861	CC1C(O)CCC1	−0.028477
Q15077	530	N:C-C:C	−0.02915
Q15077	709	C-C(C)-C-C-C	−0.030369
Q15077	464	N-C-C=C	−0.030694
Q15077	300	N-N	−0.031357
Q15077	713	Cc1ccc(C)cc1	−0.031505
Q15077	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.031756
Q15077	4	>= 1 Li	−0.032659
Q15077	490	C-C-C=C	−0.032777
Q15077	660	C-C=C-C-C	−0.03314
Q15077	12	>= 16 C	−0.033264
Q15077	28	>= 1 Si	−0.033279
Q15077	550	Cl-C-C-C	−0.033505
Q15077	800	CC1CC(N)CCC1	−0.03424
Q15077	588	O=C-C-C=O	−0.034673
Q15077	549	N-C-C:C	−0.035844
Q15077	812	NC1CC(N)CCC1	−0.036053
Q15077	616	C:C:N:N:C	−0.038125
Q15077	342	C(~C)(~Cl)	−0.038312
Q15077	507	C-C-S-C	−0.039362
Q15077	743	Oc1cc(Cl)ccc1	−0.039842
Q15077	35	>= 4 S	−0.041197
Q15077	759	Cc1c(Cl)cccc1	−0.041304
Q15077	25	>= 4 F	−0.041703
Q15077	511	S=C-N-[#1]	−0.041945
Q15077	816	ClC1CC(Br)CCC1	−0.043566
Q15077	447	C(-H)(=N)	−0.043872
Q15077	545	N-C:C-C	−0.045807
Q15077	355	C(~C)(:C)	−0.046975
Q15077	299	N-H	−0.047059
Q15077	329	C(~Br)(~H)	−0.047394
Q15077	728	Nc1ccc(N)cc1	−0.047975
Q15077	731	Clc1ccc(Cl)cc1	−0.04888
Q15077	656	C-C-N-C-C	−0.049663
Q15077	103	>= 1 Pm	−0.050308
Q15077	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.050655
Q15077	365	C(~H)(~N)	−0.050978
Q15077	382	C(~O)(:C)(:C)	−0.051449
Q15077	611	N-C-C-N-C	−0.051607
Q15077	872	SC1C(N)CCC1	−0.052747
Q15077	263	Li-H	−0.053217
Q15077	391	N(~C)(~C)(~C)	−0.053496
Q15077	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.05446
Q15077	285	C-N	−0.054672
Q15077	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.054696

Q15077	521	C:N-C-[#1]	−0.054704
Q15077	671	O=C-C=C-C	−0.055292
Q15077	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.055346
Q15077	485	N:C:C:N	−0.056017
Q15077	13	>= 32 C	−0.056408
Q15077	575	O-C-C:C-O	−0.056724
Q15077	471	S:C:C:C	−0.057604
Q15077	803	OC1CC(O)CCC1	−0.057938
Q15077	78	>= 1 Cd	−0.058041
Q15077	499	N-C:C:N	−0.058339
Q15077	480	C:S:C-C	−0.058378
Q15077	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.058427
Q15077	810	SC1CC(Cl)CCC1	−0.05855
Q15077	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.059385
Q15077	662	O-C-C-O-C	−0.060136
Q15077	67	>= 1 Kr	−0.061206
Q15077	487	N-C=N-C	−0.06132
Q15077	42	>= 2 K	−0.06209
Q15077	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.062129
Q15077	792	NC1CCC(Cl)CC1	−0.062152
Q15077	484	N-C:N:C	−0.062214
Q15077	95	>= 1 Hg	−0.062606
Q15077	106	>= 1 Gd	−0.062607
Q15077	66	>= 1 Se	−0.062723
Q15077	735	Cc1cc(O)ccc1	−0.063084
Q15077	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.063441
Q15077	110	>= 1 Er	−0.064116
Q15077	644	C-C=N-N-C	−0.064473
Q15077	26	>= 1 Na	−0.065278
Q15077	71	>= 1 Zr	−0.065706
Q15077	332	C(~C)(~C)	−0.06624
Q15077	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.066639
Q15077	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.066648
Q15077	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.066813
Q15077	86	>= 1 Lu	−0.066951
Q15077	741	Oc1cc(S)ccc1	−0.067978
Q15077	674	N-C-N-C:C	−0.069522
Q15077	729	Nc1ccc(Cl)cc1	−0.070624
Q15077	80	>= 1 Sn	−0.071313
Q15077	742	Oc1cc(N)ccc1	−0.072911
Q15077	619	O-C-C=C-C	−0.075291
Q15077	864	CC1C(Cl)CCC1	−0.076469
Q15077	558	O=N-C:C	−0.079539
Q15077	576	N=C-C:C-[#1]	−0.080215
Q15077	520	C=C-C:C	−0.082413
Q15077	373	C(~H)(:N)	−0.086826
Q15077	694	O=C-C-C-C-C=O	−0.090122
Q15077	505	Cl-C:C-O	−0.09216

Q15077	273	B-B	−0.093208
Q15077	366	C(~H)(~O)	−0.094154
Q15077	94	>= 1 Au	−0.099696
Q15077	379	C(~N)(:N)	−0.100624
Q15077	631	O-C:C-O-[#1]	−0.103456
Q15077	478	S-C=N-[#1]	−0.103577
Q15077	372	C(~H)(:C)(:N)	−0.105703
Q15077	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.107574
Q15077	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.108554
Q15077	241	>= 1 any ring size 9	−0.112191
Q15077	704	O=C-C-C-C-C-C-C	−0.112289
Q15077	270	Li-S	−0.115587
Q15077	491	C-N:C-[#1]	−0.116069
Q15077	646	O=C-N-C-[#1]	−0.116563
Q15077	24	>= 2 F	−0.123425
Q15077	374	C(~H)(~H)(~H)	−0.126586
Q15077	234	>= 2 any ring size 8	−0.127063
Q15077	693	O=C-C-C-C-C-O	−0.129124
Q15077	427	C(#C)(-C)	−0.129222
Q15077	721	Oc1ccc(N)cc1	−0.138043
Q15077	269	Li-P	−0.138723
Q15077	797	CC1CC(C)CCC1	−0.140863
Q15077	492	N-C:O:C	−0.142106
Q15077	695	O=C-C-C-C-C-N	−0.14896
Q15077	552	C:C-C:C	−0.149641
Q15077	553	O=C-C=C	−0.150325
Q15077	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.158333
Q15077	317	F-S	−0.161789
Q15077	573	O-C-C=C	−0.176791
Q15077	397	N(~C)(:C)(:C)	−0.178865
Q15077	776	CC1CCC(C)CC1	−0.186248
Q15077	351	C(~C)(~N)	−0.189267
Q15077	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.189783
Q15077	615	N-C-C-O-C	−0.189959
Q15077	766	Sc1c(S)cccc1	−0.195406
Q15077	769	Sc1c(Br)cccc1	−0.196163
Q15077	869	OC1C(Cl)CCC1	−0.196292
Q15077	323	P-H	−0.196793
Q15077	401	N(~O)(~O)	−0.197326
Q15077	333	C(~C)(~C)(~C)	−0.201247
Q15077	381	C(~O)(:C)	−0.204055
Q15077	266	Li-C	−0.212252
Q15077	583	Cl-C:C-O-C	−0.213338
Q15077	579	O=C-C-C-C	−0.218128
Q15077	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.221958
Q15077	833	NC1C(N)CCCC1	−0.222041
Q15077	465	O=S-C-C	−0.222614
Q15077	506	C-C:N:C	−0.22577

Q15077	720	Oc1ccc(S)cc1	−0.225941
Q15077	717	Cc1ccc(Cl)cc1	−0.234932
Q15077	293	C-S	−0.237646
Q15077	542	O-C:C-[#1]	−0.238202
Q15077	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.239909
Q15077	647	O=C-N-C-N	−0.241789
Q15077	353	C(~C)(~S)	−0.24753
Q15077	879	ClC1C(Br)CCC1	−0.25153
Q15077	533	S-C:C-N	−0.252059
Q15077	73	>= 1 Mo	−0.252397
Q15077	150	>= 2 any ring size 5	−0.25535
Q15077	22	>= 16 O	−0.255863
Q15077	798	CC1CC(O)CCC1	−0.256414
Q15077	83	>= 1 Xe	−0.259849
Q15077	777	CC1CCC(O)CC1	−0.264274
Q15077	714	Cc1ccc(O)cc1	−0.266701
Q15077	428	C(#C)(-H)	−0.268578
Q15077	312	O-Al	−0.272619
Q15077	258	>= 2 hetero-aromatic rings	−0.2757
Q15077	206	>= 5 any ring size 6	−0.277827
Q15077	509	Br-C:C-C	−0.283079
Q15077	528	[#1]-N-C-[#1]	−0.284445
Q15077	454	N(-C)(=O)	−0.284859
Q15077	482	C:N-C:C	−0.288562
Q15077	486	N-C:N:N	−0.290605
Q15077	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.300594
Q15077	560	N-C-N-C	−0.30715
Q15077	834	NC1C(Cl)CCCC1	−0.308225
Q15077	592	N-C-C-C-C	−0.313571
Q15077	259	>= 3 aromatic rings	−0.315359
Q15077	383	C(~S)(:C)	−0.317206
Q15077	421	C=S	−0.320954
Q15077	448	C(-H)(=O)	−0.334558
Q15077	32	>= 4 P	−0.339648
Q15077	192	>= 3 any ring size 6	−0.341955
Q15077	347	C(~C)(~H)(~O)(~O)	−0.3448
Q15077	702	O-C-C-C-C-C-N-C	−0.347995
Q15077	416	C=C	−0.351409
Q15077	461	O-C-C=N	−0.352636
Q15077	429	C(#N)(-C)	−0.355961
Q15077	612	N-C-O-C-C	−0.364364
Q15077	607	N-C-C-C:C	−0.376998
Q15077	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.378331
Q15077	497	O-C:C:N	−0.379744
Q15077	20	>= 4 O	−0.385581
Q15077	749	Nc1cc(N)ccc1	−0.388241
Q15077	556	C=C-C-C	−0.388695
Q15077	761	Oc1c(O)cccc1	−0.391985

Q15077	780	CC1CCC(Cl)CC1	−0.396112
Q15077	534	S-C:C-O	−0.402402
Q15077	376	C(~N)(:C)	−0.408664
Q15077	402	N(~O)(:O)	−0.412066
Q15077	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.416285
Q15077	456	P(-O)(=O)	−0.418653
Q15077	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.426707
Q15077	747	Sc1cc(Cl)ccc1	−0.429235
Q15077	736	Cc1cc(S)ccc1	−0.43557
Q15077	683	N-C-C-C-C-C	−0.438083
Q15077	337	C(~C)(~C)(~C)(~O)	−0.440413
Q15077	434	C(-C)(-H)(=C)	−0.440964
Q15077	681	O-C-C-C-C-O	−0.442561
Q15077	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.443076
Q15077	279	B-P	−0.444008
Q15077	667	C=C-C-O-[#1]	−0.445809
Q15077	525	[As]-C:C-[#1]	−0.446554
Q15077	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.449364
Q15077	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.45031
Q15077	288	C-Na	−0.459499
Q15077	79	>= 1 In	−0.468519
Q15077	689	O-C-C-C-C-C-C	−0.468556
Q15077	364	C(~F)(:C)	−0.475263
Q15077	322	Si-Cl	−0.486815
Q15077	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.496177
Q15077	557	N:C-O-[#1]	−0.506382
Q15077	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.506887
Q15077	453	N(-C)(=C)	−0.508098
Q15077	620	C:C-O-C-C	−0.509938
Q15077	64	>= 1 Ge	−0.513659
Q15077	604	C-O-C-C:C	−0.514582
Q15077	27	>= 2 Na	−0.515491
Q15077	338	C(~C)(~C)(~H)(~N)	−0.516376
Q15077	457	S(-C)(=O)	−0.519269
Q15077	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.522764
Q15077	823	CC1C(Br)CCCC1	−0.523292
Q15077	586	C-S-C-C-C	−0.524351
Q15077	561	Cl-C-C=O	−0.531402
Q15077	711	C-C(C)(C)-C-C	−0.534962
Q15077	623	O=C-C:C-C	−0.550015
Q15077	676	N#C-C-C-C	−0.552735
Q15077	657	C-N-C:C-C	−0.555239
Q15077	675	Br-C-C-C:C	−0.564977
Q15077	608	C-C-C-C:C	−0.565866
Q15077	90	>= 1 Re	−0.573261
Q15077	489	N-C-S-C	−0.57645
Q15077	55	>= 1 V	−0.583723
Q15077	821	CC1C(N)CCCC1	−0.592742

Q15077	618	C:C-C-C:C	−0.592831
Q15077	726	Sc1ccc(Cl)cc1	−0.596791
Q15077	518	O=C-N-N	−0.59886
Q15077	633	N-C-C:C-C	−0.601617
Q15077	199	>= 4 any ring size 6	−0.606725
Q15077	171	>= 5 any ring size 5	−0.624328
Q15077	385	C(:C)(:C)(:C)	−0.627276
Q15077	65	>= 1 As	−0.638002
Q15077	634	C-C-C:C-C	−0.644379
Q15077	10	>= 4 C	−0.647617
Q15077	791	NC1CCC(N)CC1	−0.648782
Q15077	255	>= 1 aromatic ring	−0.650245
Q15077	467	C=N-N-C	−0.653425
Q15077	661	O-C-O-C-C	−0.680681
Q15077	404	N(:C)(:C)(:C)	−0.681921
Q15077	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.682995
Q15077	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.695835
Q15077	393	N(~C)(~H)	−0.699037
Q15077	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.69985
Q15077	420	C=O	−0.700389
Q15077	439	C(-C)(-N)(=O)	−0.701941
Q15077	472	C:N:C-C	−0.7233
Q15077	606	O-C:C-C-C	−0.723886
Q15077	445	C(-H)(-N)(=C)	−0.731409
Q15077	730	Nc1ccc(Br)cc1	−0.73206
Q15077	839	CC1CC(C)CC1	−0.742406
Q15077	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.74574
Q15077	362	C(~Cl)(:C)	−0.760214
Q15077	452	C(-O)(=O)	−0.767298
Q15077	483	N-S-C:C	−0.773205
Q15077	876	NC1C(Cl)CC1	−0.776082
Q15077	309	O-O	−0.781854
Q15077	105	>= 1 Eu	−0.798042
Q15077	8	>= 4 B	−0.801562
Q15077	677	C-C=C-C:C	−0.810495
Q15077	493	O=C-C:C	−0.823219
Q15077	757	Cc1c(S)cccc1	−0.827147
Q15077	589	C-C:C-O-C	−0.83136
Q15077	845	OC1CC(O)CC1	−0.83275
Q15077	48	>= 4 I	−0.840148
Q15077	88	>= 1 Ta	−0.844979
Q15077	581	O=C-C-C-O	−0.848374
Q15077	648	O=N-C:C-N	−0.861862
Q15077	629	S-C:C:C-N	−0.87045
Q15077	826	OC1C(N)CCCC1	−0.871678
Q15077	271	Li-Cl	−0.876452
Q15077	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.876733
Q15077	44	>= 2 Br	−0.879196

Q15077	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.886837
Q15077	868	OC1C(N)CCC1	−0.896053
Q15077	6	>= 1 B	−0.914552
Q15077	68	>= 1 Rb	−0.919827
Q15077	341	C(~C)(~C)(~O)	−0.925948
Q15077	40	>= 8 Cl	−0.927637
Q15077	516	[#1]-C=C-[#1]	−0.940638
Q15077	574	O-C-C:C-C	−0.943664
Q15077	793	NC1CCC(Br)CC1	−0.956835
Q15077	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.961782
Q15077	697	C-C-C-C-C-C(C)-C	−0.964403
Q15077	390	N(~C)(~C)	−0.970608
Q15077	596	N=C-N-C-C	−0.978588
Q15077	346	C(~C)(~H)(~O)	−0.984983
Q15077	856	NC1CC(Br)CC1	−0.987034
Q15077	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.991523
Q15077	513	S:C:C-[#1]	−0.995415
Q15077	69	>= 1 Sr	−1.003476
Q15077	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−1.008911
Q15077	564	C=C-C=C	−1.031952
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Q15077	290	C-Al	−1.039857
Q15077	100	>= 1 Ce	−1.040941
Q15077	767	Sc1c(N)cccc1	−1.063168
Q15077	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−1.084648
Q15077	0	>= 4 H	−1.098676
Q15077	275	B-N	−1.109464
Q15077	755	Cc1c(C)cccc1	−1.118319
Q15077	753	Clc1cc(Br)ccc1	−1.11984
Q15077	458	S(-O)(=O)	−1.130322
Q15077	706	O=C-C-C-C-C(=O)-C	−1.142041
Q15077	765	Oc1c(Br)cccc1	−1.187191
Q15077	440	C(-C)(-O)(=O)	−1.204934
Q15077	813	NC1CC(Cl)CCC1	−1.238315
Q15077	256	>= 1 hetero-aromatic ring	−1.250984
Q15077	829	SC1C(S)CCCC1	−1.274548
Q15077	108	>= 1 Dy	−1.281393
Q15077	449	C(-N)(=C)	−1.2863
Q15077	778	CC1CCC(S)CC1	−1.349351
Q15077	867	OC1C(S)CCC1	−1.354971
Q15077	235	>= 2 saturated or aromatic carbon-only ring size 8	−1.368269
Q15077	324	P-P	−1.382104
Q15077	129	>= 1 any ring size 4	−1.396726
Q15077	193	>= 3 saturated or aromatic carbon-only ring size 6	−1.403181
Q15077	264	Li-Li	−1.459639
Q15077	51	>= 1 Al	−1.481179
Q15077	862	CC1C(S)CCC1	−1.489038
Q15077	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−1.49102

Q15077	652	O-C:C:C-N	−1.499701
Q15077	547	N-C:C-N	−1.510557
Q15077	286	C-O	−1.541643
Q15077	781	CC1CCC(Br)CC1	−1.585977
Q15077	294	C-Cl	−1.65894
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Q15077	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−1.685402
Q15077	302	N-F	−1.698864
Q15077	627	O=[As]-C:C:C	−1.724409
Q15077	143	>= 1 any ring size 5	−1.770669
Q15077	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−1.775912
Q15077	664	C-C=C-C=C	−1.782279
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Q15077	43	>= 1 Br	−2.032473
Q15077	842	CC1CC(N)CC1	−2.073615
Q15077	114	>= 1 U	−2.198573
Q15077	281	B-Cl	−2.243113
Q15077	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−2.378354
Q15077	52	>= 1 Ca	−2.419282

Fingerprints（continued)

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-0.81512766 0.0046326
-0.822862442 -0.000357
-0.829709191 0.0025621
-0.836218715 0.0048589
-0.831047889 -0.001702
-0.840142824 -5.51E-06
-0.84497319 -5.50E-06
-0.845237212 -0.003137
-0.861858523 -3.83E-06
-0.871597229 0.0011467
-0.865720111 -0.005958
-0.876445556 -5.96E-06
-0.876728226 -4.34E-06
-0.879355555 0.0001594

-0.886209621 -0.000627
-0.892373031 -0.00368
-0.919869674 0.0053178
-0.919828715 1.42E-06
-0.91916332 -0.006785
-0.927638019 1.29E-06
-0.935200776 -0.005438
-0.950169887 0.0065063
-0.956530952 -0.000304
-0.961780952 -1.50E-06
-0.97165893 0.0072557
-0.965887873 -0.00472
-0.981924646 0.003337
-0.976844651 -0.008138
-0.987027121 -6.49E-06
-0.99151835 -4.62E-06
-0.997451019 0.0020365
-1.003471246 -5.24E-06
-1.009004646 9.41E-05
-1.027466649 -0.004486
-1.034530287 -0.001679
-1.039856651 -3.92E-07
-1.040948262 7.46E-06
-1.068516114 0.0053484
-1.084659623 1.18E-05
-1.098677552 1.68E-06
-1.114562246 0.0050981
-1.110251189 -0.008068
-1.119843412 3.30E-06
-1.129194581 -0.001127
-1.14026447 -0.001777
-1.187190231 -2.71E-07
-1.207422793 0.0024888
-1.229811488 -0.008504
-1.25097887 -5.39E-06
-1.274552354 4.78E-06
-1.281398332 5.53E-06
-1.283460836 -0.002839
-1.351610124 0.0022594
-1.354978538 7.41E-06
-1.368267226 -1.38E-06
-1.38209943 -4.96E-06
-1.397511487 0.0007855
-1.403235595 5.49E-05
-1.459645889 7.18E-06
-1.481178584 -9.13E-07
-1.489037285 -1.15E-06
-1.49255685 0.0015367

-1.493794261 -0.005907
-1.514295601 0.0037383
-1.537144624 -0.004498
-1.580895026 -0.005082
-1.658834584 -0.000106
-1.676084913 -4.15E-06
-1.684243929 -0.001159
-1.698864861 7.25E-07
-1.724407358 -2.05E-06
-1.763578073 -0.007091
-1.775908301 -4.00E-06
-1.784954244 0.0026751
-1.883260075 -0.003399
-2.038895558 0.006423
-2.071211524 -0.002404
-2.198573461 6.42E-08
-2.243115681 2.27E-06
-2.378357457 3.06E-06
-2.419282005 -2.58E-07

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P41231	271	Li-Cl	3.0763782
P41231	444	C(-Cl)(=O)	2.27E+00
P41231	59	>= 1 Co	2.0376687
P41231	318	Al-H	1.8663077
P41231	854	NC1CC(N)CC1	1.7585722
P41231	852	SC1CC(Cl)CC1	1.675153
P41231	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	1.6632296
P41231	325	As-H	1.62E+00
P41231	376	C(~N)(:C)	1.6170193
P41231	520	C=C-C:C	1.6076366
P41231	85	>= 1 Ba	1.5519273
P41231	862	CC1C(S)CCC1	1.5009773
P41231	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	1.4890667
P41231	49	>= 1 Be	1.48E+00
P41231	298	C-I	1.4743373
P41231	776	CC1CCC(C)CC1	1.4311238
P41231	811	SC1CC(Br)CCC1	1.4068884
P41231	108	>= 1 Dy	1.3938075
P41231	718	Cc1ccc(Br)cc1	1.3754585
P41231	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	1.3411715
P41231	87	>= 1 Hf	1.3067009
P41231	775	Brc1c(Br)cccc1	1.296328
P41231	291	C-Si	1.2829769
P41231	112	>= 1 Yb	1.2735879
P41231	359	C(~C)(:N)(:N)	1.2602592
P41231	547	N-C:C-N	1.254171
P41231	515	N-N-C-C	1.2412363
P41231	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	1.2366863
P41231	354	C(~C)(~Si)	1.2334185
P41231	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	1.2295516
P41231	533	S-C:C-N	1.2100998
P41231	80	>= 1 Sn	1.2053855
P41231	446	C(-H)(=C)	1.2048775
P41231	527	C:C:N-[#1]	1.1860587
P41231	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	1.1826083
P41231	792	NC1CCC(Cl)CC1	1.1725035
P41231	795	ClC1CCC(Br)CC1	1.158188
P41231	522	C-N-N-[#1]	1.1351027
P41231	824	OC1C(O)CCCC1	1.1334719
P41231	283	C-H	1.1256083
P41231	812	NC1CC(N)CCC1	1.1181226
P41231	828	OC1C(Br)CCCC1	1.0813191
P41231	483	N-S-C:C	1.073191
P41231	583	Cl-C:C-O-C	1.0726948
P41231	822	CC1C(Cl)CCCC1	1.0551813
P41231	303	N-Si	1.01E+00

P41231	835	NC1C(Br)CCCC1	0.9711051
P41231	268	Li-F	0.9694811
P41231	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.9619419
P41231	739	Cc1cc(Br)ccc1	0.9600774
P41231	743	Oc1cc(Cl)ccc1	0.9543703
P41231	565	C:C-O-C	0.9172457
P41231	807	OC1CC(Br)CCC1	9.16E-01
P41231	62	>= 1 Zn	0.913827
P41231	617	C-C-C-O-[#1]	0.9034964
P41231	567	O-C-C-O	0.9015028
P41231	579	O=C-C-C-C	0.8782741
P41231	531	S-C:C-C	0.8748408
P41231	845	OC1CC(O)CC1	0.8580277
P41231	30	>= 1 P	0.8449638
P41231	276	B-O	0.8443008
P41231	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.8335468
P41231	830	SC1C(N)CCCC1	0.8179704
P41231	778	CC1CCC(S)CC1	0.8129748
P41231	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.8050808
P41231	504	N:C:N-C	0.8034393
P41231	549	N-C-C:C	0.8012577
P41231	694	O=C-C-C-C-C=O	0.7967711
P41231	327	C(~Br)(~C)	0.7967355
P41231	228	>= 1 saturated or aromatic carbon-only ring size 8	0.7766068
P41231	677	C-C=C-C:C	0.766539
P41231	275	B-N	0.7406152
P41231	691	O-C-C-C-C-C-N	0.7299495
P41231	754	Brc1cc(Br)ccc1	0.7225029
P41231	827	OC1C(Cl)CCCC1	0.7214459
P41231	31	>= 2 P	0.720346
P41231	277	B-F	0.7150483
P41231	346	C(~C)(~H)(~O)	0.7070459
P41231	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.7020402
P41231	744	Oc1cc(Br)ccc1	0.6975624
P41231	75	>= 1 Rh	0.6937533
P41231	636	C-N-C-N-C	0.6931791
P41231	836	ClC1C(Cl)CCCC1	0.6789567
P41231	389	C(:N)(:N)	0.6779865
P41231	4	>= 1 Li	0.6722311
P41231	375	C(~N)(~N)	0.6689863
P41231	206	>= 5 any ring size 6	0.6633218
P41231	445	C(-H)(-N)(=C)	0.6623892
P41231	663	O-C-C-O-[#1]	0.6510852
P41231	308	O-H	0.6464969
P41231	750	Nc1cc(Cl)ccc1	0.6452018
P41231	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.6451969
P41231	680	O-C-C-C-C-C	0.6448954
P41231	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.6439806

P41231	469	S-S-C:C	6.40E-01
P41231	760	Cc1c(Br)cccc1	0.6390967
P41231	773	Clc1c(Cl)cccc1	0.6376977
P41231	379	C(~N)(:N)	0.6372931
P41231	300	N-N	0.6369553
P41231	104	>= 1 Sm	0.6297452
P41231	340	C(~C)(~C)(~N)	0.6201613
P41231	347	C(~C)(~H)(~O)(~O)	0.6139731
P41231	123	>= 2 saturated or aromatic carbon-only ring size 3	0.6005103
P41231	503	Cl-C:C-[#1]	0.595206
P41231	814	NC1CC(Br)CCC1	0.5804641
P41231	842	CC1CC(N)CC1	0.5798612
P41231	465	O=S-C-C	0.5693042
P41231	597	O=C-C-C:C	0.5526629
P41231	479	S-C-S-C	0.5446679
P41231	395	N(~C)(~O)	0.519685
P41231	606	O-C:C-C-C	0.5168547
P41231	150	>= 2 any ring size 5	0.5168267
P41231	502	N-C=C-[#1]	0.5161682
P41231	664	C-C=C-C=C	0.5103356
P41231	164	>= 4 any ring size 5	0.5087163
P41231	398	N(~H)(~N)	0.4966364
P41231	40	>= 8 Cl	0.491655
P41231	410	P(~C)(~C)	0.4883545
P41231	282	B-Br	0.4850714
P41231	607	N-C-C-C:C	0.4775737
P41231	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.4729396
P41231	803	OC1CC(O)CCC1	0.4565908
P41231	323	P-H	0.4532614
P41231	186	>= 2 saturated or aromatic carbon-only ring size 6	0.4502066
P41231	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.448092
P41231	648	O=N-C:C-N	0.4463305
P41231	287	C-F	0.4393562
P41231	11	>= 8 C	0.4391092
P41231	542	O-C:C-[#1]	0.4376985
P41231	723	Oc1ccc(Br)cc1	0.4337793
P41231	707	O=C-C-C-C-C(N)-C	0.4332057
P41231	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.4323119
P41231	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.4276647
P41231	265	Li-B	0.4271397
P41231	106	>= 1 Gd	0.4254377
P41231	555	N=C-C=C	0.4207564
P41231	18	>= 1 O	0.4194075
P41231	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.4169803
P41231	608	C-C-C-C:C	0.4118249
P41231	573	O-C-C=C	0.4054416
P41231	876	NC1C(Cl)CC1	0.404246
P41231	296	C-Se	0.3947393

P41231	463	N:C-S-[#1]	0.3892408
P41231	295	C-As	0.386394
P41231	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.3787161
P41231	747	Sc1cc(Cl)ccc1	0.3785478
P41231	77	>= 1 Ag	0.3718327
P41231	825	OC1C(S)CCCC1	0.3701873
P41231	510	[#1]-N-N-[#1]	0.3700239
P41231	556	C=C-C-C	0.3694467
P41231	383	C(~S)(:C)	0.3674712
P41231	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.366735
P41231	478	S-C=N-[#1]	0.3616442
P41231	270	Li-S	0.3557276
P41231	729	Nc1ccc(Cl)cc1	0.3497826
P41231	696	C-C-C-C-C-C-C-C	0.3471293
P41231	658	C-C-S-C-C	0.3409628
P41231	641	O-C-C-C=C	0.3336514
P41231	785	OC1CCC(Cl)CC1	0.3294054
P41231	539	N=C-C-[#1]	0.3292666
P41231	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.3265065
P41231	847	OC1CC(N)CC1	0.3262774
P41231	32	>= 4 P	0.3250508
P41231	28	>= 1 Si	0.3217021
P41231	576	N=C-C:C-[#1]	0.3173262
P41231	151	>= 2 saturated or aromatic carbon-only ring size 5	0.3165781
P41231	717	Cc1ccc(Cl)cc1	0.3132954
P41231	429	C(#N)(-C)	0.311801
P41231	439	C(-C)(-N)(=O)	0.3103292
P41231	529	Cl-C-C-Cl	0.3100482
P41231	378	C(~N)(:C)(:N)	0.3028919
P41231	143	>= 1 any ring size 5	0.2965235
P41231	21	>= 8 O	0.292425
P41231	2	>= 16 H	0.2908559
P41231	766	Sc1c(S)cccc1	0.2875612
P41231	352	C(~C)(~O)	0.2859991
P41231	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.2805058
P41231	366	C(~H)(~O)	0.2798994
P41231	566	O-C-C-N	0.2788458
P41231	560	N-C-N-C	0.2744071
P41231	598	Cl-C:C:C-C	0.274285
P41231	289	C-Mg	0.2740366
P41231	879	ClC1C(Br)CCC1	0.2682128
P41231	462	O-C-C=O	0.261082
P41231	349	C(~C)(~H)(~S)	0.2605283
P41231	612	N-C-O-C-C	0.2549217
P41231	800	CC1CC(N)CCC1	0.2517884
P41231	633	N-C-C:C-C	0.2509575
P41231	329	C(~Br)(~H)	0.2506684
P41231	546	N-C:C-[#1]	0.2468887

P41231	404	N(:C)(:C)(:C)	0.2369976
P41231	710	C-C-C(C)-C-C	0.2340382
P41231	619	O-C-C=C-C	0.2225893
P41231	304	N-P	0.222324
P41231	427	C(#C)(-C)	0.2204288
P41231	865	CC1C(Br)CCC1	0.2201705
P41231	666	C=C-C-O-C	0.2183699
P41231	79	>= 1 In	0.2177286
P41231	611	N-C-C-N-C	0.2150782
P41231	473	S-C:N:C	0.2140657
P41231	605	O=C-C-O-C	0.2100656
P41231	737	Cc1cc(N)ccc1	0.2044007
P41231	430	C(-C)(-C)(=C)	0.201579
P41231	823	CC1C(Br)CCCC1	0.1932307
P41231	693	O=C-C-C-C-C-O	0.1925831
P41231	681	O-C-C-C-C-O	0.1920491
P41231	553	O=C-C=C	0.1906042
P41231	834	NC1C(Cl)CCCC1	0.1896453
P41231	214	>= 1 saturated or aromatic carbon-only ring size 7	0.1833576
P41231	34	>= 2 S	0.1811515
P41231	360	C(~Cl)(~Cl)	0.1807059
P41231	48	>= 4 I	0.1798712
P41231	451	C(-N)(=O)	0.1784749
P41231	870	OC1C(Br)CCC1	0.1713694
P41231	403	N(:C)(:C)	0.1673292
P41231	335	C(~C)(~C)(~C)(~H)	0.1667106
P41231	880	BrC1C(Br)CCC1	0.1633826
P41231	399	N(~H)(:C)	0.1592678
P41231	328	C(~Br)(~C)(~C)	0.1588407
P41231	477	N-N-C:C	0.1561435
P41231	858	ClC1CC(Br)CC1	1.56E-01
P41231	443	C(-C)(=O)	0.1525631
P41231	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.1505984
P41231	536	O=C-C-N	0.1500868
P41231	407	O(~C)(~P)	0.1466649
P41231	391	N(~C)(~C)(~C)	0.1457168
P41231	820	CC1C(S)CCCC1	0.1451418
P41231	501	Cl-C:C-C	0.1444788
P41231	594	C-O-C-C=C	0.143111
P41231	722	Oc1ccc(Cl)cc1	0.142573
P41231	157	>= 3 any ring size 5	0.1423305
P41231	258	>= 2 hetero-aromatic rings	0.1409046
P41231	780	CC1CCC(Cl)CC1	0.1400254
P41231	610	C-O-C-O-C	0.1383433
P41231	716	Cc1ccc(N)cc1	0.1379604
P41231	640	C=C-C-C-C	0.1326864
P41231	777	CC1CCC(O)CC1	0.130679
P41231	485	N:C:C:N	0.1270831

P41231	97	>= 1 Pb	0.1245637
P41231	538	N=C-C-C	0.1231248
P41231	592	N-C-C-C-C	0.1218369
P41231	714	Cc1ccc(O)cc1	0.1202169
P41231	341	C(~C)(~C)(~O)	0.1185917
P41231	33	>= 1 S	0.1179352
P41231	453	N(-C)(=C)	0.1174226
P41231	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.1165461
P41231	260	>= 3 hetero-aromatic rings	0.1155749
P41231	185	>= 2 any ring size 6	0.11552
P41231	390	N(~C)(~C)	0.1132272
P41231	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.1120177
P41231	269	Li-P	1.11E-01
P41231	511	S=C-N-[#1]	0.1091937
P41231	517	N-N-C-N	0.1066814
P41231	752	Clc1cc(Cl)ccc1	0.1052707
P41231	562	Br-C-C=O	0.1047271
P41231	273	B-B	0.1040762
P41231	505	Cl-C:C-O	0.1032381
P41231	639	O-C-C-C-O	0.1029392
P41231	297	C-Br	0.1028029
P41231	480	C:S:C-C	0.1011696
P41231	623	O=C-C:C-C	0.0992857
P41231	599	[#1]-C-C=C-[#1]	0.0991947
P41231	508	S=C-N-C	0.0927574
P41231	372	C(~H)(:C)(:N)	0.0907714
P41231	720	Oc1ccc(S)cc1	0.0900667
P41231	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.0876995
P41231	711	C-C(C)(C)-C-C	0.0840805
P41231	333	C(~C)(~C)(~C)	0.0837593
P41231	698	O-C-C-C-C-C-C-C	0.0823949
P41231	440	C(-C)(-O)(=O)	0.0818761
P41231	248	>= 1 any ring size 10	0.0797328
P41231	488	N-C=N-[#1]	0.0795336
P41231	506	C-C:N:C	0.0781196
P41231	322	Si-Cl	0.0767411
P41231	709	C-C(C)-C-C-C	0.0755663
P41231	382	C(~O)(:C)(:C)	0.0742837
P41231	614	C-C-O-C-C	0.0731636
P41231	452	C(-O)(=O)	0.0726278
P41231	7	>= 2 B	0.0716068
P41231	425	P=O	0.0701836
P41231	438	C(-C)(-N)(=N)	0.0701018
P41231	396	N(~C)(:C)	0.0692585
P41231	213	>= 1 any ring size 7	0.0689567
P41231	652	O-C:C:C-N	0.0680293
P41231	115	>= 1 any ring size 3	0.0671599
P41231	848	OC1CC(Cl)CC1	6.68E-02

P41231	235	>= 2 saturated or aromatic carbon-only ring size 8	0.066759
P41231	543	O-C:C-N	0.0666029
P41231	93	>= 1 Pt	0.0664634
P41231	54	>= 1 Ti	0.0660438
P41231	385	C(:C)(:C)(:C)	0.0659803
P41231	559	O-C-N-[#1]	0.0658971
P41231	102	>= 1 Nd	6.55E-02
P41231	302	N-F	0.0647064
P41231	782	OC1CCC(O)CC1	0.0646995
P41231	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	6.45E-02
P41231	428	C(#C)(-H)	0.0642119
P41231	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0641686
P41231	779	CC1CCC(N)CC1	0.0639084
P41231	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.0637292
P41231	684	O=C-C-C-C-C	0.0636452
P41231	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.06352
P41231	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.0634537
P41231	771	Nc1c(Cl)cccc1	0.0632843
P41231	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0631351
P41231	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.0622186
P41231	468	O=S-C-N	0.0614237
P41231	615	N-C-C-O-C	0.061385
P41231	401	N(~O)(~O)	0.0605024
P41231	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0604242
P41231	339	C(~C)(~C)(~H)(~O)	0.0599475
P41231	783	OC1CCC(S)CC1	0.0598952
P41231	358	C(~C)(:N)	0.057636
P41231	609	Cl-C-C-N-C	0.0565732
P41231	101	>= 1 Pr	0.0549108
P41231	804	OC1CC(S)CCC1	0.0537968
P41231	476	C-O-C=C	0.0526458
P41231	467	C=N-N-C	0.0522692
P41231	764	Oc1c(Cl)cccc1	0.0514098
P41231	334	C(~C)(~C)(~C)(~C)	0.0513873
P41231	331	C(~Br)(:N)	0.0511214
P41231	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0503142
P41231	122	>= 2 any ring size 3	0.0493751
P41231	82	>= 1 Te	0.0484386
P41231	234	>= 2 any ring size 8	0.0426144
P41231	689	O-C-C-C-C-C-C	0.0420202
P41231	489	N-C-S-C	0.0405122
P41231	171	>= 5 any ring size 5	0.0397821
P41231	837	ClC1C(Br)CCCC1	3.95E-02
P41231	849	OC1CC(Br)CC1	0.0388409
P41231	794	ClC1CCC(Cl)CC1	0.0377213
P41231	578	C-C:C-C:C	0.0375772
P41231	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.0375539
P41231	343	C(~C)(~Cl)(~H)	0.035613

P41231	797	CC1CC(C)CCC1	0.0353643
P41231	838	BrC1C(Br)CCCC1	0.0347869
P41231	435	C(-C)(-H)(=N)	0.0344837
P41231	46	>= 1 I	0.0342257
P41231	701	O-C-C-C-C-C(O)-C	0.0335467
P41231	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.0332983
P41231	574	O-C-C:C-C	0.0327416
P41231	388	C(:C)(:N)(:N)	0.0326293
P41231	314	O-P	0.0312014
P41231	326	As-As	0.0306472
P41231	839	CC1CC(C)CC1	0.0304527
P41231	336	C(~C)(~C)(~C)(~N)	0.0303596
P41231	386	C(:C)(:C)(:N)	0.0302258
P41231	26	>= 1 Na	0.0261859
P41231	10	>= 4 C	0.0256918
P41231	662	O-C-C-O-C	0.025607
P41231	819	CC1C(O)CCCC1	0.0254616
P41231	570	C:C-C-C	0.0246033
P41231	653	O-C:C:C-O	0.0245483
P41231	432	C(-C)(-C)(=O)	0.0235225
P41231	651	O-C:C:C-C	0.0234591
P41231	867	OC1C(S)CCC1	0.0234398
P41231	550	Cl-C-C-C	0.0231941
P41231	678	C-C-C=C-C	0.0231845
P41231	774	Clc1c(Br)cccc1	0.0230979
P41231	470	C:C-C=C	0.0226352
P41231	413	S(~C)(~H)	2.18E-02
P41231	787	SC1CCC(S)CC1	0.020813
P41231	15	>= 2 N	0.0204559
P41231	51	>= 1 Al	0.0204426
P41231	816	ClC1CC(Br)CCC1	0.0197752
P41231	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.0197392
P41231	630	O-C:C-O-C	0.019048
P41231	568	N#C-C-C	0.0181638
P41231	521	C:N-C-[#1]	0.0180889
P41231	770	Nc1c(N)cccc1	0.0180344
P41231	790	SC1CCC(Br)CC1	0.0179816
P41231	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0179353
P41231	305	N-S	0.0177382
P41231	315	O-K	0.0177079
P41231	627	O=[As]-C:C:C	0.0176638
P41231	734	Cc1cc(C)ccc1	0.0173483
P41231	417	C#C	0.0172313
P41231	692	O=C-C-C-C-C-C	0.0171358
P41231	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.0167664
P41231	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0161012
P41231	751	Nc1cc(Br)ccc1	0.0157147
P41231	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.0155454

P41231	12	>= 16 C	0.0152793
P41231	761	Oc1c(O)cccc1	0.0148076
P41231	27	>= 2 Na	0.0142659
P41231	16	>= 4 N	0.0140881
P41231	373	C(~H)(:N)	0.0138947
P41231	447	C(-H)(=N)	0.0136199
P41231	486	N-C:N:N	0.0133965
P41231	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.0131914
P41231	514	O-N-C-C	0.0131228
P41231	292	C-P	0.0130476
P41231	24	>= 2 F	0.0127417
P41231	513	S:C:C-[#1]	0.0126032
P41231	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0125427
P41231	821	CC1C(N)CCCC1	0.0121045
P41231	0	>= 4 H	0.0119015
P41231	493	O=C-C:C	0.0108081
P41231	316	F-P	0.010771
P41231	626	C-O-C:C-C	0.0107062
P41231	86	>= 1 Lu	0.0106901
P41231	551	Cl-C-C-O	0.0106885
P41231	851	SC1CC(N)CC1	0.0106512
P41231	798	CC1CC(O)CCC1	0.0104138
P41231	859	BrC1CC(Br)CC1	0.0100159
P41231	475	S-C=N-C	0.0095926
P41231	43	>= 1 Br	0.0094324
P41231	345	C(~C)(~H)(~N)	0.009313
P41231	39	>= 4 Cl	0.0091307
P41231	394	N(~C)(~H)(~N)	0.0090807
P41231	563	O-C-O-C	0.0090149
P41231	381	C(~O)(:C)	0.00881
P41231	53	>= 1 Sc	0.0087867
P41231	58	>= 1 Fe	0.0087683
P41231	878	ClC1C(Cl)CCC1	0.0082433
P41231	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0080527
P41231	637	O-C-C-C-C	0.0079036
P41231	558	O=N-C:C	0.0078313
P41231	103	>= 1 Pm	0.0076886
P41231	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.007186
P41231	495	C-N-C:C	0.0068452
P41231	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0065397
P41231	90	>= 1 Re	0.0059536
P41231	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.005839
P41231	5	>= 2 Li	0.005827
P41231	474	S:C:C:N	0.0056992
P41231	742	Oc1cc(N)ccc1	0.0055872
P41231	843	CC1CC(Cl)CC1	0.0051927
P41231	590	C-C:C-O-[#1]	0.0050864
P41231	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0050792

P41231	863	CC1C(N)CCC1	0.0050696
P41231	671	O=C-C=C-C	0.0049916
P41231	306	N-Cl	0.0049652
P41231	255	>= 1 aromatic ring	0.0049487
P41231	806	OC1CC(Cl)CCC1	0.0041189
P41231	35	>= 4 S	0.0039616
P41231	861	CC1C(O)CCC1	0.003936
P41231	14	>= 1 N	0.003499
P41231	591	Cl-C-C-C-C	0.0028932
P41231	61	>= 1 Cu	0.0027197
P41231	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.002397
P41231	71	>= 1 Zr	0.0023915
P41231	94	>= 1 Au	0.0022985
P41231	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.0020264
P41231	809	SC1CC(N)CCC1	0.0012645
P41231	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.0011963
P41231	654	N-C-N-C-C	0.0007046
P41231	524	C-C=C-C	0.0006656
P41231	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.0003111
P41231	83	>= 1 Xe	0.0002225
P41231	730	Nc1ccc(Br)cc1	0.0001865
P41231	207	>= 5 saturated or aromatic carbon-only ring size 6	5.42E-05
P41231	670	Br-C:C:C-C	3.01E-05
P41231	817	BrC1CC(Br)CCC1	4.83E-06
P41231	99	>= 1 La	4.48E-06
P41231	426	P=P	4.09E-06
P41231	56	>= 1 Cr	2.42E-06
P41231	871	SC1C(S)CCC1	2.36E-06
P41231	274	B-C	9.12E-07
P41231	765	Oc1c(Br)cccc1	5.96E-08
P41231	856	NC1CC(Br)CC1	4.16E-08
P41231	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	-1.24E-06
P41231	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	-2.57E-06
P41231	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	-2.74E-06
P41231	42	>= 2 K	-4.99E-06
P41231	682	O-C-C-C-C-N	-9.99E-05
P41231	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	-0.000103
P41231	313	O-Si	-0.000137
P41231	448	C(-H)(=O)	-0.000163
P41231	65	>= 1 As	-0.000168
P41231	588	O=C-C-C=O	-0.000294
P41231	571	[#1]-C-O-[#1]	-0.000468
P41231	129	>= 1 any ring size 4	-0.000545
P41231	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	-0.000573
P41231	8	>= 4 B	-0.000669
P41231	738	Cc1cc(Cl)ccc1	-0.000887
P41231	293	C-S	-0.001059
P41231	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	-0.001126

P41231	377	C(~N)(:C)(:C)	−0.001129
P41231	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.00114
P41231	840	CC1CC(O)CC1	−0.001302
P41231	644	C-C=N-N-C	−0.001408
P41231	759	Cc1c(Cl)cccc1	−0.00168
P41231	846	OC1CC(S)CC1	−0.001688
P41231	544	O-C:C-O	−1.89E−03
P41231	829	SC1C(S)CCCC1	−0.002039
P41231	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.002193
P41231	414	S(~C)(~O)	−0.002237
P41231	442	C(-C)(=N)	−0.002285
P41231	726	Sc1ccc(Cl)cc1	−0.002713
P41231	311	O-Na	−0.002778
P41231	642	O-C-C-C=O	−0.002906
P41231	36	>= 8 S	−0.003018
P41231	423	N=O	−0.003672
P41231	96	>= 1 Tl	−0.003686
P41231	25	>= 4 F	−0.003733
P41231	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.003929
P41231	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.004115
P41231	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.004126
P41231	872	SC1C(N)CCC1	−0.004412
P41231	76	>= 1 Pd	−4.79E−03
P41231	192	>= 3 any ring size 6	−0.004916
P41231	482	C:N-C:C	−0.005104
P41231	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.00545
P41231	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.005607
P41231	290	C-Al	−0.005625
P41231	393	N(~C)(~H)	−0.005725
P41231	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.005823
P41231	507	C-C-S-C	−0.005899
P41231	864	CC1C(Cl)CCC1	−0.005907
P41231	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.006048
P41231	73	>= 1 Mo	−0.006089
P41231	557	N:C-O-[#1]	−0.0061
P41231	387	C(:C)(:N)	−0.006229
P41231	620	C:C-O-C-C	−0.007373
P41231	668	C-C:C-C-C	−0.007462
P41231	873	SC1C(Cl)CCC1	−0.007733
P41231	136	>= 2 any ring size 4	−0.008105
P41231	286	C-O	−0.008243
P41231	545	N-C:C-C	−0.008482
P41231	532	S-C:C-[#1]	−0.00888
P41231	596	N=C-N-C-C	−0.00909
P41231	826	OC1C(N)CCCC1	−0.009425
P41231	745	Sc1cc(S)ccc1	−0.009541
P41231	534	S-C:C-O	−0.009587
P41231	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.009766

P41231	332	C(~C)(~C)	−9.81E−03
P41231	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.010139
P41231	672	O=C-C=C-[#1]	−0.010909
P41231	321	Si-Si	−0.011932
P41231	530	N:C-C:C	−0.012493
P41231	370	C(~H)(:C)	−0.012872
P41231	178	>= 1 any ring size 6	−0.012914
P41231	724	Sc1ccc(S)cc1	−0.013551
P41231	577	C:C-N-C:C	−0.013853
P41231	351	C(~C)(~N)	−0.014007
P41231	57	>= 1 Mn	−0.014025
P41231	457	S(-C)(=O)	−0.014087
P41231	649	O=N-C:C-O	−0.015736
P41231	319	Al-Cl	−0.018153
P41231	769	Sc1c(Br)cccc1	−0.018528
P41231	20	>= 4 O	−0.018592
P41231	1	>= 8 H	−0.019039
P41231	29	>= 2 Si	−0.019448
P41231	585	C-C:C-N-C	−0.019636
P41231	262	>= 4 hetero-aromatic rings	−0.019734
P41231	431	C(-C)(-C)(=N)	−0.019843
P41231	89	>= 1 W	−0.020823
P41231	52	>= 1 Ca	−0.021879
P41231	801	CC1CC(Cl)CCC1	−0.022114
P41231	47	>= 2 I	−0.02346
P41231	799	CC1CC(S)CCC1	−0.023571
P41231	324	P-P	−0.024817
P41231	494	O=C-C:N	−0.02489
P41231	548	O-C-C:C	−0.02505
P41231	857	ClC1CC(Cl)CC1	−0.025357
P41231	802	CC1CC(Br)CCC1	−0.02669
P41231	679	C-C-C-C-C-C	−0.026736
P41231	818	CC1C(C)CCCC1	−0.026809
P41231	657	C-N-C:C-C	−0.026887
P41231	665	N-C:C-C-C	−0.027044
P41231	109	>= 1 Ho	−0.027238
P41231	69	>= 1 Sr	−0.027347
P41231	19	>= 2 O	−0.028634
P41231	874	SC1C(Br)CCC1	−0.029905
P41231	595	C:C-C-C-C	−0.030057
P41231	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.030568
P41231	492	N-C:O:C	−0.031401
P41231	624	O=C-C:C-N	−0.031812
P41231	808	SC1CC(S)CCC1	−0.032596
P41231	646	O=C-N-C-[#1]	−0.032757
P41231	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.034065
P41231	500	C-S-C:C	−0.034837
P41231	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.037159

P41231	263	Li-H	−0.039311
P41231	466	N#C-C=C	−0.039851
P41231	3	>= 32 H	−0.039995
P41231	348	C(~C)(~H)(~P)	−0.040546
P41231	676	N#C-C-C-C	−0.040775
P41231	412	S(~C)(~C)	−0.040912
P41231	484	N-C:N:C	−0.042756
P41231	702	O-C-C-C-C-C-N-C	−0.0433
P41231	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.043715
P41231	621	N-C:C:C:N	−0.043788
P41231	767	Sc1c(N)cccc1	−0.043863
P41231	740	Oc1cc(O)ccc1	−0.043941
P41231	456	P(-O)(=O)	−0.044675
P41231	712	C-C(C)-C(C)-C	−0.046382
P41231	400	N(~H)(:C)(:C)	−0.046912
P41231	98	>= 1 Bi	−0.04767
P41231	788	SC1CCC(N)CC1	−0.048542
P41231	424	N=P	−0.049493
P41231	593	N-C-C-C-N	−0.050017
P41231	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.050923
P41231	601	N-C:C:C-N	−0.050935
P41231	875	NC1C(N)CCC1	−0.05258
P41231	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−0.053313
P41231	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.054141
P41231	257	>= 2 aromatic rings	−0.054718
P41231	877	NC1C(Br)CCC1	−0.054874
P41231	733	Brc1ccc(Br)cc1	−5.50E-02
P41231	635	N-N-C-N-[#1]	−0.056381
P41231	241	>= 1 any ring size 9	−0.057188
P41231	763	Oc1c(N)cccc1	−0.058243
P41231	700	O-C-C-C-C-C-O-C	−0.05831
P41231	111	>= 1 Tm	−0.058661
P41231	853	SC1CC(Br)CC1	−0.059303
P41231	454	N(-C)(=O)	−0.059566
P41231	645	O=C-N-C-C	−0.060108
P41231	841	CC1CC(S)CC1	−0.061614
P41231	631	O-C:C-O-[#1]	−0.061837
P41231	256	>= 1 hetero-aromatic ring	−0.062298
P41231	625	O=C-C:C-O	−0.06305
P41231	45	>= 4 Br	−6.33E-02
P41231	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.063404
P41231	278	B-Si	−0.064007
P41231	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.064733
P41231	415	Si(~C)(~C)	−0.06474
P41231	281	B-Cl	−0.064756
P41231	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.064858
P41231	786	OC1CCC(Br)CC1	−0.064909
P41231	110	>= 1 Er	−6.54E-02

P41231	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.06543
P41231	855	NC1CC(Cl)CC1	−0.065684
P41231	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.065716
P41231	100	>= 1 Ce	−0.065954
P41231	725	Sc1ccc(N)cc1	−0.066207
P41231	107	>= 1 Tb	−0.066564
P41231	687	O=C-C-C-C=O	−0.066584
P41231	312	O-Al	−6.66E-02
P41231	369	C(~H)(~Si)	−0.066669
P41231	528	[#1]-N-C-[#1]	−0.066978
P41231	768	Sc1c(Cl)cccc1	−0.067671
P41231	552	C:C-C:C	−0.068121
P41231	114	>= 1 U	−0.070162
P41231	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.070209
P41231	433	C(-C)(-Cl)(=O)	−0.074782
P41231	746	Sc1cc(N)ccc1	−0.075401
P41231	564	C=C-C=C	−0.075974
P41231	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.078287
P41231	516	[#1]-C=C-[#1]	−0.078962
P41231	434	C(-C)(-H)(=C)	−0.081107
P41231	813	NC1CC(Cl)CCC1	−0.081367
P41231	460	C-C-C#C	−0.081767
P41231	449	C(-N)(=C)	−0.082299
P41231	113	>= 1 Tc	−0.083549
P41231	634	C-C-C:C-C	−0.090549
P41231	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.090683
P41231	781	CC1CCC(Br)CC1	−0.092443
P41231	66	>= 1 Se	−0.095526
P41231	38	>= 2 Cl	−0.096233
P41231	540	C-N-C-[#1]	−0.098867
P41231	392	N(~C)(~C)(~H)	−0.100309
P41231	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.100501
P41231	355	C(~C)(:C)	−0.103765
P41231	364	C(~F)(:C)	−1.06E-01
P41231	416	C=C	−0.10786
P41231	23	>= 1 F	−0.108507
P41231	580	O=C-C-C-N	−0.108873
P41231	660	C-C=C-C-C	−0.109502
P41231	362	C(~Cl)(:C)	−0.11056
P41231	686	O=C-C-C-C-O	−0.112671
P41231	604	C-O-C-C:C	−0.114434
P41231	784	OC1CCC(N)CC1	−0.115704
P41231	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.119226
P41231	661	O-C-O-C-C	−0.121297
P41231	365	C(~H)(~N)	−0.122425
P41231	17	>= 8 N	−0.126405
P41231	455	N(-O)(=O)	−0.128818
P41231	266	Li-C	−0.131659

P41231	805	OC1CC(N)CCC1	−0.13213
P41231	721	Oc1ccc(N)cc1	−0.135519
P41231	708	C-C(C)-C-C	−0.139372
P41231	374	C(~H)(~H)(~H)	−0.140353
P41231	699	O-C-C-C-C-C(C)-C	−0.140875
P41231	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.144421
P41231	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.146859
P41231	317	F-S	−0.154713
P41231	37	>= 1 Cl	−0.157634
P41231	301	N-O	−0.158095
P41231	736	Cc1cc(S)ccc1	−0.159833
P41231	450	C(-N)(=N)	−0.16345
P41231	344	C(~C)(~H)	−0.165665
P41231	307	N-Br	−0.166531
P41231	535	O=C-C-C	−0.167084
P41231	497	O-C:C:N	−0.167868
P41231	523	N:C:C-C	−0.16827
P41231	582	C-C-C-C-C	−0.169513
P41231	409	O(:C)(:C)	−0.171846
P41231	703	O-C-C-C-C-C(N)-C	−0.181971
P41231	735	Cc1cc(O)ccc1	−0.188141
P41231	436	C(-C)(-H)(=O)	−0.188733
P41231	731	Clc1ccc(Cl)cc1	−0.189625
P41231	584	C:C-C=C-C	−0.192699
P41231	728	Nc1ccc(N)cc1	−0.195508
P41231	380	C(~O)(~O)	−0.197403
P41231	402	N(~O)(:O)	−0.20054
P41231	368	C(~H)(~S)	−0.203124
P41231	356	C(~C)(:C)(:C)	−0.211177
P41231	13	>= 32 C	−0.211995
P41231	569	N-C-C-N	−0.214348
P41231	299	N-H	−0.216021
P41231	675	Br-C-C-C:C	−0.216129
P41231	41	>= 1 K	−0.225178
P41231	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.23235
P41231	67	>= 1 Kr	−0.237287
P41231	320	Si-H	−0.242637
P41231	541	O-C:C-C	−0.245315
P41231	831	SC1C(Cl)CCCC1	−0.248651
P41231	844	CC1CC(Br)CC1	−0.248907
P41231	600	N-C:C:C-C	−0.253488
P41231	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.253995
P41231	815	ClC1CC(Cl)CCC1	−0.256604
P41231	92	>= 1 Ir	−0.257099
P41231	498	O-C=C-C	−0.258889
P41231	688	C-C-C-C-C-C-C	−0.261011
P41231	587	N-C:C-O-[#1]	−0.26205
P41231	280	B-S	−0.264234

P41231	581	O=C-C-C-O	−0.271965
P41231	509	Br-C:C-C	−0.275696
P41231	259	>= 3 aromatic rings	−0.276518
P41231	793	NC1CCC(Br)CC1	−0.278183
P41231	791	NC1CCC(N)CC1	−0.287802
P41231	397	N(~C)(:C)(:C)	−0.290444
P41231	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.292717
P41231	756	Cc1c(O)cccc1	−0.298068
P41231	353	C(~C)(~S)	−0.304973
P41231	419	C#N	−0.317558
P41231	727	Sc1ccc(Br)cc1	−0.319349
P41231	78	>= 1 Cd	−0.32168
P41231	758	Cc1c(N)cccc1	−0.326796
P41231	833	NC1C(N)CCCC1	−0.33345
P41231	481	O-S-C:C	−0.333741
P41231	371	C(~H)(:C)(:C)	−0.333969
P41231	338	C(~C)(~C)(~H)(~N)	−0.335461
P41231	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.343333
P41231	796	BrC1CCC(Br)CC1	−3.44E−01
P41231	512	C-[As]-O-[#1]	−0.359159
P41231	586	C-S-C-C-C	−0.366805
P41231	704	O=C-C-C-C-C-C-C	−0.37799
P41231	367	C(~H)(~O)(~O)	−0.388562
P41231	199	>= 4 any ring size 6	−0.390751
P41231	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.395525
P41231	74	>= 1 Ru	−0.395684
P41231	719	Oc1ccc(O)cc1	−0.4027
P41231	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.404966
P41231	361	C(~Cl)(~H)	−0.410339
P41231	705	O=C-C-C-C-C(O)-C	−0.413303
P41231	753	Clc1cc(Br)ccc1	−0.422997
P41231	441	C(-C)(=C)	−0.436798
P41231	408	O(~H)(~S)	−0.437872
P41231	44	>= 2 Br	−0.448828
P41231	88	>= 1 Ta	−0.45382
P41231	22	>= 16 O	−0.456101
P41231	613	C-N-C-C-C	−0.458196
P41231	616	C:C:N:N:C	−0.462321
P41231	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−4.72E−01
P41231	464	N-C-C=C	−0.476492
P41231	810	SC1CC(Cl)CCC1	−0.480626
P41231	220	>= 2 any ring size 7	−0.488172
P41231	697	C-C-C-C-C-C(C)-C	−0.491528
P41231	288	C-Na	−0.492849
P41231	638	O-C-C-C-N	−0.49396
P41231	309	O-O	−0.50344
P41231	832	SC1C(Br)CCCC1	−0.50839
P41231	526	Cl-C:C-Cl	−0.510297

P41231	337	C(~C)(~C)(~C)(~O)	−0.527452
P41231	264	Li-Li	−0.528884
P41231	84	>= 1 Cs	−0.539983
P41231	496	N:N-C-[#1]	−0.547044
P41231	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.555596
P41231	755	Cc1c(C)cccc1	−0.556642
P41231	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.560199
P41231	458	S(-O)(=O)	−0.560682
P41231	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.570671
P41231	647	O=C-N-C-N	−0.574038
P41231	643	[#1]-C-C-N-[#1]	−0.590034
P41231	789	SC1CCC(Cl)CC1	−0.61598
P41231	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.618617
P41231	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.619432
P41231	669	Cl-C:C-C=O	−0.624903
P41231	715	Cc1ccc(S)cc1	−0.632075
P41231	279	B-P	−0.638383
P41231	860	CC1C(C)CCC1	−0.638502
P41231	673	O=C-C=C-N	−0.642425
P41231	310	O-Mg	−0.643474
P41231	525	[As]-C:C-[#1]	−0.650389
P41231	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.654738
P41231	622	O=C-O-C:C	−0.655355
P41231	537	O=C-C-O	−0.660412
P41231	420	C=O	−0.675717
P41231	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.693112
P41231	589	C-C:C-O-C	−0.697045
P41231	418	C=N	−0.704298
P41231	406	O(~C)(~H)	−0.711516
P41231	421	C=S	−0.71201
P41231	683	N-C-C-C-C-C	−0.713456
P41231	487	N-C=N-C	−0.714008
P41231	659	O-C-C-N-C	−0.718643
P41231	63	>= 1 Ga	−7.22E-01
P41231	459	S(=O)(=O)	−0.722881
P41231	285	C-N	−0.733618
P41231	55	>= 1 V	−0.752881
P41231	632	C-C-O-C:C	−0.753784
P41231	868	OC1C(N)CCC1	−0.754198
P41231	68	>= 1 Rb	−0.770372
P41231	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.779206
P41231	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.779979
P41231	9	>= 2 C	−0.782912
P41231	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.788137
P41231	685	O=C-C-C-C-N	−0.791158
P41231	491	C-N:C-[#1]	−0.794716
P41231	294	C-Cl	−0.797418
P41231	618	C:C-C-C:C	−0.799414

P41231	650	O=C-N-C=O	−0.80849
P41231	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.809977
P41231	357	C(~C)(:C)(:N)	−0.819371
P41231	105	>= 1 Eu	−0.821827
P41231	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.825079
P41231	602	O=C-C-N-C	−0.842578
P41231	267	Li-O	−0.844689
P41231	656	C-C-N-C-C	−0.845986
P41231	6	>= 1 B	−0.856375
P41231	706	O=C-C-C-C-C(=O)-C	−0.860214
P41231	748	Sc1cc(Br)ccc1	−0.87269
P41231	342	C(~C)(~Cl)	−0.873876
P41231	461	O-C-C=N	−0.884499
P41231	762	Oc1c(S)cccc1	−0.885287
P41231	572	N:C:N:C	−0.889074
P41231	70	>= 1 Y	−0.891882
P41231	72	>= 1 Nb	−0.908444
P41231	667	C=C-C-O-[#1]	−0.910261
P41231	713	Cc1ccc(C)cc1	−0.912522
P41231	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.945455
P41231	330	C(~Br)(:C)	−0.951836
P41231	272	B-H	−0.960028
P41231	732	Clc1ccc(Br)cc1	−0.971163
P41231	363	C(~F)(~F)	−0.977323
P41231	603	C-C:C:C-C	−0.995003
P41231	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−1.007656
P41231	95	>= 1 Hg	−1.008506
P41231	50	>= 1 Mg	−1.011225
P41231	850	SC1CC(S)CC1	−1.013105
P41231	741	Oc1cc(S)ccc1	−1.020796
P41231	64	>= 1 Ge	−1.026057
P41231	261	>= 4 aromatic rings	−1.039238
P41231	757	Cc1c(S)cccc1	−1.047372
P41231	690	O-C-C-C-C-C-O	−1.047773
P41231	561	Cl-C-C=O	−1.068624
P41231	674	N-C-N-C:C	−1.072536
P41231	60	>= 1 Ni	−1.088517
P41231	519	N=C-N-C	−1.105948
P41231	471	S:C:C:C	−1.111715
P41231	411	P(~O)(~O)	−1.11228
P41231	749	Nc1cc(N)ccc1	−1.112613
P41231	384	C(:C)(:C)	−1.142023
P41231	554	Br-C-C-C	−1.147313
P41231	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−1.187156
P41231	437	C(-C)(-N)(=C)	−1.218026
P41231	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−1.236143
P41231	405	O(~C)(~C)	−1.267465
P41231	866	OC1C(O)CCC1	−1.273975

P41231	518	O=C-N-N	−1.345875
P41231	499	N-C:C:N	−1.35E+00
P41231	655	O-C-C-C:C	−1.377754
P41231	575	O-C-C:C-O	−1.38837
P41231	629	S-C:C:C-N	−1.418568
P41231	193	>= 3 saturated or aromatic carbon-only ring size 6	−1.428003
P41231	81	>= 1 Sb	−1.439525
P41231	628	C-N-C-C:C	−1.483497
P41231	422	N=N	−1.59121
P41231	695	O=C-C-C-C-C-N	−1.641888
P41231	472	C:N:C-C	−1.688602
P41231	284	C-C	−1.693065
P41231	350	C(~C)(~I)	−1.729962
P41231	227	>= 1 any ring size 8	−1.793995
P41231	91	>= 1 Os	−1.85402
P41231	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−2.043692
P41231	490	C-C-C=C	−2.066495
P41231	869	OC1C(Cl)CCC1	−2.087805
P41231	772	Nc1c(Br)cccc1	−2.334796

Fingerprints（continued)

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-1.039239905 2.40E-06
-1.044912686 -0.00246
-1.04394486 -3.83E-03
-1.068625226 7.30E-07
-1.077619718 0.0050834
-1.088519322 2.74E-06
-1.106863623 0.0009155
-1.116223296 0.0045079
-1.111524142 -0.000756
-1.110958834 -0.001654
-1.134697698 -0.007326
-1.14073664 -0.006576
-1.187159341 3.20E-06
-1.216435466 -0.00159
-1.23421964 -1.92E-03
-1.274389608 0.0069247
-1.276929069 0.0029536

-1.344808911 -0.001066
-1.368708045 0.014811
-1.38067633 0.0029227
-1.388477615 0.0001074
-1.413597675 -0.00497
-1.427667487 -3.36E-04
-1.439523416 -1.52E-06
-1.486472031 0.0029755
-1.593633573 0.0024234
-1.63957637 -0.002311
-1.685607003 -0.002995
-1.684731049 -0.008334
-1.72481174 -0.00515
-1.793995098 -4.00E-08
-1.854017974 -1.99E-06
-2.043691553 -4.26E-07
-2.068090543 0.0015951
-2.087803437 -1.34E-06
-2.334793722 -2.16E-06

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P30550	374	C(~H)(~H)(~H)	1.0358855
P30550	714	Cc1ccc(O)cc1	0.7452085
P30550	21	>= 8 O	0.6404842
P30550	694	O=C-C-C-C-C=O	0.5929253
P30550	150	>= 2 any ring size 5	0.5834642
P30550	821	CC1C(N)CCCC1	0.5201886
P30550	423	N=O	0.5162437
P30550	526	Cl-C:C-Cl	0.4894873
P30550	380	C(~O)(~O)	0.4652741
P30550	850	SC1CC(S)CC1	0.4118485
P30550	461	O-C-C=N	0.3979876
P30550	157	>= 3 any ring size 5	0.3897533
P30550	823	CC1C(Br)CCCC1	0.3663623
P30550	547	N-C:C-N	0.3241073
P30550	48	>= 4 I	0.3170422
P30550	639	O-C-C-C-O	0.3051618
P30550	579	O=C-C-C-C	0.3015035
P30550	342	C(~C)(~Cl)	0.2959864
P30550	519	N=C-N-C	0.2950817
P30550	817	BrC1CC(Br)CCC1	0.2845594
P30550	875	NC1C(N)CCC1	0.2671544
P30550	49	>= 1 Be	0.2664193
P30550	280	B-S	0.2658716
P30550	654	N-C-N-C-C	0.2656941
P30550	241	>= 1 any ring size 9	0.2644378
P30550	350	C(~C)(~I)	0.2632373
P30550	302	N-F	0.2632321
P30550	737	Cc1cc(N)ccc1	0.2607495
P30550	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.2567853
P30550	129	>= 1 any ring size 4	0.2525912
P30550	452	C(-O)(=O)	0.2448028
P30550	791	NC1CCC(N)CC1	0.2438762
P30550	297	C-Br	0.2433673
P30550	97	>= 1 Pb	0.2416057
P30550	743	Oc1cc(Cl)ccc1	0.241246
P30550	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.2398364
P30550	803	OC1CC(O)CCC1	0.2382128
P30550	760	Cc1c(Br)cccc1	0.2322414
P30550	713	Cc1ccc(C)cc1	0.2320676
P30550	727	Sc1ccc(Br)cc1	0.2252343
P30550	281	B-Cl	0.2237495
P30550	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.2230249
P30550	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.2118692
P30550	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.2106259
P30550	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.2031303
P30550	877	NC1C(Br)CCC1	0.2012537

P30550	179	>= 1 saturated or aromatic carbon-only ring size 6	0.1992155
P30550	688	C-C-C-C-C-C-C	0.1925629
P30550	583	Cl-C:C-O-C	0.1913521
P30550	456	P(-O)(=O)	0.1838798
P30550	371	C(~H)(:C)(:C)	0.1818178
P30550	27	>= 2 Na	0.1813779
P30550	405	O(~C)(~C)	0.1793027
P30550	588	O=C-C-C=O	0.1786684
P30550	11	>= 8 C	0.1775213
P30550	578	C-C:C-C:C	0.1751509
P30550	520	C=C-C:C	0.1723005
P30550	347	C(~C)(~H)(~O)(~O)	0.1714829
P30550	402	N(~O)(:O)	0.1702038
P30550	863	CC1C(N)CCC1	0.169548
P30550	442	C(-C)(=N)	0.1661997
P30550	735	Cc1cc(O)ccc1	0.1653993
P30550	802	CC1CC(Br)CCC1	0.1652802
P30550	564	C=C-C=C	0.1630073
P30550	816	ClC1CC(Br)CCC1	0.1611909
P30550	353	C(~C)(~S)	0.1589092
P30550	272	B-H	0.1570796
P30550	779	CC1CCC(N)CC1	0.1553746
P30550	559	O-C-N-[#1]	0.1547727
P30550	482	C:N-C:C	0.153866
P30550	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.1538062
P30550	385	C(:C)(:C)(:C)	0.1528277
P30550	1	>= 8 H	0.1511642
P30550	284	C-C	0.1503726
P30550	429	C(#N)(-C)	0.1447567
P30550	712	C-C(C)-C(C)-C	0.1444889
P30550	50	>= 1 Mg	0.1438832
P30550	591	Cl-C-C-C-C	0.1397889
P30550	716	Cc1ccc(N)cc1	0.1386049
P30550	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.135373
P30550	646	O=C-N-C-[#1]	0.1303495
P30550	76	>= 1 Pd	0.1295076
P30550	40	>= 8 Cl	0.128857
P30550	6	>= 1 B	0.1261253
P30550	593	N-C-C-C-N	0.1249048
P30550	255	>= 1 aromatic ring	0.1223965
P30550	759	Cc1c(Cl)cccc1	0.1208454
P30550	24	>= 2 F	0.1202497
P30550	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.1144701
P30550	527	C:C:N-[#1]	0.1139073
P30550	514	O-N-C-C	0.1138304
P30550	420	C=O	0.1133928
P30550	671	O=C-C=C-C	0.113219
P30550	266	Li-C	0.1128686

P30550	293	C-S	0.112395
P30550	108	>= 1 Dy	0.1118986
P30550	568	N#C-C-C	0.1082021
P30550	16	>= 4 N	0.1075383
P30550	348	C(~C)(~H)(~P)	0.10558
P30550	477	N-N-C:C	0.0957101
P30550	13	>= 32 C	0.0955568
P30550	828	OC1C(Br)CCCC1	0.0942241
P30550	775	Brc1c(Br)cccc1	0.09321
P30550	783	OC1CCC(S)CC1	0.091735
P30550	454	N(-C)(=O)	0.0909252
P30550	700	O-C-C-C-C-C-O-C	0.0901866
P30550	301	N-O	0.0892037
P30550	758	Cc1c(N)cccc1	0.0887393
P30550	409	O(:C)(:C)	0.0880586
P30550	249	>= 1 saturated or aromatic carbon-only ring size 10	0.0880175
P30550	417	C#C	0.0872028
P30550	730	Nc1ccc(Br)cc1	0.0866418
P30550	651	O-C:C:C-C	0.0865553
P30550	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.085677
P30550	476	C-O-C=C	0.0856211
P30550	62	>= 1 Zn	0.0849932
P30550	525	[As]-C:C-[#1]	0.0840662
P30550	337	C(~C)(~C)(~C)(~O)	0.0840302
P30550	104	>= 1 Sm	0.0840027
P30550	308	O-H	0.0837536
P30550	35	>= 4 S	0.0832311
P30550	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.0830455
P30550	17	>= 8 N	0.0821243
P30550	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0816778
P30550	101	>= 1 Pr	0.0814553
P30550	739	Cc1cc(Br)ccc1	0.0813513
P30550	69	>= 1 Sr	0.0790593
P30550	824	OC1C(O)CCCC1	0.0786934
P30550	563	O-C-O-C	0.0776321
P30550	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.0765637
P30550	475	S-C=N-C	0.0759181
P30550	287	C-F	0.0758646
P30550	778	CC1CCC(S)CC1	0.0751421
P30550	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0746152
P30550	55	>= 1 V	0.0744757
P30550	560	N-C-N-C	0.0744457
P30550	699	O-C-C-C-C-C(C)-C	0.0737183
P30550	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0730827
P30550	869	OC1C(Cl)CCC1	0.0715168
P30550	499	N-C:C:N	0.0699617
P30550	554	Br-C-C-C	0.0687291
P30550	383	C(~S)(:C)	0.0683799

P30550	763	Oc1c(N)cccc1	0.0677376
P30550	590	C-C:C-O-[#1]	0.0665987
P30550	92	>= 1 Ir	0.065764
P30550	731	Clc1ccc(Cl)cc1	0.064849
P30550	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.0594973
P30550	23	>= 1 F	0.0589798
P30550	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.0580471
P30550	325	As-H	0.0578279
P30550	376	C(~N)(:C)	0.0564968
P30550	582	C-C-C-C-C	0.0561174
P30550	657	C-N-C:C-C	0.0541006
P30550	845	OC1CC(O)CC1	0.0532425
P30550	416	C=C	0.052537
P30550	733	Brc1ccc(Br)cc1	0.0515915
P30550	507	C-C-S-C	0.0515163
P30550	542	O-C:C-[#1]	0.0511925
P30550	626	C-O-C:C-C	0.0506605
P30550	535	O=C-C-C	0.0496064
P30550	534	S-C:C-O	0.047596
P30550	749	Nc1cc(N)ccc1	0.0472247
P30550	792	NC1CCC(Cl)CC1	0.0472141
P30550	592	N-C-C-C-C	0.0468851
P30550	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.0453909
P30550	465	O=S-C-C	0.0443785
P30550	728	Nc1ccc(N)cc1	0.043386
P30550	331	C(~Br)(:N)	0.0432301
P30550	732	Clc1ccc(Br)cc1	0.0430553
P30550	789	SC1CCC(Cl)CC1	0.0430074
P30550	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0422869
P30550	843	CC1CC(Cl)CC1	0.0422364
P30550	687	O=C-C-C-C=O	0.0421888
P30550	274	B-C	0.0420921
P30550	589	C-C:C-O-C	0.0413811
P30550	12	>= 16 C	0.0400749
P30550	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.039963
P30550	360	C(~Cl)(~Cl)	0.0396467
P30550	451	C(-N)(=O)	0.0393404
P30550	695	O=C-C-C-C-C-N	0.0392721
P30550	116	>= 1 saturated or aromatic carbon-only ring size 3	0.0391175
P30550	814	NC1CC(Br)CCC1	0.038959
P30550	426	P=P	0.0388654
P30550	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.0386483
P30550	318	Al-H	0.0385323
P30550	581	O=C-C-C-O	0.0361868
P30550	769	Sc1c(Br)cccc1	0.0360672
P30550	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0356748
P30550	22	>= 16 O	0.0356696
P30550	673	O=C-C=C-N	0.0353625

P30550	459	S(=O)(=O)	0.0348659
P30550	615	N-C-C-O-C	0.0342529
P30550	375	C(~N)(~N)	0.03378
P30550	711	C-C(C)(C)-C-C	0.0337196
P30550	736	Cc1cc(S)ccc1	0.0335019
P30550	536	O=C-C-N	0.0323541
P30550	508	S=C-N-C	0.0319314
P30550	788	SC1CCC(N)CC1	0.0318916
P30550	605	O=C-C-O-C	0.0318433
P30550	171	>= 5 any ring size 5	0.0315705
P30550	530	N:C-C:C	0.0311697
P30550	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.0310924
P30550	481	O-S-C:C	0.0304246
P30550	424	N=P	0.030334
P30550	322	Si-Cl	0.0302884
P30550	781	CC1CCC(Br)CC1	0.0302086
P30550	804	OC1CC(S)CCC1	0.0290444
P30550	178	>= 1 any ring size 6	0.0287229
P30550	528	[#1]-N-C-[#1]	0.0286097
P30550	852	SC1CC(Cl)CC1	0.028537
P30550	771	Nc1c(Cl)cccc1	0.0284177
P30550	861	CC1C(O)CCC1	0.0278438
P30550	78	>= 1 Cd	0.0271457
P30550	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0269207
P30550	682	O-C-C-C-C-N	0.026666
P30550	777	CC1CCC(O)CC1	0.025895
P30550	53	>= 1 Sc	0.0254216
P30550	706	O=C-C-C-C-C(=O)-C	0.0250266
P30550	496	N:N-C-[#1]	0.025019
P30550	311	O-Na	0.0250163
P30550	391	N(~C)(~C)(~C)	0.0246452
P30550	111	>= 1 Tm	0.0236396
P30550	665	N-C:C-C-C	0.0236289
P30550	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0235858
P30550	422	N=N	0.0235458
P30550	20	>= 4 O	0.023458
P30550	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0225866
P30550	372	C(~H)(:C)(:N)	0.0216426
P30550	349	C(~C)(~H)(~S)	0.021286
P30550	74	>= 1 Ru	0.0210858
P30550	720	Oc1ccc(S)cc1	0.0209539
P30550	344	C(~C)(~H)	0.0208396
P30550	73	>= 1 Mo	0.0206348
P30550	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.0200392
P30550	685	O=C-C-C-C-N	0.0196283
P30550	421	C=S	0.019223
P30550	485	N:C:C:N	0.0191547
P30550	785	OC1CCC(Cl)CC1	0.0187942

P30550	879	ClC1C(Br)CCC1	0.0175662
P30550	799	CC1CC(S)CCC1	0.0174031
P30550	304	N-P	0.0173853
P30550	725	Sc1ccc(N)cc1	0.0172968
P30550	480	C:S:C-C	0.0171124
P30550	31	>= 2 P	0.0168516
P30550	818	CC1C(C)CCCC1	0.0164605
P30550	107	>= 1 Tb	0.0160785
P30550	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.0157546
P30550	334	C(~C)(~C)(~C)(~C)	0.0154902
P30550	614	C-C-O-C-C	0.0153912
P30550	562	Br-C-C=O	0.0153869
P30550	85	>= 1 Ba	0.0153486
P30550	784	OC1CCC(N)CC1	0.0153449
P30550	303	N-Si	0.0153034
P30550	448	C(-H)(=O)	0.01521
P30550	309	O-O	0.0151768
P30550	715	Cc1ccc(S)cc1	0.0150431
P30550	871	SC1C(S)CCC1	0.0150411
P30550	513	S:C:C-[#1]	0.0149967
P30550	543	O-C:C-N	0.0145315
P30550	645	O=C-N-C-C	0.0140785
P30550	300	N-N	0.0139664
P30550	66	>= 1 Se	0.0138615
P30550	876	NC1C(Cl)CC1	0.0136473
P30550	584	C:C-C=C-C	0.0135472
P30550	339	C(~C)(~C)(~H)(~O)	0.0135125
P30550	298	C-I	0.0135101
P30550	494	O=C-C:N	0.0133966
P30550	392	N(~C)(~C)(~H)	0.0132981
P30550	486	N-C:N:N	0.0127288
P30550	538	N=C-C-C	0.0125987
P30550	483	N-S-C:C	0.0124011
P30550	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0120589
P30550	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0119737
P30550	444	C(-Cl)(=O)	0.0119425
P30550	815	ClC1CC(Cl)CCC1	0.0118934
P30550	600	N-C:C:C-C	0.0116937
P30550	495	C-N-C:C	0.0114826
P30550	541	O-C:C-C	0.0113011
P30550	546	N-C:C-[#1]	0.0112706
P30550	696	C-C-C-C-C-C-C-C	0.0109545
P30550	773	Clc1c(Cl)cccc1	0.0107422
P30550	313	O-Si	0.0106446
P30550	504	N:C:N-C	0.0105151
P30550	319	Al-Cl	0.0103312
P30550	561	Cl-C-C=O	0.0102685
P30550	438	C(-C)(-N)(=N)	0.0102469

P30550	440	C(-C)(-O)(=O)	0.0101912
P30550	2	>= 16 H	0.0101369
P30550	841	CC1CC(S)CC1	0.0098675
P30550	220	>= 2 any ring size 7	0.0096892
P30550	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.009601
P30550	0	>= 4 H	0.0095717
P30550	722	Oc1ccc(Cl)cc1	0.0094933
P30550	806	OC1CC(Cl)CCC1	0.0094218
P30550	618	C:C-C-C:C	0.009232
P30550	701	O-C-C-C-C-C(O)-C	0.0089118
P30550	761	Oc1c(O)cccc1	0.0088221
P30550	363	C(~F)(~F)	0.0086373
P30550	367	C(~H)(~O)(~O)	0.0085345
P30550	638	O-C-C-C-N	0.0083397
P30550	656	C-C-N-C-C	0.008186
P30550	436	C(-C)(-H)(=O)	0.0080981
P30550	723	Oc1ccc(Br)cc1	0.0080349
P30550	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.007996
P30550	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0079614
P30550	443	C(-C)(=O)	0.0076885
P30550	643	[#1]-C-C-N-[#1]	0.0076157
P30550	336	C(~C)(~C)(~C)(~N)	0.0073075
P30550	33	>= 1 S	0.0071073
P30550	279	B-P	0.0069276
P30550	658	C-C-S-C-C	0.0068698
P30550	316	F-P	0.0067427
P30550	386	C(:C)(:C)(:N)	0.0065703
P30550	636	C-N-C-N-C	0.0061369
P30550	437	C(-C)(-N)(=C)	0.0061337
P30550	434	C(-C)(-H)(=C)	0.0060185
P30550	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.0059822
P30550	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0055285
P30550	846	OC1CC(S)CC1	0.0054837
P30550	729	Nc1ccc(Cl)cc1	0.0054704
P30550	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0054271
P30550	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.005346
P30550	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0053097
P30550	719	Oc1ccc(O)cc1	0.0052292
P30550	827	OC1C(Cl)CCCC1	0.005208
P30550	79	>= 1 In	0.0051927
P30550	382	C(~O)(:C)(:C)	0.0051738
P30550	115	>= 1 any ring size 3	0.0051321
P30550	259	>= 3 aromatic rings	0.0051233
P30550	446	C(-H)(=C)	0.0049572
P30550	484	N-C:N:C	0.0047439
P30550	755	Cc1c(C)cccc1	0.0047371
P30550	512	C-[As]-O-[#1]	0.0046368
P30550	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.0045603

P30550	317	F-S	0.0044135
P30550	404	N(:C)(:C)(:C)	0.0044058
P30550	44	>= 2 Br	0.0043109
P30550	594	C-O-C-C=C	0.004251
P30550	813	NC1CC(Cl)CCC1	0.0041077
P30550	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.0039884
P30550	457	S(-C)(=O)	0.0039374
P30550	631	O-C:C-O-[#1]	0.0037854
P30550	286	C-O	0.0036529
P30550	261	>= 4 aromatic rings	0.0035683
P30550	335	C(~C)(~C)(~C)(~H)	0.0035538
P30550	414	S(~C)(~O)	0.0035273
P30550	575	O-C-C:C-O	0.003206
P30550	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0031265
P30550	458	S(-O)(=O)	0.0029931
P30550	518	O=C-N-N	0.0029807
P30550	235	>= 2 saturated or aromatic carbon-only ring size 8	0.0029043
P30550	859	BrC1CC(Br)CC1	0.0028891
P30550	844	CC1CC(Br)CC1	0.0028356
P30550	637	O-C-C-C-C	0.0028316
P30550	419	C#N	0.0028055
P30550	835	NC1C(Br)CCCC1	0.0026567
P30550	398	N(~H)(~N)	0.002599
P30550	63	>= 1 Ga	0.0025943
P30550	395	N(~C)(~O)	0.0025154
P30550	610	C-O-C-O-C	0.0024986
P30550	839	CC1CC(C)CC1	0.0024043
P30550	726	Sc1ccc(Cl)cc1	0.0023943
P30550	653	O-C:C:C-O	0.0023473
P30550	609	Cl-C-C-N-C	0.0023247
P30550	80	>= 1 Sn	0.0022842
P30550	271	Li-Cl	0.0022328
P30550	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0020471
P30550	323	P-H	0.0019089
P30550	798	CC1CC(O)CCC1	0.0018316
P30550	98	>= 1 Bi	0.001636
P30550	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.0016263
P30550	820	CC1C(S)CCCC1	0.0015232
P30550	327	C(~Br)(~C)	0.0014848
P30550	867	OC1C(S)CCC1	0.0014631
P30550	338	C(~C)(~C)(~H)(~N)	0.0011743
P30550	754	Brc1cc(Br)ccc1	0.0011571
P30550	683	N-C-C-C-C-C	0.0010958
P30550	874	SC1C(Br)CCC1	0.0010762
P30550	690	O-C-C-C-C-C-O	0.0010563
P30550	721	Oc1ccc(N)cc1	0.0010473
P30550	268	Li-F	0.0010045
P30550	373	C(~H)(:N)	0.0009757

P30550	745	Sc1cc(S)ccc1	0.0009679
P30550	213	>= 1 any ring size 7	0.0009585
P30550	321	Si-Si	0.0009174
P30550	670	Br-C:C:C-C	0.0008364
P30550	328	C(~Br)(~C)(~C)	0.0008354
P30550	87	>= 1 Hf	0.0008267
P30550	330	C(~Br)(:C)	0.0008249
P30550	71	>= 1 Zr	0.0008172
P30550	509	Br-C:C-C	0.0008117
P30550	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0007957
P30550	740	Oc1cc(O)ccc1	0.0006536
P30550	4	>= 1 Li	0.0006068
P30550	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.000539
P30550	65	>= 1 As	0.0004764
P30550	137	>= 2 saturated or aromatic carbon-only ring size 4	0.000282
P30550	123	>= 2 saturated or aromatic carbon-only ring size 3	0.0002504
P30550	39	>= 4 Cl	0.0002471
P30550	505	Cl-C:C-O	0.0001293
P30550	822	CC1C(Cl)CCCC1	8.29E-05
P30550	750	Nc1cc(Cl)ccc1	4.16E-05
P30550	361	C(~Cl)(~H)	3.47E-05
P30550	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	3.36E-05
P30550	864	CC1C(Cl)CCC1	2.95E-05
P30550	5	>= 2 Li	2.29E-05
P30550	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	2.17E-05
P30550	257	>= 2 aromatic rings	1.87E-05
P30550	744	Oc1cc(Br)ccc1	1.59E-05
P30550	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	1.48E-05
P30550	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	1.44E-05
P30550	795	ClC1CCC(Br)CC1	1.42E-05
P30550	3	>= 32 H	1.38E-05
P30550	786	OC1CCC(Br)CC1	9.58E-06
P30550	275	B-N	6.92E-06
P30550	122	>= 2 any ring size 3	6.81E-06
P30550	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	5.75E-06
P30550	258	>= 2 hetero-aromatic rings	5.06E-06
P30550	30	>= 1 P	5.03E-06
P30550	463	N:C-S-[#1]	3.39E-06
P30550	47	>= 2 I	3.13E-06
P30550	200	>= 4 saturated or aromatic carbon-only ring size 6	3.04E-06
P30550	825	OC1C(S)CCCC1	1.80E-06
P30550	427	C(#C)(-C)	-1.02E-07
P30550	102	>= 1 Nd	-4.82E-07
P30550	158	>= 3 saturated or aromatic carbon-only ring size 5	-6.72E-07
P30550	64	>= 1 Ge	-3.94E-06
P30550	854	NC1CC(N)CC1	-4.05E-06
P30550	796	BrC1CCC(Br)CC1	-4.40E-06
P30550	762	Oc1c(S)cccc1	-5.23E-06

P30550	748	Sc1cc(Br)ccc1	-5.73E-06
P30550	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	-7.48E-06
P30550	29	>= 2 Si	-1.01E-05
P30550	106	>= 1 Gd	-1.04E-05
P30550	26	>= 1 Na	-1.04E-05
P30550	870	OC1C(Br)CCC1	-1.15E-05
P30550	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	-1.16E-05
P30550	54	>= 1 Ti	-1.19E-05
P30550	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	-1.26E-05
P30550	82	>= 1 Te	-1.45E-05
P30550	110	>= 1 Er	-1.46E-05
P30550	77	>= 1 Ag	-1.61E-05
P30550	479	S-C-S-C	-1.66E-05
P30550	717	Cc1ccc(Cl)cc1	-1.69E-05
P30550	774	Clc1c(Br)cccc1	-1.70E-05
P30550	7	>= 2 B	-1.82E-05
P30550	61	>= 1 Cu	-2.22E-05
P30550	625	O=C-C:C-O	-2.87E-05
P30550	873	SC1C(Cl)CCC1	-3.05E-05
P30550	627	O=[As]-C:C:C	-4.34E-05
P30550	277	B-F	-8.15E-05
P30550	93	>= 1 Pt	-8.99E-05
P30550	425	P=O	-0.00018
P30550	296	C-Se	-0.000186
P30550	267	Li-O	-0.000237
P30550	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	-0.000288
P30550	606	O-C:C-C-C	-0.000328
P30550	312	O-Al	-0.000333
P30550	764	Oc1c(Cl)cccc1	-0.000374
P30550	99	>= 1 La	-0.000387
P30550	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	-0.000426
P30550	450	C(-N)(=N)	-0.000577
P30550	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	-0.000602
P30550	572	N:C:N:C	-0.000704
P30550	488	N-C=N-[#1]	-0.000707
P30550	604	C-O-C-C:C	-0.000748
P30550	260	>= 3 hetero-aromatic rings	-0.00075
P30550	624	O=C-C:C-N	-0.000805
P30550	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	-0.000916
P30550	262	>= 4 hetero-aromatic rings	-0.000952
P30550	675	Br-C-C-C:C	-0.001012
P30550	462	O-C-C=O	-0.001287
P30550	278	B-Si	-0.001434
P30550	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-0.0015
P30550	41	>= 1 K	-0.001663
P30550	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.00167
P30550	766	Sc1c(S)cccc1	-0.001694
P30550	326	As-As	-0.001921

P30550	500	C-S-C:C	−0.00203
P30550	746	Sc1cc(N)ccc1	−0.002133
P30550	91	>= 1 Os	−0.002227
P30550	805	OC1CC(N)CCC1	−0.002252
P30550	599	[#1]-C-C=C-[#1]	−0.002376
P30550	644	C-C=N-N-C	−0.002523
P30550	199	>= 4 any ring size 6	−0.002557
P30550	368	C(~H)(~S)	−0.002728
P30550	498	O-C=C-C	−0.002808
P30550	164	>= 4 any ring size 5	−0.002958
P30550	523	N:C:C-C	−0.003141
P30550	630	O-C:C-O-C	−0.003212
P30550	295	C-As	−0.003529
P30550	641	O-C-C-C=C	−0.003542
P30550	396	N(~C)(:C)	−0.003665
P30550	52	>= 1 Ca	−0.003699
P30550	577	C:C-N-C:C	−0.003887
P30550	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.003887
P30550	672	O=C-C=C-[#1]	−0.004048
P30550	394	N(~C)(~H)(~N)	−0.004063
P30550	550	Cl-C-C-C	−0.004091
P30550	598	Cl-C:C:C-C	−0.004093
P30550	642	O-C-C-C=O	−0.00411
P30550	377	C(~N)(:C)(:C)	−0.00412
P30550	576	N=C-C:C-[#1]	−0.004124
P30550	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.004146
P30550	521	C:N-C-[#1]	−0.004187
P30550	143	>= 1 any ring size 5	−0.004445
P30550	471	S:C:C:C	−0.004549
P30550	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.004971
P30550	472	C:N:C-C	−0.005128
P30550	352	C(~C)(~O)	−0.005221
P30550	829	SC1C(S)CCCC1	−0.005368
P30550	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.005437
P30550	640	C=C-C-C-C	−0.005544
P30550	780	CC1CCC(Cl)CC1	−0.005582
P30550	529	Cl-C-C-Cl	−0.005606
P30550	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.00564
P30550	68	>= 1 Rb	−0.005674
P30550	470	C:C-C=C	−0.005821
P30550	67	>= 1 Kr	−0.005866
P30550	467	C=N-N-C	−0.005977
P30550	497	O-C:C:N	−0.00623
P30550	265	Li-B	−0.006236
P30550	621	N-C:C:C:N	−0.006294
P30550	502	N-C=C-[#1]	−0.006462
P30550	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−0.006535
P30550	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.006936

P30550	677	C-C=C-C:C	−0.006937
P30550	418	C=N	−0.006966
P30550	306	N-Cl	−0.007062
P30550	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.00709
P30550	136	>= 2 any ring size 4	−0.007306
P30550	664	C-C=C-C=C	−0.007351
P30550	842	CC1CC(N)CC1	−0.007387
P30550	345	C(~C)(~H)(~N)	−0.0075
P30550	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.007923
P30550	676	N#C-C-C-C	−0.008009
P30550	607	N-C-C-C:C	−0.008055
P30550	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.008211
P30550	770	Nc1c(N)cccc1	−0.008237
P30550	613	C-N-C-C-C	−0.008253
P30550	674	N-C-N-C:C	−0.008411
P30550	751	Nc1cc(Br)ccc1	−0.008413
P30550	648	O=N-C:C-N	−0.008586
P30550	473	S-C:N:C	−0.008688
P30550	411	P(~O)(~O)	−0.008709
P30550	285	C-N	−0.008841
P30550	10	>= 4 C	−0.008853
P30550	14	>= 1 N	−0.008853
P30550	439	C(-C)(-N)(=O)	−0.008982
P30550	608	C-C-C-C:C	−0.008993
P30550	469	S-S-C:C	−0.009061
P30550	362	C(~Cl)(:C)	−0.009064
P30550	390	N(~C)(~C)	−0.009108
P30550	840	CC1CC(O)CC1	−0.009341
P30550	45	>= 4 Br	−0.009493
P30550	595	C:C-C-C-C	−0.009601
P30550	227	>= 1 any ring size 8	−0.009749
P30550	105	>= 1 Eu	−0.009839
P30550	466	N#C-C=C	−0.00986
P30550	574	O-C-C:C-C	−0.00989
P30550	612	N-C-O-C-C	−0.010009
P30550	678	C-C-C=C-C	−0.010185
P30550	629	S-C:C:C-N	−0.010213
P30550	793	NC1CCC(Br)CC1	−0.010347
P30550	32	>= 4 P	−0.010521
P30550	403	N(:C)(:C)	−0.010662
P30550	449	C(-N)(=C)	−0.011004
P30550	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.011015
P30550	492	N-C:O:C	−0.011452
P30550	659	O-C-C-N-C	−0.011548
P30550	765	Oc1c(Br)cccc1	−0.011708
P30550	724	Sc1ccc(S)cc1	−0.011819
P30550	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.01183
P30550	633	N-C-C:C-C	−0.011872

P30550	556	C=C-C-C	−0.012074
P30550	393	N(~C)(~H)	−0.012162
P30550	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.012197
P30550	812	NC1CC(N)CCC1	−0.01226
P30550	652	O-C:C:C-N	−0.012454
P30550	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.013043
P30550	747	Sc1cc(Cl)ccc1	−0.013048
P30550	38	>= 2 Cl	−0.013312
P30550	333	C(~C)(~C)(~C)	−0.013443
P30550	647	O=C-N-C-N	−0.013692
P30550	603	C-C:C:C-C	−0.013709
P30550	359	C(~C)(:N)(:N)	−0.014036
P30550	587	N-C:C-O-[#1]	−0.014055
P30550	628	C-N-C-C:C	−0.014095
P30550	666	C=C-C-O-C	−0.014125
P30550	290	C-Al	−0.014146
P30550	602	O=C-C-N-C	−0.01421
P30550	433	C(-C)(-Cl)(=O)	−0.014248
P30550	619	O-C-C=C-C	−0.014316
P30550	667	C=C-C-O-[#1]	−0.014354
P30550	555	N=C-C=C	−0.014522
P30550	620	C:C-O-C-C	−0.014536
P30550	57	>= 1 Mn	−0.014832
P30550	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.014985
P30550	109	>= 1 Ho	−0.015013
P30550	551	Cl-C-C-O	−0.0152
P30550	738	Cc1cc(Cl)ccc1	−0.01523
P30550	206	>= 5 any ring size 6	−0.015485
P30550	782	OC1CCC(O)CC1	−0.015994
P30550	539	N=C-C-[#1]	−0.016037
P30550	378	C(~N)(:C)(:N)	−0.016472
P30550	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.016689
P30550	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.016912
P30550	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.017094
P30550	548	O-C-C:C	−0.017244
P30550	487	N-C=N-C	−0.017505
P30550	332	C(~C)(~C)	−0.017683
P30550	838	BrC1C(Br)CCCC1	−0.017978
P30550	501	Cl-C:C-C	−0.01824
P30550	468	O=S-C-N	−0.018378
P30550	872	SC1C(N)CCC1	−0.018533
P30550	611	N-C-C-N-C	−0.018635
P30550	460	C-C-C#C	−0.018814
P30550	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.018967
P30550	399	N(~H)(:C)	−0.019131
P30550	868	OC1C(N)CCC1	−0.019156
P30550	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.019281
P30550	8	>= 4 B	−0.019544

P30550	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.019898
P30550	809	SC1CC(N)CCC1	−0.020222
P30550	549	N-C-C:C	−0.020482
P30550	103	>= 1 Pm	−0.020643
P30550	689	O-C-C-C-C-C-C	−0.021258
P30550	288	C-Na	−0.021309
P30550	865	CC1C(Br)CCC1	−0.021374
P30550	72	>= 1 Nb	−0.021613
P30550	517	N-N-C-N	−0.021853
P30550	532	S-C:C-[#1]	−0.022054
P30550	708	C-C(C)-C-C	−0.022185
P30550	571	[#1]-C-O-[#1]	−0.022229
P30550	354	C(~C)(~Si)	−0.022258
P30550	282	B-Br	−0.022491
P30550	474	S:C:C:N	−0.022544
P30550	632	C-C-O-C:C	−0.022755
P30550	668	C-C:C-C-C	−0.023401
P30550	680	O-C-C-C-C-C	−0.0235
P30550	340	C(~C)(~C)(~N)	−0.023587
P30550	42	>= 2 K	−0.02369
P30550	703	O-C-C-C-C-C(N)-C	−0.02377
P30550	831	SC1C(Cl)CCCC1	−0.024095
P30550	851	SC1CC(N)CC1	−0.02434
P30550	684	O=C-C-C-C-C	−0.024526
P30550	59	>= 1 Co	−0.024646
P30550	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.024741
P30550	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.024891
P30550	346	C(~C)(~H)(~O)	−0.025111
P30550	464	N-C-C=C	−0.02517
P30550	692	O=C-C-C-C-C-C	−0.025292
P30550	787	SC1CCC(S)CC1	−0.025643
P30550	320	Si-H	−0.02606
P30550	601	N-C:C:C-N	−0.026742
P30550	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.027051
P30550	649	O=N-C:C-O	−0.027135
P30550	185	>= 2 any ring size 6	−0.027216
P30550	113	>= 1 Tc	−0.027364
P30550	734	Cc1cc(C)ccc1	−0.027673
P30550	807	OC1CC(Br)CCC1	−0.028181
P30550	291	C-Si	−0.02824
P30550	860	CC1C(C)CCC1	−0.028309
P30550	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.028435
P30550	397	N(~C)(:C)(:C)	−0.028499
P30550	294	C-Cl	−0.02887
P30550	83	>= 1 Xe	−0.02909
P30550	833	NC1C(N)CCCC1	−0.030285
P30550	28	>= 1 Si	−0.030537
P30550	289	C-Mg	−0.031031

P30550	545	N-C:C-C	−0.031375
P30550	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.032376
P30550	36	>= 8 S	−0.033846
P30550	533	S-C:C-N	−0.034169
P30550	366	C(~H)(~O)	−0.034192
P30550	553	O=C-C=C	−0.034565
P30550	94	>= 1 Au	−0.034627
P30550	88	>= 1 Ta	−0.034748
P30550	616	C:C:N:N:C	−0.03558
P30550	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.035791
P30550	314	O-P	−0.036019
P30550	663	O-C-C-O-[#1]	−0.036071
P30550	356	C(~C)(:C)(:C)	−0.036124
P30550	704	O=C-C-C-C-C-C-C	−0.037695
P30550	767	Sc1c(N)cccc1	−0.03785
P30550	768	Sc1c(Cl)cccc1	−0.038004
P30550	801	CC1CC(Cl)CCC1	−0.038314
P30550	401	N(~O)(~O)	−0.038884
P30550	811	SC1CC(Br)CCC1	−0.039525
P30550	75	>= 1 Rh	−0.040021
P30550	56	>= 1 Cr	−0.040176
P30550	635	N-N-C-N-[#1]	−0.04035
P30550	310	O-Mg	−0.041222
P30550	515	N-N-C-C	−0.041357
P30550	407	O(~C)(~P)	−0.041925
P30550	693	O=C-C-C-C-C-O	−0.041937
P30550	849	OC1CC(Br)CC1	−0.042576
P30550	753	Clc1cc(Br)ccc1	−0.042942
P30550	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.044077
P30550	19	>= 2 O	−0.046749
P30550	586	C-S-C-C-C	−0.04678
P30550	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.046811
P30550	431	C(-C)(-C)(=N)	−0.046839
P30550	718	Cc1ccc(Br)cc1	−0.04822
P30550	413	S(~C)(~H)	−0.048279
P30550	634	C-C-C:C-C	−0.04914
P30550	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.049681
P30550	836	ClC1C(Cl)CCCC1	−0.049956
P30550	70	>= 1 Y	−0.050164
P30550	866	OC1C(O)CCC1	−0.050245
P30550	307	N-Br	−0.05165
P30550	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.052205
P30550	264	Li-Li	−0.054391
P30550	445	C(-H)(-N)(=C)	−0.055363
P30550	837	ClC1C(Br)CCCC1	−0.056075
P30550	453	N(-C)(=C)	−0.056248
P30550	270	Li-S	−0.056405
P30550	567	O-C-C-O	−0.058775

P30550	566	O-C-C-N	−0.05948
P30550	757	Cc1c(S)cccc1	−0.059941
P30550	478	S-C=N-[#1]	−0.060095
P30550	329	C(~Br)(~H)	−0.06059
P30550	51	>= 1 Al	−0.061225
P30550	379	C(~N)(:N)	−0.061307
P30550	552	C:C-C:C	−0.061531
P30550	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.062967
P30550	89	>= 1 W	−0.063228
P30550	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.064196
P30550	596	N=C-N-C-C	−0.066017
P30550	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.067673
P30550	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.06768
P30550	511	S=C-N-[#1]	−0.068415
P30550	655	O-C-C-C:C	−0.071799
P30550	364	C(~F)(:C)	−0.072357
P30550	248	>= 1 any ring size 10	−0.073304
P30550	292	C-P	−0.073742
P30550	569	N-C-C-N	−0.074002
P30550	384	C(:C)(:C)	−0.074208
P30550	558	O=N-C:C	−0.075473
P30550	370	C(~H)(:C)	−0.076352
P30550	269	Li-P	−0.078578
P30550	585	C-C:C-N-C	−0.079033
P30550	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.079293
P30550	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.079603
P30550	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.079952
P30550	276	B-O	−0.080362
P30550	381	C(~O)(:C)	−0.080676
P30550	81	>= 1 Sb	−0.080719
P30550	341	C(~C)(~C)(~O)	−0.080937
P30550	455	N(-O)(=O)	−0.081361
P30550	524	C-C=C-C	−0.081749
P30550	34	>= 2 S	−0.083058
P30550	365	C(~H)(~N)	−0.084102
P30550	95	>= 1 Hg	−0.085047
P30550	669	Cl-C:C-C=O	−0.086071
P30550	880	BrC1C(Br)CCC1	−0.086259
P30550	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.086272
P30550	100	>= 1 Ce	−0.086552
P30550	858	ClC1CC(Br)CC1	−0.086842
P30550	570	C:C-C-C	−0.086995
P30550	830	SC1C(N)CCCC1	−0.087044
P30550	826	OC1C(N)CCCC1	−0.087396
P30550	810	SC1CC(Cl)CCC1	−0.087684
P30550	862	CC1C(S)CCC1	−0.088553
P30550	772	Nc1c(Br)cccc1	−0.088569
P30550	90	>= 1 Re	−0.088637

P30550	617	C-C-C-O-[#1]	−0.09018
P30550	698	O-C-C-C-C-C-C-C	−0.092499
P30550	273	B-B	−0.092825
P30550	697	C-C-C-C-C-C(C)-C	−0.093031
P30550	686	O=C-C-C-C-O	−0.093123
P30550	522	C-N-N-[#1]	−0.09472
P30550	283	C-H	−0.097268
P30550	389	C(:N)(:N)	−0.098764
P30550	834	NC1C(Cl)CCCC1	−0.099194
P30550	441	C(-C)(=C)	−0.099864
P30550	752	Clc1cc(Cl)ccc1	−0.100178
P30550	516	[#1]-C=C-[#1]	−0.104424
P30550	412	S(~C)(~C)	−0.10829
P30550	490	C-C-C=C	−0.1084
P30550	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.108461
P30550	573	O-C-C=C	−0.108998
P30550	263	Li-H	−0.111039
P30550	415	Si(~C)(~C)	−0.113479
P30550	18	>= 1 O	−0.113581
P30550	46	>= 1 I	−0.114172
P30550	756	Cc1c(O)cccc1	−0.114535
P30550	709	C-C(C)-C-C-C	−0.11678
P30550	351	C(~C)(~N)	−0.119044
P30550	710	C-C-C(C)-C-C	−0.123655
P30550	794	ClC1CCC(Cl)CC1	−0.125099
P30550	430	C(-C)(-C)(=C)	−0.125244
P30550	544	O-C:C-O	−0.126617
P30550	343	C(~C)(~Cl)(~H)	−0.126882
P30550	114	>= 1 U	−0.128196
P30550	428	C(#C)(-H)	−0.129838
P30550	503	Cl-C:C-[#1]	−0.131745
P30550	691	O-C-C-C-C-C-N	−0.145714
P30550	447	C(-H)(=N)	−0.151778
P30550	679	C-C-C-C-C-C	−0.153753
P30550	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.158843
P30550	388	C(:C)(:N)(:N)	−0.16185
P30550	60	>= 1 Ni	−0.169215
P30550	531	S-C:C-C	−0.173053
P30550	192	>= 3 any ring size 6	−0.174015
P30550	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.174151
P30550	857	ClC1CC(Cl)CC1	−0.174166
P30550	819	CC1C(O)CCCC1	−0.17544
P30550	565	C:C-O-C	−0.17828
P30550	432	C(-C)(-C)(=O)	−0.189982
P30550	408	O(~H)(~S)	−0.197876
P30550	790	SC1CCC(Br)CC1	−0.200636
P30550	662	O-C-C-O-C	−0.203172
P30550	623	O=C-C:C-C	−0.208792

P30550	410	P(~C)(~C)	-0.210519
P30550	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	-0.212289
P30550	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	-0.214549
P30550	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.215658
P30550	681	O-C-C-C-C-O	-0.217073
P30550	256	>= 1 hetero-aromatic ring	-0.221611
P30550	355	C(~C)(:C)	-0.222081
P30550	25	>= 4 F	-0.222715
P30550	369	C(~H)(~Si)	-0.226916
P30550	622	O=C-O-C:C	-0.227703
P30550	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.228201
P30550	58	>= 1 Fe	-0.229374
P30550	800	CC1CC(N)CCC1	-0.233418
P30550	705	O=C-C-C-C-C(O)-C	-0.236724
P30550	9	>= 2 C	-0.238166
P30550	37	>= 1 Cl	-0.238437
P30550	742	Oc1cc(N)ccc1	-0.239051
P30550	776	CC1CCC(C)CC1	-0.239239
P30550	557	N:C-O-[#1]	-0.242159
P30550	707	O=C-C-C-C-C(N)-C	-0.242541
P30550	510	[#1]-N-N-[#1]	-0.242714
P30550	84	>= 1 Cs	-0.2437
P30550	43	>= 1 Br	-0.248692
P30550	702	O-C-C-C-C-C-N-C	-0.249959
P30550	324	P-P	-0.251064
P30550	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	-0.251511
P30550	144	>= 1 saturated or aromatic carbon-only ring size 5	-0.251875
P30550	650	O=C-N-C=O	-0.253251
P30550	661	O-C-O-C-C	-0.254189
P30550	741	Oc1cc(S)ccc1	-0.257194
P30550	808	SC1CC(S)CCC1	-0.257392
P30550	234	>= 2 any ring size 8	-0.25762
P30550	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-0.260343
P30550	832	SC1C(Br)CCCC1	-0.260898
P30550	86	>= 1 Lu	-0.260938
P30550	847	OC1CC(N)CC1	-0.261838
P30550	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	-0.262045
P30550	878	ClC1C(Cl)CCC1	-0.262746
P30550	489	N-C-S-C	-0.265036
P30550	357	C(~C)(:C)(:N)	-0.265842
P30550	96	>= 1 Tl	-0.265867
P30550	112	>= 1 Yb	-0.266377
P30550	848	OC1CC(Cl)CC1	-0.266542
P30550	855	NC1CC(Cl)CC1	-0.266947
P30550	305	N-S	-0.281142
P30550	358	C(~C)(:N)	-0.306961
P30550	491	C-N:C-[#1]	-0.310845
P30550	15	>= 2 N	-0.31147

P30550	387	C(:C)(:N)	−0.322158
P30550	540	C-N-C-[#1]	−0.333887
P30550	299	N-H	−0.33601
P30550	315	O-K	−0.336654
P30550	660	C-C=C-C-C	−0.351127
P30550	506	C-C:N:C	−0.353919
P30550	435	C(-C)(-H)(=N)	−0.364942
P30550	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.370362
P30550	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.400839
P30550	580	O=C-C-C-N	−0.439741
P30550	406	O(~C)(~H)	−0.4405
P30550	537	O=C-C-O	−0.441509
P30550	797	CC1CC(C)CCC1	−0.466346
P30550	493	O=C-C:C	−0.483445
P30550	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.537619
P30550	597	O=C-C-C:C	−0.553702
P30550	856	NC1CC(Br)CC1	−0.748843
P30550	853	SC1CC(Br)CC1	−0.823187
P30550	400	N(~H)(:C)(:C)	−1.246562

Fingerprints（continued)

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0.3412029	-0.0171
0.3170265	1.57E-05
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0.3139282	-0.01242
0.300093	-0.00411
0.2903426	0.004739
0.2845439	1.55E-05
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0.2658757	-4.13E-06
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0.263242	-4.69E-06
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0.231817	0.009429
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0.2237347	1.48E-05
0.2230431	-1.82E-05
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0.2012875	-3.39E-05

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0.1702047	-9.35E-07
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0.1611979	-7.01E-06
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0.1592263	-0.00885
0.1440282	0.000729
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0.0195633	-0.00696
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0.0119515	-8.98E-06
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-0.007523	0.019217
0.0189926	-0.00751
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0.0106822	-3.76E-05
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0.010324	7.21E-06
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0.0101551	-1.82E-05
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0.009606	-5.02E-06
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-2.20E-05	0.009444
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0.0080499	-1.50E-05
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0.0024813	0.005134
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0	0.005229
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-1.239391 -0.00717

Data S1. Ranking of importance of substructure features from Pubchem Fingerp

GPCR ID	Bit Posit	Bit Substructure	W	P
P28336	336	C(~C)(~C)(~C)(~N)	1.033324	1.003512
P28336	21	>= 8 O	0.917344	0.899491
P28336	17	>= 8 N	0.89847	0.880659
P28336	179	>= 1 saturated or aromatic carbon-only ring size 6	0.791978	0.753458
P28336	829	SC1C(S)CCCC1	0.759341	0.759254
P28336	605	O=C-C-O-C	0.526397	0.503005
P28336	716	Cc1ccc(N)cc1	0.521133	0.483797
P28336	844	CC1CC(Br)CC1	0.421485	0.421407
P28336	645	O=C-N-C-C	0.387829	0.394158
P28336	639	O-C-C-C-O	0.370302	0.360383
P28336	581	O=C-C-C-O	0.353787	0.358905
P28336	623	O=C-C:C-C	0.337774	0.33712
P28336	792	NC1CCC(Cl)CC1	0.320663	0.309679
P28336	440	C(-C)(-O)(=O)	0.315402	0.332713
P28336	368	C(~H)(~S)	0.307211	0.302873
P28336	558	O=N-C:C	0.292565	0.291304
P28336	728	Nc1ccc(N)cc1	0.287007	0.256905
P28336	568	N#C-C-C	0.285382	0.269133
P28336	689	O-C-C-C-C-C-C	0.277237	0.288344
P28336	18	>= 1 O	0.271749	0.250966
P28336	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.271324	0.262668
P28336	367	C(~H)(~O)(~O)	0.268728	0.264746
P28336	827	OC1C(Cl)CCCC1	0.26865	0.267961
P28336	84	>= 1 Cs	0.266946	0.266995
P28336	465	O=S-C-C	0.266012	0.259156
P28336	122	>= 2 any ring size 3	0.264186	0.264239
P28336	165	>= 4 saturated or aromatic carbon-only ring size 5	0.264136	0.264186
P28336	407	O(~C)(~P)	0.262946	0.262999
P28336	785	OC1CCC(Cl)CC1	0.262718	0.263863
P28336	361	C(~Cl)(~H)	0.26152	0.261564
P28336	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.260858	0.260906
P28336	868	OC1C(N)CCC1	0.259254	0.259303
P28336	778	CC1CCC(S)CC1	0.253257	0.262089
P28336	113	>= 1 Tc	0.253	0.253046
P28336	313	O-Si	0.248887	0.248937
P28336	510	[#1]-N-N-[#1]	0.246137	0.251792
P28336	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.238518	0.238557
P28336	600	N-C:C:C-C	0.237191	0.217758
P28336	80	>= 1 Sn	0.232061	0.232108
P28336	775	Brc1c(Br)cccc1	0.229729	0.229773
P28336	55	>= 1 V	0.225582	0.225642
P28336	824	OC1C(O)CCCC1	0.223235	0.219757
P28336	543	O-C:C-N	0.222045	0.223529
P28336	666	C=C-C-O-C	0.220898	0.212544
P28336	480	C:S:C-C	0.218459	0.219729
P28336	823	CC1C(Br)CCCC1	0.216028	0.216071

P28336	699	O-C-C-C-C-C(C)-C	0.213229	0.190247
P28336	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.208806	0.214766
P28336	766	Sc1c(S)cccc1	0.208768	0.208817
P28336	545	N-C:C-C	0.206647	0.214277
P28336	677	C-C=C-C:C	0.2061	0.213729
P28336	706	O=C-C-C-C-C(=O)-C	0.204621	0.204662
P28336	575	O-C-C:C-O	0.201541	0.200192
P28336	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.201327	0.201373
P28336	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.200228	0.20027
P28336	290	C-Al	0.198978	0.199021
P28336	416	C=C	0.198754	0.206383
P28336	353	C(~C)(~S)	0.198676	0.177262
P28336	108	>= 1 Dy	0.197287	0.197326
P28336	472	C:N:C-C	0.196443	0.214213
P28336	760	Cc1c(Br)cccc1	0.196275	0.196319
P28336	374	C(~H)(~H)(~H)	0.193262	0.165046
P28336	540	C-N-C-[#1]	0.192345	0.214824
P28336	434	C(-C)(-H)(=C)	0.19175	0.188246
P28336	95	>= 1 Hg	0.191115	0.191158
P28336	5	>= 2 Li	0.190602	0.190639
P28336	652	O-C:C:C-N	0.189345	0.194728
P28336	10	>= 4 C	0.189289	0.196799
P28336	560	N-C-N-C	0.188142	0.185673
P28336	335	C(~C)(~C)(~C)(~H)	0.18461	0.155314
P28336	321	Si-Si	0.18121	0.181251
P28336	712	C-C(C)-C(C)-C	0.176756	0.188766
P28336	272	B-H	0.17538	0.175414
P28336	631	O-C:C-O-[#1]	0.175195	0.175236
P28336	563	O-C-O-C	0.170931	0.175629
P28336	869	OC1C(Cl)CCC1	0.168396	0.168457
P28336	514	O-N-C-C	0.167386	0.169793
P28336	500	C-S-C:C	0.165425	0.16945
P28336	571	[#1]-C-O-[#1]	0.160839	0.183888
P28336	671	O=C-C=C-C	0.157311	0.150768
P28336	674	N-C-N-C:C	0.155483	0.124397
P28336	375	C(~N)(~N)	0.150359	0.128568
P28336	279	B-P	0.144981	0.145017
P28336	341	C(~C)(~C)(~O)	0.144532	0.144819
P28336	593	N-C-C-C-N	0.143624	0.104306
P28336	483	N-S-C:C	0.14216	0.138741
P28336	758	Cc1c(N)cccc1	0.140554	0.122938
P28336	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.139102	0.141323
P28336	616	C:C:N:N:C	0.130557	0.127228
P28336	759	Cc1c(Cl)cccc1	0.130457	0.128809
P28336	144	>= 1 saturated or aromatic carbon-only ring size 5	0.127281	0.120112
P28336	806	OC1CC(Cl)CCC1	0.124352	0.125483
P28336	754	Brc1cc(Br)ccc1	0.12425	0.124313
P28336	319	Al-Cl	0.124178	0.12422

P28336	25	>= 4 F	0.122289	0.092601
P28336	334	C(~C)(~C)(~C)(~C)	0.118521	0.077627
P28336	487	N-C=N-C	0.117101	0.127526
P28336	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.115841	0.1159
P28336	632	C-C-O-C:C	0.115823	0.11481
P28336	427	C(#C)(-C)	0.11479	0.114826
P28336	192	>= 3 any ring size 6	0.113927	0.07694
P28336	412	S(~C)(~C)	0.112893	0.095479
P28336	322	Si-Cl	0.11283	0.112869
P28336	377	C(~N)(:C)(:C)	0.109855	0.097619
P28336	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.10838	0.108315
P28336	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.107928	0.108752
P28336	834	NC1C(Cl)CCCC1	0.106902	0.095808
P28336	859	BrC1CC(Br)CC1	0.09952	0.099556
P28336	265	Li-B	0.096998	0.097037
P28336	842	CC1CC(N)CC1	0.093963	0.085016
P28336	687	O=C-C-C-C=O	0.092063	0.065115
P28336	130	>= 1 saturated or aromatic carbon-only ring size 4	0.091354	0.085898
P28336	555	N=C-C=C	0.089899	0.081343
P28336	60	>= 1 Ni	0.089357	0.089398
P28336	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.08774	0.087714
P28336	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.085215	0.085187
P28336	402	N(~O)(:O)	0.085082	0.085054
P28336	262	>= 4 hetero-aromatic rings	0.084734	0.084705
P28336	534	S-C:C-O	0.084586	0.073179
P28336	862	CC1C(S)CCC1	0.084178	0.084149
P28336	628	C-N-C-C:C	0.083795	0.079404
P28336	711	C-C(C)(C)-C-C	0.083477	0.04017
P28336	83	>= 1 Xe	0.082117	0.082076
P28336	636	C-N-C-N-C	0.081473	0.058879
P28336	701	O-C-C-C-C-C(O)-C	0.080376	0.078966
P28336	798	CC1CC(O)CCC1	0.08009	0.084253
P28336	268	Li-F	0.078517	0.07849
P28336	106	>= 1 Gd	0.078005	0.077974
P28336	508	S=C-N-C	0.077556	0.074242
P28336	822	CC1C(Cl)CCCC1	0.077151	0.075451
P28336	101	>= 1 Pr	0.075694	0.075662
P28336	473	S-C:N:C	0.075019	0.081096
P28336	702	O-C-C-C-C-C-N-C	0.072991	0.066952
P28336	627	O=[As]-C:C:C	0.071923	0.071893
P28336	516	[#1]-C=C-[#1]	0.071552	0.067981
P28336	624	O=C-C:C-N	0.07131	0.071284
P28336	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.071031	0.071008
P28336	836	ClC1C(Cl)CCCC1	0.069209	0.068087
P28336	378	C(~N)(:C)(:N)	0.068747	0.082937
P28336	719	Oc1ccc(O)cc1	0.068501	0.06779
P28336	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.068422	0.068457
P28336	762	Oc1c(S)cccc1	0.068145	0.068115

P28336	572	N:C:N:C	0.06813	0.059458
P28336	750	Nc1cc(Cl)ccc1	0.06809	0.066928
P28336	621	N-C:C:C:N	0.067573	0.051808
P28336	708	C-C(C)-C-C	0.067427	0.074591
P28336	742	Oc1cc(N)ccc1	0.066736	0.068239
P28336	349	C(~C)(~H)(~S)	0.064729	0.061973
P28336	352	C(~C)(~O)	0.064243	0.046568
P28336	150	>= 2 any ring size 5	0.063886	0.053475
P28336	590	C-C:C-O-[#1]	0.062851	0.06169
P28336	665	N-C:C-C-C	0.062503	0.070062
P28336	397	N(~C)(:C)(:C)	0.062461	0.043511
P28336	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.061505	0.061477
P28336	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.061256	0.06123
P28336	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.061118	0.061096
P28336	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.061063	0.061093
P28336	303	N-Si	0.060869	0.060847
P28336	385	C(:C)(:C)(:C)	0.060586	0.050167
P28336	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.058695	0.065995
P28336	259	>= 3 aromatic rings	0.058632	0.05861
P28336	542	O-C:C-[#1]	0.058258	0.046861
P28336	462	O-C-C=O	0.05772	0.037548
P28336	280	B-S	0.056947	0.05699
P28336	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.055953	0.055929
P28336	526	Cl-C:C-Cl	0.055422	0.054367
P28336	537	O=C-C-O	0.052632	0.032443
P28336	388	C(:C)(:N)(:N)	0.052147	0.065442
P28336	791	NC1CCC(N)CC1	0.051186	0.04006
P28336	96	>= 1 Tl	0.049873	0.04984
P28336	589	C-C:C-O-C	0.049606	0.024123
P28336	604	C-O-C-C:C	0.049017	0.04064
P28336	640	C=C-C-C-C	0.048899	0.056523
P28336	722	Oc1ccc(Cl)cc1	0.048444	0.049573
P28336	655	O-C-C-C:C	0.048361	0.055433
P28336	696	C-C-C-C-C-C-C-C	0.048359	0.03634
P28336	670	Br-C:C:C-C	0.046941	0.037741
P28336	569	N-C-C-N	0.044108	0.049427
P28336	787	SC1CCC(S)CC1	0.043756	0.043817
P28336	417	C#C	0.043105	0.04313
P28336	36	>= 8 S	0.042488	0.042551
P28336	744	Oc1cc(Br)ccc1	0.04248	0.042502
P28336	221	>= 2 saturated or aromatic carbon-only ring size 7	0.042225	0.042244
P28336	391	N(~C)(~C)(~C)	0.042222	0.011515
P28336	89	>= 1 W	0.042185	0.042205
P28336	329	C(~Br)(~H)	0.042113	0.042136
P28336	13	>= 32 C	0.041979	-0.00982
P28336	260	>= 3 hetero-aromatic rings	0.041734	0.041719
P28336	298	C-I	0.041719	0.041742
P28336	463	N:C-S-[#1]	0.041473	0.04149

P28336	72	>= 1 Nb	0.04106	0.041075
P28336	41	>= 1 K	0.038501	0.038528
P28336	426	P=P	0.037561	0.03758
P28336	29	>= 2 Si	0.037124	0.037095
P28336	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.036904	0.02828
P28336	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.036843	0.036817
P28336	58	>= 1 Fe	0.036533	0.036561
P28336	837	ClC1C(Br)CCCC1	0.036369	0.036342
P28336	461	O-C-C=N	0.035391	0.038335
P28336	703	O-C-C-C-C-C(N)-C	0.035248	0.031965
P28336	592	N-C-C-C-C	0.034376	0.041972
P28336	841	CC1CC(S)CC1	0.034324	0.034333
P28336	499	N-C:C:N	0.034127	0.028248
P28336	3	>= 32 H	0.034005	0.034016
P28336	734	Cc1cc(C)ccc1	0.033992	0.004961
P28336	642	O-C-C-C=O	0.033193	0.038268
P28336	489	N-C-S-C	0.032558	0.038689
P28336	723	Oc1ccc(Br)cc1	0.032325	0.032298
P28336	292	C-P	0.032096	0.032063
P28336	333	C(~C)(~C)(~C)	0.031007	0.040051
P28336	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.030465	0.030501
P28336	821	CC1C(N)CCCC1	0.030083	0.015422
P28336	464	N-C-C=C	0.030041	0.006829
P28336	551	Cl-C-C-O	0.030026	0.0293
P28336	81	>= 1 Sb	0.029821	0.0298
P28336	698	O-C-C-C-C-C-C-C	0.029666	0.049041
P28336	654	N-C-N-C-C	0.029067	0.026548
P28336	38	>= 2 Cl	0.028517	0.019929
P28336	37	>= 1 Cl	0.027508	0.02285
P28336	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.027115	0.024791
P28336	316	F-P	0.026997	0.027018
P28336	808	SC1CC(S)CCC1	0.026783	0.0268
P28336	541	O-C:C-C	0.026669	0
P28336	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0262	0.026221
P28336	363	C(~F)(~F)	0.026068	0.001432
P28336	724	Sc1ccc(S)cc1	0.025792	0.025762
P28336	476	C-O-C=C	0.025612	0.000162
P28336	565	C:C-O-C	0.025456	0
P28336	626	C-O-C:C-C	0.025454	0
P28336	606	O-C:C-C-C	0.025386	-0.00521
P28336	507	C-C-S-C	0.025325	0.00795
P28336	577	C:C-N-C:C	0.024807	0.031327
P28336	384	C(:C)(:C)	0.024762	0.032368
P28336	733	Brc1ccc(Br)cc1	0.024569	0.024554
P28336	379	C(~N)(:N)	0.023943	0.006492
P28336	241	>= 1 any ring size 9	0.023664	0.023651
P28336	872	SC1C(N)CCC1	0.023108	0.023125
P28336	676	N#C-C-C-C	0.021704	0.005437

P28336	257	>= 2 aromatic rings	0.021421	0.021442
P28336	562	Br-C-C=O	0.021234	0.02125
P28336	644	C-C=N-N-C	0.021161	0
P28336	30	>= 1 P	0.020739	0.020732
P28336	769	Sc1c(Br)cccc1	0.020129	0.020116
P28336	424	N=P	0.019993	0.019976
P28336	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.019967	0.019956
P28336	443	C(-C)(=O)	0.019716	-0.00031
P28336	865	CC1C(Br)CCC1	0.019564	0.019549
P28336	53	>= 1 Sc	0.019495	0.019517
P28336	281	B-Cl	0.019155	0.019136
P28336	726	Sc1ccc(Cl)cc1	0.018578	0.018561
P28336	731	Clc1ccc(Cl)cc1	0.018565	0.018531
P28336	591	Cl-C-C-C-C	0.018315	0.013699
P28336	420	C=O	0.018135	0
P28336	43	>= 1 Br	0.017521	0.008315
P28336	598	Cl-C:C:C-C	0.017387	0.012766
P28336	264	Li-Li	0.017255	0.017234
P28336	586	C-S-C-C-C	0.017156	-0.00023
P28336	104	>= 1 Sm	0.016946	0.016921
P28336	853	SC1CC(Br)CC1	0.016791	0.016765
P28336	116	>= 1 saturated or aromatic carbon-only ring size 3	0.01665	0.010262
P28336	22	>= 16 O	0.01642	0
P28336	860	CC1C(C)CCC1	0.016267	0.002217
P28336	649	O=N-C:C-O	0.015511	0.015532
P28336	82	>= 1 Te	0.015337	0.015347
P28336	557	N:C-O-[#1]	0.015302	0
P28336	651	O-C:C:C-C	0.01524	-4.46E-05
P28336	394	N(~C)(~H)(~N)	0.015196	0.018234
P28336	789	SC1CCC(Cl)CC1	0.015161	0.015143
P28336	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.014944	0.014962
P28336	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.014898	0.022948
P28336	185	>= 2 any ring size 6	0.014821	0.00424
P28336	815	ClC1CC(Cl)CCC1	0.014747	0.005498
P28336	485	N:C:C:N	0.014692	-0.0011
P28336	494	O=C-C:N	0.014586	0.001277
P28336	695	O=C-C-C-C-C-N	0.013858	0.010657
P28336	49	>= 1 Be	0.013796	0.013814
P28336	773	Clc1c(Cl)cccc1	0.013755	0.012657
P28336	136	>= 2 any ring size 4	0.013435	0.013444
P28336	28	>= 1 Si	0.013294	0.012995
P28336	439	C(-C)(-N)(=O)	0.013257	0
P28336	544	O-C:C-O	0.013216	0.009696
P28336	293	C-S	0.013069	0
P28336	261	>= 4 aromatic rings	0.012956	0.012962
P28336	482	C:N-C:C	0.012903	0.021426
P28336	56	>= 1 Cr	0.012876	0.012892
P28336	459	S(=O)(=O)	0.012795	0.001919

P28336	92	>= 1 Ir	0.012505	0.012522
P28336	52	>= 1 Ca	0.012245	0.012208
P28336	673	O=C-C=C-N	0.012207	0.003632
P28336	692	O=C-C-C-C-C-C	0.011682	0.001097
P28336	535	O=C-C-C	0.011496	0.010911
P28336	550	Cl-C-C-C	0.011417	0.006767
P28336	594	C-O-C-C=C	0.011131	0.002751
P28336	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.011067	-0.00053
P28336	771	Nc1c(Cl)cccc1	0.011062	0
P28336	450	C(-N)(=N)	0.010869	0.005341
P28336	826	OC1C(N)CCCC1	0.010637	0.012761
P28336	729	Nc1ccc(Cl)cc1	0.010361	-0.00054
P28336	720	Oc1ccc(S)cc1	0.010234	0.004862
P28336	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.009775	0.009759
P28336	525	[As]-C:C-[#1]	0.009733	0.009719
P28336	220	>= 2 any ring size 7	0.009689	0.00968
P28336	359	C(~C)(:N)(:N)	0.009632	0.020648
P28336	115	>= 1 any ring size 3	0.009622	0.003256
P28336	451	C(-N)(=O)	0.009619	-0.00179
P28336	781	CC1CCC(Br)CC1	0.009404	0.000179
P28336	714	Cc1ccc(O)cc1	0.009371	-0.0015
P28336	328	C(~Br)(~C)(~C)	0.009233	0
P28336	675	Br-C-C-C:C	0.009228	0
P28336	718	Cc1ccc(Br)cc1	0.009227	0
P28336	330	C(~Br)(:C)	0.009225	0
P28336	554	Br-C-C-C	0.009223	0
P28336	327	C(~Br)(~C)	0.009222	0
P28336	129	>= 1 any ring size 4	0.00922	0.003798
P28336	59	>= 1 Co	0.0092	0.009184
P28336	458	S(-O)(=O)	0.009194	0
P28336	373	C(~H)(:N)	0.009103	0.025491
P28336	818	CC1C(C)CCCC1	0.009071	0.004406
P28336	880	BrC1C(Br)CCC1	0.009064	0.009054
P28336	831	SC1C(Cl)CCCC1	0.008943	0.008973
P28336	713	Cc1ccc(C)cc1	0.008917	0.026322
P28336	466	N#C-C=C	0.008814	-0.00468
P28336	511	S=C-N-[#1]	0.008741	0.005446
P28336	289	C-Mg	0.008707	0.0087
P28336	286	C-O	0.008691	0
P28336	504	N:C:N-C	0.008675	0
P28336	386	C(:C)(:C)(:N)	0.00788	-0.01141
P28336	816	ClC1CC(Br)CCC1	0.007653	0.007667
P28336	691	O-C-C-C-C-C-N	0.007627	-0.00525
P28336	519	N=C-N-C	0.007546	0.002372
P28336	784	OC1CCC(N)CC1	0.007429	0.014694
P28336	389	C(:N)(:N)	0.007229	-0.00145
P28336	110	>= 1 Er	0.00692	0.006934
P28336	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.006679	0.006669

P28336	683	N-C-C-C-C-C	0.006657	0.014216
P28336	248	>= 1 any ring size 10	0.0062	0.006211
P28336	456	P(-O)(=O)	0.006138	0.006119
P28336	553	O=C-C=C	0.006039	-0.0005
P28336	850	SC1CC(S)CC1	0.006029	0.006037
P28336	573	O-C-C=C	0.005967	0.00655
P28336	641	O-C-C-C=C	0.005833	0.012923
P28336	387	C(:C)(:N)	0.005458	0.013986
P28336	536	O=C-C-N	0.005286	-0.00476
P28336	688	C-C-C-C-C-C-C	0.00525	0
P28336	861	CC1C(O)CCC1	0.005231	0.009168
P28336	596	N=C-N-C-C	0.005183	0
P28336	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.004972	0.004963
P28336	362	C(~Cl)(:C)	0.004651	0
P28336	730	Nc1ccc(Br)cc1	0.004605	0.004598
P28336	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.004535	0.004526
P28336	761	Oc1c(O)cccc1	0.004507	0.001024
P28336	475	S-C=N-C	0.004483	0.010583
P28336	419	C#N	0.003746	-0.01253
P28336	446	C(-H)(=C)	0.003639	9.06E-05
P28336	401	N(~O)(~O)	0.003523	0.002249
P28336	213	>= 1 any ring size 7	0.003465	-0.00103
P28336	393	N(~C)(~H)	0.003183	0.019378
P28336	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.003146	0.003161
P28336	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.002792	0.002781
P28336	793	NC1CCC(Br)CC1	0.002738	0.002731
P28336	813	NC1CC(Cl)CCC1	0.002622	0.001467
P28336	783	OC1CCC(S)CC1	0.002563	-0.0028
P28336	740	Oc1cc(O)ccc1	0.002471	0.001074
P28336	354	C(~C)(~Si)	0.002059	0.001744
P28336	772	Nc1c(Br)cccc1	0.002025	0.002037
P28336	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.001857	-0.00359
P28336	370	C(~H)(:C)	0.001857	-0.0017
P28336	288	C-Na	0.001799	0.001808
P28336	777	CC1CCC(O)CC1	0.001765	-0.00911
P28336	794	ClC1CCC(Cl)CC1	0.001641	0.00165
P28336	484	N-C:N:C	0.001492	0
P28336	529	Cl-C-C-Cl	0.001082	0
P28336	858	ClC1CC(Br)CC1	0.001036	0.00104
P28336	270	Li-S	0.000994	0.000999
P28336	42	>= 2 K	0.000842	0.000835
P28336	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.000841	0.000814
P28336	602	O=C-C-N-C	0.000772	-2.63E-05
P28336	505	Cl-C:C-O	0.000739	0
P28336	493	O=C-C:C	0.000702	0
P28336	68	>= 1 Rb	0.0007	0.00071
P28336	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.000569	0.000575
P28336	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.000462	0

P28336	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.000453	0.000465
P28336	423	N=O	0.000363	0.002771
P28336	399	N(~H)(:C)	0.000319	-0.00229
P28336	71	>= 1 Zr	3.76E-05	4.74E-05
P28336	425	P=O	8.90E-06	0
P28336	845	OC1CC(O)CC1	8.84E-06	0
P28336	87	>= 1 Hf	8.21E-06	0
P28336	54	>= 1 Ti	7.76E-06	0
P28336	588	O=C-C-C=O	7.33E-06	0
P28336	51	>= 1 Al	7.16E-06	0
P28336	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	6.70E-06	0
P28336	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	6.28E-06	0
P28336	786	OC1CCC(Br)CC1	6.08E-06	0
P28336	105	>= 1 Eu	5.16E-06	0
P28336	874	SC1C(Br)CCC1	4.60E-06	0
P28336	109	>= 1 Ho	3.74E-06	0
P28336	302	N-F	3.63E-06	0
P28336	93	>= 1 Pt	3.25E-06	0
P28336	873	SC1C(Cl)CCC1	3.20E-06	0
P28336	200	>= 4 saturated or aromatic carbon-only ring size 6	2.96E-06	0
P28336	854	NC1CC(N)CC1	2.92E-06	0
P28336	103	>= 1 Pm	2.34E-06	0
P28336	66	>= 1 Se	2.17E-06	0
P28336	727	Sc1ccc(Br)cc1	1.20E-06	0
P28336	267	Li-O	9.94E-07	0
P28336	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	7.75E-07	0
P28336	45	>= 4 Br	7.05E-07	0
P28336	63	>= 1 Ga	4.40E-07	0
P28336	102	>= 1 Nd	1.22E-07	0
P28336	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	-2.51E-07	0
P28336	732	Clc1ccc(Br)cc1	-7.43E-07	0
P28336	838	BrC1C(Br)CCCC1	-1.06E-06	0
P28336	4	>= 1 Li	-1.19E-06	0
P28336	802	CC1CC(Br)CCC1	-1.30E-06	0
P28336	318	Al-H	-1.66E-06	0
P28336	433	C(-C)(-Cl)(=O)	-1.75E-06	0
P28336	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	-2.21E-06	0
P28336	8	>= 4 B	-2.37E-06	0
P28336	114	>= 1 U	-2.37E-06	0
P28336	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	-2.41E-06	0
P28336	811	SC1CC(Br)CCC1	-2.45E-06	0
P28336	469	S-S-C:C	-2.79E-06	0
P28336	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	-3.77E-06	0
P28336	849	OC1CC(Br)CC1	-4.36E-06	0
P28336	317	F-S	-4.62E-06	0
P28336	814	NC1CC(Br)CCC1	-5.03E-06	0
P28336	62	>= 1 Zn	-5.09E-06	0
P28336	90	>= 1 Re	-5.21E-06	0

P28336	40	>= 8 Cl	-5.28E-06	0
P28336	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	-5.45E-06	0
P28336	234	>= 2 any ring size 8	-5.65E-06	0
P28336	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	-5.84E-06	0
P28336	39	>= 4 Cl	-5.91E-06	0
P28336	625	O=C-C:C-O	-8.02E-06	0
P28336	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	-9.43E-06	0
P28336	807	OC1CC(Br)CCC1	-1.02E-05	0
P28336	271	Li-Cl	-1.16E-05	0
P28336	320	Si-H	-2.76E-05	-3.99E-05
P28336	400	N(~H)(:C)(:C)	-3.42E-05	0.005778
P28336	99	>= 1 La	-6.71E-05	-6.73E-05
P28336	347	C(~C)(~H)(~O)(~O)	-7.18E-05	-7.53E-05
P28336	430	C(-C)(-C)(=C)	-9.41E-05	0.000149
P28336	857	ClC1CC(Cl)CC1	-0.00013	-0.00013
P28336	86	>= 1 Lu	-0.00017	-0.00019
P28336	47	>= 2 I	-0.00042	-0.00041
P28336	804	OC1CC(S)CCC1	-0.00056	-0.00055
P28336	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	-0.00059	0
P28336	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.00059	0
P28336	735	Cc1cc(O)ccc1	-0.00061	-0.00038
P28336	312	O-Al	-0.00076	-0.00076
P28336	266	Li-C	-0.00087	-0.00087
P28336	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	-0.00094	-0.00095
P28336	743	Oc1cc(Cl)ccc1	-0.00108	0
P28336	91	>= 1 Os	-0.00119	-0.0012
P28336	830	SC1C(N)CCCC1	-0.00135	0
P28336	686	O=C-C-C-C-O	-0.0014	0.01348
P28336	863	CC1C(N)CCC1	-0.00145	-0.01037
P28336	767	Sc1c(N)cccc1	-0.00166	-0.0003
P28336	164	>= 4 any ring size 5	-0.00185	0
P28336	871	SC1C(S)CCC1	-0.00207	-0.00206
P28336	301	N-O	-0.00214	0.000272
P28336	123	>= 2 saturated or aromatic carbon-only ring size 3	-0.00226	-0.00223
P28336	629	S-C:C:C-N	-0.00236	-0.00684
P28336	438	C(-C)(-N)(=N)	-0.00238	-0.00382
P28336	48	>= 4 I	-0.00249	-0.00247
P28336	757	Cc1c(S)cccc1	-0.00274	0
P28336	57	>= 1 Mn	-0.00301	-0.00301
P28336	796	BrC1CCC(Br)CC1	-0.00321	-0.00323
P28336	492	N-C:O:C	-0.00331	-0.00329
P28336	870	OC1C(Br)CCC1	-0.00351	-0.0035
P28336	228	>= 1 saturated or aromatic carbon-only ring size 8	-0.00364	-0.00365
P28336	490	C-C-C=C	-0.00377	0.003824
P28336	454	N(-C)(=O)	-0.00386	-0.00145
P28336	788	SC1CCC(N)CC1	-0.004	-0.00399
P28336	736	Cc1cc(S)ccc1	-0.00404	-0.00403
P28336	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	-0.00427	-0.00424

P28336	157	>= 3 any ring size 5	−0.00434	0
P28336	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.0045	−0.01097
P28336	437	C(-C)(-N)(=C)	−0.00464	6.30E−05
P28336	704	O=C-C-C-C-C-C-C	−0.00472	0.002048
P28336	324	P-P	−0.00492	−0.00491
P28336	609	Cl-C-C-N-C	−0.00493	−0.00209
P28336	410	P(~C)(~C)	−0.00499	−0.00498
P28336	382	C(~O)(:C)(:C)	−0.00501	−0.00085
P28336	97	>= 1 Pb	−0.00514	−0.00512
P28336	548	O-C-C:C	−0.00525	−0.00467
P28336	78	>= 1 Cd	−0.00546	−0.00544
P28336	345	C(~C)(~H)(~N)	−0.00554	0.001607
P28336	269	Li-P	−0.00562	−0.00566
P28336	365	C(~H)(~N)	−0.00575	0.001389
P28336	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.00577	−0.00576
P28336	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−0.00592	0
P28336	693	O=C-C-C-C-C-O	−0.00604	0
P28336	64	>= 1 Ge	−0.00605	−0.00606
P28336	295	C-As	−0.00608	−0.00609
P28336	282	B-Br	−0.00622	−0.00624
P28336	11	>= 8 C	−0.00637	0.001217
P28336	612	N-C-O-C-C	−0.00637	−0.00082
P28336	755	Cc1c(C)cccc1	−0.00645	−0.01108
P28336	780	CC1CCC(Cl)CC1	−0.00655	−0.00198
P28336	479	S-C-S-C	−0.00677	−0.00082
P28336	31	>= 2 P	−0.00692	−0.00688
P28336	503	Cl-C:C-[#1]	−0.00695	−0.00431
P28336	24	>= 2 F	−0.00701	−0.00523
P28336	339	C(~C)(~C)(~H)(~O)	−0.00712	0.005828
P28336	275	B-N	−0.00725	−0.00726
P28336	657	C-N-C:C-C	−0.00727	0.000304
P28336	587	N-C:C-O-[#1]	−0.0073	−0.00518
P28336	421	C=S	−0.00734	0.000408
P28336	15	>= 2 N	−0.00744	0.000148
P28336	520	C=C-C:C	−0.00756	2.46E−05
P28336	603	C-C:C:C-C	−0.00758	0
P28336	595	C:C-C-C-C	−0.00759	0
P28336	570	C:C-C-C	−0.0076	0
P28336	478	S-C=N-[#1]	−0.00773	−0.00529
P28336	497	O-C:C:N	−0.00773	−0.00843
P28336	812	NC1CC(N)CCC1	−0.00774	−0.01496
P28336	481	O-S-C:C	−0.00784	−0.00785
P28336	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.00804	−0.00803
P28336	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.00809	−0.00808
P28336	617	C-C-C-O-[#1]	−0.0081	0
P28336	69	>= 1 Sr	−0.0081	−0.00809
P28336	564	C=C-C=C	−0.0081	−0.00052
P28336	471	S:C:C:C	−0.00833	0

P28336	356	C(~C)(:C)(:C)	-0.00835	-0.0081
P28336	746	Sc1cc(N)ccc1	-0.00857	-0.00855
P28336	502	N-C=C-[#1]	-0.0086	3.98E-05
P28336	524	C-C=C-C	-0.00867	-0.00107
P28336	366	C(~H)(~O)	-0.00868	-0.00847
P28336	552	C:C-C:C	-0.00869	-0.0011
P28336	715	Cc1ccc(S)cc1	-0.00878	0
P28336	457	S(-C)(=O)	-0.00886	-0.01578
P28336	477	N-N-C:C	-0.00889	0.002126
P28336	300	N-N	-0.00893	0.001223
P28336	390	N(~C)(~C)	-0.00911	-0.00149
P28336	694	O=C-C-C-C-C=O	-0.00938	0.008591
P28336	76	>= 1 Pd	-0.00952	-0.00954
P28336	357	C(~C)(:C)(:N)	-0.00961	-0.00991
P28336	178	>= 1 any ring size 6	-0.0097	-0.00212
P28336	668	C-C:C-C-C	-0.00974	-0.00217
P28336	283	C-H	-0.00988	-0.0023
P28336	531	S-C:C-C	-0.00993	0
P28336	308	O-H	-0.01007	0.001757
P28336	832	SC1C(Br)CCCC1	-0.01011	-0.0101
P28336	65	>= 1 As	-0.01015	-0.01018
P28336	705	O=C-C-C-C-C(O)-C	-0.01018	0
P28336	846	OC1CC(S)CC1	-0.01027	-0.01033
P28336	608	C-C-C-C:C	-0.01033	-0.00276
P28336	61	>= 1 Cu	-0.01035	-0.01034
P28336	344	C(~C)(~H)	-0.01059	-0.00297
P28336	274	B-C	-0.01072	0
P28336	6	>= 1 B	-0.01074	0
P28336	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	-0.01074	-0.01072
P28336	748	Sc1cc(Br)ccc1	-0.01085	-0.01084
P28336	453	N(-C)(=C)	-0.01086	0.001903
P28336	325	As-H	-0.01152	-0.01155
P28336	406	O(~C)(~H)	-0.01182	0
P28336	661	O-C-O-C-C	-0.01189	-0.00723
P28336	27	>= 2 Na	-0.0122	-0.01218
P28336	725	Sc1ccc(N)cc1	-0.01248	-0.0125
P28336	360	C(~Cl)(~Cl)	-0.01259	-0.01252
P28336	647	O=C-N-C-N	-0.01263	-0.00596
P28336	663	O-C-C-O-[#1]	-0.01286	-0.00955
P28336	297	C-Br	-0.01293	-0.02218
P28336	546	N-C:C-[#1]	-0.01343	-0.00483
P28336	186	>= 2 saturated or aromatic carbon-only ring size 6	-0.0135	-0.01037
P28336	538	N=C-C-C	-0.01351	-0.00076
P28336	549	N-C-C:C	-0.01354	-0.01676
P28336	578	C-C:C-C:C	-0.01363	-0.00606
P28336	635	N-N-C-N-[#1]	-0.014	-0.00353
P28336	284	C-C	-0.01423	-0.00663
P28336	73	>= 1 Mo	-0.01443	-0.01444

P28336	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.01484	−0.01486
P28336	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.01498	−0.00045
P28336	331	C(~Br)(:N)	−0.01525	−0.01526
P28336	495	C-N-C:C	−0.01526	−0.00767
P28336	776	CC1CCC(C)CC1	−0.01549	−0.00639
P28336	276	B-O	−0.01562	−0.01564
P28336	878	ClC1C(Cl)CCC1	−0.01563	−0.01564
P28336	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.01615	−0.01617
P28336	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.01659	0
P28336	658	C-C-S-C-C	−0.01726	−0.00443
P28336	372	C(~H)(:C)(:N)	−0.01768	−0.00125
P28336	819	CC1C(O)CCCC1	−0.01778	−0.0033
P28336	455	N(-O)(=O)	−0.01792	−0.01919
P28336	380	C(~O)(~O)	−0.01803	0.009379
P28336	19	>= 2 O	−0.01805	−0.01418
P28336	763	Oc1c(N)cccc1	−0.01823	−0.01614
P28336	67	>= 1 Kr	−0.01849	−0.01848
P28336	294	C-Cl	−0.01864	−0.0233
P28336	305	N-S	−0.01867	−0.02219
P28336	444	C(-Cl)(=O)	−0.01898	−0.01901
P28336	700	O-C-C-C-C-C-O-C	−0.01942	−0.01117
P28336	85	>= 1 Ba	−0.01984	−0.01982
P28336	530	N:C-C:C	−0.02004	−0.00864
P28336	601	N-C:C:C-N	−0.02018	−0.02741
P28336	506	C-C:N:C	−0.0203	−0.00256
P28336	533	S-C:C-N	−0.02053	−0.04036
P28336	681	O-C-C-C-C-O	−0.02064	−0.0214
P28336	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.02135	−0.02134
P28336	452	C(-O)(=O)	−0.0215	0.001317
P28336	396	N(~C)(:C)	−0.02252	−0.01403
P28336	672	O=C-C=C-[#1]	−0.02283	−0.00121
P28336	369	C(~H)(~Si)	−0.02289	−0.02288
P28336	348	C(~C)(~H)(~P)	−0.02321	−0.02323
P28336	619	O-C-C=C-C	−0.02329	−0.02437
P28336	521	C:N-C-[#1]	−0.02353	−0.01618
P28336	143	>= 1 any ring size 5	−0.02369	−0.00463
P28336	843	CC1CC(Cl)CC1	−0.02427	−0.02426
P28336	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.02428	−0.02426
P28336	467	C=N-N-C	−0.02437	−0.03763
P28336	765	Oc1c(Br)cccc1	−0.02445	−0.02443
P28336	610	C-O-C-O-C	−0.02458	−0.01996
P28336	199	>= 4 any ring size 6	−0.02461	−0.00317
P28336	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.0247	−0.01431
P28336	256	>= 1 hetero-aromatic ring	−0.0248	−0.02478
P28336	877	NC1C(Br)CCC1	−0.02497	−0.02496
P28336	840	CC1CC(O)CC1	−0.02554	−0.02161
P28336	684	O=C-C-C-C-C	−0.02562	−0.03618
P28336	809	SC1CC(N)CCC1	−0.02577	−0.02579

P28336	810	SC1CC(Cl)CCC1	-0.02618	-0.02616
P28336	77	>= 1 Ag	-0.02618	-0.02615
P28336	404	N(:C)(:C)(:C)	-0.0265	-0.02654
P28336	774	Clc1c(Br)cccc1	-0.02708	-0.0271
P28336	255	>= 1 aromatic ring	-0.02726	-0.02724
P28336	583	Cl-C:C-O-C	-0.02738	-0.02815
P28336	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	-0.02805	0
P28336	782	OC1CCC(O)CC1	-0.02981	-0.03058
P28336	522	C-N-N-[#1]	-0.03057	-0.04008
P28336	442	C(-C)(=N)	-0.03073	-0.01798
P28336	445	C(-H)(-N)(=C)	-0.03121	-0.0148
P28336	582	C-C-C-C-C	-0.03139	-0.02379
P28336	413	S(~C)(~H)	-0.03161	-0.02385
P28336	825	OC1C(S)CCCC1	-0.03186	-0.03183
P28336	112	>= 1 Yb	-0.03283	-0.03285
P28336	527	C:C:N-[#1]	-0.03286	-0.02548
P28336	547	N-C:C-N	-0.0337	3.89E-05
P28336	383	C(~S)(:C)	-0.03411	-0.03948
P28336	679	C-C-C-C-C-C	-0.03412	-0.03177
P28336	638	O-C-C-C-N	-0.03421	-0.02942
P28336	395	N(~C)(~O)	-0.03453	-0.03215
P28336	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-0.03467	-0.0347
P28336	630	O-C:C-O-C	-0.03476	-0.03831
P28336	800	CC1CC(N)CCC1	-0.03556	-0.00527
P28336	34	>= 2 S	-0.0356	-0.01166
P28336	315	O-K	-0.03599	-0.03597
P28336	75	>= 1 Rh	-0.03647	-0.03643
P28336	566	O-C-C-N	-0.03681	0
P28336	856	NC1CC(Br)CC1	-0.03751	-0.03753
P28336	839	CC1CC(C)CC1	-0.03843	-0.03152
P28336	501	Cl-C:C-C	-0.0387	-0.04329
P28336	74	>= 1 Ru	-0.03898	-0.039
P28336	584	C:C-C=C-C	-0.03908	-0.03148
P28336	747	Sc1cc(Cl)ccc1	-0.04101	-0.04105
P28336	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	-0.04103	-0.04105
P28336	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	-0.04105	-0.04107
P28336	620	C:C-O-C-C	-0.04126	-0.0423
P28336	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	-0.04133	-0.04135
P28336	285	C-N	-0.0415	-0.03389
P28336	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	-0.04205	-0.04208
P28336	678	C-C-C=C-C	-0.04216	-0.03455
P28336	660	C-C=C-C-C	-0.04246	-0.03484
P28336	306	N-Cl	-0.04263	-0.04264
P28336	614	C-C-O-C-C	-0.04286	-0.02914
P28336	435	C(-C)(-H)(=N)	-0.0429	-0.04175
P28336	23	>= 1 F	-0.04338	-0.01314
P28336	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	-0.04392	-0.03893
P28336	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	-0.0445	-0.04447

P28336	79	>= 1 In	−0.04455	−0.04459
P28336	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.04462	−0.03423
P28336	576	N=C-C:C-[#1]	−0.04512	−0.05119
P28336	441	C(-C)(=C)	−0.04534	−0.03779
P28336	9	>= 2 C	−0.04662	−0.03906
P28336	346	C(~C)(~H)(~O)	−0.04706	−0.03951
P28336	408	O(~H)(~S)	−0.04749	−0.05665
P28336	403	N(:C)(:C)	−0.04827	−0.03049
P28336	646	O=C-N-C-[#1]	−0.04831	−0.0503
P28336	263	Li-H	−0.04905	−0.04908
P28336	338	C(~C)(~C)(~H)(~N)	−0.04955	−0.00361
P28336	258	>= 2 hetero-aromatic rings	−0.04956	−0.04959
P28336	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−0.04983	−0.04987
P28336	273	B-B	−0.04985	−0.04988
P28336	764	Oc1c(Cl)cccc1	−0.05023	−0.05095
P28336	449	C(-N)(=C)	−0.05236	−0.04474
P28336	828	OC1C(Br)CCCC1	−0.05327	−0.05324
P28336	664	C-C=C-C=C	−0.05329	−0.04568
P28336	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.05528	−0.05526
P28336	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.05618	−0.05615
P28336	411	P(~O)(~O)	−0.05625	−0.05623
P28336	643	[#1]-C-C-N-[#1]	−0.05647	−0.0354
P28336	866	OC1C(O)CCC1	−0.05669	−0.05666
P28336	709	C-C(C)-C-C-C	−0.05686	−0.04965
P28336	392	N(~C)(~C)(~H)	−0.05794	−0.03135
P28336	409	O(:C)(:C)	−0.0592	−0.07472
P28336	518	O=C-N-N	−0.05922	−0.05421
P28336	756	Cc1c(O)cccc1	−0.06018	−0.04955
P28336	599	[#1]-C-C=C-[#1]	−0.06254	−0.07348
P28336	448	C(-H)(=O)	−0.06294	−0.07845
P28336	662	O-C-C-O-C	−0.06396	−0.06498
P28336	611	N-C-C-N-C	−0.06497	−0.05046
P28336	358	C(~C)(:N)	−0.06551	−0.05703
P28336	637	O-C-C-C-C	−0.06555	−0.05333
P28336	468	O=S-C-N	−0.06562	−0.06167
P28336	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.06573	−0.05876
P28336	597	O=C-C-C:C	−0.0677	−0.04921
P28336	44	>= 2 Br	−0.0678	−0.06783
P28336	311	O-Na	−0.06902	−0.06899
P28336	697	C-C-C-C-C-C(C)-C	−0.07138	−0.06573
P28336	337	C(~C)(~C)(~C)(~O)	−0.07199	−0.08016
P28336	304	N-P	−0.07218	−0.07216
P28336	613	C-N-C-C-C	−0.0728	−0.06519
P28336	710	C-C-C(C)-C-C	−0.0729	−0.06829
P28336	875	NC1C(N)CCC1	−0.07308	−0.07305
P28336	431	C(-C)(-C)(=N)	−0.07317	−0.08453
P28336	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.07327	−0.07325
P28336	100	>= 1 Ce	−0.07329	−0.07327

P28336	847	OC1CC(N)CC1	−0.07386	−0.07383
P28336	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.07488	−0.07716
P28336	364	C(~F)(:C)	−0.07517	−0.04357
P28336	864	CC1C(Cl)CCC1	−0.0755	−0.07547
P28336	685	O=C-C-C-C-N	−0.07555	−0.0666
P28336	852	SC1CC(Cl)CC1	−0.07633	−0.07631
P28336	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.07796	−0.07083
P28336	867	OC1C(S)CCC1	−0.0782	−0.07817
P28336	659	O-C-C-N-C	−0.07919	−0.03414
P28336	817	BrC1CC(Br)CCC1	−0.08134	−0.08132
P28336	607	N-C-C-C:C	−0.0823	−0.07119
P28336	835	NC1C(Br)CCCC1	−0.08257	−0.08254
P28336	309	O-O	−0.0832	−0.08317
P28336	790	SC1CCC(Br)CC1	−0.08324	−0.08322
P28336	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−0.0833	−0.08327
P28336	803	OC1CC(O)CCC1	−0.08491	−0.08627
P28336	428	C(#C)(-H)	−0.08532	−0.08529
P28336	879	ClC1C(Br)CCC1	−0.08599	−0.08596
P28336	745	Sc1cc(S)ccc1	−0.08692	−0.08689
P28336	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.08741	−0.08738
P28336	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.08745	−0.08742
P28336	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.08751	−0.08748
P28336	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.08772	−0.08769
P28336	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.08793	−0.0879
P28336	532	S-C:C-[#1]	−0.08836	−0.0811
P28336	690	O-C-C-C-C-C-O	−0.08901	−0.08071
P28336	517	N-N-C-N	−0.0905	−0.06812
P28336	323	P-H	−0.0925	−0.09255
P28336	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.09303	−0.09309
P28336	1	>= 8 H	−0.09504	−0.09508
P28336	14	>= 1 N	−0.09757	−0.09002
P28336	539	N=C-C-[#1]	−0.09799	−0.09534
P28336	447	C(-H)(=N)	−0.09883	−0.09768
P28336	801	CC1CC(Cl)CCC1	−0.1008	−0.10077
P28336	35	>= 4 S	−0.10204	−0.10211
P28336	567	O-C-C-O	−0.10259	−0.10032
P28336	299	N-H	−0.10294	−0.08672
P28336	405	O(~C)(~C)	−0.10406	−0.08849
P28336	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.10453	−0.10457
P28336	171	>= 5 any ring size 5	−0.10548	−0.10044
P28336	752	Clc1cc(Cl)ccc1	−0.10567	−0.11494
P28336	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.10756	−0.10805
P28336	94	>= 1 Au	−0.10761	−0.10764
P28336	515	N-N-C-C	−0.10807	−0.1099
P28336	851	SC1CC(N)CC1	−0.10915	−0.10918
P28336	737	Cc1cc(N)ccc1	−0.10987	−0.09764
P28336	277	B-F	−0.11108	−0.10027
P28336	667	C=C-C-O-[#1]	−0.11353	−0.09733

P28336	376	C(~N)(:C)	−0.11542	−0.10777
P28336	332	C(~C)(~C)	−0.11871	−0.11116
P28336	33	>= 1 S	−0.11967	−0.1328
P28336	429	C(#N)(-C)	−0.12219	−0.13853
P28336	721	Oc1ccc(N)cc1	−0.12243	−0.11512
P28336	16	>= 4 N	−0.12371	−0.11378
P28336	650	O=C-N-C=O	−0.12577	−0.12583
P28336	512	C-[As]-O-[#1]	−0.12794	−0.128
P28336	580	O=C-C-C-N	−0.12944	−0.09908
P28336	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.13089	−0.13092
P28336	615	N-C-C-O-C	−0.13121	−0.14625
P28336	559	O-C-N-[#1]	−0.13196	−0.14168
P28336	98	>= 1 Bi	−0.13214	−0.13218
P28336	680	O-C-C-C-C-C	−0.13325	−0.12099
P28336	717	Cc1ccc(Cl)cc1	−0.13454	−0.12994
P28336	498	O-C=C-C	−0.13457	−0.16122
P28336	579	O=C-C-C-C	−0.13599	−0.13392
P28336	799	CC1CC(S)CCC1	−0.1401	−0.14014
P28336	20	>= 4 O	−0.14058	−0.14228
P28336	739	Cc1cc(Br)ccc1	−0.14149	−0.14153
P28336	556	C=C-C-C	−0.14304	−0.13553
P28336	343	C(~C)(~Cl)(~H)	−0.14504	−0.14508
P28336	682	O-C-C-C-C-N	−0.1478	−0.13553
P28336	32	>= 4 P	−0.15327	−0.1533
P28336	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.15502	−0.16949
P28336	805	OC1CC(N)CCC1	−0.15661	−0.15518
P28336	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.15997	−0.15143
P28336	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.16518	−0.16523
P28336	770	Nc1c(N)cccc1	−0.16548	−0.12138
P28336	307	N-Br	−0.16843	−0.16847
P28336	855	NC1CC(Cl)CC1	−0.1693	−0.16936
P28336	355	C(~C)(:C)	−0.17005	−0.1625
P28336	287	C-F	−0.1706	−0.1508
P28336	876	NC1C(Cl)CC1	−0.17279	−0.17282
P28336	751	Nc1cc(Br)ccc1	−0.17719	−0.17723
P28336	340	C(~C)(~C)(~N)	−0.18173	−0.18004
P28336	12	>= 16 C	−0.18684	−0.18093
P28336	585	C-C:C-N-C	−0.1888	−0.18125
P28336	46	>= 1 I	−0.19091	−0.19095
P28336	381	C(~O)(:C)	−0.19304	−0.20977
P28336	474	S:C:C:N	−0.19327	−0.2022
P28336	513	S:C:C-[#1]	−0.19557	−0.1873
P28336	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.19563	−0.20422
P28336	326	As-As	−0.21098	−0.21091
P28336	415	Si(~C)(~C)	−0.21172	−0.21208
P28336	833	NC1C(N)CCCC1	−0.21417	−0.17004
P28336	496	N:N-C-[#1]	−0.21472	−0.20588
P28336	779	CC1CCC(N)CC1	−0.21882	−0.21521

P28336	669	Cl-C:C-C=O	-0.21906	-0.21911
P28336	158	>= 3 saturated or aromatic carbon-only ring size 5	-0.21926	-0.21931
P28336	486	N-C:N:N	-0.21933	-0.2273
P28336	88	>= 1 Ta	-0.21946	-0.21951
P28336	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	-0.21964	-0.21111
P28336	242	>= 1 saturated or aromatic carbon-only ring size 9	-0.2232	-0.22325
P28336	795	ClC1CCC(Br)CC1	-0.22329	-0.22335
P28336	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	-0.22702	-0.22707
P28336	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	-0.22834	-0.22839
P28336	460	C-C-C#C	-0.23227	-0.23231
P28336	561	Cl-C-C=O	-0.23793	-0.23798
P28336	633	N-C-C:C-C	-0.23823	-0.24148
P28336	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	-0.2408	-0.24086
P28336	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	-0.24081	-0.23719
P28336	622	O=C-O-C:C	-0.24359	-0.25323
P28336	291	C-Si	-0.24644	-0.2468
P28336	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	-0.24654	-0.24657
P28336	653	O-C:C:C-O	-0.24687	-0.24831
P28336	278	B-Si	-0.24704	-0.24709
P28336	50	>= 1 Mg	-0.24793	-0.24797
P28336	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.25191	-0.25194
P28336	414	S(~C)(~O)	-0.25195	-0.2589
P28336	206	>= 5 any ring size 6	-0.25304	-0.21494
P28336	70	>= 1 Y	-0.25368	-0.25373
P28336	749	Nc1cc(N)ccc1	-0.25597	-0.26327
P28336	350	C(~C)(~I)	-0.25666	-0.25671
P28336	0	>= 4 H	-0.25695	-0.25701
P28336	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.25714	-0.25719
P28336	753	Clc1cc(Br)ccc1	-0.26013	-0.26017
P28336	314	O-P	-0.26118	-0.26122
P28336	2	>= 16 H	-0.26253	-0.26257
P28336	7	>= 2 B	-0.26455	-0.2646
P28336	26	>= 1 Na	-0.26485	-0.2649
P28336	296	C-Se	-0.26541	-0.26546
P28336	436	C(-C)(-H)(=O)	-0.26617	-0.28175
P28336	768	Sc1c(Cl)cccc1	-0.26709	-0.26714
P28336	227	>= 1 any ring size 8	-0.26742	-0.26747
P28336	523	N:C:C-C	-0.27704	-0.26858
P28336	432	C(-C)(-C)(=O)	-0.29497	-0.30132
P28336	509	Br-C:C-C	-0.30212	-0.31139
P28336	342	C(~C)(~Cl)	-0.30407	-0.30875
P28336	470	C:C-C=C	-0.30421	-0.29667
P28336	574	O-C-C:C-C	-0.3044	-0.30555
P28336	422	N=N	-0.3075	-0.31976
P28336	820	CC1C(S)CCCC1	-0.31026	-0.30755
P28336	371	C(~H)(:C)(:C)	-0.32019	-0.32379
P28336	491	C-N:C-[#1]	-0.32609	-0.30973
P28336	634	C-C-C:C-C	-0.3261	-0.31858

P28336	351	C(~C)(~N)	-0.32965	-0.32212
P28336	618	C:C-C-C:C	-0.33653	-0.329
P28336	656	C-C-N-C-C	-0.35247	-0.34324
P28336	398	N(~H)(~N)	-0.36591	-0.36345
P28336	848	OC1CC(Cl)CC1	-0.41923	-0.41915
P28336	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	-0.42519	-0.42022
P28336	111	>= 1 Tm	-0.43107	-0.43099
P28336	418	C=N	-0.44168	-0.42896
P28336	488	N-C=N-[#1]	-0.46714	-0.45645
P28336	107	>= 1 Tb	-0.52447	-0.52439
P28336	528	[#1]-N-C-[#1]	-0.57936	-0.57133
P28336	741	Oc1cc(S)ccc1	-0.60336	-0.60328
P28336	738	Cc1cc(Cl)ccc1	-0.61601	-0.61595
P28336	310	O-Mg	-0.63827	-0.63817
P28336	648	O=N-C:C-N	-0.77351	-0.74388
P28336	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	-0.79461	-0.75224
P28336	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	-0.92652	-0.91936
P28336	797	CC1CC(C)CCC1	-0.97051	-0.96903
P28336	707	O=C-C-C-C-C(N)-C	-1.03325	-0.99564

rints（continued)

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-0.03761

Data S1. Ranking of importance of substructure features from Pubchem Fingerpı

GPCR ID	Bit Posit	Bit Substructure	W	P
P32247	695	O=C-C-C-C-C-N	0.9622178	0.868863
P32247	213	>= 1 any ring size 7	0.9006924	0.807261
P32247	144	>= 1 saturated or aromatic carbon-only ring size 5	0.540545	0.450811
P32247	192	>= 3 any ring size 6	0.5387484	0.423132
P32247	539	N=C-C-[#1]	0.5232268	0.439581
P32247	364	C(~F)(:C)	0.4895942	0.367322
P32247	338	C(~C)(~C)(~H)(~N)	0.4738122	0.423568
P32247	720	Oc1ccc(S)cc1	0.4732839	0.455631
P32247	484	N-C:N:C	0.4616958	0.378978
P32247	597	O=C-C-C:C	0.3942852	0.223446
P32247	632	C-C-O-C:C	0.3471782	0.301371
P32247	25	>= 4 F	0.3378911	0.299945
P32247	640	C=C-C-C-C	0.3327117	0.374022
P32247	434	C(-C)(-H)(=C)	0.3325268	0.374192
P32247	549	N-C-C:C	0.3266483	0.393342
P32247	461	O-C-C=N	0.3234828	0.180052
P32247	826	OC1C(N)CCCC1	0.3222396	0.306695
P32247	738	Cc1cc(Cl)ccc1	0.2983153	0.292572
P32247	485	N:C:C:N	0.2959672	0.148919
P32247	510	[#1]-N-N-[#1]	0.2725768	0.128447
P32247	24	>= 2 F	0.2691409	0.121983
P32247	543	O-C:C-N	0.2689695	0.084012
P32247	472	C:N:C-C	0.2684328	0.248979
P32247	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.268136	0.268195
P32247	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.2678534	0.267901
P32247	854	NC1CC(N)CC1	0.2657798	0.265832
P32247	856	NC1CC(Br)CC1	0.2637133	0.263748
P32247	248	>= 1 any ring size 10	0.262573	0.262607
P32247	324	P-P	0.2595158	0.259583
P32247	714	Cc1ccc(O)cc1	0.2585018	0.109127
P32247	560	N-C-N-C	0.2564864	0.127595
P32247	87	>= 1 Hf	0.2527683	0.252821
P32247	346	C(~C)(~H)(~O)	0.2525815	0.11359
P32247	273	B-B	0.2510152	0.25105
P32247	105	>= 1 Eu	0.2486638	0.248731
P32247	75	>= 1 Rh	0.2480517	0.248096
P32247	627	O=[As]-C:C:C	0.2461274	0.246155
P32247	654	N-C-N-C-C	0.2460509	0.117146
P32247	823	CC1C(Br)CCCC1	0.2428182	0.242838
P32247	448	C(-H)(=O)	0.2418411	0.218768
P32247	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.2396816	0.239744
P32247	27	>= 2 Na	0.2370178	0.237052
P32247	831	SC1C(Cl)CCCC1	0.2351189	0.235155
P32247	104	>= 1 Sm	0.234974	0.235037
P32247	37	>= 1 Cl	0.2346268	0.231372
P32247	609	Cl-C-C-N-C	0.232973	0.266813

P32247	52	>= 1 Ca	0.2243981	0.224448
P32247	334	C(~C)(~C)(~C)(~C)	0.2222125	0.115365
P32247	257	>= 2 aromatic rings	0.2210781	0.221104
P32247	789	SC1CCC(Cl)CC1	0.2140146	0.214077
P32247	711	C-C(C)(C)-C-C	0.2139868	0.135283
P32247	642	O-C-C-C=O	0.2069953	0.133734
P32247	307	N-Br	0.2069029	0.206947
P32247	573	O-C-C=C	0.2041956	0.134852
P32247	106	>= 1 Gd	0.2026093	0.202647
P32247	482	C:N-C:C	0.2023081	0.188192
P32247	114	>= 1 U	0.1995962	0.199659
P32247	808	SC1CC(S)CCC1	0.1969704	0.197006
P32247	598	Cl-C:C:C-C	0.1961096	0.192851
P32247	28	>= 1 Si	0.194469	0.219769
P32247	488	N-C=N-[#1]	0.1926213	0.078815
P32247	404	N(:C)(:C)(:C)	0.192436	0.192368
P32247	527	C:C:N-[#1]	0.1875703	0.085571
P32247	779	CC1CCC(N)CC1	0.1863318	0.074199
P32247	793	NC1CCC(Br)CC1	0.1778304	0.177874
P32247	497	O-C:C:N	0.1758526	0.00648
P32247	777	CC1CCC(O)CC1	0.1746553	0.025262
P32247	716	Cc1ccc(N)cc1	0.1726604	0.056529
P32247	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.1723834	0.172311
P32247	116	>= 1 saturated or aromatic carbon-only ring size 3	0.1714772	0.091337
P32247	171	>= 5 any ring size 5	0.1713923	0.118849
P32247	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.166442	0.136851
P32247	286	C-O	0.1662222	0.072466
P32247	816	ClC1CC(Br)CCC1	0.1621566	0.162198
P32247	605	O=C-C-O-C	0.1605867	0.072217
P32247	745	Sc1cc(S)ccc1	0.1604233	0.160438
P32247	499	N-C:C:N	0.1585116	0.028519
P32247	635	N-N-C-N-[#1]	0.1580269	0.030148
P32247	16	>= 4 N	0.1572729	0.107469
P32247	462	O-C-C=O	0.1559433	0.094172
P32247	400	N(~H)(:C)(:C)	0.1556712	0
P32247	770	Nc1c(N)cccc1	0.1545321	0.238485
P32247	705	O=C-C-C-C-C(O)-C	0.1526445	0.014864
P32247	614	C-C-O-C-C	0.1522449	0.062212
P32247	537	O=C-C-O	0.1495185	0.087736
P32247	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.1477614	0.076753
P32247	515	N-N-C-C	0.1442902	0.036923
P32247	616	C:C:N:N:C	0.1441182	0.013055
P32247	357	C(~C)(:C)(:N)	0.1434939	0.07746
P32247	431	C(-C)(-C)(=N)	0.1432611	0.062081
P32247	601	N-C:C:C-N	0.1388089	0.05332
P32247	544	O-C:C-O	0.1382217	0.10686
P32247	260	>= 3 hetero-aromatic rings	0.1361457	0.136196
P32247	822	CC1C(Cl)CCCC1	0.1312218	0.093755

P32247	824	OC1C(O)CCCC1	0.1304131	0.099041
P32247	693	O=C-C-C-C-C-O	0.1287732	0.018831
P32247	277	B-F	0.1246479	0.124657
P32247	409	O(:C)(:C)	0.1245959	0.053956
P32247	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.1239299	0.063219
P32247	766	Sc1c(S)cccc1	0.1236857	0.123752
P32247	80	>= 1 Sn	0.1223572	0.122396
P32247	740	Oc1cc(O)ccc1	0.1205301	0.129908
P32247	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.120155	0.007908
P32247	185	>= 2 any ring size 6	0.1199151	-0.00362
P32247	702	O-C-C-C-C-C-N-C	0.1195465	0.044253
P32247	506	C-C:N:C	0.1189235	0.099381
P32247	522	C-N-N-[#1]	0.1176339	0
P32247	424	N=P	0.1171024	0.117136
P32247	305	N-S	0.1164179	0.077541
P32247	311	O-Na	0.1150459	0.115072
P32247	746	Sc1cc(N)ccc1	0.1141666	0.1142
P32247	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.112968	0.030539
P32247	645	O=C-N-C-C	0.1127051	0.064397
P32247	478	S-C=N-[#1]	0.1096029	0.067506
P32247	115	>= 1 any ring size 3	0.1078081	0.027678
P32247	150	>= 2 any ring size 5	0.1061696	0.021999
P32247	432	C(-C)(-C)(=O)	0.1047747	0.05531
P32247	692	O=C-C-C-C-C-C	0.1046903	0.034423
P32247	498	O-C=C-C	0.1042187	0.076697
P32247	374	C(~H)(~H)(~H)	0.1039472	0
P32247	26	>= 1 Na	0.1023134	0.10235
P32247	143	>= 1 any ring size 5	0.1012225	0.03793
P32247	584	C:C-C=C-C	0.0976514	0.139098
P32247	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.0971245	0.041728
P32247	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.0939184	0.093944
P32247	771	Nc1c(Cl)cccc1	0.0933424	0.071789
P32247	594	C-O-C-C=C	0.093022	0.095777
P32247	621	N-C:C:C:N	0.0915007	0.004597
P32247	393	N(~C)(~H)	0.0910532	0.080388
P32247	574	O-C-C:C-C	0.091034	0.035378
P32247	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.0877509	0.087702
P32247	343	C(~C)(~Cl)(~H)	0.0874851	0.087432
P32247	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0866075	0.086581
P32247	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0865468	0.086507
P32247	325	As-H	0.0858645	0.085843
P32247	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.0855588	0.085525
P32247	737	Cc1cc(N)ccc1	0.0842985	0.001314
P32247	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0828695	0.050847
P32247	5	>= 2 Li	0.0825488	0.082596
P32247	97	>= 1 Pb	0.081834	0.08183
P32247	278	B-Si	0.0815072	0.081478
P32247	103	>= 1 Pm	0.0812827	0.081267

P32247	684	O=C-C-C-C-C	0.0810018	0.010717
P32247	102	>= 1 Nd	0.0805281	0.080546
P32247	783	OC1CCC(S)CC1	0.0799036	0.06214
P32247	392	N(~C)(~C)(~H)	0.0793926	-0.00291
P32247	880	BrC1C(Br)CCC1	0.0792684	0.079219
P32247	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0787787	0.026446
P32247	2	>= 16 H	0.0782998	0.078296
P32247	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0779421	0.011912
P32247	411	P(~O)(~O)	0.0776875	0.077678
P32247	697	C-C-C-C-C-C(C)-C	0.0775137	0.008108
P32247	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.0760349	0.064284
P32247	529	Cl-C-C-Cl	0.0747217	0.073864
P32247	398	N(~H)(~N)	0.0733265	0.048848
P32247	313	O-Si	0.0727751	0.072756
P32247	650	O=C-N-C=O	0.0727495	0.076368
P32247	668	C-C:C-C-C	0.0726789	0.114133
P32247	36	>= 8 S	0.0726161	0.07259
P32247	335	C(~C)(~C)(~C)(~H)	0.0725503	-0.00732
P32247	548	O-C-C:C	0.0717321	0.002333
P32247	517	N-N-C-N	0.0711206	0.051497
P32247	436	C(-C)(-H)(=O)	0.0706656	0
P32247	17	>= 8 N	0.0687873	0.097234
P32247	524	C-C=C-C	0.0682753	0.109716
P32247	67	>= 1 Kr	0.0671944	0.067186
P32247	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.0662547	0.016035
P32247	648	O=N-C:C-N	0.0651448	0.073041
P32247	864	CC1C(Cl)CCC1	0.0649935	0.064987
P32247	765	Oc1c(Br)cccc1	0.0645747	0.064539
P32247	677	C-C=C-C:C	0.0645038	0.105812
P32247	447	C(-H)(=N)	0.0629003	0.095754
P32247	878	ClC1C(Cl)CCC1	0.0625748	0.062531
P32247	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0620645	-0.00898
P32247	662	O-C-C-O-C	0.0620563	0
P32247	415	Si(~C)(~C)	0.0620281	0.087252
P32247	519	N=C-N-C	0.061637	-0.02097
P32247	759	Cc1c(Cl)cccc1	0.0614001	0.023973
P32247	849	OC1CC(Br)CC1	0.0609796	0.060992
P32247	546	N-C:C-[#1]	0.0603361	0.014294
P32247	873	SC1C(Cl)CCC1	0.0602792	0.060255
P32247	827	OC1C(Cl)CCCC1	0.0600266	0.035538
P32247	596	N=C-N-C-C	0.0581819	-0.02443
P32247	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.05812	0.058113
P32247	475	S-C=N-C	0.0568531	0.014768
P32247	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0565461	0.050644
P32247	703	O-C-C-C-C-C(N)-C	0.0563512	-0.00955
P32247	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0560218	0.000608
P32247	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.0552858	0.002742
P32247	874	SC1C(Br)CCC1	0.055203	0.05526

P32247	590	C-C:C-O-[#1]	0.0545309	-0.00133
P32247	638	O-C-C-C-N	0.0543373	0.000745
P32247	577	C:C-N-C:C	0.0535343	0.000772
P32247	508	S=C-N-C	0.0533562	-0.00713
P32247	7	>= 2 B	0.0531395	0.05313
P32247	622	O=C-O-C:C	0.0525813	0.003327
P32247	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.0517952	-0.00076
P32247	289	C-Mg	0.0516205	0.051628
P32247	378	C(~N)(:C)(:N)	0.050107	0.000496
P32247	35	>= 4 S	0.0499095	0.049846
P32247	758	Cc1c(N)cccc1	0.0493177	0
P32247	576	N=C-C:C-[#1]	0.0488365	0
P32247	530	N:C-C:C	0.0485963	0
P32247	820	CC1C(S)CCCC1	0.0481893	0.060815
P32247	271	Li-Cl	0.048118	0.048096
P32247	559	O-C-N-[#1]	0.0470687	0.030604
P32247	489	N-C-S-C	0.0468521	0.00844
P32247	523	N:C:C-C	0.0467445	0.032603
P32247	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0464258	0.010253
P32247	846	OC1CC(S)CC1	0.0456913	0.045683
P32247	341	C(~C)(~C)(~O)	0.0456446	0.004128
P32247	47	>= 2 I	0.0441148	0.044152
P32247	729	Nc1ccc(Cl)cc1	0.0435427	0.108175
P32247	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.0434116	-0.00911
P32247	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0430907	0.043105
P32247	40	>= 8 Cl	0.0425327	0.042493
P32247	602	O=C-C-N-C	0.0424442	0.051837
P32247	274	B-C	0.0424332	0.042402
P32247	0	>= 4 H	0.0421269	0.042131
P32247	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0418617	0.041898
P32247	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.0416142	0.041638
P32247	581	O=C-C-C-O	0.0415952	-0.0317
P32247	547	N-C:C-N	0.0412636	0.004942
P32247	31	>= 2 P	0.040723	0.04073
P32247	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0406724	0.040696
P32247	502	N-C=C-[#1]	0.0398324	-0.00629
P32247	473	S-C:N:C	0.0397586	-0.00229
P32247	270	Li-S	0.0394725	0.039479
P32247	835	NC1C(Br)CCCC1	0.0390732	0.039062
P32247	483	N-S-C:C	0.0388281	0
P32247	587	N-C:C-O-[#1]	0.0387402	0.015268
P32247	77	>= 1 Ag	0.0384337	0.038446
P32247	511	S=C-N-[#1]	0.0379763	-0.02254
P32247	11	>= 8 C	0.0379688	0.079368
P32247	42	>= 2 K	0.0374228	0.037452
P32247	550	Cl-C-C-C	0.0373781	0.034082
P32247	800	CC1CC(N)CCC1	0.0372633	0.001247
P32247	781	CC1CCC(Br)CC1	0.0364026	0.041776

P32247	406	O(~C)(~H)	0.0358197	-0.00068
P32247	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.035796	0.035798
P32247	504	N:C:N-C	0.0357268	0.002739
P32247	567	O-C-C-O	0.0354655	0
P32247	733	Brc1ccc(Br)cc1	0.0346584	0.034694
P32247	663	O-C-C-O-[#1]	0.0339946	0.029244
P32247	788	SC1CCC(N)CC1	0.0338797	0.033896
P32247	571	[#1]-C-O-[#1]	0.0338543	0.001936
P32247	487	N-C=N-C	0.0337948	0.045389
P32247	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0335553	0
P32247	389	C(:N)(:N)	0.0333846	0.000415
P32247	308	O-H	0.032944	-0.00353
P32247	630	O-C:C-O-C	0.0313603	0
P32247	348	C(~C)(~H)(~P)	0.0308254	0.030792
P32247	787	SC1CCC(S)CC1	0.0305817	0.016695
P32247	629	S-C:C:C-N	0.0301402	-0.01582
P32247	109	>= 1 Ho	0.0296697	0.029698
P32247	453	N(-C)(=C)	0.0293128	0
P32247	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.0289646	0.017191
P32247	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.0274834	0.027502
P32247	513	S:C:C-[#1]	0.0270466	0.090379
P32247	836	ClC1C(Cl)CCCC1	0.0267203	0.025859
P32247	798	CC1CC(O)CCC1	0.0265618	0
P32247	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0260506	0.013712
P32247	735	Cc1cc(O)ccc1	0.0259244	-0.0006
P32247	867	OC1C(S)CCC1	0.0251531	0.025128
P32247	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0250399	0.025003
P32247	659	O-C-C-N-C	0.0245537	-0.04467
P32247	877	NC1C(Br)CCC1	0.024545	0.024524
P32247	764	Oc1c(Cl)cccc1	0.0245277	0
P32247	551	Cl-C-C-O	0.0244854	0
P32247	34	>= 2 S	0.0235546	2.54E-05
P32247	30	>= 1 P	0.0235378	0.023496
P32247	53	>= 1 Sc	0.022546	0.022544
P32247	98	>= 1 Bi	0.0225077	0.022509
P32247	331	C(~Br)(:N)	0.0224958	0.022487
P32247	778	CC1CCC(S)CC1	0.0224922	-0.00559
P32247	784	OC1CCC(N)CC1	0.0224711	0.009574
P32247	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0223309	0.02235
P32247	12	>= 16 C	0.0223263	0.002472
P32247	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0222172	0.022246
P32247	421	C=S	0.0219068	0
P32247	293	C-S	0.0218729	0.007097
P32247	610	C-O-C-O-C	0.0217375	-0.00459
P32247	739	Cc1cc(Br)ccc1	0.0217113	0.021688
P32247	572	N:C:N:C	0.0216208	-0.01132
P32247	295	C-As	0.0211946	0.021155
P32247	442	C(-C)(=N)	0.0209531	-0.00838

P32247	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.0202276	0.020236
P32247	555	N=C-C=C	0.0202112	0.008333
P32247	712	C-C(C)-C(C)-C	0.0198813	0
P32247	403	N(:C)(:C)	0.0195264	0
P32247	445	C(-H)(-N)(=C)	0.0194473	0.000995
P32247	563	O-C-O-C	0.0185225	-0.00777
P32247	29	>= 2 Si	0.0183933	0.018372
P32247	288	C-Na	0.0182066	0.01819
P32247	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.0176344	0.017606
P32247	316	F-P	0.017453	0.017479
P32247	413	S(~C)(~H)	0.0169473	0.02467
P32247	749	Nc1cc(N)ccc1	0.0168247	0.009153
P32247	298	C-I	0.0167374	0.016699
P32247	722	Oc1ccc(Cl)cc1	0.0165084	0
P32247	661	O-C-O-C-C	0.0163767	-0.00995
P32247	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0159759	0.016035
P32247	86	>= 1 Lu	0.0158492	0.015876
P32247	678	C-C-C=C-C	0.0154749	0.056855
P32247	569	N-C-C-N	0.0153956	0.009451
P32247	553	O=C-C=C	0.0153252	-0.01717
P32247	443	C(-C)(=O)	0.0149229	0.058024
P32247	682	O-C-C-C-C-N	0.0149211	-0.00054
P32247	33	>= 1 S	0.0147287	0
P32247	267	Li-O	0.0145692	0.014578
P32247	541	O-C:C-C	0.0145478	-0.01294
P32247	724	Sc1ccc(S)cc1	0.013862	-1.08E-05
P32247	72	>= 1 Nb	0.0133718	0.013379
P32247	304	N-P	0.0131682	0.013184
P32247	112	>= 1 Yb	0.0131063	0.013118
P32247	700	O-C-C-C-C-C-O-C	0.0130262	0
P32247	721	Oc1ccc(N)cc1	0.0125989	-0.00033
P32247	122	>= 2 any ring size 3	0.0123744	0.012388
P32247	164	>= 4 any ring size 5	0.0123039	-0.0154
P32247	58	>= 1 Fe	0.012051	0.012023
P32247	337	C(~C)(~C)(~C)(~O)	0.011819	0.013337
P32247	391	N(~C)(~C)(~C)	0.0113728	0.020537
P32247	611	N-C-C-N-C	0.0113021	0
P32247	469	S-S-C:C	0.0112764	0.011295
P32247	646	O=C-N-C-[#1]	0.0111367	-0.00398
P32247	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.0107755	0.010777
P32247	829	SC1C(S)CCCC1	0.0106232	0.01062
P32247	299	N-H	0.010596	-3.51E-05
P32247	869	OC1C(Cl)CCC1	0.0105038	0.010467
P32247	62	>= 1 Zn	0.0098726	0.009849
P32247	797	CC1CC(C)CCC1	0.0094481	0.026629
P32247	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0094406	-0.00262
P32247	45	>= 4 Br	0.0092159	0.009224
P32247	837	ClC1C(Br)CCCC1	0.0090943	0.009108

P32247	345	C(~C)(~H)(~N)	0.0086016	0.032664
P32247	387	C(:C)(:N)	0.0084217	-0.00575
P32247	769	Sc1c(Br)cccc1	0.0080638	0.008054
P32247	812	NC1CC(N)CCC1	0.0079739	0.000314
P32247	679	C-C-C-C-C-C	0.0078865	-0.00225
P32247	386	C(:C)(:C)(:N)	0.0078101	-0.03584
P32247	99	>= 1 La	0.0076702	0.007704
P32247	802	CC1CC(Br)CCC1	0.0073172	0.007331
P32247	859	BrC1CC(Br)CC1	0.0072533	0.007255
P32247	101	>= 1 Pr	0.0071266	0.007144
P32247	401	N(~O)(~O)	0.007098	0
P32247	425	P=O	0.0069466	0.006966
P32247	310	O-Mg	0.0066662	0.00666
P32247	129	>= 1 any ring size 4	0.0064314	0.001269
P32247	367	C(~H)(~O)(~O)	0.0064007	-0.02786
P32247	69	>= 1 Sr	0.0061836	0.006146
P32247	256	>= 1 hetero-aromatic ring	0.0059953	0.005994
P32247	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0057545	0.005758
P32247	631	O-C:C-O-[#1]	0.0052764	0.005235
P32247	623	O=C-C:C-C	0.0050109	0.005332
P32247	641	O-C-C-C=C	0.0049556	0.036352
P32247	803	OC1CC(O)CCC1	0.0047707	0.014122
P32247	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.0047578	0.004741
P32247	688	C-C-C-C-C-C-C	0.004752	-0.00368
P32247	269	Li-P	0.0044272	0.00443
P32247	446	C(-H)(=C)	0.0044141	0.046013
P32247	44	>= 2 Br	0.0043685	0.004392
P32247	857	ClC1CC(Cl)CC1	0.0043273	0.004328
P32247	728	Nc1ccc(N)cc1	0.0041167	-0.00489
P32247	617	C-C-C-O-[#1]	0.0036289	-0.02146
P32247	107	>= 1 Tb	0.0035146	0.003548
P32247	294	C-Cl	0.0030014	-0.00027
P32247	261	>= 4 aromatic rings	0.0029477	0.002944
P32247	715	Cc1ccc(S)cc1	0.0027429	-0.02532
P32247	408	O(~H)(~S)	0.002624	0.021178
P32247	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.0025478	0.04612
P32247	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0024846	-0.00267
P32247	751	Nc1cc(Br)ccc1	0.002376	0.002393
P32247	474	S:C:C:N	0.0023218	0.002302
P32247	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.0020385	0.002026
P32247	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0016923	0.001676
P32247	317	F-S	0.001513	0.001538
P32247	258	>= 2 hetero-aromatic rings	0.0015008	0.00151
P32247	457	S(-C)(=O)	0.0014452	0
P32247	320	Si-H	0.0014209	0.00145
P32247	753	Clc1cc(Br)ccc1	0.0013302	0.001343
P32247	534	S-C:C-O	0.001208	0.001196
P32247	39	>= 4 Cl	0.0012071	0.00121

P32247	43	>= 1 Br	0.0010157	0.00638
P32247	526	Cl-C:C-Cl	0.000849	0
P32247	852	SC1CC(Cl)CC1	0.0008342	0.000852
P32247	60	>= 1 Ni	0.0008276	0.000817
P32247	309	O-O	0.0007942	0.000786
P32247	865	CC1C(Br)CCC1	0.0007548	0.000765
P32247	828	OC1C(Br)CCCC1	0.0007094	0.00068
P32247	402	N(~O)(:O)	0.0005227	0.000496
P32247	89	>= 1 W	0.0004414	0.000441
P32247	272	B-H	0.0003633	0.0004
P32247	479	S-C-S-C	0.0002302	0.000229
P32247	1	>= 8 H	0.0002269	0.000201
P32247	81	>= 1 Sb	0.0001602	0.000154
P32247	810	SC1CC(Cl)CCC1	5.09E-05	0
P32247	876	NC1C(Cl)CC1	4.31E-05	0
P32247	557	N:C-O-[#1]	3.66E-05	0
P32247	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	3.59E-05	0
P32247	460	C-C-C#C	3.10E-05	0
P32247	809	SC1CC(N)CCC1	2.45E-05	0
P32247	49	>= 1 Be	2.24E-05	1.18E-05
P32247	744	Oc1cc(Br)ccc1	2.12E-05	0
P32247	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	1.94E-05	0
P32247	71	>= 1 Zr	1.58E-05	0
P32247	50	>= 1 Mg	1.52E-05	0
P32247	268	Li-F	1.52E-05	0
P32247	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	1.49E-05	0
P32247	207	>= 5 saturated or aromatic carbon-only ring size 6	1.16E-05	0
P32247	807	OC1CC(Br)CCC1	1.07E-05	0
P32247	444	C(-Cl)(=O)	1.04E-05	0
P32247	79	>= 1 In	9.86E-06	0
P32247	276	B-O	8.79E-06	0
P32247	318	Al-H	5.01E-06	0
P32247	427	C(#C)(-C)	3.60E-06	0
P32247	76	>= 1 Pd	3.41E-06	0
P32247	845	OC1CC(O)CC1	2.64E-06	-3.28E-05
P32247	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	3.03E-07	0
P32247	280	B-S	-6.66E-07	0
P32247	726	Sc1ccc(Cl)cc1	-8.25E-07	0
P32247	82	>= 1 Te	-1.76E-06	0
P32247	847	OC1CC(N)CC1	-3.14E-06	0
P32247	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	-3.38E-06	0
P32247	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	-3.44E-06	0
P32247	266	Li-C	-4.02E-06	0
P32247	73	>= 1 Mo	-4.05E-06	0
P32247	481	O-S-C:C	-5.11E-06	0
P32247	319	Al-Cl	-6.90E-06	0
P32247	796	BrC1CCC(Br)CC1	-7.27E-06	0
P32247	57	>= 1 Mn	-7.99E-06	0

P32247	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	-8.64E-06	0
P32247	525	[As]-C:C-[#1]	-8.87E-06	0
P32247	512	C-[As]-O-[#1]	-1.10E-05	0
P32247	200	>= 4 saturated or aromatic carbon-only ring size 6	-1.17E-05	0
P32247	562	Br-C-C=O	-1.29E-05	0
P32247	61	>= 1 Cu	-1.77E-05	0
P32247	110	>= 1 Er	-1.85E-05	0
P32247	843	CC1CC(Cl)CC1	-1.85E-05	0
P32247	303	N-Si	-2.39E-05	0
P32247	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	-2.42E-05	0
P32247	875	NC1C(N)CCC1	-2.69E-05	0
P32247	66	>= 1 Se	-2.88E-05	0
P32247	292	C-P	-4.87E-05	-5.50E-05
P32247	32	>= 4 P	-8.45E-05	-0.00011
P32247	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	-0.000101	-8.00E-05
P32247	493	O=C-C:C	-0.000323	0
P32247	762	Oc1c(S)cccc1	-0.00036	-0.00034
P32247	234	>= 2 any ring size 8	-0.000372	-0.00037
P32247	64	>= 1 Ge	-0.000429	-0.00041
P32247	804	OC1CC(S)CCC1	-0.000462	-0.00043
P32247	681	O-C-C-C-C-O	-0.00048	-0.00224
P32247	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	-0.000751	-0.00076
P32247	853	SC1CC(Br)CC1	-0.000882	-0.00086
P32247	760	Cc1c(Br)cccc1	-0.000891	-0.00089
P32247	113	>= 1 Tc	-0.000924	-0.0009
P32247	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-0.001016	-0.00103
P32247	825	OC1C(S)CCCC1	-0.001161	-0.00115
P32247	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.001164	-0.00118
P32247	347	C(~C)(~H)(~O)(~O)	-0.001236	-0.00123
P32247	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	-0.001371	-0.00139
P32247	840	CC1CC(O)CC1	-0.001452	-0.00148
P32247	768	Sc1c(Cl)cccc1	-0.001475	-0.00148
P32247	727	Sc1ccc(Br)cc1	-0.001514	-0.00149
P32247	361	C(~Cl)(~H)	-0.001531	-0.00151
P32247	51	>= 1 Al	-0.001889	-0.00192
P32247	872	SC1C(N)CCC1	-0.001914	-0.00195
P32247	18	>= 1 O	-0.001952	0.070657
P32247	282	B-Br	-0.001981	-0.00197
P32247	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	-0.002004	-0.00203
P32247	666	C=C-C-O-C	-0.002024	0.000673
P32247	535	O=C-C-C	-0.002036	2.84E-05
P32247	428	C(#C)(-H)	-0.002103	-0.00207
P32247	227	>= 1 any ring size 8	-0.002212	-0.01397
P32247	136	>= 2 any ring size 4	-0.002297	-0.00229
P32247	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	-0.00277	-0.00279
P32247	41	>= 1 K	-0.00289	-0.0029
P32247	279	B-P	-0.002931	-0.00294
P32247	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.002974	-0.00298

P32247	492	N-C:O:C	−0.003022	−0.00301
P32247	589	C-C:C-O-C	−0.003422	0.024927
P32247	396	N(~C)(:C)	−0.003531	−0.01766
P32247	326	As-As	−0.00374	−0.00374
P32247	861	CC1C(O)CCC1	−0.003911	−0.0039
P32247	363	C(~F)(~F)	−0.003929	−0.00141
P32247	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.004115	−0.0041
P32247	670	Br-C:C:C-C	−0.004291	0.001097
P32247	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.004678	−0.0047
P32247	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.004721	−0.00476
P32247	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.004736	−0.00475
P32247	747	Sc1cc(Cl)ccc1	−0.005112	−0.00512
P32247	819	CC1C(O)CCCC1	−0.005118	0.016336
P32247	375	C(~N)(~N)	−0.005204	−0.01772
P32247	830	SC1C(N)CCCC1	−0.005332	−0.01032
P32247	718	Cc1ccc(Br)cc1	−0.00535	0
P32247	327	C(~Br)(~C)	−0.005355	0
P32247	509	Br-C:C-C	−0.005385	0
P32247	862	CC1C(S)CCC1	−0.005828	−0.00582
P32247	748	Sc1cc(Br)ccc1	−0.005993	−0.006
P32247	59	>= 1 Co	−0.006098	−0.00609
P32247	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.006807	−0.00682
P32247	834	NC1C(Cl)CCCC1	−0.006967	−0.02844
P32247	281	B-Cl	−0.007016	−0.00704
P32247	255	>= 1 aromatic ring	−0.0073	−0.00732
P32247	592	N-C-C-C-C	−0.007357	0.034028
P32247	763	Oc1c(N)cccc1	−0.007711	−0.02328
P32247	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.008058	0
P32247	420	C=O	−0.008152	0
P32247	637	O-C-C-C-C	−0.008357	0.010091
P32247	719	Oc1ccc(O)cc1	−0.008863	−0.03334
P32247	699	O-C-C-C-C-C(C)-C	−0.009003	−0.00883
P32247	575	O-C-C:C-O	−0.009312	0
P32247	858	ClC1CC(Br)CC1	−0.009333	−0.00931
P32247	691	O-C-C-C-C-C-N	−0.009607	0
P32247	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.009698	−0.00969
P32247	606	O-C:C-C-C	−0.010173	−0.03768
P32247	690	O-C-C-C-C-C-O	−0.010246	−0.00046
P32247	579	O=C-C-C-C	−0.010259	0.006445
P32247	701	O-C-C-C-C-C(O)-C	−0.010361	−0.00104
P32247	241	>= 1 any ring size 9	−0.010564	−0.01059
P32247	178	>= 1 any ring size 6	−0.010867	0.030547
P32247	767	Sc1c(N)cccc1	−0.011142	−0.01612
P32247	817	BrC1CC(Br)CCC1	−0.01131	−0.0113
P32247	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.011485	−0.00168
P32247	74	>= 1 Ru	−0.01174	−0.01173
P32247	868	OC1C(N)CCC1	−0.011884	−0.01187
P32247	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.011958	−0.01199

P32247	360	C(~Cl)(~Cl)	−0.012135	−0.01212
P32247	330	C(~Br)(:C)	−0.012314	−0.00695
P32247	410	P(~C)(~C)	−0.012823	−0.0128
P32247	554	Br-C-C-C	−0.012841	−0.00749
P32247	815	ClC1CC(Cl)CCC1	−0.013005	−0.00767
P32247	591	Cl-C-C-C-C	−0.013075	−0.01635
P32247	838	BrC1C(Br)CCCC1	−0.013864	−0.0139
P32247	199	>= 4 any ring size 6	−0.01394	0
P32247	372	C(~H)(:C)(:N)	−0.014276	−0.03276
P32247	850	SC1CC(S)CC1	−0.014795	−0.01477
P32247	111	>= 1 Tm	−0.015461	−0.01548
P32247	369	C(~H)(~Si)	−0.015587	−0.01558
P32247	582	C-C-C-C-C	−0.016113	0.025274
P32247	647	O=C-N-C-N	−0.016504	0.019731
P32247	821	CC1C(N)CCCC1	−0.016752	0
P32247	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.017787	−0.01778
P32247	756	Cc1c(O)cccc1	−0.018151	0.00329
P32247	422	N=N	−0.018223	0.075572
P32247	680	O-C-C-C-C-C	−0.01845	0
P32247	613	C-N-C-C-C	−0.020595	0.020819
P32247	265	Li-B	−0.020866	−0.02084
P32247	438	C(-C)(-N)(=N)	−0.021057	−0.02029
P32247	322	Si-Cl	−0.021324	−0.02133
P32247	520	C=C-C:C	−0.021514	0.019931
P32247	465	O=S-C-C	−0.021731	−0.02318
P32247	521	C:N-C-[#1]	−0.021936	0.007229
P32247	93	>= 1 Pt	−0.021947	−0.02196
P32247	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.02203	−0.02204
P32247	667	C=C-C-O-[#1]	−0.022132	−0.04809
P32247	314	O-P	−0.022523	−0.02255
P32247	698	O-C-C-C-C-C-C-C	−0.02253	0.030285
P32247	624	O=C-C:C-N	−0.022538	−0.02251
P32247	63	>= 1 Ga	−0.022566	−0.02254
P32247	604	C-O-C-C:C	−0.02266	−0.01996
P32247	55	>= 1 V	−0.022674	−0.02266
P32247	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.023	−0.02294
P32247	805	OC1CC(N)CCC1	−0.023094	−0.0485
P32247	761	Oc1c(O)cccc1	−0.024001	−0.0553
P32247	296	C-Se	−0.024563	−0.02455
P32247	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.02473	−0.02472
P32247	291	C-Si	−0.025223	0
P32247	466	N#C-C=C	−0.025231	0.009036
P32247	354	C(~C)(~Si)	−0.025265	0
P32247	14	>= 1 N	−0.02561	0.015812
P32247	625	O=C-C:C-O	−0.026547	−0.02654
P32247	643	[#1]-C-C-N-[#1]	−0.027132	0.006492
P32247	368	C(~H)(~S)	−0.027887	−0.00021
P32247	312	O-Al	−0.028786	−0.02882

P32247	92	>= 1 Ir	-0.02886	-0.02889
P32247	249	>= 1 saturated or aromatic carbon-only ring size 10	-0.028921	-0.02887
P32247	284	C-C	-0.028925	0.012448
P32247	491	C-N:C-[#1]	-0.02916	-2.61E-05
P32247	384	C(:C)(:C)	-0.029296	0.012093
P32247	639	O-C-C-C-O	-0.029591	0.002948
P32247	297	C-Br	-0.029646	-0.02429
P32247	419	C#N	-0.02993	0.006648
P32247	158	>= 3 saturated or aromatic carbon-only ring size 5	-0.030412	-0.03045
P32247	655	O-C-C-C:C	-0.030416	0.000957
P32247	342	C(~C)(~Cl)	-0.030811	-0.03413
P32247	83	>= 1 Xe	-0.031372	-0.03145
P32247	405	O(~C)(~C)	-0.031737	0.003193
P32247	359	C(~C)(:N)(:N)	-0.031908	0
P32247	673	O=C-C=C-N	-0.03213	0
P32247	108	>= 1 Dy	-0.034243	-0.03426
P32247	672	O=C-C=C-[#1]	-0.034924	-0.00677
P32247	750	Nc1cc(Cl)ccc1	-0.034953	-0.00046
P32247	507	C-C-S-C	-0.035578	0
P32247	429	C(#N)(-C)	-0.035679	0.00088
P32247	676	N#C-C-C-C	-0.036567	0
P32247	352	C(~C)(~O)	-0.036617	-0.00452
P32247	743	Oc1cc(Cl)ccc1	-0.037413	-0.05385
P32247	813	NC1CC(Cl)CCC1	-0.037464	-0.00299
P32247	585	C-C:C-N-C	-0.038166	-0.00041
P32247	455	N(-O)(=O)	-0.038399	-0.04548
P32247	785	OC1CCC(Cl)CC1	-0.038445	-0.05493
P32247	315	O-K	-0.038549	-0.03857
P32247	471	S:C:C:C	-0.038564	0
P32247	696	C-C-C-C-C-C-C-C	-0.039205	0.010187
P32247	516	[#1]-C=C-[#1]	-0.039209	0.002408
P32247	262	>= 4 hetero-aromatic rings	-0.039415	-0.03939
P32247	791	NC1CCC(N)CC1	-0.039594	-0.02671
P32247	723	Oc1ccc(Br)cc1	-0.039742	-0.03972
P32247	355	C(~C)(:C)	-0.040113	0.001293
P32247	774	Clc1c(Br)cccc1	-0.040145	-0.0401
P32247	356	C(~C)(:C)(:C)	-0.040656	-0.0211
P32247	518	O=C-N-N	-0.040817	-0.01267
P32247	321	Si-Si	-0.040825	-0.04082
P32247	782	OC1CCC(O)CC1	-0.040828	-0.06532
P32247	564	C=C-C=C	-0.040867	0.000537
P32247	664	C-C=C-C=C	-0.041027	0.000364
P32247	752	Clc1cc(Cl)ccc1	-0.041119	-0.03574
P32247	634	C-C-C:C-C	-0.041344	3.12E-05
P32247	470	C:C-C=C	-0.041401	0
P32247	556	C=C-C-C	-0.041407	0
P32247	390	N(~C)(~C)	-0.041412	0
P32247	10	>= 4 C	-0.041492	-8.81E-05

P32247	879	ClC1C(Br)CCC1	−0.041703	−0.04172
P32247	323	P-H	−0.042253	−0.04227
P32247	353	C(~C)(~S)	−0.042688	0.003047
P32247	612	N-C-O-C-C	−0.042999	−0.0115
P32247	463	N:C-S-[#1]	−0.043071	−0.04308
P32247	382	C(~O)(:C)(:C)	−0.043136	0
P32247	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.043599	0
P32247	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.043631	0.049449
P32247	283	C-H	−0.043632	−0.00224
P32247	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.047074	−0.08059
P32247	349	C(~C)(~H)(~S)	−0.047154	0
P32247	328	C(~Br)(~C)(~C)	−0.047534	−0.0422
P32247	370	C(~H)(:C)	−0.047894	−0.00627
P32247	48	>= 4 I	−0.047918	−0.04787
P32247	96	>= 1 Tl	−0.04823	−0.04822
P32247	626	C-O-C:C-C	−0.049205	−0.0208
P32247	9	>= 2 C	−0.049365	−0.00795
P32247	468	O=S-C-N	−0.049513	−0.0766
P32247	416	C=C	−0.051081	−0.00966
P32247	540	C-N-C-[#1]	−0.051156	−0.03078
P32247	285	C-N	−0.051316	−0.0099
P32247	383	C(~S)(:C)	−0.052048	0.00629
P32247	458	S(-O)(=O)	−0.052208	−0.03366
P32247	600	N-C:C:C-C	−0.052912	0
P32247	599	[#1]-C-C=C-[#1]	−0.053711	−0.00191
P32247	615	N-C-C-O-C	−0.054692	−0.00816
P32247	366	C(~H)(~O)	−0.057502	0.008578
P32247	423	N=O	−0.05824	0.000191
P32247	578	C-C:C-C:C	−0.059011	−0.01758
P32247	531	S-C:C-C	−0.059398	−0.00107
P32247	514	O-N-C-C	−0.061221	−0.00278
P32247	686	O=C-C-C-C-O	−0.06191	−0.05747
P32247	344	C(~C)(~H)	−0.062807	−0.02139
P32247	786	OC1CCC(Br)CC1	−0.062808	−0.06276
P32247	694	O=C-C-C-C-C=O	−0.063457	−0.00946
P32247	456	P(-O)(=O)	−0.063816	−0.06378
P32247	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.06396	−0.00501
P32247	773	Clc1c(Cl)cccc1	−0.064118	−0.06493
P32247	851	SC1CC(N)CC1	−0.064698	−0.06473
P32247	542	O-C:C-[#1]	−0.065375	−0.09293
P32247	536	O=C-C-N	−0.065497	−0.05073
P32247	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.065697	−0.00188
P32247	644	C-C=N-N-C	−0.066344	0.083231
P32247	38	>= 2 Cl	−0.066674	3.68E−05
P32247	437	C(-C)(-N)(=C)	−0.0669	−0.11305
P32247	503	Cl-C:C-[#1]	−0.066978	−0.07939
P32247	533	S-C:C-N	−0.067876	−0.00105
P32247	839	CC1CC(C)CC1	−0.067932	−0.0019

P32247	734	Cc1cc(C)ccc1	−0.068043	−0.00705
P32247	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.069411	0
P32247	287	C-F	−0.069581	−0.06557
P32247	754	Brc1cc(Br)ccc1	−0.069824	−0.06979
P32247	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.072694	−0.07266
P32247	732	Clc1ccc(Br)cc1	−0.074285	−0.07432
P32247	373	C(~H)(:N)	−0.074722	−0.04558
P32247	395	N(~C)(~O)	−0.074793	−0.01633
P32247	755	Cc1c(C)cccc1	−0.075219	0
P32247	656	C-C-N-C-C	−0.075739	−0.02304
P32247	394	N(~C)(~H)(~N)	−0.075984	0.012495
P32247	376	C(~N)(:C)	−0.076708	−0.0389
P32247	619	O-C-C=C-C	−0.077353	−0.13309
P32247	832	SC1C(Br)CCCC1	−0.079013	−0.07904
P32247	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.079253	−0.07923
P32247	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.079371	−0.07935
P32247	552	C:C-C:C	−0.079663	−0.03828
P32247	595	C:C-C-C-C	−0.079682	−0.0383
P32247	710	C-C-C(C)-C-C	−0.079777	0
P32247	593	N-C-C-C-N	−0.079808	−0.03235
P32247	94	>= 1 Au	−0.080084	−0.08005
P32247	792	NC1CCC(Cl)CC1	−0.080199	−0.01557
P32247	56	>= 1 Cr	−0.080539	−0.08051
P32247	46	>= 1 I	−0.081151	−0.08109
P32247	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.081747	−0.0818
P32247	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.082234	−0.08219
P32247	350	C(~C)(~I)	−0.082308	−0.08228
P32247	841	CC1CC(S)CC1	−0.082429	−0.08245
P32247	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.082441	−0.08243
P32247	70	>= 1 Y	−0.082623	−0.08258
P32247	15	>= 2 N	−0.083449	−0.04205
P32247	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.083776	−0.08374
P32247	586	C-S-C-C-C	−0.084499	−0.0489
P32247	54	>= 1 Ti	−0.084649	−0.08458
P32247	68	>= 1 Rb	−0.08547	−0.08546
P32247	23	>= 1 F	−0.085481	−0.05629
P32247	709	C-C(C)-C-C-C	−0.085676	−0.00588
P32247	561	Cl-C-C=O	−0.085755	−0.08572
P32247	731	Clc1ccc(Cl)cc1	−0.085772	−0.08579
P32247	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.085879	−0.08586
P32247	848	OC1CC(Cl)CC1	−0.086068	−0.08605
P32247	333	C(~C)(~C)(~C)	−0.086249	−0.08184
P32247	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.086268	−0.08625
P32247	441	C(-C)(=C)	−0.086306	−0.04492
P32247	653	O-C:C:C-O	−0.086312	−0.07701
P32247	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.086347	−0.08633
P32247	451	C(-N)(=O)	−0.086552	−0.00078
P32247	397	N(~C)(:C)(:C)	−0.087124	−0.08711

P32247	855	NC1CC(Cl)CC1	−0.087431	−0.08746
P32247	407	O(~C)(~P)	−0.087567	−0.08752
P32247	741	Oc1cc(S)ccc1	−0.087771	−0.08778
P32247	706	O=C-C-C-C-C(=O)-C	−0.088099	−0.08806
P32247	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.088127	−0.08809
P32247	100	>= 1 Ce	−0.08814	−0.08811
P32247	657	C-N-C:C-C	−0.088158	−0.05041
P32247	78	>= 1 Cd	−0.088315	−0.08827
P32247	568	N#C-C-C	−0.088627	−0.05208
P32247	633	N-C-C:C-C	−0.089657	0.001656
P32247	301	N-O	−0.091292	−0.03284
P32247	658	C-C-S-C-C	−0.092296	−0.00776
P32247	435	C(-C)(-H)(=N)	−0.092399	−0.10722
P32247	454	N(-C)(=O)	−0.092531	−0.0341
P32247	340	C(~C)(~C)(~N)	−0.093505	0.023549
P32247	430	C(-C)(-C)(=C)	−0.093829	−0.07421
P32247	414	S(~C)(~O)	−0.096508	−0.09796
P32247	22	>= 16 O	−0.096512	−0.01143
P32247	371	C(~H)(:C)(:C)	−0.097126	−0.05552
P32247	565	C:C-O-C	−0.097705	−0.06933
P32247	871	SC1C(S)CCC1	−0.097852	−0.09789
P32247	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.098208	−0.03925
P32247	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.099444	−0.03564
P32247	459	S(=O)(=O)	−0.099611	−0.07386
P32247	275	B-N	−0.09966	−0.09966
P32247	450	C(-N)(=N)	−0.10079	−0.07066
P32247	708	C-C(C)-C-C	−0.100833	−0.02107
P32247	381	C(~O)(:C)	−0.101161	−0.06196
P32247	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.10156	−0.15411
P32247	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.10159	−0.09177
P32247	365	C(~H)(~N)	−0.102315	−0.07825
P32247	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.103833	−0.03781
P32247	290	C-Al	−0.104149	−0.10419
P32247	379	C(~N)(:N)	−0.104513	−0.16864
P32247	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.105331	−0.08882
P32247	336	C(~C)(~C)(~C)(~N)	−0.110467	0.007919
P32247	730	Nc1ccc(Br)cc1	−0.112312	−0.11239
P32247	863	CC1C(N)CCC1	−0.113841	−0.02004
P32247	660	C-C=C-C-C	−0.11785	−0.07643
P32247	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.118024	−0.11804
P32247	19	>= 2 O	−0.118256	−0.01794
P32247	570	C:C-C-C	−0.118367	−0.07693
P32247	707	O=C-C-C-C-C(N)-C	−0.118925	−0.06466
P32247	417	C#C	−0.119541	−0.11958
P32247	814	NC1CC(Br)CCC1	−0.124283	−0.12424
P32247	580	O=C-C-C-N	−0.12762	−0.10367
P32247	620	C:C-O-C-C	−0.130325	−0.17621
P32247	776	CC1CCC(C)CC1	−0.131179	0.016255

P32247	449	C(-N)(=C)	−0.13125	−0.09348
P32247	528	[#1]-N-C-[#1]	−0.131655	−0.04533
P32247	618	C:C-C-C:C	−0.133679	−0.09225
P32247	302	N-F	−0.137282	−0.13731
P32247	486	N-C:N:N	−0.140323	0
P32247	157	>= 3 any ring size 5	−0.141394	−0.00372
P32247	20	>= 4 O	−0.142173	−0.10775
P32247	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.144155	−0.14419
P32247	439	C(-C)(-N)(=O)	−0.144699	−0.02398
P32247	95	>= 1 Hg	−0.144863	−0.14487
P32247	636	C-N-C-N-C	−0.145437	0.005143
P32247	91	>= 1 Os	−0.146787	−0.14683
P32247	339	C(~C)(~C)(~H)(~O)	−0.148352	−0.07171
P32247	608	C-C-C-C:C	−0.1485	−0.10708
P32247	8	>= 4 B	−0.14876	−0.1488
P32247	380	C(~O)(~O)	−0.149216	−0.02038
P32247	21	>= 8 O	−0.149629	−0.12124
P32247	377	C(~N)(:C)(:C)	−0.149776	−0.05827
P32247	495	C-N-C:C	−0.150882	−0.11307
P32247	496	N:N-C-[#1]	−0.152028	−0.05436
P32247	452	C(-O)(=O)	−0.155154	0
P32247	464	N-C-C=C	−0.155517	−0.05215
P32247	665	N-C:C-C-C	−0.155545	−0.11778
P32247	85	>= 1 Ba	−0.156651	−0.15673
P32247	505	Cl-C:C-O	−0.157507	−0.18207
P32247	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.159142	−0.09054
P32247	90	>= 1 Re	−0.161433	−0.16145
P32247	801	CC1CC(Cl)CCC1	−0.161579	−0.1674
P32247	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.16884	−0.16885
P32247	685	O=C-C-C-C-N	−0.171775	−0.10678
P32247	780	CC1CCC(Cl)CC1	−0.174695	−0.02734
P32247	842	CC1CC(N)CC1	−0.176976	−0.08324
P32247	736	Cc1cc(S)ccc1	−0.17764	−0.1777
P32247	742	Oc1cc(N)ccc1	−0.178415	−0.20386
P32247	772	Nc1c(Br)cccc1	−0.178495	−0.17851
P32247	501	Cl-C:C-C	−0.182392	−0.18576
P32247	818	CC1C(C)CCCC1	−0.182698	−0.08804
P32247	649	O=N-C:C-O	−0.1916	−0.19164
P32247	65	>= 1 As	−0.196724	−0.19673
P32247	399	N(~H)(:C)	−0.197325	−0.30134
P32247	500	C-S-C:C	−0.19795	−0.11466
P32247	480	C:S:C-C	−0.200404	−0.1159
P32247	362	C(~Cl)(:C)	−0.206148	−0.20951
P32247	418	C=N	−0.212146	−0.24148
P32247	833	NC1C(N)CCCC1	−0.212694	−0.12881
P32247	558	O=N-C:C	−0.213066	−0.22024
P32247	220	>= 2 any ring size 7	−0.214375	−0.21442
P32247	545	N-C:C-C	−0.21711	−0.17932

P32247	264	Li-Li	−0.217632	−0.2177
P32247	607	N-C-C-C:C	−0.217838	−0.08695
P32247	583	Cl-C:C-O-C	−0.217863	−0.2424
P32247	671	O=C-C=C-C	−0.217963	−0.25053
P32247	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.222879	−0.25729
P32247	675	Br-C-C-C:C	−0.227877	−0.22244
P32247	717	Cc1ccc(Cl)cc1	−0.22895	−0.08162
P32247	358	C(~C)(:N)	−0.229171	−0.24336
P32247	651	O-C:C:C-C	−0.23039	−0.25781
P32247	669	Cl-C:C-C=O	−0.231964	−0.23202
P32247	263	Li-H	−0.233014	−0.23308
P32247	566	O-C-C-N	−0.233409	−0.16744
P32247	440	C(-C)(-O)(=O)	−0.234498	−0.06094
P32247	494	O=C-C:N	−0.235552	−0.17677
P32247	351	C(~C)(~N)	−0.235707	−0.19436
P32247	790	SC1CCC(Br)CC1	−0.236057	−0.23613
P32247	794	ClC1CCC(Cl)CC1	−0.237492	−0.23753
P32247	88	>= 1 Ta	−0.238356	−0.2384
P32247	4	>= 1 Li	−0.239706	−0.23975
P32247	3	>= 32 H	−0.240839	−0.24092
P32247	300	N-N	−0.245236	−0.25951
P32247	6	>= 1 B	−0.246084	−0.24614
P32247	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.246613	−0.24665
P32247	538	N=C-C-C	−0.246709	−0.27606
P32247	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.251666	−0.25166
P32247	433	C(-C)(-Cl)(=O)	−0.252464	−0.2525
P32247	84	>= 1 Cs	−0.252994	−0.25303
P32247	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.255916	−0.25594
P32247	588	O=C-C-C=O	−0.256807	−0.25685
P32247	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.257645	−0.2577
P32247	683	N-C-C-C-C-C	−0.258184	−0.21681
P32247	689	O-C-C-C-C-C-C	−0.259282	−0.30232
P32247	259	>= 3 aromatic rings	−0.259528	−0.25954
P32247	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.263685	−0.26371
P32247	866	OC1C(O)CCC1	−0.265525	−0.26554
P32247	329	C(~Br)(~H)	−0.266112	−0.26615
P32247	775	Brc1c(Br)cccc1	−0.266144	−0.26618
P32247	725	Sc1ccc(N)cc1	−0.266169	−0.26621
P32247	306	N-Cl	−0.266396	−0.26642
P32247	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.266656	−0.26669
P32247	426	P=P	−0.266658	−0.2667
P32247	870	OC1C(Br)CCC1	−0.266704	−0.26675
P32247	795	ClC1CCC(Br)CC1	−0.267186	−0.26722
P32247	799	CC1CC(S)CCC1	−0.267654	−0.26771
P32247	652	O-C:C:C-N	−0.285107	−0.15149
P32247	467	C=N-N-C	−0.29858	−0.09334
P32247	628	C-N-C-C:C	−0.301644	−0.19141
P32247	603	C-C:C:C-C	−0.301919	−0.26055

P32247	860	CC1C(C)CCC1	−0.303911	−0.21019
P32247	332	C(~C)(~C)	−0.317929	−0.27657
P32247	206	>= 5 any ring size 6	−0.320244	−0.31804
P32247	477	N-N-C:C	−0.32861	−0.25048
P32247	412	S(~C)(~C)	−0.341365	−0.30581
P32247	806	OC1CC(Cl)CCC1	−0.342823	−0.35939
P32247	713	Cc1ccc(C)cc1	−0.35921	−0.29084
P32247	811	SC1CC(Br)CCC1	−0.360661	−0.3606
P32247	388	C(:C)(:N)(:N)	−0.361681	−0.31309
P32247	385	C(:C)(:C)(:C)	−0.385298	−0.37074
P32247	532	S-C:C-[#1]	−0.397523	−0.31451
P32247	490	C-C-C=C	−0.42541	−0.38408
P32247	476	C-O-C=C	−0.525502	−0.49717
P32247	704	O=C-C-C-C-C-C-C	−0.577172	−0.43946
P32247	13	>= 32 C	−0.636554	−0.47769
P32247	844	CC1CC(Br)CC1	−0.771681	−0.77159
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P32247	757	Cc1c(S)cccc1	−0.876516	−0.86375
P32247	687	O=C-C-C-C=O	−0.888976	−0.77865

rints（continued)

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Data S1. Ranking of importance of substructure features from Pubchem Fingerp

GPCR ID	Bit Posit	Bit Substructure	W	P
P32302	97	>= 1 Pb	2.663471	2.663472
P32302	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	2.36526	2.365258
P32302	731	Clc1ccc(Cl)cc1	2.356772	2.356964
P32302	491	C-N:C-[#1]	2.283236	2.285269
P32302	450	C(-N)(=N)	2.126823	2.129814
P32302	330	C(~Br)(:C)	2.051355	2.048593
P32302	846	OC1CC(S)CC1	1.928019	1.92802
P32302	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	1.886224	1.886225
P32302	507	C-C-S-C	1.841769	1.842998
P32302	274	B-C	1.714127	1.714125
P32302	331	C(~Br)(:N)	1.639919	1.639987
P32302	3	>= 32 H	1.511189	1.511191
P32302	99	>= 1 La	1.504033	1.504032
P32302	673	O=C-C=C-N	1.498365	1.492243
P32302	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	1.488145	1.487863
P32302	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	1.485345	1.485791
P32302	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	1.460923	1.460124
P32302	632	C-C-O-C:C	1.372963	1.37403
P32302	747	Sc1cc(Cl)ccc1	1.352068	1.354744
P32302	870	OC1C(Br)CCC1	1.316154	1.316154
P32302	389	C(:N)(:N)	1.29993	1.299383
P32302	437	C(-C)(-N)(=C)	1.25752	1.251554
P32302	144	>= 1 saturated or aromatic carbon-only ring size 5	1.255342	1.252426
P32302	577	C:C-N-C:C	1.253013	1.245683
P32302	625	O=C-C:C-O	1.248275	1.252161
P32302	405	O(~C)(~C)	1.248123	1.250118
P32302	859	BrC1CC(Br)CC1	1.227649	1.227648
P32302	451	C(-N)(=O)	1.221779	1.228945
P32302	509	Br-C:C-C	1.214739	1.212411
P32302	249	>= 1 saturated or aromatic carbon-only ring size 10	1.2008	1.200803
P32302	591	Cl-C-C-C-C	1.175746	1.177742
P32302	465	O=S-C-C	1.156905	1.155299
P32302	791	NC1CCC(N)CC1	1.148031	1.144417
P32302	662	O-C-C-O-C	1.142079	1.138588
P32302	542	O-C:C-[#1]	1.135292	1.135094
P32302	694	O=C-C-C-C-C=O	1.125303	1.117968
P32302	698	O-C-C-C-C-C-C-C	1.116033	1.119075
P32302	478	S-C=N-[#1]	1.099978	1.098062
P32302	71	>= 1 Zr	1.076935	1.076937
P32302	797	CC1CC(C)CCC1	1.050071	1.045405
P32302	351	C(~C)(~N)	1.04013	1.044241
P32302	423	N=O	1.031789	1.037641
P32302	697	C-C-C-C-C-C(C)-C	1.029999	1.02643
P32302	769	Sc1c(Br)cccc1	1.028771	1.028766
P32302	687	O=C-C-C-C=O	1.021434	1.014922
P32302	866	OC1C(O)CCC1	1.016699	1.016741

P32302	30	>= 1 P	1.011074	1.011391
P32302	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	1.002695	1.002035
P32302	227	>= 1 any ring size 8	0.965197	0.964238
P32302	525	[As]-C:C-[#1]	0.958077	0.958077
P32302	728	Nc1ccc(N)cc1	0.946963	0.953897
P32302	96	>= 1 Tl	0.944802	0.944802
P32302	606	O-C:C-C-C	0.944367	0.949046
P32302	526	Cl-C:C-Cl	0.942452	0.951556
P32302	364	C(~F)(:C)	0.942106	0.943739
P32302	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.929504	0.927092
P32302	650	O=C-N-C=O	0.926574	0.910653
P32302	661	O-C-O-C-C	0.910355	0.912094
P32302	722	Oc1ccc(Cl)cc1	0.910157	0.91709
P32302	122	>= 2 any ring size 3	0.897628	0.897564
P32302	800	CC1CC(N)CCC1	0.871647	0.872842
P32302	85	>= 1 Ba	0.866715	0.866716
P32302	520	C=C-C:C	0.866541	0.86638
P32302	528	[#1]-N-C-[#1]	0.861487	0.863713
P32302	839	CC1CC(C)CC1	0.860873	0.861494
P32302	55	>= 1 V	0.858617	0.858618
P32302	668	C-C:C-C-C	0.857778	0.856281
P32302	476	C-O-C=C	0.846016	0.84596
P32302	95	>= 1 Hg	0.821299	0.821298
P32302	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.820168	0.82017
P32302	34	>= 2 S	0.818319	0.812084
P32302	506	C-C:N:C	0.810931	0.808354
P32302	727	Sc1ccc(Br)cc1	0.8104	0.812715
P32302	259	>= 3 aromatic rings	0.807877	0.807877
P32302	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.792322	0.792321
P32302	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.789029	0.780815
P32302	193	>= 3 saturated or aromatic carbon-only ring size 6	0.783265	0.78433
P32302	314	O-P	0.780994	0.780798
P32302	670	Br-C:C:C-C	0.77505	0.772725
P32302	494	O=C-C:N	0.747565	0.754244
P32302	283	C-H	0.737304	0.757981
P32302	726	Sc1ccc(Cl)cc1	0.725776	0.729816
P32302	559	O-C-N-[#1]	0.723681	0.726823
P32302	281	B-Cl	0.715934	0.715933
P32302	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.714666	0.71485
P32302	539	N=C-C-[#1]	0.711269	0.717023
P32302	795	ClC1CCC(Br)CC1	0.70765	0.707647
P32302	235	>= 2 saturated or aromatic carbon-only ring size 8	0.702227	0.702227
P32302	875	NC1C(N)CCC1	0.683645	0.683645
P32302	448	C(-H)(=O)	0.656965	0.666903
P32302	130	>= 1 saturated or aromatic carbon-only ring size 4	0.647217	0.649859
P32302	801	CC1CC(Cl)CCC1	0.646648	0.648108
P32302	77	>= 1 Ag	0.640391	0.64039
P32302	413	S(~C)(~H)	0.639708	0.639706

P32302	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.632977	0.632978
P32302	23	>= 1 F	0.626174	0.624661
P32302	574	O-C-C:C-C	0.608751	0.603455
P32302	792	NC1CCC(Cl)CC1	0.606297	0.601329
P32302	294	C-Cl	0.599533	0.61052
P32302	54	>= 1 Ti	0.59927	0.599268
P32302	76	>= 1 Pd	0.59267	0.592669
P32302	273	B-B	0.568918	0.568918
P32302	804	OC1CC(S)CCC1	0.564479	0.557545
P32302	647	O=C-N-C-N	0.543169	0.544452
P32302	861	CC1C(O)CCC1	0.541403	0.542784
P32302	372	C(~H)(:C)(:N)	0.536378	0.535807
P32302	829	SC1C(S)CCCC1	0.533799	0.533798
P32302	304	N-P	0.533378	0.533378
P32302	844	CC1CC(Br)CC1	0.532525	0.532527
P32302	306	N-Cl	0.526332	0.526331
P32302	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.521766	0.52015
P32302	803	OC1CC(O)CCC1	0.512875	0.516649
P32302	627	O=[As]-C:C:C	0.512172	0.51217
P32302	39	>= 4 Cl	0.510361	0.50774
P32302	380	C(~O)(~O)	0.499655	0.497871
P32302	466	N#C-C=C	0.499199	0.503237
P32302	425	P=O	0.497734	0.497538
P32302	569	N-C-C-N	0.49564	0.495183
P32302	671	O=C-C=C-C	0.486138	0.478959
P32302	83	>= 1 Xe	0.481939	0.48194
P32302	567	O-C-C-O	0.478482	0.475396
P32302	32	>= 4 P	0.475163	0.475166
P32302	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.474233	0.474234
P32302	486	N-C:N:N	0.470989	0.471779
P32302	483	N-S-C:C	0.469505	0.471959
P32302	555	N=C-C=C	0.467129	0.464801
P32302	513	S:C:C-[#1]	0.464034	0.467112
P32302	463	N:C-S-[#1]	0.446193	0.446193
P32302	442	C(-C)(=N)	0.438673	0.44257
P32302	82	>= 1 Te	0.436699	0.4367
P32302	845	OC1CC(O)CC1	0.428621	0.428621
P32302	100	>= 1 Ce	0.426573	0.426573
P32302	17	>= 8 N	0.424526	0.427923
P32302	79	>= 1 In	0.419995	0.419995
P32302	257	>= 2 aromatic rings	0.418962	0.41896
P32302	833	NC1C(N)CCCC1	0.409742	0.407133
P32302	475	S-C=N-C	0.402298	0.39844
P32302	279	B-P	0.401663	0.401662
P32302	643	[#1]-C-C-N-[#1]	0.399972	0.38862
P32302	848	OC1CC(Cl)CC1	0.397743	0.39774
P32302	593	N-C-C-C-N	0.393486	0.402873
P32302	521	C:N-C-[#1]	0.380894	0.381002

P32302	811	SC1CC(Br)CCC1	0.375365	0.375367
P32302	108	>= 1 Dy	0.375315	0.375315
P32302	199	>= 4 any ring size 6	0.370111	0.368972
P32302	583	Cl-C:C-O-C	0.367203	0.360554
P32302	629	S-C:C:C-N	0.364984	0.363059
P32302	261	>= 4 aromatic rings	0.363466	0.363466
P32302	749	Nc1cc(N)ccc1	0.362398	0.376768
P32302	571	[#1]-C-O-[#1]	0.359648	0.359307
P32302	43	>= 1 Br	0.358666	0.359555
P32302	868	OC1C(N)CCC1	0.347699	0.347678
P32302	369	C(~H)(~Si)	0.347213	0.347212
P32302	561	Cl-C-C=O	0.34519	0.345803
P32302	778	CC1CCC(S)CC1	0.34119	0.33421
P32302	558	O=N-C:C	0.340783	0.349225
P32302	362	C(~Cl)(:C)	0.340151	0.354247
P32302	599	[#1]-C-C=C-[#1]	0.339225	0.339096
P32302	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.333752	0.333753
P32302	402	N(~O)(:O)	0.328491	0.32849
P32302	794	ClC1CCC(Cl)CC1	0.326626	0.326815
P32302	16	>= 4 N	0.325527	0.324446
P32302	80	>= 1 Sn	0.323238	0.323239
P32302	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.318518	0.318516
P32302	20	>= 4 O	0.3091	0.309264
P32302	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.307339	0.306323
P32302	716	Cc1ccc(N)cc1	0.299314	0.303582
P32302	352	C(~C)(~O)	0.296792	0.309061
P32302	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.295691	0.295993
P32302	338	C(~C)(~C)(~H)(~N)	0.295237	0.30367
P32302	24	>= 2 F	0.29111	0.291142
P32302	25	>= 4 F	0.289561	0.293566
P32302	22	>= 16 O	0.286468	0.286456
P32302	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.278861	0.278798
P32302	672	O=C-C=C-[#1]	0.278129	0.274048
P32302	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.276658	0.279947
P32302	461	O-C-C=N	0.273715	0.276819
P32302	602	O=C-C-N-C	0.257144	0.248288
P32302	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.254755	0.254757
P32302	393	N(~C)(~H)	0.254354	0.256741
P32302	81	>= 1 Sb	0.251109	0.251111
P32302	499	N-C:C:N	0.248945	0.241545
P32302	518	O=C-N-N	0.24459	0.235345
P32302	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.240362	0.241076
P32302	767	Sc1c(N)cccc1	0.23602	0.231614
P32302	318	Al-H	0.232311	0.232314
P32302	137	>= 2 saturated or aromatic carbon-only ring size 4	0.230038	0.23004
P32302	185	>= 2 any ring size 6	0.217186	0.21639
P32302	398	N(~H)(~N)	0.214115	0.213579
P32302	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.213062	0.206872

P32302	214	>= 1 saturated or aromatic carbon-only ring size 7	0.210438	0.207199
P32302	270	Li-S	0.199636	0.199639
P32302	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.198041	0.198043
P32302	220	>= 2 any ring size 7	0.195551	0.195551
P32302	484	N-C:N:C	0.183276	0.18511
P32302	374	C(~H)(~H)(~H)	0.180296	0.182609
P32302	818	CC1C(C)CCCC1	0.177934	0.186799
P32302	564	C=C-C=C	0.175399	0.174553
P32302	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.170213	0.170215
P32302	535	O=C-C-C	0.169868	0.173031
P32302	10	>= 4 C	0.166851	0.187529
P32302	734	Cc1cc(C)ccc1	0.163809	0.164648
P32302	400	N(~H)(:C)(:C)	0.16334	0.169719
P32302	659	O-C-C-N-C	0.161136	0.162793
P32302	754	Brc1cc(Br)ccc1	0.160372	0.160123
P32302	445	C(-H)(-N)(=C)	0.149057	0.148799
P32302	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.148429	0.148429
P32302	291	C-Si	0.146539	0.146536
P32302	388	C(:C)(:N)(:N)	0.144703	0.136912
P32302	18	>= 1 O	0.138206	0.141793
P32302	68	>= 1 Rb	0.136465	0.136468
P32302	358	C(~C)(:N)	0.129751	0.124097
P32302	51	>= 1 Al	0.127989	0.127989
P32302	880	BrC1C(Br)CCC1	0.127673	0.12767
P32302	101	>= 1 Pr	0.12545	0.125448
P32302	633	N-C-C:C-C	0.12126	0.119117
P32302	256	>= 1 hetero-aromatic ring	0.120974	0.120973
P32302	64	>= 1 Ge	0.119487	0.119485
P32302	371	C(~H)(:C)(:C)	0.115697	0.112344
P32302	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.113491	0.11349
P32302	646	O=C-N-C-[#1]	0.112703	0.116206
P32302	449	C(-N)(=C)	0.110526	0.101888
P32302	426	P=P	0.110377	0.110379
P32302	7	>= 2 B	0.108513	0.108513
P32302	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.099305	0.102546
P32302	608	C-C-C-C:C	0.098073	0.100979
P32302	683	N-C-C-C-C-C	0.095325	0.087948
P32302	12	>= 16 C	0.094861	0.10448
P32302	285	C-N	0.092708	0.096819
P32302	552	C:C-C:C	0.091462	0.091299
P32302	532	S-C:C-[#1]	0.09025	0.092845
P32302	529	Cl-C-C-Cl	0.088914	0.098017
P32302	335	C(~C)(~C)(~C)(~H)	0.083987	0.091273
P32302	860	CC1C(C)CCC1	0.083143	0.08093
P32302	544	O-C:C-O	0.07725	0.071178
P32302	111	>= 1 Tm	0.074784	0.074784
P32302	397	N(~C)(:C)(:C)	0.073475	0.066018
P32302	490	C-C-C=C	0.068391	0.06164

P32302	660	C-C=C-C-C	0.067839	0.064305
P32302	588	O=C-C-C=O	0.067206	0.065872
P32302	562	Br-C-C=O	0.067163	0.066675
P32302	315	O-K	0.06714	0.067139
P32302	739	Cc1cc(Br)ccc1	0.06688	0.063289
P32302	272	B-H	0.066874	0.066874
P32302	837	ClC1C(Br)CCCC1	0.066609	0.066607
P32302	2	>= 16 H	0.065908	0.06591
P32302	473	S-C:N:C	0.065412	0.062226
P32302	343	C(~C)(~Cl)(~H)	0.065332	0.061542
P32302	321	Si-Si	0.06505	0.065049
P32302	640	C=C-C-C-C	0.064974	0.064369
P32302	566	O-C-C-N	0.064766	0.070335
P32302	360	C(~Cl)(~Cl)	0.06463	0.0647
P32302	91	>= 1 Os	0.064438	0.064437
P32302	474	S:C:C:N	0.063466	0.065622
P32302	228	>= 1 saturated or aromatic carbon-only ring size 8	0.062852	0.06272
P32302	337	C(~C)(~C)(~C)(~O)	0.061139	0.063494
P32302	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.060887	0.060647
P32302	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.059884	0.059886
P32302	377	C(~N)(:C)(:C)	0.059681	0.054512
P32302	390	N(~C)(~C)	0.058746	0.051381
P32302	313	O-Si	0.058042	0.05804
P32302	706	O=C-C-C-C-C(=O)-C	0.057659	0.050357
P32302	644	C-C=N-N-C	0.056819	0.055633
P32302	723	Oc1ccc(Br)cc1	0.056713	0.060658
P32302	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.055993	0.05638
P32302	780	CC1CCC(Cl)CC1	0.054048	0.056259
P32302	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.053385	0.053383
P32302	418	C=N	0.053122	0.052608
P32302	601	N-C:C:C-N	0.052275	0.052633
P32302	361	C(~Cl)(~H)	0.050768	0.046981
P32302	123	>= 2 saturated or aromatic carbon-only ring size 3	0.048663	0.048667
P32302	508	S=C-N-C	0.04827	0.050791
P32302	348	C(~C)(~H)(~P)	0.048251	0.048567
P32302	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.047796	0.043002
P32302	805	OC1CC(N)CCC1	0.047232	0.051025
P32302	533	S-C:C-N	0.047041	0.050699
P32302	502	N-C=C-[#1]	0.046557	0.043553
P32302	112	>= 1 Yb	0.046463	0.046461
P32302	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.045673	0.045675
P32302	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.045465	0.045466
P32302	495	C-N-C:C	0.044971	0.040108
P32302	592	N-C-C-C-C	0.04484	0.044741
P32302	363	C(~F)(~F)	0.044671	0.043615
P32302	724	Sc1ccc(S)cc1	0.043752	0.047712
P32302	325	As-H	0.043469	0.043467
P32302	408	O(~H)(~S)	0.043229	0.045008

P32302	401	N(~O)(~O)	0.043	0.042405
P32302	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.04247	0.043881
P32302	4	>= 1 Li	0.042415	0.042417
P32302	843	CC1CC(Cl)CC1	0.041749	0.042857
P32302	656	C-C-N-C-C	0.041498	0.037677
P32302	356	C(~C)(:C)(:C)	0.039877	0.029903
P32302	618	C:C-C-C:C	0.039684	0.036869
P32302	60	>= 1 Ni	0.038778	0.038778
P32302	864	CC1C(Cl)CCC1	0.038408	0.038409
P32302	384	C(:C)(:C)	0.035689	0.0364
P32302	452	C(-O)(=O)	0.034789	0.028699
P32302	113	>= 1 Tc	0.034393	0.034393
P32302	653	O-C:C:C-O	0.034024	0.037432
P32302	695	O=C-C-C-C-C-N	0.033484	0.032424
P32302	851	SC1CC(N)CC1	0.032664	0.031497
P32302	691	O-C-C-C-C-C-N	0.031411	0.031494
P32302	406	O(~C)(~H)	0.030933	0.02597
P32302	603	C-C:C:C-C	0.030446	0.028455
P32302	537	O=C-C-O	0.029573	0.028794
P32302	326	As-As	0.028106	0.028107
P32302	493	O=C-C:C	0.028031	0.033559
P32302	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.027403	0.027406
P32302	654	N-C-N-C-C	0.027296	0.026207
P32302	11	>= 8 C	0.025922	0.04392
P32302	340	C(~C)(~C)(~N)	0.02556	0.02143
P32302	316	F-P	0.025351	0.025349
P32302	0	>= 4 H	0.025346	0.025347
P32302	684	O=C-C-C-C-C	0.025072	0.028043
P32302	847	OC1CC(N)CC1	0.0245	0.025541
P32302	382	C(~O)(:C)(:C)	0.024484	0.020505
P32302	584	C:C-C=C-C	0.024478	0.022328
P32302	344	C(~C)(~H)	0.024237	0.044417
P32302	771	Nc1c(Cl)cccc1	0.023272	0.021025
P32302	675	Br-C-C-C:C	0.023033	0.020427
P32302	458	S(-O)(=O)	0.022988	0.025562
P32302	807	OC1CC(Br)CCC1	0.022646	0.023702
P32302	702	O-C-C-C-C-C-N-C	0.022408	0.027455
P32302	379	C(~N)(:N)	0.022026	0.023008
P32302	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.021823	0.021563
P32302	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.021806	0.021809
P32302	87	>= 1 Hf	0.021385	0.021385
P32302	773	Clc1c(Cl)cccc1	0.020902	0.019849
P32302	94	>= 1 Au	0.02042	0.020418
P32302	109	>= 1 Ho	0.020162	0.020163
P32302	822	CC1C(Cl)CCCC1	0.020012	0.016967
P32302	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.019742	0.019745
P32302	333	C(~C)(~C)(~C)	0.019498	0.020399
P32302	5	>= 2 Li	0.019452	0.019448

P32302	582	C-C-C-C-C	0.019223	0.022626
P32302	329	C(~Br)(~H)	0.019002	0.018724
P32302	143	>= 1 any ring size 5	0.018584	0.012496
P32302	49	>= 1 Be	0.018514	0.018512
P32302	114	>= 1 U	0.018477	0.018476
P32302	165	>= 4 saturated or aromatic carbon-only ring size 5	0.018275	0.018276
P32302	742	Oc1cc(N)ccc1	0.018103	0.021896
P32302	808	SC1CC(S)CCC1	0.018083	0.018087
P32302	70	>= 1 Y	0.018076	0.018075
P32302	634	C-C-C:C-C	0.017249	0.015751
P32302	686	O=C-C-C-C-O	0.017076	0.015341
P32302	157	>= 3 any ring size 5	0.016639	0.014934
P32302	432	C(-C)(-C)(=O)	0.016602	0.011297
P32302	297	C-Br	0.015545	0.012503
P32302	511	S=C-N-[#1]	0.015174	0.022279
P32302	690	O-C-C-C-C-C-O	0.014982	0.022733
P32302	530	N:C-C:C	0.014839	0.009201
P32302	579	O=C-C-C-C	0.014631	0.016113
P32302	534	S-C:C-O	0.01274	0.013107
P32302	587	N-C:C-O-[#1]	0.012667	0.012322
P32302	387	C(:C)(:N)	0.012288	0.006814
P32302	489	N-C-S-C	0.01138	0.010384
P32302	785	OC1CCC(Cl)CC1	0.011259	0.018191
P32302	700	O-C-C-C-C-C-O-C	0.010642	0.011696
P32302	312	O-Al	0.010488	0.010488
P32302	278	B-Si	0.010466	0.010467
P32302	200	>= 4 saturated or aromatic carbon-only ring size 6	0.010227	0.007682
P32302	260	>= 3 hetero-aromatic rings	0.010012	0.010012
P32302	482	C:N-C:C	0.009948	0.007161
P32302	638	O-C-C-C-N	0.009694	0.004658
P32302	826	OC1C(N)CCCC1	0.009415	0.003276
P32302	536	O=C-C-N	0.00903	0.001577
P32302	296	C-Se	0.008997	0.009
P32302	705	O=C-C-C-C-C(O)-C	0.008683	0.005614
P32302	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.008674	0.008674
P32302	589	C-C:C-O-C	0.008495	0.005628
P32302	467	C=N-N-C	0.00833	0.005935
P32302	357	C(~C)(:C)(:N)	0.007947	0.007229
P32302	676	N#C-C-C-C	0.007717	0.009482
P32302	472	C:N:C-C	0.007264	0.004683
P32302	365	C(~H)(~N)	0.006835	0.008608
P32302	708	C-C(C)-C-C	0.006715	0
P32302	13	>= 32 C	0.006627	-0.00021
P32302	522	C-N-N-[#1]	0.006342	0.006554
P32302	850	SC1CC(S)CC1	0.006224	0.006225
P32302	412	S(~C)(~C)	0.005321	0.006301
P32302	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.005099	0.005475
P32302	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.005093	0.002069

P32302	106	>= 1 Gd	0.004775	0.004773
P32302	678	C-C-C=C-C	0.004749	0.001218
P32302	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.004344	0.003333
P32302	613	C-N-C-C-C	0.004029	-0.00103
P32302	681	O-C-C-C-C-O	0.003879	0.006599
P32302	693	O=C-C-C-C-C-O	0.003816	0.00064
P32302	828	OC1C(Br)CCCC1	0.003704	0.006143
P32302	624	O=C-C:C-N	0.003648	0
P32302	524	C-C=C-C	0.003458	0.000838
P32302	768	Sc1c(Cl)cccc1	0.00327	0.004889
P32302	717	Cc1ccc(Cl)cc1	0.003027	0.005242
P32302	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.003002	0.002742
P32302	715	Cc1ccc(S)cc1	0.002843	-0.00413
P32302	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.002705	-1.63E-05
P32302	1	>= 8 H	0.002577	0.002579
P32302	568	N#C-C-C	0.002548	0.006793
P32302	27	>= 2 Na	0.002512	0.002513
P32302	696	C-C-C-C-C-C-C-C	0.002259	-0.00996
P32302	565	C:C-O-C	0.002173	-0.00045
P32302	857	ClC1CC(Cl)CC1	0.001901	0.001903
P32302	479	S-C-S-C	0.00187	-0.00562
P32302	305	N-S	0.001788	0.002344
P32302	674	N-C-N-C:C	0.001562	0.004063
P32302	446	C(-H)(=C)	0.001298	0.000729
P32302	616	C:C:N:N:C	0.001147	0.00375
P32302	789	SC1CCC(Cl)CC1	0.00077	0.004807
P32302	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.000754	0
P32302	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.000617	0.00111
P32302	8	>= 4 B	0.000547	0.000548
P32302	241	>= 1 any ring size 9	0.000521	0.00026
P32302	497	O-C:C:N	0.0005	0.004919
P32302	680	O-C-C-C-C-C	0.000347	0.001634
P32302	303	N-Si	0.000246	0.000245
P32302	874	SC1C(Br)CCC1	0.000157	0.000156
P32302	93	>= 1 Pt	2.63E-05	2.66E-05
P32302	262	>= 4 hetero-aromatic rings	2.44E-06	0
P32302	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	1.34E-06	0
P32302	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	7.81E-07	0
P32302	255	>= 1 aromatic ring	7.44E-07	0
P32302	865	CC1C(Br)CCC1	6.75E-07	0
P32302	65	>= 1 As	6.71E-07	0
P32302	428	C(#C)(-H)	1.45E-07	0
P32302	319	Al-Cl	-3.02E-07	0
P32302	415	Si(~C)(~C)	-8.70E-07	0
P32302	28	>= 1 Si	-1.25E-06	0
P32302	84	>= 1 Cs	-1.49E-06	0
P32302	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-7.27E-05	-7.25E-05
P32302	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	-0.00025	-0.00025

P32302	560	N-C-N-C	−0.00028	−0.00386
P32302	248	>= 1 any ring size 10	−0.0003	0
P32302	42	>= 2 K	−0.00032	−0.00032
P32302	813	NC1CC(Cl)CCC1	−0.00063	−0.00096
P32302	258	>= 2 hetero-aromatic rings	−0.00072	−0.00072
P32302	835	NC1C(Br)CCCC1	−0.00073	−0.00099
P32302	554	Br-C-C-C	−0.0008	−0.00341
P32302	271	Li-Cl	−0.00081	−0.00081
P32302	669	Cl-C:C-C=O	−0.00089	−0.01006
P32302	35	>= 4 S	−0.0009	0.000783
P32302	92	>= 1 Ir	−0.00108	−0.00108
P32302	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.00112	0.000676
P32302	787	SC1CCC(S)CC1	−0.00123	0.002733
P32302	626	C-O-C:C-C	−0.00138	−0.00425
P32302	523	N:C:C-C	−0.00149	−0.00038
P32302	679	C-C-C-C-C-C	−0.00151	0.003489
P32302	464	N-C-C=C	−0.00156	0.002313
P32302	840	CC1CC(O)CC1	−0.0017	−0.00013
P32302	58	>= 1 Fe	−0.00176	−0.00176
P32302	862	CC1C(S)CCC1	−0.00214	−0.0088
P32302	47	>= 2 I	−0.00216	−0.0028
P32302	790	SC1CCC(Br)CC1	−0.0023	9.47E−06
P32302	610	C-O-C-O-C	−0.00245	0.000134
P32302	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.0026	−0.0026
P32302	50	>= 1 Mg	−0.00285	−0.00285
P32302	553	O=C-C=C	−0.00293	−0.00663
P32302	770	Nc1c(N)cccc1	−0.00295	−0.0047
P32302	546	N-C:C-[#1]	−0.00295	−0.00232
P32302	710	C-C-C(C)-C-C	−0.00309	−0.00049
P32302	527	C:C:N-[#1]	−0.0031	0
P32302	841	CC1CC(S)CC1	−0.00327	−0.00327
P32302	439	C(-C)(-N)(=O)	−0.00358	0
P32302	711	C-C(C)(C)-C-C	−0.00373	−0.0049
P32302	213	>= 1 any ring size 7	−0.00383	−0.01183
P32302	103	>= 1 Pm	−0.00389	−0.00389
P32302	815	ClC1CC(Cl)CCC1	−0.00395	−0.00388
P32302	849	OC1CC(Br)CC1	−0.00397	−0.00397
P32302	812	NC1CC(N)CCC1	−0.00406	−0.00371
P32302	664	C-C=C-C=C	−0.00417	−0.007
P32302	635	N-N-C-N-[#1]	−0.00431	−0.0016
P32302	299	N-H	−0.00449	−0.00141
P32302	430	C(-C)(-C)(=C)	−0.00455	−0.01032
P32302	288	C-Na	−0.00463	−0.00463
P32302	540	C-N-C-[#1]	−0.00467	−0.00428
P32302	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.00482	−0.0029
P32302	350	C(~C)(~I)	−0.00497	−0.00026
P32302	621	N-C:C:C:N	−0.00508	−0.01218
P32302	802	CC1CC(Br)CCC1	−0.00524	−0.00883

P32302	298	C-I	−0.00547	−0.00076
P32302	308	O-H	−0.00566	−0.01162
P32302	733	Brc1ccc(Br)cc1	−0.00574	−0.00574
P32302	703	O-C-C-C-C-C(N)-C	−0.00576	−0.00608
P32302	701	O-C-C-C-C-C(O)-C	−0.00576	0.004949
P32302	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.00578	−0.00578
P32302	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.00579	−0.00579
P32302	383	C(~S)(:C)	−0.00622	−0.00411
P32302	367	C(~H)(~O)(~O)	−0.00628	−0.00567
P32302	309	O-O	−0.00653	−0.00653
P32302	334	C(~C)(~C)(~C)(~C)	−0.00702	−0.0143
P32302	394	N(~C)(~H)(~N)	−0.00763	−0.00891
P32302	355	C(~C)(:C)	−0.0077	−0.00275
P32302	107	>= 1 Tb	−0.00784	−0.00784
P32302	468	O=S-C-N	−0.00802	−0.01392
P32302	824	OC1C(O)CCCC1	−0.00854	−0.01584
P32302	63	>= 1 Ga	−0.00892	−0.00892
P32302	453	N(-C)(=C)	−0.00901	−0.0001
P32302	323	P-H	−0.00912	−0.00911
P32302	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.0094	−0.0094
P32302	721	Oc1ccc(N)cc1	−0.0094	−0.00057
P32302	178	>= 1 any ring size 6	−0.00959	−0.00784
P32302	738	Cc1cc(Cl)ccc1	−0.0097	−0.00824
P32302	639	O-C-C-C-O	−0.0101	−0.01473
P32302	263	Li-H	−0.01055	−0.01055
P32302	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.01059	−0.01059
P32302	342	C(~C)(~Cl)	−0.0107	0.000288
P32302	655	O-C-C-C:C	−0.01084	−0.0068
P32302	550	Cl-C-C-C	−0.01086	−0.00544
P32302	410	P(~C)(~C)	−0.01088	−0.01056
P32302	821	CC1C(N)CCCC1	−0.01108	−0.00553
P32302	879	ClC1C(Br)CCC1	−0.01146	−0.01145
P32302	720	Oc1ccc(S)cc1	−0.01211	−0.01355
P32302	269	Li-P	−0.01293	−0.01293
P32302	863	CC1C(N)CCC1	−0.01326	−0.00632
P32302	586	C-S-C-C-C	−0.01383	−0.0123
P32302	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.01399	−0.00987
P32302	685	O=C-C-C-C-N	−0.01429	−0.01282
P32302	485	N:C:C:N	−0.01444	−0.01077
P32302	782	OC1CCC(O)CC1	−0.01542	−0.02204
P32302	781	CC1CCC(Br)CC1	−0.01572	−0.01804
P32302	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.01608	−0.01363
P32302	666	C=C-C-O-C	−0.01675	−0.02272
P32302	816	ClC1CC(Br)CCC1	−0.01684	−0.01684
P32302	667	C=C-C-O-[#1]	−0.01718	−0.01696
P32302	434	C(-C)(-H)(=C)	−0.01734	−0.01878
P32302	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.0176	−0.0176
P32302	810	SC1CC(Cl)CCC1	−0.01815	−0.01548

P32302	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.01822	−0.02116
P32302	718	Cc1ccc(Br)cc1	−0.01879	−0.02111
P32302	105	>= 1 Eu	−0.02016	−0.02016
P32302	612	N-C-O-C-C	−0.02036	−0.02989
P32302	346	C(~C)(~H)(~O)	−0.02094	−0.01896
P32302	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.02119	−0.02119
P32302	302	N-F	−0.02125	−0.02125
P32302	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.02135	−0.02135
P32302	543	O-C:C-N	−0.02182	−0.01331
P32302	396	N(~C)(:C)	−0.02192	−0.01915
P32302	45	>= 4 Br	−0.02206	−0.02206
P32302	37	>= 1 Cl	−0.02394	−0.02237
P32302	712	C-C(C)-C(C)-C	−0.02475	−0.02441
P32302	665	N-C:C-C-C	−0.02508	−0.02163
P32302	648	O=N-C:C-N	−0.02577	−0.02615
P32302	677	C-C=C-C:C	−0.02617	−0.02832
P32302	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.027	−0.027
P32302	459	S(=O)(=O)	−0.02722	−0.02024
P32302	604	C-O-C-C:C	−0.02805	−0.03271
P32302	192	>= 3 any ring size 6	−0.02859	−0.02328
P32302	607	N-C-C-C:C	−0.03125	−0.04046
P32302	596	N=C-N-C-C	−0.03129	−0.02984
P32302	471	S:C:C:C	−0.03139	−0.03533
P32302	642	O-C-C-C=O	−0.03151	−0.03555
P32302	56	>= 1 Cr	−0.03271	−0.03271
P32302	809	SC1CC(N)CCC1	−0.03281	−0.03353
P32302	793	NC1CCC(Br)CC1	−0.03429	−0.03704
P32302	877	NC1C(Br)CCC1	−0.03437	−0.03438
P32302	289	C-Mg	−0.03477	−0.03477
P32302	264	Li-Li	−0.03586	−0.03586
P32302	519	N=C-N-C	−0.03602	−0.03713
P32302	757	Cc1c(S)cccc1	−0.03612	−0.03327
P32302	311	O-Na	−0.03778	−0.03778
P32302	817	BrC1CC(Br)CCC1	−0.03794	−0.03819
P32302	820	CC1C(S)CCCC1	−0.03859	−0.03637
P32302	67	>= 1 Kr	−0.0395	−0.0395
P32302	57	>= 1 Mn	−0.04082	−0.04082
P32302	570	C:C-C-C	−0.04194	−0.04518
P32302	470	C:C-C=C	−0.04482	−0.04498
P32302	265	Li-B	−0.04513	−0.04513
P32302	617	C-C-C-O-[#1]	−0.04553	−0.05082
P32302	395	N(~C)(~O)	−0.04562	−0.04006
P32302	328	C(~Br)(~C)(~C)	−0.04595	−0.04878
P32302	454	N(-C)(=O)	−0.04602	−0.04016
P32302	743	Oc1cc(Cl)ccc1	−0.04907	−0.06198
P32302	512	C-[As]-O-[#1]	−0.05039	−0.05039
P32302	36	>= 8 S	−0.0504	−0.0504
P32302	276	B-O	−0.05103	−0.05103

P32302	692	O=C-C-C-C-C-C	−0.05109	−0.05306
P32302	41	>= 1 K	−0.05277	−0.05277
P32302	290	C-Al	−0.05301	−0.05301
P32302	745	Sc1cc(S)ccc1	−0.05321	−0.05321
P32302	836	ClC1C(Cl)CCCC1	−0.05322	−0.05427
P32302	631	O-C:C-O-[#1]	−0.05474	−0.0558
P32302	487	N-C=N-C	−0.05512	−0.04855
P32302	736	Cc1cc(S)ccc1	−0.05582	−0.06132
P32302	600	N-C:C:C-C	−0.05667	−0.06057
P32302	164	>= 4 any ring size 5	−0.05678	−0.05446
P32302	763	Oc1c(N)cccc1	−0.05779	−0.06425
P32302	46	>= 1 I	−0.05792	−0.05497
P32302	38	>= 2 Cl	−0.05814	−0.05502
P32302	110	>= 1 Er	−0.05924	−0.05924
P32302	52	>= 1 Ca	−0.06042	−0.06042
P32302	416	C=C	−0.06056	−0.0548
P32302	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.06103	−0.06104
P32302	373	C(~H)(:N)	−0.06104	−0.06191
P32302	317	F-S	−0.06205	−0.06204
P32302	90	>= 1 Re	−0.06313	−0.06313
P32302	585	C-C:C-N-C	−0.06318	−0.06341
P32302	447	C(-H)(=N)	−0.06369	−0.05873
P32302	557	N:C-O-[#1]	−0.06388	−0.05973
P32302	766	Sc1c(S)cccc1	−0.06428	−0.06428
P32302	6	>= 1 B	−0.06537	−0.06537
P32302	867	OC1C(S)CCC1	−0.06551	−0.06551
P32302	853	SC1CC(Br)CC1	−0.06571	−0.06571
P32302	104	>= 1 Sm	−0.06643	−0.06644
P32302	320	Si-H	−0.06657	−0.06657
P32302	102	>= 1 Nd	−0.06683	−0.06683
P32302	652	O-C:C:C-N	−0.06746	−0.06561
P32302	751	Nc1cc(Br)ccc1	−0.06792	−0.06634
P32302	831	SC1C(Cl)CCCC1	−0.06848	−0.06686
P32302	500	C-S-C:C	−0.06934	−0.07462
P32302	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.06983	−0.06304
P32302	349	C(~C)(~H)(~S)	−0.07133	−0.0738
P32302	737	Cc1cc(N)ccc1	−0.07233	−0.06966
P32302	460	C-C-C#C	−0.07247	−0.07058
P32302	21	>= 8 O	−0.07329	−0.07782
P32302	827	OC1C(Cl)CCCC1	−0.07369	−0.07569
P32302	764	Oc1c(Cl)cccc1	−0.07467	−0.07667
P32302	457	S(-C)(=O)	−0.07635	−0.07614
P32302	286	C-O	−0.07978	−0.07929
P32302	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.08079	−0.081
P32302	551	Cl-C-C-O	−0.08174	−0.08369
P32302	341	C(~C)(~C)(~O)	−0.08592	−0.08025
P32302	663	O-C-C-O-[#1]	−0.08802	−0.10106
P32302	752	Clc1cc(Cl)ccc1	−0.08936	−0.08928

P32302	420	C=O	−0.09062	−0.09286
P32302	878	ClC1C(Cl)CCC1	−0.09191	−0.09191
P32302	637	O-C-C-C-C	−0.09377	−0.09396
P32302	614	C-C-O-C-C	−0.09689	−0.09597
P32302	516	[#1]-C=C-[#1]	−0.09757	−0.10218
P32302	504	N:C:N-C	−0.10407	−0.10478
P32302	15	>= 2 N	−0.10466	−0.11037
P32302	548	O-C-C:C	−0.10708	−0.11162
P32302	714	Cc1ccc(O)cc1	−0.10718	−0.10189
P32302	531	S-C:C-C	−0.11083	−0.11062
P32302	427	C(#C)(-C)	−0.11782	−0.11602
P32302	435	C(-C)(-H)(=N)	−0.1192	−0.11394
P32302	735	Cc1cc(O)ccc1	−0.12036	−0.10674
P32302	386	C(:C)(:C)(:N)	−0.12069	−0.12543
P32302	641	O-C-C-C=C	−0.12128	−0.11641
P32302	481	O-S-C:C	−0.12298	−0.1263
P32302	628	C-N-C-C:C	−0.12573	−0.12843
P32302	150	>= 2 any ring size 5	−0.12635	−0.12607
P32302	649	O=N-C:C-O	−0.12798	−0.1207
P32302	510	[#1]-N-N-[#1]	−0.12863	−0.13347
P32302	854	NC1CC(N)CC1	−0.12863	−0.12435
P32302	469	S-S-C:C	−0.13053	−0.13003
P32302	66	>= 1 Se	−0.13313	−0.13313
P32302	547	N-C:C-N	−0.13611	−0.1441
P32302	462	O-C-C=O	−0.13836	−0.13913
P32302	48	>= 4 I	−0.13987	−0.13981
P32302	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.15024	−0.15025
P32302	576	N=C-C:C-[#1]	−0.15054	−0.14371
P32302	421	C=S	−0.15061	−0.1466
P32302	33	>= 1 S	−0.15659	−0.13969
P32302	422	N=N	−0.15788	−0.15326
P32302	455	N(-O)(=O)	−0.16216	−0.16276
P32302	779	CC1CCC(N)CC1	−0.16403	−0.15977
P32302	753	Clc1cc(Br)ccc1	−0.16745	−0.16745
P32302	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.16897	−0.16537
P32302	777	CC1CCC(O)CC1	−0.16919	−0.16474
P32302	730	Nc1ccc(Br)cc1	−0.17231	−0.17507
P32302	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.17862	−0.16559
P32302	368	C(~H)(~S)	−0.1847	−0.18734
P32302	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.18613	−0.18325
P32302	876	NC1C(Cl)CC1	−0.18644	−0.18644
P32302	759	Cc1c(Cl)cccc1	−0.18694	−0.18999
P32302	292	C-P	−0.19372	−0.1934
P32302	378	C(~N)(:C)(:N)	−0.19638	−0.19118
P32302	758	Cc1c(N)cccc1	−0.19828	−0.19161
P32302	709	C-C(C)-C-C-C	−0.20214	−0.20432
P32302	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.20354	−0.20354
P32302	496	N:N-C-[#1]	−0.20714	−0.20133

P32302	88	>= 1 Ta	−0.21084	−0.21084
P32302	775	Brc1c(Br)cccc1	−0.21119	−0.21119
P32302	505	Cl-C:C-O	−0.22598	−0.22792
P32302	707	O=C-C-C-C-C(N)-C	−0.22988	−0.23376
P32302	756	Cc1c(O)cccc1	−0.23025	−0.22624
P32302	594	C-O-C-C=C	−0.23038	−0.23635
P32302	424	N=P	−0.24098	−0.24097
P32302	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.24158	−0.24158
P32302	171	>= 5 any ring size 5	−0.24324	−0.25125
P32302	825	OC1C(S)CCCC1	−0.24613	−0.24718
P32302	376	C(~N)(:C)	−0.24624	−0.24732
P32302	732	Clc1ccc(Br)cc1	−0.24989	−0.24989
P32302	713	Cc1ccc(C)cc1	−0.25207	−0.23819
P32302	115	>= 1 any ring size 3	−0.26238	−0.25881
P32302	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.26294	−0.26256
P32302	44	>= 2 Br	−0.26767	−0.26764
P32302	433	C(-C)(-Cl)(=O)	−0.27766	−0.27766
P32302	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.27854	−0.27853
P32302	590	C-C:C-O-[#1]	−0.28191	−0.28105
P32302	517	N-N-C-N	−0.28417	−0.27977
P32302	295	C-As	−0.28526	−0.28526
P32302	776	CC1CCC(C)CC1	−0.28631	−0.29014
P32302	336	C(~C)(~C)(~C)(~N)	−0.28692	−0.28224
P32302	411	P(~O)(~O)	−0.29129	−0.29149
P32302	280	B-S	−0.2919	−0.2919
P32302	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.29282	−0.29662
P32302	855	NC1CC(Cl)CC1	−0.29412	−0.29412
P32302	477	N-N-C:C	−0.30035	−0.29785
P32302	282	B-Br	−0.30041	−0.30041
P32302	761	Oc1c(O)cccc1	−0.30368	−0.30975
P32302	541	O-C:C-C	−0.30479	−0.30022
P32302	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.30649	−0.30649
P32302	725	Sc1ccc(N)cc1	−0.30811	−0.31134
P32302	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.30849	−0.30465
P32302	480	C:S:C-C	−0.31103	−0.31104
P32302	657	C-N-C:C-C	−0.31184	−0.31207
P32302	549	N-C-C:C	−0.31371	−0.3161
P32302	399	N(~H)(:C)	−0.32812	−0.32511
P32302	852	SC1CC(Cl)CC1	−0.32962	−0.32962
P32302	98	>= 1 Bi	−0.33625	−0.33624
P32302	581	O=C-C-C-O	−0.34446	−0.3485
P32302	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.3454	−0.34541
P32302	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.36431	−0.36433
P32302	414	S(~C)(~O)	−0.36706	−0.36685
P32302	750	Nc1cc(Cl)ccc1	−0.36839	−0.36872
P32302	206	>= 5 any ring size 6	−0.36871	−0.3776
P32302	704	O=C-C-C-C-C-C-C	−0.37022	−0.36128
P32302	69	>= 1 Sr	−0.37106	−0.37106

P32302	784	OC1CCC(N)CC1	−0.41312	−0.41036
P32302	819	CC1C(O)CCCC1	−0.41739	−0.41477
P32302	409	O(:C)(:C)	−0.42252	−0.42768
P32302	740	Oc1cc(O)ccc1	−0.43389	−0.43048
P32302	407	O(~C)(~P)	−0.43529	−0.43531
P32302	623	O=C-C:C-C	−0.43962	−0.43697
P32302	385	C(:C)(:C)(:C)	−0.4398	−0.43814
P32302	619	O-C-C=C-C	−0.44145	−0.44016
P32302	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.44419	−0.44419
P32302	324	P-P	−0.4496	−0.4496
P32302	856	NC1CC(Br)CC1	−0.45059	−0.45059
P32302	234	>= 2 any ring size 8	−0.45284	−0.45284
P32302	359	C(~C)(:N)(:N)	−0.45418	−0.45742
P32302	307	N-Br	−0.45717	−0.45718
P32302	501	Cl-C:C-C	−0.45747	−0.44888
P32302	440	C(-C)(-O)(=O)	−0.46112	−0.46328
P32302	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.46191	−0.46191
P32302	658	C-C-S-C-C	−0.46304	−0.46427
P32302	300	N-N	−0.4664	−0.46075
P32302	129	>= 1 any ring size 4	−0.46719	−0.46729
P32302	636	C-N-C-N-C	−0.46728	−0.47373
P32302	605	O=C-C-O-C	−0.4707	−0.46728
P32302	19	>= 2 O	−0.49243	−0.48389
P32302	834	NC1C(Cl)CCCC1	−0.49418	−0.49643
P32302	284	C-C	−0.49493	−0.47424
P32302	760	Cc1c(Br)cccc1	−0.5028	−0.50285
P32302	366	C(~H)(~O)	−0.50323	−0.50231
P32302	744	Oc1cc(Br)ccc1	−0.50388	−0.50283
P32302	573	O-C-C=C	−0.50462	−0.50257
P32302	322	Si-Cl	−0.50603	−0.50603
P32302	688	C-C-C-C-C-C-C	−0.50632	−0.50416
P32302	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.52201	−0.52201
P32302	842	CC1CC(N)CC1	−0.52369	−0.52626
P32302	441	C(-C)(=C)	−0.53103	−0.52629
P32302	503	Cl-C:C-[#1]	−0.54107	−0.53365
P32302	429	C(#N)(-C)	−0.54429	−0.54005
P32302	9	>= 2 C	−0.55251	−0.53183
P32302	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.55508	−0.55508
P32302	630	O-C:C-O-C	−0.56263	−0.5687
P32302	871	SC1C(S)CCC1	−0.56473	−0.56473
P32302	29	>= 2 Si	−0.56524	−0.56524
P32302	332	C(~C)(~C)	−0.57497	−0.55925
P32302	823	CC1C(Br)CCCC1	−0.57814	−0.57819
P32302	492	N-C:O:C	−0.58091	−0.59092
P32302	392	N(~C)(~C)(~H)	−0.58439	−0.57992
P32302	620	C:C-O-C-C	−0.58457	−0.58351
P32302	431	C(-C)(-C)(=N)	−0.58636	−0.59094
P32302	59	>= 1 Co	−0.58833	−0.58833

P32302	615	N-C-C-O-C	−0.59617	−0.59189
P32302	645	O=C-N-C-C	−0.60194	−0.60201
P32302	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.60734	−0.60226
P32302	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.61361	−0.6136
P32302	86	>= 1 Lu	−0.61993	−0.61993
P32302	53	>= 1 Sc	−0.62092	−0.62092
P32302	873	SC1C(Cl)CCC1	−0.62375	−0.62375
P32302	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.62846	−0.63398
P32302	699	O-C-C-C-C-C(C)-C	−0.63294	−0.64555
P32302	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.636	−0.636
P32302	78	>= 1 Cd	−0.63986	−0.63986
P32302	74	>= 1 Ru	−0.64231	−0.64231
P32302	498	O-C=C-C	−0.6475	−0.64321
P32302	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.6597	−0.66113
P32302	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.67528	−0.67498
P32302	682	O-C-C-C-C-N	−0.68044	−0.68153
P32302	73	>= 1 Mo	−0.68395	−0.68395
P32302	762	Oc1c(S)cccc1	−0.68411	−0.68517
P32302	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.68613	−0.68613
P32302	403	N(:C)(:C)	−0.68932	−0.69289
P32302	266	Li-C	−0.69555	−0.69555
P32302	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.70031	−0.70031
P32302	268	Li-F	−0.71396	−0.71396
P32302	858	ClC1CC(Br)CC1	−0.71549	−0.71549
P32302	783	OC1CCC(S)CC1	−0.71848	−0.71993
P32302	339	C(~C)(~C)(~H)(~O)	−0.72316	−0.73034
P32302	417	C#C	−0.73063	−0.72883
P32302	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.73451	−0.73451
P32302	796	BrC1CCC(Br)CC1	−0.75194	−0.75194
P32302	275	B-N	−0.7643	−0.7643
P32302	443	C(-C)(=O)	−0.77152	−0.77429
P32302	345	C(~C)(~H)(~N)	−0.77228	−0.76345
P32302	545	N-C:C-C	−0.77757	−0.77371
P32302	689	O-C-C-C-C-C-C	−0.77836	−0.77899
P32302	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.77988	−0.78904
P32302	838	BrC1C(Br)CCCC1	−0.78185	−0.78185
P32302	741	Oc1cc(S)ccc1	−0.78185	−0.78879
P32302	287	C-F	−0.78979	−0.7913
P32302	381	C(~O)(:C)	−0.79366	−0.79066
P32302	40	>= 8 Cl	−0.80073	−0.80073
P32302	444	C(-Cl)(=O)	−0.80268	−0.80268
P32302	375	C(~N)(~N)	−0.81404	−0.81029
P32302	293	C-S	−0.8183	−0.80149
P32302	597	O=C-C-C:C	−0.8311	−0.8351
P32302	806	OC1CC(Cl)CCC1	−0.84103	−0.85393
P32302	404	N(:C)(:C)(:C)	−0.84303	−0.84194
P32302	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.8478	−0.85914
P32302	310	O-Mg	−0.85174	−0.85174

P32302	538	N=C-C-C	−0.85809	−0.85631
P32302	814	NC1CC(Br)CCC1	−0.86056	−0.85898
P32302	755	Cc1c(C)cccc1	−0.86635	−0.85681
P32302	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.8682	−0.86212
P32302	578	C-C:C-C:C	−0.87008	−0.87223
P32302	788	SC1CCC(N)CC1	−0.88336	−0.88659
P32302	419	C#N	−0.89591	−0.8917
P32302	277	B-F	−0.90675	−0.90675
P32302	765	Oc1c(Br)cccc1	−0.9074	−0.90496
P32302	515	N-N-C-C	−0.90901	−0.90997
P32302	799	CC1CC(S)CCC1	−0.92949	−0.93499
P32302	563	O-C-O-C	−0.93455	−0.93282
P32302	347	C(~C)(~H)(~O)(~O)	−0.9454	−0.94598
P32302	598	Cl-C:C:C-C	−0.94735	−0.94535
P32302	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.94806	−0.9452
P32302	729	Nc1ccc(Cl)cc1	−0.98418	−0.98915
P32302	514	O-N-C-C	−0.99397	−0.99088
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P32302	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−1.00402	−1.00403
P32302	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−1.00898	−1.00898
P32302	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−1.00956	−1.01555
P32302	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−1.01749	−1.01815
P32302	267	Li-O	−1.03842	−1.03843
P32302	136	>= 2 any ring size 4	−1.04496	−1.04272
P32302	62	>= 1 Zn	−1.04536	−1.04536
P32302	772	Nc1c(Br)cccc1	−1.04726	−1.04751
P32302	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−1.04851	−1.05185
P32302	89	>= 1 W	−1.05525	−1.05525
P32302	456	P(-O)(=O)	−1.0765	−1.0767
P32302	353	C(~C)(~S)	−1.07873	−1.0669
P32302	611	N-C-C-N-C	−1.11074	−1.10886
P32302	746	Sc1cc(N)ccc1	−1.11343	−1.11415
P32302	391	N(~C)(~C)(~C)	−1.13893	−1.13173
P32302	207	>= 5 saturated or aromatic carbon-only ring size 6	−1.16333	−1.16333
P32302	72	>= 1 Nb	−1.16669	−1.16669
P32302	830	SC1C(N)CCCC1	−1.18891	−1.19331
P32302	14	>= 1 N	−1.19732	−1.19321
P32302	719	Oc1ccc(O)cc1	−1.21322	−1.21988
P32302	327	C(~Br)(~C)	−1.21959	−1.22263
P32302	872	SC1C(N)CCC1	−1.23925	−1.23925
P32302	438	C(-C)(-N)(=N)	−1.24142	−1.23328
P32302	575	O-C-C:C-O	−1.2655	−1.26552
P32302	26	>= 1 Na	−1.3077	−1.30949
P32302	651	O-C:C:C-C	−1.31716	−1.31658
P32302	832	SC1C(Br)CCCC1	−1.32296	−1.32296
P32302	572	N:C:N:C	−1.33187	−1.33498
P32302	354	C(~C)(~Si)	−1.34754	−1.34753
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P32302	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−1.38605	−1.38922
P32302	172	>= 5 saturated or aromatic carbon-only ring size 5	−1.40012	−1.40011
P32302	869	OC1C(Cl)CCC1	−1.43753	−1.43753
P32302	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.4412	−1.4412
P32302	61	>= 1 Cu	−1.52367	−1.52367
P32302	580	O=C-C-C-N	−1.54052	−1.53531
P32302	75	>= 1 Rh	−1.56914	−1.56914
P32302	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−1.60389	−1.60389
P32302	622	O=C-O-C:C	−1.62184	−1.62596
P32302	436	C(-C)(-H)(=O)	−1.65832	−1.65622
P32302	488	N-C=N-[#1]	−1.67627	−1.67389
P32302	31	>= 2 P	−1.69767	−1.69766
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P32302	370	C(~H)(:C)	−1.74198	−1.7458
P32302	609	Cl-C-C-N-C	−1.84291	−1.84333
P32302	774	Clc1c(Br)cccc1	−1.89416	−1.89416
P32302	301	N-O	−1.98865	−1.98309
P32302	556	C=C-C-C	−2.17867	−2.18542
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2.54E-08

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P51685	76	>= 1 Pd	2.7364583
P51685	172	>= 5 saturated or aromatic carbon-only ring size 5	2.5137869
P51685	808	SC1CC(S)CCC1	2.4099704
P51685	275	B-N	2.3575393
P51685	631	O-C:C-O-[#1]	2.3062034
P51685	828	OC1C(Br)CCCC1	2.3060444
P51685	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	2.288039
P51685	733	Brc1ccc(Br)cc1	2.2321985
P51685	265	Li-B	2.1780815
P51685	498	O-C=C-C	2.1590903
P51685	482	C:N-C:C	2.1563183
P51685	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	2.1374623
P51685	868	OC1C(N)CCC1	2.0613935
P51685	715	Cc1ccc(S)cc1	2.0573075
P51685	111	>= 1 Tm	2.02842
P51685	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	2.0264755
P51685	534	S-C:C-O	1.9721979
P51685	619	O-C-C=C-C	1.690754
P51685	661	O-C-O-C-C	1.68816
P51685	793	NC1CCC(Br)CC1	1.6876777
P51685	878	ClC1C(Cl)CCC1	1.6791399
P51685	833	NC1C(N)CCCC1	1.6622959
P51685	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	1.6469636
P51685	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	1.6374688
P51685	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	1.6283225
P51685	403	N(:C)(:C)	1.6106807
P51685	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	1.5916241
P51685	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	1.55787
P51685	856	NC1CC(Br)CC1	1.5529879
P51685	612	N-C-O-C-C	1.5508166
P51685	98	>= 1 Bi	1.5371712
P51685	583	Cl-C:C-O-C	1.527061
P51685	56	>= 1 Cr	1.494217
P51685	681	O-C-C-C-C-O	1.4721899
P51685	646	O=C-N-C-[#1]	1.4695107
P51685	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	1.4610531
P51685	737	Cc1cc(N)ccc1	1.4453138
P51685	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	1.4445371
P51685	0	>= 4 H	1.4205031
P51685	541	O-C:C-C	1.397745
P51685	279	B-P	1.3930812
P51685	851	SC1CC(N)CC1	1.3833191
P51685	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	1.3771651
P51685	9	>= 2 C	1.3700723
P51685	345	C(~C)(~H)(~N)	1.3526097
P51685	768	Sc1c(Cl)cccc1	1.3381974

P51685	97	>= 1 Pb	1.3381452
P51685	772	Nc1c(Br)cccc1	1.3310104
P51685	709	C-C(C)-C-C-C	1.3270175
P51685	789	SC1CCC(Cl)CC1	1.2774944
P51685	757	Cc1c(S)cccc1	1.2754667
P51685	379	C(~N)(:N)	1.2583827
P51685	1	>= 8 H	1.2324152
P51685	609	Cl-C-C-N-C	1.217181
P51685	86	>= 1 Lu	1.217009
P51685	626	C-O-C:C-C	1.2086727
P51685	662	O-C-C-O-C	1.1985515
P51685	645	O=C-N-C-C	1.1980701
P51685	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	1.1870408
P51685	492	N-C:O:C	1.1820095
P51685	5	>= 2 Li	1.1765762
P51685	332	C(~C)(~C)	1.1728839
P51685	322	Si-Cl	1.1681172
P51685	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	1.1566535
P51685	327	C(~Br)(~C)	1.1557931
P51685	561	Cl-C-C=O	1.1551291
P51685	682	O-C-C-C-C-N	1.1515714
P51685	102	>= 1 Nd	1.1479178
P51685	836	ClC1C(Cl)CCCC1	1.1293481
P51685	453	N(-C)(=C)	1.1213455
P51685	688	C-C-C-C-C-C-C	1.1157673
P51685	262	>= 4 hetero-aromatic rings	1.1124699
P51685	137	>= 2 saturated or aromatic carbon-only ring size 4	1.1054273
P51685	862	CC1C(S)CCC1	1.1045584
P51685	28	>= 1 Si	1.0828129
P51685	105	>= 1 Eu	1.0828082
P51685	527	C:C:N-[#1]	1.0604459
P51685	573	O-C-C=C	1.0588964
P51685	837	ClC1C(Br)CCCC1	1.0451241
P51685	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	1.0172846
P51685	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	1.0095728
P51685	755	Cc1c(C)cccc1	1.0039915
P51685	781	CC1CCC(Br)CC1	0.9950336
P51685	34	>= 2 S	0.9949024
P51685	616	C:C:N:N:C	0.9855835
P51685	499	N-C:C:N	0.9738916
P51685	822	CC1C(Cl)CCCC1	0.9713024
P51685	475	S-C=N-C	0.9647806
P51685	643	[#1]-C-C-N-[#1]	0.9543819
P51685	458	S(-O)(=O)	0.9491368
P51685	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.9472318
P51685	270	Li-S	0.9448656
P51685	734	Cc1cc(C)ccc1	0.9405441
P51685	747	Sc1cc(Cl)ccc1	0.9289767

P51685	438	C(-C)(-N)(=N)	0.9137119
P51685	89	>= 1 W	0.9042778
P51685	545	N-C:C-C	0.8907883
P51685	812	NC1CC(N)CCC1	0.8869734
P51685	365	C(~H)(~N)	0.8863778
P51685	749	Nc1cc(N)ccc1	0.8861976
P51685	280	B-S	0.8778943
P51685	27	>= 2 Na	0.8752722
P51685	490	C-C-C=C	0.875223
P51685	692	O=C-C-C-C-C-C	0.8696225
P51685	740	Oc1cc(O)ccc1	0.8615977
P51685	623	O=C-C:C-C	0.8575976
P51685	535	O=C-C-C	0.8525505
P51685	473	S-C:N:C	0.8404676
P51685	179	>= 1 saturated or aromatic carbon-only ring size 6	0.834597
P51685	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.8332789
P51685	375	C(~N)(~N)	0.83261
P51685	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.8183036
P51685	7	>= 2 B	0.8171756
P51685	373	C(~H)(:N)	0.8113015
P51685	68	>= 1 Rb	0.8099246
P51685	866	OC1C(O)CCC1	0.8029262
P51685	512	C-[As]-O-[#1]	0.7942435
P51685	477	N-N-C:C	0.788913
P51685	829	SC1C(S)CCCC1	0.7873134
P51685	584	C:C-C=C-C	0.7871816
P51685	505	Cl-C:C-O	0.7859674
P51685	791	NC1CCC(N)CC1	0.7849742
P51685	746	Sc1cc(N)ccc1	0.7809064
P51685	448	C(-H)(=O)	0.7803499
P51685	794	ClC1CCC(Cl)CC1	0.7721097
P51685	659	O-C-C-N-C	0.7673046
P51685	762	Oc1c(S)cccc1	0.7643622
P51685	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.7611458
P51685	550	Cl-C-C-C	0.7588981
P51685	67	>= 1 Kr	0.7570074
P51685	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.7538001
P51685	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.7534642
P51685	377	C(~N)(:C)(:C)	0.748177
P51685	109	>= 1 Ho	0.7393612
P51685	314	O-P	0.7380488
P51685	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.7335299
P51685	46	>= 1 I	0.7287361
P51685	74	>= 1 Ru	0.7242261
P51685	91	>= 1 Os	0.7231294
P51685	725	Sc1ccc(N)cc1	0.7220198
P51685	356	C(~C)(:C)(:C)	0.7190185
P51685	106	>= 1 Gd	0.7186427

P51685	259	>= 3 aromatic rings	0.7185185
P51685	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.7168124
P51685	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.71652
P51685	528	[#1]-N-C-[#1]	0.7160669
P51685	858	ClC1CC(Br)CC1	0.7111231
P51685	743	Oc1cc(Cl)ccc1	0.7087581
P51685	60	>= 1 Ni	0.7082043
P51685	805	OC1CC(N)CCC1	0.705052
P51685	591	Cl-C-C-C-C	0.689734
P51685	399	N(~H)(:C)	0.6868785
P51685	722	Oc1ccc(Cl)cc1	0.6863669
P51685	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.6857681
P51685	555	N=C-C=C	0.6845683
P51685	408	O(~H)(~S)	0.6832704
P51685	872	SC1C(N)CCC1	0.6811356
P51685	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.6729121
P51685	795	ClC1CCC(Br)CC1	0.6715711
P51685	569	N-C-C-N	0.6709636
P51685	346	C(~C)(~H)(~O)	0.6674332
P51685	130	>= 1 saturated or aromatic carbon-only ring size 4	0.6586718
P51685	719	Oc1ccc(O)cc1	0.6402976
P51685	249	>= 1 saturated or aromatic carbon-only ring size 10	0.6395471
P51685	267	Li-O	0.6379012
P51685	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.6363777
P51685	826	OC1C(N)CCCC1	0.6343392
P51685	718	Cc1ccc(Br)cc1	0.6340467
P51685	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.6339107
P51685	774	Clc1c(Br)cccc1	0.629841
P51685	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.6281684
P51685	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.612738
P51685	825	OC1C(S)CCCC1	0.6126551
P51685	761	Oc1c(O)cccc1	0.6105154
P51685	110	>= 1 Er	0.606633
P51685	525	[As]-C:C-[#1]	0.6056791
P51685	816	ClC1CC(Br)CCC1	0.6032484
P51685	351	C(~C)(~N)	0.5967504
P51685	389	C(:N)(:N)	0.5943964
P51685	321	Si-Si	0.5936749
P51685	107	>= 1 Tb	0.5836642
P51685	635	N-N-C-N-[#1]	0.5699686
P51685	752	Clc1cc(Cl)ccc1	0.5636324
P51685	283	C-H	0.5614527
P51685	679	C-C-C-C-C-C	0.5599575
P51685	221	>= 2 saturated or aromatic carbon-only ring size 7	0.558129
P51685	425	P=O	0.5575205
P51685	546	N-C:C-[#1]	0.5551851
P51685	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.5504026
P51685	627	O=[As]-C:C:C	0.550334

P51685	328	C(~Br)(~C)(~C)	0.5418111
P51685	200	>= 4 saturated or aromatic carbon-only ring size 6	0.5392142
P51685	317	F-S	0.5383673
P51685	342	C(~C)(~Cl)	0.5382154
P51685	644	C-C=N-N-C	0.5350114
P51685	305	N-S	0.5309913
P51685	574	O-C-C:C-C	0.5296037
P51685	558	O=N-C:C	0.526528
P51685	671	O=C-C=C-C	0.519171
P51685	777	CC1CCC(O)CC1	0.5052374
P51685	684	O=C-C-C-C-C	0.5036781
P51685	730	Nc1ccc(Br)cc1	0.4999643
P51685	329	C(~Br)(~H)	0.4955068
P51685	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.4914883
P51685	678	C-C-C=C-C	0.4883203
P51685	637	O-C-C-C-C	0.4772173
P51685	374	C(~H)(~H)(~H)	0.4692775
P51685	115	>= 1 any ring size 3	0.4619256
P51685	536	O=C-C-N	0.4611196
P51685	285	C-N	0.4606839
P51685	594	C-O-C-C=C	0.4600348
P51685	854	NC1CC(N)CC1	0.4467155
P51685	843	CC1CC(Cl)CC1	0.4462122
P51685	694	O=C-C-C-C-C=O	0.441684
P51685	672	O=C-C=C-[#1]	0.4364651
P51685	587	N-C:C-O-[#1]	0.4350576
P51685	650	O=C-N-C=O	0.4323503
P51685	708	C-C(C)-C-C	0.4244948
P51685	529	Cl-C-C-Cl	0.4213388
P51685	313	O-Si	0.415148
P51685	481	O-S-C:C	0.4117113
P51685	81	>= 1 Sb	0.4009096
P51685	199	>= 4 any ring size 6	0.3980418
P51685	88	>= 1 Ta	0.3960155
P51685	330	C(~Br)(:C)	0.3946255
P51685	648	O=N-C:C-N	0.3902125
P51685	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.3898539
P51685	26	>= 1 Na	0.3883282
P51685	306	N-Cl	0.3767115
P51685	873	SC1C(Cl)CCC1	0.3747231
P51685	667	C=C-C-O-[#1]	0.369469
P51685	600	N-C:C:C-C	0.3674953
P51685	266	Li-C	0.3648215
P51685	308	O-H	0.364563
P51685	726	Sc1ccc(Cl)cc1	0.3626917
P51685	289	C-Mg	0.3626664
P51685	630	O-C:C-O-C	0.3610024
P51685	712	C-C(C)-C(C)-C	0.3601592

P51685	449	C(-N)(=C)	0.3542483
P51685	78	>= 1 Cd	0.3513704
P51685	355	C(~C)(:C)	0.3497036
P51685	707	O=C-C-C-C-C(N)-C	0.3486201
P51685	613	C-N-C-C-C	0.3475322
P51685	804	OC1CC(S)CCC1	0.3474389
P51685	520	C=C-C:C	0.343585
P51685	830	SC1C(N)CCCC1	0.3388352
P51685	764	Oc1c(Cl)cccc1	0.3373235
P51685	444	C(-Cl)(=O)	0.3331685
P51685	552	C:C-C:C	0.328586
P51685	113	>= 1 Tc	0.3281585
P51685	657	C-N-C:C-C	0.32441
P51685	471	S:C:C:C	0.3219453
P51685	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.3214035
P51685	248	>= 1 any ring size 10	0.3174382
P51685	803	OC1CC(O)CCC1	0.3156421
P51685	228	>= 1 saturated or aromatic carbon-only ring size 8	0.31013
P51685	416	C=C	0.3089518
P51685	685	O=C-C-C-C-N	0.3075836
P51685	474	S:C:C:N	0.3073517
P51685	235	>= 2 saturated or aromatic carbon-only ring size 8	0.3022152
P51685	549	N-C-C:C	0.3013325
P51685	362	C(~Cl)(:C)	0.2970795
P51685	819	CC1C(O)CCCC1	0.2957678
P51685	41	>= 1 K	0.2912203
P51685	514	O-N-C-C	0.2879243
P51685	443	C(-C)(=O)	0.2876773
P51685	820	CC1C(S)CCCC1	0.2857143
P51685	763	Oc1c(N)cccc1	0.28073
P51685	54	>= 1 Ti	0.2759643
P51685	293	C-S	0.274367
P51685	38	>= 2 Cl	0.2637631
P51685	641	O-C-C-C=C	0.2637379
P51685	33	>= 1 S	0.2633189
P51685	506	C-C:N:C	0.2519378
P51685	697	C-C-C-C-C-C(C)-C	0.2518453
P51685	562	Br-C-C=O	0.2505233
P51685	303	N-Si	0.2463935
P51685	171	>= 5 any ring size 5	0.2432905
P51685	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.2414389
P51685	680	O-C-C-C-C-C	0.2405352
P51685	673	O=C-C=C-N	0.2357587
P51685	390	N(~C)(~C)	0.2352567
P51685	51	>= 1 Al	0.232449
P51685	44	>= 2 Br	0.2319137
P51685	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.2266084
P51685	511	S=C-N-[#1]	0.2194776

P51685	429	C(#N)(-C)	0.2159044
P51685	8	>= 4 B	0.2154989
P51685	487	N-C=N-C	0.215375
P51685	370	C(~H)(:C)	0.202418
P51685	486	N-C:N:N	0.1977313
P51685	838	BrC1C(Br)CCCC1	0.1957038
P51685	617	C-C-C-O-[#1]	0.1931469
P51685	588	O=C-C-C=O	0.1920279
P51685	537	O=C-C-O	0.1845639
P51685	759	Cc1c(Cl)cccc1	0.1836339
P51685	241	>= 1 any ring size 9	0.1804269
P51685	515	N-N-C-C	0.1763657
P51685	441	C(-C)(=C)	0.17624
P51685	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.1745211
P51685	568	N#C-C-C	0.1739451
P51685	614	C-C-O-C-C	0.1624554
P51685	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.1587539
P51685	263	Li-H	0.1464514
P51685	432	C(-C)(-C)(=O)	0.1453271
P51685	214	>= 1 saturated or aromatic carbon-only ring size 7	0.1447458
P51685	483	N-S-C:C	0.1324579
P51685	136	>= 2 any ring size 4	0.1265342
P51685	407	O(~C)(~P)	0.1182374
P51685	349	C(~C)(~H)(~S)	0.1173685
P51685	302	N-F	0.1164959
P51685	560	N-C-N-C	0.1153795
P51685	462	O-C-C=O	0.1152927
P51685	446	C(-H)(=C)	0.1110118
P51685	593	N-C-C-C-N	0.1098606
P51685	452	C(-O)(=O)	0.106922
P51685	85	>= 1 Ba	0.1026864
P51685	404	N(:C)(:C)(:C)	0.1002906
P51685	466	N#C-C=C	0.0962175
P51685	450	C(-N)(=N)	0.090015
P51685	711	C-C(C)(C)-C-C	0.0887183
P51685	542	O-C:C-[#1]	0.0833139
P51685	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0832551
P51685	326	As-As	0.0820935
P51685	23	>= 1 F	0.0778351
P51685	463	N:C-S-[#1]	0.0724386
P51685	567	O-C-C-O	0.0719435
P51685	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0712384
P51685	823	CC1C(Br)CCCC1	0.0703543
P51685	451	C(-N)(=O)	0.0674461
P51685	294	C-Cl	0.0656929
P51685	547	N-C:C-N	0.061718
P51685	455	N(-O)(=O)	0.0615809
P51685	484	N-C:N:C	0.060258

P51685	360	C(~Cl)(~Cl)	0.0593353
P51685	277	B-F	0.057105
P51685	503	Cl-C:C-[#1]	0.0532588
P51685	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.0522324
P51685	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0489279
P51685	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0477598
P51685	539	N=C-C-[#1]	0.0473062
P51685	509	Br-C:C-C	0.0469261
P51685	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.0426782
P51685	796	BrC1CCC(Br)CC1	0.0417572
P51685	785	OC1CCC(Cl)CC1	0.0414643
P51685	445	C(-H)(-N)(=C)	0.0410535
P51685	496	N:N-C-[#1]	0.036269
P51685	608	C-C-C-C:C	0.0358912
P51685	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0348538
P51685	760	Cc1c(Br)cccc1	0.0347378
P51685	337	C(~C)(~C)(~C)(~O)	0.0345458
P51685	649	O=N-C:C-O	0.0339601
P51685	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0336583
P51685	430	C(-C)(-C)(=C)	0.0335244
P51685	595	C:C-C-C-C	0.0334456
P51685	71	>= 1 Zr	0.0332824
P51685	271	Li-Cl	0.0331793
P51685	380	C(~O)(~O)	0.0331334
P51685	347	C(~C)(~H)(~O)(~O)	0.0324906
P51685	427	C(#C)(-C)	0.0324187
P51685	227	>= 1 any ring size 8	0.031558
P51685	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.0308142
P51685	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.030779
P51685	702	O-C-C-C-C-C-N-C	0.0302239
P51685	470	C:C-C=C	0.0301227
P51685	255	>= 1 aromatic ring	0.0297278
P51685	880	BrC1C(Br)CCC1	0.0286103
P51685	771	Nc1c(Cl)cccc1	0.0274138
P51685	339	C(~C)(~C)(~H)(~O)	0.0272655
P51685	721	Oc1ccc(N)cc1	0.0267709
P51685	261	>= 4 aromatic rings	0.0263431
P51685	299	N-H	0.0252809
P51685	521	C:N-C-[#1]	0.0234571
P51685	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0224114
P51685	42	>= 2 K	0.0213065
P51685	497	O-C:C:N	0.0203545
P51685	598	Cl-C:C:C-C	0.0191884
P51685	530	N:C-C:C	0.0187165
P51685	101	>= 1 Pr	0.0183479
P51685	653	O-C:C:C-O	0.0180919
P51685	750	Nc1cc(Cl)ccc1	0.017973
P51685	601	N-C:C:C-N	0.0179163

P51685	350	C(~C)(~I)	0.0171076
P51685	361	C(~Cl)(~H)	0.0160549
P51685	336	C(~C)(~C)(~C)(~N)	0.0160198
P51685	401	N(~O)(~O)	0.0146771
P51685	840	CC1CC(O)CC1	0.0136687
P51685	334	C(~C)(~C)(~C)(~C)	0.0129436
P51685	422	N=N	0.0121435
P51685	433	C(-C)(-Cl)(=O)	0.0107964
P51685	634	C-C-C:C-C	0.0105057
P51685	300	N-N	0.0102441
P51685	775	Brc1c(Br)cccc1	0.0100504
P51685	287	C-F	0.009089
P51685	2	>= 16 H	0.0084852
P51685	4	>= 1 Li	0.0078617
P51685	476	C-O-C=C	0.0077505
P51685	489	N-C-S-C	0.0076151
P51685	779	CC1CCC(N)CC1	0.006457
P51685	69	>= 1 Sr	0.0048836
P51685	309	O-O	0.00448
P51685	824	OC1C(O)CCCC1	0.0041129
P51685	434	C(-C)(-H)(=C)	0.0038594
P51685	43	>= 1 Br	0.0038298
P51685	83	>= 1 Xe	0.0037535
P51685	292	C-P	0.0034511
P51685	417	C#C	0.0033961
P51685	164	>= 4 any ring size 5	0.0032317
P51685	65	>= 1 As	0.0030558
P51685	72	>= 1 Nb	0.0022417
P51685	459	S(=O)(=O)	0.0020275
P51685	849	OC1CC(Br)CC1	0.0019625
P51685	297	C-Br	0.0018025
P51685	234	>= 2 any ring size 8	0.0016708
P51685	478	S-C=N-[#1]	0.0014373
P51685	766	Sc1c(S)cccc1	0.0013497
P51685	100	>= 1 Ce	0.0013309
P51685	323	P-H	0.0011919
P51685	367	C(~H)(~O)(~O)	0.0010645
P51685	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0010146
P51685	66	>= 1 Se	0.0009204
P51685	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.0009009
P51685	344	C(~C)(~H)	0.0005522
P51685	853	SC1CC(Br)CC1	0.0005494
P51685	442	C(-C)(=N)	0.0004341
P51685	753	Clc1cc(Br)ccc1	0.0002902
P51685	52	>= 1 Ca	0.0001453
P51685	876	NC1C(Cl)CC1	4.71E-05
P51685	84	>= 1 Cs	3.34E-05
P51685	80	>= 1 Sn	1.37E-05

P51685	319	Al-Cl	4.10E-07
P51685	258	>= 2 hetero-aromatic rings	1.12E-07
P51685	879	ClC1C(Br)CCC1	-1.12E-07
P51685	844	CC1CC(Br)CC1	-1.82E-05
P51685	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	-0.000321
P51685	353	C(~C)(~S)	-0.000458
P51685	790	SC1CCC(Br)CC1	-0.000787
P51685	769	Sc1c(Br)cccc1	-0.001184
P51685	316	F-P	-0.001297
P51685	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.001416
P51685	99	>= 1 La	-0.001619
P51685	582	C-C-C-C-C	-0.001672
P51685	92	>= 1 Ir	-0.001733
P51685	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	-0.001883
P51685	668	C-C:C-C-C	-0.002127
P51685	413	S(~C)(~H)	-0.002708
P51685	47	>= 2 I	-0.002752
P51685	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	-0.002915
P51685	491	C-N:C-[#1]	-0.003124
P51685	343	C(~C)(~Cl)(~H)	-0.003594
P51685	624	O=C-C:C-N	-0.004148
P51685	295	C-As	-0.00461
P51685	639	O-C-C-C-O	-0.005197
P51685	615	N-C-C-O-C	-0.005485
P51685	578	C-C:C-C:C	-0.005748
P51685	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	-0.006591
P51685	807	OC1CC(Br)CCC1	-0.006754
P51685	426	P=P	-0.006984
P51685	621	N-C:C:C:N	-0.00708
P51685	447	C(-H)(=N)	-0.007841
P51685	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	-0.007988
P51685	572	N:C:N:C	-0.008396
P51685	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.008598
P51685	90	>= 1 Re	-0.008906
P51685	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	-0.008932
P51685	77	>= 1 Ag	-0.009149
P51685	398	N(~H)(~N)	-0.009437
P51685	157	>= 3 any ring size 5	-0.009656
P51685	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	-0.009666
P51685	331	C(~Br)(:N)	-0.010504
P51685	736	Cc1cc(S)ccc1	-0.010669
P51685	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	-0.010851
P51685	460	C-C-C#C	-0.010912
P51685	423	N=O	-0.011159
P51685	298	C-I	-0.011995
P51685	304	N-P	-0.014039
P51685	735	Cc1cc(O)ccc1	-0.014132
P51685	193	>= 3 saturated or aromatic carbon-only ring size 6	-0.014175

P51685	406	O(~C)(~H)	−0.01482
P51685	129	>= 1 any ring size 4	−0.014861
P51685	683	N-C-C-C-C-C	−0.016693
P51685	62	>= 1 Zn	−0.017024
P51685	494	O=C-C:N	−0.017459
P51685	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.018613
P51685	96	>= 1 Tl	−0.020053
P51685	783	OC1CCC(S)CC1	−0.020279
P51685	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.021742
P51685	516	[#1]-C=C-[#1]	−0.02176
P51685	744	Oc1cc(Br)ccc1	−0.022194
P51685	352	C(~C)(~O)	−0.022578
P51685	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.02283
P51685	606	O-C:C-C-C	−0.023229
P51685	376	C(~N)(:C)	−0.023532
P51685	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.024031
P51685	340	C(~C)(~C)(~N)	−0.0242
P51685	731	Clc1ccc(Cl)cc1	−0.024599
P51685	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.024996
P51685	21	>= 8 O	−0.026176
P51685	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.027819
P51685	832	SC1C(Br)CCCC1	−0.028723
P51685	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.028764
P51685	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.031106
P51685	220	>= 2 any ring size 7	−0.031171
P51685	863	CC1C(N)CCC1	−0.03135
P51685	811	SC1CC(Br)CCC1	−0.031777
P51685	792	NC1CCC(Cl)CC1	−0.032449
P51685	687	O=C-C-C-C=O	−0.032966
P51685	282	B-Br	−0.03343
P51685	324	P-P	−0.033535
P51685	504	N:C:N-C	−0.033682
P51685	391	N(~C)(~C)(~C)	−0.034379
P51685	660	C-C=C-C-C	−0.034687
P51685	580	O=C-C-C-N	−0.03483
P51685	418	C=N	−0.041431
P51685	519	N=C-N-C	−0.041696
P51685	669	Cl-C:C-C=O	−0.041724
P51685	532	S-C:C-[#1]	−0.041962
P51685	143	>= 1 any ring size 5	−0.047703
P51685	690	O-C-C-C-C-C-O	−0.050365
P51685	388	C(:C)(:N)(:N)	−0.051326
P51685	696	C-C-C-C-C-C-C-C	−0.051745
P51685	773	Clc1c(Cl)cccc1	−0.053178
P51685	472	C:N:C-C	−0.054023
P51685	780	CC1CCC(Cl)CC1	−0.055324
P51685	513	S:C:C-[#1]	−0.056013
P51685	150	>= 2 any ring size 5	−0.057681

P51685	524	C-C=C-C	−0.057987
P51685	846	OC1CC(S)CC1	−0.058172
P51685	431	C(-C)(-C)(=N)	−0.059071
P51685	607	N-C-C-C:C	−0.061444
P51685	291	C-Si	−0.065291
P51685	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.065359
P51685	357	C(~C)(:C)(:N)	−0.066117
P51685	290	C-Al	−0.069811
P51685	713	Cc1ccc(C)cc1	−0.070369
P51685	359	C(~C)(:N)(:N)	−0.072114
P51685	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.073298
P51685	381	C(~O)(:C)	−0.074495
P51685	579	O=C-C-C-C	−0.076798
P51685	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.077201
P51685	787	SC1CCC(S)CC1	−0.077804
P51685	500	C-S-C:C	−0.080893
P51685	383	C(~S)(:C)	−0.081046
P51685	286	C-O	−0.081492
P51685	700	O-C-C-C-C-C-O-C	−0.081988
P51685	665	N-C:C-C-C	−0.082409
P51685	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.087606
P51685	717	Cc1ccc(Cl)cc1	−0.087969
P51685	24	>= 2 F	−0.089981
P51685	480	C:S:C-C	−0.09065
P51685	666	C=C-C-O-C	−0.091084
P51685	658	C-C-S-C-C	−0.09109
P51685	817	BrC1CC(Br)CCC1	−0.091621
P51685	605	O=C-C-O-C	−0.094222
P51685	369	C(~H)(~Si)	−0.095804
P51685	788	SC1CCC(N)CC1	−0.097841
P51685	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.100126
P51685	738	Cc1cc(Cl)ccc1	−0.104764
P51685	395	N(~C)(~O)	−0.104931
P51685	813	NC1CC(Cl)CCC1	−0.106047
P51685	440	C(-C)(-O)(=O)	−0.107016
P51685	372	C(~H)(:C)(:N)	−0.108444
P51685	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.10913
P51685	801	CC1CC(Cl)CCC1	−0.110257
P51685	335	C(~C)(~C)(~C)(~H)	−0.114083
P51685	464	N-C-C=C	−0.117024
P51685	834	NC1C(Cl)CCCC1	−0.121756
P51685	745	Sc1cc(S)ccc1	−0.124528
P51685	570	C:C-C-C	−0.12453
P51685	531	S-C:C-C	−0.126494
P51685	714	Cc1ccc(O)cc1	−0.127433
P51685	855	NC1CC(Cl)CC1	−0.131723
P51685	495	C-N-C:C	−0.132888
P51685	14	>= 1 N	−0.133294

P51685	274	B-C	−0.13762
P51685	457	S(-C)(=O)	−0.13931
P51685	603	C-C:C:C-C	−0.142653
P51685	770	Nc1c(N)cccc1	−0.144533
P51685	636	C-N-C-N-C	−0.148707
P51685	698	O-C-C-C-C-C-C-C	−0.158432
P51685	695	O=C-C-C-C-C-N	−0.159562
P51685	12	>= 16 C	−0.160958
P51685	192	>= 3 any ring size 6	−0.165297
P51685	575	O-C-C:C-O	−0.175102
P51685	48	>= 4 I	−0.176641
P51685	25	>= 4 F	−0.180441
P51685	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.186097
P51685	857	ClC1CC(Cl)CC1	−0.195067
P51685	523	N:C:C-C	−0.197605
P51685	53	>= 1 Sc	−0.206392
P51685	16	>= 4 N	−0.210535
P51685	421	C=S	−0.216545
P51685	518	O=C-N-N	−0.220941
P51685	767	Sc1c(N)cccc1	−0.221356
P51685	566	O-C-C-N	−0.223096
P51685	39	>= 4 Cl	−0.235749
P51685	40	>= 8 Cl	−0.238145
P51685	384	C(:C)(:C)	−0.240351
P51685	739	Cc1cc(Br)ccc1	−0.240765
P51685	272	B-H	−0.246212
P51685	30	>= 1 P	−0.250767
P51685	112	>= 1 Yb	−0.251901
P51685	638	O-C-C-C-N	−0.252915
P51685	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.263589
P51685	590	C-C:C-O-[#1]	−0.263856
P51685	363	C(~F)(~F)	−0.267368
P51685	847	OC1CC(N)CC1	−0.278321
P51685	456	P(-O)(=O)	−0.279339
P51685	815	ClC1CC(Cl)CCC1	−0.279872
P51685	724	Sc1ccc(S)cc1	−0.280647
P51685	307	N-Br	−0.28891
P51685	859	BrC1CC(Br)CC1	−0.293238
P51685	122	>= 2 any ring size 3	−0.293547
P51685	311	O-Na	−0.298644
P51685	592	N-C-C-C-C	−0.300055
P51685	877	NC1C(Br)CCC1	−0.301154
P51685	281	B-Cl	−0.304033
P51685	870	OC1C(Br)CCC1	−0.306056
P51685	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.306477
P51685	419	C#N	−0.310478
P51685	703	O-C-C-C-C-C(N)-C	−0.319088
P51685	312	O-Al	−0.320744

P51685	585	C-C:C-N-C	−0.321404
P51685	586	C-S-C-C-C	−0.322248
P51685	806	OC1CC(Cl)CCC1	−0.323175
P51685	800	CC1CC(N)CCC1	−0.323506
P51685	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.324256
P51685	748	Sc1cc(Br)ccc1	−0.32746
P51685	602	O=C-C-N-C	−0.330982
P51685	664	C-C=C-C=C	−0.334696
P51685	522	C-N-N-[#1]	−0.334751
P51685	385	C(:C)(:C)(:C)	−0.338932
P51685	469	S-S-C:C	−0.345302
P51685	269	Li-P	−0.346859
P51685	454	N(-C)(=O)	−0.348647
P51685	507	C-C-S-C	−0.35381
P51685	765	Oc1c(Br)cccc1	−0.354753
P51685	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.363535
P51685	382	C(~O)(:C)(:C)	−0.365694
P51685	642	O-C-C-C=O	−0.371597
P51685	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.373323
P51685	36	>= 8 S	−0.376516
P51685	396	N(~C)(:C)	−0.388287
P51685	611	N-C-C-N-C	−0.392809
P51685	701	O-C-C-C-C-C(O)-C	−0.410692
P51685	341	C(~C)(~C)(~O)	−0.417062
P51685	814	NC1CC(Br)CCC1	−0.427556
P51685	13	>= 32 C	−0.427829
P51685	296	C-Se	−0.430182
P51685	276	B-O	−0.448585
P51685	741	Oc1cc(S)ccc1	−0.453051
P51685	348	C(~C)(~H)(~P)	−0.458149
P51685	371	C(~H)(:C)(:C)	−0.459522
P51685	556	C=C-C-C	−0.463435
P51685	874	SC1C(Br)CCC1	−0.466402
P51685	599	[#1]-C-C=C-[#1]	−0.476495
P51685	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.477491
P51685	411	P(~O)(~O)	−0.48035
P51685	670	Br-C:C-C-C	−0.48111
P51685	865	CC1C(Br)CCC1	−0.482478
P51685	17	>= 8 N	−0.485059
P51685	501	Cl-C:C-C	−0.486654
P51685	786	OC1CCC(Br)CC1	−0.489256
P51685	465	O=S-C-C	−0.489741
P51685	467	C=N-N-C	−0.497217
P51685	104	>= 1 Sm	−0.498595
P51685	409	O(:C)(:C)	−0.500514
P51685	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.501407
P51685	620	C:C-O-C-C	−0.50652
P51685	368	C(~H)(~S)	−0.515946

P51685	651	O-C:C:C-C	−0.518568
P51685	742	Oc1cc(N)ccc1	−0.520032
P51685	485	N:C:C:N	−0.520171
P51685	656	C-C-N-C-C	−0.523144
P51685	610	C-O-C-O-C	−0.527055
P51685	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.528489
P51685	49	>= 1 Be	−0.529308
P51685	437	C(-C)(-N)(=C)	−0.533063
P51685	20	>= 4 O	−0.536829
P51685	577	C:C-N-C:C	−0.539305
P51685	728	Nc1ccc(N)cc1	−0.546735
P51685	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.548407
P51685	18	>= 1 O	−0.552503
P51685	461	O-C-C=N	−0.563381
P51685	797	CC1CC(C)CCC1	−0.563474
P51685	784	OC1CCC(N)CC1	−0.564274
P51685	32	>= 4 P	−0.567796
P51685	676	N#C-C-C-C	−0.571124
P51685	493	O=C-C:C	−0.572326
P51685	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−0.575562
P51685	776	CC1CCC(C)CC1	−0.58804
P51685	260	>= 3 hetero-aromatic rings	−0.589087
P51685	597	O=C-C-C:C	−0.590857
P51685	565	C:C-O-C	−0.593192
P51685	301	N-O	−0.60602
P51685	675	Br-C-C-C:C	−0.606912
P51685	686	O=C-C-C-C-O	−0.60784
P51685	548	O-C-C:C	−0.607855
P51685	185	>= 2 any ring size 6	−0.616386
P51685	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.61964
P51685	213	>= 1 any ring size 7	−0.622108
P51685	839	CC1CC(C)CC1	−0.630334
P51685	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.631286
P51685	571	[#1]-C-O-[#1]	−0.632124
P51685	386	C(:C)(:C)(:N)	−0.633372
P51685	581	O=C-C-C-O	−0.636677
P51685	436	C(-C)(-H)(=O)	−0.637908
P51685	663	O-C-C-O-[#1]	−0.645782
P51685	108	>= 1 Dy	−0.648272
P51685	691	O-C-C-C-C-C-N	−0.650414
P51685	284	C-C	−0.654672
P51685	543	O-C:C-N	−0.663106
P51685	629	S-C:C-C-N	−0.665113
P51685	632	C-C-O-C:C	−0.665145
P51685	674	N-C-N-C:C	−0.668154
P51685	871	SC1C(S)CCC1	−0.668488
P51685	394	N(~C)(~H)(~N)	−0.668757
P51685	325	As-H	−0.686174

P51685	799	CC1CC(S)CCC1	−0.688724
P51685	278	B-Si	−0.69594
P51685	758	Cc1c(N)cccc1	−0.700035
P51685	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−0.700947
P51685	818	CC1C(C)CCCC1	−0.70281
P51685	693	O=C-C-C-C-C-O	−0.704664
P51685	553	O=C-C=C	−0.705829
P51685	19	>= 2 O	−0.706544
P51685	538	N=C-C-C	−0.710283
P51685	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.712648
P51685	310	O-Mg	−0.714285
P51685	729	Nc1ccc(Cl)cc1	−0.723121
P51685	35	>= 4 S	−0.723366
P51685	576	N=C-C:C-[#1]	−0.725724
P51685	428	C(#C)(-H)	−0.738445
P51685	273	B-B	−0.7404
P51685	50	>= 1 Mg	−0.740988
P51685	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.742979
P51685	70	>= 1 Y	−0.746064
P51685	114	>= 1 U	−0.754574
P51685	751	Nc1cc(Br)ccc1	−0.755895
P51685	827	OC1C(Cl)CCCC1	−0.760514
P51685	45	>= 4 Br	−0.762377
P51685	29	>= 2 Si	−0.772381
P51685	782	OC1CCC(O)CC1	−0.773923
P51685	364	C(~F)(:C)	−0.777047
P51685	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.779692
P51685	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.787057
P51685	63	>= 1 Ga	−0.791999
P51685	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.792942
P51685	392	N(~C)(~C)(~H)	−0.81025
P51685	589	C-C:C-O-C	−0.820328
P51685	10	>= 4 C	−0.822237
P51685	95	>= 1 Hg	−0.833814
P51685	852	SC1CC(Cl)CC1	−0.834175
P51685	654	N-C-N-C-C	−0.839221
P51685	841	CC1CC(S)CC1	−0.839446
P51685	848	OC1CC(Cl)CC1	−0.84384
P51685	677	C-C=C-C:C	−0.852652
P51685	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.854169
P51685	79	>= 1 In	−0.861207
P51685	689	O-C-C-C-C-C-C	−0.862043
P51685	22	>= 16 O	−0.863652
P51685	869	OC1C(Cl)CCC1	−0.866549
P51685	412	S(~C)(~C)	−0.866851
P51685	831	SC1C(Cl)CCCC1	−0.870523
P51685	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.87202
P51685	864	CC1C(Cl)CCC1	−0.876396

P51685	551	Cl-C-C-O	−0.888427
P51685	378	C(~N)(:C)(:N)	−0.889386
P51685	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.896695
P51685	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.902298
P51685	704	O=C-C-C-C-C-C-C	−0.902419
P51685	206	>= 5 any ring size 6	−0.911623
P51685	178	>= 1 any ring size 6	−0.911984
P51685	402	N(~O)(:O)	−0.919823
P51685	850	SC1CC(S)CC1	−0.920615
P51685	540	C-N-C-[#1]	−0.92514
P51685	727	Sc1ccc(Br)cc1	−0.933599
P51685	338	C(~C)(~C)(~H)(~N)	−0.943419
P51685	720	Oc1ccc(S)cc1	−0.944031
P51685	64	>= 1 Ge	−0.944508
P51685	625	O=C-C:C-O	−0.946681
P51685	11	>= 8 C	−0.946967
P51685	414	S(~C)(~O)	−0.947653
P51685	810	SC1CC(Cl)CCC1	−0.949065
P51685	716	Cc1ccc(N)cc1	−0.94923
P51685	508	S=C-N-C	−0.952869
P51685	15	>= 2 N	−0.957101
P51685	655	O-C-C-C:C	−0.96587
P51685	366	C(~H)(~O)	−0.966849
P51685	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.974593
P51685	699	O-C-C-C-C-C(C)-C	−0.999569
P51685	544	O-C:C-O	−1.011128
P51685	31	>= 2 P	−1.023985
P51685	604	C-O-C-C:C	−1.024629
P51685	622	O=C-O-C:C	−1.029772
P51685	596	N=C-N-C-C	−1.032819
P51685	510	[#1]-N-N-[#1]	−1.036681
P51685	55	>= 1 V	−1.074056
P51685	526	Cl-C:C-Cl	−1.098486
P51685	502	N-C=C-[#1]	−1.100671
P51685	57	>= 1 Mn	−1.102055
P51685	633	N-C-C:C-C	−1.10675
P51685	93	>= 1 Pt	−1.107224
P51685	628	C-N-C-C:C	−1.109191
P51685	563	O-C-O-C	−1.110263
P51685	652	O-C:C:C-N	−1.137634
P51685	333	C(~C)(~C)(~C)	−1.146266
P51685	821	CC1C(N)CCCC1	−1.151908
P51685	867	OC1C(S)CCC1	−1.155505
P51685	842	CC1CC(N)CC1	−1.162668
P51685	354	C(~C)(~Si)	−1.170626
P51685	875	NC1C(N)CCC1	−1.171333
P51685	861	CC1C(O)CCC1	−1.172014
P51685	59	>= 1 Co	−1.178792

P51685	439	C(-C)(-N)(=O)	−1.187387
P51685	802	CC1CC(Br)CCC1	−1.192946
P51685	103	>= 1 Pm	−1.196596
P51685	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−1.21367
P51685	415	Si(~C)(~C)	−1.219716
P51685	400	N(~H)(:C)(:C)	−1.221416
P51685	710	C-C-C(C)-C-C	−1.222841
P51685	288	C-Na	−1.230141
P51685	73	>= 1 Mo	−1.235541
P51685	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−1.256727
P51685	3	>= 32 H	−1.264646
P51685	94	>= 1 Au	−1.283811
P51685	257	>= 2 aromatic rings	−1.296026
P51685	798	CC1CC(O)CCC1	−1.300385
P51685	435	C(-C)(-H)(=N)	−1.30802
P51685	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−1.318846
P51685	405	O(~C)(~C)	−1.325486
P51685	564	C=C-C=C	−1.327539
P51685	397	N(~C)(:C)(:C)	−1.328826
P51685	6	>= 1 B	−1.330606
P51685	835	NC1C(Br)CCCC1	−1.334231
P51685	517	N-N-C-N	−1.335021
P51685	61	>= 1 Cu	−1.339965
P51685	186	>= 2 saturated or aromatic carbon-only ring size 6	−1.34449
P51685	393	N(~C)(~H)	−1.362398
P51685	410	P(~C)(~C)	−1.384061
P51685	706	O=C-C-C-C-C(=O)-C	−1.387853
P51685	647	O=C-N-C-N	−1.388457
P51685	488	N-C=N-[#1]	−1.399408
P51685	468	O=S-C-N	−1.422968
P51685	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−1.440399
P51685	420	C=O	−1.455502
P51685	809	SC1CC(N)CCC1	−1.456587
P51685	778	CC1CCC(S)CC1	−1.470196
P51685	165	>= 4 saturated or aromatic carbon-only ring size 5	−1.474632
P51685	756	Cc1c(O)cccc1	−1.504818
P51685	358	C(~C)(:N)	−1.542842
P51685	723	Oc1ccc(Br)cc1	−1.542937
P51685	732	Clc1ccc(Br)cc1	−1.543668
P51685	424	N=P	−1.584706
P51685	87	>= 1 Hf	−1.630092
P51685	58	>= 1 Fe	−1.634285
P51685	151	>= 2 saturated or aromatic carbon-only ring size 5	−1.637628
P51685	318	Al-H	−1.643743
P51685	479	S-C-S-C	−1.643894
P51685	82	>= 1 Te	−1.649406
P51685	75	>= 1 Rh	−1.655499
P51685	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−1.659549

P51685	860	CC1C(C)CCC1	−1.660126
P51685	618	C:C-C-C:C	−1.662101
P51685	554	Br-C-C-C	−1.68638
P51685	320	Si-H	−1.686457
P51685	559	O-C-N-[#1]	−1.689372
P51685	315	O-K	−1.703929
P51685	387	C(:C)(:N)	−1.709581
P51685	754	Brc1cc(Br)ccc1	−1.72785
P51685	640	C=C-C-C-C	−1.738277
P51685	533	S-C:C-N	−1.78131
P51685	256	>= 1 hetero-aromatic ring	−1.797274
P51685	705	O=C-C-C-C-C(O)-C	−1.892234
P51685	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−1.988111
P51685	268	Li-F	−2.1092
P51685	845	OC1CC(O)CC1	−2.273421
P51685	37	>= 1 Cl	−2.277324
P51685	557	N:C-O-[#1]	−2.438497
P51685	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−2.650913
P51685	264	Li-Li	−2.89246

Fingerprints（continued)

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-1.389068 -0.01034
-1.432912 0.0099439
-1.440398 -1.03E-06
-1.449078 -0.006423
-1.451395 -0.005192
-1.459013 -0.011183
-1.474631 -7.54E-07
-1.494612 -0.010206
-1.545532 0.0026902
-1.540078 -0.002859
-1.543667 -5.95E-07
-1.584706 -4.79E-07
-1.630091 -5.44E-07
-1.634284 -9.29E-07
-1.632999 -0.004629
-1.643742 -9.18E-07
-1.643996 0.0001023
-1.649405 -1.03E-06
-1.655497 -1.06E-06
-1.658563 -0.000986

-1.668136 0.0080102
-1.660427 -0.001675
-1.687369 0.0009891
-1.686457 -5.85E-07
-1.695003 0.0056316
-1.703928 -8.48E-07
-1.712859 0.003278
-1.727849 -8.01E-07
-1.736007 -0.00227
-1.784394 0.0030843
-1.797273 -1.06E-06
-1.892364 0.0001303
-1.98811 -1.30E-06
-2.109199 -8.80E-07
-2.27342 -1.23E-06
-2.283701 0.0063773
-2.438878 0.0003815
-2.653944 0.0030306
-2.892459 -1.40E-06

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P51684	86	>= 1 Lu	3.227842
P51684	843	CC1CC(Cl)CC1	2.5119209
P51684	846	OC1CC(S)CC1	2.1123502
P51684	809	SC1CC(N)CCC1	1.9640312
P51684	551	Cl-C-C-O	1.8518053
P51684	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	1.7407533
P51684	463	N:C-S-[#1]	1.6537598
P51684	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	1.6304911
P51684	151	>= 2 saturated or aromatic carbon-only ring size 5	1.5850454
P51684	594	C-O-C-C=C	1.5201878
P51684	321	Si-Si	1.4752699
P51684	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	1.4449745
P51684	53	>= 1 Sc	1.4333953
P51684	469	S-S-C:C	1.371849
P51684	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	1.3604973
P51684	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	1.3072262
P51684	655	O-C-C-C:C	1.2478465
P51684	263	Li-H	1.2347349
P51684	75	>= 1 Rh	1.1653391
P51684	262	>= 4 hetero-aromatic rings	1.1614429
P51684	618	C:C-C-C:C	1.1351118
P51684	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	1.107035
P51684	631	O-C:C-O-[#1]	1.0877884
P51684	832	SC1C(Br)CCCC1	1.0853391
P51684	851	SC1CC(N)CC1	1.0837728
P51684	311	O-Na	1.0768219
P51684	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	1.0623664
P51684	661	O-C-O-C-C	1.0614605
P51684	549	N-C-C:C	1.0208185
P51684	363	C(~F)(~F)	1.0197417
P51684	669	Cl-C:C-C=O	0.9900563
P51684	14	>= 1 N	0.9748971
P51684	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.9724186
P51684	442	C(-C)(=N)	0.9690782
P51684	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.9644436
P51684	564	C=C-C=C	0.94288
P51684	769	Sc1c(Br)cccc1	0.9378138
P51684	289	C-Mg	0.9114926
P51684	2	>= 16 H	0.8976251
P51684	613	C-N-C-C-C	0.8965019
P51684	703	O-C-C-C-C-C(N)-C	0.8907882
P51684	865	CC1C(Br)CCC1	0.8777218
P51684	7	>= 2 B	0.867966
P51684	36	>= 8 S	0.8669127
P51684	611	N-C-C-N-C	0.8586812
P51684	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.8576233

P51684	833	NC1C(N)CCCC1	0.8571706
P51684	639	O-C-C-C-O	0.8289949
P51684	107	>= 1 Tb	0.815344
P51684	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.7826059
P51684	320	Si-H	0.7511072
P51684	95	>= 1 Hg	0.7460373
P51684	49	>= 1 Be	0.7184131
P51684	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.7179824
P51684	657	C-N-C:C-C	0.7169878
P51684	495	C-N-C:C	0.7132337
P51684	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.6860149
P51684	529	Cl-C-C-Cl	0.6843205
P51684	21	>= 8 O	0.6794555
P51684	825	OC1C(S)CCCC1	0.6774075
P51684	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.6749218
P51684	369	C(~H)(~Si)	0.6728775
P51684	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.672447
P51684	10	>= 4 C	0.6705503
P51684	768	Sc1c(Cl)cccc1	0.6692936
P51684	830	SC1C(N)CCCC1	0.669206
P51684	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.666735
P51684	807	OC1CC(Br)CCC1	0.6627048
P51684	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.6546599
P51684	18	>= 1 O	0.6219593
P51684	272	B-H	0.620474
P51684	596	N=C-N-C-C	0.6195935
P51684	790	SC1CCC(Br)CC1	0.6179977
P51684	652	O-C:C:C-N	0.6154798
P51684	298	C-I	0.6123309
P51684	315	O-K	0.6118904
P51684	877	NC1C(Br)CCC1	0.6118468
P51684	523	N:C:C-C	0.6052902
P51684	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.6036874
P51684	686	O=C-C-C-C-O	0.5927397
P51684	772	Nc1c(Br)cccc1	0.5888562
P51684	571	[#1]-C-O-[#1]	0.579842
P51684	318	Al-H	0.5710859
P51684	424	N=P	0.5704286
P51684	601	N-C:C:C-N	0.5660574
P51684	820	CC1C(S)CCCC1	0.565735
P51684	441	C(-C)(=C)	0.5622241
P51684	867	OC1C(S)CCC1	0.5596873
P51684	557	N:C-O-[#1]	0.5550174
P51684	457	S(-C)(=O)	0.5510525
P51684	430	C(-C)(-C)(=C)	0.5497349
P51684	20	>= 4 O	0.5473041
P51684	402	N(~O)(:O)	0.52942
P51684	828	OC1C(Br)CCCC1	0.5217993

P51684	705	O=C-C-C-C-C(O)-C	0.5157317
P51684	102	>= 1 Nd	0.5135689
P51684	299	N-H	0.5125489
P51684	540	C-N-C-[#1]	0.5098117
P51684	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.5067355
P51684	698	O-C-C-C-C-C-C-C	0.4893304
P51684	429	C(#N)(-C)	0.4859755
P51684	535	O=C-C-C	0.4846966
P51684	848	OC1CC(Cl)CC1	0.4759499
P51684	503	Cl-C:C-[#1]	0.4719977
P51684	462	O-C-C=O	0.4693173
P51684	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.4691163
P51684	561	Cl-C-C=O	0.4674361
P51684	818	CC1C(C)CCCC1	0.4662892
P51684	508	S=C-N-C	0.462053
P51684	476	C-O-C=C	0.460776
P51684	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.4546481
P51684	637	O-C-C-C-C	0.4446887
P51684	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.4398002
P51684	255	>= 1 aromatic ring	0.4230139
P51684	16	>= 4 N	0.4147668
P51684	362	C(~Cl)(:C)	0.4080446
P51684	675	Br-C-C-C:C	0.4049903
P51684	111	>= 1 Tm	0.4017825
P51684	470	C:C-C=C	0.3925572
P51684	388	C(:C)(:N)(:N)	0.3913904
P51684	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.3840048
P51684	479	S-C-S-C	0.383897
P51684	819	CC1C(O)CCCC1	0.3827768
P51684	879	ClC1C(Br)CCC1	0.3817982
P51684	547	N-C:C-N	0.3751499
P51684	679	C-C-C-C-C-C	0.3731579
P51684	821	CC1C(N)CCCC1	0.3687922
P51684	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.3670756
P51684	805	OC1CC(N)CCC1	0.3651196
P51684	834	NC1C(Cl)CCCC1	0.3620435
P51684	330	C(~Br)(:C)	0.3548512
P51684	273	B-B	0.3494468
P51684	343	C(~C)(~Cl)(~H)	0.345298
P51684	475	S-C=N-C	0.3377128
P51684	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.3358604
P51684	737	Cc1cc(N)ccc1	0.3308023
P51684	823	CC1C(Br)CCCC1	0.3306194
P51684	220	>= 2 any ring size 7	0.3287242
P51684	249	>= 1 saturated or aromatic carbon-only ring size 10	0.3257343
P51684	797	CC1CC(C)CCC1	0.3227446
P51684	804	OC1CC(S)CCC1	0.3210953
P51684	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.3209875

P51684	397	N(~C)(:C)(:C)	0.3174363
P51684	382	C(~O)(:C)(:C)	0.310715
P51684	87	>= 1 Hf	0.3084306
P51684	588	O=C-C-C=O	0.3080726
P51684	654	N-C-N-C-C	0.3067707
P51684	440	C(-C)(-O)(=O)	0.3013935
P51684	62	>= 1 Zn	0.3003029
P51684	307	N-Br	0.299555
P51684	491	C-N:C-[#1]	0.2986392
P51684	277	B-F	0.2955071
P51684	632	C-C-O-C:C	0.2918623
P51684	694	O=C-C-C-C-C=O	0.2881299
P51684	849	OC1CC(Br)CC1	0.2848054
P51684	144	>= 1 saturated or aromatic carbon-only ring size 5	0.282616
P51684	351	C(~C)(~N)	0.282513
P51684	389	C(:N)(:N)	0.2824192
P51684	428	C(#C)(-H)	0.2777291
P51684	816	ClC1CC(Br)CCC1	0.2775936
P51684	504	N:C:N-C	0.2769155
P51684	748	Sc1cc(Br)ccc1	0.2737483
P51684	677	C-C=C-C:C	0.2736908
P51684	602	O=C-C-N-C	0.2720763
P51684	334	C(~C)(~C)(~C)(~C)	0.2668302
P51684	333	C(~C)(~C)(~C)	0.2626038
P51684	681	O-C-C-C-C-O	0.2598149
P51684	690	O-C-C-C-C-C-O	0.2546745
P51684	345	C(~C)(~H)(~N)	0.2545746
P51684	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.248045
P51684	403	N(:C)(:C)	0.2463101
P51684	383	C(~S)(:C)	0.2441426
P51684	46	>= 1 I	0.2434744
P51684	92	>= 1 Ir	0.2373511
P51684	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.2325717
P51684	38	>= 2 Cl	0.2317565
P51684	97	>= 1 Pb	0.2302671
P51684	394	N(~C)(~H)(~N)	0.2299664
P51684	502	N-C=C-[#1]	0.2298962
P51684	766	Sc1c(S)cccc1	0.228178
P51684	630	O-C:C-O-C	0.2271074
P51684	560	N-C-N-C	0.2270607
P51684	511	S=C-N-[#1]	0.2253034
P51684	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.2213905
P51684	609	Cl-C-C-N-C	0.2162545
P51684	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.2132618
P51684	787	SC1CCC(S)CC1	0.2124132
P51684	157	>= 3 any ring size 5	0.2099762
P51684	666	C=C-C-O-C	0.2087298
P51684	532	S-C:C-[#1]	0.2067982

P51684	857	ClC1CC(Cl)CC1	0.2030817
P51684	704	O=C-C-C-C-C-C-C	0.1999371
P51684	401	N(~O)(~O)	0.1980901
P51684	552	C:C-C:C	0.1959463
P51684	129	>= 1 any ring size 4	0.1955131
P51684	422	N=N	0.1935673
P51684	221	>= 2 saturated or aromatic carbon-only ring size 7	0.1929111
P51684	758	Cc1c(N)cccc1	0.1923943
P51684	438	C(-C)(-N)(=N)	0.1857545
P51684	810	SC1CC(Cl)CCC1	0.185728
P51684	115	>= 1 any ring size 3	0.1837738
P51684	265	Li-B	0.1817842
P51684	400	N(~H)(:C)(:C)	0.1775282
P51684	437	C(-C)(-N)(=C)	0.1734466
P51684	405	O(~C)(~C)	0.1716108
P51684	406	O(~C)(~H)	0.1715504
P51684	353	C(~C)(~S)	0.1657021
P51684	600	N-C:C:C-C	0.1619157
P51684	136	>= 2 any ring size 4	0.1599324
P51684	815	ClC1CC(Cl)CCC1	0.159616
P51684	706	O=C-C-C-C-C(=O)-C	0.159543
P51684	40	>= 8 Cl	0.1580889
P51684	186	>= 2 saturated or aromatic carbon-only ring size 6	0.1579102
P51684	531	S-C:C-C	0.1570781
P51684	267	Li-O	0.1569835
P51684	730	Nc1ccc(Br)cc1	0.1521878
P51684	474	S:C:C:N	0.1513808
P51684	379	C(~N)(:N)	0.1499494
P51684	488	N-C=N-[#1]	0.1439515
P51684	788	SC1CCC(N)CC1	0.1431705
P51684	300	N-N	0.1418302
P51684	786	OC1CCC(Br)CC1	0.141756
P51684	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.1414128
P51684	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.1410945
P51684	5	>= 2 Li	0.1400709
P51684	683	N-C-C-C-C-C	0.1379344
P51684	514	O-N-C-C	0.1372061
P51684	44	>= 2 Br	0.1346706
P51684	257	>= 2 aromatic rings	0.1334591
P51684	15	>= 2 N	0.1327784
P51684	626	C-O-C:C-C	0.1306974
P51684	799	CC1CC(S)CCC1	0.1284484
P51684	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.128162
P51684	622	O=C-O-C:C	0.1268132
P51684	831	SC1C(Cl)CCCC1	0.12509
P51684	553	O=C-C=C	0.1241987
P51684	520	C=C-C:C	0.1239984
P51684	282	B-Br	0.1194235

P51684	615	N-C-C-O-C	0.1183355
P51684	25	>= 4 F	0.1163731
P51684	305	N-S	0.1162133
P51684	308	O-H	0.1160649
P51684	427	C(#C)(-C)	0.1154772
P51684	649	O=N-C:C-O	0.1134136
P51684	77	>= 1 Ag	0.1120671
P51684	836	ClC1C(Cl)CCCC1	0.1116327
P51684	539	N=C-C-[#1]	0.1112431
P51684	801	CC1CC(Cl)CCC1	0.1111405
P51684	793	NC1CCC(Br)CC1	0.1093352
P51684	860	CC1C(C)CCC1	0.1053822
P51684	591	Cl-C-C-C-C	0.1024152
P51684	501	Cl-C:C-C	0.0989766
P51684	392	N(~C)(~C)(~H)	0.0970865
P51684	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0969453
P51684	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0962729
P51684	234	>= 2 any ring size 8	0.0943504
P51684	381	C(~O)(:C)	0.0911708
P51684	206	>= 5 any ring size 6	0.0906978
P51684	731	Clc1ccc(Cl)cc1	0.0885823
P51684	359	C(~C)(:N)(:N)	0.0882998
P51684	598	Cl-C:C:C-C	0.0880979
P51684	566	O-C-C-N	0.086956
P51684	720	Oc1ccc(S)cc1	0.0852622
P51684	579	O=C-C-C-C	0.0841476
P51684	750	Nc1cc(Cl)ccc1	0.0822107
P51684	116	>= 1 saturated or aromatic carbon-only ring size 3	0.0815835
P51684	361	C(~Cl)(~H)	0.0810639
P51684	586	C-S-C-C-C	0.0801716
P51684	447	C(-H)(=N)	0.0799142
P51684	776	CC1CCC(C)CC1	0.0795172
P51684	303	N-Si	0.0773722
P51684	665	N-C:C-C-C	0.0752882
P51684	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0716548
P51684	472	C:N:C-C	0.0707049
P51684	213	>= 1 any ring size 7	0.0705698
P51684	623	O=C-C:C-C	0.0703894
P51684	721	Oc1ccc(N)cc1	0.0694269
P51684	749	Nc1cc(N)ccc1	0.0674323
P51684	380	C(~O)(~O)	0.0671742
P51684	450	C(-N)(=N)	0.0670933
P51684	37	>= 1 Cl	0.0670018
P51684	338	C(~C)(~C)(~H)(~N)	0.0668988
P51684	760	Cc1c(Br)cccc1	0.0668545
P51684	324	P-P	0.0668046
P51684	774	Clc1c(Br)cccc1	0.0667476
P51684	278	B-Si	0.0666218

P51684	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0665994
P51684	399	N(~H)(:C)	0.0664183
P51684	426	P=P	0.0662587
P51684	372	C(~H)(:C)(:N)	0.0648218
P51684	498	O-C=C-C	0.064584
P51684	368	C(~H)(~S)	0.0644702
P51684	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0642683
P51684	644	C-C=N-N-C	0.0641171
P51684	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0641135
P51684	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.0639914
P51684	513	S:C:C-[#1]	0.0638337
P51684	515	N-N-C-C	0.0634989
P51684	473	S-C:N:C	0.0619342
P51684	65	>= 1 As	0.0617848
P51684	451	C(-N)(=O)	0.0612493
P51684	329	C(~Br)(~H)	0.0610939
P51684	617	C-C-C-O-[#1]	0.0608542
P51684	89	>= 1 W	0.0604302
P51684	784	OC1CCC(N)CC1	0.0602133
P51684	55	>= 1 V	0.060197
P51684	82	>= 1 Te	0.0596963
P51684	200	>= 4 saturated or aromatic carbon-only ring size 6	0.0590206
P51684	448	C(-H)(=O)	0.0572556
P51684	660	C-C=C-C-C	0.0560616
P51684	576	N=C-C:C-[#1]	0.0558922
P51684	674	N-C-N-C:C	0.0556257
P51684	47	>= 2 I	0.0555592
P51684	517	N-N-C-N	0.0553837
P51684	57	>= 1 Mn	0.0550921
P51684	587	N-C:C-O-[#1]	0.0545632
P51684	268	Li-F	0.0542043
P51684	521	C:N-C-[#1]	0.0537645
P51684	271	Li-Cl	0.0533363
P51684	590	C-C:C-O-[#1]	0.0532105
P51684	385	C(:C)(:C)(:C)	0.0527307
P51684	806	OC1CC(Cl)CCC1	0.052481
P51684	477	N-N-C:C	0.052222
P51684	81	>= 1 Sb	0.0521414
P51684	306	N-Cl	0.052001
P51684	733	Brc1ccc(Br)cc1	0.0512747
P51684	242	>= 1 saturated or aromatic carbon-only ring size 9	0.0503588
P51684	42	>= 2 K	0.0498423
P51684	241	>= 1 any ring size 9	0.0497643
P51684	554	Br-C-C-C	0.0472021
P51684	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.0467457
P51684	113	>= 1 Tc	0.0452701
P51684	687	O=C-C-C-C=O	0.0449007
P51684	96	>= 1 Tl	0.04472

P51684	337	C(~C)(~C)(~C)(~O)	0.043951
P51684	409	O(:C)(:C)	0.0439446
P51684	651	O-C:C:C-C	0.043645
P51684	781	CC1CCC(Br)CC1	0.0431998
P51684	558	O=N-C:C	0.0414
P51684	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0411566
P51684	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.0409204
P51684	658	C-C-S-C-C	0.0402548
P51684	589	C-C:C-O-C	0.0397934
P51684	486	N-C:N:N	0.0394074
P51684	19	>= 2 O	0.0391405
P51684	67	>= 1 Kr	0.0389199
P51684	506	C-C:N:C	0.0383602
P51684	812	NC1CC(N)CCC1	0.0377277
P51684	811	SC1CC(Br)CCC1	0.0371791
P51684	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0364934
P51684	835	NC1C(Br)CCCC1	0.0364162
P51684	866	OC1C(O)CCC1	0.0361405
P51684	83	>= 1 Xe	0.035756
P51684	398	N(~H)(~N)	0.0351334
P51684	765	Oc1c(Br)cccc1	0.0348715
P51684	384	C(:C)(:C)	0.0346883
P51684	327	C(~Br)(~C)	0.0346654
P51684	839	CC1CC(C)CC1	0.0345136
P51684	688	C-C-C-C-C-C-C	0.0338548
P51684	709	C-C(C)-C-C-C	0.0326805
P51684	556	C=C-C-C	0.032427
P51684	293	C-S	0.0322556
P51684	543	O-C:C-N	0.0314524
P51684	570	C:C-C-C	0.0311536
P51684	487	N-C=N-C	0.0311
P51684	494	O=C-C:N	0.0304992
P51684	285	C-N	0.0301506
P51684	340	C(~C)(~C)(~N)	0.0299529
P51684	667	C=C-C-O-[#1]	0.029925
P51684	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.0286443
P51684	354	C(~C)(~Si)	0.0281717
P51684	614	C-C-O-C-C	0.0273502
P51684	616	C:C:N:N:C	0.0266755
P51684	109	>= 1 Ho	0.0262161
P51684	467	C=N-N-C	0.0258279
P51684	522	C-N-N-[#1]	0.0254382
P51684	728	Nc1ccc(N)cc1	0.0252219
P51684	387	C(:C)(:N)	0.0247465
P51684	395	N(~C)(~O)	0.0241141
P51684	50	>= 1 Mg	0.0239574
P51684	715	Cc1ccc(S)cc1	0.0232724
P51684	228	>= 1 saturated or aromatic carbon-only ring size 8	0.0226085

P51684	483	N-S-C:C	0.0217681
P51684	108	>= 1 Dy	0.0217328
P51684	344	C(~C)(~H)	0.0214054
P51684	565	C:C-O-C	0.0204835
P51684	396	N(~C)(:C)	0.0203328
P51684	528	[#1]-N-C-[#1]	0.0202861
P51684	90	>= 1 Re	0.0198935
P51684	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0196109
P51684	485	N:C:C:N	0.0193519
P51684	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0187635
P51684	856	NC1CC(Br)CC1	0.0184089
P51684	367	C(~H)(~O)(~O)	0.0183459
P51684	757	Cc1c(S)cccc1	0.0167606
P51684	544	O-C:C-O	0.0163843
P51684	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0159657
P51684	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0159526
P51684	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0153651
P51684	743	Oc1cc(Cl)ccc1	0.0145106
P51684	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.0144227
P51684	500	C-S-C:C	0.0142518
P51684	864	CC1C(Cl)CCC1	0.0126504
P51684	527	C:C:N-[#1]	0.0124874
P51684	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.0120871
P51684	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.0119719
P51684	682	O-C-C-C-C-N	0.0114776
P51684	727	Sc1ccc(Br)cc1	0.0108248
P51684	283	C-H	0.0106028
P51684	98	>= 1 Bi	0.0105062
P51684	41	>= 1 K	0.0104906
P51684	507	C-C-S-C	0.0102439
P51684	446	C(-H)(=C)	0.0100041
P51684	645	O=C-N-C-C	0.0097202
P51684	276	B-O	0.0096967
P51684	707	O=C-C-C-C-C(N)-C	0.0093244
P51684	608	C-C-C-C:C	0.0089553
P51684	509	Br-C:C-C	0.0084344
P51684	782	OC1CCC(O)CC1	0.0081614
P51684	325	As-H	0.0080151
P51684	85	>= 1 Ba	0.0078123
P51684	640	C=C-C-C-C	0.0076445
P51684	863	CC1C(N)CCC1	0.007477
P51684	530	N:C-C:C	0.0072999
P51684	297	C-Br	0.0069241
P51684	31	>= 2 P	0.0069126
P51684	465	O=S-C-C	0.00648
P51684	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0060725
P51684	699	O-C-C-C-C-C(C)-C	0.0057898
P51684	796	BrC1CCC(Br)CC1	0.0056722

P51684	106	>= 1 Gd	0.005366
P51684	754	Brc1cc(Br)ccc1	0.0051685
P51684	54	>= 1 Ti	0.004529
P51684	653	O-C:C:C-O	0.0043685
P51684	292	C-P	0.0042946
P51684	584	C:C-C=C-C	0.0041809
P51684	739	Cc1cc(Br)ccc1	0.0041216
P51684	861	CC1C(O)CCC1	0.0040659
P51684	798	CC1CC(O)CCC1	0.0040442
P51684	290	C-Al	0.0039828
P51684	850	SC1CC(S)CC1	0.0038752
P51684	875	NC1C(N)CCC1	0.0033475
P51684	693	O=C-C-C-C-C-O	0.0029923
P51684	227	>= 1 any ring size 8	0.0025881
P51684	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0025178
P51684	91	>= 1 Os	0.0023834
P51684	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0022195
P51684	310	O-Mg	0.0021506
P51684	326	As-As	0.0020087
P51684	207	>= 5 saturated or aromatic carbon-only ring size 6	0.0017403
P51684	78	>= 1 Cd	0.0015087
P51684	248	>= 1 any ring size 10	0.0014691
P51684	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0014404
P51684	646	O=C-N-C-[#1]	0.00075
P51684	52	>= 1 Ca	0.0006472
P51684	453	N(-C)(=C)	0.0005675
P51684	673	O=C-C=C-N	0.00041
P51684	301	N-O	0.0003149
P51684	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0002972
P51684	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.0002906
P51684	323	P-H	7.10E-07
P51684	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	3.99E-07
P51684	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	3.11E-07
P51684	165	>= 4 saturated or aromatic carbon-only ring size 5	8.17E-08
P51684	845	OC1CC(O)CC1	1.23E-08
P51684	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	-9.18E-08
P51684	873	SC1C(Cl)CCC1	-3.44E-07
P51684	444	C(-Cl)(=O)	-4.51E-07
P51684	270	Li-S	-8.72E-07
P51684	876	NC1C(Cl)CC1	-0.000198
P51684	753	Clc1cc(Br)ccc1	-0.000205
P51684	808	SC1CC(S)CCC1	-0.000226
P51684	537	O=C-C-O	-0.000461
P51684	32	>= 4 P	-0.000545
P51684	112	>= 1 Yb	-0.000769
P51684	346	C(~C)(~H)(~O)	-0.00098
P51684	275	B-N	-0.001064
P51684	854	NC1CC(N)CC1	-0.001714

P51684	80	>= 1 Sn	−0.001821
P51684	76	>= 1 Pd	−0.002395
P51684	425	P=O	−0.002437
P51684	331	C(~Br)(:N)	−0.002461
P51684	264	Li-Li	−0.002587
P51684	279	B-P	−0.002606
P51684	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.00262
P51684	68	>= 1 Rb	−0.002781
P51684	312	O-Al	−0.002928
P51684	22	>= 16 O	−0.00304
P51684	288	C-Na	−0.003133
P51684	314	O-P	−0.003252
P51684	712	C-C(C)-C(C)-C	−0.003533
P51684	412	S(~C)(~C)	−0.003563
P51684	761	Oc1c(O)cccc1	−0.003692
P51684	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.003813
P51684	663	O-C-C-O-[#1]	−0.003874
P51684	377	C(~N)(:C)(:C)	−0.003878
P51684	328	C(~Br)(~C)(~C)	−0.003941
P51684	296	C-Se	−0.00397
P51684	751	Nc1cc(Br)ccc1	−0.003972
P51684	742	Oc1cc(N)ccc1	−0.004073
P51684	60	>= 1 Ni	−0.004736
P51684	484	N-C:N:C	−0.005329
P51684	605	O=C-C-O-C	−0.005404
P51684	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.00591
P51684	70	>= 1 Y	−0.006054
P51684	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.006144
P51684	349	C(~C)(~H)(~S)	−0.006339
P51684	763	Oc1c(N)cccc1	−0.006433
P51684	456	P(-O)(=O)	−0.007387
P51684	633	N-C-C:C-C	−0.007462
P51684	541	O-C:C-C	−0.007633
P51684	376	C(~N)(:C)	−0.008457
P51684	726	Sc1ccc(Cl)cc1	−0.008686
P51684	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.008931
P51684	104	>= 1 Sm	−0.009586
P51684	741	Oc1cc(S)ccc1	−0.00974
P51684	619	O-C-C=C-C	−0.009794
P51684	30	>= 1 P	−0.009805
P51684	789	SC1CCC(Cl)CC1	−0.009807
P51684	676	N#C-C-C-C	−0.009915
P51684	671	O=C-C=C-C	−0.01012
P51684	322	Si-Cl	−0.010177
P51684	39	>= 4 Cl	−0.010525
P51684	745	Sc1cc(S)ccc1	−0.011742
P51684	35	>= 4 S	−0.011845
P51684	546	N-C:C-[#1]	−0.012147

P51684	4	>= 1 Li	−0.012169
P51684	443	C(-C)(=O)	−0.012611
P51684	266	Li-C	−0.012827
P51684	435	C(-C)(-H)(=N)	−0.012833
P51684	582	C-C-C-C-C	−0.014508
P51684	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.01489
P51684	11	>= 8 C	−0.015062
P51684	0	>= 4 H	−0.01514
P51684	636	C-N-C-N-C	−0.015208
P51684	414	S(~C)(~O)	−0.015701
P51684	624	O=C-C:C-N	−0.015769
P51684	578	C-C:C-C:C	−0.01622
P51684	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.016488
P51684	606	O-C:C-C-C	−0.017366
P51684	603	C-C:C:C-C	−0.017679
P51684	595	C:C-C-C-C	−0.017885
P51684	597	O=C-C-C:C	−0.018555
P51684	844	CC1CC(Br)CC1	−0.018791
P51684	407	O(~C)(~P)	−0.019044
P51684	58	>= 1 Fe	−0.019088
P51684	350	C(~C)(~I)	−0.020509
P51684	103	>= 1 Pm	−0.020921
P51684	496	N:N-C-[#1]	−0.021064
P51684	61	>= 1 Cu	−0.02128
P51684	795	ClC1CCC(Br)CC1	−0.021661
P51684	855	NC1CC(Cl)CC1	−0.021703
P51684	364	C(~F)(:C)	−0.022097
P51684	69	>= 1 Sr	−0.022116
P51684	533	S-C:C-N	−0.022563
P51684	538	N=C-C-C	−0.023295
P51684	708	C-C(C)-C-C	−0.026393
P51684	822	CC1C(Cl)CCCC1	−0.02649
P51684	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.026637
P51684	779	CC1CCC(N)CC1	−0.028364
P51684	853	SC1CC(Br)CC1	−0.029097
P51684	827	OC1C(Cl)CCCC1	−0.029765
P51684	567	O-C-C-O	−0.029848
P51684	461	O-C-C=N	−0.030179
P51684	732	Clc1ccc(Br)cc1	−0.030244
P51684	261	>= 4 aromatic rings	−0.03054
P51684	723	Oc1ccc(Br)cc1	−0.030608
P51684	580	O=C-C-C-N	−0.030616
P51684	581	O=C-C-C-O	−0.031382
P51684	280	B-S	−0.031796
P51684	650	O=C-N-C=O	−0.032089
P51684	423	N=O	−0.032244
P51684	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.032726
P51684	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.032862

P51684	26	>= 1 Na	−0.033204
P51684	493	O=C-C:C	−0.033214
P51684	454	N(-C)(=O)	−0.033277
P51684	550	Cl-C-C-C	−0.033799
P51684	762	Oc1c(S)cccc1	−0.034248
P51684	73	>= 1 Mo	−0.034346
P51684	662	O-C-C-O-C	−0.034849
P51684	12	>= 16 C	−0.035307
P51684	729	Nc1ccc(Cl)cc1	−0.037469
P51684	813	NC1CC(Cl)CCC1	−0.037556
P51684	878	ClC1C(Cl)CCC1	−0.037619
P51684	100	>= 1 Ce	−0.038049
P51684	701	O-C-C-C-C-C(O)-C	−0.038582
P51684	740	Oc1cc(O)ccc1	−0.038965
P51684	23	>= 1 F	−0.039421
P51684	185	>= 2 any ring size 6	−0.040848
P51684	714	Cc1ccc(O)cc1	−0.040883
P51684	656	C-C-N-C-C	−0.043154
P51684	641	O-C-C-C=C	−0.043472
P51684	747	Sc1cc(Cl)ccc1	−0.043533
P51684	287	C-F	−0.043734
P51684	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.044088
P51684	516	[#1]-C=C-[#1]	−0.044438
P51684	460	C-C-C#C	−0.044623
P51684	773	Clc1c(Cl)cccc1	−0.044668
P51684	717	Cc1ccc(Cl)cc1	−0.045409
P51684	840	CC1CC(O)CC1	−0.045756
P51684	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.04594
P51684	6	>= 1 B	−0.047308
P51684	577	C:C-N-C:C	−0.049063
P51684	711	C-C(C)(C)-C-C	−0.049482
P51684	478	S-C=N-[#1]	−0.049871
P51684	27	>= 2 Na	−0.05062
P51684	659	O-C-C-N-C	−0.051653
P51684	700	O-C-C-C-C-C-O-C	−0.052558
P51684	105	>= 1 Eu	−0.052786
P51684	348	C(~C)(~H)(~P)	−0.053567
P51684	870	OC1C(Br)CCC1	−0.056009
P51684	492	N-C:O:C	−0.056191
P51684	122	>= 2 any ring size 3	−0.058731
P51684	48	>= 4 I	−0.05919
P51684	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.05935
P51684	28	>= 1 Si	−0.059874
P51684	512	C-[As]-O-[#1]	−0.059986
P51684	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.061275
P51684	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.061466
P51684	852	SC1CC(Cl)CC1	−0.061492
P51684	410	P(~C)(~C)	−0.062534

P51684	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.063051
P51684	713	Cc1ccc(C)cc1	−0.063086
P51684	171	>= 5 any ring size 5	−0.063335
P51684	164	>= 4 any ring size 5	−0.063416
P51684	370	C(~H)(:C)	−0.063741
P51684	114	>= 1 U	−0.064029
P51684	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.064394
P51684	482	C:N-C:C	−0.064562
P51684	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.064918
P51684	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.065682
P51684	635	N-N-C-N-[#1]	−0.065967
P51684	621	N-C:C:C:N	−0.066186
P51684	413	S(~C)(~H)	−0.066601
P51684	612	N-C-O-C-C	−0.066629
P51684	697	C-C-C-C-C-C(C)-C	−0.066946
P51684	548	O-C-C:C	−0.06826
P51684	638	O-C-C-C-N	−0.068307
P51684	610	C-O-C-O-C	−0.068986
P51684	316	F-P	−0.069739
P51684	625	O=C-C:C-O	−0.072562
P51684	792	NC1CCC(Cl)CC1	−0.072595
P51684	668	C-C:C-C-C	−0.078003
P51684	643	[#1]-C-C-N-[#1]	−0.078015
P51684	536	O=C-C-N	−0.0787
P51684	574	O-C-C:C-C	−0.081492
P51684	9	>= 2 C	−0.082285
P51684	497	O-C:C:N	−0.083871
P51684	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.085526
P51684	360	C(~Cl)(~Cl)	−0.086041
P51684	752	Clc1cc(Cl)ccc1	−0.086351
P51684	471	S:C:C:C	−0.088144
P51684	302	N-F	−0.09055
P51684	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.090628
P51684	352	C(~C)(~O)	−0.091409
P51684	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.093484
P51684	17	>= 8 N	−0.09475
P51684	759	Cc1c(Cl)cccc1	−0.095933
P51684	505	Cl-C:C-O	−0.098164
P51684	51	>= 1 Al	−0.098361
P51684	868	OC1C(N)CCC1	−0.099995
P51684	510	[#1]-N-N-[#1]	−0.101394
P51684	526	Cl-C:C-Cl	−0.102177
P51684	29	>= 2 Si	−0.10249
P51684	568	N#C-C-C	−0.104844
P51684	481	O-S-C:C	−0.107898
P51684	371	C(~H)(:C)(:C)	−0.110461
P51684	390	N(~C)(~C)	−0.110513
P51684	434	C(-C)(-H)(=C)	−0.111182

P51684	691	O-C-C-C-C-C-N	−0.115223
P51684	420	C=O	−0.11536
P51684	45	>= 4 Br	−0.11608
P51684	722	Oc1ccc(Cl)cc1	−0.116665
P51684	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.117241
P51684	294	C-Cl	−0.119643
P51684	710	C-C-C(C)-C-C	−0.120635
P51684	374	C(~H)(~H)(~H)	−0.121661
P51684	696	C-C-C-C-C-C-C-C	−0.12207
P51684	695	O=C-C-C-C-C-N	−0.12359
P51684	433	C(-C)(-Cl)(=O)	−0.123784
P51684	88	>= 1 Ta	−0.128507
P51684	559	O-C-N-[#1]	−0.130437
P51684	678	C-C-C=C-C	−0.131029
P51684	607	N-C-C-C:C	−0.133221
P51684	791	NC1CCC(N)CC1	−0.137709
P51684	756	Cc1c(O)cccc1	−0.145841
P51684	13	>= 32 C	−0.146443
P51684	286	C-O	−0.151111
P51684	647	O=C-N-C-N	−0.154764
P51684	432	C(-C)(-C)(=O)	−0.155979
P51684	313	O-Si	−0.156618
P51684	583	Cl-C:C-O-C	−0.164225
P51684	101	>= 1 Pr	−0.164905
P51684	735	Cc1cc(O)ccc1	−0.17568
P51684	627	O=[As]-C:C:C	−0.175958
P51684	672	O=C-C=C-[#1]	−0.179632
P51684	738	Cc1cc(Cl)ccc1	−0.179672
P51684	680	O-C-C-C-C-C	−0.180334
P51684	356	C(~C)(:C)(:C)	−0.181167
P51684	824	OC1C(O)CCCC1	−0.183433
P51684	785	OC1CCC(Cl)CC1	−0.187319
P51684	778	CC1CCC(S)CC1	−0.188767
P51684	562	Br-C-C=O	−0.190127
P51684	459	S(=O)(=O)	−0.190696
P51684	347	C(~C)(~H)(~O)(~O)	−0.193408
P51684	684	O=C-C-C-C-C	−0.201876
P51684	391	N(~C)(~C)(~C)	−0.205182
P51684	43	>= 1 Br	−0.2074
P51684	755	Cc1c(C)cccc1	−0.217211
P51684	719	Oc1ccc(O)cc1	−0.220037
P51684	692	O=C-C-C-C-C-C	−0.220833
P51684	34	>= 2 S	−0.232047
P51684	358	C(~C)(:N)	−0.234771
P51684	480	C:S:C-C	−0.236732
P51684	519	N=C-N-C	−0.237909
P51684	634	C-C-C:C-C	−0.237987
P51684	524	C-C=C-C	−0.244414

P51684	826	OC1C(N)CCCC1	−0.245043
P51684	94	>= 1 Au	−0.245355
P51684	780	CC1CCC(Cl)CC1	−0.248155
P51684	736	Cc1cc(S)ccc1	−0.257615
P51684	421	C=S	−0.266764
P51684	378	C(~N)(:C)(:N)	−0.2678
P51684	702	O-C-C-C-C-C-N-C	−0.271089
P51684	431	C(-C)(-C)(=N)	−0.271932
P51684	458	S(-O)(=O)	−0.274568
P51684	357	C(~C)(:C)(:N)	−0.275013
P51684	366	C(~H)(~O)	−0.275234
P51684	93	>= 1 Pt	−0.282156
P51684	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.28667
P51684	620	C:C-O-C-C	−0.30434
P51684	150	>= 2 any ring size 5	−0.305353
P51684	466	N#C-C=C	−0.307857
P51684	56	>= 1 Cr	−0.311727
P51684	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.313494
P51684	489	N-C-S-C	−0.318919
P51684	777	CC1CCC(O)CC1	−0.331259
P51684	685	O=C-C-C-C-N	−0.331438
P51684	71	>= 1 Zr	−0.334471
P51684	365	C(~H)(~N)	−0.335867
P51684	642	O-C-C-C=O	−0.339528
P51684	192	>= 3 any ring size 6	−0.343063
P51684	803	OC1CC(O)CCC1	−0.350213
P51684	99	>= 1 La	−0.352134
P51684	629	S-C:C:C-N	−0.358523
P51684	555	N=C-C=C	−0.366817
P51684	419	C#N	−0.372015
P51684	404	N(:C)(:C)(:C)	−0.387412
P51684	386	C(:C)(:C)(:N)	−0.392415
P51684	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.392573
P51684	802	CC1CC(Br)CCC1	−0.392901
P51684	1	>= 8 H	−0.39682
P51684	464	N-C-C=C	−0.399052
P51684	847	OC1CC(N)CC1	−0.399477
P51684	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.400873
P51684	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.409636
P51684	841	CC1CC(S)CC1	−0.412261
P51684	518	O=C-N-N	−0.412924
P51684	281	B-Cl	−0.413185
P51684	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.424935
P51684	862	CC1C(S)CCC1	−0.424991
P51684	734	Cc1cc(C)ccc1	−0.428635
P51684	563	O-C-O-C	−0.436802
P51684	859	BrC1CC(Br)CC1	−0.441464
P51684	664	C-C=C-C=C	−0.456652

P51684	874	SC1C(Br)CCC1	−0.469844
P51684	718	Cc1ccc(Br)cc1	−0.470837
P51684	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.474539
P51684	445	C(-H)(-N)(=C)	−0.477934
P51684	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.480984
P51684	670	Br-C:C-C	−0.482389
P51684	8	>= 4 B	−0.48497
P51684	716	Cc1ccc(N)cc1	−0.495697
P51684	829	SC1C(S)CCCC1	−0.498025
P51684	869	OC1C(Cl)CCC1	−0.502802
P51684	439	C(-C)(-N)(=O)	−0.507941
P51684	767	Sc1c(N)cccc1	−0.518098
P51684	373	C(~H)(:N)	−0.520878
P51684	569	N-C-C-N	−0.520987
P51684	33	>= 1 S	−0.523704
P51684	335	C(~C)(~C)(~C)(~H)	−0.527807
P51684	256	>= 1 hetero-aromatic ring	−0.528246
P51684	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.528967
P51684	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.529
P51684	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.538297
P51684	628	C-N-C-C:C	−0.540126
P51684	341	C(~C)(~C)(~O)	−0.542868
P51684	800	CC1CC(N)CCC1	−0.549314
P51684	79	>= 1 In	−0.551908
P51684	775	Brc1c(Br)cccc1	−0.554481
P51684	199	>= 4 any ring size 6	−0.563697
P51684	417	C#C	−0.57299
P51684	436	C(-C)(-H)(=O)	−0.588846
P51684	599	[#1]-C-C=C-[#1]	−0.60337
P51684	291	C-Si	−0.604536
P51684	490	C-C-C=C	−0.612146
P51684	449	C(-N)(=C)	−0.618969
P51684	545	N-C:C-C	−0.624228
P51684	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.641117
P51684	838	BrC1C(Br)CCCC1	−0.667345
P51684	393	N(~C)(~H)	−0.669805
P51684	408	O(~H)(~S)	−0.675131
P51684	455	N(-O)(=O)	−0.68324
P51684	542	O-C:C-[#1]	−0.688263
P51684	66	>= 1 Se	−0.697386
P51684	269	Li-P	−0.698161
P51684	593	N-C-C-C-N	−0.698598
P51684	842	CC1CC(N)CC1	−0.698614
P51684	143	>= 1 any ring size 5	−0.699355
P51684	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.707143
P51684	411	P(~O)(~O)	−0.709652
P51684	770	Nc1c(N)cccc1	−0.71308
P51684	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.720944

P51684	872	SC1C(N)CCC1	−0.727566
P51684	309	O-O	−0.733375
P51684	525	[As]-C:C-[#1]	−0.774025
P51684	573	O-C-C=C	−0.781334
P51684	499	N-C:C:N	−0.80773
P51684	814	NC1CC(Br)CCC1	−0.826593
P51684	858	ClC1CC(Br)CC1	−0.838717
P51684	24	>= 2 F	−0.863301
P51684	771	Nc1c(Cl)cccc1	−0.877678
P51684	880	BrC1C(Br)CCC1	−0.88128
P51684	64	>= 1 Ge	−0.885866
P51684	592	N-C-C-C-C	−0.904918
P51684	74	>= 1 Ru	−0.910541
P51684	295	C-As	−0.922837
P51684	317	F-S	−0.925406
P51684	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.927478
P51684	572	N:C:N:C	−0.928507
P51684	648	O=N-C:C-N	−0.943314
P51684	274	B-C	−0.950094
P51684	178	>= 1 any ring size 6	−0.95612
P51684	452	C(-O)(=O)	−0.960837
P51684	418	C=N	−0.961717
P51684	871	SC1C(S)CCC1	−0.965963
P51684	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.995348
P51684	415	Si(~C)(~C)	−1.003046
P51684	744	Oc1cc(Br)ccc1	−1.018886
P51684	689	O-C-C-C-C-C-C	−1.028294
P51684	817	BrC1CC(Br)CCC1	−1.034257
P51684	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−1.043859
P51684	342	C(~C)(~Cl)	−1.055541
P51684	59	>= 1 Co	−1.056576
P51684	339	C(~C)(~C)(~H)(~O)	−1.082512
P51684	724	Sc1ccc(S)cc1	−1.085221
P51684	258	>= 2 hetero-aromatic rings	−1.08868
P51684	259	>= 3 aromatic rings	−1.096105
P51684	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−1.117587
P51684	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−1.155981
P51684	585	C-C:C-N-C	−1.156788
P51684	158	>= 3 saturated or aromatic carbon-only ring size 5	−1.160939
P51684	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−1.163491
P51684	63	>= 1 Ga	−1.179868
P51684	468	O=S-C-N	−1.200892
P51684	604	C-O-C-C:C	−1.202931
P51684	332	C(~C)(~C)	−1.24971
P51684	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−1.275386
P51684	375	C(~N)(~N)	−1.285285
P51684	72	>= 1 Nb	−1.294059
P51684	3	>= 32 H	−1.298625

P51684	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−1.306399
P51684	355	C(~C)(:C)	−1.368265
P51684	336	C(~C)(~C)(~C)(~N)	−1.381317
P51684	725	Sc1ccc(N)cc1	−1.389371
P51684	575	O-C-C:C-O	−1.41766
P51684	746	Sc1cc(N)ccc1	−1.423236
P51684	783	OC1CCC(S)CC1	−1.43629
P51684	110	>= 1 Er	−1.461934
P51684	304	N-P	−1.519541
P51684	260	>= 3 hetero-aromatic rings	−1.586162
P51684	794	ClC1CCC(Cl)CC1	−1.586486
P51684	764	Oc1c(Cl)cccc1	−1.595902
P51684	416	C=C	−1.653239
P51684	319	Al-Cl	−1.709698
P51684	837	ClC1C(Br)CCCC1	−1.768297
P51684	235	>= 2 saturated or aromatic carbon-only ring size 8	−1.966693
P51684	284	C-C	−2.240843
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Fingerprints（continued)

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
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P51679	375	C(~N)(~N)	2.2216914
P51679	278	B-Si	2.1208767
P51679	269	Li-P	1.8944966
P51679	414	S(~C)(~O)	1.8530009
P51679	876	NC1C(Cl)CC1	1.814854
P51679	769	Sc1c(Br)cccc1	1.7305074
P51679	492	N-C:O:C	1.7192602
P51679	42	>= 2 K	1.7024358
P51679	290	C-Al	1.6599801
P51679	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	1.6516248
P51679	200	>= 4 saturated or aromatic carbon-only ring size 6	1.6515175
P51679	315	O-K	1.5898435
P51679	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	1.5425725
P51679	731	Clc1ccc(Cl)cc1	1.4962439
P51679	622	O=C-O-C:C	1.4948508
P51679	874	SC1C(Br)CCC1	1.4854502
P51679	581	O=C-C-C-O	1.47467
P51679	687	O=C-C-C-C=O	1.4544361
P51679	53	>= 1 Sc	1.4298773
P51679	214	>= 1 saturated or aromatic carbon-only ring size 7	1.3853641
P51679	767	Sc1c(N)cccc1	1.3594642
P51679	745	Sc1cc(S)ccc1	1.3474586
P51679	29	>= 2 Si	1.3265231
P51679	61	>= 1 Cu	1.3177437
P51679	629	S-C:C:C-N	1.3056268
P51679	44	>= 2 Br	1.3053582
P51679	801	CC1CC(Cl)CCC1	1.2999508
P51679	143	>= 1 any ring size 5	1.2978198
P51679	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	1.2901436
P51679	803	OC1CC(O)CCC1	1.2891728
P51679	877	NC1C(Br)CCC1	1.2808853
P51679	45	>= 4 Br	1.2757022
P51679	870	OC1C(Br)CCC1	1.2624134
P51679	248	>= 1 any ring size 10	1.235361
P51679	739	Cc1cc(Br)ccc1	1.2174434
P51679	390	N(~C)(~C)	1.2113385
P51679	68	>= 1 Rb	1.2078395
P51679	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	1.1927867
P51679	24	>= 2 F	1.1803948
P51679	435	C(-C)(-H)(=N)	1.177421
P51679	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	1.1632789
P51679	791	NC1CCC(N)CC1	1.1356497
P51679	2	>= 16 H	1.1316346
P51679	439	C(-C)(-N)(=O)	1.1284164
P51679	817	BrC1CC(Br)CCC1	1.1274382

P51679	66	>= 1 Se	1.1217491
P51679	424	N=P	1.116968
P51679	21	>= 8 O	1.0976386
P51679	368	C(~H)(~S)	1.0840428
P51679	594	C-O-C-C=C	1.0816567
P51679	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.07489
P51679	651	O-C:C:C-C	1.074382
P51679	87	>= 1 Hf	1.0680718
P51679	867	OC1C(S)CCC1	1.0673222
P51679	427	C(#C)(-C)	1.0536314
P51679	275	B-N	1.0410867
P51679	282	B-Br	1.0367804
P51679	352	C(~C)(~O)	1.0340188
P51679	851	SC1CC(N)CC1	1.0322777
P51679	89	>= 1 W	1.0278325
P51679	347	C(~C)(~H)(~O)(~O)	1.0228482
P51679	60	>= 1 Ni	1.0225578
P51679	531	S-C:C-C	1.018927
P51679	773	Clc1c(Cl)cccc1	1.0058924
P51679	265	Li-B	1.0042776
P51679	6	>= 1 B	0.9847768
P51679	815	ClC1CC(Cl)CCC1	0.9817351
P51679	466	N#C-C=C	0.975354
P51679	526	Cl-C:C-Cl	0.965821
P51679	272	B-H	0.9634844
P51679	341	C(~C)(~C)(~O)	0.9626621
P51679	274	B-C	0.9605291
P51679	97	>= 1 Pb	0.957664
P51679	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.957274
P51679	393	N(~C)(~H)	0.9417374
P51679	178	>= 1 any ring size 6	0.9349623
P51679	330	C(~Br)(:C)	0.9338198
P51679	485	N:C:C:N	0.9298036
P51679	540	C-N-C-[#1]	0.9275438
P51679	663	O-C-C-O-[#1]	0.9189303
P51679	661	O-C-O-C-C	0.9167584
P51679	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.9060625
P51679	386	C(:C)(:C)(:N)	0.899056
P51679	284	C-C	0.8804299
P51679	717	Cc1ccc(Cl)cc1	0.8693002
P51679	834	NC1C(Cl)CCCC1	0.8644986
P51679	805	OC1CC(N)CCC1	0.8633999
P51679	560	N-C-N-C	0.8613346
P51679	468	O=S-C-N	0.8517406
P51679	372	C(~H)(:C)(:N)	0.8478965
P51679	151	>= 2 saturated or aromatic carbon-only ring size 5	0.8266601
P51679	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.8223168
P51679	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.8176493

P51679	825	OC1C(S)CCCC1	0.8165958
P51679	484	N-C:N:C	0.8113068
P51679	778	CC1CCC(S)CC1	0.8109661
P51679	660	C-C=C-C-C	0.8069246
P51679	106	>= 1 Gd	0.8039489
P51679	681	O-C-C-C-C-O	0.803132
P51679	480	C:S:C-C	0.7954813
P51679	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.7833941
P51679	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.7782038
P51679	5	>= 2 Li	0.7766803
P51679	818	CC1C(C)CCCC1	0.7744774
P51679	93	>= 1 Pt	0.7590864
P51679	537	O=C-C-O	0.7588829
P51679	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.7586228
P51679	658	C-C-S-C-C	0.7581168
P51679	829	SC1C(S)CCCC1	0.7533254
P51679	688	C-C-C-C-C-C-C	0.7517357
P51679	598	Cl-C:C:C-C	0.7465749
P51679	376	C(~N)(:C)	0.7382923
P51679	266	Li-C	0.7339743
P51679	186	>= 2 saturated or aromatic carbon-only ring size 6	0.7278179
P51679	23	>= 1 F	0.7244299
P51679	677	C-C=C-C:C	0.7169501
P51679	832	SC1C(Br)CCCC1	0.7085603
P51679	505	Cl-C:C-O	0.7047269
P51679	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.6959981
P51679	487	N-C=N-C	0.6921153
P51679	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.6908827
P51679	619	O-C-C=C-C	0.6898062
P51679	396	N(~C)(:C)	0.6855333
P51679	737	Cc1cc(N)ccc1	0.6820891
P51679	404	N(:C)(:C)(:C)	0.6811565
P51679	361	C(~Cl)(~H)	0.6790087
P51679	518	O=C-N-N	0.6763144
P51679	839	CC1CC(C)CC1	0.6726729
P51679	334	C(~C)(~C)(~C)(~C)	0.6714781
P51679	847	OC1CC(N)CC1	0.6711349
P51679	668	C-C:C-C-C	0.6711055
P51679	878	ClC1C(Cl)CCC1	0.6704662
P51679	841	CC1CC(S)CC1	0.6681506
P51679	718	Cc1ccc(Br)cc1	0.6633864
P51679	562	Br-C-C=O	0.6606668
P51679	358	C(~C)(:N)	0.6596998
P51679	473	S-C:N:C	0.6586266
P51679	32	>= 4 P	0.655498
P51679	476	C-O-C=C	0.6480279
P51679	544	O-C:C-O	0.6459718
P51679	57	>= 1 Mn	0.6447552

P51679	500	C-S-C:C	0.6401766
P51679	719	Oc1ccc(O)cc1	0.6382061
P51679	116	>= 1 saturated or aromatic carbon-only ring size 3	0.6373333
P51679	628	C-N-C-C:C	0.632336
P51679	555	N=C-C=C	0.6321711
P51679	751	Nc1cc(Br)ccc1	0.6318002
P51679	726	Sc1ccc(Cl)cc1	0.6283902
P51679	316	F-P	0.6257439
P51679	525	[As]-C:C-[#1]	0.6218645
P51679	524	C-C=C-C	0.6150827
P51679	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.6118836
P51679	652	O-C:C:C-N	0.6111282
P51679	578	C-C:C-C:C	0.6057589
P51679	261	>= 4 aromatic rings	0.603277
P51679	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.6006258
P51679	714	Cc1ccc(O)cc1	0.6000006
P51679	596	N=C-N-C-C	0.5951048
P51679	310	O-Mg	0.5898613
P51679	527	C:C:N-[#1]	0.5897629
P51679	474	S:C:C:N	0.5843246
P51679	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.582409
P51679	8	>= 4 B	0.5782074
P51679	185	>= 2 any ring size 6	0.5733986
P51679	479	S-C-S-C	0.5634699
P51679	413	S(~C)(~H)	0.5601995
P51679	511	S=C-N-[#1]	0.5486768
P51679	838	BrC1C(Br)CCCC1	0.5445244
P51679	501	Cl-C:C-C	0.544444
P51679	545	N-C:C-C	0.5388609
P51679	172	>= 5 saturated or aromatic carbon-only ring size 5	0.5376765
P51679	873	SC1C(Cl)CCC1	0.5353791
P51679	425	P=O	0.5338683
P51679	549	N-C-C:C	0.531268
P51679	848	OC1CC(Cl)CC1	0.5303419
P51679	83	>= 1 Xe	0.5302904
P51679	835	NC1C(Br)CCCC1	0.5252408
P51679	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.5220394
P51679	796	BrC1CCC(Br)CC1	0.5104719
P51679	486	N-C:N:N	0.506958
P51679	821	CC1C(N)CCCC1	0.5015391
P51679	689	O-C-C-C-C-C-C	0.5005745
P51679	551	Cl-C-C-O	0.4987862
P51679	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.4973084
P51679	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.4940072
P51679	729	Nc1ccc(Cl)cc1	0.4878615
P51679	324	P-P	0.4761046
P51679	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.4747219
P51679	776	CC1CCC(C)CC1	0.4746833

P51679	495	C-N-C:C	0.4742855
P51679	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.4666622
P51679	318	Al-H	0.462657
P51679	478	S-C=N-[#1]	0.4588178
P51679	671	O=C-C=C-C	0.4563213
P51679	461	O-C-C=N	0.4513211
P51679	682	O-C-C-C-C-N	0.4509828
P51679	339	C(~C)(~C)(~H)(~O)	0.4501674
P51679	451	C(-N)(=O)	0.4473132
P51679	808	SC1CC(S)CCC1	0.4470275
P51679	799	CC1CC(S)CCC1	0.4446786
P51679	419	C#N	0.4410244
P51679	78	>= 1 Cd	0.4358165
P51679	543	O-C:C-N	0.4354108
P51679	76	>= 1 Pd	0.4325778
P51679	517	N-N-C-N	0.4294355
P51679	77	>= 1 Ag	0.4137501
P51679	785	OC1CCC(Cl)CC1	0.4036525
P51679	749	Nc1cc(N)ccc1	0.4018682
P51679	503	Cl-C:C-[#1]	0.3966087
P51679	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.3952498
P51679	623	O=C-C:C-C	0.3940657
P51679	36	>= 8 S	0.3905312
P51679	716	Cc1ccc(N)cc1	0.3891747
P51679	320	Si-H	0.3882715
P51679	416	C=C	0.386853
P51679	809	SC1CC(N)CCC1	0.3807764
P51679	406	O(~C)(~H)	0.3784109
P51679	4	>= 1 Li	0.3762495
P51679	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.3752479
P51679	104	>= 1 Sm	0.3706022
P51679	591	Cl-C-C-C-C	0.3701789
P51679	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.3678034
P51679	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.3674583
P51679	431	C(-C)(-C)(=N)	0.3629301
P51679	615	N-C-C-O-C	0.3587857
P51679	657	C-N-C:C-C	0.3573946
P51679	810	SC1CC(Cl)CCC1	0.346698
P51679	46	>= 1 I	0.3436668
P51679	506	C-C:N:C	0.3387263
P51679	74	>= 1 Ru	0.3365597
P51679	609	Cl-C-C-N-C	0.3363498
P51679	787	SC1CCC(S)CC1	0.3362522
P51679	92	>= 1 Ir	0.3331509
P51679	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.3298116
P51679	595	C:C-C-C-C	0.3233348
P51679	732	Clc1ccc(Br)cc1	0.321229
P51679	635	N-N-C-N-[#1]	0.319578

P51679	401	N(~O)(~O)	0.3112751
P51679	831	SC1C(Cl)CCCC1	0.3081649
P51679	408	O(~H)(~S)	0.3058057
P51679	797	CC1CC(C)CCC1	0.3035099
P51679	22	>= 16 O	0.3033401
P51679	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.3027643
P51679	587	N-C:C-O-[#1]	0.300907
P51679	798	CC1CC(O)CCC1	0.2955852
P51679	469	S-S-C:C	0.2952364
P51679	317	F-S	0.2928193
P51679	748	Sc1cc(Br)ccc1	0.2915756
P51679	91	>= 1 Os	0.2877175
P51679	546	N-C:C-[#1]	0.282766
P51679	73	>= 1 Mo	0.2789373
P51679	644	C-C=N-N-C	0.277372
P51679	389	C(:N)(:N)	0.2772222
P51679	868	OC1C(N)CCC1	0.2762431
P51679	684	O=C-C-C-C-C	0.276166
P51679	692	O=C-C-C-C-C-C	0.2757678
P51679	634	C-C-C:C-C	0.2741054
P51679	712	C-C(C)-C(C)-C	0.2723342
P51679	804	OC1CC(S)CCC1	0.2611742
P51679	354	C(~C)(~Si)	0.2593451
P51679	95	>= 1 Hg	0.2584961
P51679	569	N-C-C-N	0.2570968
P51679	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.2550934
P51679	852	SC1CC(Cl)CC1	0.249165
P51679	593	N-C-C-C-N	0.2475121
P51679	448	C(-H)(=O)	0.2469232
P51679	667	C=C-C-O-[#1]	0.2415446
P51679	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.240759
P51679	669	Cl-C:C-C=O	0.2393998
P51679	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.2372366
P51679	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.2368202
P51679	754	Brc1cc(Br)ccc1	0.236546
P51679	16	>= 4 N	0.2356736
P51679	820	CC1C(S)CCCC1	0.2307773
P51679	327	C(~Br)(~C)	0.2306567
P51679	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.2298243
P51679	733	Brc1ccc(Br)cc1	0.221461
P51679	301	N-O	0.2199595
P51679	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.2178403
P51679	542	O-C:C-[#1]	0.2088216
P51679	577	C:C-N-C:C	0.2077513
P51679	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.2048114
P51679	553	O=C-C=C	0.2039686
P51679	364	C(~F)(:C)	0.2005524
P51679	356	C(~C)(:C)(:C)	0.1999346

P51679	426	P=P	0.1996106
P51679	308	O-H	0.1872471
P51679	88	>= 1 Ta	0.1866408
P51679	536	O=C-C-N	0.1811855
P51679	428	C(#C)(-H)	0.1776073
P51679	454	N(-C)(=O)	0.1774927
P51679	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.1763328
P51679	335	C(~C)(~C)(~C)(~H)	0.1739301
P51679	588	O=C-C-C=O	0.173725
P51679	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.172216
P51679	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.1699883
P51679	625	O=C-C:C-O	0.1688637
P51679	570	C:C-C-C	0.1674161
P51679	192	>= 3 any ring size 6	0.1672429
P51679	342	C(~C)(~Cl)	0.1645499
P51679	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.1622103
P51679	417	C#C	0.1615468
P51679	112	>= 1 Yb	0.1588693
P51679	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.1573746
P51679	388	C(:C)(:N)(:N)	0.1564776
P51679	273	B-B	0.1562457
P51679	559	O-C-N-[#1]	0.1553287
P51679	20	>= 4 O	0.1550473
P51679	482	C:N-C:C	0.1537851
P51679	3	>= 32 H	0.1537082
P51679	607	N-C-C-C:C	0.1519799
P51679	632	C-C-O-C:C	0.1502024
P51679	340	C(~C)(~C)(~N)	0.1499796
P51679	371	C(~H)(:C)(:C)	0.1480927
P51679	655	O-C-C-C:C	0.1426663
P51679	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.1385294
P51679	813	NC1CC(Cl)CCC1	0.1382848
P51679	472	C:N:C-C	0.1312881
P51679	258	>= 2 hetero-aromatic rings	0.1312591
P51679	735	Cc1cc(O)ccc1	0.1304916
P51679	336	C(~C)(~C)(~C)(~N)	0.1251572
P51679	612	N-C-O-C-C	0.1246137
P51679	13	>= 32 C	0.1244381
P51679	362	C(~Cl)(:C)	0.121892
P51679	538	N=C-C-C	0.1207888
P51679	648	O=N-C:C-N	0.1189695
P51679	47	>= 2 I	0.1172643
P51679	12	>= 16 C	0.1170746
P51679	756	Cc1c(O)cccc1	0.1151436
P51679	377	C(~N)(:C)(:C)	0.1143217
P51679	602	O=C-C-N-C	0.1113933
P51679	221	>= 2 saturated or aromatic carbon-only ring size 7	0.1097915
P51679	64	>= 1 Ge	0.1096318

P51679	662	O-C-C-O-C	0.1080492
P51679	592	N-C-C-C-C	0.1075293
P51679	583	Cl-C:C-O-C	0.1019915
P51679	659	O-C-C-N-C	0.1016119
P51679	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0968521
P51679	399	N(~H)(:C)	0.0960568
P51679	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0946073
P51679	567	O-C-C-O	0.0920353
P51679	691	O-C-C-C-C-C-N	0.0908172
P51679	747	Sc1cc(Cl)ccc1	0.0904092
P51679	467	C=N-N-C	0.0871011
P51679	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0862641
P51679	576	N=C-C:C-[#1]	0.0816966
P51679	103	>= 1 Pm	0.0807783
P51679	621	N-C:C:C:N	0.0755558
P51679	402	N(~O)(:O)	0.0727941
P51679	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0724183
P51679	72	>= 1 Nb	0.0715139
P51679	630	O-C:C-O-C	0.068004
P51679	683	N-C-C-C-C-C	0.0629416
P51679	698	O-C-C-C-C-C-C-C	0.0618231
P51679	462	O-C-C=O	0.0611782
P51679	442	C(-C)(=N)	0.0594472
P51679	452	C(-O)(=O)	0.0591943
P51679	400	N(~H)(:C)(:C)	0.0565006
P51679	513	S:C:C-[#1]	0.0551574
P51679	837	ClC1C(Br)CCCC1	0.0542533
P51679	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.0540523
P51679	512	C-[As]-O-[#1]	0.0525154
P51679	438	C(-C)(-N)(=N)	0.049661
P51679	43	>= 1 Br	0.0492376
P51679	242	>= 1 saturated or aromatic carbon-only ring size 9	0.0445142
P51679	665	N-C:C-C-C	0.0430189
P51679	676	N#C-C-C-C	0.0412185
P51679	257	>= 2 aromatic rings	0.0400248
P51679	227	>= 1 any ring size 8	0.0394043
P51679	483	N-S-C:C	0.0388989
P51679	762	Oc1c(S)cccc1	0.037087
P51679	407	O(~C)(~P)	0.0355104
P51679	666	C=C-C-O-C	0.0351917
P51679	558	O=N-C:C	0.0334959
P51679	760	Cc1c(Br)cccc1	0.0334774
P51679	55	>= 1 V	0.0332562
P51679	741	Oc1cc(S)ccc1	0.0324461
P51679	137	>= 2 saturated or aromatic carbon-only ring size 4	0.0324145
P51679	302	N-F	0.0322243
P51679	378	C(~N)(:C)(:N)	0.0321256
P51679	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.0320708

P51679	7	>= 2 B	0.0317787
P51679	397	N(~C)(:C)(:C)	0.0309353
P51679	746	Sc1cc(N)ccc1	0.0309022
P51679	369	C(~H)(~Si)	0.0299497
P51679	49	>= 1 Be	0.0298687
P51679	722	Oc1ccc(Cl)cc1	0.0298489
P51679	879	ClC1C(Br)CCC1	0.0295144
P51679	440	C(-C)(-O)(=O)	0.0294686
P51679	556	C=C-C-C	0.0287599
P51679	430	C(-C)(-C)(=C)	0.0287079
P51679	80	>= 1 Sn	0.0286386
P51679	552	C:C-C:C	0.0279723
P51679	604	C-O-C-C:C	0.0277468
P51679	696	C-C-C-C-C-C-C-C	0.0272892
P51679	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0271613
P51679	811	SC1CC(Br)CCC1	0.0269344
P51679	150	>= 2 any ring size 5	0.0267625
P51679	641	O-C-C-C=C	0.0263859
P51679	114	>= 1 U	0.0243617
P51679	31	>= 2 P	0.0232409
P51679	744	Oc1cc(Br)ccc1	0.0215455
P51679	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0207052
P51679	470	C:C-C=C	0.0203826
P51679	673	O=C-C=C-N	0.0193197
P51679	845	OC1CC(O)CC1	0.0187326
P51679	582	C-C-C-C-C	0.0179166
P51679	420	C=O	0.0174224
P51679	62	>= 1 Zn	0.015554
P51679	353	C(~C)(~S)	0.0152746
P51679	709	C-C(C)-C-C-C	0.0149785
P51679	674	N-C-N-C:C	0.014718
P51679	277	B-F	0.0145431
P51679	37	>= 1 Cl	0.0144331
P51679	585	C-C:C-N-C	0.0143843
P51679	463	N:C-S-[#1]	0.0109776
P51679	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0105347
P51679	862	CC1C(S)CCC1	0.010467
P51679	63	>= 1 Ga	0.0103323
P51679	781	CC1CCC(Br)CC1	0.0094369
P51679	793	NC1CCC(Br)CC1	0.0091151
P51679	387	C(:C)(:N)	0.0085849
P51679	860	CC1C(C)CCC1	0.0082337
P51679	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.0081663
P51679	101	>= 1 Pr	0.0060536
P51679	654	N-C-N-C-C	0.0057021
P51679	298	C-I	0.0055323
P51679	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.0053016
P51679	550	Cl-C-C-C	0.0048023

P51679	763	Oc1c(N)cccc1	0.0044083
P51679	723	Oc1ccc(Br)cc1	0.0041796
P51679	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.0040412
P51679	498	O-C=C-C	0.0039459
P51679	759	Cc1c(Cl)cccc1	0.0039448
P51679	220	>= 2 any ring size 7	0.0037094
P51679	314	O-P	0.0024853
P51679	814	NC1CC(Br)CCC1	0.0020945
P51679	48	>= 4 I	0.0017611
P51679	429	C(#N)(-C)	0.0014035
P51679	864	CC1C(Cl)CCC1	0.0013898
P51679	742	Oc1cc(N)ccc1	0.0013652
P51679	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.0010967
P51679	557	N:C-O-[#1]	0.0010376
P51679	844	CC1CC(Br)CC1	0.0009319
P51679	343	C(~C)(~Cl)(~H)	0.000835
P51679	639	O-C-C-C-O	0.0002079
P51679	643	[#1]-C-C-N-[#1]	0.0001735
P51679	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	3.90E-05
P51679	279	B-P	2.44E-06
P51679	859	BrC1CC(Br)CC1	2.58E-09
P51679	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	-9.80E-10
P51679	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	-1.13E-09
P51679	307	N-Br	-2.22E-09
P51679	82	>= 1 Te	-2.62E-09
P51679	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	-3.11E-09
P51679	326	As-As	-2.34E-05
P51679	783	OC1CCC(S)CC1	-0.000284
P51679	784	OC1CCC(N)CC1	-0.000301
P51679	802	CC1CC(Br)CCC1	-0.000628
P51679	631	O-C:C-O-[#1]	-0.000833
P51679	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	-0.00108
P51679	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	-0.001124
P51679	296	C-Se	-0.001512
P51679	863	CC1C(N)CCC1	-0.001599
P51679	880	BrC1C(Br)CCC1	-0.00188
P51679	332	C(~C)(~C)	-0.001885
P51679	392	N(~C)(~C)(~H)	-0.001919
P51679	865	CC1C(Br)CCC1	-0.001962
P51679	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.002031
P51679	768	Sc1c(Cl)cccc1	-0.00223
P51679	256	>= 1 hetero-aromatic ring	-0.002529
P51679	418	C=N	-0.002656
P51679	344	C(~C)(~H)	-0.00308
P51679	477	N-N-C:C	-0.003567
P51679	380	C(~O)(~O)	-0.003652
P51679	584	C:C-C=C-C	-0.003868
P51679	313	O-Si	-0.003911

P51679	771	Nc1c(Cl)cccc1	−0.003912
P51679	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.004193
P51679	708	C-C(C)-C-C	−0.004349
P51679	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.004401
P51679	437	C(-C)(-N)(=C)	−0.004578
P51679	281	B-Cl	−0.004616
P51679	309	O-O	−0.004708
P51679	786	OC1CCC(Br)CC1	−0.004745
P51679	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.004844
P51679	725	Sc1ccc(N)cc1	−0.004914
P51679	303	N-Si	−0.00504
P51679	627	O=[As]-C:C:C	−0.005062
P51679	721	Oc1ccc(N)cc1	−0.005122
P51679	102	>= 1 Nd	−0.005372
P51679	306	N-Cl	−0.005468
P51679	610	C-O-C-O-C	−0.00553
P51679	26	>= 1 Na	−0.005582
P51679	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.006031
P51679	493	O=C-C:C	−0.006847
P51679	58	>= 1 Fe	−0.007033
P51679	255	>= 1 aromatic ring	−0.008206
P51679	858	ClC1CC(Br)CC1	−0.009119
P51679	359	C(~C)(:N)(:N)	−0.009235
P51679	697	C-C-C-C-C-C(C)-C	−0.010177
P51679	789	SC1CCC(Cl)CC1	−0.010417
P51679	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.013849
P51679	297	C-Br	−0.015436
P51679	565	C:C-O-C	−0.016339
P51679	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.017021
P51679	640	C=C-C-C-C	−0.017168
P51679	94	>= 1 Au	−0.01881
P51679	111	>= 1 Tm	−0.019598
P51679	710	C-C-C(C)-C-C	−0.020435
P51679	345	C(~C)(~H)(~N)	−0.020541
P51679	71	>= 1 Zr	−0.020989
P51679	672	O=C-C=C-[#1]	−0.024208
P51679	600	N-C:C:C-C	−0.024305
P51679	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.024306
P51679	617	C-C-C-O-[#1]	−0.024758
P51679	720	Oc1ccc(S)cc1	−0.024789
P51679	295	C-As	−0.025015
P51679	411	P(~O)(~O)	−0.025096
P51679	855	NC1CC(Cl)CC1	−0.02592
P51679	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.026486
P51679	580	O=C-C-C-N	−0.027577
P51679	624	O=C-C:C-N	−0.027732
P51679	515	N-N-C-C	−0.027905
P51679	14	>= 1 N	−0.02822

P51679	365	C(~H)(~N)	−0.028578
P51679	775	Brc1c(Br)cccc1	−0.02885
P51679	79	>= 1 In	−0.029133
P51679	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.02945
P51679	554	Br-C-C-C	−0.030375
P51679	35	>= 4 S	−0.030804
P51679	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.031067
P51679	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.031567
P51679	105	>= 1 Eu	−0.031589
P51679	260	>= 3 hetero-aromatic rings	−0.032595
P51679	38	>= 2 Cl	−0.032808
P51679	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.032975
P51679	270	Li-S	−0.033299
P51679	289	C-Mg	−0.033322
P51679	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.033373
P51679	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.034135
P51679	18	>= 1 O	−0.035009
P51679	300	N-N	−0.037325
P51679	510	[#1]-N-N-[#1]	−0.037347
P51679	822	CC1C(Cl)CCCC1	−0.037924
P51679	367	C(~H)(~O)(~O)	−0.038978
P51679	321	Si-Si	−0.039871
P51679	680	O-C-C-C-C-C	−0.040936
P51679	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.041385
P51679	701	O-C-C-C-C-C(O)-C	−0.045399
P51679	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.046648
P51679	670	Br-C:C-C	−0.046703
P51679	826	OC1C(N)CCCC1	−0.04709
P51679	383	C(~S)(:C)	−0.052854
P51679	432	C(-C)(-C)(=O)	−0.054051
P51679	690	O-C-C-C-C-C-O	−0.054405
P51679	489	N-C-S-C	−0.056986
P51679	421	C=S	−0.061148
P51679	637	O-C-C-C-C	−0.062791
P51679	535	O=C-C-C	−0.064168
P51679	782	OC1CCC(O)CC1	−0.066196
P51679	700	O-C-C-C-C-C-O-C	−0.069186
P51679	15	>= 2 N	−0.076205
P51679	405	O(~C)(~C)	−0.078531
P51679	30	>= 1 P	−0.080842
P51679	694	O=C-C-C-C-C=O	−0.081345
P51679	647	O=C-N-C-N	−0.086395
P51679	614	C-C-O-C-C	−0.087056
P51679	338	C(~C)(~C)(~H)(~N)	−0.090467
P51679	866	OC1C(O)CCC1	−0.090782
P51679	507	C-C-S-C	−0.092498
P51679	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.094218
P51679	638	O-C-C-C-N	−0.096168

P51679	705	O=C-C-C-C-C(O)-C	−0.098456
P51679	374	C(~H)(~H)(~H)	−0.1004
P51679	693	O=C-C-C-C-C-O	−0.101002
P51679	90	>= 1 Re	−0.101775
P51679	259	>= 3 aromatic rings	−0.103737
P51679	458	S(-O)(=O)	−0.104418
P51679	446	C(-H)(=C)	−0.104931
P51679	516	[#1]-C=C-[#1]	−0.109647
P51679	753	Clc1cc(Br)ccc1	−0.115385
P51679	730	Nc1ccc(Br)cc1	−0.117576
P51679	734	Cc1cc(C)ccc1	−0.122319
P51679	436	C(-C)(-H)(=O)	−0.12281
P51679	85	>= 1 Ba	−0.123384
P51679	563	O-C-O-C	−0.127654
P51679	17	>= 8 N	−0.128135
P51679	56	>= 1 Cr	−0.128352
P51679	566	O-C-C-N	−0.128397
P51679	40	>= 8 Cl	−0.129007
P51679	633	N-C-C:C-C	−0.131326
P51679	806	OC1CC(Cl)CCC1	−0.138358
P51679	514	O-N-C-C	−0.138527
P51679	109	>= 1 Ho	−0.142276
P51679	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.14429
P51679	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.146294
P51679	616	C:C:N:N:C	−0.151374
P51679	599	[#1]-C-C=C-[#1]	−0.156443
P51679	129	>= 1 any ring size 4	−0.156795
P51679	491	C-N:C-[#1]	−0.16116
P51679	727	Sc1ccc(Br)cc1	−0.162486
P51679	50	>= 1 Mg	−0.162984
P51679	656	C-C-N-C-C	−0.163548
P51679	391	N(~C)(~C)(~C)	−0.166935
P51679	494	O=C-C:N	−0.167194
P51679	304	N-P	−0.167534
P51679	465	O=S-C-C	−0.169221
P51679	840	CC1CC(O)CC1	−0.170668
P51679	846	OC1CC(S)CC1	−0.171389
P51679	807	OC1CC(Br)CCC1	−0.173016
P51679	65	>= 1 As	−0.182387
P51679	107	>= 1 Tb	−0.183007
P51679	611	N-C-C-N-C	−0.194279
P51679	459	S(=O)(=O)	−0.196122
P51679	27	>= 2 Na	−0.199271
P51679	164	>= 4 any ring size 5	−0.202589
P51679	750	Nc1cc(Cl)ccc1	−0.202898
P51679	434	C(-C)(-H)(=C)	−0.203024
P51679	872	SC1C(N)CCC1	−0.20477
P51679	346	C(~C)(~H)(~O)	−0.205093

P51679	603	C-C:C:C-C	−0.206848
P51679	853	SC1CC(Br)CC1	−0.207339
P51679	457	S(-C)(=O)	−0.209933
P51679	572	N:C:N:C	−0.210203
P51679	508	S=C-N-C	−0.212579
P51679	312	O-Al	−0.21456
P51679	471	S:C:C:C	−0.215799
P51679	39	>= 4 Cl	−0.217928
P51679	268	Li-F	−0.220077
P51679	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.221776
P51679	267	Li-O	−0.223507
P51679	98	>= 1 Bi	−0.224784
P51679	816	ClC1CC(Br)CCC1	−0.226392
P51679	283	C-H	−0.233041
P51679	403	N(:C)(:C)	−0.234526
P51679	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.237491
P51679	571	[#1]-C-O-[#1]	−0.240506
P51679	115	>= 1 any ring size 3	−0.240556
P51679	496	N:N-C-[#1]	−0.241237
P51679	449	C(-N)(=C)	−0.244238
P51679	409	O(:C)(:C)	−0.245973
P51679	350	C(~C)(~I)	−0.249098
P51679	263	Li-H	−0.250779
P51679	792	NC1CCC(Cl)CC1	−0.250927
P51679	856	NC1CC(Br)CC1	−0.254461
P51679	766	Sc1c(S)cccc1	−0.255839
P51679	695	O=C-C-C-C-C-N	−0.256235
P51679	743	Oc1cc(Cl)ccc1	−0.266715
P51679	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.266724
P51679	329	C(~Br)(~H)	−0.267726
P51679	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.273219
P51679	444	C(-Cl)(=O)	−0.273916
P51679	790	SC1CCC(Br)CC1	−0.274875
P51679	423	N=O	−0.283815
P51679	736	Cc1cc(S)ccc1	−0.285094
P51679	586	C-S-C-C-C	−0.285328
P51679	280	B-S	−0.286237
P51679	715	Cc1ccc(S)cc1	−0.28876
P51679	645	O=C-N-C-C	−0.291426
P51679	288	C-Na	−0.294625
P51679	522	C-N-N-[#1]	−0.295602
P51679	579	O=C-C-C-C	−0.299523
P51679	33	>= 1 S	−0.300194
P51679	757	Cc1c(S)cccc1	−0.301778
P51679	777	CC1CCC(O)CC1	−0.30503
P51679	711	C-C(C)(C)-C-C	−0.313728
P51679	366	C(~H)(~O)	−0.313759
P51679	52	>= 1 Ca	−0.315785

P51679	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.316163
P51679	850	SC1CC(S)CC1	−0.325338
P51679	875	NC1C(N)CCC1	−0.327744
P51679	833	NC1C(N)CCCC1	−0.331288
P51679	521	C:N-C-[#1]	−0.337279
P51679	779	CC1CCC(N)CC1	−0.341665
P51679	539	N=C-C-[#1]	−0.341714
P51679	849	OC1CC(Br)CC1	−0.343033
P51679	455	N(-O)(=O)	−0.350508
P51679	830	SC1C(N)CCCC1	−0.351385
P51679	385	C(:C)(:C)(:C)	−0.358192
P51679	795	ClC1CCC(Br)CC1	−0.358685
P51679	678	C-C-C=C-C	−0.364593
P51679	51	>= 1 Al	−0.365905
P51679	601	N-C:C:C-N	−0.366314
P51679	234	>= 2 any ring size 8	−0.36836
P51679	861	CC1C(O)CCC1	−0.368963
P51679	325	As-H	−0.379709
P51679	355	C(~C)(:C)	−0.380176
P51679	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.383443
P51679	704	O=C-C-C-C-C-C-C	−0.391041
P51679	532	S-C:C-[#1]	−0.395511
P51679	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.396356
P51679	199	>= 4 any ring size 6	−0.402097
P51679	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.410911
P51679	99	>= 1 La	−0.411416
P51679	443	C(-C)(=O)	−0.419701
P51679	702	O-C-C-C-C-C-N-C	−0.421231
P51679	110	>= 1 Er	−0.423529
P51679	605	O=C-C-O-C	−0.424704
P51679	415	Si(~C)(~C)	−0.428993
P51679	520	C=C-C:C	−0.434568
P51679	10	>= 4 C	−0.445944
P51679	780	CC1CCC(Cl)CC1	−0.455977
P51679	509	Br-C:C-C	−0.458575
P51679	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.461139
P51679	360	C(~Cl)(~Cl)	−0.461742
P51679	755	Cc1c(C)cccc1	−0.462152
P51679	529	Cl-C-C-Cl	−0.465119
P51679	122	>= 2 any ring size 3	−0.465949
P51679	328	C(~Br)(~C)(~C)	−0.466203
P51679	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.466629
P51679	206	>= 5 any ring size 6	−0.477835
P51679	11	>= 8 C	−0.478061
P51679	412	S(~C)(~C)	−0.479316
P51679	19	>= 2 O	−0.491812
P51679	706	O=C-C-C-C-C(=O)-C	−0.492756
P51679	69	>= 1 Sr	−0.507158

P51679	649	O=N-C:C-O	-0.512647
P51679	770	Nc1c(N)cccc1	-0.530479
P51679	869	OC1C(Cl)CCC1	-0.530543
P51679	664	C-C=C-C=C	-0.531411
P51679	373	C(~H)(:N)	-0.533259
P51679	548	O-C-C:C	-0.536066
P51679	679	C-C-C-C-C-C	-0.543425
P51679	398	N(~H)(~N)	-0.545534
P51679	70	>= 1 Y	-0.551638
P51679	395	N(~C)(~O)	-0.555758
P51679	333	C(~C)(~C)(~C)	-0.567517
P51679	653	O-C:C:C-O	-0.568523
P51679	445	C(-H)(-N)(=C)	-0.57061
P51679	824	OC1C(O)CCCC1	-0.571056
P51679	573	O-C-C=C	-0.574554
P51679	81	>= 1 Sb	-0.57511
P51679	685	O=C-C-C-C-N	-0.580801
P51679	499	N-C:C:N	-0.583597
P51679	422	N=N	-0.586958
P51679	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	-0.59673
P51679	171	>= 5 any ring size 5	-0.597375
P51679	25	>= 4 F	-0.600188
P51679	453	N(-C)(=C)	-0.600682
P51679	394	N(~C)(~H)(~N)	-0.601739
P51679	528	[#1]-N-C-[#1]	-0.611863
P51679	370	C(~H)(:C)	-0.625303
P51679	752	Clc1cc(Cl)ccc1	-0.625728
P51679	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	-0.632481
P51679	561	Cl-C-C=O	-0.63598
P51679	349	C(~C)(~H)(~S)	-0.643604
P51679	575	O-C-C:C-O	-0.644085
P51679	606	O-C:C-C-C	-0.646232
P51679	686	O=C-C-C-C-O	-0.646485
P51679	823	CC1C(Br)CCCC1	-0.654281
P51679	618	C:C-C-C:C	-0.655996
P51679	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	-0.65677
P51679	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	-0.666168
P51679	381	C(~O)(:C)	-0.669096
P51679	608	C-C-C-C:C	-0.673745
P51679	740	Oc1cc(O)ccc1	-0.675206
P51679	481	O-S-C:C	-0.679878
P51679	761	Oc1c(O)cccc1	-0.683156
P51679	379	C(~N)(:N)	-0.684685
P51679	764	Oc1c(Cl)cccc1	-0.686621
P51679	59	>= 1 Co	-0.692942
P51679	363	C(~F)(~F)	-0.700504
P51679	713	Cc1ccc(C)cc1	-0.703519
P51679	728	Nc1ccc(N)cc1	-0.70648

P51679	597	O=C-C-C:C	−0.710725
P51679	34	>= 2 S	−0.711151
P51679	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.712038
P51679	305	N-S	−0.718794
P51679	827	OC1C(Cl)CCCC1	−0.719716
P51679	410	P(~C)(~C)	−0.729524
P51679	530	N:C-C:C	−0.732402
P51679	590	C-C:C-O-[#1]	−0.735761
P51679	843	CC1CC(Cl)CC1	−0.736309
P51679	724	Sc1ccc(S)cc1	−0.736706
P51679	337	C(~C)(~C)(~C)(~O)	−0.741634
P51679	812	NC1CC(N)CCC1	−0.742294
P51679	384	C(:C)(:C)	−0.757271
P51679	319	Al-Cl	−0.762429
P51679	213	>= 1 any ring size 7	−0.764516
P51679	758	Cc1c(N)cccc1	−0.771602
P51679	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.78309
P51679	738	Cc1cc(Cl)ccc1	−0.791524
P51679	504	N:C:N-C	−0.800186
P51679	564	C=C-C=C	−0.802593
P51679	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.810712
P51679	351	C(~C)(~N)	−0.822352
P51679	857	ClC1CC(Cl)CC1	−0.831031
P51679	285	C-N	−0.843576
P51679	490	C-C-C=C	−0.848184
P51679	547	N-C:C-N	−0.84966
P51679	772	Nc1c(Br)cccc1	−0.852863
P51679	828	OC1C(Br)CCCC1	−0.854531
P51679	113	>= 1 Tc	−0.857999
P51679	699	O-C-C-C-C-C(C)-C	−0.858665
P51679	523	N:C:C-C	−0.871643
P51679	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.87516
P51679	534	S-C:C-O	−0.876087
P51679	788	SC1CCC(N)CC1	−0.876993
P51679	519	N=C-N-C	−0.87971
P51679	299	N-H	−0.886371
P51679	541	O-C:C-C	−0.898668
P51679	287	C-F	−0.899135
P51679	502	N-C=C-[#1]	−0.900751
P51679	9	>= 2 C	−0.903083
P51679	262	>= 4 hetero-aromatic rings	−0.929313
P51679	136	>= 2 any ring size 4	−0.935407
P51679	707	O=C-C-C-C-C(N)-C	−0.935923
P51679	108	>= 1 Dy	−0.93965
P51679	774	Clc1c(Br)cccc1	−0.948419
P51679	293	C-S	−0.973
P51679	819	CC1C(O)CCCC1	−0.987276
P51679	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−1.003288

P51679	854	NC1CC(N)CC1	-1.028969
P51679	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	-1.03294
P51679	842	CC1CC(N)CC1	-1.037498
P51679	291	C-Si	-1.055101
P51679	86	>= 1 Lu	-1.056214
P51679	456	P(-O)(=O)	-1.068929
P51679	75	>= 1 Rh	-1.072107
P51679	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	-1.073884
P51679	488	N-C=N-[#1]	-1.076036
P51679	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	-1.077117
P51679	357	C(~C)(:C)(:N)	-1.079332
P51679	497	O-C:C:N	-1.094298
P51679	533	S-C:C-N	-1.097183
P51679	475	S-C=N-C	-1.109261
P51679	286	C-O	-1.113038
P51679	123	>= 2 saturated or aromatic carbon-only ring size 3	-1.113172
P51679	589	C-C:C-O-C	-1.123769
P51679	144	>= 1 saturated or aromatic carbon-only ring size 5	-1.123986
P51679	382	C(~O)(:C)(:C)	-1.126052
P51679	703	O-C-C-C-C-C(N)-C	-1.135521
P51679	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	-1.140055
P51679	464	N-C-C=C	-1.153545
P51679	646	O=C-N-C-[#1]	-1.157026
P51679	1	>= 8 H	-1.159907
P51679	28	>= 1 Si	-1.167669
P51679	447	C(-H)(=N)	-1.192097
P51679	84	>= 1 Cs	-1.224253
P51679	568	N#C-C-C	-1.226026
P51679	636	C-N-C-N-C	-1.226367
P51679	433	C(-C)(-Cl)(=O)	-1.238953
P51679	800	CC1CC(N)CCC1	-1.251355
P51679	574	O-C-C:C-C	-1.26162
P51679	441	C(-C)(=C)	-1.277646
P51679	675	Br-C-C-C:C	-1.284292
P51679	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	-1.299767
P51679	271	Li-Cl	-1.320785
P51679	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	-1.348946
P51679	96	>= 1 Tl	-1.365782
P51679	100	>= 1 Ce	-1.394794
P51679	620	C:C-O-C-C	-1.402778
P51679	460	C-C-C#C	-1.409986
P51679	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	-1.416531
P51679	650	O=C-N-C=O	-1.475481
P51679	241	>= 1 any ring size 9	-1.479334
P51679	41	>= 1 K	-1.487392
P51679	331	C(~Br)(:N)	-1.489162
P51679	642	O-C-C-C=O	-1.541835
P51679	292	C-P	-1.569059

P51679	871	SC1C(S)CCC1	−1.578478
P51679	67	>= 1 Kr	−1.586503
P51679	0	>= 4 H	−1.63788
P51679	322	Si-Cl	−1.691904
P51679	836	ClC1C(Cl)CCCC1	−1.697855
P51679	54	>= 1 Ti	−1.787789
P51679	613	C-N-C-C-C	−1.806796
P51679	765	Oc1c(Br)cccc1	−1.813759
P51679	323	P-H	−1.882899
P51679	311	O-Na	−1.909929
P51679	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−1.966846
P51679	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.976901
P51679	294	C-Cl	−2.003384
P51679	157	>= 3 any ring size 5	−2.016153
P51679	794	ClC1CCC(Cl)CC1	−2.033071
P51679	276	B-O	−2.083632
P51679	264	Li-Li	−2.101654
P51679	450	C(-N)(=N)	−2.121713
P51679	348	C(~C)(~H)(~P)	−2.369751

Fingerprints（continued)

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1.7024358	-4.73E-09
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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P49019	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	1.6619822
P49019	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	1.4765256
P49019	399	N(~H)(:C)	1.1468988
P49019	596	N=C-N-C-C	1.1415391
P49019	422	N=N	1.1250648
P49019	35	>= 4 S	1.1203377
P49019	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	1.060244
P49019	558	O=N-C:C	1.0374596
P49019	459	S(=O)(=O)	0.9828844
P49019	607	N-C-C-C:C	0.9735433
P49019	865	CC1C(Br)CCC1	0.9226156
P49019	500	C-S-C:C	0.9167507
P49019	464	N-C-C=C	0.8354953
P49019	285	C-N	0.8226611
P49019	814	NC1CC(Br)CCC1	0.8160731
P49019	543	O-C:C-N	0.810005
P49019	111	>= 1 Tm	0.7746243
P49019	559	O-C-N-[#1]	0.7660063
P49019	21	>= 8 O	0.74803
P49019	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.745199
P49019	51	>= 1 Al	0.7262624
P49019	656	C-C-N-C-C	0.6862409
P49019	540	C-N-C-[#1]	0.6821645
P49019	355	C(~C)(:C)	0.6350724
P49019	845	OC1CC(O)CC1	0.6252923
P49019	714	Cc1ccc(O)cc1	0.6107902
P49019	483	N-S-C:C	0.5964144
P49019	676	N#C-C-C-C	0.5949656
P49019	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.5930902
P49019	671	O=C-C=C-C	0.5866815
P49019	802	CC1CC(Br)CCC1	0.5809563
P49019	560	N-C-N-C	0.5798774
P49019	856	NC1CC(Br)CC1	0.5667213
P49019	309	O-O	0.5653812
P49019	650	O=C-N-C=O	0.5495367
P49019	564	C=C-C=C	0.4764785
P49019	214	>= 1 saturated or aromatic carbon-only ring size 7	0.4763933
P49019	703	O-C-C-C-C-C(N)-C	0.4744066
P49019	674	N-C-N-C:C	0.4727788
P49019	737	Cc1cc(N)ccc1	0.4652748
P49019	695	O=C-C-C-C-C-N	0.4523665
P49019	277	B-F	0.4373702
P49019	113	>= 1 Tc	0.4256462
P49019	165	>= 4 saturated or aromatic carbon-only ring size 5	0.4247393
P49019	725	Sc1ccc(N)cc1	0.4045802
P49019	840	CC1CC(O)CC1	0.4030397

P49019	62	>= 1 Zn	0.3917896
P49019	536	O=C-C-N	0.3881414
P49019	599	[#1]-C-C=C-[#1]	0.3835341
P49019	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.3827375
P49019	712	C-C(C)-C(C)-C	0.3818154
P49019	407	O(~C)(~P)	0.3701974
P49019	831	SC1C(Cl)CCCC1	0.3670608
P49019	324	P-P	0.3579619
P49019	634	C-C-C:C-C	0.3575223
P49019	603	C-C:C:C-C	0.3478285
P49019	834	NC1C(Cl)CCCC1	0.3467975
P49019	93	>= 1 Pt	0.3381299
P49019	487	N-C=N-C	0.3336841
P49019	171	>= 5 any ring size 5	0.3265824
P49019	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.3254308
P49019	390	N(~C)(~C)	0.3206924
P49019	586	C-S-C-C-C	0.3199497
P49019	532	S-C:C-[#1]	0.3151453
P49019	380	C(~O)(~O)	0.3051129
P49019	179	>= 1 saturated or aromatic carbon-only ring size 6	0.2933081
P49019	580	O=C-C-C-N	0.2881088
P49019	449	C(-N)(=C)	0.2878514
P49019	752	Clc1cc(Cl)ccc1	0.2818927
P49019	597	O=C-C-C:C	0.2774186
P49019	122	>= 2 any ring size 3	0.2708429
P49019	336	C(~C)(~C)(~C)(~N)	0.2552048
P49019	551	Cl-C-C-O	0.2485502
P49019	830	SC1C(N)CCCC1	0.2389188
P49019	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.2372924
P49019	618	C:C-C-C:C	0.230567
P49019	772	Nc1c(Br)cccc1	0.2038766
P49019	61	>= 1 Cu	0.2022207
P49019	693	O=C-C-C-C-C-O	0.1951051
P49019	583	Cl-C:C-O-C	0.1892617
P49019	20	>= 4 O	0.1871774
P49019	689	O-C-C-C-C-C-C	0.1833909
P49019	34	>= 2 S	0.1830591
P49019	625	O=C-C:C-O	0.1821492
P49019	235	>= 2 saturated or aromatic carbon-only ring size 8	0.181715
P49019	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.1809189
P49019	110	>= 1 Er	0.1784474
P49019	573	O-C-C=C	0.1773878
P49019	356	C(~C)(:C)(:C)	0.1756253
P49019	400	N(~H)(:C)(:C)	0.1737478
P49019	702	O-C-C-C-C-C-N-C	0.169803
P49019	333	C(~C)(~C)(~C)	0.1691527
P49019	531	S-C:C-C	0.1653561
P49019	780	CC1CCC(Cl)CC1	0.165266

P49019	783	OC1CCC(S)CC1	0.1525639
P49019	363	C(~F)(~F)	0.151049
P49019	130	>= 1 saturated or aromatic carbon-only ring size 4	0.1502973
P49019	412	S(~C)(~C)	0.1428962
P49019	442	C(-C)(=N)	0.1384955
P49019	468	O=S-C-N	0.1357737
P49019	404	N(:C)(:C)(:C)	0.1341295
P49019	606	O-C:C-C-C	0.1338889
P49019	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.1335954
P49019	199	>= 4 any ring size 6	0.1329819
P49019	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.132873
P49019	866	OC1C(O)CCC1	0.1327968
P49019	424	N=P	0.1327273
P49019	104	>= 1 Sm	0.1321994
P49019	432	C(-C)(-C)(=O)	0.1320051
P49019	760	Cc1c(Br)cccc1	0.1316235
P49019	137	>= 2 saturated or aromatic carbon-only ring size 4	0.1312948
P49019	85	>= 1 Ba	0.1311899
P49019	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.1307472
P49019	843	CC1CC(Cl)CC1	0.1307087
P49019	213	>= 1 any ring size 7	0.1305481
P49019	518	O=C-N-N	0.1305433
P49019	282	B-Br	0.1304757
P49019	53	>= 1 Sc	0.1299464
P49019	854	NC1CC(N)CC1	0.1298416
P49019	759	Cc1c(Cl)cccc1	0.1296875
P49019	829	SC1C(S)CCCC1	0.1289176
P49019	799	CC1CC(S)CCC1	0.1287314
P49019	347	C(~C)(~H)(~O)(~O)	0.1283519
P49019	325	As-H	0.1275438
P49019	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.1267278
P49019	323	P-H	0.1258724
P49019	629	S-C:C:C-N	0.1258188
P49019	782	OC1CCC(O)CC1	0.1248145
P49019	65	>= 1 As	0.1244157
P49019	762	Oc1c(S)cccc1	0.1241474
P49019	263	Li-H	0.1210967
P49019	44	>= 2 Br	0.1206588
P49019	688	C-C-C-C-C-C-C	0.1203376
P49019	33	>= 1 S	0.1192748
P49019	823	CC1C(Br)CCCC1	0.116847
P49019	84	>= 1 Cs	0.1167807
P49019	441	C(-C)(=C)	0.1164639
P49019	614	C-C-O-C-C	0.1145203
P49019	701	O-C-C-C-C-C(O)-C	0.1134804
P49019	164	>= 4 any ring size 5	0.1130948
P49019	425	P=O	0.1127502
P49019	286	C-O	0.1088973

P49019	681	O-C-C-C-C-O	0.108313
P49019	704	O=C-C-C-C-C-C-C	0.1059298
P49019	63	>= 1 Ga	0.1056482
P49019	374	C(~H)(~H)(~H)	0.1054853
P49019	342	C(~C)(~Cl)	0.104942
P49019	262	>= 4 hetero-aromatic rings	0.1048861
P49019	98	>= 1 Bi	0.1041451
P49019	680	O-C-C-C-C-C	0.1030876
P49019	386	C(:C)(:C)(:N)	0.1018203
P49019	715	Cc1ccc(S)cc1	0.101686
P49019	88	>= 1 Ta	0.1016026
P49019	360	C(~Cl)(~Cl)	0.1015693
P49019	675	Br-C-C-C:C	0.1001511
P49019	795	ClC1CCC(Br)CC1	0.1001145
P49019	123	>= 2 saturated or aromatic carbon-only ring size 3	0.100066
P49019	297	C-Br	0.0993182
P49019	362	C(~Cl)(:C)	0.0992166
P49019	621	N-C:C:C:N	0.099104
P49019	686	O=C-C-C-C-O	0.0990533
P49019	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0988902
P49019	719	Oc1ccc(O)cc1	0.0984775
P49019	465	O=S-C-C	0.0975084
P49019	570	C:C-C-C	0.096255
P49019	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.096153
P49019	405	O(~C)(~C)	0.0959241
P49019	479	S-C-S-C	0.095005
P49019	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0947243
P49019	746	Sc1cc(N)ccc1	0.0942204
P49019	415	Si(~C)(~C)	0.0932888
P49019	56	>= 1 Cr	0.0921504
P49019	409	O(:C)(:C)	0.0920028
P49019	474	S:C:C:N	0.0915317
P49019	96	>= 1 Tl	0.0906209
P49019	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0903018
P49019	267	Li-O	0.0893008
P49019	533	S-C:C-N	0.089243
P49019	718	Cc1ccc(Br)cc1	0.0873585
P49019	10	>= 4 C	0.087097
P49019	443	C(-C)(=O)	0.0870813
P49019	12	>= 16 C	0.0869414
P49019	624	O=C-C:C-N	0.0862154
P49019	357	C(~C)(:C)(:N)	0.0848737
P49019	773	Clc1c(Cl)cccc1	0.0842812
P49019	329	C(~Br)(~H)	0.0833521
P49019	249	>= 1 saturated or aromatic carbon-only ring size 10	0.0819648
P49019	818	CC1C(C)CCCC1	0.0803031
P49019	192	>= 3 any ring size 6	0.0802457
P49019	859	BrC1CC(Br)CC1	0.0799509

P49019	816	ClC1CC(Br)CCC1	0.0797816
P49019	796	BrC1CCC(Br)CC1	0.0779369
P49019	256	>= 1 hetero-aromatic ring	0.0761269
P49019	394	N(~C)(~H)(~N)	0.075692
P49019	345	C(~C)(~H)(~N)	0.0729096
P49019	482	C:N-C:C	0.0729025
P49019	382	C(~O)(:C)(:C)	0.0727947
P49019	855	NC1CC(Cl)CC1	0.0720868
P49019	846	OC1CC(S)CC1	0.0716903
P49019	584	C:C-C=C-C	0.0715983
P49019	740	Oc1cc(O)ccc1	0.071091
P49019	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.0708435
P49019	92	>= 1 Ir	0.0706602
P49019	697	C-C-C-C-C-C(C)-C	0.0704407
P49019	368	C(~H)(~S)	0.0689822
P49019	677	C-C=C-C:C	0.0682277
P49019	733	Brc1ccc(Br)cc1	0.0681349
P49019	644	C-C=N-N-C	0.0678643
P49019	776	CC1CCC(C)CC1	0.067297
P49019	821	CC1C(N)CCCC1	0.0661939
P49019	516	[#1]-C=C-[#1]	0.0645433
P49019	228	>= 1 saturated or aromatic carbon-only ring size 8	0.0636564
P49019	537	O=C-C-O	0.0621121
P49019	308	O-H	0.0620047
P49019	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.0608439
P49019	870	OC1C(Br)CCC1	0.0603808
P49019	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.0590873
P49019	544	O-C:C-O	0.0577412
P49019	255	>= 1 aromatic ring	0.0562234
P49019	287	C-F	0.0556828
P49019	440	C(-C)(-O)(=O)	0.0546366
P49019	785	OC1CCC(Cl)CC1	0.0538185
P49019	691	O-C-C-C-C-C-N	0.0524337
P49019	835	NC1C(Br)CCCC1	0.0516669
P49019	43	>= 1 Br	0.0514732
P49019	38	>= 2 Cl	0.0509678
P49019	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.0508533
P49019	609	Cl-C-C-N-C	0.0507279
P49019	545	N-C:C-C	0.0449678
P49019	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.044368
P49019	444	C(-Cl)(=O)	0.0440457
P49019	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0439654
P49019	649	O=N-C:C-O	0.0439412
P49019	304	N-P	0.0434368
P49019	768	Sc1c(Cl)cccc1	0.0433052
P49019	602	O=C-C-N-C	0.0429804
P49019	234	>= 2 any ring size 8	0.0427991
P49019	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0427926

P49019	87	>= 1 Hf	0.042783
P49019	76	>= 1 Pd	0.0424858
P49019	513	S:C:C-[#1]	0.0424338
P49019	64	>= 1 Ge	0.0423202
P49019	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.0423125
P49019	52	>= 1 Ca	0.0420616
P49019	872	SC1C(N)CCC1	0.0419978
P49019	242	>= 1 saturated or aromatic carbon-only ring size 9	0.0411776
P49019	136	>= 2 any ring size 4	0.0406751
P49019	46	>= 1 I	0.0396443
P49019	665	N-C:C-C-C	0.0394332
P49019	507	C-C-S-C	0.0392027
P49019	754	Brc1cc(Br)ccc1	0.0385242
P49019	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.037022
P49019	129	>= 1 any ring size 4	0.0367264
P49019	739	Cc1cc(Br)ccc1	0.0364082
P49019	692	O=C-C-C-C-C-C	0.0362546
P49019	337	C(~C)(~C)(~C)(~O)	0.0361614
P49019	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.0361001
P49019	385	C(:C)(:C)(:C)	0.0359241
P49019	827	OC1C(Cl)CCCC1	0.0342553
P49019	241	>= 1 any ring size 9	0.033899
P49019	555	N=C-C=C	0.0334207
P49019	841	CC1CC(S)CC1	0.0330509
P49019	13	>= 32 C	0.0327356
P49019	709	C-C(C)-C-C-C	0.0327209
P49019	598	Cl-C:C:C-C	0.0323167
P49019	384	C(:C)(:C)	0.0321999
P49019	103	>= 1 Pm	0.0321708
P49019	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0320453
P49019	763	Oc1c(N)cccc1	0.0319023
P49019	9	>= 2 C	0.0317064
P49019	861	CC1C(O)CCC1	0.0312143
P49019	571	[#1]-C-O-[#1]	0.0307197
P49019	340	C(~C)(~C)(~N)	0.0305392
P49019	352	C(~C)(~O)	0.0305171
P49019	495	C-N-C:C	0.0295577
P49019	74	>= 1 Ru	0.0268274
P49019	395	N(~C)(~O)	0.0267333
P49019	82	>= 1 Te	0.0247979
P49019	811	SC1CC(Br)CCC1	0.0245877
P49019	502	N-C=C-[#1]	0.0236808
P49019	706	O=C-C-C-C-C(=O)-C	0.0236693
P49019	578	C-C:C-C:C	0.0234224
P49019	710	C-C-C(C)-C-C	0.0229097
P49019	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.0226979
P49019	828	OC1C(Br)CCCC1	0.0225283
P49019	471	S:C:C:C	0.0225065

P49019	466	N#C-C=C	0.0224532
P49019	857	ClC1CC(Cl)CC1	0.0219102
P49019	0	>= 4 H	0.0216234
P49019	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.0214085
P49019	730	Nc1ccc(Br)cc1	0.0211397
P49019	698	O-C-C-C-C-C-C-C	0.0211198
P49019	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.0210471
P49019	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.0210385
P49019	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.0210276
P49019	26	>= 1 Na	0.0210128
P49019	787	SC1CCC(S)CC1	0.0209175
P49019	80	>= 1 Sn	0.0207467
P49019	742	Oc1cc(N)ccc1	0.0207117
P49019	320	Si-H	0.020651
P49019	734	Cc1cc(C)ccc1	0.0206447
P49019	344	C(~C)(~H)	0.0205494
P49019	556	C=C-C-C	0.0203762
P49019	279	B-P	0.0197204
P49019	791	NC1CCC(N)CC1	0.0193868
P49019	761	Oc1c(O)cccc1	0.0192651
P49019	484	N-C:N:C	0.0191244
P49019	510	[#1]-N-N-[#1]	0.018656
P49019	682	O-C-C-C-C-N	0.0184623
P49019	848	OC1CC(Cl)CC1	0.018353
P49019	264	Li-Li	0.0183445
P49019	528	[#1]-N-C-[#1]	0.018337
P49019	301	N-O	0.0181144
P49019	454	N(-C)(=O)	0.0180805
P49019	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.0176682
P49019	662	O-C-C-O-C	0.0176204
P49019	576	N=C-C:C-[#1]	0.0169283
P49019	266	Li-C	0.0166528
P49019	593	N-C-C-C-N	0.016619
P49019	265	Li-B	0.0150306
P49019	700	O-C-C-C-C-C-O-C	0.0144887
P49019	661	O-C-O-C-C	0.0142556
P49019	95	>= 1 Hg	0.0140375
P49019	673	O=C-C=C-N	0.0133473
P49019	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0131945
P49019	467	C=N-N-C	0.0127844
P49019	716	Cc1ccc(N)cc1	0.0125014
P49019	779	CC1CCC(N)CC1	0.0123549
P49019	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.0122938
P49019	805	OC1CC(N)CCC1	0.0122321
P49019	862	CC1C(S)CCC1	0.0120025
P49019	771	Nc1c(Cl)cccc1	0.0119689
P49019	289	C-Mg	0.0117186
P49019	306	N-Cl	0.0115688

P49019	257	>= 2 aromatic rings	0.0114921
P49019	431	C(-C)(-C)(=N)	0.0111031
P49019	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0110142
P49019	478	S-C=N-[#1]	0.0109614
P49019	636	C-N-C-N-C	0.0107937
P49019	116	>= 1 saturated or aromatic carbon-only ring size 3	0.0105004
P49019	860	CC1C(C)CCC1	0.0101236
P49019	312	O-Al	0.0098972
P49019	694	O=C-C-C-C-C=O	0.00875
P49019	514	O-N-C-C	0.0086285
P49019	11	>= 8 C	0.0082663
P49019	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.0082627
P49019	765	Oc1c(Br)cccc1	0.0082428
P49019	453	N(-C)(=C)	0.0082214
P49019	387	C(:C)(:N)	0.0080878
P49019	100	>= 1 Ce	0.0080163
P49019	314	O-P	0.0079462
P49019	654	N-C-N-C-C	0.007868
P49019	293	C-S	0.007751
P49019	797	CC1CC(C)CCC1	0.0074885
P49019	748	Sc1cc(Br)ccc1	0.0073985
P49019	460	C-C-C#C	0.0072127
P49019	667	C=C-C-O-[#1]	0.0070722
P49019	36	>= 8 S	0.0070719
P49019	557	N:C-O-[#1]	0.0064016
P49019	647	O=C-N-C-N	0.00572
P49019	853	SC1CC(Br)CC1	0.0052641
P49019	669	Cl-C:C-C=O	0.0050461
P49019	402	N(~O)(:O)	0.0050387
P49019	736	Cc1cc(S)ccc1	0.0050209
P49019	439	C(-C)(-N)(=O)	0.0047979
P49019	299	N-H	0.0045742
P49019	663	O-C-C-O-[#1]	0.0045504
P49019	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0042543
P49019	200	>= 4 saturated or aromatic carbon-only ring size 6	0.004116
P49019	6	>= 1 B	0.0040588
P49019	107	>= 1 Tb	0.0034595
P49019	653	O-C:C:C-O	0.0034074
P49019	178	>= 1 any ring size 6	0.0032602
P49019	812	NC1CC(N)CCC1	0.0031839
P49019	67	>= 1 Kr	0.0027119
P49019	396	N(~C)(:C)	0.0026208
P49019	433	C(-C)(-Cl)(=O)	0.0024594
P49019	150	>= 2 any ring size 5	0.0024494
P49019	503	Cl-C:C-[#1]	0.0024088
P49019	339	C(~C)(~C)(~H)(~O)	0.0023944
P49019	605	O=C-C-O-C	0.0023028
P49019	397	N(~C)(:C)(:C)	0.0022516

P49019	417	C#C	0.00222
P49019	359	C(~C)(:N)(:N)	0.002219
P49019	144	>= 1 saturated or aromatic carbon-only ring size 5	0.0022015
P49019	475	S-C=N-C	0.0021375
P49019	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0021276
P49019	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0020772
P49019	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.0020445
P49019	641	O-C-C-C=C	0.0019253
P49019	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0019223
P49019	601	N-C:C:C-N	0.0018274
P49019	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.0017189
P49019	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.0016848
P49019	679	C-C-C-C-C-C	0.0015744
P49019	546	N-C:C-[#1]	0.0014353
P49019	879	ClC1C(Br)CCC1	0.0012618
P49019	79	>= 1 In	0.0012282
P49019	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.0011832
P49019	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0011089
P49019	450	C(-N)(=N)	0.0009622
P49019	370	C(~H)(:C)	0.00092
P49019	476	C-O-C=C	0.0006968
P49019	435	C(-C)(-H)(=N)	0.0006215
P49019	59	>= 1 Co	0.0005189
P49019	81	>= 1 Sb	0.0005151
P49019	341	C(~C)(~C)(~O)	0.0004391
P49019	515	N-N-C-C	0.000409
P49019	770	Nc1c(N)cccc1	0.000342
P49019	684	O=C-C-C-C-C	0.0002952
P49019	711	C-C(C)(C)-C-C	0.0002933
P49019	569	N-C-C-N	0.0002894
P49019	77	>= 1 Ag	0.0002751
P49019	489	N-C-S-C	0.0002341
P49019	722	Oc1ccc(Cl)cc1	0.0002272
P49019	520	C=C-C:C	0.0002272
P49019	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0002146
P49019	806	OC1CC(Cl)CCC1	0.0001626
P49019	741	Oc1cc(S)ccc1	0.0001437
P49019	804	OC1CC(S)CCC1	0.0001437
P49019	529	Cl-C-C-Cl	0.0001087
P49019	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	6.44E-05
P49019	530	N:C-C:C	6.25E-05
P49019	526	Cl-C:C-Cl	1.39E-05
P49019	630	O-C:C-O-C	5.39E-06
P49019	193	>= 3 saturated or aromatic carbon-only ring size 6	4.48E-06
P49019	864	CC1C(Cl)CCC1	4.72E-09
P49019	874	SC1C(Br)CCC1	3.78E-09
P49019	310	O-Mg	3.39E-09
P49019	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	2.44E-09

P49019	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	1.48E-09
P49019	258	>= 2 hetero-aromatic rings	1.11E-09
P49019	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	1.05E-09
P49019	5	>= 2 Li	8.72E-10
P49019	71	>= 1 Zr	5.41E-10
P49019	54	>= 1 Ti	1.83E-10
P49019	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	1.62E-10
P49019	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	1.29E-11
P49019	32	>= 4 P	-2.72E-10
P49019	317	F-S	-3.89E-10
P49019	269	Li-P	-7.90E-10
P49019	271	Li-Cl	-8.91E-10
P49019	627	O=[As]-C:C:C	-1.04E-09
P49019	90	>= 1 Re	-1.07E-09
P49019	825	OC1C(S)CCCC1	-1.34E-09
P49019	280	B-S	-1.42E-09
P49019	276	B-O	-1.48E-09
P49019	525	[As]-C:C-[#1]	-1.51E-09
P49019	348	C(~C)(~H)(~P)	-1.63E-09
P49019	788	SC1CCC(N)CC1	-2.15E-09
P49019	810	SC1CC(Cl)CCC1	-3.37E-09
P49019	278	B-Si	-3.93E-09
P49019	29	>= 2 Si	-4.68E-09
P49019	414	S(~C)(~O)	-2.57E-06
P49019	322	Si-Cl	-8.12E-06
P49019	418	C=N	-1.30E-05
P49019	610	C-O-C-O-C	-0.000102
P49019	494	O=C-C:N	-0.000224
P49019	445	C(-H)(-N)(=C)	-0.000244
P49019	447	C(-H)(=N)	-0.000246
P49019	294	C-Cl	-0.000259
P49019	248	>= 1 any ring size 10	-0.000303
P49019	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	-0.000332
P49019	416	C=C	-0.000486
P49019	185	>= 2 any ring size 6	-0.000527
P49019	565	C:C-O-C	-0.000558
P49019	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	-0.00058
P49019	406	O(~C)(~H)	-0.000589
P49019	869	OC1C(Cl)CCC1	-0.000593
P49019	16	>= 4 N	-0.000601
P49019	102	>= 1 Nd	-0.00061
P49019	777	CC1CCC(O)CC1	-0.00067
P49019	705	O=C-C-C-C-C(O)-C	-0.000679
P49019	389	C(:N)(:N)	-0.000733
P49019	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	-0.000753
P49019	774	Clc1c(Br)cccc1	-0.000774
P49019	388	C(:C)(:N)(:N)	-0.000821
P49019	509	Br-C:C-C	-0.000824

P49019	469	S-S-C:C	−0.000896
P49019	786	OC1CCC(Br)CC1	−0.000948
P49019	808	SC1CC(S)CCC1	−0.000956
P49019	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.000983
P49019	849	OC1CC(Br)CC1	−0.001006
P49019	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.001233
P49019	89	>= 1 W	−0.001467
P49019	623	O=C-C:C-C	−0.001647
P49019	707	O=C-C-C-C-C(N)-C	−0.001749
P49019	807	OC1CC(Br)CCC1	−0.002298
P49019	350	C(~C)(~I)	−0.002363
P49019	504	N:C:N-C	−0.002445
P49019	724	Sc1ccc(S)cc1	−0.0025
P49019	508	S=C-N-C	−0.002523
P49019	781	CC1CCC(Br)CC1	−0.00258
P49019	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.002633
P49019	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.002707
P49019	290	C-Al	−0.002724
P49019	283	C-H	−0.002791
P49019	749	Nc1cc(N)ccc1	−0.00282
P49019	114	>= 1 U	−0.003112
P49019	378	C(~N)(:C)(:N)	−0.003185
P49019	666	C=C-C-O-C	−0.003218
P49019	745	Sc1cc(S)ccc1	−0.003281
P49019	657	C-N-C:C-C	−0.003539
P49019	2	>= 16 H	−0.003675
P49019	330	C(~Br)(:C)	−0.003724
P49019	651	O-C:C:C-C	−0.003737
P49019	14	>= 1 N	−0.003801
P49019	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.00407
P49019	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.004261
P49019	106	>= 1 Gd	−0.004268
P49019	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.004289
P49019	868	OC1C(N)CCC1	−0.00452
P49019	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.004747
P49019	45	>= 4 Br	−0.004904
P49019	839	CC1CC(C)CC1	−0.004915
P49019	498	O-C=C-C	−0.005168
P49019	778	CC1CCC(S)CC1	−0.005207
P49019	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.005282
P49019	379	C(~N)(:N)	−0.005348
P49019	566	O-C-C-N	−0.005703
P49019	550	Cl-C-C-C	−0.005726
P49019	522	C-N-N-[#1]	−0.006108
P49019	497	O-C:C:N	−0.006284
P49019	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.006399
P49019	429	C(#N)(-C)	−0.006783
P49019	512	C-[As]-O-[#1]	−0.006938

P49019	68	>= 1 Rb	-0.007385
P49019	755	Cc1c(C)cccc1	-0.007539
P49019	295	C-As	-0.007623
P49019	22	>= 16 O	-0.007746
P49019	91	>= 1 Os	-0.008035
P49019	638	O-C-C-C-N	-0.008084
P49019	143	>= 1 any ring size 5	-0.008549
P49019	729	Nc1ccc(Cl)cc1	-0.008599
P49019	542	O-C:C-[#1]	-0.008679
P49019	803	OC1CC(O)CCC1	-0.008994
P49019	94	>= 1 Au	-0.009482
P49019	744	Oc1cc(Br)ccc1	-0.009918
P49019	311	O-Na	-0.009965
P49019	275	B-N	-0.010044
P49019	632	C-C-O-C:C	-0.010279
P49019	491	C-N:C-[#1]	-0.010914
P49019	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.011052
P49019	493	O=C-C:C	-0.01171
P49019	844	CC1CC(Br)CC1	-0.01209
P49019	820	CC1C(S)CCCC1	-0.012144
P49019	622	O=C-O-C:C	-0.012309
P49019	721	Oc1ccc(N)cc1	-0.012311
P49019	270	Li-S	-0.012405
P49019	206	>= 5 any ring size 6	-0.012711
P49019	458	S(-O)(=O)	-0.01315
P49019	490	C-C-C=C	-0.013174
P49019	423	N=O	-0.013212
P49019	462	O-C-C=O	-0.013301
P49019	585	C-C:C-N-C	-0.013406
P49019	408	O(~H)(~S)	-0.013708
P49019	567	O-C-C-O	-0.014
P49019	822	CC1C(Cl)CCCC1	-0.015513
P49019	548	O-C-C:C	-0.015986
P49019	798	CC1CC(O)CCC1	-0.016072
P49019	658	C-C-S-C-C	-0.016475
P49019	383	C(~S)(:C)	-0.016631
P49019	794	ClC1CCC(Cl)CC1	-0.016644
P49019	850	SC1CC(S)CC1	-0.016847
P49019	708	C-C(C)-C-C	-0.01699
P49019	539	N=C-C-[#1]	-0.017731
P49019	470	C:C-C=C	-0.017734
P49019	481	O-S-C:C	-0.018361
P49019	115	>= 1 any ring size 3	-0.018858
P49019	775	Brc1c(Br)cccc1	-0.018924
P49019	626	C-O-C:C-C	-0.019052
P49019	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	-0.019352
P49019	826	OC1C(N)CCCC1	-0.019785
P49019	430	C(-C)(-C)(=C)	-0.02003

P49019	720	Oc1ccc(S)cc1	−0.020058
P49019	837	ClC1C(Br)CCCC1	−0.020454
P49019	272	B-H	−0.02058
P49019	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.020686
P49019	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.020742
P49019	633	N-C-C:C-C	−0.020766
P49019	750	Nc1cc(Cl)ccc1	−0.020966
P49019	315	O-K	−0.021118
P49019	615	N-C-C-O-C	−0.021247
P49019	678	C-C-C=C-C	−0.021514
P49019	351	C(~C)(~N)	−0.021872
P49019	353	C(~C)(~S)	−0.02212
P49019	15	>= 2 N	−0.022385
P49019	764	Oc1c(Cl)cccc1	−0.022867
P49019	358	C(~C)(:N)	−0.023661
P49019	326	As-As	−0.02367
P49019	83	>= 1 Xe	−0.024354
P49019	553	O=C-C=C	−0.024703
P49019	645	O=C-N-C-C	−0.025528
P49019	562	Br-C-C=O	−0.02624
P49019	371	C(~H)(:C)(:C)	−0.027202
P49019	505	Cl-C:C-O	−0.027439
P49019	731	Clc1ccc(Cl)cc1	−0.028187
P49019	660	C-C=C-C-C	−0.028261
P49019	78	>= 1 Cd	−0.028421
P49019	354	C(~C)(~Si)	−0.029585
P49019	438	C(-C)(-N)(=N)	−0.030335
P49019	27	>= 2 Na	−0.030441
P49019	369	C(~H)(~Si)	−0.030617
P49019	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.032539
P49019	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.032573
P49019	305	N-S	−0.032633
P49019	590	C-C:C-O-[#1]	−0.032767
P49019	619	O-C-C=C-C	−0.033727
P49019	640	C=C-C-C-C	−0.034589
P49019	535	O=C-C-C	−0.034595
P49019	554	Br-C-C-C	−0.036068
P49019	588	O=C-C-C=O	−0.036077
P49019	751	Nc1cc(Br)ccc1	−0.03615
P49019	403	N(:C)(:C)	−0.036411
P49019	288	C-Na	−0.036927
P49019	587	N-C:C-O-[#1]	−0.037761
P49019	547	N-C:C-N	−0.037965
P49019	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.038347
P49019	833	NC1C(N)CCCC1	−0.039541
P49019	757	Cc1c(S)cccc1	−0.039749
P49019	25	>= 4 F	−0.040256
P49019	732	Clc1ccc(Br)cc1	−0.040359

P49019	376	C(~N)(:C)	−0.040577
P49019	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.041461
P49019	55	>= 1 V	−0.041478
P49019	39	>= 4 Cl	−0.041728
P49019	758	Cc1c(N)cccc1	−0.042082
P49019	563	O-C-O-C	−0.042701
P49019	112	>= 1 Yb	−0.043075
P49019	819	CC1C(O)CCCC1	−0.043217
P49019	876	NC1C(Cl)CC1	−0.04326
P49019	852	SC1CC(Cl)CC1	−0.043414
P49019	101	>= 1 Pr	−0.043497
P49019	260	>= 3 hetero-aromatic rings	−0.043615
P49019	817	BrC1CC(Br)CCC1	−0.043722
P49019	631	O-C:C-O-[#1]	−0.043861
P49019	3	>= 32 H	−0.043889
P49019	316	F-P	−0.044289
P49019	274	B-C	−0.045733
P49019	436	C(-C)(-H)(=O)	−0.04644
P49019	519	N=C-N-C	−0.04946
P49019	690	O-C-C-C-C-C-O	−0.050347
P49019	268	Li-F	−0.050631
P49019	485	N:C:C:N	−0.051477
P49019	303	N-Si	−0.053167
P49019	541	O-C:C-C	−0.054696
P49019	800	CC1CC(N)CCC1	−0.054819
P49019	581	O=C-C-C-O	−0.055246
P49019	366	C(~H)(~O)	−0.055279
P49019	592	N-C-C-C-C	−0.055333
P49019	437	C(-C)(-N)(=C)	−0.056449
P49019	313	O-Si	−0.056903
P49019	836	ClC1C(Cl)CCCC1	−0.056988
P49019	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.057696
P49019	23	>= 1 F	−0.058748
P49019	635	N-N-C-N-[#1]	−0.060124
P49019	455	N(-O)(=O)	−0.060135
P49019	75	>= 1 Rh	−0.060858
P49019	863	CC1C(N)CCC1	−0.061029
P49019	30	>= 1 P	−0.061599
P49019	343	C(~C)(~Cl)(~H)	−0.061791
P49019	699	O-C-C-C-C-C(C)-C	−0.064417
P49019	69	>= 1 Sr	−0.064824
P49019	594	C-O-C-C=C	−0.064892
P49019	652	O-C:C:C-N	−0.065077
P49019	696	C-C-C-C-C-C-C-C	−0.065607
P49019	832	SC1C(Br)CCCC1	−0.066018
P49019	659	O-C-C-N-C	−0.06635
P49019	670	Br-C:C:C-C	−0.067641
P49019	648	O=N-C:C-N	−0.069076

P49019	411	P(~O)(~O)	-0.07005
P49019	639	O-C-C-C-O	-0.070525
P49019	617	C-C-C-O-[#1]	-0.071191
P49019	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	-0.071274
P49019	70	>= 1 Y	-0.071337
P49019	349	C(~C)(~H)(~S)	-0.071712
P49019	496	N:N-C-[#1]	-0.072355
P49019	685	O=C-C-C-C-N	-0.072623
P49019	824	OC1C(O)CCCC1	-0.073313
P49019	47	>= 2 I	-0.073832
P49019	735	Cc1cc(O)ccc1	-0.074641
P49019	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	-0.076363
P49019	506	C-C:N:C	-0.076436
P49019	642	O-C-C-C=O	-0.076699
P49019	381	C(~O)(:C)	-0.077033
P49019	421	C=S	-0.078304
P49019	767	Sc1c(N)cccc1	-0.079301
P49019	877	NC1C(Br)CCC1	-0.079921
P49019	410	P(~C)(~C)	-0.079965
P49019	296	C-Se	-0.080639
P49019	611	N-C-C-N-C	-0.080914
P49019	672	O=C-C=C-[#1]	-0.082232
P49019	426	P=P	-0.082561
P49019	523	N:C:C-C	-0.084511
P49019	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	-0.08458
P49019	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	-0.084856
P49019	428	C(#C)(-H)	-0.086081
P49019	809	SC1CC(N)CCC1	-0.086231
P49019	18	>= 1 O	-0.087167
P49019	456	P(-O)(=O)	-0.087471
P49019	801	CC1CC(Cl)CCC1	-0.088254
P49019	575	O-C-C:C-O	-0.08851
P49019	1	>= 8 H	-0.088566
P49019	723	Oc1ccc(Br)cc1	-0.08887
P49019	319	Al-Cl	-0.091386
P49019	50	>= 1 Mg	-0.093182
P49019	628	C-N-C-C:C	-0.093185
P49019	713	Cc1ccc(C)cc1	-0.093847
P49019	419	C#N	-0.094699
P49019	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	-0.094723
P49019	858	ClC1CC(Br)CC1	-0.094896
P49019	792	NC1CCC(Cl)CC1	-0.096796
P49019	48	>= 4 I	-0.097668
P49019	511	S=C-N-[#1]	-0.098086
P49019	604	C-O-C-C:C	-0.098669
P49019	501	Cl-C:C-C	-0.098828
P49019	434	C(-C)(-H)(=C)	-0.099856
P49019	747	Sc1cc(Cl)ccc1	-0.100614

P49019	461	O-C-C=N	−0.100922
P49019	40	>= 8 Cl	−0.102091
P49019	300	N-N	−0.102268
P49019	847	OC1CC(N)CC1	−0.102692
P49019	72	>= 1 Nb	−0.103523
P49019	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.106984
P49019	472	C:N:C-C	−0.108146
P49019	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.109362
P49019	24	>= 2 F	−0.113155
P49019	367	C(~H)(~O)(~O)	−0.113909
P49019	17	>= 8 N	−0.114492
P49019	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.114631
P49019	302	N-F	−0.116023
P49019	743	Oc1cc(Cl)ccc1	−0.116629
P49019	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.117575
P49019	838	BrC1C(Br)CCCC1	−0.118901
P49019	73	>= 1 Mo	−0.12
P49019	643	[#1]-C-C-N-[#1]	−0.121431
P49019	220	>= 2 any ring size 7	−0.123113
P49019	413	S(~C)(~H)	−0.124142
P49019	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.124532
P49019	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.125195
P49019	574	O-C-C:C-C	−0.126073
P49019	227	>= 1 any ring size 8	−0.126747
P49019	616	C:C:N:N:C	−0.128616
P49019	99	>= 1 La	−0.128904
P49019	753	Clc1cc(Br)ccc1	−0.129215
P49019	291	C-Si	−0.129345
P49019	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.131121
P49019	726	Sc1ccc(Cl)cc1	−0.131243
P49019	157	>= 3 any ring size 5	−0.132516
P49019	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.132556
P49019	871	SC1C(S)CCC1	−0.132609
P49019	393	N(~C)(~H)	−0.133147
P49019	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.133202
P49019	307	N-Br	−0.133226
P49019	784	OC1CCC(N)CC1	−0.133243
P49019	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.133258
P49019	332	C(~C)(~C)	−0.133397
P49019	60	>= 1 Ni	−0.133618
P49019	259	>= 3 aromatic rings	−0.133702
P49019	108	>= 1 Dy	−0.134085
P49019	452	C(-O)(=O)	−0.134222
P49019	591	Cl-C-C-C-C	−0.138276
P49019	668	C-C:C-C-C	−0.142968
P49019	327	C(~Br)(~C)	−0.143948
P49019	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.145624
P49019	346	C(~C)(~H)(~O)	−0.146775

P49019	582	C-C-C-C-C	−0.148558
P49019	637	O-C-C-C-C	−0.149514
P49019	664	C-C=C-C=C	−0.153149
P49019	37	>= 1 Cl	−0.161483
P49019	756	Cc1c(O)cccc1	−0.16162
P49019	298	C-I	−0.166167
P49019	373	C(~H)(:N)	−0.167095
P49019	446	C(-H)(=C)	−0.168525
P49019	334	C(~C)(~C)(~C)(~C)	−0.177347
P49019	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.196901
P49019	717	Cc1ccc(Cl)cc1	−0.200031
P49019	521	C:N-C-[#1]	−0.20493
P49019	398	N(~H)(~N)	−0.205209
P49019	273	B-B	−0.207539
P49019	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.208428
P49019	613	C-N-C-C-C	−0.214022
P49019	335	C(~C)(~C)(~C)(~H)	−0.219049
P49019	766	Sc1c(S)cccc1	−0.220944
P49019	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.227055
P49019	281	B-Cl	−0.232248
P49019	793	NC1CCC(Br)CC1	−0.235919
P49019	549	N-C-C:C	−0.247511
P49019	486	N-C:N:N	−0.252413
P49019	867	OC1C(S)CCC1	−0.254779
P49019	738	Cc1cc(Cl)ccc1	−0.257597
P49019	338	C(~C)(~C)(~H)(~N)	−0.262107
P49019	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.277086
P49019	595	C:C-C-C-C	−0.278955
P49019	457	S(-C)(=O)	−0.285772
P49019	463	N:C-S-[#1]	−0.307493
P49019	19	>= 2 O	−0.310139
P49019	365	C(~H)(~N)	−0.328029
P49019	321	Si-Si	−0.339043
P49019	473	S-C:N:C	−0.348322
P49019	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.35245
P49019	646	O=C-N-C-[#1]	−0.355355
P49019	538	N=C-C-C	−0.363682
P49019	57	>= 1 Mn	−0.368651
P49019	488	N-C=N-[#1]	−0.378541
P49019	448	C(-H)(=O)	−0.38211
P49019	612	N-C-O-C-C	−0.386526
P49019	683	N-C-C-C-C-C	−0.408482
P49019	579	O=C-C-C-C	−0.424504
P49019	727	Sc1ccc(Br)cc1	−0.428046
P49019	480	C:S:C-C	−0.429542
P49019	364	C(~F)(:C)	−0.432707
P49019	105	>= 1 Eu	−0.434729
P49019	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.439677

P49019	28	>= 1 Si	−0.444472
P49019	815	ClC1CC(Cl)CCC1	−0.445505
P49019	568	N#C-C-C	−0.453036
P49019	377	C(~N)(:C)(:C)	−0.471799
P49019	392	N(~C)(~C)(~H)	−0.486998
P49019	318	Al-H	−0.488206
P49019	789	SC1CCC(Cl)CC1	−0.506764
P49019	561	Cl-C-C=O	−0.511017
P49019	589	C-C:C-O-C	−0.516312
P49019	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.529895
P49019	451	C(-N)(=O)	−0.534701
P49019	7	>= 2 B	−0.538949
P49019	328	C(~Br)(~C)(~C)	−0.539398
P49019	687	O=C-C-C-C=O	−0.542629
P49019	577	C:C-N-C:C	−0.550811
P49019	873	SC1C(Cl)CCC1	−0.564583
P49019	517	N-N-C-N	−0.574537
P49019	813	NC1CC(Cl)CCC1	−0.585918
P49019	58	>= 1 Fe	−0.590721
P49019	851	SC1CC(N)CC1	−0.591693
P49019	375	C(~N)(~N)	−0.597562
P49019	527	C:C:N-[#1]	−0.610362
P49019	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.619083
P49019	552	C:C-C:C	−0.637856
P49019	728	Nc1ccc(N)cc1	−0.68411
P49019	620	C:C-O-C-C	−0.690266
P49019	31	>= 2 P	−0.69578
P49019	655	O-C-C-C:C	−0.70691
P49019	492	N-C:O:C	−0.712992
P49019	534	S-C:C-O	−0.731836
P49019	8	>= 4 B	−0.748932
P49019	600	N-C:C:C-C	−0.765765
P49019	97	>= 1 Pb	−0.770749
P49019	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.789469
P49019	608	C-C-C-C:C	−0.793756
P49019	361	C(~Cl)(~H)	−0.795604
P49019	42	>= 2 K	−0.807453
P49019	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.822038
P49019	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.824604
P49019	572	N:C:N:C	−0.844438
P49019	769	Sc1c(Br)cccc1	−0.845914
P49019	109	>= 1 Ho	−0.892825
P49019	427	C(#C)(-C)	−0.915799
P49019	875	NC1C(N)CCC1	−0.915919
P49019	49	>= 1 Be	−0.916799
P49019	477	N-N-C:C	−0.936215
P49019	4	>= 1 Li	−0.940811
P49019	842	CC1CC(N)CC1	−1.014489

P49019	331	C(~Br)(:N)	-1.042319
P49019	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-1.128585
P49019	41	>= 1 K	-1.136463
P49019	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	-1.19559
P49019	66	>= 1 Se	-1.21105
P49019	391	N(~C)(~C)(~C)	-1.223254
P49019	499	N-C:C:N	-1.223507
P49019	372	C(~H)(:C)(:N)	-1.26543
P49019	292	C-P	-1.283935
P49019	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	-1.331368
P49019	420	C=O	-1.39333
P49019	401	N(~O)(~O)	-1.410329
P49019	880	BrC1C(Br)CCC1	-1.472602
P49019	86	>= 1 Lu	-1.489015
P49019	524	C-C=C-C	-1.841403
P49019	878	ClC1C(Cl)CCC1	-1.860881
P49019	284	C-C	-2.021383
P49019	261	>= 4 aromatic rings	-2.325148
P49019	790	SC1CCC(Br)CC1	-2.781955

Fingerprints（continued)

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0.822789	-0.0001275
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0.726262	-3.65E-09
0.686231	9.58E-06
0.682163	1.64E-06
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0.625292	3.40E-10
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0.596315	9.91E-05
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0.476476	2.69E-06
0.476421	-2.78E-05
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0.473136	-0.0003567
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0.452827	-0.0004601
0.43737	-1.73E-09
0.425646	2.49E-09
0.424739	2.84E-09
0.40458	5.93E-10
0.403583	-0.0005428

0.39179	1.12E-10
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0.383488	4.60E-05
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0.367061	3.06E-09
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0.320752	-5.96E-05
0.320033	-8.38E-05
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0.255206	-1.02E-06
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0.230784	-0.0002165
0.20389	-1.38E-05
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0.022528	4.12E-11
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0.021028	-0.0006522
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0.01926	5.39E-06
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0.018365	-0.0002847
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-8.12E-06	-1.17E-09
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-0.00096	-6.90E-10
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-0.13362	1.03E-09
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-0.13409	1.27E-09
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-0.13782	-0.0004551
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-0.16197	0.00035462
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-0.19985	-0.0001834
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-0.20843	-1.24E-09
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-0.21831	-0.0007376
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-0.23225	-1.06E-09
-0.23593	7.32E-06
-0.24748	-3.61E-05
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-0.25478	-1.29E-11
-0.25783	0.00023762
-0.262	-0.0001035
-0.27709	-2.13E-09
-0.27958	0.0006281
-0.28577	-2.57E-06
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-0.31044	0.00030324
-0.32792	-0.0001046
-0.33904	-1.17E-09
-0.34814	-0.0001798
-0.35245	-3.92E-11
-0.35475	-0.0006014
-0.36367	-1.30E-05
-0.36865	-1.44E-10
-0.37819	-0.0003524
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-0.38662	9.88E-05
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-0.42471	0.00020488
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-0.43238	-0.0003242
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-0.43968	-2.91E-09

-0.44447	-2.14E-09
-0.44549	-1.10E-05
-0.45283	-0.0002012
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-0.48722	0.00022107
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-0.50676	-1.58E-09
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-0.57493	0.00038875
-0.58593	1.08E-05
-0.59072	-1.38E-09
-0.59169	-2.04E-09
-0.59754	-2.46E-05
-0.60968	-0.000681
-0.61908	-2.67E-09
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-0.68411	-1.86E-09
-0.68971	-0.000552
-0.69578	-6.23E-10
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-0.71275	-0.0002398
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-0.74893	-2.14E-09
-0.76535	-0.0004184
-0.77075	-2.86E-09
-0.78947	1.25E-09
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-0.79581	0.00020473
-0.80745	4.51E-09
-0.82204	9.41E-10
-0.82461	4.48E-06
-0.84407	-0.0003707
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-0.9168	3.78E-10
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-1.01468	0.00019419

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-1.12858	-1.96E-10
-1.13646	1.07E-09
-1.19559	-3.04E-10
-1.21105	-3.11E-09
-1.2232	-5.52E-05
-1.22332	-0.0001832
-1.26519	-0.0002445
-1.28394	-5.37E-09
-1.33137	-7.98E-10
-1.39295	-0.0003772
-1.41031	-1.64E-05
-1.4726	-5.43E-09
-1.48902	-2.04E-09
-1.84061	-0.0007966
-1.86088	-4.51E-09
-2.02088	-0.0005052
-2.32515	-1.32E-10
-2.78195	-3.70E-09

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q9BXC0	453	N(-C)(=C)	2.1764661
Q9BXC0	428	C(#C)(-H)	0.6808973
Q9BXC0	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.6764152
Q9BXC0	717	Cc1ccc(Cl)cc1	0.4029469
Q9BXC0	637	O-C-C-C-C	0.3711044
Q9BXC0	780	CC1CCC(Cl)CC1	0.370168
Q9BXC0	822	CC1C(Cl)CCCC1	0.3375893
Q9BXC0	438	C(-C)(-N)(=N)	0.2987208
Q9BXC0	761	Oc1c(O)cccc1	0.2933891
Q9BXC0	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.2792292
Q9BXC0	449	C(-N)(=C)	0.2777311
Q9BXC0	392	N(~C)(~C)(~H)	0.2616051
Q9BXC0	389	C(:N)(:N)	0.2614982
Q9BXC0	59	>= 1 Co	0.2607886
Q9BXC0	787	SC1CCC(S)CC1	0.2606873
Q9BXC0	725	Sc1ccc(N)cc1	0.260333
Q9BXC0	783	OC1CCC(S)CC1	0.2598284
Q9BXC0	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.2585246
Q9BXC0	86	>= 1 Lu	0.257742
Q9BXC0	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.2576761
Q9BXC0	326	As-As	0.2576364
Q9BXC0	769	Sc1c(Br)cccc1	0.2575976
Q9BXC0	320	Si-H	0.2564594
Q9BXC0	448	C(-H)(=O)	0.2554851
Q9BXC0	61	>= 1 Cu	0.2551714
Q9BXC0	27	>= 2 Na	0.2542853
Q9BXC0	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.2541355
Q9BXC0	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.2501118
Q9BXC0	759	Cc1c(Cl)cccc1	0.2469288
Q9BXC0	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.2465049
Q9BXC0	302	N-F	0.245797
Q9BXC0	727	Sc1ccc(Br)cc1	0.2439459
Q9BXC0	103	>= 1 Pm	0.2430496
Q9BXC0	266	Li-C	0.242711
Q9BXC0	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.2404367
Q9BXC0	570	C:C-C-C	0.2389085
Q9BXC0	76	>= 1 Pd	0.2379381
Q9BXC0	92	>= 1 Ir	0.2354189
Q9BXC0	870	OC1C(Br)CCC1	0.232421
Q9BXC0	719	Oc1ccc(O)cc1	0.2322894
Q9BXC0	474	S:C:C:N	0.2304578
Q9BXC0	771	Nc1c(Cl)cccc1	0.2289374
Q9BXC0	41	>= 1 K	0.2264256
Q9BXC0	684	O=C-C-C-C-C	0.2262317
Q9BXC0	689	O-C-C-C-C-C-C	0.2248283
Q9BXC0	806	OC1CC(Cl)CCC1	0.2242643

Q9BXC0	60	>= 1 Ni	0.2227913
Q9BXC0	788	SC1CCC(N)CC1	0.2198713
Q9BXC0	459	S(=O)(=O)	0.2178096
Q9BXC0	300	N-N	0.2167608
Q9BXC0	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.2147652
Q9BXC0	385	C(:C)(:C)(:C)	0.2141493
Q9BXC0	371	C(~H)(:C)(:C)	0.2137247
Q9BXC0	454	N(-C)(=O)	0.2125194
Q9BXC0	530	N:C-C:C	0.2124451
Q9BXC0	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.2112441
Q9BXC0	80	>= 1 Sn	0.2088735
Q9BXC0	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.2031641
Q9BXC0	742	Oc1cc(N)ccc1	0.1984301
Q9BXC0	335	C(~C)(~C)(~C)(~H)	0.1964377
Q9BXC0	322	Si-Cl	0.1956366
Q9BXC0	489	N-C-S-C	0.1897915
Q9BXC0	67	>= 1 Kr	0.186938
Q9BXC0	737	Cc1cc(N)ccc1	0.1862776
Q9BXC0	609	Cl-C-C-N-C	0.1848155
Q9BXC0	656	C-C-N-C-C	0.1844933
Q9BXC0	104	>= 1 Sm	0.1815265
Q9BXC0	349	C(~C)(~H)(~S)	0.1805829
Q9BXC0	37	>= 1 Cl	0.1787765
Q9BXC0	307	N-Br	0.177107
Q9BXC0	643	[#1]-C-C-N-[#1]	0.1763714
Q9BXC0	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.1757327
Q9BXC0	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.1708043
Q9BXC0	750	Nc1cc(Cl)ccc1	0.1682948
Q9BXC0	471	S:C:C:C	0.1673549
Q9BXC0	249	>= 1 saturated or aromatic carbon-only ring size 10	0.1650692
Q9BXC0	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.1611362
Q9BXC0	414	S(~C)(~O)	0.159937
Q9BXC0	355	C(~C)(:C)	0.1572512
Q9BXC0	817	BrC1CC(Br)CCC1	0.1548357
Q9BXC0	626	C-O-C:C-C	0.1546986
Q9BXC0	467	C=N-N-C	0.1537647
Q9BXC0	399	N(~H)(:C)	0.1518113
Q9BXC0	507	C-C-S-C	0.1516015
Q9BXC0	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.1511374
Q9BXC0	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.1492428
Q9BXC0	721	Oc1ccc(N)cc1	0.1452196
Q9BXC0	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.1371521
Q9BXC0	675	Br-C-C-C:C	0.1360866
Q9BXC0	834	NC1C(Cl)CCCC1	0.1355603
Q9BXC0	744	Oc1cc(Br)ccc1	0.1352078
Q9BXC0	24	>= 2 F	0.1350434
Q9BXC0	164	>= 4 any ring size 5	0.1345416
Q9BXC0	859	BrC1CC(Br)CC1	0.1333638

Q9BXC0	634	C-C-C:C-C	0.1311963
Q9BXC0	793	NC1CCC(Br)CC1	0.1311766
Q9BXC0	432	C(-C)(-C)(=O)	0.1300223
Q9BXC0	539	N=C-C-[#1]	0.1292049
Q9BXC0	38	>= 2 Cl	0.1279306
Q9BXC0	29	>= 2 Si	0.1271396
Q9BXC0	680	O-C-C-C-C-C	0.1267114
Q9BXC0	671	O=C-C=C-C	0.1174859
Q9BXC0	543	O-C:C-N	0.116699
Q9BXC0	758	Cc1c(N)cccc1	0.1164001
Q9BXC0	734	Cc1cc(C)ccc1	0.1160435
Q9BXC0	377	C(~N)(:C)(:C)	0.1141779
Q9BXC0	593	N-C-C-C-N	0.1136091
Q9BXC0	544	O-C:C-O	0.1134998
Q9BXC0	801	CC1CC(Cl)CCC1	0.1134762
Q9BXC0	601	N-C:C:C-N	0.1134011
Q9BXC0	129	>= 1 any ring size 4	0.1129619
Q9BXC0	800	CC1CC(N)CCC1	0.1123828
Q9BXC0	810	SC1CC(Cl)CCC1	0.1110343
Q9BXC0	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.1092123
Q9BXC0	227	>= 1 any ring size 8	0.1080899
Q9BXC0	757	Cc1c(S)cccc1	0.1073191
Q9BXC0	357	C(~C)(:C)(:N)	0.1049823
Q9BXC0	566	O-C-C-N	0.1042601
Q9BXC0	612	N-C-O-C-C	0.1036301
Q9BXC0	137	>= 2 saturated or aromatic carbon-only ring size 4	0.1024145
Q9BXC0	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0989096
Q9BXC0	464	N-C-C=C	0.097275
Q9BXC0	505	Cl-C:C-O	0.0962092
Q9BXC0	437	C(-C)(-N)(=C)	0.0955269
Q9BXC0	113	>= 1 Tc	0.0934126
Q9BXC0	87	>= 1 Hf	0.0928592
Q9BXC0	858	ClC1CC(Br)CC1	0.0927985
Q9BXC0	814	NC1CC(Br)CCC1	0.0925116
Q9BXC0	313	O-Si	0.0924268
Q9BXC0	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.0917247
Q9BXC0	382	C(~O)(:C)(:C)	0.0910371
Q9BXC0	720	Oc1ccc(S)cc1	0.0904678
Q9BXC0	488	N-C=N-[#1]	0.0902479
Q9BXC0	508	S=C-N-C	0.090217
Q9BXC0	285	C-N	0.0897874
Q9BXC0	260	>= 3 hetero-aromatic rings	0.0896852
Q9BXC0	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.0895751
Q9BXC0	422	N=N	0.0875098
Q9BXC0	281	B-Cl	0.08526
Q9BXC0	602	O=C-C-N-C	0.0850662
Q9BXC0	784	OC1CCC(N)CC1	0.0847347
Q9BXC0	524	C-C=C-C	0.0846143

Q9BXC0	348	C(~C)(~H)(~P)	0.0845143
Q9BXC0	450	C(-N)(=N)	0.0845017
Q9BXC0	786	OC1CCC(Br)CC1	0.0844187
Q9BXC0	636	C-N-C-N-C	0.0836211
Q9BXC0	333	C(~C)(~C)(~C)	0.082925
Q9BXC0	809	SC1CC(N)CCC1	0.0826511
Q9BXC0	475	S-C=N-C	0.0819943
Q9BXC0	547	N-C:C-N	0.0819485
Q9BXC0	590	C-C:C-O-[#1]	0.080151
Q9BXC0	376	C(~N)(:C)	0.080046
Q9BXC0	565	C:C-O-C	0.0785512
Q9BXC0	545	N-C:C-C	0.0779178
Q9BXC0	826	OC1C(N)CCCC1	0.0774179
Q9BXC0	433	C(-C)(-Cl)(=O)	0.0772797
Q9BXC0	404	N(:C)(:C)(:C)	0.0753379
Q9BXC0	50	>= 1 Mg	0.074921
Q9BXC0	309	O-O	0.0746357
Q9BXC0	777	CC1CCC(O)CC1	0.0728987
Q9BXC0	673	O=C-C=C-N	0.0721959
Q9BXC0	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0716407
Q9BXC0	779	CC1CCC(N)CC1	0.0714863
Q9BXC0	42	>= 2 K	0.0707631
Q9BXC0	329	C(~Br)(~H)	0.0695029
Q9BXC0	716	Cc1ccc(N)cc1	0.0670464
Q9BXC0	871	SC1C(S)CCC1	0.066397
Q9BXC0	692	O=C-C-C-C-C-C	0.0662765
Q9BXC0	596	N=C-N-C-C	0.06602
Q9BXC0	381	C(~O)(:C)	0.0645177
Q9BXC0	383	C(~S)(:C)	0.0644193
Q9BXC0	569	N-C-C-N	0.0641398
Q9BXC0	659	O-C-C-N-C	0.0639806
Q9BXC0	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.063635
Q9BXC0	55	>= 1 V	0.0611793
Q9BXC0	343	C(~C)(~Cl)(~H)	0.0585458
Q9BXC0	529	Cl-C-C-Cl	0.0575752
Q9BXC0	99	>= 1 La	0.0569739
Q9BXC0	456	P(-O)(=O)	0.0561183
Q9BXC0	752	Clc1cc(Cl)ccc1	0.055905
Q9BXC0	798	CC1CC(O)CCC1	0.0549994
Q9BXC0	555	N=C-C=C	0.0535543
Q9BXC0	367	C(~H)(~O)(~O)	0.0521353
Q9BXC0	778	CC1CCC(S)CC1	0.0512714
Q9BXC0	824	OC1C(O)CCCC1	0.05117
Q9BXC0	686	O=C-C-C-C-O	0.0480926
Q9BXC0	372	C(~H)(:C)(:N)	0.0479098
Q9BXC0	672	O=C-C=C-[#1]	0.0468725
Q9BXC0	242	>= 1 saturated or aromatic carbon-only ring size 9	0.0454105
Q9BXC0	579	O=C-C-C-C	0.0446694

Q9BXC0	703	O-C-C-C-C-C(N)-C	0.0443694
Q9BXC0	17	>= 8 N	0.0439791
Q9BXC0	1	>= 8 H	0.0421739
Q9BXC0	418	C=N	0.0417625
Q9BXC0	470	C:C-C=C	0.0411883
Q9BXC0	289	C-Mg	0.0411114
Q9BXC0	576	N=C-C:C-[#1]	0.0410267
Q9BXC0	794	ClC1CCC(Cl)CC1	0.0408112
Q9BXC0	697	C-C-C-C-C-C(C)-C	0.0402449
Q9BXC0	553	O=C-C=C	0.0395414
Q9BXC0	451	C(-N)(=O)	0.0390632
Q9BXC0	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.0389206
Q9BXC0	88	>= 1 Ta	0.0380741
Q9BXC0	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.037835
Q9BXC0	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.0377158
Q9BXC0	271	Li-Cl	0.0376599
Q9BXC0	325	As-H	0.037559
Q9BXC0	654	N-C-N-C-C	0.0374364
Q9BXC0	662	O-C-C-O-C	0.0363273
Q9BXC0	297	C-Br	0.0361383
Q9BXC0	255	>= 1 aromatic ring	0.0361092
Q9BXC0	518	O=C-N-N	0.0355921
Q9BXC0	457	S(-C)(=O)	0.0352266
Q9BXC0	340	C(~C)(~C)(~N)	0.0351319
Q9BXC0	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0348066
Q9BXC0	455	N(-O)(=O)	0.0345557
Q9BXC0	11	>= 8 C	0.0343041
Q9BXC0	525	[As]-C:C-[#1]	0.0339167
Q9BXC0	314	O-P	0.0336916
Q9BXC0	661	O-C-O-C-C	0.0335375
Q9BXC0	872	SC1C(N)CCC1	0.0328583
Q9BXC0	652	O-C:C:C-N	0.0324483
Q9BXC0	504	N:C:N-C	0.0324236
Q9BXC0	439	C(-C)(-N)(=O)	0.0322532
Q9BXC0	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0321467
Q9BXC0	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.0319975
Q9BXC0	600	N-C:C:C-C	0.0309165
Q9BXC0	71	>= 1 Zr	0.0307804
Q9BXC0	493	O=C-C:C	0.0307137
Q9BXC0	660	C-C=C-C-C	0.0299126
Q9BXC0	863	CC1C(N)CCC1	0.0293722
Q9BXC0	269	Li-P	0.0284729
Q9BXC0	213	>= 1 any ring size 7	0.028416
Q9BXC0	685	O=C-C-C-C-N	0.0283731
Q9BXC0	393	N(~C)(~H)	0.0277033
Q9BXC0	844	CC1CC(Br)CC1	0.0273673
Q9BXC0	708	C-C(C)-C-C	0.0262454
Q9BXC0	429	C(#N)(-C)	0.0260134

Q9BXC0	732	Clc1ccc(Br)cc1	0.0258289
Q9BXC0	394	N(~C)(~H)(~N)	0.0248522
Q9BXC0	546	N-C:C-[#1]	0.0246415
Q9BXC0	405	O(~C)(~C)	0.0243828
Q9BXC0	77	>= 1 Ag	0.0242962
Q9BXC0	79	>= 1 In	0.0240385
Q9BXC0	85	>= 1 Ba	0.0239453
Q9BXC0	39	>= 4 Cl	0.0238946
Q9BXC0	877	NC1C(Br)CCC1	0.0238661
Q9BXC0	830	SC1C(N)CCCC1	0.0237997
Q9BXC0	10	>= 4 C	0.0235244
Q9BXC0	270	Li-S	0.0231267
Q9BXC0	540	C-N-C-[#1]	0.0230162
Q9BXC0	730	Nc1ccc(Br)cc1	0.0217334
Q9BXC0	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0213931
Q9BXC0	400	N(~H)(:C)(:C)	0.0213166
Q9BXC0	419	C#N	0.0212151
Q9BXC0	533	S-C:C-N	0.0211533
Q9BXC0	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0209922
Q9BXC0	328	C(~Br)(~C)(~C)	0.0202232
Q9BXC0	378	C(~N)(:C)(:N)	0.0197973
Q9BXC0	532	S-C:C-[#1]	0.0191467
Q9BXC0	751	Nc1cc(Br)ccc1	0.0188178
Q9BXC0	841	CC1CC(S)CC1	0.0185884
Q9BXC0	687	O=C-C-C-C=O	0.0185205
Q9BXC0	670	Br-C:C-C	0.0182993
Q9BXC0	262	>= 4 hetero-aromatic rings	0.0182943
Q9BXC0	388	C(:C)(:N)(:N)	0.0177181
Q9BXC0	14	>= 1 N	0.0177013
Q9BXC0	427	C(#C)(-C)	0.0176503
Q9BXC0	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0172227
Q9BXC0	486	N-C:N:N	0.0166225
Q9BXC0	395	N(~C)(~O)	0.0163367
Q9BXC0	386	C(:C)(:C)(:N)	0.0162257
Q9BXC0	417	C#C	0.0162057
Q9BXC0	30	>= 1 P	0.0158931
Q9BXC0	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.0155424
Q9BXC0	331	C(~Br)(:N)	0.0154785
Q9BXC0	234	>= 2 any ring size 8	0.0154002
Q9BXC0	327	C(~Br)(~C)	0.0151521
Q9BXC0	850	SC1CC(S)CC1	0.014954
Q9BXC0	62	>= 1 Zn	0.0148643
Q9BXC0	491	C-N:C-[#1]	0.0148477
Q9BXC0	358	C(~C)(:N)	0.0147814
Q9BXC0	484	N-C:N:C	0.014579
Q9BXC0	442	C(-C)(=N)	0.0145278
Q9BXC0	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0143335
Q9BXC0	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0143293

Q9BXC0	773	Clc1c(Cl)cccc1	0.0142829
Q9BXC0	538	N=C-C-C	0.0139418
Q9BXC0	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.013779
Q9BXC0	864	CC1C(Cl)CCC1	0.0136533
Q9BXC0	855	NC1CC(Cl)CC1	0.0133552
Q9BXC0	51	>= 1 Al	0.0131208
Q9BXC0	767	Sc1c(N)cccc1	0.0129279
Q9BXC0	75	>= 1 Rh	0.0129242
Q9BXC0	816	ClC1CC(Br)CCC1	0.0127665
Q9BXC0	324	P-P	0.0126014
Q9BXC0	678	C-C-C=C-C	0.0125782
Q9BXC0	835	NC1C(Br)CCCC1	0.012304
Q9BXC0	531	S-C:C-C	0.01228
Q9BXC0	292	C-P	0.0122561
Q9BXC0	36	>= 8 S	0.0120505
Q9BXC0	396	N(~C)(:C)	0.0119912
Q9BXC0	485	N:C:C:N	0.0119394
Q9BXC0	509	Br-C:C-C	0.011548
Q9BXC0	54	>= 1 Ti	0.011335
Q9BXC0	53	>= 1 Sc	0.0112807
Q9BXC0	435	C(-C)(-H)(=N)	0.0109544
Q9BXC0	25	>= 4 F	0.0105241
Q9BXC0	621	N-C:C:C:N	0.0104988
Q9BXC0	361	C(~Cl)(~H)	0.0102424
Q9BXC0	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.0101471
Q9BXC0	665	N-C:C-C-C	0.0101447
Q9BXC0	263	Li-H	0.0100498
Q9BXC0	387	C(:C)(:N)	0.0096001
Q9BXC0	683	N-C-C-C-C-C	0.0093774
Q9BXC0	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0093248
Q9BXC0	583	Cl-C:C-O-C	0.0092925
Q9BXC0	101	>= 1 Pr	0.0091146
Q9BXC0	702	O-C-C-C-C-C-N-C	0.009092
Q9BXC0	640	C=C-C-C-C	0.0090053
Q9BXC0	490	C-C-C=C	0.0089365
Q9BXC0	473	S-C:N:C	0.0088038
Q9BXC0	390	N(~C)(~C)	0.0086939
Q9BXC0	495	C-N-C:C	0.0086513
Q9BXC0	568	N#C-C-C	0.0085911
Q9BXC0	403	N(:C)(:C)	0.0084449
Q9BXC0	765	Oc1c(Br)cccc1	0.0080602
Q9BXC0	82	>= 1 Te	0.0079391
Q9BXC0	410	P(~C)(~C)	0.0078618
Q9BXC0	472	C:N:C-C	0.0077665
Q9BXC0	445	C(-H)(-N)(=C)	0.0076372
Q9BXC0	628	C-N-C-C:C	0.0074461
Q9BXC0	869	OC1C(Cl)CCC1	0.0072108
Q9BXC0	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0071064

Q9BXC0	551	Cl-C-C-O	0.0070525
Q9BXC0	838	BrC1C(Br)CCCC1	0.0069891
Q9BXC0	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0068099
Q9BXC0	96	>= 1 Tl	0.0064247
Q9BXC0	49	>= 1 Be	0.006417
Q9BXC0	28	>= 1 Si	0.0063507
Q9BXC0	360	C(~Cl)(~Cl)	0.0059181
Q9BXC0	713	Cc1ccc(C)cc1	0.0057056
Q9BXC0	776	CC1CCC(C)CC1	0.0056584
Q9BXC0	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.0056103
Q9BXC0	4	>= 1 Li	0.0056054
Q9BXC0	487	N-C=N-C	0.0054945
Q9BXC0	549	N-C-C:C	0.0054575
Q9BXC0	444	C(-Cl)(=O)	0.0053861
Q9BXC0	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0053858
Q9BXC0	304	N-P	0.0053194
Q9BXC0	733	Brc1ccc(Br)cc1	0.005269
Q9BXC0	7	>= 2 B	0.0051935
Q9BXC0	458	S(-O)(=O)	0.0050977
Q9BXC0	644	C-C=N-N-C	0.0050314
Q9BXC0	536	O=C-C-N	0.0050214
Q9BXC0	463	N:C-S-[#1]	0.0047715
Q9BXC0	851	SC1CC(N)CC1	0.0045327
Q9BXC0	468	O=S-C-N	0.0043871
Q9BXC0	819	CC1C(O)CCCC1	0.0043022
Q9BXC0	620	C:C-O-C-C	0.0041741
Q9BXC0	248	>= 1 any ring size 10	0.0041586
Q9BXC0	879	ClC1C(Br)CCC1	0.0041223
Q9BXC0	321	Si-Si	0.0039991
Q9BXC0	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.0039147
Q9BXC0	336	C(~C)(~C)(~C)(~N)	0.0038944
Q9BXC0	764	Oc1c(Cl)cccc1	0.003708
Q9BXC0	878	ClC1C(Cl)CCC1	0.0036984
Q9BXC0	630	O-C:C-O-C	0.0035035
Q9BXC0	312	O-Al	0.0033393
Q9BXC0	572	N:C:N:C	0.0032723
Q9BXC0	391	N(~C)(~C)(~C)	0.0032623
Q9BXC0	105	>= 1 Eu	0.0032254
Q9BXC0	446	C(-H)(=C)	0.0029969
Q9BXC0	273	B-B	0.0028326
Q9BXC0	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.0028206
Q9BXC0	748	Sc1cc(Br)ccc1	0.0028164
Q9BXC0	280	B-S	0.0027716
Q9BXC0	107	>= 1 Tb	0.0027446
Q9BXC0	303	N-Si	0.0027055
Q9BXC0	58	>= 1 Fe	0.0026353
Q9BXC0	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0026247
Q9BXC0	496	N:N-C-[#1]	0.0025633

Q9BXC0	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.0025628
Q9BXC0	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.0025106
Q9BXC0	43	>= 1 Br	0.0025044
Q9BXC0	812	NC1CC(N)CCC1	0.0024368
Q9BXC0	722	Oc1ccc(Cl)cc1	0.0024008
Q9BXC0	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0023707
Q9BXC0	592	N-C-C-C-C	0.0022522
Q9BXC0	728	Nc1ccc(N)cc1	0.0022081
Q9BXC0	35	>= 4 S	0.0022046
Q9BXC0	705	O=C-C-C-C-C(O)-C	0.0021753
Q9BXC0	804	OC1CC(S)CCC1	0.0021323
Q9BXC0	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0020905
Q9BXC0	65	>= 1 As	0.0020764
Q9BXC0	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.0020681
Q9BXC0	267	Li-O	0.0020446
Q9BXC0	402	N(~O)(:O)	0.0020045
Q9BXC0	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.0019349
Q9BXC0	698	O-C-C-C-C-C-C-C	0.0017679
Q9BXC0	261	>= 4 aromatic rings	0.0016816
Q9BXC0	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0016012
Q9BXC0	500	C-S-C:C	0.0015006
Q9BXC0	781	CC1CCC(Br)CC1	0.0014749
Q9BXC0	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.0014701
Q9BXC0	334	C(~C)(~C)(~C)(~C)	0.0014129
Q9BXC0	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0013838
Q9BXC0	241	>= 1 any ring size 9	0.0013648
Q9BXC0	811	SC1CC(Br)CCC1	0.0013298
Q9BXC0	369	C(~H)(~Si)	0.0012496
Q9BXC0	766	Sc1c(S)cccc1	0.0011804
Q9BXC0	70	>= 1 Y	0.0010977
Q9BXC0	200	>= 4 saturated or aromatic carbon-only ring size 6	0.0010423
Q9BXC0	256	>= 1 hetero-aromatic ring	0.000984
Q9BXC0	736	Cc1cc(S)ccc1	0.0009651
Q9BXC0	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.0009522
Q9BXC0	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.000892
Q9BXC0	843	CC1CC(Cl)CC1	0.0008492
Q9BXC0	880	BrC1C(Br)CCC1	0.0007753
Q9BXC0	785	OC1CCC(Cl)CC1	0.0007383
Q9BXC0	411	P(~O)(~O)	0.0007281
Q9BXC0	832	SC1C(Br)CCCC1	0.000699
Q9BXC0	825	OC1C(S)CCCC1	0.0006825
Q9BXC0	648	O=N-C:C-N	0.0005279
Q9BXC0	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0004771
Q9BXC0	171	>= 5 any ring size 5	0.0004147
Q9BXC0	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.0004081
Q9BXC0	64	>= 1 Ge	0.0004064
Q9BXC0	799	CC1CC(S)CCC1	0.0003857
Q9BXC0	556	C=C-C-C	0.0003805

Q9BXC0	68	>= 1 Rb	0.0003085
Q9BXC0	586	C-S-C-C-C	0.0002991
Q9BXC0	707	O=C-C-C-C-C(N)-C	0.0002671
Q9BXC0	264	Li-Li	0.0002239
Q9BXC0	265	Li-B	0.0002067
Q9BXC0	136	>= 2 any ring size 4	0.0002051
Q9BXC0	695	O=C-C-C-C-C-N	5.31E-05
Q9BXC0	279	B-P	1.53E-05
Q9BXC0	66	>= 1 Se	2.29E-06
Q9BXC0	723	Oc1ccc(Br)cc1	-3.90E-05
Q9BXC0	753	Clc1cc(Br)ccc1	-8.14E-05
Q9BXC0	8	>= 4 B	-8.53E-05
Q9BXC0	73	>= 1 Mo	-0.000128
Q9BXC0	74	>= 1 Ru	-0.000136
Q9BXC0	874	SC1C(Br)CCC1	-0.000201
Q9BXC0	272	B-H	-0.000259
Q9BXC0	317	F-S	-0.000268
Q9BXC0	828	OC1C(Br)CCCC1	-0.000302
Q9BXC0	22	>= 16 O	-0.000336
Q9BXC0	789	SC1CCC(Cl)CC1	-0.000352
Q9BXC0	100	>= 1 Ce	-0.000394
Q9BXC0	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	-0.000451
Q9BXC0	6	>= 1 B	-0.000477
Q9BXC0	726	Sc1ccc(Cl)cc1	-0.000497
Q9BXC0	645	O=C-N-C-C	-0.000578
Q9BXC0	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	-0.000579
Q9BXC0	873	SC1C(Cl)CCC1	-0.000609
Q9BXC0	338	C(~C)(~C)(~H)(~N)	-0.000662
Q9BXC0	351	C(~C)(~N)	-0.000679
Q9BXC0	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	-0.000707
Q9BXC0	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	-0.000714
Q9BXC0	598	Cl-C:C:C-C	-0.000738
Q9BXC0	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	-0.000799
Q9BXC0	102	>= 1 Nd	-0.000819
Q9BXC0	296	C-Se	-0.00088
Q9BXC0	91	>= 1 Os	-0.000881
Q9BXC0	856	NC1CC(Br)CC1	-0.001008
Q9BXC0	310	O-Mg	-0.001076
Q9BXC0	511	S=C-N-[#1]	-0.00108
Q9BXC0	865	CC1C(Br)CCC1	-0.001165
Q9BXC0	316	F-P	-0.001167
Q9BXC0	479	S-C-S-C	-0.001183
Q9BXC0	235	>= 2 saturated or aromatic carbon-only ring size 8	-0.001187
Q9BXC0	257	>= 2 aromatic rings	-0.001345
Q9BXC0	749	Nc1cc(N)ccc1	-0.001357
Q9BXC0	108	>= 1 Dy	-0.001421
Q9BXC0	290	C-Al	-0.001485
Q9BXC0	57	>= 1 Mn	-0.001495

Q9BXC0	93	>= 1 Pt	-0.001497
Q9BXC0	714	Cc1ccc(O)cc1	-0.001518
Q9BXC0	562	Br-C-C=O	-0.001586
Q9BXC0	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.001592
Q9BXC0	831	SC1C(Cl)CCCC1	-0.001652
Q9BXC0	795	ClC1CCC(Br)CC1	-0.00168
Q9BXC0	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-0.001693
Q9BXC0	561	Cl-C-C=O	-0.001842
Q9BXC0	277	B-F	-0.001968
Q9BXC0	78	>= 1 Cd	-0.00206
Q9BXC0	591	Cl-C-C-C-C	-0.002123
Q9BXC0	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-0.002214
Q9BXC0	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	-0.002286
Q9BXC0	852	SC1CC(Cl)CC1	-0.002289
Q9BXC0	84	>= 1 Cs	-0.002315
Q9BXC0	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	-0.002463
Q9BXC0	700	O-C-C-C-C-C-O-C	-0.002494
Q9BXC0	848	OC1CC(Cl)CC1	-0.00251
Q9BXC0	754	Brc1cc(Br)ccc1	-0.002613
Q9BXC0	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	-0.002708
Q9BXC0	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	-0.002763
Q9BXC0	527	C:C:N-[#1]	-0.002764
Q9BXC0	613	C-N-C-C-C	-0.002793
Q9BXC0	691	O-C-C-C-C-C-N	-0.002803
Q9BXC0	478	S-C=N-[#1]	-0.002813
Q9BXC0	510	[#1]-N-N-[#1]	-0.002853
Q9BXC0	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	-0.002931
Q9BXC0	668	C-C:C-C-C	-0.003144
Q9BXC0	681	O-C-C-C-C-O	-0.003188
Q9BXC0	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	-0.003368
Q9BXC0	123	>= 2 saturated or aromatic carbon-only ring size 3	-0.003425
Q9BXC0	424	N=P	-0.003438
Q9BXC0	791	NC1CCC(N)CC1	-0.003464
Q9BXC0	746	Sc1cc(N)ccc1	-0.003518
Q9BXC0	207	>= 5 saturated or aromatic carbon-only ring size 6	-0.003907
Q9BXC0	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.004074
Q9BXC0	605	O=C-C-O-C	-0.004116
Q9BXC0	323	P-H	-0.004125
Q9BXC0	365	C(~H)(~N)	-0.004189
Q9BXC0	44	>= 2 Br	-0.004225
Q9BXC0	743	Oc1cc(Cl)ccc1	-0.004276
Q9BXC0	268	Li-F	-0.004304
Q9BXC0	476	C-O-C=C	-0.004428
Q9BXC0	46	>= 1 I	-0.00447
Q9BXC0	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	-0.004628
Q9BXC0	762	Oc1c(S)cccc1	-0.004773
Q9BXC0	709	C-C(C)-C-C-C	-0.004864
Q9BXC0	301	N-O	-0.004899

Q9BXC0	667	C=C-C-O-[#1]	−0.004914
Q9BXC0	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.004916
Q9BXC0	354	C(~C)(~Si)	−0.005159
Q9BXC0	514	O-N-C-C	−0.005508
Q9BXC0	706	O=C-C-C-C-C(=O)-C	−0.00565
Q9BXC0	775	Brc1c(Br)cccc1	−0.0057
Q9BXC0	466	N#C-C=C	−0.005722
Q9BXC0	618	C:C-C-C:C	−0.005782
Q9BXC0	718	Cc1ccc(Br)cc1	−0.005951
Q9BXC0	90	>= 1 Re	−0.006103
Q9BXC0	494	O=C-C:N	−0.006248
Q9BXC0	122	>= 2 any ring size 3	−0.006313
Q9BXC0	492	N-C:O:C	−0.006606
Q9BXC0	693	O=C-C-C-C-C-O	−0.006634
Q9BXC0	497	O-C:C:N	−0.006729
Q9BXC0	876	NC1C(Cl)CC1	−0.007069
Q9BXC0	436	C(-C)(-H)(=O)	−0.007177
Q9BXC0	610	C-O-C-O-C	−0.007525
Q9BXC0	469	S-S-C:C	−0.007561
Q9BXC0	12	>= 16 C	−0.007739
Q9BXC0	0	>= 4 H	−0.007867
Q9BXC0	829	SC1C(S)CCCC1	−0.008214
Q9BXC0	625	O=C-C:C-O	−0.008673
Q9BXC0	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.008871
Q9BXC0	735	Cc1cc(O)ccc1	−0.008905
Q9BXC0	106	>= 1 Gd	−0.008939
Q9BXC0	578	C-C:C-C:C	−0.009003
Q9BXC0	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.009005
Q9BXC0	580	O=C-C-C-N	−0.009029
Q9BXC0	554	Br-C-C-C	−0.009032
Q9BXC0	379	C(~N)(:N)	−0.009237
Q9BXC0	853	SC1CC(Br)CC1	−0.009281
Q9BXC0	694	O=C-C-C-C-C=O	−0.009594
Q9BXC0	291	C-Si	−0.009786
Q9BXC0	21	>= 8 O	−0.009816
Q9BXC0	711	C-C(C)(C)-C-C	−0.009834
Q9BXC0	315	O-K	−0.009847
Q9BXC0	178	>= 1 any ring size 6	−0.009873
Q9BXC0	770	Nc1c(N)cccc1	−0.009879
Q9BXC0	409	O(:C)(:C)	−0.009902
Q9BXC0	651	O-C:C:C-C	−0.009982
Q9BXC0	696	C-C-C-C-C-C-C-C	−0.009992
Q9BXC0	588	O=C-C-C=O	−0.010216
Q9BXC0	815	ClC1CC(Cl)CCC1	−0.010648
Q9BXC0	603	C-C:C:C-C	−0.010798
Q9BXC0	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.010873
Q9BXC0	364	C(~F)(:C)	−0.01095
Q9BXC0	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.01104

Q9BXC0	866	OC1C(O)CCC1	−0.011409
Q9BXC0	513	S:C:C-[#1]	−0.011441
Q9BXC0	564	C=C-C=C	−0.011643
Q9BXC0	635	N-N-C-N-[#1]	−0.011789
Q9BXC0	34	>= 2 S	−0.012393
Q9BXC0	745	Sc1cc(S)ccc1	−0.012761
Q9BXC0	608	C-C-C-C:C	−0.012921
Q9BXC0	534	S-C:C-O	−0.012976
Q9BXC0	423	N=O	−0.013053
Q9BXC0	72	>= 1 Nb	−0.013061
Q9BXC0	401	N(~O)(~O)	−0.013171
Q9BXC0	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.013266
Q9BXC0	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.013273
Q9BXC0	31	>= 2 P	−0.013361
Q9BXC0	857	ClC1CC(Cl)CC1	−0.013374
Q9BXC0	520	C=C-C:C	−0.013686
Q9BXC0	860	CC1C(C)CCC1	−0.013869
Q9BXC0	558	O=N-C:C	−0.01404
Q9BXC0	282	B-Br	−0.014516
Q9BXC0	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.01452
Q9BXC0	666	C=C-C-O-C	−0.014807
Q9BXC0	629	S-C:C:C-N	−0.015133
Q9BXC0	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−0.015256
Q9BXC0	109	>= 1 Ho	−0.015307
Q9BXC0	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.015781
Q9BXC0	577	C:C-N-C:C	−0.016142
Q9BXC0	584	C:C-C=C-C	−0.016337
Q9BXC0	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.017056
Q9BXC0	415	Si(~C)(~C)	−0.017208
Q9BXC0	710	C-C-C(C)-C-C	−0.017213
Q9BXC0	574	O-C-C:C-C	−0.01758
Q9BXC0	594	C-O-C-C=C	−0.01769
Q9BXC0	642	O-C-C-C=O	−0.017985
Q9BXC0	521	C:N-C-[#1]	−0.018
Q9BXC0	842	CC1CC(N)CC1	−0.018291
Q9BXC0	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.018551
Q9BXC0	526	Cl-C:C-Cl	−0.018871
Q9BXC0	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.01892
Q9BXC0	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.019173
Q9BXC0	32	>= 4 P	−0.019216
Q9BXC0	646	O=C-N-C-[#1]	−0.019677
Q9BXC0	699	O-C-C-C-C-C(C)-C	−0.019797
Q9BXC0	421	C=S	−0.020315
Q9BXC0	616	C:C:N:N:C	−0.020643
Q9BXC0	522	C-N-N-[#1]	−0.021317
Q9BXC0	498	O-C=C-C	−0.021534
Q9BXC0	425	P=O	−0.021776
Q9BXC0	658	C-C-S-C-C	−0.022268

Q9BXC0	373	C(~H)(:N)	-0.022355
Q9BXC0	368	C(~H)(~S)	-0.022569
Q9BXC0	756	Cc1c(O)cccc1	-0.022621
Q9BXC0	151	>= 2 saturated or aromatic carbon-only ring size 5	-0.022805
Q9BXC0	447	C(-H)(=N)	-0.023524
Q9BXC0	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	-0.023901
Q9BXC0	501	Cl-C:C-C	-0.024359
Q9BXC0	295	C-As	-0.024747
Q9BXC0	157	>= 3 any ring size 5	-0.02548
Q9BXC0	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	-0.025598
Q9BXC0	158	>= 3 saturated or aromatic carbon-only ring size 5	-0.02568
Q9BXC0	712	C-C(C)-C(C)-C	-0.0258
Q9BXC0	581	O=C-C-C-O	-0.026496
Q9BXC0	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.026631
Q9BXC0	867	OC1C(S)CCC1	-0.026742
Q9BXC0	33	>= 1 S	-0.02679
Q9BXC0	81	>= 1 Sb	-0.027314
Q9BXC0	747	Sc1cc(Cl)ccc1	-0.027601
Q9BXC0	192	>= 3 any ring size 6	-0.027885
Q9BXC0	542	O-C:C-[#1]	-0.027965
Q9BXC0	13	>= 32 C	-0.028455
Q9BXC0	617	C-C-C-O-[#1]	-0.029435
Q9BXC0	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	-0.029515
Q9BXC0	875	NC1C(N)CCC1	-0.030527
Q9BXC0	790	SC1CCC(Br)CC1	-0.030844
Q9BXC0	845	OC1CC(O)CC1	-0.030944
Q9BXC0	632	C-C-O-C:C	-0.031448
Q9BXC0	374	C(~H)(~H)(~H)	-0.031571
Q9BXC0	669	Cl-C:C-C=O	-0.032983
Q9BXC0	330	C(~Br)(:C)	-0.0331
Q9BXC0	52	>= 1 Ca	-0.033764
Q9BXC0	837	ClC1C(Br)CCCC1	-0.03391
Q9BXC0	861	CC1C(O)CCC1	-0.034249
Q9BXC0	318	Al-H	-0.034408
Q9BXC0	430	C(-C)(-C)(=C)	-0.034723
Q9BXC0	116	>= 1 saturated or aromatic carbon-only ring size 3	-0.034859
Q9BXC0	833	NC1C(N)CCCC1	-0.035351
Q9BXC0	363	C(~F)(~F)	-0.035667
Q9BXC0	288	C-Na	-0.036822
Q9BXC0	56	>= 1 Cr	-0.037264
Q9BXC0	502	N-C=C-[#1]	-0.037316
Q9BXC0	619	O-C-C=C-C	-0.037878
Q9BXC0	407	O(~C)(~P)	-0.038373
Q9BXC0	641	O-C-C-C=C	-0.039006
Q9BXC0	293	C-S	-0.03901
Q9BXC0	597	O=C-C-C:C	-0.039662
Q9BXC0	47	>= 2 I	-0.040357
Q9BXC0	563	O-C-O-C	-0.040784

Q9BXC0	347	C(~C)(~H)(~O)(~O)	-0.041135
Q9BXC0	214	>= 1 saturated or aromatic carbon-only ring size 7	-0.041282
Q9BXC0	821	CC1C(N)CCCC1	-0.041287
Q9BXC0	350	C(~C)(~I)	-0.042065
Q9BXC0	595	C:C-C-C-C	-0.043066
Q9BXC0	481	O-S-C:C	-0.043819
Q9BXC0	95	>= 1 Hg	-0.044308
Q9BXC0	186	>= 2 saturated or aromatic carbon-only ring size 6	-0.044311
Q9BXC0	362	C(~Cl)(:C)	-0.044332
Q9BXC0	23	>= 1 F	-0.044621
Q9BXC0	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	-0.04486
Q9BXC0	276	B-O	-0.046046
Q9BXC0	573	O-C-C=C	-0.046476
Q9BXC0	840	CC1CC(O)CC1	-0.046654
Q9BXC0	112	>= 1 Yb	-0.047033
Q9BXC0	259	>= 3 aromatic rings	-0.047694
Q9BXC0	664	C-C=C-C=C	-0.048144
Q9BXC0	557	N:C-O-[#1]	-0.048934
Q9BXC0	412	S(~C)(~C)	-0.04928
Q9BXC0	622	O=C-O-C:C	-0.049326
Q9BXC0	589	C-C:C-O-C	-0.049876
Q9BXC0	20	>= 4 O	-0.05085
Q9BXC0	110	>= 1 Er	-0.051142
Q9BXC0	541	O-C:C-C	-0.051431
Q9BXC0	623	O=C-C:C-C	-0.052395
Q9BXC0	818	CC1C(C)CCCC1	-0.052558
Q9BXC0	820	CC1C(S)CCCC1	-0.053471
Q9BXC0	655	O-C-C-C:C	-0.053614
Q9BXC0	849	OC1CC(Br)CC1	-0.05493
Q9BXC0	199	>= 4 any ring size 6	-0.055793
Q9BXC0	19	>= 2 O	-0.05611
Q9BXC0	582	C-C-C-C-C	-0.056515
Q9BXC0	715	Cc1ccc(S)cc1	-0.056602
Q9BXC0	548	O-C-C:C	-0.056636
Q9BXC0	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	-0.057298
Q9BXC0	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	-0.060135
Q9BXC0	738	Cc1cc(Cl)ccc1	-0.061839
Q9BXC0	345	C(~C)(~H)(~N)	-0.06325
Q9BXC0	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	-0.065863
Q9BXC0	657	C-N-C:C-C	-0.066103
Q9BXC0	287	C-F	-0.06631
Q9BXC0	854	NC1CC(N)CC1	-0.066372
Q9BXC0	796	BrC1CCC(Br)CC1	-0.066672
Q9BXC0	729	Nc1ccc(Cl)cc1	-0.066879
Q9BXC0	2	>= 16 H	-0.066988
Q9BXC0	638	O-C-C-C-N	-0.067858
Q9BXC0	366	C(~H)(~O)	-0.069023
Q9BXC0	599	[#1]-C-C=C-[#1]	-0.069886

Q9BXC0	356	C(~C)(:C)(:C)	−0.070585
Q9BXC0	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.072086
Q9BXC0	97	>= 1 Pb	−0.072341
Q9BXC0	89	>= 1 W	−0.073369
Q9BXC0	813	NC1CC(Cl)CCC1	−0.074273
Q9BXC0	384	C(:C)(:C)	−0.074915
Q9BXC0	397	N(~C)(:C)(:C)	−0.075308
Q9BXC0	299	N-H	−0.075707
Q9BXC0	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.077101
Q9BXC0	587	N-C:C-O-[#1]	−0.077655
Q9BXC0	552	C:C-C:C	−0.080712
Q9BXC0	803	OC1CC(O)CCC1	−0.082065
Q9BXC0	650	O=C-N-C=O	−0.082436
Q9BXC0	220	>= 2 any ring size 7	−0.083982
Q9BXC0	627	O=[As]-C:C:C	−0.084014
Q9BXC0	774	Clc1c(Br)cccc1	−0.084069
Q9BXC0	868	OC1C(N)CCC1	−0.086453
Q9BXC0	16	>= 4 N	−0.089515
Q9BXC0	615	N-C-C-O-C	−0.089589
Q9BXC0	275	B-N	−0.089603
Q9BXC0	45	>= 4 Br	−0.089604
Q9BXC0	98	>= 1 Bi	−0.089738
Q9BXC0	836	ClC1C(Cl)CCCC1	−0.089838
Q9BXC0	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.08991
Q9BXC0	649	O=N-C:C-O	−0.090024
Q9BXC0	69	>= 1 Sr	−0.090288
Q9BXC0	306	N-Cl	−0.091255
Q9BXC0	339	C(~C)(~C)(~H)(~O)	−0.091631
Q9BXC0	465	O=S-C-C	−0.092061
Q9BXC0	688	C-C-C-C-C-C-C	−0.094715
Q9BXC0	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.09604
Q9BXC0	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.096472
Q9BXC0	571	[#1]-C-O-[#1]	−0.098115
Q9BXC0	185	>= 2 any ring size 6	−0.098396
Q9BXC0	676	N#C-C-C-C	−0.098608
Q9BXC0	416	C=C	−0.099955
Q9BXC0	679	C-C-C-C-C-C	−0.10308
Q9BXC0	839	CC1CC(C)CC1	−0.107063
Q9BXC0	792	NC1CCC(Cl)CC1	−0.107533
Q9BXC0	704	O=C-C-C-C-C-C-C	−0.108712
Q9BXC0	731	Clc1ccc(Cl)cc1	−0.111072
Q9BXC0	604	C-O-C-C:C	−0.111266
Q9BXC0	337	C(~C)(~C)(~C)(~O)	−0.111548
Q9BXC0	460	C-C-C#C	−0.116616
Q9BXC0	701	O-C-C-C-C-C(O)-C	−0.116629
Q9BXC0	477	N-N-C:C	−0.117098
Q9BXC0	639	O-C-C-C-O	−0.117335
Q9BXC0	406	O(~C)(~H)	−0.118638

Q9BXC0	3	>= 32 H	-0.118646
Q9BXC0	258	>= 2 hetero-aromatic rings	-0.120255
Q9BXC0	550	Cl-C-C-C	-0.124946
Q9BXC0	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	-0.132883
Q9BXC0	653	O-C:C:C-O	-0.135284
Q9BXC0	690	O-C-C-C-C-C-O	-0.136698
Q9BXC0	760	Cc1c(Br)cccc1	-0.138129
Q9BXC0	380	C(~O)(~O)	-0.138208
Q9BXC0	308	O-H	-0.139979
Q9BXC0	575	O-C-C:C-O	-0.141181
Q9BXC0	611	N-C-C-N-C	-0.143895
Q9BXC0	298	C-I	-0.14647
Q9BXC0	802	CC1CC(Br)CCC1	-0.1465
Q9BXC0	5	>= 2 Li	-0.146701
Q9BXC0	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	-0.147419
Q9BXC0	370	C(~H)(:C)	-0.147761
Q9BXC0	346	C(~C)(~H)(~O)	-0.149172
Q9BXC0	341	C(~C)(~C)(~O)	-0.149906
Q9BXC0	633	N-C-C:C-C	-0.151692
Q9BXC0	375	C(~N)(~N)	-0.153492
Q9BXC0	461	O-C-C=N	-0.154863
Q9BXC0	503	Cl-C:C-[#1]	-0.159362
Q9BXC0	624	O=C-C:C-N	-0.16065
Q9BXC0	359	C(~C)(:N)(:N)	-0.165784
Q9BXC0	115	>= 1 any ring size 3	-0.165913
Q9BXC0	40	>= 8 Cl	-0.166889
Q9BXC0	823	CC1C(Br)CCCC1	-0.167368
Q9BXC0	805	OC1CC(N)CCC1	-0.167801
Q9BXC0	647	O=C-N-C-N	-0.16815
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Q9BXC0	682	O-C-C-C-C-N	-0.180663
Q9BXC0	441	C(-C)(=C)	-0.182308
Q9BXC0	607	N-C-C-C:C	-0.184027
Q9BXC0	674	N-C-N-C:C	-0.185751
Q9BXC0	353	C(~C)(~S)	-0.187733
Q9BXC0	274	B-C	-0.188561
Q9BXC0	480	C:S:C-C	-0.191501
Q9BXC0	512	C-[As]-O-[#1]	-0.194214
Q9BXC0	772	Nc1c(Br)cccc1	-0.198441
Q9BXC0	398	N(~H)(~N)	-0.198703
Q9BXC0	528	[#1]-N-C-[#1]	-0.199445
Q9BXC0	413	S(~C)(~H)	-0.201451
Q9BXC0	26	>= 1 Na	-0.20635
Q9BXC0	228	>= 1 saturated or aromatic carbon-only ring size 8	-0.206886
Q9BXC0	677	C-C=C-C:C	-0.210701
Q9BXC0	724	Sc1ccc(S)cc1	-0.2108
Q9BXC0	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	-0.2131
Q9BXC0	150	>= 2 any ring size 5	-0.213315

Q9BXC0	499	N-C:C:N	-0.215029
Q9BXC0	294	C-Cl	-0.216911
Q9BXC0	111	>= 1 Tm	-0.220989
Q9BXC0	515	N-N-C-C	-0.221751
Q9BXC0	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	-0.222472
Q9BXC0	143	>= 1 any ring size 5	-0.223256
Q9BXC0	482	C:N-C:C	-0.224207
Q9BXC0	847	OC1CC(N)CC1	-0.224508
Q9BXC0	319	Al-Cl	-0.224835
Q9BXC0	506	C-C:N:C	-0.224931
Q9BXC0	431	C(-C)(-C)(=N)	-0.225352
Q9BXC0	434	C(-C)(-H)(=C)	-0.225466
Q9BXC0	483	N-S-C:C	-0.228933
Q9BXC0	342	C(~C)(~Cl)	-0.23096
Q9BXC0	560	N-C-N-C	-0.231153
Q9BXC0	739	Cc1cc(Br)ccc1	-0.232871
Q9BXC0	862	CC1C(S)CCC1	-0.233111
Q9BXC0	15	>= 2 N	-0.233714
Q9BXC0	585	C-C:C-N-C	-0.235033
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Q9BXC0	408	O(~H)(~S)	-0.242436
Q9BXC0	517	N-N-C-N	-0.245461
Q9BXC0	631	O-C:C-O-[#1]	-0.247682
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Q9BXC0	768	Sc1c(Cl)cccc1	-0.248486
Q9BXC0	808	SC1CC(S)CCC1	-0.248585
Q9BXC0	452	C(-O)(=O)	-0.249029
Q9BXC0	426	P=P	-0.251711
Q9BXC0	827	OC1C(Cl)CCCC1	-0.251755
Q9BXC0	94	>= 1 Au	-0.254557
Q9BXC0	63	>= 1 Ga	-0.255005
Q9BXC0	782	OC1CCC(O)CC1	-0.255872
Q9BXC0	305	N-S	-0.256336
Q9BXC0	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	-0.256634
Q9BXC0	48	>= 4 I	-0.257701
Q9BXC0	83	>= 1 Xe	-0.259949
Q9BXC0	206	>= 5 any ring size 6	-0.260138
Q9BXC0	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	-0.260191
Q9BXC0	284	C-C	-0.260312
Q9BXC0	846	OC1CC(S)CC1	-0.263089
Q9BXC0	567	O-C-C-O	-0.270699
Q9BXC0	797	CC1CC(C)CCC1	-0.278045
Q9BXC0	763	Oc1c(N)cccc1	-0.283855
Q9BXC0	535	O=C-C-C	-0.283998
Q9BXC0	606	O-C:C-C-C	-0.284617
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Q9BXC0	462	O-C-C=O	-0.313235
Q9BXC0	443	C(-C)(=O)	-0.313263
Q9BXC0	283	C-H	-0.318853
Q9BXC0	344	C(~C)(~H)	-0.319291
Q9BXC0	352	C(~C)(~O)	-0.32739
Q9BXC0	332	C(~C)(~C)	-0.327978
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Q9BXC0	9	>= 2 C	-0.337322
Q9BXC0	18	>= 1 O	-0.341491
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Q9BXC0	440	C(-C)(-O)(=O)	-0.355435
Q9BXC0	537	O=C-C-O	-0.359748
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Q9BXC0	740	Oc1cc(O)ccc1	-0.412936
Q9BXC0	114	>= 1 U	-0.445102
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Fingerprints（continued)

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Data S1. Ranking of importance of substructure features from Pubchem Fingerpı

GPCR ID	Bit Posit	Bit Substructure	W	P
O95838	756	Cc1c(O)cccc1	2.6739905	2.6737528
O95838	779	CC1CCC(N)CC1	2.2091756	2.2088255
O95838	649	O=N-C:C-O	2.1223161	2.1228171
O95838	684	O=C-C-C-C-C	2.0573518	2.057352
O95838	100	>= 1 Ce	2.0509729	2.0509729
O95838	696	C-C-C-C-C-C-C-C	1.9035488	1.9036891
O95838	538	N=C-C-C	1.8489898	1.8490991
O95838	261	>= 4 aromatic rings	1.8286286	1.8286286
O95838	320	Si-H	1.7415014	1.7415015
O95838	871	SC1C(S)CCC1	1.6909633	1.6909633
O95838	55	>= 1 V	1.62744	1.6274401
O95838	76	>= 1 Pd	1.6129342	1.6129342
O95838	635	N-N-C-N-[#1]	1.5690502	1.5692868
O95838	200	>= 4 saturated or aromatic carbon-only ring size 6	1.5492592	1.5492593
O95838	510	[#1]-N-N-[#1]	1.5457996	1.5458868
O95838	626	C-O-C:C-C	1.5284141	1.5283163
O95838	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	1.518078	1.5180781
O95838	278	B-Si	1.5128115	1.5128116
O95838	398	N(~H)(~N)	1.49784	1.4978417
O95838	553	O=C-C=C	1.4441838	1.4441674
O95838	570	C:C-C-C	1.4069941	1.4072592
O95838	516	[#1]-C=C-[#1]	1.3940429	1.3942943
O95838	702	O-C-C-C-C-C-N-C	1.349306	1.3491559
O95838	567	O-C-C-O	1.3313332	1.3313889
O95838	540	C-N-C-[#1]	1.2842893	1.2844547
O95838	301	N-O	1.2399821	1.2399494
O95838	98	>= 1 Bi	1.2363634	1.2363633
O95838	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	1.1813016	1.1813923
O95838	565	C:C-O-C	1.1742298	1.1742807
O95838	608	C-C-C-C:C	1.1576885	1.1579536
O95838	842	CC1CC(N)CC1	1.1542585	1.1541608
O95838	731	Clc1ccc(Cl)cc1	1.150502	1.1507249
O95838	805	OC1CC(N)CCC1	1.1500146	1.1499188
O95838	586	C-S-C-C-C	1.1277519	1.1277384
O95838	349	C(~C)(~H)(~S)	1.1268805	1.1269168
O95838	810	SC1CC(Cl)CCC1	1.1248105	1.1246551
O95838	542	O-C:C-[#1]	1.1202484	1.1204978
O95838	207	>= 5 saturated or aromatic carbon-only ring size 6	1.1064094	1.1064095
O95838	534	S-C:C-O	1.1012526	1.1011437
O95838	714	Cc1ccc(O)cc1	1.0957189	1.0961948
O95838	531	S-C:C-C	1.0909043	1.0910576
O95838	105	>= 1 Eu	1.0430512	1.0430512
O95838	880	BrC1C(Br)CCC1	1.0421839	1.042184
O95838	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	1.0317464	1.0317464
O95838	825	OC1C(S)CCCC1	1.0251956	1.0250867
O95838	445	C(-H)(-N)(=C)	1.0142868	1.0140033

O95838	868	OC1C(N)CCC1	1.0064176	1.0064176
O95838	425	P=O	1.005804	1.005804
O95838	760	Cc1c(Br)cccc1	1.0032063	1.0033722
O95838	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.9991617	0.9992982
O95838	762	Oc1c(S)cccc1	0.9971229	0.9970141
O95838	488	N-C=N-[#1]	0.9936557	0.9937422
O95838	790	SC1CCC(Br)CC1	0.9923059	0.9923059
O95838	831	SC1C(Cl)CCCC1	0.9884653	0.9884653
O95838	164	>= 4 any ring size 5	0.9856519	0.9857885
O95838	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.9785028	0.978583
O95838	700	O-C-C-C-C-C-O-C	0.9633824	0.963495
O95838	824	OC1C(O)CCCC1	0.9454009	0.945442
O95838	822	CC1C(Cl)CCCC1	0.9431039	0.9432051
O95838	464	N-C-C=C	0.9382977	0.9385704
O95838	378	C(~N)(:C)(:N)	0.9339259	0.9339344
O95838	315	O-K	0.9294736	0.9294735
O95838	812	NC1CC(N)CCC1	0.9203795	0.9203831
O95838	3	>= 32 H	0.898754	0.8987542
O95838	719	Oc1ccc(O)cc1	0.8678432	0.8677661
O95838	123	>= 2 saturated or aromatic carbon-only ring size 3	0.8590197	0.8590197
O95838	276	B-O	0.8571908	0.8571909
O95838	679	C-C-C-C-C-C	0.8460148	0.8462093
O95838	429	C(#N)(-C)	0.8267078	0.8264927
O95838	476	C-O-C=C	0.8175395	0.8175904
O95838	407	O(~C)(~P)	0.8129953	0.8129954
O95838	298	C-I	0.8108531	0.810795
O95838	533	S-C:C-N	0.8098297	0.8097397
O95838	113	>= 1 Tc	0.8052333	0.8052333
O95838	33	>= 1 S	0.7965843	0.796552
O95838	374	C(~H)(~H)(~H)	0.7907931	0.7907474
O95838	199	>= 4 any ring size 6	0.7878068	0.7878771
O95838	873	SC1C(Cl)CCC1	0.779755	0.7797551
O95838	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.7592427	0.7592428
O95838	24	>= 2 F	0.7556229	0.7557841
O95838	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.7528585	0.7528585
O95838	455	N(-O)(=O)	0.7446489	0.7447056
O95838	761	Oc1c(O)cccc1	0.7364848	0.736529
O95838	395	N(~C)(~O)	0.730393	0.7303603
O95838	754	Brc1cc(Br)ccc1	0.7299987	0.7299988
O95838	625	O=C-C:C-O	0.7265086	0.7264161
O95838	90	>= 1 Re	0.7262044	0.7262046
O95838	348	C(~C)(~H)(~P)	0.7185753	0.7185752
O95838	813	NC1CC(Cl)CCC1	0.7185517	0.7183426
O95838	426	P=P	0.7164728	0.7164728
O95838	63	>= 1 Ga	0.7121908	0.7121908
O95838	647	O=C-N-C-N	0.7002638	0.7005642
O95838	432	C(-C)(-C)(=O)	0.6999739	0.7000272
O95838	622	O=C-O-C:C	0.6937973	0.6937974

O95838	582	C-C-C-C-C	0.6882628	0.6885278
O95838	655	O-C-C-C:C	0.6825131	0.6824269
O95838	841	CC1CC(S)CC1	0.6800378	0.6800378
O95838	6	>= 1 B	0.6489741	0.6489741
O95838	764	Oc1c(Cl)cccc1	0.6485368	0.6481963
O95838	781	CC1CCC(Br)CC1	0.622608	0.622764
O95838	62	>= 1 Zn	0.617545	0.617545
O95838	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.6120982	0.6120983
O95838	855	NC1CC(Cl)CC1	0.6105438	0.6105439
O95838	334	C(~C)(~C)(~C)(~C)	0.6098508	0.6098855
O95838	640	C=C-C-C-C	0.6065968	0.6068619
O95838	355	C(~C)(:C)	0.6011491	0.6014141
O95838	706	O=C-C-C-C-C(=O)-C	0.5994661	0.5995627
O95838	23	>= 1 F	0.5834747	0.5835445
O95838	493	O=C-C:C	0.5796213	0.5796608
O95838	49	>= 1 Be	0.5701393	0.5701393
O95838	559	O-C-N-[#1]	0.5644154	0.5644155
O95838	274	B-C	0.5626898	0.56269
O95838	519	N=C-N-C	0.5576318	0.557703
O95838	227	>= 1 any ring size 8	0.5569858	0.5569857
O95838	1	>= 8 H	0.5563899	0.55639
O95838	713	Cc1ccc(C)cc1	0.555252	0.5553702
O95838	402	N(~O)(:O)	0.5535453	0.5535453
O95838	260	>= 3 hetero-aromatic rings	0.5481859	0.5481859
O95838	465	O=S-C-C	0.5481714	0.5482842
O95838	36	>= 8 S	0.5418403	0.5418404
O95838	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.5359309	0.5362015
O95838	549	N-C-C:C	0.5171688	0.5174415
O95838	58	>= 1 Fe	0.5169412	0.5169412
O95838	81	>= 1 Sb	0.515267	0.515267
O95838	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.51359	0.51359
O95838	525	[As]-C:C-[#1]	0.5094965	0.5094966
O95838	30	>= 1 P	0.5064788	0.5064789
O95838	610	C-O-C-O-C	0.5052866	0.5055917
O95838	312	O-Al	0.5028942	0.5028941
O95838	78	>= 1 Cd	0.5010327	0.5010328
O95838	409	O(:C)(:C)	0.4968346	0.4969517
O95838	428	C(#C)(-H)	0.4954804	0.4954804
O95838	591	Cl-C-C-C-C	0.4836473	0.48373
O95838	777	CC1CCC(O)CC1	0.477239	0.4777118
O95838	279	B-P	0.4734529	0.473453
O95838	554	Br-C-C-C	0.4702791	0.4701619
O95838	518	O=C-N-N	0.4679367	0.4680051
O95838	296	C-Se	0.4666434	0.4666433
O95838	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.4586781	0.4586781
O95838	314	O-P	0.4579444	0.4579446
O95838	452	C(-O)(=O)	0.4464147	0.4463617
O95838	613	C-N-C-C-C	0.4408338	0.4407027

O95838	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.4406044	0.4404647
O95838	571	[#1]-C-O-[#1]	0.437442	0.437629
O95838	421	C=S	0.4265124	0.426318
O95838	544	O-C:C-O	0.424711	0.4247552
O95838	326	As-As	0.4213793	0.4213793
O95838	691	O-C-C-C-C-C-N	0.4187405	0.4184751
O95838	427	C(#C)(-C)	0.4170541	0.4170543
O95838	703	O-C-C-C-C-C(N)-C	0.4150809	0.4150194
O95838	874	SC1C(Br)CCC1	0.4133353	0.4133353
O95838	248	>= 1 any ring size 10	0.4096522	0.4096523
O95838	151	>= 2 saturated or aromatic carbon-only ring size 5	0.4035536	0.4037194
O95838	594	C-O-C-C=C	0.390742	0.3908013
O95838	19	>= 2 O	0.3886228	0.3887869
O95838	662	O-C-C-O-C	0.3828245	0.3827646
O95838	418	C=N	0.3808352	0.3809672
O95838	443	C(-C)(=O)	0.3800403	0.3801942
O95838	44	>= 2 Br	0.3742733	0.3742733
O95838	589	C-C:C-O-C	0.372399	0.3723012
O95838	7	>= 2 B	0.368884	0.368884
O95838	65	>= 1 As	0.3684687	0.3684689
O95838	46	>= 1 I	0.3665679	0.3665099
O95838	103	>= 1 Pm	0.3649167	0.3649167
O95838	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.3646021	0.3646022
O95838	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.3524156	0.3524155
O95838	352	C(~C)(~O)	0.3500453	0.3500458
O95838	393	N(~C)(~H)	0.3361112	0.3363577
O95838	283	C-H	0.3347081	0.3349731
O95838	839	CC1CC(C)CC1	0.3313565	0.3309545
O95838	528	[#1]-N-C-[#1]	0.3263889	0.3262579
O95838	849	OC1CC(Br)CC1	0.3172299	0.3172299
O95838	537	O=C-C-O	0.311367	0.3114981
O95838	367	C(~H)(~O)(~O)	0.3103831	0.3103832
O95838	634	C-C-C:C-C	0.3083937	0.3086587
O95838	249	>= 1 saturated or aromatic carbon-only ring size 10	0.3036598	0.3036598
O95838	282	B-Br	0.3003164	0.3003163
O95838	590	C-C:C-O-[#1]	0.3001314	0.2998162
O95838	99	>= 1 La	0.2979638	0.2979639
O95838	475	S-C=N-C	0.2949891	0.294902
O95838	484	N-C:N:C	0.2932349	0.2929635
O95838	68	>= 1 Rb	0.2905089	0.2905089
O95838	310	O-Mg	0.2823986	0.2823987
O95838	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.2801158	0.2801158
O95838	602	O=C-C-N-C	0.2792739	0.2795399
O95838	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.2749707	0.275269
O95838	785	OC1CCC(Cl)CC1	0.2714691	0.2713796
O95838	769	Sc1c(Br)cccc1	0.2703969	0.2707407
O95838	654	N-C-N-C-C	0.2687373	0.268303
O95838	144	>= 1 saturated or aromatic carbon-only ring size 5	0.2665146	0.2663356

O95838	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.2660969	0.2660969
O95838	578	C-C:C-C:C	0.2618287	0.262094
O95838	721	Oc1ccc(N)cc1	0.2557296	0.2559908
O95838	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.2509406	0.2509374
O95838	876	NC1C(Cl)CC1	0.2459374	0.2459374
O95838	681	O-C-C-C-C-O	0.243617	0.2433748
O95838	829	SC1C(S)CCCC1	0.2435396	0.2435397
O95838	37	>= 1 Cl	0.2432788	0.2434191
O95838	369	C(~H)(~Si)	0.2385821	0.238582
O95838	419	C#N	0.235704	0.2354888
O95838	733	Brc1ccc(Br)cc1	0.2335236	0.2335237
O95838	52	>= 1 Ca	0.2244245	0.2244247
O95838	864	CC1C(Cl)CCC1	0.2168243	0.2168245
O95838	447	C(-H)(=N)	0.2167535	0.2164511
O95838	560	N-C-N-C	0.2136663	0.2132317
O95838	380	C(~O)(~O)	0.2096239	0.2095711
O95838	595	C:C-C-C-C	0.2004914	0.2007565
O95838	711	C-C(C)(C)-C-C	0.1982356	0.1982837
O95838	588	O=C-C-C=O	0.1824818	0.1824817
O95838	93	>= 1 Pt	0.1811102	0.1811102
O95838	512	C-[As]-O-[#1]	0.1806165	0.1806166
O95838	306	N-Cl	0.1779785	0.1779785
O95838	4	>= 1 Li	0.1727635	0.1727635
O95838	365	C(~H)(~N)	0.171939	0.172098
O95838	668	C-C:C-C-C	0.1716995	0.1719646
O95838	653	O-C:C:C-O	0.1710965	0.171219
O95838	643	[#1]-C-C-N-[#1]	0.1684242	0.1679587
O95838	273	B-B	0.1598959	0.159896
O95838	8	>= 4 B	0.1588861	0.158886
O95838	686	O=C-C-C-C-O	0.1576345	0.1575221
O95838	523	N:C:C-C	0.1524489	0.1522689
O95838	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.1499884	0.1499884
O95838	850	SC1CC(S)CC1	0.1458477	0.1458478
O95838	110	>= 1 Er	0.1294646	0.1294646
O95838	95	>= 1 Hg	0.1287063	0.1287064
O95838	397	N(~C)(:C)(:C)	0.1213853	0.1214614
O95838	338	C(~C)(~C)(~H)(~N)	0.1127435	0.112111
O95838	389	C(:N)(:N)	0.1098998	0.1100832
O95838	67	>= 1 Kr	0.1058817	0.1058818
O95838	77	>= 1 Ag	0.1042743	0.1042743
O95838	485	N:C:C:N	0.1035694	0.1036669
O95838	59	>= 1 Co	0.1023883	0.1023883
O95838	636	C-N-C-N-C	0.1002068	0.1000972
O95838	354	C(~C)(~Si)	0.0980878	0.0980877
O95838	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0892898	0.0892114
O95838	766	Sc1c(S)cccc1	0.0801168	0.0801168
O95838	546	N-C:C-[#1]	0.0766113	0.0769505
O95838	442	C(-C)(=N)	0.0690182	0.068941

O95838	683	N-C-C-C-C-C	0.0681173	0.06839
O95838	285	C-N	0.0676393	0.0677011
O95838	860	CC1C(C)CCC1	0.0675086	0.0675229
O95838	618	C:C-C-C:C	0.0673669	0.0675257
O95838	593	N-C-C-C-N	0.0673527	0.0674362
O95838	394	N(~C)(~H)(~N)	0.0671557	0.0671886
O95838	743	Oc1cc(Cl)ccc1	0.0667747	0.0667894
O95838	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0667274	0.0676136
O95838	511	S=C-N-[#1]	0.0666932	0.0666274
O95838	869	OC1C(Cl)CCC1	0.0666212	0.0666212
O95838	107	>= 1 Tb	0.0661914	0.0661915
O95838	746	Sc1cc(N)ccc1	0.0661812	0.0665313
O95838	879	ClC1C(Br)CCC1	0.0659884	0.0659885
O95838	468	O=S-C-N	0.065703	0.0657031
O95838	47	>= 2 I	0.0656544	0.0656544
O95838	91	>= 1 Os	0.0655708	0.0655709
O95838	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.0650753	0.0650753
O95838	171	>= 5 any ring size 5	0.0647025	0.0648392
O95838	457	S(-C)(=O)	0.0636886	0.0638013
O95838	325	As-H	0.0636653	0.0636652
O95838	562	Br-C-C=O	0.062756	0.0627559
O95838	641	O-C-C-C=C	0.0623191	0.062233
O95838	431	C(-C)(-C)(=N)	0.0619024	0.0621919
O95838	548	O-C-C:C	0.0604183	0.0603321
O95838	235	>= 2 saturated or aromatic carbon-only ring size 8	0.0598735	0.0598734
O95838	564	C=C-C=C	0.059849	0.0601141
O95838	809	SC1CC(N)CCC1	0.0592818	0.0594146
O95838	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.0587061	0.058706
O95838	667	C=C-C-O-[#1]	0.0584529	0.0582427
O95838	396	N(~C)(:C)	0.0584197	0.0582552
O95838	356	C(~C)(:C)(:C)	0.0576174	0.0578825
O95838	499	N-C:C:N	0.0567041	0.0566317
O95838	143	>= 1 any ring size 5	0.0565041	0.0567653
O95838	612	N-C-O-C-C	0.0553359	0.0553243
O95838	157	>= 3 any ring size 5	0.0553063	0.055369
O95838	313	O-Si	0.0546221	0.0546222
O95838	288	C-Na	0.0539388	0.053939
O95838	847	OC1CC(N)CC1	0.0539121	0.053912
O95838	536	O=C-C-N	0.0534687	0.053822
O95838	366	C(~H)(~O)	0.053071	0.0528347
O95838	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0530418	0.0530419
O95838	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.0529008	0.0526366
O95838	318	Al-H	0.0519411	0.0519411
O95838	89	>= 1 W	0.0508686	0.0508686
O95838	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.0504666	0.0504665
O95838	478	S-C=N-[#1]	0.0498133	0.0499571
O95838	479	S-C-S-C	0.0495511	0.049551
O95838	390	N(~C)(~C)	0.0490759	0.0492512

O95838	336	C(~C)(~C)(~C)(~N)	0.0489947	0.0491731
O95838	309	O-O	0.0487502	0.0487501
O95838	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.0479271	0.0479272
O95838	220	>= 2 any ring size 7	0.0477068	0.0477067
O95838	430	C(-C)(-C)(=C)	0.046697	0.046962
O95838	497	O-C:C:N	0.0459938	0.0460769
O95838	616	C:C:N:N:C	0.0459922	0.0459841
O95838	289	C-Mg	0.04561	0.0456099
O95838	851	SC1CC(N)CC1	0.0452692	0.0452692
O95838	460	C-C-C#C	0.0451207	0.0451206
O95838	64	>= 1 Ge	0.0448918	0.0448918
O95838	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.0444661	0.0444662
O95838	257	>= 2 aromatic rings	0.0441459	0.044146
O95838	623	O=C-C:C-C	0.0429576	0.0429972
O95838	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.041916	0.041916
O95838	388	C(:C)(:N)(:N)	0.0418638	0.0417707
O95838	458	S(-O)(=O)	0.041272	0.041323
O95838	265	Li-B	0.040481	0.040481
O95838	329	C(~Br)(~H)	0.0399516	0.0399515
O95838	495	C-N-C:C	0.0383173	0.0386379
O95838	206	>= 5 any ring size 6	0.0363353	0.0365301
O95838	627	O=[As]-C:C:C	0.0361496	0.0361496
O95838	14	>= 1 N	0.0361259	0.0361876
O95838	677	C-C=C-C:C	0.036118	0.036383
O95838	577	C:C-N-C:C	0.0354904	0.0352458
O95838	515	N-N-C-C	0.0344668	0.034431
O95838	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.0342997	0.0342997
O95838	70	>= 1 Y	0.0338814	0.0338813
O95838	434	C(-C)(-H)(=C)	0.0337433	0.0339021
O95838	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.033397	0.0333969
O95838	48	>= 4 I	0.0326853	0.0326852
O95838	259	>= 3 aromatic rings	0.0317364	0.0317364
O95838	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.0316539	0.0316539
O95838	241	>= 1 any ring size 9	0.0314052	0.0314052
O95838	328	C(~Br)(~C)(~C)	0.0300471	0.0299083
O95838	12	>= 16 C	0.0291316	0.02917
O95838	606	O-C:C-C-C	0.0267564	0.0267627
O95838	490	C-C-C=C	0.0264393	0.0267042
O95838	79	>= 1 In	0.0264259	0.0264258
O95838	22	>= 16 O	0.0246632	0.0246236
O95838	114	>= 1 U	0.0238622	0.0238622
O95838	797	CC1CC(C)CCC1	0.0235649	0.0235682
O95838	377	C(~N)(:C)(:C)	0.0230836	0.0231506
O95838	213	>= 1 any ring size 7	0.0228366	0.0228335
O95838	678	C-C-C=C-C	0.0226328	0.0228978
O95838	675	Br-C-C-C:C	0.0224312	0.0224484
O95838	408	O(~H)(~S)	0.0221909	0.022242
O95838	609	Cl-C-C-N-C	0.0220291	0.0220618

O95838	423	N=O	0.0218408	0.0218356
O95838	29	>= 2 Si	0.0218012	0.0218013
O95838	807	OC1CC(Br)CCC1	0.0213491	0.0213223
O95838	768	Sc1c(Cl)cccc1	0.0208304	0.0208305
O95838	417	C#C	0.0206907	0.0206908
O95838	722	Oc1ccc(Cl)cc1	0.019988	0.0198987
O95838	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.0193105	0.0194166
O95838	453	N(-C)(=C)	0.0187797	0.0187557
O95838	307	N-Br	0.018272	0.018272
O95838	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.018054	0.0181215
O95838	172	>= 5 saturated or aromatic carbon-only ring size 5	0.0178831	0.0178832
O95838	424	N=P	0.0177443	0.0177443
O95838	599	[#1]-C-C=C-[#1]	0.0175249	0.0177762
O95838	551	Cl-C-C-O	0.0167928	0.0164525
O95838	316	F-P	0.0160754	0.0160754
O95838	605	O=C-C-O-C	0.0143425	0.0142367
O95838	422	N=N	0.0135875	0.0139065
O95838	115	>= 1 any ring size 3	0.0130416	0.0130109
O95838	620	C:C-O-C-C	0.0125206	0.0124422
O95838	857	ClC1CC(Cl)CC1	0.0121598	0.0121598
O95838	255	>= 1 aromatic ring	0.0112283	0.0112283
O95838	632	C-C-O-C:C	0.0107822	0.0107037
O95838	844	CC1CC(Br)CC1	0.0105239	0.0105239
O95838	550	Cl-C-C-C	0.0105154	0.010598
O95838	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.010478	0.010478
O95838	401	N(~O)(~O)	0.0101709	0.0102274
O95838	856	NC1CC(Br)CC1	0.0100878	0.0100878
O95838	271	Li-Cl	0.0096744	0.0096744
O95838	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.0096218	0.0096218
O95838	607	N-C-C-C:C	0.009046	0.0093186
O95838	399	N(~H)(:C)	0.0089812	0.0088798
O95838	669	Cl-C:C-C=O	0.0089808	0.0090536
O95838	687	O=C-C-C-C=O	0.0085823	0.0085427
O95838	85	>= 1 Ba	0.0085041	0.0085041
O95838	787	SC1CCC(S)CC1	0.0085038	0.0085037
O95838	579	O=C-C-C-C	0.0084768	0.0085522
O95838	748	Sc1cc(Br)ccc1	0.0083911	0.0083911
O95838	383	C(~S)(:C)	0.0082663	0.0084196
O95838	757	Cc1c(S)cccc1	0.0080479	0.008174
O95838	31	>= 2 P	0.0080281	0.008028
O95838	699	O-C-C-C-C-C(C)-C	0.0075462	0.0075126
O95838	303	N-Si	0.0074263	0.0074262
O95838	372	C(~H)(:C)(:N)	0.0073804	0.0070969
O95838	820	CC1C(S)CCCC1	0.0073221	0.0072663
O95838	345	C(~C)(~H)(~N)	0.007172	0.0073547
O95838	674	N-C-N-C:C	0.0068633	0.0067742
O95838	185	>= 2 any ring size 6	0.0066021	0.0067155
O95838	693	O=C-C-C-C-C-O	0.00631	0.0064379

O95838	496	N:N-C-[#1]	0.006093	0.006085
O95838	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0060308	0.0061447
O95838	690	O-C-C-C-C-C-O	0.0059637	0.0060761
O95838	481	O-S-C:C	0.0059325	0.0059324
O95838	524	C-C=C-C	0.0058157	0.0060808
O95838	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0058085	0.0058085
O95838	603	C-C:C:C-C	0.0057621	0.0060272
O95838	406	O(~C)(~H)	0.0056239	0.005529
O95838	34	>= 2 S	0.0053952	0.0050693
O95838	774	Clc1c(Br)cccc1	0.0052558	0.0052558
O95838	784	OC1CCC(N)CC1	0.0051203	0.0053816
O95838	664	C-C=C-C=C	0.0050114	0.0052766
O95838	371	C(~H)(:C)(:C)	0.0046592	0.0048181
O95838	742	Oc1cc(N)ccc1	0.0046243	0.0045285
O95838	472	C:N:C-C	0.0042924	0.0040981
O95838	364	C(~F)(:C)	0.0041191	0.0035852
O95838	701	O-C-C-C-C-C(O)-C	0.0038152	0.0038405
O95838	477	N-N-C:C	0.0035646	0.0035565
O95838	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0033727	0.0033695
O95838	330	C(~Br)(:C)	0.0029021	0.0027849
O95838	712	C-C(C)-C(C)-C	0.0026823	0.0022169
O95838	835	NC1C(Br)CCCC1	0.0026075	0.0026075
O95838	500	C-S-C:C	0.0022779	0.0025865
O95838	280	B-S	0.002078	0.0020779
O95838	727	Sc1ccc(Br)cc1	0.0017816	0.0017815
O95838	521	C:N-C-[#1]	0.0017396	0.0014811
O95838	373	C(~H)(:N)	0.0015294	0.001246
O95838	293	C-S	0.0012117	0.0011794
O95838	340	C(~C)(~C)(~N)	0.001196	0.001253
O95838	732	Clc1ccc(Br)cc1	0.00112	0.00112
O95838	836	ClC1C(Cl)CCCC1	0.0007238	0
O95838	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0006733	0.00067
O95838	597	O=C-C-C:C	0.0006477	0.0006874
O95838	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.0006134	0.0007686
O95838	192	>= 3 any ring size 6	0.0004544	0.000717
O95838	471	S:C:C:C	0.0004257	0.0003214
O95838	799	CC1CC(S)CCC1	0.0003074	0
O95838	751	Nc1cc(Br)ccc1	0.0002764	0
O95838	568	N#C-C-C	0.0002152	0
O95838	645	O=C-N-C-C	0.0001946	0.0003982
O95838	659	O-C-C-N-C	0.0001799	0.0007062
O95838	744	Oc1cc(Br)ccc1	0.0001797	0.000153
O95838	704	O=C-C-C-C-C-C-C	0.0001391	0.0001195
O95838	295	C-As	0.0001253	0.0001252
O95838	819	CC1C(O)CCCC1	0.0001081	-0.000133
O95838	878	ClC1C(Cl)CCC1	4.64E-05	4.63E-05
O95838	509	Br-C:C-C	4.19E-05	-7.53E-05
O95838	741	Oc1cc(S)ccc1	3.86E-05	3.88E-05

O95838	728	Nc1ccc(N)cc1	3.63E-05	0
O95838	692	O=C-C-C-C-C-C	1.94E-05	0
O95838	492	N-C:O:C	1.16E-05	0
O95838	461	O-C-C=N	1.01E-05	0
O95838	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	1.46E-07	0
O95838	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	8.36E-08	0
O95838	319	Al-Cl	8.23E-08	0
O95838	415	Si(~C)(~C)	7.93E-08	0
O95838	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	5.35E-08	0
O95838	837	ClC1C(Br)CCCC1	4.10E-08	0
O95838	304	N-P	3.90E-08	0
O95838	267	Li-O	3.33E-08	0
O95838	101	>= 1 Pr	2.39E-08	0
O95838	772	Nc1c(Br)cccc1	1.53E-08	0
O95838	221	>= 2 saturated or aromatic carbon-only ring size 7	1.26E-08	0
O95838	343	C(~C)(~Cl)(~H)	-3.85E-09	0
O95838	361	C(~Cl)(~H)	-1.52E-08	0
O95838	102	>= 1 Nd	-7.85E-08	0
O95838	228	>= 1 saturated or aromatic carbon-only ring size 8	-9.90E-08	0
O95838	337	C(~C)(~C)(~C)(~O)	-2.53E-05	0
O95838	242	>= 1 saturated or aromatic carbon-only ring size 9	-2.56E-05	-2.56E-05
O95838	513	S:C:C-[#1]	-7.28E-05	-7.81E-05
O95838	771	Nc1c(Cl)cccc1	-9.38E-05	-0.000118
O95838	541	O-C:C-C	-0.000128	-0.000122
O95838	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	-0.000137	0
O95838	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	-0.00023	-0.00023
O95838	332	C(~C)(~C)	-0.000265	0
O95838	539	N=C-C-[#1]	-0.000296	0
O95838	178	>= 1 any ring size 6	-0.000326	-0.000131
O95838	745	Sc1cc(S)ccc1	-0.000402	-0.000402
O95838	867	OC1C(S)CCC1	-0.000448	-0.000448
O95838	697	C-C-C-C-C-C(C)-C	-0.000525	0.0001894
O95838	342	C(~C)(~Cl)	-0.000548	-0.000408
O95838	853	SC1CC(Br)CC1	-0.000554	-0.000554
O95838	437	C(-C)(-N)(=C)	-0.000599	-0.000548
O95838	449	C(-N)(=C)	-0.000638	-0.000392
O95838	454	N(-C)(=O)	-0.000831	-0.000836
O95838	833	NC1C(N)CCCC1	-0.000931	-0.00089
O95838	508	S=C-N-C	-0.000957	-0.001113
O95838	854	NC1CC(N)CC1	-0.001112	-0.001112
O95838	333	C(~C)(~C)(~C)	-0.00135	-0.001085
O95838	792	NC1CCC(Cl)CC1	-0.001379	-0.000917
O95838	866	OC1C(O)CCC1	-0.001457	-0.00146
O95838	505	Cl-C:C-O	-0.001537	-0.001877
O95838	483	N-S-C:C	-0.001559	-0.001715
O95838	846	OC1CC(S)CC1	-0.001657	-0.001657
O95838	9	>= 2 C	-0.001824	-0.001559
O95838	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	-0.002071	-0.001731

O95838	112	>= 1 Yb	−0.002124	−0.002124
O95838	800	CC1CC(N)CCC1	−0.00213	−0.002241
O95838	284	C-C	−0.002142	−0.001877
O95838	555	N=C-C=C	−0.002143	−0.002209
O95838	865	CC1C(Br)CCC1	−0.002146	−0.002146
O95838	740	Oc1cc(O)ccc1	−0.00223	−0.002107
O95838	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.00228	−0.00228
O95838	752	Clc1cc(Cl)ccc1	−0.002405	−0.002456
O95838	308	O-H	−0.002582	−0.00248
O95838	517	N-N-C-N	−0.002631	−0.002374
O95838	795	ClC1CCC(Br)CC1	−0.002665	−0.002665
O95838	368	C(~H)(~S)	−0.003028	−0.002739
O95838	725	Sc1ccc(N)cc1	−0.003044	−0.00313
O95838	585	C-C:C-N-C	−0.003164	−0.003022
O95838	767	Sc1c(N)cccc1	−0.003231	−0.003231
O95838	466	N#C-C=C	−0.003247	−0.003462
O95838	56	>= 1 Cr	−0.003467	−0.003467
O95838	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.003529	−0.003529
O95838	726	Sc1ccc(Cl)cc1	−0.003655	−0.003791
O95838	803	OC1CC(O)CCC1	−0.003671	−0.003551
O95838	74	>= 1 Ru	−0.003709	−0.003709
O95838	363	C(~F)(~F)	−0.003723	−0.003798
O95838	705	O=C-C-C-C-C(O)-C	−0.003835	−0.003656
O95838	277	B-F	−0.003844	−0.003844
O95838	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.003896	−0.003896
O95838	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.003967	−0.003967
O95838	724	Sc1ccc(S)cc1	−0.004054	−0.004054
O95838	710	C-C-C(C)-C-C	−0.004272	−0.004007
O95838	780	CC1CCC(Cl)CC1	−0.004625	−0.004989
O95838	717	Cc1ccc(Cl)cc1	−0.004886	−0.00525
O95838	529	Cl-C-C-Cl	−0.004907	−0.005631
O95838	698	O-C-C-C-C-C-C-C	−0.005077	−0.005135
O95838	73	>= 1 Mo	−0.005125	−0.005125
O95838	21	>= 8 O	−0.005671	−0.005915
O95838	86	>= 1 Lu	−0.00589	−0.00589
O95838	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.005967	−0.005967
O95838	875	NC1C(N)CCC1	−0.006063	−0.006063
O95838	494	O=C-C:N	−0.00611	−0.005789
O95838	791	NC1CCC(N)CC1	−0.006651	−0.006688
O95838	297	C-Br	−0.006802	−0.006919
O95838	0	>= 4 H	−0.006926	−0.006926
O95838	547	N-C:C-N	−0.007411	−0.007483
O95838	642	O-C-C-C=O	−0.00751	−0.007642
O95838	150	>= 2 any ring size 5	−0.007605	−0.007591
O95838	414	S(~C)(~O)	−0.007839	−0.007726
O95838	789	SC1CCC(Cl)CC1	−0.008307	−0.008442
O95838	651	O-C:C:C-C	−0.008452	−0.008352
O95838	709	C-C(C)-C-C-C	−0.00873	−0.008465

O95838	459	S(=O)(=O)	−0.009342	−0.009631
O95838	358	C(~C)(:N)	−0.009609	−0.009834
O95838	545	N-C:C-C	−0.009814	−0.009746
O95838	770	Nc1c(N)cccc1	−0.009922	−0.009882
O95838	572	N:C:N:C	−0.00996	−0.009873
O95838	82	>= 1 Te	−0.010137	−0.010137
O95838	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.010194	−0.010222
O95838	436	C(-C)(-H)(=O)	−0.010379	−0.010318
O95838	467	C=N-N-C	−0.010533	−0.010544
O95838	621	N-C:C:C:N	−0.010576	−0.010601
O95838	695	O=C-C-C-C-C-N	−0.011149	−0.011581
O95838	802	CC1CC(Br)CCC1	−0.011527	−0.011854
O95838	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.012277	−0.012277
O95838	381	C(~O)(:C)	−0.013964	−0.01381
O95838	10	>= 4 C	−0.014499	−0.014234
O95838	735	Cc1cc(O)ccc1	−0.015035	−0.015314
O95838	13	>= 32 C	−0.015944	−0.01563
O95838	413	S(~C)(~H)	−0.016072	−0.016072
O95838	737	Cc1cc(N)ccc1	−0.016515	−0.016337
O95838	580	O=C-C-C-N	−0.016719	−0.01701
O95838	522	C-N-N-[#1]	−0.016963	−0.016735
O95838	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.016994	−0.016994
O95838	351	C(~C)(~N)	−0.017194	−0.017133
O95838	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.018379	−0.018379
O95838	347	C(~C)(~H)(~O)(~O)	−0.019071	−0.019071
O95838	450	C(-N)(=N)	−0.019104	−0.019139
O95838	730	Nc1ccc(Br)cc1	−0.019356	−0.019356
O95838	630	O-C:C-O-C	−0.019562	−0.019441
O95838	106	>= 1 Gd	−0.019674	−0.019674
O95838	456	P(-O)(=O)	−0.019952	−0.019952
O95838	32	>= 4 P	−0.020116	−0.020116
O95838	729	Nc1ccc(Cl)cc1	−0.02077	−0.020307
O95838	611	N-C-C-N-C	−0.020856	−0.021116
O95838	506	C-C:N:C	−0.02115	−0.021345
O95838	676	N#C-C-C-C	−0.021179	−0.021394
O95838	793	NC1CCC(Br)CC1	−0.021843	−0.021843
O95838	26	>= 1 Na	−0.022063	−0.022063
O95838	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.024157	−0.024157
O95838	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.024434	−0.024434
O95838	362	C(~Cl)(:C)	−0.024547	−0.024407
O95838	5	>= 2 Li	−0.024773	−0.024773
O95838	474	S:C:C:N	−0.024979	−0.025069
O95838	646	O=C-N-C-[#1]	−0.02913	−0.02891
O95838	501	Cl-C:C-C	−0.03169	−0.031607
O95838	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.033927	−0.033927
O95838	379	C(~N)(:N)	−0.034904	−0.034921
O95838	763	Oc1c(N)cccc1	−0.035952	−0.036009
O95838	439	C(-C)(-N)(=O)	−0.036299	−0.036268

O95838	290	C-Al	−0.036655	−0.036655
O95838	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.038831	−0.038742
O95838	462	O-C-C=O	−0.039367	−0.039236
O95838	391	N(~C)(~C)(~C)	−0.039748	−0.039617
O95838	859	BrC1CC(Br)CC1	−0.041059	−0.041059
O95838	104	>= 1 Sm	−0.04285	−0.04285
O95838	604	C-O-C-C:C	−0.042995	−0.042936
O95838	281	B-Cl	−0.043148	−0.043148
O95838	738	Cc1cc(Cl)ccc1	−0.043189	−0.043367
O95838	359	C(~C)(:N)(:N)	−0.044374	−0.044377
O95838	657	C-N-C:C-C	−0.044554	−0.044412
O95838	420	C=O	−0.044722	−0.044568
O95838	331	C(~Br)(:N)	−0.044952	−0.044952
O95838	773	Clc1c(Cl)cccc1	−0.045354	−0.046078
O95838	275	B-N	−0.045827	−0.045827
O95838	650	O=C-N-C=O	−0.046673	−0.046424
O95838	405	O(~C)(~C)	−0.046865	−0.046641
O95838	66	>= 1 Se	−0.047364	−0.047365
O95838	122	>= 2 any ring size 3	−0.049459	−0.049459
O95838	346	C(~C)(~H)(~O)	−0.050049	−0.050112
O95838	344	C(~C)(~H)	−0.050173	−0.049908
O95838	327	C(~Br)(~C)	−0.050215	−0.050332
O95838	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.05084	−0.05084
O95838	448	C(-H)(=O)	−0.051226	−0.051166
O95838	758	Cc1c(N)cccc1	−0.051257	−0.051204
O95838	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.052207	−0.052071
O95838	637	O-C-C-C-C	−0.054496	−0.054478
O95838	796	BrC1CCC(Br)CC1	−0.055055	−0.055054
O95838	294	C-Cl	−0.055592	−0.055452
O95838	339	C(~C)(~C)(~H)(~O)	−0.055667	−0.05566
O95838	656	C-C-N-C-C	−0.055902	−0.055672
O95838	840	CC1CC(O)CC1	−0.057411	−0.057414
O95838	87	>= 1 Hf	−0.057594	−0.057594
O95838	287	C-F	−0.05812	−0.058051
O95838	665	N-C:C-C-C	−0.058729	−0.05861
O95838	614	C-C-O-C-C	−0.058751	−0.05865
O95838	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.059251	−0.059251
O95838	300	N-N	−0.059406	−0.059225
O95838	264	Li-Li	−0.059741	−0.05974
O95838	311	O-Na	−0.059808	−0.059808
O95838	317	F-S	−0.059901	−0.059901
O95838	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.060356	−0.060356
O95838	286	C-O	−0.06118	−0.061179
O95838	581	O=C-C-C-O	−0.061599	−0.061731
O95838	234	>= 2 any ring size 8	−0.06172	−0.06172
O95838	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.061763	−0.061763
O95838	718	Cc1ccc(Br)cc1	−0.061779	−0.061623
O95838	561	Cl-C-C=O	−0.061886	−0.061886

O95838	716	Cc1ccc(N)cc1	−0.062475	−0.062751
O95838	28	>= 1 Si	−0.062564	−0.062564
O95838	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.062569	−0.06257
O95838	350	C(~C)(~I)	−0.062635	−0.062693
O95838	491	C-N:C-[#1]	−0.0628	−0.06316
O95838	60	>= 1 Ni	−0.062893	−0.062893
O95838	335	C(~C)(~C)(~C)(~H)	−0.063746	−0.063593
O95838	502	N-C=C-[#1]	−0.063985	−0.063645
O95838	527	C:C:N-[#1]	−0.064176	−0.064294
O95838	387	C(:C)(:N)	−0.064824	−0.064943
O95838	821	CC1C(N)CCCC1	−0.064858	−0.065004
O95838	617	C-C-C-O-[#1]	−0.065054	−0.065243
O95838	672	O=C-C=C-[#1]	−0.065178	−0.064915
O95838	341	C(~C)(~C)(~O)	−0.065227	−0.065179
O95838	633	N-C-C:C-C	−0.065237	−0.064965
O95838	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.065418	−0.064965
O95838	806	OC1CC(Cl)CCC1	−0.066226	−0.066211
O95838	262	>= 4 hetero-aromatic rings	−0.066304	−0.066303
O95838	673	O=C-C=C-N	−0.066388	−0.066471
O95838	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.066404	−0.0665
O95838	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.066534	−0.066534
O95838	558	O=N-C:C	−0.066537	−0.066481
O95838	753	Clc1cc(Br)ccc1	−0.0667	−0.0667
O95838	80	>= 1 Sn	−0.066772	−0.066772
O95838	94	>= 1 Au	−0.06695	−0.06695
O95838	57	>= 1 Mn	−0.067147	−0.067147
O95838	619	O-C-C=C-C	−0.069074	−0.06916
O95838	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.070325	−0.070325
O95838	552	C:C-C:C	−0.076367	−0.076102
O95838	862	CC1C(S)CCC1	−0.079985	−0.079985
O95838	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.080952	−0.080953
O95838	827	OC1C(Cl)CCCC1	−0.084204	−0.084544
O95838	375	C(~N)(~N)	−0.085241	−0.085582
O95838	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.08556	−0.08556
O95838	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.086503	−0.08612
O95838	451	C(-N)(=O)	−0.089478	−0.089416
O95838	11	>= 8 C	−0.091068	−0.090803
O95838	798	CC1CC(O)CCC1	−0.096529	−0.096812
O95838	324	P-P	−0.098062	−0.098062
O95838	680	O-C-C-C-C-C	−0.100155	−0.100251
O95838	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.101057	−0.101057
O95838	72	>= 1 Nb	−0.104199	−0.104199
O95838	54	>= 1 Ti	−0.10493	−0.10493
O95838	648	O=N-C:C-N	−0.107647	−0.107647
O95838	631	O-C:C-O-[#1]	−0.107712	−0.107745
O95838	720	Oc1ccc(S)cc1	−0.109347	−0.109303
O95838	592	N-C-C-C-C	−0.10986	−0.109643
O95838	357	C(~C)(:C)(:N)	−0.111735	−0.111676

O95838	788	SC1CCC(N)CC1	-0.111744	-0.111829
O95838	444	C(-Cl)(=O)	-0.118407	-0.118407
O95838	786	OC1CCC(Br)CC1	-0.120113	-0.120068
O95838	35	>= 4 S	-0.121051	-0.121051
O95838	385	C(:C)(:C)(:C)	-0.127574	-0.127078
O95838	108	>= 1 Dy	-0.134343	-0.134343
O95838	598	Cl-C:C:C-C	-0.136233	-0.13615
O95838	688	C-C-C-C-C-C-C	-0.136756	-0.136562
O95838	69	>= 1 Sr	-0.137041	-0.137041
O95838	765	Oc1c(Br)cccc1	-0.140253	-0.140253
O95838	480	C:S:C-C	-0.142322	-0.142517
O95838	382	C(~O)(:C)(:C)	-0.149729	-0.149453
O95838	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	-0.149872	-0.149872
O95838	470	C:C-C=C	-0.155724	-0.155459
O95838	269	Li-P	-0.157121	-0.157121
O95838	638	O-C-C-C-N	-0.16117	-0.161027
O95838	575	O-C-C:C-O	-0.163662	-0.163189
O95838	671	O=C-C=C-C	-0.181973	-0.181989
O95838	794	ClC1CCC(Cl)CC1	-0.18482	-0.184597
O95838	266	Li-C	-0.187492	-0.187492
O95838	384	C(:C)(:C)	-0.188677	-0.188412
O95838	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	-0.194704	-0.194704
O95838	486	N-C:N:N	-0.202745	-0.202604
O95838	503	Cl-C:C-[#1]	-0.204504	-0.204462
O95838	624	O=C-C:C-N	-0.207611	-0.207695
O95838	658	C-C-S-C-C	-0.209556	-0.209441
O95838	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	-0.210182	-0.210182
O95838	734	Cc1cc(C)ccc1	-0.2195	-0.219493
O95838	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	-0.229805	-0.229668
O95838	441	C(-C)(=C)	-0.238649	-0.238383
O95838	556	C=C-C-C	-0.24773	-0.247465
O95838	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	-0.24798	-0.24798
O95838	755	Cc1c(C)cccc1	-0.249187	-0.24939
O95838	305	N-S	-0.253632	-0.253787
O95838	392	N(~C)(~C)(~H)	-0.255304	-0.255194
O95838	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	-0.257443	-0.257632
O95838	84	>= 1 Cs	-0.260964	-0.260964
O95838	828	OC1C(Br)CCCC1	-0.26537	-0.26537
O95838	601	N-C:C:C-N	-0.267116	-0.267086
O95838	482	C:N-C:C	-0.273963	-0.273997
O95838	863	CC1C(N)CCC1	-0.278398	-0.278653
O95838	816	ClC1CC(Br)CCC1	-0.286912	-0.286912
O95838	71	>= 1 Zr	-0.286947	-0.286947
O95838	670	Br-C:C:C-C	-0.291078	-0.291196
O95838	520	C=C-C:C	-0.292374	-0.292109
O95838	50	>= 1 Mg	-0.298245	-0.298245
O95838	136	>= 2 any ring size 4	-0.301522	-0.301522
O95838	826	OC1C(N)CCCC1	-0.310386	-0.310443

O95838	292	C-P	−0.312655	−0.312655
O95838	600	N-C:C:C-C	−0.314575	−0.314461
O95838	433	C(-C)(-Cl)(=O)	−0.314583	−0.314584
O95838	75	>= 1 Rh	−0.315674	−0.315674
O95838	27	>= 2 Na	−0.318808	−0.318808
O95838	411	P(~O)(~O)	−0.322851	−0.322851
O95838	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.327786	−0.327786
O95838	412	S(~C)(~C)	−0.328356	−0.32837
O95838	18	>= 1 O	−0.33521	−0.335256
O95838	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.338547	−0.338547
O95838	323	P-H	−0.34332	−0.34332
O95838	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.347907	−0.347907
O95838	848	OC1CC(Cl)CC1	−0.353927	−0.353927
O95838	573	O-C-C=C	−0.356047	−0.356133
O95838	815	ClC1CC(Cl)CCC1	−0.356289	−0.356341
O95838	838	BrC1C(Br)CCCC1	−0.358999	−0.358999
O95838	834	NC1C(Cl)CCCC1	−0.360062	−0.360087
O95838	660	C-C=C-C-C	−0.362554	−0.362289
O95838	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.362833	−0.362833
O95838	644	C-C=N-N-C	−0.372234	−0.372221
O95838	25	>= 4 F	−0.373127	−0.373706
O95838	685	O=C-C-C-C-N	−0.37457	−0.374668
O95838	473	S-C:N:C	−0.377467	−0.377554
O95838	43	>= 1 Br	−0.377542	−0.377659
O95838	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.378811	−0.378811
O95838	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.391063	−0.390927
O95838	45	>= 4 Br	−0.394056	−0.394056
O95838	487	N-C=N-C	−0.394289	−0.394578
O95838	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.404467	−0.404467
O95838	40	>= 8 Cl	−0.410331	−0.410331
O95838	268	Li-F	−0.416089	−0.416089
O95838	370	C(~H)(:C)	−0.422655	−0.422496
O95838	83	>= 1 Xe	−0.425603	−0.425603
O95838	782	OC1CCC(O)CC1	−0.427638	−0.427718
O95838	400	N(~H)(:C)(:C)	−0.433302	−0.433419
O95838	111	>= 1 Tm	−0.436993	−0.436993
O95838	801	CC1CC(Cl)CCC1	−0.437757	−0.437935
O95838	569	N-C-C-N	−0.446207	−0.446467
O95838	852	SC1CC(Cl)CC1	−0.447696	−0.447696
O95838	628	C-N-C-C:C	−0.45542	−0.455424
O95838	739	Cc1cc(Br)ccc1	−0.457685	−0.458011
O95838	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.459218	−0.459218
O95838	861	CC1C(O)CCC1	−0.474898	−0.474901
O95838	563	O-C-O-C	−0.479333	−0.479028
O95838	463	N:C-S-[#1]	−0.481196	−0.481196
O95838	823	CC1C(Br)CCCC1	−0.485735	−0.485569
O95838	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.489283	−0.489147
O95838	51	>= 1 Al	−0.492254	−0.492254

O95838	814	NC1CC(Br)CCC1	−0.492609	−0.492886
O95838	20	>= 4 O	−0.493119	−0.493163
O95838	410	P(~C)(~C)	−0.499057	−0.499057
O95838	749	Nc1cc(N)ccc1	−0.501039	−0.501036
O95838	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.501568	−0.501387
O95838	845	OC1CC(O)CC1	−0.502686	−0.502685
O95838	750	Nc1cc(Cl)ccc1	−0.504696	−0.504905
O95838	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.507635	−0.507635
O95838	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.508123	−0.508123
O95838	629	S-C:C:C-N	−0.512892	−0.512542
O95838	446	C(-H)(=C)	−0.517508	−0.517349
O95838	258	>= 2 hetero-aromatic rings	−0.523787	−0.523787
O95838	88	>= 1 Ta	−0.52488	−0.52488
O95838	403	N(:C)(:C)	−0.552874	−0.553068
O95838	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.55717	−0.557834
O95838	715	Cc1ccc(S)cc1	−0.561339	−0.56113
O95838	299	N-H	−0.570472	−0.570381
O95838	489	N-C-S-C	−0.57621	−0.576363
O95838	587	N-C:C-O-[#1]	−0.583249	−0.583323
O95838	404	N(:C)(:C)(:C)	−0.586226	−0.586226
O95838	97	>= 1 Pb	−0.590955	−0.590955
O95838	583	Cl-C:C-O-C	−0.595598	−0.595865
O95838	386	C(:C)(:C)(:N)	−0.603106	−0.60296
O95838	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.610968	−0.610968
O95838	129	>= 1 any ring size 4	−0.616531	−0.616275
O95838	61	>= 1 Cu	−0.617788	−0.617788
O95838	682	O-C-C-C-C-N	−0.620659	−0.620517
O95838	302	N-F	−0.631603	−0.631603
O95838	16	>= 4 N	−0.639619	−0.639996
O95838	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.651075	−0.651075
O95838	689	O-C-C-C-C-C-C	−0.65562	−0.655822
O95838	438	C(-C)(-N)(=N)	−0.655804	−0.655633
O95838	15	>= 2 N	−0.656009	−0.655795
O95838	707	O=C-C-C-C-C(N)-C	−0.678938	−0.679551
O95838	514	O-N-C-C	−0.680918	−0.680951
O95838	321	Si-Si	−0.686127	−0.686127
O95838	440	C(-C)(-O)(=O)	−0.688461	−0.688514
O95838	39	>= 4 Cl	−0.693937	−0.693865
O95838	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.711324	−0.711324
O95838	652	O-C:C:C-N	−0.72174	−0.721881
O95838	708	C-C(C)-C-C	−0.727311	−0.727046
O95838	736	Cc1cc(S)ccc1	−0.728021	−0.728364
O95838	2	>= 16 H	−0.728406	−0.728406
O95838	322	Si-Cl	−0.730884	−0.730884
O95838	96	>= 1 Tl	−0.736854	−0.736854
O95838	109	>= 1 Ho	−0.746063	−0.746063
O95838	747	Sc1cc(Cl)ccc1	−0.748492	−0.748647
O95838	817	BrC1CC(Br)CCC1	−0.748569	−0.748569

O95838	530	N:C-C:C	−0.753281 −0.753163
O95838	804	OC1CC(S)CCC1	−0.765082 −0.765082
O95838	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.769161 −0.769161
O95838	872	SC1C(N)CCC1	−0.781602 −0.781602
O95838	17	>= 8 N	−0.789039 −0.789051
O95838	53	>= 1 Sc	−0.789094 −0.789094
O95838	291	C-Si	−0.793224 −0.793225
O95838	584	C:C-C=C-C	−0.794237 −0.793973
O95838	41	>= 1 K	−0.799642 −0.799642
O95838	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.804394 −0.804394
O95838	272	B-H	−0.806843 −0.806843
O95838	723	Oc1ccc(Br)cc1	−0.818797 −0.818751
O95838	532	S-C:C-[#1]	−0.822832 −0.823004
O95838	830	SC1C(N)CCCC1	−0.823795 −0.823795
O95838	877	NC1C(Br)CCC1	−0.826606 −0.826606
O95838	808	SC1CC(S)CCC1	−0.857064 −0.857064
O95838	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.876064 −0.875808
O95838	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.897689 −0.897689
O95838	535	O=C-C-C	−0.915326 −0.915119
O95838	663	O-C-C-O-[#1]	−0.915961 −0.915805
O95838	811	SC1CC(Br)CCC1	−0.920784 −0.920784
O95838	42	>= 2 K	−0.93084 −0.93084
O95838	843	CC1CC(Cl)CC1	−0.966472 −0.966472
O95838	435	C(-C)(-H)(=N)	−1.011661 −1.011939
O95838	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−1.029801 −1.029801
O95838	858	ClC1CC(Br)CC1	−1.030757 −1.030757
O95838	353	C(~C)(~S)	−1.035487 −1.035519
O95838	596	N=C-N-C-C	−1.035979 −1.035908
O95838	775	Brc1c(Br)cccc1	−1.04264 −1.04264
O95838	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−1.096904 −1.096904
O95838	256	>= 1 hetero-aromatic ring	−1.097868 −1.097868
O95838	783	OC1CCC(S)CC1	−1.137506 −1.137462
O95838	832	SC1C(Br)CCCC1	−1.138482 −1.138139
O95838	666	C=C-C-O-C	−1.146272 −1.146212
O95838	639	O-C-C-C-O	−1.147445 −1.147208
O95838	759	Cc1c(Cl)cccc1	−1.154633 −1.154532
O95838	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−1.170448 −1.170448
O95838	186	>= 2 saturated or aromatic carbon-only ring size 6	−1.226912 −1.227034
O95838	376	C(~N)(:C)	−1.233173 −1.232927
O95838	360	C(~Cl)(~Cl)	−1.2337 −1.2337
O95838	615	N-C-C-O-C	−1.234785 −1.234778
O95838	92	>= 1 Ir	−1.250571 −1.250571
O95838	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−1.270004 −1.270004
O95838	469	S-S-C:C	−1.274585 −1.274585
O95838	566	O-C-C-N	−1.325393 −1.32542
O95838	504	N:C:N-C	−1.338892 −1.338805
O95838	507	C-C-S-C	−1.382483 −1.382497
O95838	574	O-C-C:C-C	−1.405728 −1.405814

O95838	498	O-C=C-C	-1.405813	-1.405807
O95838	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	-1.430846	-1.430846
O95838	870	OC1C(Br)CCC1	-1.49	-1.49
O95838	543	O-C:C-N	-1.509541	-1.509649
O95838	38	>= 2 Cl	-1.588132	-1.588759
O95838	818	CC1C(C)CCCC1	-1.618386	-1.618592
O95838	263	Li-H	-1.682629	-1.682629
O95838	576	N=C-C:C-[#1]	-1.687154	-1.687377
O95838	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	-1.758553	-1.758553
O95838	416	C=C	-1.784752	-1.784487
O95838	270	Li-S	-1.826822	-1.826822
O95838	557	N:C-O-[#1]	-1.858109	-1.858109
O95838	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	-1.903606	-1.903411
O95838	776	CC1CCC(C)CC1	-1.938041	-1.93789
O95838	778	CC1CCC(S)CC1	-2.066551	-2.066341
O95838	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	-2.100522	-2.100522
O95838	694	O=C-C-C-C-C=O	-2.267871	-2.267863
O95838	526	Cl-C:C-Cl	-2.269853	-2.270577
O95838	661	O-C-O-C-C	-2.544993	-2.544688

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P48546	720	Oc1ccc(S)cc1	2.4710232
P48546	606	O-C:C-C-C	1.8896524
P48546	864	CC1C(Cl)CCC1	1.8036411
P48546	281	B-Cl	1.4700691
P48546	260	>= 3 hetero-aromatic rings	1.4560577
P48546	185	>= 2 any ring size 6	1.3927663
P48546	855	NC1CC(Cl)CC1	1.3496825
P48546	524	C-C=C-C	1.3042982
P48546	583	Cl-C:C-O-C	1.2880773
P48546	467	C=N-N-C	1.250815
P48546	678	C-C-C=C-C	1.2452486
P48546	854	NC1CC(N)CC1	1.230341
P48546	263	Li-H	1.2297822
P48546	580	O=C-C-C-N	1.2205586
P48546	466	N#C-C=C	1.2177761
P48546	39	>= 4 Cl	1.2086159
P48546	612	N-C-O-C-C	1.2049487
P48546	578	C-C:C-C:C	1.1832062
P48546	516	[#1]-C=C-[#1]	1.1788808
P48546	608	C-C-C-C:C	1.1767564
P48546	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.1707858
P48546	401	N(~O)(~O)	1.1692158
P48546	814	NC1CC(Br)CCC1	1.1364807
P48546	41	>= 1 K	1.1284036
P48546	99	>= 1 La	1.0930372
P48546	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	1.0839294
P48546	721	Oc1ccc(N)cc1	1.0671437
P48546	272	B-H	1.0575764
P48546	786	OC1CCC(Br)CC1	1.0151978
P48546	370	C(~H)(:C)	1.014657
P48546	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	1.0019005
P48546	726	Sc1ccc(Cl)cc1	0.9960662
P48546	738	Cc1cc(Cl)ccc1	0.992295
P48546	430	C(-C)(-C)(=C)	0.9915691
P48546	730	Nc1ccc(Br)cc1	0.9912824
P48546	453	N(-C)(=C)	0.9831802
P48546	491	C-N:C-[#1]	0.9787285
P48546	819	CC1C(O)CCCC1	0.9525259
P48546	421	C=S	0.9367303
P48546	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.9338609
P48546	653	O-C:C-C-O	0.9259134
P48546	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.9031417
P48546	813	NC1CC(Cl)CCC1	0.8995408
P48546	279	B-P	0.8862866
P48546	274	B-C	0.8786944
P48546	270	Li-S	0.8662451

P48546	603	C-C:C:C-C	0.8578881
P48546	774	Clc1c(Br)cccc1	0.8528451
P48546	871	SC1C(S)CCC1	0.8511101
P48546	0	>= 4 H	0.8455339
P48546	591	Cl-C-C-C-C	0.83861
P48546	568	N#C-C-C	0.8350908
P48546	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.8320285
P48546	845	OC1CC(O)CC1	0.8291113
P48546	710	C-C-C(C)-C-C	0.8281783
P48546	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.8199309
P48546	292	C-P	0.813619
P48546	795	ClC1CCC(Br)CC1	0.7975911
P48546	863	CC1C(N)CCC1	0.797014
P48546	641	O-C-C-C=C	0.7966018
P48546	552	C:C-C:C	0.7956729
P48546	24	>= 2 F	0.7925267
P48546	531	S-C:C-C	0.7890235
P48546	868	OC1C(N)CCC1	0.7841342
P48546	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.7765945
P48546	546	N-C:C-[#1]	0.7725817
P48546	384	C(:C)(:C)	0.756057
P48546	747	Sc1cc(Cl)ccc1	0.74658
P48546	725	Sc1ccc(N)cc1	0.7462202
P48546	406	O(~C)(~H)	0.7427439
P48546	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.7398115
P48546	623	O=C-C:C-C	0.7281766
P48546	307	N-Br	0.7129149
P48546	632	C-C-O-C:C	0.7111256
P48546	872	SC1C(N)CCC1	0.7016961
P48546	536	O=C-C-N	0.7015322
P48546	96	>= 1 Tl	0.6883483
P48546	794	ClC1CCC(Cl)CC1	0.6831352
P48546	461	O-C-C=N	0.6798416
P48546	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.6791665
P48546	852	SC1CC(Cl)CC1	0.6783397
P48546	313	O-Si	0.6732706
P48546	261	>= 4 aromatic rings	0.6626133
P48546	787	SC1CCC(S)CC1	0.6556969
P48546	200	>= 4 saturated or aromatic carbon-only ring size 6	0.6477287
P48546	396	N(~C)(:C)	0.6473109
P48546	799	CC1CC(S)CCC1	0.6458856
P48546	856	NC1CC(Br)CC1	0.6456268
P48546	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.6451261
P48546	458	S(-O)(=O)	0.6366697
P48546	298	C-I	0.6337844
P48546	867	OC1C(S)CCC1	0.6262881
P48546	768	Sc1c(Cl)cccc1	0.6193701
P48546	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.6164037

P48546	772	Nc1c(Br)cccc1	0.6134678
P48546	481	O-S-C:C	0.6103231
P48546	97	>= 1 Pb	0.6073942
P48546	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.6002314
P48546	539	N=C-C-[#1]	0.5941863
P48546	433	C(-C)(-Cl)(=O)	0.5850949
P48546	716	Cc1ccc(N)cc1	0.5779693
P48546	509	Br-C:C-C	0.5776515
P48546	810	SC1CC(Cl)CCC1	0.5762775
P48546	171	>= 5 any ring size 5	0.5747397
P48546	220	>= 2 any ring size 7	0.5697086
P48546	754	Brc1cc(Br)ccc1	0.565864
P48546	297	C-Br	0.5600146
P48546	193	>= 3 saturated or aromatic carbon-only ring size 6	0.5585657
P48546	673	O=C-C=C-N	0.5555153
P48546	687	O=C-C-C-C=O	0.553629
P48546	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.551913
P48546	532	S-C:C-[#1]	0.5509883
P48546	835	NC1C(Br)CCCC1	0.5485943
P48546	853	SC1CC(Br)CC1	0.5386756
P48546	729	Nc1ccc(Cl)cc1	0.5355968
P48546	807	OC1CC(Br)CCC1	0.5355607
P48546	221	>= 2 saturated or aromatic carbon-only ring size 7	0.5290137
P48546	338	C(~C)(~C)(~H)(~N)	0.5273786
P48546	766	Sc1c(S)cccc1	0.5251784
P48546	482	C:N-C:C	0.5181545
P48546	363	C(~F)(~F)	0.5167742
P48546	30	>= 1 P	0.5093559
P48546	704	O=C-C-C-C-C-C-C	0.5064688
P48546	328	C(~Br)(~C)(~C)	0.4927722
P48546	81	>= 1 Sb	0.4783307
P48546	804	OC1CC(S)CCC1	0.4718513
P48546	438	C(-C)(-N)(=N)	0.4696497
P48546	29	>= 2 Si	0.4660546
P48546	123	>= 2 saturated or aromatic carbon-only ring size 3	0.461396
P48546	770	Nc1c(N)cccc1	0.4613239
P48546	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.4612919
P48546	691	O-C-C-C-C-C-N	0.4607708
P48546	670	Br-C:C:C-C	0.4523225
P48546	731	Clc1ccc(Cl)cc1	0.4471856
P48546	92	>= 1 Ir	0.4464264
P48546	534	S-C:C-O	0.4377046
P48546	645	O=C-N-C-C	0.4363512
P48546	403	N(:C)(:C)	0.435002
P48546	444	C(-Cl)(=O)	0.4346574
P48546	671	O=C-C=C-C	0.4321916
P48546	395	N(~C)(~O)	0.428871
P48546	523	N:C:C-C	0.4182132

P48546	572	N:C:N:C	0.4161614
P48546	684	O=C-C-C-C-C	0.4120623
P48546	734	Cc1cc(C)ccc1	0.4092544
P48546	790	SC1CCC(Br)CC1	0.3961194
P48546	526	Cl-C:C-Cl	0.3952145
P48546	744	Oc1cc(Br)ccc1	0.3932557
P48546	303	N-Si	0.3868985
P48546	489	N-C-S-C	0.3856369
P48546	447	C(-H)(=N)	0.378793
P48546	573	O-C-C=C	0.3694489
P48546	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.361571
P48546	199	>= 4 any ring size 6	0.3597432
P48546	705	O=C-C-C-C-C(O)-C	0.358593
P48546	339	C(~C)(~C)(~H)(~O)	0.354888
P48546	409	O(:C)(:C)	0.3512435
P48546	873	SC1C(Cl)CCC1	0.3505575
P48546	129	>= 1 any ring size 4	0.3497713
P48546	699	O-C-C-C-C-C(C)-C	0.3488651
P48546	832	SC1C(Br)CCCC1	0.3421841
P48546	800	CC1CC(N)CCC1	0.3402823
P48546	487	N-C=N-C	0.3378586
P48546	446	C(-H)(=C)	0.3373213
P48546	345	C(~C)(~H)(~N)	0.3240801
P48546	777	CC1CCC(O)CC1	0.3218221
P48546	36	>= 8 S	0.3200887
P48546	681	O-C-C-C-C-O	0.31635
P48546	77	>= 1 Ag	0.3018285
P48546	826	OC1C(N)CCCC1	0.300676
P48546	718	Cc1ccc(Br)cc1	0.292072
P48546	717	Cc1ccc(Cl)cc1	0.2898296
P48546	839	CC1CC(C)CC1	0.2890285
P48546	741	Oc1cc(S)ccc1	0.2852597
P48546	685	O=C-C-C-C-N	0.2766249
P48546	636	C-N-C-N-C	0.2742072
P48546	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.263937
P48546	346	C(~C)(~H)(~O)	0.2606227
P48546	815	ClC1CC(Cl)CCC1	0.2540024
P48546	102	>= 1 Nd	0.2493424
P48546	317	F-S	0.2487672
P48546	47	>= 2 I	0.2466106
P48546	79	>= 1 In	0.2463936
P48546	728	Nc1ccc(N)cc1	0.2456721
P48546	525	[As]-C:C-[#1]	0.2423761
P48546	554	Br-C-C-C	0.2394505
P48546	733	Brc1ccc(Br)cc1	0.2329558
P48546	719	Oc1ccc(O)cc1	0.2306413
P48546	486	N-C:N:N	0.2284759
P48546	343	C(~C)(~Cl)(~H)	0.2267238

P48546	529	Cl-C-C-Cl	0.2266546
P48546	179	>= 1 saturated or aromatic carbon-only ring size 6	0.2208309
P48546	78	>= 1 Cd	0.2191605
P48546	116	>= 1 saturated or aromatic carbon-only ring size 3	0.2180444
P48546	818	CC1C(C)CCCC1	0.2134715
P48546	35	>= 4 S	0.2082088
P48546	859	BrC1CC(Br)CC1	0.2068769
P48546	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.2013482
P48546	585	C-C:C-N-C	0.1984573
P48546	172	>= 5 saturated or aromatic carbon-only ring size 5	0.1843365
P48546	605	O=C-C-O-C	0.1780229
P48546	20	>= 4 O	0.1763712
P48546	763	Oc1c(N)cccc1	0.1752935
P48546	802	CC1CC(Br)CCC1	0.1727039
P48546	83	>= 1 Xe	0.1703744
P48546	104	>= 1 Sm	0.1667376
P48546	709	C-C(C)-C-C-C	0.1627991
P48546	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.1623248
P48546	792	NC1CCC(Cl)CC1	0.1610301
P48546	278	B-Si	0.1563196
P48546	757	Cc1c(S)cccc1	0.1561922
P48546	541	O-C:C-C	0.1547513
P48546	353	C(~C)(~S)	0.1497991
P48546	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.1471366
P48546	549	N-C-C:C	0.1467258
P48546	779	CC1CCC(N)CC1	0.1446933
P48546	335	C(~C)(~C)(~C)(~H)	0.1426542
P48546	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.1416424
P48546	711	C-C(C)(C)-C-C	0.1370147
P48546	441	C(-C)(=C)	0.1342327
P48546	448	C(-H)(=O)	0.1309812
P48546	861	CC1C(O)CCC1	0.1304345
P48546	13	>= 32 C	0.1303954
P48546	473	S-C:N:C	0.1300985
P48546	825	OC1C(S)CCCC1	0.1279841
P48546	295	C-As	0.1272397
P48546	654	N-C-N-C-C	0.1237825
P48546	499	N-C:C:N	0.1229325
P48546	507	C-C-S-C	0.1227515
P48546	566	O-C-C-N	0.1224938
P48546	17	>= 8 N	0.1222022
P48546	618	C:C-C-C:C	0.1138719
P48546	1	>= 8 H	0.1131024
P48546	743	Oc1cc(Cl)ccc1	0.1094409
P48546	680	O-C-C-C-C-C	0.1009318
P48546	452	C(-O)(=O)	0.1007353
P48546	249	>= 1 saturated or aromatic carbon-only ring size 10	0.0986843
P48546	676	N#C-C-C-C	0.0983174

P48546	457	S(-C)(=O)	0.0982322
P48546	143	>= 1 any ring size 5	0.0977798
P48546	276	B-O	0.0944519
P48546	366	C(~H)(~O)	0.0930186
P48546	712	C-C(C)-C(C)-C	0.0857562
P48546	638	O-C-C-C-N	0.0837665
P48546	693	O=C-C-C-C-C-O	0.0793251
P48546	698	O-C-C-C-C-C-C-C	0.0780585
P48546	784	OC1CCC(N)CC1	0.0756712
P48546	538	N=C-C-C	0.0753533
P48546	610	C-O-C-O-C	0.071988
P48546	256	>= 1 hetero-aromatic ring	0.0705753
P48546	472	C:N:C-C	0.07054
P48546	382	C(~O)(:C)(:C)	0.0703596
P48546	697	C-C-C-C-C-C(C)-C	0.0673675
P48546	85	>= 1 Ba	0.0663392
P48546	510	[#1]-N-N-[#1]	0.0657589
P48546	837	ClC1C(Br)CCCC1	0.0657086
P48546	479	S-C-S-C	0.065306
P48546	477	N-N-C:C	0.0649858
P48546	84	>= 1 Cs	0.0649469
P48546	575	O-C-C:C-O	0.0646381
P48546	736	Cc1cc(S)ccc1	0.0646303
P48546	282	B-Br	0.0645068
P48546	463	N:C-S-[#1]	0.0640014
P48546	422	N=N	0.0635953
P48546	661	O-C-O-C-C	0.0630169
P48546	596	N=C-N-C-C	0.0622493
P48546	765	Oc1c(Br)cccc1	0.0618992
P48546	8	>= 4 B	0.0607578
P48546	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.0604155
P48546	639	O-C-C-C-O	0.0595725
P48546	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0594438
P48546	459	S(=O)(=O)	0.0590062
P48546	402	N(~O)(:O)	0.0579644
P48546	619	O-C-C=C-C	0.057661
P48546	740	Oc1cc(O)ccc1	0.0575387
P48546	242	>= 1 saturated or aromatic carbon-only ring size 9	0.0566788
P48546	329	C(~Br)(~H)	0.0557515
P48546	337	C(~C)(~C)(~C)(~O)	0.0549851
P48546	848	OC1CC(Cl)CC1	0.0546895
P48546	521	C:N-C-[#1]	0.054563
P48546	782	OC1CCC(O)CC1	0.052856
P48546	648	O=N-C:C-N	0.0526874
P48546	840	CC1CC(O)CC1	0.0523374
P48546	150	>= 2 any ring size 5	0.0512717
P48546	101	>= 1 Pr	0.0500669
P48546	764	Oc1c(Cl)cccc1	0.0490686

P48546	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0484163
P48546	806	OC1CC(Cl)CCC1	0.0483268
P48546	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.0478463
P48546	599	[#1]-C-C=C-[#1]	0.0478381
P48546	493	O=C-C:C	0.0477994
P48546	611	N-C-C-N-C	0.0467015
P48546	492	N-C:O:C	0.0463645
P48546	558	O=N-C:C	0.046086
P48546	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.0458751
P48546	470	C:C-C=C	0.0457027
P48546	846	OC1CC(S)CC1	0.0455687
P48546	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0455441
P48546	817	BrC1CC(Br)CCC1	0.0451848
P48546	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0449269
P48546	294	C-Cl	0.0441918
P48546	551	Cl-C-C-O	0.0439318
P48546	151	>= 2 saturated or aromatic carbon-only ring size 5	0.0438209
P48546	563	O-C-O-C	0.0435647
P48546	746	Sc1cc(N)ccc1	0.043016
P48546	349	C(~C)(~H)(~S)	0.0426056
P48546	404	N(:C)(:C)(:C)	0.0405547
P48546	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.0401532
P48546	564	C=C-C=C	0.0399604
P48546	63	>= 1 Ga	0.0394524
P48546	545	N-C:C-C	0.0390249
P48546	285	C-N	0.0388969
P48546	98	>= 1 Bi	0.0388704
P48546	388	C(:C)(:N)(:N)	0.0381863
P48546	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.0370586
P48546	586	C-S-C-C-C	0.036937
P48546	579	O=C-C-C-C	0.0359963
P48546	265	Li-B	0.0356933
P48546	830	SC1C(N)CCCC1	0.0343198
P48546	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.0339139
P48546	570	C:C-C-C	0.0330188
P48546	115	>= 1 any ring size 3	0.032523
P48546	829	SC1C(S)CCCC1	0.0293682
P48546	652	O-C:C:C-N	0.0290593
P48546	192	>= 3 any ring size 6	0.0288134
P48546	847	OC1CC(N)CC1	0.0285508
P48546	644	C-C=N-N-C	0.0282475
P48546	735	Cc1cc(O)ccc1	0.0279103
P48546	56	>= 1 Cr	0.0263469
P48546	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0254962
P48546	454	N(-C)(=O)	0.0243801
P48546	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0224103
P48546	857	ClC1CC(Cl)CC1	0.022139
P48546	437	C(-C)(-N)(=C)	0.0214492

P48546	321	Si-Si	0.0213288
P48546	760	Cc1c(Br)cccc1	0.0211325
P48546	761	Oc1c(O)cccc1	0.0207782
P48546	318	Al-H	0.0206306
P48546	876	NC1C(Cl)CC1	0.0204432
P48546	332	C(~C)(~C)	0.0204421
P48546	365	C(~H)(~N)	0.0201883
P48546	553	O=C-C=C	0.0187046
P48546	547	N-C:C-N	0.0186056
P48546	620	C:C-O-C-C	0.0183525
P48546	416	C=C	0.0181972
P48546	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0181654
P48546	75	>= 1 Rh	0.0179962
P48546	413	S(~C)(~H)	0.0164527
P48546	22	>= 16 O	0.0161641
P48546	106	>= 1 Gd	0.0152883
P48546	471	S:C:C:C	0.0145829
P48546	662	O-C-C-O-C	0.0133969
P48546	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0132188
P48546	617	C-C-C-O-[#1]	0.0132075
P48546	320	Si-H	0.0130272
P48546	665	N-C:C-C-C	0.0127824
P48546	707	O=C-C-C-C-C(N)-C	0.0125086
P48546	16	>= 4 N	0.0122771
P48546	7	>= 2 B	0.0122629
P48546	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.012225
P48546	373	C(~H)(:N)	0.011658
P48546	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.0115578
P48546	576	N=C-C:C-[#1]	0.0110816
P48546	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.0108723
P48546	377	C(~N)(:C)(:C)	0.0108085
P48546	537	O=C-C-O	0.0107537
P48546	255	>= 1 aromatic ring	0.0105525
P48546	59	>= 1 Co	0.010513
P48546	361	C(~Cl)(~H)	0.0105001
P48546	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0104364
P48546	45	>= 4 Br	0.010415
P48546	675	Br-C-C-C:C	0.0103917
P48546	544	O-C:C-O	0.0103533
P48546	248	>= 1 any ring size 10	0.0097955
P48546	50	>= 1 Mg	0.0097078
P48546	362	C(~Cl)(:C)	0.0095234
P48546	71	>= 1 Zr	0.009209
P48546	785	OC1CCC(Cl)CC1	0.0091769
P48546	700	O-C-C-C-C-C-O-C	0.008673
P48546	657	C-N-C:C-C	0.008603
P48546	727	Sc1ccc(Br)cc1	0.0079472
P48546	107	>= 1 Tb	0.0072767

P48546	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0068787
P48546	723	Oc1ccc(Br)cc1	0.00675
P48546	412	S(~C)(~C)	0.0066219
P48546	478	S-C=N-[#1]	0.0065864
P48546	701	O-C-C-C-C-C(O)-C	0.0065821
P48546	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0060471
P48546	378	C(~N)(:C)(:N)	0.0050392
P48546	783	OC1CCC(S)CC1	0.0050297
P48546	109	>= 1 Ho	0.0046433
P48546	359	C(~C)(:N)(:N)	0.0044719
P48546	713	Cc1ccc(C)cc1	0.0043183
P48546	136	>= 2 any ring size 4	0.004225
P48546	594	C-O-C-C=C	0.0041827
P48546	869	OC1C(Cl)CCC1	0.0038225
P48546	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0037971
P48546	434	C(-C)(-H)(=C)	0.0037779
P48546	667	C=C-C-O-[#1]	0.0037701
P48546	405	O(~C)(~C)	0.0033832
P48546	389	C(:N)(:N)	0.003188
P48546	820	CC1C(S)CCCC1	0.0031003
P48546	780	CC1CCC(Cl)CC1	0.0028325
P48546	460	C-C-C#C	0.0026776
P48546	356	C(~C)(:C)(:C)	0.0022586
P48546	58	>= 1 Fe	0.0021036
P48546	627	O=[As]-C:C:C	0.001911
P48546	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.001758
P48546	708	C-C(C)-C-C	0.0015232
P48546	533	S-C:C-N	0.0012938
P48546	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0012223
P48546	688	C-C-C-C-C-C-C	0.0011311
P48546	860	CC1C(C)CCC1	0.0011193
P48546	666	C=C-C-O-C	0.0011002
P48546	484	N-C:N:C	0.0010778
P48546	60	>= 1 Ni	0.0009345
P48546	450	C(-N)(=N)	0.0009097
P48546	878	ClC1C(Cl)CCC1	0.0008222
P48546	299	N-H	0.0005502
P48546	555	N=C-C=C	0.000527
P48546	850	SC1CC(S)CC1	0.0004464
P48546	485	N:C:C:N	0.0004308
P48546	394	N(~C)(~H)(~N)	0.0004044
P48546	348	C(~C)(~H)(~P)	0.0003221
P48546	350	C(~C)(~I)	0.0002833
P48546	264	Li-Li	0.0002206
P48546	767	Sc1c(N)cccc1	0.0001892
P48546	311	O-Na	5.06E-05
P48546	590	C-C:C-O-[#1]	1.77E-05
P48546	227	>= 1 any ring size 8	2.63E-08

P48546	273	B-B	2.59E-08
P48546	858	ClC1CC(Br)CC1	2.02E-08
P48546	62	>= 1 Zn	1.88E-08
P48546	410	P(~C)(~C)	1.15E-08
P48546	326	As-As	4.60E-09
P48546	88	>= 1 Ta	3.65E-09
P48546	879	ClC1C(Br)CCC1	2.19E-09
P48546	559	O-C-N-[#1]	4.86E-10
P48546	67	>= 1 Kr	-8.02E-09
P48546	512	C-[As]-O-[#1]	-8.22E-09
P48546	456	P(-O)(=O)	-9.15E-09
P48546	100	>= 1 Ce	-1.74E-08
P48546	4	>= 1 Li	-1.89E-08
P48546	870	OC1C(Br)CCC1	-2.13E-08
P48546	74	>= 1 Ru	-4.50E-08
P48546	89	>= 1 W	-4.74E-08
P48546	214	>= 1 saturated or aromatic carbon-only ring size 7	-5.23E-05
P48546	2	>= 16 H	-9.85E-05
P48546	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	-0.000245
P48546	414	S(~C)(~O)	-0.000267
P48546	31	>= 2 P	-0.00041
P48546	488	N-C=N-[#1]	-0.000424
P48546	498	O-C=C-C	-0.000499
P48546	495	C-N-C:C	-0.000788
P48546	468	O=S-C-N	-0.000922
P48546	604	C-O-C-C:C	-0.001495
P48546	385	C(:C)(:C)(:C)	-0.001582
P48546	12	>= 16 C	-0.001786
P48546	344	C(~C)(~H)	-0.00193
P48546	626	C-O-C:C-C	-0.002043
P48546	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	-0.002058
P48546	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	-0.002228
P48546	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	-0.002284
P48546	213	>= 1 any ring size 7	-0.002317
P48546	355	C(~C)(:C)	-0.002328
P48546	28	>= 1 Si	-0.002398
P48546	391	N(~C)(~C)(~C)	-0.002534
P48546	280	B-S	-0.003265
P48546	621	N-C:C:C:N	-0.003265
P48546	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	-0.003324
P48546	588	O=C-C-C=O	-0.003566
P48546	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	-0.00357
P48546	574	O-C-C:C-C	-0.003762
P48546	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-0.003821
P48546	360	C(~Cl)(~Cl)	-0.003821
P48546	658	C-C-S-C-C	-0.003866
P48546	371	C(~H)(:C)(:C)	-0.003949
P48546	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	-0.004034

P48546	351	C(~C)(~N)	−0.004137
P48546	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.004146
P48546	581	O=C-C-C-O	−0.004233
P48546	425	P=O	−0.004622
P48546	497	O-C:C:N	−0.004635
P48546	304	N-P	−0.004983
P48546	277	B-F	−0.005411
P48546	674	N-C-N-C:C	−0.005531
P48546	61	>= 1 Cu	−0.005542
P48546	528	[#1]-N-C-[#1]	−0.005543
P48546	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.005619
P48546	758	Cc1c(N)cccc1	−0.005728
P48546	522	C-N-N-[#1]	−0.00588
P48546	293	C-S	−0.006381
P48546	407	O(~C)(~P)	−0.006396
P48546	565	C:C-O-C	−0.006459
P48546	833	NC1C(N)CCCC1	−0.006488
P48546	775	Brc1c(Br)cccc1	−0.006877
P48546	530	N:C-C:C	−0.007166
P48546	651	O-C:C:C-C	−0.007613
P48546	347	C(~C)(~H)(~O)(~O)	−0.008039
P48546	577	C:C-N-C:C	−0.008088
P48546	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.008128
P48546	797	CC1CC(C)CCC1	−0.00897
P48546	690	O-C-C-C-C-C-O	−0.009404
P48546	324	P-P	−0.009653
P48546	462	O-C-C=O	−0.009717
P48546	53	>= 1 Sc	−0.009825
P48546	38	>= 2 Cl	−0.010174
P48546	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.010556
P48546	609	Cl-C-C-N-C	−0.010569
P48546	562	Br-C-C=O	−0.010821
P48546	418	C=N	−0.011023
P48546	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.011419
P48546	475	S-C=N-C	−0.0115
P48546	715	Cc1ccc(S)cc1	−0.012116
P48546	598	Cl-C:C:C-C	−0.012143
P48546	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.012704
P48546	683	N-C-C-C-C-C	−0.012931
P48546	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.013439
P48546	556	C=C-C-C	−0.01356
P48546	752	Clc1cc(Cl)ccc1	−0.01454
P48546	672	O=C-C=C-[#1]	−0.014788
P48546	722	Oc1ccc(Cl)cc1	−0.014868
P48546	592	N-C-C-C-C	−0.014951
P48546	284	C-C	−0.015007
P48546	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.015237
P48546	751	Nc1cc(Br)ccc1	−0.016413

P48546	287	C-F	−0.01656
P48546	637	O-C-C-C-C	−0.01661
P48546	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.017209
P48546	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.017387
P48546	455	N(-O)(=O)	−0.017869
P48546	809	SC1CC(N)CCC1	−0.018117
P48546	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.018418
P48546	417	C#C	−0.01857
P48546	322	Si-Cl	−0.018798
P48546	21	>= 8 O	−0.01892
P48546	442	C(-C)(=N)	−0.019257
P48546	76	>= 1 Pd	−0.019753
P48546	411	P(~O)(~O)	−0.019774
P48546	724	Sc1ccc(S)cc1	−0.020384
P48546	689	O-C-C-C-C-C-C	−0.020499
P48546	27	>= 2 Na	−0.020656
P48546	649	O=N-C:C-O	−0.020671
P48546	668	C-C:C-C-C	−0.021342
P48546	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.021515
P48546	271	Li-Cl	−0.021557
P48546	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.021673
P48546	664	C-C=C-C=C	−0.021703
P48546	82	>= 1 Te	−0.021782
P48546	86	>= 1 Lu	−0.021949
P48546	432	C(-C)(-C)(=O)	−0.022676
P48546	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.023005
P48546	334	C(~C)(~C)(~C)(~C)	−0.023686
P48546	393	N(~C)(~H)	−0.024337
P48546	469	S-S-C:C	−0.024884
P48546	113	>= 1 Tc	−0.026614
P48546	357	C(~C)(:C)(:N)	−0.027183
P48546	68	>= 1 Rb	−0.02733
P48546	379	C(~N)(:N)	−0.027391
P48546	266	Li-C	−0.027775
P48546	331	C(~Br)(:N)	−0.0287
P48546	342	C(~C)(~Cl)	−0.029902
P48546	635	N-N-C-N-[#1]	−0.029965
P48546	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.030049
P48546	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.031341
P48546	300	N-N	−0.031618
P48546	682	O-C-C-C-C-N	−0.032381
P48546	40	>= 8 Cl	−0.033261
P48546	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.034198
P48546	368	C(~H)(~S)	−0.034589
P48546	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.035598
P48546	94	>= 1 Au	−0.036057
P48546	375	C(~N)(~N)	−0.036381
P48546	677	C-C=C-C:C	−0.037409

P48546	46	>= 1 I	−0.037795
P48546	381	C(~O)(:C)	−0.038187
P48546	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.03849
P48546	838	BrC1C(Br)CCCC1	−0.041556
P48546	15	>= 2 N	−0.042566
P48546	600	N-C:C:C-C	−0.043301
P48546	262	>= 4 hetero-aromatic rings	−0.043653
P48546	616	C:C:N:N:C	−0.044416
P48546	310	O-Mg	−0.045493
P48546	646	O=C-N-C-[#1]	−0.045793
P48546	423	N=O	−0.04714
P48546	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.047635
P48546	506	C-C:N:C	−0.047968
P48546	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.048558
P48546	464	N-C-C=C	−0.048695
P48546	567	O-C-C-O	−0.049721
P48546	543	O-C:C-N	−0.051687
P48546	290	C-Al	−0.051787
P48546	400	N(~H)(:C)(:C)	−0.052767
P48546	625	O=C-C:C-O	−0.052964
P48546	781	CC1CCC(Br)CC1	−0.053718
P48546	624	O=C-C:C-N	−0.05491
P48546	26	>= 1 Na	−0.054991
P48546	501	Cl-C:C-C	−0.055295
P48546	490	C-C-C=C	−0.055852
P48546	449	C(-N)(=C)	−0.056007
P48546	291	C-Si	−0.057288
P48546	288	C-Na	−0.057519
P48546	65	>= 1 As	−0.057781
P48546	72	>= 1 Nb	−0.058879
P48546	54	>= 1 Ti	−0.059208
P48546	301	N-O	−0.05947
P48546	540	C-N-C-[#1]	−0.059629
P48546	426	P=P	−0.05974
P48546	831	SC1C(Cl)CCCC1	−0.060013
P48546	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.06037
P48546	851	SC1CC(N)CC1	−0.060799
P48546	302	N-F	−0.060966
P48546	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.061002
P48546	90	>= 1 Re	−0.061943
P48546	542	O-C:C-[#1]	−0.062195
P48546	769	Sc1c(Br)cccc1	−0.062227
P48546	37	>= 1 Cl	−0.063851
P48546	57	>= 1 Mn	−0.06405
P48546	275	B-N	−0.064712
P48546	435	C(-C)(-H)(=N)	−0.065301
P48546	796	BrC1CCC(Br)CC1	−0.065424
P48546	93	>= 1 Pt	−0.065436

P48546	369	C(~H)(~Si)	−0.065761
P48546	267	Li-O	−0.066154
P48546	844	CC1CC(Br)CC1	−0.066255
P48546	111	>= 1 Tm	−0.066486
P48546	325	As-H	−0.066611
P48546	257	>= 2 aromatic rings	−0.066933
P48546	340	C(~C)(~C)(~N)	−0.067577
P48546	206	>= 5 any ring size 6	−0.068207
P48546	513	S:C:C-[#1]	−0.068629
P48546	309	O-O	−0.068772
P48546	702	O-C-C-C-C-C-N-C	−0.069866
P48546	374	C(~H)(~H)(~H)	−0.069937
P48546	341	C(~C)(~C)(~O)	−0.070431
P48546	439	C(-C)(-N)(=O)	−0.072964
P48546	584	C:C-C=C-C	−0.073595
P48546	703	O-C-C-C-C-C(N)-C	−0.077136
P48546	376	C(~N)(:C)	−0.079237
P48546	776	CC1CCC(C)CC1	−0.081183
P48546	520	C=C-C:C	−0.081742
P48546	660	C-C=C-C-C	−0.081932
P48546	14	>= 1 N	−0.08346
P48546	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.083875
P48546	602	O=C-C-N-C	−0.084081
P48546	742	Oc1cc(N)ccc1	−0.085302
P48546	122	>= 2 any ring size 3	−0.085381
P48546	679	C-C-C-C-C-C	−0.086297
P48546	178	>= 1 any ring size 6	−0.088335
P48546	613	C-N-C-C-C	−0.089217
P48546	34	>= 2 S	−0.090112
P48546	508	S=C-N-C	−0.092482
P48546	398	N(~H)(~N)	−0.09617
P48546	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.096926
P48546	364	C(~F)(:C)	−0.097577
P48546	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.098005
P48546	25	>= 4 F	−0.098159
P48546	789	SC1CCC(Cl)CC1	−0.105395
P48546	762	Oc1c(S)cccc1	−0.10751
P48546	550	Cl-C-C-C	−0.107552
P48546	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.110969
P48546	773	Clc1c(Cl)cccc1	−0.113371
P48546	6	>= 1 B	−0.114746
P48546	595	C:C-C-C-C	−0.116762
P48546	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.119555
P48546	91	>= 1 Os	−0.119851
P48546	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.129285
P48546	390	N(~C)(~C)	−0.13062
P48546	64	>= 1 Ge	−0.135736
P48546	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.138435

P48546	834	NC1C(Cl)CCCC1	−0.138737
P48546	737	Cc1cc(N)ccc1	−0.144481
P48546	793	NC1CCC(Br)CC1	−0.145812
P48546	3	>= 32 H	−0.151145
P48546	52	>= 1 Ca	−0.153101
P48546	798	CC1CC(O)CCC1	−0.155537
P48546	821	CC1C(N)CCCC1	−0.159282
P48546	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.164912
P48546	696	C-C-C-C-C-C-C-C	−0.165829
P48546	69	>= 1 Sr	−0.167966
P48546	9	>= 2 C	−0.168594
P48546	383	C(~S)(:C)	−0.177728
P48546	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.179843
P48546	527	C:C:N-[#1]	−0.180642
P48546	108	>= 1 Dy	−0.183037
P48546	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.183489
P48546	305	N-S	−0.189465
P48546	316	F-P	−0.190345
P48546	157	>= 3 any ring size 5	−0.193105
P48546	502	N-C=C-[#1]	−0.194144
P48546	10	>= 4 C	−0.194406
P48546	43	>= 1 Br	−0.195146
P48546	18	>= 1 O	−0.198677
P48546	415	Si(~C)(~C)	−0.213443
P48546	480	C:S:C-C	−0.214801
P48546	496	N:N-C-[#1]	−0.215624
P48546	824	OC1C(O)CCCC1	−0.216695
P48546	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.217351
P48546	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.221737
P48546	827	OC1C(Cl)CCCC1	−0.225259
P48546	656	C-C-N-C-C	−0.231619
P48546	865	CC1C(Br)CCC1	−0.232435
P48546	663	O-C-C-O-[#1]	−0.234078
P48546	408	O(~H)(~S)	−0.234655
P48546	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.242427
P48546	753	Clc1cc(Br)ccc1	−0.244179
P48546	517	N-N-C-N	−0.247661
P48546	622	O=C-O-C:C	−0.250289
P48546	788	SC1CCC(N)CC1	−0.250526
P48546	749	Nc1cc(N)ccc1	−0.252577
P48546	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.263485
P48546	352	C(~C)(~O)	−0.263569
P48546	399	N(~H)(:C)	−0.272491
P48546	571	[#1]-C-O-[#1]	−0.273237
P48546	629	S-C:C:C-N	−0.273813
P48546	805	OC1CC(N)CCC1	−0.3081
P48546	535	O=C-C-C	−0.309491
P48546	569	N-C-C-N	−0.320616

P48546	849	OC1CC(Br)CC1	−0.322171
P48546	80	>= 1 Sn	−0.322211
P48546	874	SC1C(Br)CCC1	−0.32566
P48546	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.327375
P48546	511	S=C-N-[#1]	−0.329021
P48546	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.334286
P48546	424	N=P	−0.335421
P48546	66	>= 1 Se	−0.349523
P48546	694	O=C-C-C-C-C=O	−0.362711
P48546	500	C-S-C:C	−0.368526
P48546	686	O=C-C-C-C-O	−0.372952
P48546	315	O-K	−0.378382
P48546	103	>= 1 Pm	−0.378702
P48546	647	O=C-N-C-N	−0.384887
P48546	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.388507
P48546	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.390472
P48546	750	Nc1cc(Cl)ccc1	−0.391925
P48546	631	O-C:C-O-[#1]	−0.39403
P48546	451	C(-N)(=O)	−0.394575
P48546	801	CC1CC(Cl)CCC1	−0.402319
P48546	327	C(~Br)(~C)	−0.408214
P48546	822	CC1C(Cl)CCCC1	−0.411238
P48546	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.425386
P48546	386	C(:C)(:C)(:N)	−0.435231
P48546	443	C(-C)(=O)	−0.436636
P48546	95	>= 1 Hg	−0.437593
P48546	420	C=O	−0.439654
P48546	607	N-C-C-C:C	−0.442923
P48546	739	Cc1cc(Br)ccc1	−0.457208
P48546	561	Cl-C-C=O	−0.471043
P48546	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.487439
P48546	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.498819
P48546	655	O-C-C-C:C	−0.504935
P48546	440	C(-C)(-O)(=O)	−0.527469
P48546	714	Cc1ccc(O)cc1	−0.532849
P48546	812	NC1CC(N)CCC1	−0.536682
P48546	778	CC1CCC(S)CC1	−0.537068
P48546	354	C(~C)(~Si)	−0.541282
P48546	494	O=C-C:N	−0.541625
P48546	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.55746
P48546	269	Li-P	−0.564122
P48546	336	C(~C)(~C)(~C)(~N)	−0.578729
P48546	843	CC1CC(Cl)CC1	−0.580128
P48546	5	>= 2 Li	−0.59055
P48546	289	C-Mg	−0.59182
P48546	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.597163
P48546	19	>= 2 O	−0.598784
P48546	505	Cl-C:C-O	−0.605097

P48546	164	>= 4 any ring size 5	−0.60984
P48546	518	O=C-N-N	−0.613644
P48546	771	Nc1c(Cl)cccc1	−0.614506
P48546	866	OC1C(O)CCC1	−0.628096
P48546	323	P-H	−0.633495
P48546	659	O-C-C-N-C	−0.635041
P48546	803	OC1CC(O)CCC1	−0.636694
P48546	862	CC1C(S)CCC1	−0.642228
P48546	601	N-C:C-C-N	−0.644846
P48546	392	N(~C)(~C)(~H)	−0.646986
P48546	823	CC1C(Br)CCCC1	−0.64765
P48546	759	Cc1c(Cl)cccc1	−0.65174
P48546	842	CC1CC(N)CC1	−0.652758
P48546	427	C(#C)(-C)	−0.65635
P48546	49	>= 1 Be	−0.665646
P48546	283	C-H	−0.676192
P48546	429	C(#N)(-C)	−0.67687
P48546	70	>= 1 Y	−0.67895
P48546	732	Clc1ccc(Br)cc1	−0.679215
P48546	515	N-N-C-C	−0.691118
P48546	695	O=C-C-C-C-C-N	−0.692089
P48546	748	Sc1cc(Br)ccc1	−0.694695
P48546	387	C(:C)(:N)	−0.705301
P48546	73	>= 1 Mo	−0.707066
P48546	519	N=C-N-C	−0.707353
P48546	234	>= 2 any ring size 8	−0.733327
P48546	755	Cc1c(C)cccc1	−0.746464
P48546	877	NC1C(Br)CCC1	−0.755206
P48546	642	O-C-C-C=O	−0.756098
P48546	582	C-C-C-C-C	−0.776091
P48546	669	Cl-C:C-C=O	−0.781098
P48546	114	>= 1 U	−0.790172
P48546	557	N:C-O-[#1]	−0.794721
P48546	333	C(~C)(~C)(~C)	−0.809564
P48546	836	ClC1C(Cl)CCCC1	−0.811064
P48546	503	Cl-C:C-[#1]	−0.814495
P48546	634	C-C-C:C-C	−0.816665
P48546	44	>= 2 Br	−0.821471
P48546	308	O-H	−0.828071
P48546	587	N-C:C-O-[#1]	−0.830949
P48546	816	ClC1CC(Br)CCC1	−0.831797
P48546	474	S:C:C:N	−0.832811
P48546	828	OC1C(Br)CCCC1	−0.833238
P48546	358	C(~C)(:N)	−0.835538
P48546	319	Al-Cl	−0.836448
P48546	643	[#1]-C-C-N-[#1]	−0.839611
P48546	314	O-P	−0.845508
P48546	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.852281

P48546	880	BrC1C(Br)CCC1	−0.853657
P48546	483	N-S-C:C	−0.854795
P48546	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.861574
P48546	241	>= 1 any ring size 9	−0.86556
P48546	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.874868
P48546	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.881588
P48546	268	Li-F	−0.884353
P48546	367	C(~H)(~O)(~O)	−0.887298
P48546	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.89835
P48546	33	>= 1 S	−0.899763
P48546	112	>= 1 Yb	−0.905994
P48546	23	>= 1 F	−0.930553
P48546	640	C=C-C-C-C	−0.936583
P48546	87	>= 1 Hf	−0.942165
P48546	548	O-C-C:C	−0.950811
P48546	745	Sc1cc(S)ccc1	−0.9584
P48546	614	C-C-O-C-C	−0.967487
P48546	593	N-C-C-C-N	−0.979481
P48546	431	C(-C)(-C)(=N)	−0.996933
P48546	259	>= 3 aromatic rings	−1.01006
P48546	428	C(#C)(-H)	−1.010457
P48546	756	Cc1c(O)cccc1	−1.019226
P48546	875	NC1C(N)CCC1	−1.037213
P48546	476	C-O-C=C	−1.046157
P48546	105	>= 1 Eu	−1.05653
P48546	560	N-C-N-C	−1.081371
P48546	51	>= 1 Al	−1.085077
P48546	55	>= 1 V	−1.102153
P48546	633	N-C-C:C-C	−1.115446
P48546	372	C(~H)(:C)(:N)	−1.123062
P48546	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−1.124584
P48546	110	>= 1 Er	−1.156437
P48546	589	C-C:C-O-C	−1.157314
P48546	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.160016
P48546	808	SC1CC(S)CCC1	−1.164709
P48546	841	CC1CC(S)CC1	−1.191834
P48546	258	>= 2 hetero-aromatic rings	−1.192856
P48546	397	N(~C)(:C)(:C)	−1.248372
P48546	445	C(-H)(-N)(=C)	−1.25947
P48546	504	N:C:N-C	−1.284641
P48546	165	>= 4 saturated or aromatic carbon-only ring size 5	−1.319596
P48546	11	>= 8 C	−1.345672
P48546	436	C(-C)(-H)(=O)	−1.396524
P48546	628	C-N-C-C:C	−1.399863
P48546	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−1.40258
P48546	706	O=C-C-C-C-C(=O)-C	−1.43118
P48546	306	N-Cl	−1.466796
P48546	32	>= 4 P	−1.508758

P48546	615	N-C-C-O-C	−1.541304
P48546	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−1.546209
P48546	465	O=S-C-C	−1.564963
P48546	630	O-C:C-O-C	−1.570026
P48546	811	SC1CC(Br)CCC1	−1.57371
P48546	597	O=C-C-C:C	−1.594154
P48546	312	O-Al	−1.603352
P48546	419	C#N	−1.644369
P48546	514	O-N-C-C	−1.686025
P48546	791	NC1CCC(N)CC1	−1.699399
P48546	286	C-O	−1.709976
P48546	380	C(~O)(~O)	−1.769668
P48546	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−1.796033
P48546	42	>= 2 K	−1.810317
P48546	692	O=C-C-C-C-C-C	−1.815593
P48546	650	O=C-N-C=O	−1.984711
P48546	48	>= 4 I	−2.016429
P48546	296	C-Se	−2.873785
P48546	330	C(~Br)(:C)	−2.922176

Fingerprints（continued)

P	Q
2.4714037	-0.00038
1.8898463	-0.00019
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-0.065424	-1.54E-08
-0.065436	4.20E-08

-0.065674 -8.64E-05
-0.066154 -8.92E-08
-0.066255 1.43E-08
-0.066486 -1.52E-08
-0.066611 5.62E-08
-0.066933 -3.26E-08
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 -0.06821 2.26E-06
-0.068897 0.000268
-0.068772 2.40E-08
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 -0.06926 -0.00068
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-0.072357 -0.00061
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 -0.08102 -0.00016
-0.081518 -0.00022
-0.081709 -0.00022
-0.083946 0.000486
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-0.085381 8.79E-09
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-0.089374 0.000158
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-0.097267 0.000341
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-0.098695 0.000536
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-0.114746 2.26E-08
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-0.119177 -0.00038
-0.119851 1.58E-08
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-0.135736 9.25E-08
-0.138551 0.000115

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-0.164912	2.61E-08
-0.165281	-0.00055
-0.167966	-2.70E-08
-0.16837	-0.00022
-0.178222	0.000494
-0.179843	-1.81E-08
-0.180331	-0.00031
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-0.183489	1.10E-08
-0.189547	8.20E-05
-0.190345	4.80E-08
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-0.194627	0.000482
-0.194182	-0.00022
-0.195191	4.47E-05
-0.199336	0.000659
-0.213357	-8.64E-05
-0.214781	-1.99E-05
-0.215399	-0.00023
-0.216524	-0.00017
-0.216942	-0.00041
-0.221344	-0.00039
-0.225366	0.000107
-0.231617	-2.22E-06
-0.232435	-1.85E-08
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-0.235644	0.000989
-0.242427	3.73E-08
-0.244179	1.63E-08
-0.248013	0.000352
-0.250289	4.58E-08
-0.25097	0.000444
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-0.32049	-0.00013

-0.322171	-2.41E-08
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-0.334111	-0.00018
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-0.394559	-1.65E-05
-0.402334	1.49E-05
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-0.411209	-2.99E-05
-0.425386	1.12E-08
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-0.442495	-0.00043
-0.457049	-0.00016
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-0.487439	7.24E-08
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-0.527905	0.000436
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-0.536841	0.000159
-0.536819	-0.00025
-0.541196	-8.63E-05
-0.541923	0.000298
-0.55746	-5.54E-08
-0.564122	1.19E-08
-0.578306	-0.00042
-0.580128	2.01E-09
-0.59055	6.26E-08
-0.59182	1.08E-08
-0.597162	-1.63E-08
-0.598605	-0.00018
-0.605204	0.000107

-0.609664	-0.00018
-0.612934	-0.00071
-0.614177	-0.00033
-0.628043	-5.23E-05
-0.633495	3.37E-08
-0.635485	0.000444
-0.637006	0.000312
-0.642228	2.82E-08
-0.64458	-0.00027
-0.646853	-0.00013
-0.647146	-0.0005
-0.65171	-2.99E-05
-0.65202	-0.00074
-0.65635	3.65E-08
-0.665646	-1.24E-09
-0.675969	-0.00022
-0.677128	0.000258
-0.67895	8.14E-08
-0.679215	9.75E-09
-0.691844	0.000725
-0.692362	0.000274
-0.694695	-8.66E-09
-0.705263	-3.85E-05
-0.707067	5.45E-08
-0.708233	0.00088
-0.733327	1.52E-09
-0.74608	-0.00038
-0.755206	2.80E-08
-0.755377	-0.00072
-0.775868	-0.00022
-0.781726	0.000628
-0.790172	5.50E-08
-0.794721	3.52E-08
-0.80934	-0.00022
-0.811363	0.000299
-0.814818	0.000323
-0.816442	-0.00022
-0.821471	9.07E-09
-0.827335	-0.00074
-0.830705	-0.00024
-0.831797	-5.80E-08
-0.833484	0.000673
-0.833238	9.48E-08
-0.836737	0.001199
-0.836448	2.19E-08
-0.838664	-0.00095
-0.845508	4.52E-09
-0.852281	-3.61E-08

-0.853657	5.42E-08
-0.854877	8.19E-05
-0.861574	4.91E-08
-0.86556	3.05E-08
-0.875233	0.000366
-0.881588	-1.60E-08
-0.884353	-5.23E-08
-0.887298	5.61E-08
-0.89835	-4.76E-08
-0.899997	0.000234
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-0.930436	-0.00012
-0.936359	-0.00022
-0.942165	-1.94E-08
-0.95129	0.000479
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-0.967394	-9.29E-05
-0.978849	-0.00063
-0.997524	0.000591
-1.01006	9.22E-08
-1.010457	5.26E-08
-1.0195	0.000275
-1.037213	3.71E-08
-1.045736	-0.00042
-1.05653	6.92E-08
-1.08202	0.000649
-1.085077	8.52E-08
-1.102153	4.48E-08
-1.115018	-0.00043
-1.122412	-0.00065
-1.124584	-6.62E-08
-1.156437	3.07E-08
-1.15704	-0.00027
-1.160016	-1.47E-08
-1.16471	7.90E-08
-1.191834	-4.91E-09
-1.192856	6.70E-08
-1.248068	-0.0003
-1.258819	-0.00065
-1.284147	-0.00049
-1.319596	7.86E-08
-1.345448	-0.00022
-1.396972	0.000448
-1.399807	-5.63E-05
-1.40258	4.21E-08
-1.430423	-0.00076
-1.466796	2.21E-09
-1.508758	2.96E-08

-1.541195	-0.00011
-1.546209	5.05E-08
-1.564749	-0.00021
-1.570371	0.000345
-1.57371	8.44E-08
-1.593888	-0.00027
-1.603352	3.75E-08
-1.644627	0.000258
-1.685789	-0.00024
-1.6989	-0.0005
-1.709951	-2.58E-05
-1.770103	0.000436
-1.796033	6.17E-08
-1.810317	6.60E-08
-1.815564	-2.90E-05
-1.98444	-0.00027
-2.016429	8.52E-08
-2.873785	4.37E-08
-2.92222	4.47E-05

Data S1. Ranking of importance of substructure features from Pubchem Fingerpı

GPCR ID	Bit Posit	Bit Substructure	W	P
Q14831	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	2.825405	2.8254045
Q14831	515	N-N-C-C	2.591174	2.5883188
Q14831	529	Cl-C-C-Cl	2.337395	2.3380974
Q14831	624	O=C-C:C-N	2.254718	2.2526344
Q14831	526	Cl-C:C-Cl	1.982255	1.982956
Q14831	40	>= 8 Cl	1.86008	1.8600795
Q14831	340	C(~C)(~C)(~N)	1.8194	1.8198117
Q14831	87	>= 1 Hf	1.791444	1.7914429
Q14831	731	Clc1ccc(Cl)cc1	1.762459	1.7624592
Q14831	856	NC1CC(Br)CC1	1.726581	1.7265799
Q14831	818	CC1C(C)CCCC1	1.718109	1.7166744
Q14831	24	>= 2 F	1.676768	1.6799845
Q14831	419	C#N	1.67486	1.6724805
Q14831	104	>= 1 Sm	1.664731	1.6647316
Q14831	12	>= 16 C	1.607496	1.6061527
Q14831	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	1.576704	1.5781036
Q14831	547	N-C:C-N	1.555734	1.5546214
Q14831	242	>= 1 saturated or aromatic carbon-only ring size 9	1.550334	1.5503341
Q14831	629	S-C:C-C-N	1.537978	1.5386851
Q14831	848	OC1CC(Cl)CC1	1.532833	1.5328326
Q14831	779	CC1CCC(N)CC1	1.528579	1.5265127
Q14831	342	C(~C)(~Cl)	1.520936	1.5194652
Q14831	853	SC1CC(Br)CC1	1.464266	1.4642654
Q14831	742	Oc1cc(N)ccc1	1.449481	1.448754
Q14831	755	Cc1c(C)cccc1	1.444531	1.4401643
Q14831	566	O-C-C-N	1.42508	1.4252208
Q14831	542	O-C:C-[#1]	1.41692	1.4178256
Q14831	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	1.398092	1.401189
Q14831	491	C-N:C-[#1]	1.392331	1.3892201
Q14831	850	SC1CC(S)CC1	1.358031	1.3580299
Q14831	44	>= 2 Br	1.356986	1.3569605
Q14831	641	O-C-C-C=C	1.348654	1.3484661
Q14831	370	C(~H)(:C)	1.34592	1.3455137
Q14831	555	N=C-C=C	1.345631	1.3479071
Q14831	302	N-F	1.32484	1.3248405
Q14831	506	C-C:N:C	1.324465	1.3250648
Q14831	22	>= 16 O	1.319716	1.3197148
Q14831	686	O=C-C-C-C-O	1.311418	1.3101993
Q14831	604	C-O-C-C:C	1.310069	1.3093
Q14831	821	CC1C(N)CCCC1	1.303313	1.3062534
Q14831	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	1.302615	1.300416
Q14831	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	1.302178	1.3021785
Q14831	708	C-C(C)-C-C	1.296082	1.2957358
Q14831	722	Oc1ccc(Cl)cc1	1.295145	1.2949977
Q14831	367	C(~H)(~O)(~O)	1.277222	1.2773035
Q14831	33	>= 1 S	1.268988	1.2695899

Q14831	94	>= 1 Au	1.263722	1.2637206
Q14831	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	1.255674	1.2556741
Q14831	787	SC1CCC(S)CC1	1.206498	1.206496
Q14831	863	CC1C(N)CCC1	1.173691	1.1661481
Q14831	677	C-C=C-C:C	1.17367	1.17291
Q14831	364	C(~F)(:C)	1.170031	1.1733442
Q14831	417	C#C	1.155336	1.1546293
Q14831	740	Oc1cc(O)ccc1	1.150229	1.1517176
Q14831	46	>= 1 I	1.148195	1.147067
Q14831	840	CC1CC(O)CC1	1.144263	1.1442662
Q14831	484	N-C:N:C	1.139161	1.1372148
Q14831	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	1.120882	1.1208831
Q14831	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	1.115544	1.1155439
Q14831	874	SC1C(Br)CCC1	1.115214	1.1152142
Q14831	431	C(-C)(-C)(=N)	1.104871	1.1076281
Q14831	449	C(-N)(=C)	1.102898	1.1022626
Q14831	867	OC1C(S)CCC1	1.100282	1.1002799
Q14831	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	1.096623	1.0979871
Q14831	516	[#1]-C=C-[#1]	1.095683	1.0993501
Q14831	4	>= 1 Li	1.094758	1.0947583
Q14831	726	Sc1ccc(Cl)cc1	1.080285	1.0804583
Q14831	507	C-C-S-C	1.07751	1.0753721
Q14831	407	O(~C)(~P)	1.074635	1.0744713
Q14831	648	O=N-C:C-N	1.062234	1.0625516
Q14831	644	C-C=N-N-C	1.060024	1.0614658
Q14831	610	C-O-C-O-C	1.057785	1.0578662
Q14831	460	C-C-C#C	1.056946	1.056574
Q14831	598	Cl-C:C:C-C	1.054121	1.0537069
Q14831	553	O=C-C=C	1.050014	1.0490666
Q14831	663	O-C-C-O-[#1]	1.048354	1.0508241
Q14831	743	Oc1cc(Cl)ccc1	1.04431	1.0444357
Q14831	310	O-Mg	1.043995	1.0439923
Q14831	116	>= 1 saturated or aromatic carbon-only ring size 3	1.041218	1.0407921
Q14831	837	ClC1C(Br)CCCC1	1.040544	1.0405438
Q14831	49	>= 1 Be	1.031327	1.031328
Q14831	864	CC1C(Cl)CCC1	1.015813	1.0158114
Q14831	241	>= 1 any ring size 9	1.008377	1.0083778
Q14831	771	Nc1c(Cl)cccc1	0.981449	0.9796527
Q14831	517	N-N-C-N	0.976492	0.9748476
Q14831	746	Sc1cc(N)ccc1	0.974408	0.9771581
Q14831	685	O=C-C-C-C-N	0.972769	0.9741328
Q14831	35	>= 4 S	0.96897	0.9689696
Q14831	583	Cl-C:C-O-C	0.968374	0.9686368
Q14831	628	C-N-C-C:C	0.967693	0.9722252
Q14831	268	Li-F	0.962863	0.962864
Q14831	533	S-C:C-N	0.962344	0.9618178
Q14831	472	C:N:C-C	0.958409	0.9590097
Q14831	461	O-C-C=N	0.947309	0.9485855

Q14831	763	Oc1c(N)cccc1	0.936818	0.9369035
Q14831	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.929719	0.9297171
Q14831	64	>= 1 Ge	0.927511	0.9275125
Q14831	317	F-S	0.923316	0.9233173
Q14831	401	N(~O)(~O)	0.909633	0.9099486
Q14831	78	>= 1 Cd	0.898984	0.8989826
Q14831	678	C-C-C=C-C	0.895194	0.8962459
Q14831	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.879836	0.8798375
Q14831	702	O-C-C-C-C-C-N-C	0.877878	0.8799436
Q14831	546	N-C:C-[#1]	0.861244	0.8561443
Q14831	446	C(-H)(=C)	0.856675	0.8560013
Q14831	783	OC1CCC(S)CC1	0.85413	0.8544964
Q14831	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.852614	0.8526137
Q14831	860	CC1C(C)CCC1	0.845664	0.8455357
Q14831	698	O-C-C-C-C-C-C-C	0.82299	0.8192016
Q14831	579	O=C-C-C-C	0.822206	0.8257429
Q14831	371	C(~H)(:C)(:C)	0.82103	0.8187097
Q14831	751	Nc1cc(Br)ccc1	0.805082	0.8052253
Q14831	652	O-C:C:C-N	0.800935	0.7982844
Q14831	570	C:C-C-C	0.798937	0.7997865
Q14831	354	C(~C)(~Si)	0.795037	0.7950365
Q14831	509	Br-C:C-C	0.791356	0.7918854
Q14831	764	Oc1c(Cl)cccc1	0.791272	0.791536
Q14831	543	O-C:C-N	0.772659	0.7738386
Q14831	227	>= 1 any ring size 8	0.768176	0.7671137
Q14831	259	>= 3 aromatic rings	0.764922	0.7649219
Q14831	602	O=C-C-N-C	0.758961	0.7544697
Q14831	291	C-Si	0.753312	0.7533109
Q14831	458	S(-O)(=O)	0.75216	0.7563237
Q14831	378	C(~N)(:C)(:N)	0.750903	0.7515761
Q14831	503	Cl-C:C-[#1]	0.750569	0.7502445
Q14831	535	O=C-C-C	0.748381	0.7459369
Q14831	695	O=C-C-C-C-C-N	0.745685	0.7480834
Q14831	206	>= 5 any ring size 6	0.723551	0.7244802
Q14831	811	SC1CC(Br)CCC1	0.722743	0.7232241
Q14831	456	P(-O)(=O)	0.721617	0.7215927
Q14831	581	O=C-C-C-O	0.720501	0.7216873
Q14831	69	>= 1 Sr	0.718892	0.7188925
Q14831	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.717842	0.7194141
Q14831	857	ClC1CC(Cl)CC1	0.714526	0.7145253
Q14831	376	C(~N)(:C)	0.712248	0.7104113
Q14831	256	>= 1 hetero-aromatic ring	0.710687	0.7106872
Q14831	5	>= 2 Li	0.708814	0.7088132
Q14831	803	OC1CC(O)CCC1	0.701625	0.7031108
Q14831	724	Sc1ccc(S)cc1	0.701602	0.7016014
Q14831	60	>= 1 Ni	0.698483	0.6984815
Q14831	455	N(-O)(=O)	0.695148	0.6954638
Q14831	772	Nc1c(Br)cccc1	0.691502	0.6915023

Q14831	645	O=C-N-C-C	0.69143	0.6910358
Q14831	258	>= 2 hetero-aromatic rings	0.691184	0.6911837
Q14831	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.689823	0.6898229
Q14831	442	C(-C)(=N)	0.689302	0.6890389
Q14831	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.688596	0.6885953
Q14831	711	C-C(C)(C)-C-C	0.684396	0.6857696
Q14831	754	Brc1cc(Br)ccc1	0.683695	0.683694
Q14831	96	>= 1 Tl	0.683192	0.6831924
Q14831	609	Cl-C-C-N-C	0.68152	0.6796993
Q14831	632	C-C-O-C:C	0.67718	0.680212
Q14831	571	[#1]-C-O-[#1]	0.672746	0.6763815
Q14831	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.665446	0.665447
Q14831	492	N-C:O:C	0.661859	0.6604815
Q14831	65	>= 1 As	0.654701	0.6547017
Q14831	345	C(~C)(~H)(~N)	0.650909	0.6531141
Q14831	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.650254	0.6502556
Q14831	512	C-[As]-O-[#1]	0.643605	0.6436026
Q14831	262	>= 4 hetero-aromatic rings	0.639385	0.6393851
Q14831	839	CC1CC(C)CC1	0.637415	0.636262
Q14831	833	NC1C(N)CCCC1	0.631013	0.6312606
Q14831	400	N(~H)(:C)(:C)	0.630474	0.6298261
Q14831	688	C-C-C-C-C-C-C	0.629152	0.6299286
Q14831	28	>= 1 Si	0.614781	0.6147814
Q14831	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.611789	0.6116341
Q14831	689	O-C-C-C-C-C-C	0.609224	0.6097518
Q14831	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.607283	0.6072831
Q14831	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.603785	0.6058579
Q14831	537	O=C-C-O	0.602665	0.6041778
Q14831	416	C=C	0.59779	0.600104
Q14831	289	C-Mg	0.586994	0.5869934
Q14831	559	O-C-N-[#1]	0.585312	0.585735
Q14831	483	N-S-C:C	0.584393	0.5830376
Q14831	823	CC1C(Br)CCCC1	0.58092	0.5830215
Q14831	363	C(~F)(~F)	0.580885	0.5808539
Q14831	486	N-C:N:N	0.576894	0.5752302
Q14831	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.572529	0.5728019
Q14831	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.57209	0.5716073
Q14831	671	O=C-C=C-C	0.57031	0.5739078
Q14831	466	N#C-C=C	0.568683	0.5708502
Q14831	463	N:C-S-[#1]	0.566254	0.566253
Q14831	670	Br-C:C-C-C	0.565311	0.5658417
Q14831	511	S=C-N-[#1]	0.554484	0.5540296
Q14831	630	O-C:C-O-C	0.548317	0.5474617
Q14831	294	C-Cl	0.54717	0.5451663
Q14831	200	>= 4 saturated or aromatic carbon-only ring size 6	0.546559	0.5464286
Q14831	10	>= 4 C	0.536791	0.534761
Q14831	651	O-C:C:C-C	0.536548	0.5365293
Q14831	568	N#C-C-C	0.530028	0.5286485

Q14831	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.518223	0.5182236
Q14831	737	Cc1cc(N)ccc1	0.511091	0.5085169
Q14831	786	OC1CCC(Br)CC1	0.507753	0.5077538
Q14831	30	>= 1 P	0.49869	0.4986691
Q14831	16	>= 4 N	0.495045	0.4986042
Q14831	25	>= 4 F	0.493159	0.4940068
Q14831	585	C-C:C-N-C	0.491259	0.4899982
Q14831	75	>= 1 Rh	0.488092	0.4880923
Q14831	862	CC1C(S)CCC1	0.481076	0.4820267
Q14831	157	>= 3 any ring size 5	0.476598	0.4728874
Q14831	101	>= 1 Pr	0.474059	0.4740578
Q14831	447	C(-H)(=N)	0.469698	0.4690427
Q14831	336	C(~C)(~C)(~C)(~N)	0.46745	0.4681644
Q14831	842	CC1CC(N)CC1	0.466586	0.4673878
Q14831	548	O-C-C:C	0.454128	0.4557603
Q14831	765	Oc1c(Br)cccc1	0.453245	0.4532464
Q14831	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.451923	0.4522404
Q14831	360	C(~Cl)(~Cl)	0.451182	0.4511815
Q14831	634	C-C-C:C-C	0.450896	0.4519479
Q14831	464	N-C-C=C	0.446963	0.4441684
Q14831	572	N:C:N:C	0.445407	0.445484
Q14831	633	N-C-C:C-C	0.434473	0.4336455
Q14831	551	Cl-C-C-O	0.43443	0.4331721
Q14831	277	B-F	0.417519	0.4175187
Q14831	576	N=C-C:C-[#1]	0.41457	0.4131312
Q14831	255	>= 1 aromatic ring	0.413413	0.4134133
Q14831	475	S-C=N-C	0.413133	0.4120155
Q14831	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.405867	0.4058676
Q14831	741	Oc1cc(S)ccc1	0.404643	0.4046443
Q14831	625	O=C-C:C-O	0.402388	0.4005586
Q14831	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.399355	0.3991469
Q14831	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.396448	0.3958929
Q14831	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.390747	0.3907484
Q14831	45	>= 4 Br	0.3904	0.3904001
Q14831	710	C-C-C(C)-C-C	0.388983	0.3855467
Q14831	495	C-N-C:C	0.387106	0.3871211
Q14831	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.384186	0.3841838
Q14831	861	CC1C(O)CCC1	0.380191	0.380031
Q14831	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.375613	0.3738877
Q14831	829	SC1C(S)CCCC1	0.37198	0.3719795
Q14831	34	>= 2 S	0.369835	0.3693261
Q14831	756	Cc1c(O)cccc1	0.36975	0.3727494
Q14831	501	Cl-C:C-C	0.366804	0.3650716
Q14831	788	SC1CCC(N)CC1	0.361317	0.3631887
Q14831	418	C=N	0.358912	0.3620235
Q14831	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.352795	0.3510672
Q14831	59	>= 1 Co	0.352408	0.3524074
Q14831	311	O-Na	0.348003	0.3480027

Q14831	518	O=C-N-N	0.338686	0.3370138
Q14831	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.335089	0.3350903
Q14831	573	O-C-C=C	0.333156	0.3348389
Q14831	826	OC1C(N)CCCC1	0.331224	0.3326215
Q14831	480	C:S:C-C	0.330697	0.3274498
Q14831	9	>= 2 C	0.327494	0.3251652
Q14831	832	SC1C(Br)CCCC1	0.326426	0.3264225
Q14831	13	>= 32 C	0.324147	0.3241479
Q14831	768	Sc1c(Cl)cccc1	0.313502	0.3135015
Q14831	701	O-C-C-C-C-C(O)-C	0.305182	0.3029692
Q14831	51	>= 1 Al	0.299178	0.2991786
Q14831	665	N-C:C-C-C	0.297048	0.2977874
Q14831	469	S-S-C:C	0.296428	0.2964284
Q14831	85	>= 1 Ba	0.28521	0.2852107
Q14831	699	O-C-C-C-C-C(C)-C	0.281764	0.2874774
Q14831	164	>= 4 any ring size 5	0.279293	0.2806927
Q14831	2	>= 16 H	0.275825	0.2758246
Q14831	815	ClC1CC(Cl)CCC1	0.271105	0.2738633
Q14831	207	>= 5 saturated or aromatic carbon-only ring size 6	0.26799	0.2679886
Q14831	790	SC1CCC(Br)CC1	0.260494	0.2604926
Q14831	334	C(~C)(~C)(~C)(~C)	0.260009	0.2618079
Q14831	398	N(~H)(~N)	0.258025	0.2578251
Q14831	406	O(~C)(~H)	0.256435	0.2569624
Q14831	421	C=S	0.250716	0.2504804
Q14831	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.249502	0.2495002
Q14831	89	>= 1 W	0.247783	0.2477829
Q14831	88	>= 1 Ta	0.24669	0.24669
Q14831	471	S:C:C:C	0.244706	0.2466062
Q14831	38	>= 2 Cl	0.239511	0.243519
Q14831	76	>= 1 Pd	0.236362	0.2363623
Q14831	780	CC1CCC(Cl)CC1	0.233151	0.2338233
Q14831	485	N:C:C:N	0.223733	0.2223036
Q14831	588	O=C-C-C=O	0.220543	0.2183135
Q14831	356	C(~C)(:C)(:C)	0.220449	0.2219586
Q14831	343	C(~C)(~Cl)(~H)	0.220399	0.2203986
Q14831	450	C(-N)(=N)	0.21824	0.2177536
Q14831	235	>= 2 saturated or aromatic carbon-only ring size 8	0.213906	0.2139058
Q14831	329	C(~Br)(~H)	0.213691	0.2136924
Q14831	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.205651	0.2059559
Q14831	279	B-P	0.205619	0.2056208
Q14831	74	>= 1 Ru	0.193164	0.1931664
Q14831	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.190479	0.1904792
Q14831	390	N(~C)(~C)	0.187491	0.1870082
Q14831	479	S-C-S-C	0.185513	0.1872361
Q14831	48	>= 4 I	0.180387	0.1803857
Q14831	691	O-C-C-C-C-C-N	0.177305	0.1776084
Q14831	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.175484	0.175483
Q14831	690	O-C-C-C-C-C-O	0.174703	0.1790922

Q14831	611	N-C-C-N-C	0.166264	0.1673474
Q14831	525	[As]-C:C-[#1]	0.161983	0.161983
Q14831	324	P-P	0.161687	0.1616876
Q14831	659	O-C-C-N-C	0.1607	0.1596986
Q14831	836	ClC1C(Cl)CCCC1	0.155392	0.1560942
Q14831	734	Cc1cc(C)ccc1	0.154665	0.1488633
Q14831	607	N-C-C-C:C	0.15098	0.1490178
Q14831	327	C(~Br)(~C)	0.150688	0.1505294
Q14831	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.149853	0.1498533
Q14831	248	>= 1 any ring size 10	0.149106	0.149106
Q14831	750	Nc1cc(Cl)ccc1	0.149079	0.1472967
Q14831	595	C:C-C-C-C	0.147484	0.1484389
Q14831	328	C(~Br)(~C)(~C)	0.134364	0.1348129
Q14831	643	[#1]-C-C-N-[#1]	0.129068	0.1345406
Q14831	106	>= 1 Gd	0.112945	0.1129437
Q14831	870	OC1C(Br)CCC1	0.110178	0.110179
Q14831	642	O-C-C-C=O	0.109829	0.1110174
Q14831	95	>= 1 Hg	0.10776	0.1077602
Q14831	346	C(~C)(~H)(~O)	0.106163	0.1026025
Q14831	381	C(~O)(:C)	0.099059	0.1008478
Q14831	438	C(-C)(-N)(=N)	0.098659	0.1001593
Q14831	582	C-C-C-C-C	0.09777	0.096868
Q14831	774	Clc1c(Br)cccc1	0.096193	0.0961936
Q14831	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.091215	0.0912156
Q14831	584	C:C-C=C-C	0.087234	0.086475
Q14831	640	C=C-C-C-C	0.086186	0.0868758
Q14831	606	O-C:C-C-C	0.078405	0.0829932
Q14831	14	>= 1 N	0.077198	0.0764861
Q14831	676	N#C-C-C-C	0.076246	0.075361
Q14831	875	NC1C(N)CCC1	0.07484	0.0748387
Q14831	362	C(~Cl)(:C)	0.074578	0.0731072
Q14831	618	C:C-C-C:C	0.073246	0.0761779
Q14831	123	>= 2 saturated or aromatic carbon-only ring size 3	0.072869	0.075385
Q14831	646	O=C-N-C-[#1]	0.072348	0.0700102
Q14831	565	C:C-O-C	0.069574	0.0696671
Q14831	93	>= 1 Pt	0.068332	0.0683299
Q14831	528	[#1]-N-C-[#1]	0.067312	0.0708139
Q14831	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.066083	0.0660821
Q14831	15	>= 2 N	0.060312	0.0567365
Q14831	580	O=C-C-C-N	0.058157	0.0563933
Q14831	439	C(-C)(-N)(=O)	0.055381	0.0553744
Q14831	295	C-As	0.052295	0.0522948
Q14831	98	>= 1 Bi	0.043523	0.0435245
Q14831	759	Cc1c(Cl)cccc1	0.04254	0.0444767
Q14831	626	C-O-C:C-C	0.041704	0.0409281
Q14831	11	>= 8 C	0.041473	0.0386457
Q14831	355	C(~C)(:C)	0.041324	0.0396525
Q14831	704	O=C-C-C-C-C-C-C	0.038545	0.0373137

Q14831	300	N-N	0.035545	0.0326985
Q14831	814	NC1CC(Br)CCC1	0.035244	0.0353917
Q14831	578	C-C:C-C:C	0.034788	0.0340286
Q14831	287	C-F	0.034491	0.0322795
Q14831	383	C(~S)(:C)	0.033955	0.0307148
Q14831	71	>= 1 Zr	0.033502	0.0335032
Q14831	808	SC1CC(S)CCC1	0.032967	0.0329673
Q14831	827	OC1C(Cl)CCCC1	0.032807	0.0330698
Q14831	273	B-B	0.032672	0.0326724
Q14831	257	>= 2 aromatic rings	0.032208	0.0322084
Q14831	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.03035	0.0303508
Q14831	621	N-C:C:C:N	0.029933	0.0312226
Q14831	79	>= 1 In	0.029841	0.0298435
Q14831	508	S=C-N-C	0.029774	0.0325433
Q14831	90	>= 1 Re	0.02828	0.0282788
Q14831	785	OC1CCC(Cl)CC1	0.028158	0.0280122
Q14831	817	BrC1CC(Br)CCC1	0.027807	0.0278072
Q14831	422	N=N	0.027677	0.0240209
Q14831	715	Cc1ccc(S)cc1	0.027199	0.0271928
Q14831	739	Cc1cc(Br)ccc1	0.026374	0.0282969
Q14831	129	>= 1 any ring size 4	0.025519	0.024686
Q14831	847	OC1CC(N)CC1	0.025377	0.0244954
Q14831	220	>= 2 any ring size 7	0.024558	0.0245593
Q14831	114	>= 1 U	0.024136	0.0241353
Q14831	430	C(-C)(-C)(=C)	0.023851	0.0232506
Q14831	770	Nc1c(N)cccc1	0.023183	0.023405
Q14831	657	C-N-C:C-C	0.022259	0.0209976
Q14831	350	C(~C)(~I)	0.021535	0.0204055
Q14831	478	S-C=N-[#1]	0.020686	0.0251169
Q14831	834	NC1C(Cl)CCCC1	0.019921	0.0181226
Q14831	308	O-H	0.018799	0.0181088
Q14831	316	F-P	0.018179	0.0181803
Q14831	260	>= 3 hetero-aromatic rings	0.01793	0.0179292
Q14831	57	>= 1 Mn	0.017546	0.0175462
Q14831	496	N:N-C-[#1]	0.017488	0.0206589
Q14831	298	C-I	0.01643	0.0153008
Q14831	679	C-C-C-C-C-C	0.016244	0.0163109
Q14831	359	C(~C)(:N)(:N)	0.015514	0.0162589
Q14831	47	>= 2 I	0.014634	0.0146334
Q14831	784	OC1CCC(N)CC1	0.014266	0.0133731
Q14831	144	>= 1 saturated or aromatic carbon-only ring size 5	0.013785	0.0136317
Q14831	429	C(#N)(-C)	0.013035	0.0106541
Q14831	810	SC1CC(Cl)CCC1	0.012719	0.0123079
Q14831	729	Nc1ccc(Cl)cc1	0.012639	0.0137559
Q14831	745	Sc1cc(S)ccc1	0.012585	0.0125866
Q14831	394	N(~C)(~H)(~N)	0.01228	0.0122074
Q14831	605	O=C-C-O-C	0.011888	0.0095098
Q14831	228	>= 1 saturated or aromatic carbon-only ring size 8	0.011528	0.0106207

Q14831	477	N-N-C:C	0.01147	0.0086067
Q14831	179	>= 1 saturated or aromatic carbon-only ring size 6	0.011358	0.0106178
Q14831	261	>= 4 aromatic rings	0.010912	0.0109124
Q14831	83	>= 1 Xe	0.010877	0.0108763
Q14831	534	S-C:C-O	0.010839	0.0108396
Q14831	831	SC1C(Cl)CCCC1	0.010296	0.0102954
Q14831	444	C(-Cl)(=O)	0.010251	0.0102527
Q14831	556	C=C-C-C	0.009509	0.0100907
Q14831	877	NC1C(Br)CCC1	0.00928	0.0092788
Q14831	326	As-As	0.009255	0.0092553
Q14831	653	O-C:C:C-O	0.009065	0.0103364
Q14831	499	N-C:C:N	0.008696	0.0075357
Q14831	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.008631	0.0086302
Q14831	445	C(-H)(-N)(=C)	0.00847	0.0103228
Q14831	389	C(:N)(:N)	0.008163	0.0083993
Q14831	109	>= 1 Ho	0.008163	0.0081635
Q14831	638	O-C-C-C-N	0.007633	0.0089579
Q14831	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.007262	0.0072624
Q14831	42	>= 2 K	0.006339	0.0063383
Q14831	352	C(~C)(~O)	0.006152	0.0061145
Q14831	351	C(~C)(~N)	0.005963	0.0052503
Q14831	99	>= 1 La	0.005911	0.0059102
Q14831	32	>= 4 P	0.005736	0.0057356
Q14831	413	S(~C)(~H)	0.005303	0.0053047
Q14831	271	Li-Cl	0.005185	0.0051855
Q14831	721	Oc1ccc(N)cc1	0.005038	0.0041457
Q14831	470	C:C-C=C	0.005025	0.0041195
Q14831	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.004901	0.0047456
Q14831	332	C(~C)(~C)	0.004842	0.0025117
Q14831	432	C(-C)(-C)(=O)	0.004465	0.0049798
Q14831	505	Cl-C:C-O	0.004074	0.0028176
Q14831	706	O=C-C-C-C-C(=O)-C	0.003984	0.0032262
Q14831	575	O-C-C:C-O	0.003821	0.0055092
Q14831	459	S(=O)(=O)	0.003818	0.0034148
Q14831	748	Sc1cc(Br)ccc1	0.003816	0.004297
Q14831	684	O=C-C-C-C-C	0.003536	0.0025391
Q14831	859	BrC1CC(Br)CC1	0.003032	0.0030306
Q14831	500	C-S-C:C	0.00284	0.0011125
Q14831	399	N(~H)(:C)	0.002467	0
Q14831	713	Cc1ccc(C)cc1	0.002428	0.0043366
Q14831	36	>= 8 S	0.002318	0.0023177
Q14831	841	CC1CC(S)CC1	0.002156	0.0031067
Q14831	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.002021	0.0018121
Q14831	487	N-C=N-C	0.002015	0.0014114
Q14831	392	N(~C)(~C)(~H)	0.001745	-0.001289
Q14831	592	N-C-C-C-C	0.001545	0.0024041
Q14831	497	O-C:C:N	0.001471	4.93E-06
Q14831	589	C-C:C-O-C	0.001267	0.0004885

Q14831	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.001248	0.0012481
Q14831	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.00105	0.0010518
Q14831	660	C-C=C-C-C	0.001032	0.002086
Q14831	758	Cc1c(N)cccc1	0.000989	-0.000576
Q14831	410	P(~C)(~C)	0.000961	0.0006768
Q14831	635	N-N-C-N-[#1]	0.000771	0.0014781
Q14831	373	C(~H)(:N)	0.000735	0
Q14831	27	>= 2 Na	0.000716	0.0007145
Q14831	412	S(~C)(~C)	0.000592	-0.001547
Q14831	524	C-C=C-C	0.000485	0.0013908
Q14831	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.000483	-0.002924
Q14831	386	C(:C)(:C)(:N)	0.000322	0
Q14831	481	O-S-C:C	0.00013	0.0001285
Q14831	320	Si-H	5.51E-05	5.50E-05
Q14831	0	>= 4 H	2.87E-06	0
Q14831	307	N-Br	1.21E-06	0
Q14831	796	BrC1CCC(Br)CC1	4.57E-07	0
Q14831	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	2.21E-07	0
Q14831	165	>= 4 saturated or aromatic carbon-only ring size 5	1.30E-07	0
Q14831	70	>= 1 Y	-5.51E-07	0
Q14831	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	-1.50E-06	0
Q14831	727	Sc1ccc(Br)cc1	-1.57E-06	0
Q14831	80	>= 1 Sn	-1.84E-06	0
Q14831	433	C(-C)(-Cl)(=O)	-2.00E-06	0
Q14831	700	O-C-C-C-C-C-O-C	-3.08E-05	-0.001758
Q14831	86	>= 1 Lu	-4.01E-05	-3.98E-05
Q14831	791	NC1CCC(N)CC1	-0.00017	0
Q14831	369	C(~H)(~Si)	-0.00029	-0.000288
Q14831	391	N(~C)(~C)(~C)	-0.00034	0.0016905
Q14831	292	C-P	-0.00038	-0.000237
Q14831	672	O=C-C=C-[#1]	-0.00039	0.0002466
Q14831	789	SC1CCC(Cl)CC1	-0.00046	-0.000286
Q14831	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	-0.00055	0.0020022
Q14831	601	N-C:C:C-N	-0.00066	-1.63E-05
Q14831	136	>= 2 any ring size 4	-0.00078	0
Q14831	361	C(~Cl)(~H)	-0.00084	-0.000844
Q14831	290	C-Al	-0.00094	-0.00094
Q14831	627	O=[As]-C:C:C	-0.001	-0.001005
Q14831	270	Li-S	-0.00109	-0.001092
Q14831	39	>= 4 Cl	-0.0014	-0.001466
Q14831	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	-0.00143	-0.001429
Q14831	612	N-C-O-C-C	-0.00182	0
Q14831	6	>= 1 B	-0.00211	-0.002112
Q14831	263	Li-H	-0.00214	-0.002143
Q14831	800	CC1CC(N)CCC1	-0.00243	0.0016223
Q14831	561	Cl-C-C=O	-0.00263	-0.004151
Q14831	296	C-Se	-0.00275	-0.002747
Q14831	735	Cc1cc(O)ccc1	-0.00289	-0.003655

Q14831	738	Cc1cc(Cl)ccc1	−0.00292	−0.001149
Q14831	280	B-S	−0.00297	−0.002975
Q14831	110	>= 1 Er	−0.00309	−0.003088
Q14831	798	CC1CC(O)CCC1	−0.00352	−0.006131
Q14831	339	C(~C)(~C)(~H)(~O)	−0.00415	−0.007863
Q14831	693	O=C-C-C-C-C-O	−0.00466	−0.003578
Q14831	293	C-S	−0.00485	−0.00419
Q14831	760	Cc1c(Br)cccc1	−0.00519	−0.003089
Q14831	514	O-N-C-C	−0.00555	−0.003114
Q14831	830	SC1C(N)CCCC1	−0.00584	−0.008746
Q14831	358	C(~C)(:N)	−0.00596	−0.005625
Q14831	567	O-C-C-O	−0.00612	−0.005546
Q14831	436	C(-C)(-H)(=O)	−0.00618	−0.005248
Q14831	728	Nc1ccc(N)cc1	−0.00668	−0.006662
Q14831	649	O=N-C:C-O	−0.0072	−0.007196
Q14831	62	>= 1 Zn	−0.00728	−0.007276
Q14831	63	>= 1 Ga	−0.00843	−0.008429
Q14831	733	Brc1ccc(Br)cc1	−0.00847	−0.008464
Q14831	408	O(~H)(~S)	−0.00881	−0.004682
Q14831	552	C:C-C:C	−0.00882	−0.00972
Q14831	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−0.00897	−0.008972
Q14831	812	NC1CC(N)CCC1	−0.00935	−0.007994
Q14831	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.00943	−0.009435
Q14831	599	[#1]-C-C=C-[#1]	−0.00985	−0.010445
Q14831	306	N-Cl	−0.01001	−0.010013
Q14831	425	P=O	−0.01012	−0.010141
Q14831	54	>= 1 Ti	−0.01017	−0.010166
Q14831	102	>= 1 Nd	−0.01052	−0.010518
Q14831	843	CC1CC(Cl)CC1	−0.0106	−0.010599
Q14831	423	N=O	−0.01064	−0.010836
Q14831	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.01089	−0.010893
Q14831	655	O-C-C-C:C	−0.011	−0.011187
Q14831	802	CC1CC(Br)CCC1	−0.01154	−0.00962
Q14831	871	SC1C(S)CCC1	−0.01177	−0.01177
Q14831	873	SC1C(Cl)CCC1	−0.01206	−0.01206
Q14831	122	>= 2 any ring size 3	−0.01345	−0.010934
Q14831	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.01626	−0.016264
Q14831	489	N-C-S-C	−0.01663	−0.018366
Q14831	322	Si-Cl	−0.01717	−0.017168
Q14831	108	>= 1 Dy	−0.01746	−0.01746
Q14831	876	NC1C(Cl)CC1	−0.01748	−0.017476
Q14831	368	C(~H)(~S)	−0.01753	−0.018134
Q14831	725	Sc1ccc(N)cc1	−0.01816	−0.016288
Q14831	825	OC1C(S)CCCC1	−0.01833	−0.018335
Q14831	707	O=C-C-C-C-C(N)-C	−0.01967	−0.020466
Q14831	213	>= 1 any ring size 7	−0.01993	−0.018557
Q14831	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.02034	−0.018787
Q14831	536	O=C-C-N	−0.0208	−0.018604

Q14831	465	O=S-C-C	-0.02127	-0.020024
Q14831	596	N=C-N-C-C	-0.02155	-0.016997
Q14831	58	>= 1 Fe	-0.0231	-0.023098
Q14831	53	>= 1 Sc	-0.0231	-0.023098
Q14831	330	C(~Br)(:C)	-0.02313	-0.023288
Q14831	50	>= 1 Mg	-0.02328	-0.02328
Q14831	865	CC1C(Br)CCC1	-0.02339	-0.02339
Q14831	668	C-C:C-C-C	-0.02349	-0.02244
Q14831	819	CC1C(O)CCCC1	-0.02414	-0.020462
Q14831	820	CC1C(S)CCCC1	-0.0252	-0.027462
Q14831	531	S-C:C-C	-0.02531	-0.023453
Q14831	858	ClC1CC(Br)CC1	-0.02565	-0.025646
Q14831	824	OC1C(O)CCCC1	-0.02567	-0.026702
Q14831	723	Oc1ccc(Br)cc1	-0.02623	-0.026232
Q14831	849	OC1CC(Br)CC1	-0.02643	-0.026433
Q14831	288	C-Na	-0.02797	-0.02797
Q14831	639	O-C-C-C-O	-0.0287	-0.025798
Q14831	105	>= 1 Eu	-0.02872	-0.02872
Q14831	615	N-C-C-O-C	-0.02882	-0.031103
Q14831	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	-0.02882	-0.028826
Q14831	77	>= 1 Ag	-0.02944	-0.029441
Q14831	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	-0.02999	-0.029994
Q14831	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	-0.03169	-0.032168
Q14831	694	O=C-C-C-C-C=O	-0.03239	-0.03123
Q14831	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	-0.03256	-0.032557
Q14831	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	-0.03262	-0.032616
Q14831	435	C(-C)(-H)(=N)	-0.03334	-0.03141
Q14831	272	B-H	-0.03335	-0.033349
Q14831	82	>= 1 Te	-0.03348	-0.033481
Q14831	687	O=C-C-C-C=O	-0.03357	-0.031603
Q14831	301	N-O	-0.03417	-0.032932
Q14831	636	C-N-C-N-C	-0.03432	-0.033458
Q14831	474	S:C:C:N	-0.0354	-0.036532
Q14831	544	O-C:C-O	-0.03634	-0.037101
Q14831	637	O-C-C-C-C	-0.04245	-0.04246
Q14831	623	O=C-C:C-C	-0.04289	-0.03929
Q14831	426	P=P	-0.04532	-0.045321
Q14831	353	C(~C)(~S)	-0.04622	-0.045998
Q14831	453	N(-C)(=C)	-0.05745	-0.057671
Q14831	773	Clc1c(Cl)cccc1	-0.05978	-0.05908
Q14831	305	N-S	-0.06064	-0.062342
Q14831	375	C(~N)(~N)	-0.06252	-0.064287
Q14831	457	S(-C)(=O)	-0.06371	-0.062877
Q14831	521	C:N-C-[#1]	-0.06483	-0.065346
Q14831	415	Si(~C)(~C)	-0.06639	-0.06639
Q14831	532	S-C:C-[#1]	-0.06655	-0.068031
Q14831	697	C-C-C-C-C-C(C)-C	-0.0735	-0.075989
Q14831	608	C-C-C-C:C	-0.0737	-0.072748

Q14831	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	-0.07664	-0.076522
Q14831	18	>= 1 O	-0.07907	-0.08173
Q14831	777	CC1CCC(O)CC1	-0.08144	-0.081944
Q14831	650	O=C-N-C=O	-0.0821	-0.081562
Q14831	137	>= 2 saturated or aromatic carbon-only ring size 4	-0.08225	-0.081483
Q14831	782	OC1CCC(O)CC1	-0.08397	-0.083783
Q14831	7	>= 2 B	-0.08784	-0.087841
Q14831	428	C(#C)(-H)	-0.09282	-0.094214
Q14831	286	C-O	-0.09332	-0.095648
Q14831	178	>= 1 any ring size 6	-0.09348	-0.095983
Q14831	666	C=C-C-O-C	-0.09395	-0.09472
Q14831	348	C(~C)(~H)(~P)	-0.09411	-0.093957
Q14831	427	C(#C)(-C)	-0.10252	-0.103224
Q14831	366	C(~H)(~O)	-0.10379	-0.109053
Q14831	562	Br-C-C=O	-0.10726	-0.107258
Q14831	766	Sc1c(S)cccc1	-0.10775	-0.107754
Q14831	199	>= 4 any ring size 6	-0.11341	-0.110598
Q14831	488	N-C=N-[#1]	-0.12271	-0.12439
Q14831	278	B-Si	-0.12324	-0.123242
Q14831	761	Oc1c(O)cccc1	-0.125	-0.126028
Q14831	388	C(:C)(:N)(:N)	-0.12686	-0.129231
Q14831	662	O-C-C-O-C	-0.12789	-0.127917
Q14831	714	Cc1ccc(O)cc1	-0.13022	-0.131951
Q14831	365	C(~H)(~N)	-0.13552	-0.13414
Q14831	234	>= 2 any ring size 8	-0.14593	-0.145924
Q14831	747	Sc1cc(Cl)ccc1	-0.14668	-0.147095
Q14831	312	O-Al	-0.14923	-0.149227
Q14831	304	N-P	-0.15193	-0.151933
Q14831	560	N-C-N-C	-0.15204	-0.151767
Q14831	151	>= 2 saturated or aromatic carbon-only ring size 5	-0.15667	-0.154925
Q14831	325	As-H	-0.1612	-0.161201
Q14831	185	>= 2 any ring size 6	-0.16263	-0.159166
Q14831	111	>= 1 Tm	-0.16486	-0.164858
Q14831	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	-0.16795	-0.167949
Q14831	622	O=C-O-C:C	-0.17082	-0.170958
Q14831	303	N-Si	-0.17191	-0.171906
Q14831	550	Cl-C-C-C	-0.17754	-0.179276
Q14831	792	NC1CCC(Cl)CC1	-0.17936	-0.178246
Q14831	749	Nc1cc(N)ccc1	-0.18063	-0.17893
Q14831	591	Cl-C-C-C-C	-0.18109	-0.183029
Q14831	297	C-Br	-0.18121	-0.180975
Q14831	467	C=N-N-C	-0.18275	-0.180049
Q14831	107	>= 1 Tb	-0.18435	-0.18435
Q14831	527	C:C:N-[#1]	-0.18827	-0.189543
Q14831	113	>= 1 Tc	-0.18875	-0.188745
Q14831	807	OC1CC(Br)CCC1	-0.19066	-0.190664
Q14831	409	O(:C)(:C)	-0.19314	-0.194753
Q14831	379	C(~N)(:N)	-0.19815	-0.199841

Q14831	347	C(~C)(~H)(~O)(~O)	−0.1999	−0.199901
Q14831	115	>= 1 any ring size 3	−0.21115	−0.211582
Q14831	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.21841	−0.215751
Q14831	97	>= 1 Pb	−0.2201	−0.220106
Q14831	813	NC1CC(Cl)CCC1	−0.22724	−0.229022
Q14831	476	C-O-C=C	−0.22857	−0.228479
Q14831	675	Br-C-C-C:C	−0.22871	−0.228096
Q14831	852	SC1CC(Cl)CC1	−0.22944	−0.229445
Q14831	753	Clc1cc(Br)ccc1	−0.23182	−0.231823
Q14831	387	C(:C)(:N)	−0.23783	−0.235681
Q14831	265	Li-B	−0.23834	−0.238344
Q14831	620	C:C-O-C-C	−0.23953	−0.236494
Q14831	564	C=C-C=C	−0.24074	−0.241649
Q14831	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.24171	−0.240799
Q14831	656	C-C-N-C-C	−0.24233	−0.243505
Q14831	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.25373	−0.253728
Q14831	454	N(-C)(=O)	−0.2656	−0.265798
Q14831	682	O-C-C-C-C-N	−0.26966	−0.273092
Q14831	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.2735	−0.273503
Q14831	275	B-N	−0.27418	−0.274181
Q14831	744	Oc1cc(Br)ccc1	−0.27713	−0.277127
Q14831	281	B-Cl	−0.28901	−0.28901
Q14831	437	C(-C)(-N)(=C)	−0.29218	−0.295188
Q14831	468	O=S-C-N	−0.29581	−0.295809
Q14831	333	C(~C)(~C)(~C)	−0.30536	−0.304936
Q14831	473	S-C:N:C	−0.30984	−0.311138
Q14831	341	C(~C)(~C)(~O)	−0.31789	−0.321229
Q14831	872	SC1C(N)CCC1	−0.31841	−0.31841
Q14831	405	O(~C)(~C)	−0.32041	−0.322243
Q14831	716	Cc1ccc(N)cc1	−0.3255	−0.320009
Q14831	692	O=C-C-C-C-C-C	−0.33351	−0.33684
Q14831	674	N-C-N-C:C	−0.33658	−0.335465
Q14831	513	S:C:C-[#1]	−0.33997	−0.338067
Q14831	752	Clc1cc(Cl)ccc1	−0.34165	−0.338888
Q14831	498	O-C=C-C	−0.34317	−0.344785
Q14831	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.34591	−0.345905
Q14831	838	BrC1C(Br)CCCC1	−0.34995	−0.349952
Q14831	709	C-C(C)-C-C-C	−0.35041	−0.354544
Q14831	73	>= 1 Mo	−0.35499	−0.354987
Q14831	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.36123	−0.362039
Q14831	828	OC1C(Br)CCCC1	−0.36597	−0.365969
Q14831	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.36641	−0.36988
Q14831	266	Li-C	−0.37342	−0.373419
Q14831	393	N(~C)(~H)	−0.37353	−0.372265
Q14831	539	N=C-C-[#1]	−0.3778	−0.381669
Q14831	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.37929	−0.379251
Q14831	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.3841	−0.384105
Q14831	313	O-Si	−0.38458	−0.384581

Q14831	793	NC1CCC(Br)CC1	−0.38765	−0.388424
Q14831	372	C(~H)(:C)(:N)	−0.38888	−0.387027
Q14831	775	Brc1c(Br)cccc1	−0.39277	−0.392775
Q14831	717	Cc1ccc(Cl)cc1	−0.39294	−0.392265
Q14831	597	O=C-C-C:C	−0.39675	−0.397102
Q14831	3	>= 32 H	−0.39936	−0.399361
Q14831	37	>= 1 Cl	−0.41327	−0.41027
Q14831	549	N-C-C:C	−0.41397	−0.416764
Q14831	29	>= 2 Si	−0.41834	−0.418338
Q14831	72	>= 1 Nb	−0.42671	−0.426706
Q14831	440	C(-C)(-O)(=O)	−0.42793	−0.43046
Q14831	55	>= 1 V	−0.42999	−0.429988
Q14831	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.43198	−0.432627
Q14831	338	C(~C)(~C)(~H)(~N)	−0.43855	−0.437197
Q14831	557	N:C-O-[#1]	−0.44084	−0.441262
Q14831	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.44528	−0.445286
Q14831	314	O-P	−0.4471	−0.447122
Q14831	441	C(-C)(=C)	−0.44969	−0.451628
Q14831	719	Oc1ccc(O)cc1	−0.45587	−0.455692
Q14831	264	Li-Li	−0.45672	−0.45672
Q14831	541	O-C:C-C	−0.46349	−0.465103
Q14831	282	B-Br	−0.46536	−0.465359
Q14831	482	C:N-C:C	−0.46749	−0.469571
Q14831	17	>= 8 N	−0.47263	−0.47278
Q14831	805	OC1CC(N)CCC1	−0.47707	−0.478606
Q14831	806	OC1CC(Cl)CCC1	−0.47909	−0.478966
Q14831	323	P-H	−0.48123	−0.481227
Q14831	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.48576	−0.485758
Q14831	781	CC1CCC(Br)CC1	−0.49151	−0.492326
Q14831	402	N(~O)(:O)	−0.49367	−0.493667
Q14831	720	Oc1ccc(S)cc1	−0.49631	−0.49594
Q14831	614	C-C-O-C-C	−0.4976	−0.498858
Q14831	631	O-C:C-O-[#1]	−0.50817	−0.507999
Q14831	66	>= 1 Se	−0.51381	−0.513809
Q14831	794	ClC1CCC(Cl)CC1	−0.51515	−0.515148
Q14831	703	O-C-C-C-C-C(N)-C	−0.51577	−0.51436
Q14831	683	N-C-C-C-C-C	−0.52184	−0.520463
Q14831	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.52211	−0.525452
Q14831	100	>= 1 Ce	−0.52214	−0.522145
Q14831	845	OC1CC(O)CC1	−0.53084	−0.530843
Q14831	68	>= 1 Rb	−0.54181	−0.541811
Q14831	41	>= 1 K	−0.54956	−0.549563
Q14831	712	C-C(C)-C(C)-C	−0.55634	−0.55824
Q14831	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.57237	−0.572374
Q14831	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.57628	−0.57628
Q14831	795	ClC1CCC(Br)CC1	−0.57699	−0.576991
Q14831	411	P(~O)(~O)	−0.57874	−0.578764
Q14831	593	N-C-C-C-N	−0.5828	−0.584732

Q14831	451	C(-N)(=O)	-0.58639	-0.586753
Q14831	769	Sc1c(Br)cccc1	-0.59123	-0.591233
Q14831	285	C-N	-0.59593	-0.596644
Q14831	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.60232	-0.602319
Q14831	61	>= 1 Cu	-0.60449	-0.604492
Q14831	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	-0.61213	-0.612129
Q14831	661	O-C-O-C-C	-0.6139	-0.61382
Q14831	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	-0.62685	-0.622684
Q14831	337	C(~C)(~C)(~C)(~O)	-0.62892	-0.631227
Q14831	851	SC1CC(N)CC1	-0.62892	-0.627974
Q14831	540	C-N-C-[#1]	-0.63118	-0.631924
Q14831	171	>= 5 any ring size 5	-0.63403	-0.63403
Q14831	545	N-C:C-C	-0.6348	-0.638579
Q14831	673	O=C-C=C-N	-0.63531	-0.63739
Q14831	647	O=C-N-C-N	-0.64163	-0.64056
Q14831	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	-0.64439	-0.64439
Q14831	374	C(~H)(~H)(~H)	-0.64923	-0.644062
Q14831	801	CC1CC(Cl)CCC1	-0.652	-0.650228
Q14831	844	CC1CC(Br)CC1	-0.65472	-0.654713
Q14831	669	Cl-C:C-C=O	-0.65564	-0.655306
Q14831	776	CC1CCC(C)CC1	-0.65957	-0.660378
Q14831	809	SC1CC(N)CCC1	-0.6627	-0.658994
Q14831	395	N(~C)(~O)	-0.66668	-0.665437
Q14831	569	N-C-C-N	-0.67263	-0.67199
Q14831	420	C=O	-0.67705	-0.679046
Q14831	384	C(:C)(:C)	-0.68328	-0.685297
Q14831	530	N:C-C:C	-0.68597	-0.685353
Q14831	835	NC1C(Br)CCCC1	-0.70322	-0.703218
Q14831	403	N(:C)(:C)	-0.70554	-0.704858
Q14831	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-0.70556	-0.705562
Q14831	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	-0.70825	-0.70825
Q14831	81	>= 1 Sb	-0.70948	-0.709483
Q14831	554	Br-C-C-C	-0.71241	-0.711877
Q14831	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	-0.71395	-0.714375
Q14831	172	>= 5 saturated or aromatic carbon-only ring size 5	-0.71561	-0.715611
Q14831	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	-0.71614	-0.716135
Q14831	664	C-C=C-C=C	-0.72757	-0.728327
Q14831	619	O-C-C=C-C	-0.73151	-0.728594
Q14831	868	OC1C(N)CCC1	-0.7328	-0.731491
Q14831	20	>= 4 O	-0.73492	-0.734507
Q14831	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	-0.73816	-0.738157
Q14831	522	C-N-N-[#1]	-0.74553	-0.745734
Q14831	84	>= 1 Cs	-0.74984	-0.749839
Q14831	276	B-O	-0.75778	-0.757775
Q14831	31	>= 2 P	-0.76771	-0.76771
Q14831	1	>= 8 H	-0.76801	-0.768008
Q14831	563	O-C-O-C	-0.76978	-0.769695
Q14831	397	N(~C)(:C)(:C)	-0.77394	-0.773472

Q14831	681	O-C-C-C-C-O	−0.7773	−0.773498
Q14831	284	C-C	−0.78227	−0.784598
Q14831	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.78295	−0.782953
Q14831	504	N:C:N-C	−0.79165	−0.791568
Q14831	880	BrC1C(Br)CCC1	−0.79914	−0.799136
Q14831	424	N=P	−0.80627	−0.806268
Q14831	357	C(~C)(:C)(:N)	−0.80823	−0.80595
Q14831	267	Li-O	−0.81406	−0.814058
Q14831	91	>= 1 Os	−0.82238	−0.822382
Q14831	112	>= 1 Yb	−0.83363	−0.833628
Q14831	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.8349	−0.834899
Q14831	299	N-H	−0.85113	−0.853441
Q14831	380	C(~O)(~O)	−0.85758	−0.856421
Q14831	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.85979	−0.859791
Q14831	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.87294	−0.872935
Q14831	667	C=C-C-O-[#1]	−0.87346	−0.873164
Q14831	490	C-C-C=C	−0.87565	−0.87507
Q14831	344	C(~C)(~H)	−0.87603	−0.878361
Q14831	797	CC1CC(C)CCC1	−0.88155	−0.880482
Q14831	510	[#1]-N-N-[#1]	−0.88251	−0.882515
Q14831	462	O-C-C=O	−0.88393	−0.882417
Q14831	718	Cc1ccc(Br)cc1	−0.89711	−0.897928
Q14831	558	O=N-C:C	−0.90407	−0.904918
Q14831	443	C(-C)(=O)	−0.90501	−0.907707
Q14831	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.91628	−0.916276
Q14831	92	>= 1 Ir	−0.91628	−0.91628
Q14831	822	CC1C(Cl)CCCC1	−0.93683	−0.934889
Q14831	335	C(~C)(~C)(~C)(~H)	−0.93693	−0.936256
Q14831	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.93778	−0.937778
Q14831	377	C(~N)(:C)(:C)	−0.93896	−0.936278
Q14831	730	Nc1ccc(Br)cc1	−0.94666	−0.947432
Q14831	396	N(~C)(:C)	−0.95038	−0.955653
Q14831	617	C-C-C-O-[#1]	−0.95058	−0.948195
Q14831	654	N-C-N-C-C	−0.95162	−0.95218
Q14831	846	OC1CC(S)CC1	−0.9607	−0.960702
Q14831	434	C(-C)(-H)(=C)	−0.96698	−0.969304
Q14831	658	C-C-S-C-C	−0.9672	−0.965386
Q14831	519	N=C-N-C	−0.97297	−0.97342
Q14831	19	>= 2 O	−0.9812	−0.980655
Q14831	778	CC1CCC(S)CC1	−1.01692	−1.016922
Q14831	855	NC1CC(Cl)CC1	−1.03373	−1.033734
Q14831	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−1.0368	−1.036805
Q14831	414	S(~C)(~O)	−1.03956	−1.038722
Q14831	494	O=C-C:N	−1.04274	−1.042758
Q14831	767	Sc1c(N)cccc1	−1.04384	−1.044468
Q14831	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−1.04721	−1.043281
Q14831	321	Si-Si	−1.07815	−1.078152
Q14831	866	OC1C(O)CCC1	−1.0793	−1.079304

Q14831	382	C(~O)(:C)(:C)	-1.08374	-1.083278
Q14831	448	C(-H)(=O)	-1.08438	-1.085221
Q14831	854	NC1CC(N)CC1	-1.08878	-1.08892
Q14831	523	N:C:C-C	-1.09246	-1.092719
Q14831	757	Cc1c(S)cccc1	-1.10169	-1.102824
Q14831	8	>= 4 B	-1.1044	-1.104396
Q14831	502	N-C=C-[#1]	-1.11729	-1.12088
Q14831	192	>= 3 any ring size 6	-1.12942	-1.128543
Q14831	52	>= 1 Ca	-1.13565	-1.135649
Q14831	613	C-N-C-C-C	-1.1401	-1.140624
Q14831	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	-1.14017	-1.138802
Q14831	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	-1.14637	-1.146373
Q14831	452	C(-O)(=O)	-1.14976	-1.148684
Q14831	732	Clc1ccc(Br)cc1	-1.15695	-1.15695
Q14831	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	-1.15719	-1.156435
Q14831	586	C-S-C-C-C	-1.16044	-1.155795
Q14831	736	Cc1cc(S)ccc1	-1.16065	-1.161127
Q14831	150	>= 2 any ring size 5	-1.16829	-1.166961
Q14831	43	>= 1 Br	-1.19193	-1.191694
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Q14831	799	CC1CC(S)CCC1	-1.24367	-1.243186
Q14831	274	B-C	-1.25695	-1.256946
Q14831	594	C-O-C-C=C	-1.27419	-1.274961
Q14831	318	Al-H	-1.29354	-1.293535
Q14831	21	>= 8 O	-1.30389	-1.306307
Q14831	56	>= 1 Cr	-1.30698	-1.306979
Q14831	538	N=C-C-C	-1.32007	-1.320519
Q14831	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	-1.32874	-1.328742
Q14831	158	>= 3 saturated or aromatic carbon-only ring size 5	-1.35478	-1.354778
Q14831	283	C-H	-1.36971	-1.372045
Q14831	878	ClC1C(Cl)CCC1	-1.38895	-1.388947
Q14831	385	C(:C)(:C)(:C)	-1.40652	-1.409131
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Q14831	804	OC1CC(S)CCC1	-1.40992	-1.40992
Q14831	603	C-C:C:C-C	-1.43002	-1.430777
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Q14831	577	C:C-N-C:C	-1.45603	-1.457473
Q14831	186	>= 2 saturated or aromatic carbon-only ring size 6	-1.46029	-1.460342
Q14831	319	Al-Cl	-1.47515	-1.475152
Q14831	493	O=C-C:C	-1.47997	-1.480963
Q14831	762	Oc1c(S)cccc1	-1.48577	-1.485772
Q14831	816	ClC1CC(Br)CCC1	-1.50659	-1.506593
Q14831	574	O-C-C:C-C	-1.53616	-1.532778
Q14831	67	>= 1 Kr	-1.54503	-1.545031
Q14831	590	C-C:C-O-[#1]	-1.5552	-1.555143
Q14831	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	-1.57152	-1.57152
Q14831	404	N(:C)(:C)(:C)	-1.59087	-1.5906

Q14831	680	O-C-C-C-C-C	−1.61067	−1.611767
Q14831	705	O=C-C-C-C-C(O)-C	−1.61169	−1.610908
Q14831	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−1.62442	−1.62285
Q14831	600	N-C:C:C-C	−1.62732	−1.628881
Q14831	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−1.70879	−1.708788
Q14831	616	C:C:N:N:C	−1.72607	−1.728181
Q14831	349	C(~C)(~H)(~S)	−1.7701	−1.765459
Q14831	309	O-O	−1.77949	−1.779494
Q14831	269	Li-P	−1.81498	−1.814976
Q14831	26	>= 1 Na	−1.84461	−1.844615
Q14831	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−1.91356	−1.915694
Q14831	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−1.92101	−1.921011
Q14831	23	>= 1 F	−1.96561	−1.967822
Q14831	143	>= 1 any ring size 5	−2.00179	−1.996717
Q14831	331	C(~Br)(:N)	−2.19921	−2.19944
Q14831	869	OC1C(Cl)CCC1	−2.22321	−2.22321
Q14831	696	C-C-C-C-C-C-C-C	−2.55603	−2.557363
Q14831	221	>= 2 saturated or aromatic carbon-only ring size 7	−2.79883	−2.798836
Q14831	103	>= 1 Pm	−2.9469	−2.9469

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1.44E-06
-0.000273

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
O00222	310	O-Mg	2.8447725
O00222	475	S-C=N-C	2.5003889
O00222	279	B-P	2.4446798
O00222	76	>= 1 Pd	2.4013684
O00222	739	Cc1cc(Br)ccc1	2.3336311
O00222	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	2.2260335
O00222	415	Si(~C)(~C)	2.2158173
O00222	94	>= 1 Au	2.2058843
O00222	628	C-N-C-C:C	2.0921195
O00222	546	N-C:C-[#1]	2.0635598
O00222	87	>= 1 Hf	2.0426197
O00222	206	>= 5 any ring size 6	2.0235673
O00222	525	[As]-C:C-[#1]	1.976988
O00222	862	CC1C(S)CCC1	1.9489215
O00222	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	1.932853
O00222	715	Cc1ccc(S)cc1	1.9201871
O00222	774	Clc1c(Br)cccc1	1.900947
O00222	20	>= 4 O	1.88012
O00222	78	>= 1 Cd	1.8689544
O00222	480	C:S:C-C	1.8135916
O00222	769	Sc1c(Br)cccc1	1.7957345
O00222	400	N(~H)(:C)(:C)	1.7884658
O00222	471	S:C:C:C	1.7877062
O00222	858	ClC1CC(Br)CC1	1.7583607
O00222	620	C:C-O-C-C	1.7487607
O00222	115	>= 1 any ring size 3	1.6507263
O00222	261	>= 4 aromatic rings	1.6471405
O00222	442	C(-C)(=N)	1.6466951
O00222	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	1.59779
O00222	274	B-C	1.5942257
O00222	685	O=C-C-C-C-N	1.5863258
O00222	460	C-C-C#C	1.5761976
O00222	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	1.562981
O00222	734	Cc1cc(C)ccc1	1.5617988
O00222	581	O=C-C-C-O	1.5609501
O00222	64	>= 1 Ge	1.5483115
O00222	269	Li-P	1.5207975
O00222	281	B-Cl	1.5203296
O00222	768	Sc1c(Cl)cccc1	1.5036296
O00222	340	C(~C)(~C)(~N)	1.4993605
O00222	292	C-P	1.4833799
O00222	264	Li-Li	1.4824991
O00222	298	C-I	1.473063
O00222	654	N-C-N-C-C	1.4706647
O00222	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	1.4546931
O00222	200	>= 4 saturated or aromatic carbon-only ring size 6	1.4241318

O00222	817	BrC1CC(Br)CCC1	1.4174746
O00222	258	>= 2 hetero-aromatic rings	1.4131376
O00222	854	NC1CC(N)CC1	1.4088282
O00222	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	1.3877764
O00222	692	O=C-C-C-C-C-C	1.3870802
O00222	674	N-C-N-C:C	1.3844832
O00222	683	N-C-C-C-C-C	1.3762372
O00222	499	N-C:C:N	1.3598213
O00222	373	C(~H)(:N)	1.3477805
O00222	520	C=C-C:C	1.3475995
O00222	801	CC1CC(Cl)CCC1	1.3227157
O00222	112	>= 1 Yb	1.3122114
O00222	644	C-C=N-N-C	1.3112808
O00222	672	O=C-C=C-[#1]	1.3071987
O00222	802	CC1CC(Br)CCC1	1.3062263
O00222	690	O-C-C-C-C-C-O	1.3027808
O00222	472	C:N:C-C	1.2842831
O00222	52	>= 1 Ca	1.2766759
O00222	347	C(~C)(~H)(~O)(~O)	1.2760855
O00222	270	Li-S	1.2721114
O00222	396	N(~C)(:C)	1.2395129
O00222	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	1.2301591
O00222	736	Cc1cc(S)ccc1	1.2218933
O00222	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.2215308
O00222	11	>= 8 C	1.2016583
O00222	510	[#1]-N-N-[#1]	1.198522
O00222	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	1.1915757
O00222	66	>= 1 Se	1.1880698
O00222	316	F-P	1.1869256
O00222	361	C(~Cl)(~H)	1.1830429
O00222	626	C-O-C:C-C	1.1745952
O00222	144	>= 1 saturated or aromatic carbon-only ring size 5	1.1622669
O00222	716	Cc1ccc(N)cc1	1.1582413
O00222	563	O-C-O-C	1.1495553
O00222	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	1.145114
O00222	102	>= 1 Nd	1.1274862
O00222	566	O-C-C-N	1.1251738
O00222	583	Cl-C:C-O-C	1.123526
O00222	511	S=C-N-[#1]	1.1223975
O00222	364	C(~F)(:C)	1.1125595
O00222	151	>= 2 saturated or aromatic carbon-only ring size 5	1.1108901
O00222	865	CC1C(Br)CCC1	1.1088475
O00222	164	>= 4 any ring size 5	1.1038267
O00222	762	Oc1c(S)cccc1	1.1036848
O00222	579	O=C-C-C-C	1.0872479
O00222	8	>= 4 B	1.0861556
O00222	561	Cl-C-C=O	1.0784605
O00222	587	N-C:C-O-[#1]	1.0692869

O00222	14	>= 1 N	1.0544069
O00222	562	Br-C-C=O	1.0529342
O00222	22	>= 16 O	1.0507233
O00222	618	C:C-C-C:C	1.0284333
O00222	29	>= 2 Si	1.026247
O00222	370	C(~H)(:C)	1.0244678
O00222	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	1.0192194
O00222	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	1.0187701
O00222	686	O=C-C-C-C-O	1.0110743
O00222	40	>= 8 Cl	1.0056366
O00222	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	1.0020803
O00222	228	>= 1 saturated or aromatic carbon-only ring size 8	0.9942891
O00222	590	C-C:C-O-[#1]	0.9883336
O00222	39	>= 4 Cl	0.9853693
O00222	44	>= 2 Br	0.9831398
O00222	705	O=C-C-C-C-C(O)-C	0.9805927
O00222	441	C(-C)(=C)	0.9681091
O00222	824	OC1C(O)CCCC1	0.9660099
O00222	406	O(~C)(~H)	0.9642103
O00222	677	C-C=C-C:C	0.9602495
O00222	879	ClC1C(Br)CCC1	0.9412376
O00222	425	P=O	0.9408296
O00222	805	OC1CC(N)CCC1	0.9360531
O00222	467	C=N-N-C	0.9319453
O00222	95	>= 1 Hg	0.9271616
O00222	712	C-C(C)-C(C)-C	0.925103
O00222	778	CC1CCC(S)CC1	0.9220604
O00222	864	CC1C(Cl)CCC1	0.9188494
O00222	97	>= 1 Pb	0.9126736
O00222	306	N-Cl	0.907819
O00222	816	ClC1CC(Br)CCC1	0.9057088
O00222	761	Oc1c(O)cccc1	0.8931709
O00222	309	O-O	0.8890803
O00222	744	Oc1cc(Br)ccc1	0.8860251
O00222	812	NC1CC(N)CCC1	0.882751
O00222	669	Cl-C:C-C=O	0.8818931
O00222	852	SC1CC(Cl)CC1	0.8811374
O00222	311	O-Na	0.8804615
O00222	776	CC1CCC(C)CC1	0.8546955
O00222	508	S=C-N-C	0.8532877
O00222	645	O=C-N-C-C	0.848414
O00222	752	Clc1cc(Cl)ccc1	0.8473285
O00222	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.8453756
O00222	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.8450613
O00222	664	C-C=C-C=C	0.8444653
O00222	558	O=N-C:C	0.844112
O00222	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.8400477
O00222	604	C-O-C-C:C	0.8378973

O00222	528	[#1]-N-C-[#1]	0.8364122
O00222	784	OC1CCC(N)CC1	0.8327282
O00222	567	O-C-C-O	0.8317578
O00222	872	SC1C(N)CCC1	0.8305119
O00222	276	B-O	0.827175
O00222	100	>= 1 Ce	0.8208131
O00222	514	O-N-C-C	0.8069173
O00222	849	OC1CC(Br)CC1	0.8059395
O00222	294	C-Cl	0.8044373
O00222	847	OC1CC(N)CC1	0.8033727
O00222	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.7933143
O00222	673	O=C-C=C-N	0.792683
O00222	474	S:C:C:N	0.7925574
O00222	810	SC1CC(Cl)CCC1	0.7896402
O00222	573	O-C-C=C	0.7871556
O00222	570	C:C-C-C	0.7825048
O00222	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.7750599
O00222	859	BrC1CC(Br)CC1	0.77385
O00222	486	N-C:N:N	0.7618167
O00222	312	O-Al	0.7480453
O00222	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.745466
O00222	809	SC1CC(N)CCC1	0.7430592
O00222	129	>= 1 any ring size 4	0.7378892
O00222	437	C(-C)(-N)(=C)	0.7378209
O00222	497	O-C:C:N	0.7371245
O00222	6	>= 1 B	0.7296867
O00222	192	>= 3 any ring size 6	0.7242053
O00222	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.7177352
O00222	304	N-P	0.7166377
O00222	330	C(~Br)(:C)	0.716212
O00222	560	N-C-N-C	0.7013248
O00222	820	CC1C(S)CCCC1	0.7002081
O00222	318	Al-H	0.6953677
O00222	57	>= 1 Mn	0.6942741
O00222	303	N-Si	0.689574
O00222	389	C(:N)(:N)	0.6868357
O00222	754	Brc1cc(Br)ccc1	0.6863844
O00222	25	>= 4 F	0.6856802
O00222	444	C(-Cl)(=O)	0.6845699
O00222	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.6823716
O00222	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.6800715
O00222	165	>= 4 saturated or aromatic carbon-only ring size 5	0.6792135
O00222	554	Br-C-C-C	0.6744108
O00222	671	O=C-C=C-C	0.67037
O00222	213	>= 1 any ring size 7	0.6644073
O00222	367	C(~H)(~O)(~O)	0.661841
O00222	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.6522897
O00222	760	Cc1c(Br)cccc1	0.6452759

O00222	98	>= 1 Bi	0.6418377
O00222	838	BrC1C(Br)CCCC1	0.6397181
O00222	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.6392439
O00222	331	C(~Br)(:N)	0.6383985
O00222	571	[#1]-C-O-[#1]	0.6370846
O00222	853	SC1CC(Br)CC1	0.6271285
O00222	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.6248785
O00222	722	Oc1ccc(Cl)cc1	0.6200812
O00222	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.6179645
O00222	419	C#N	0.6165105
O00222	296	C-Se	0.5993648
O00222	656	C-C-N-C-C	0.5944577
O00222	465	O=S-C-C	0.5907164
O00222	429	C(#N)(-C)	0.5870484
O00222	580	O=C-C-C-N	0.578223
O00222	745	Sc1cc(S)ccc1	0.5776677
O00222	500	C-S-C:C	0.5760557
O00222	193	>= 3 saturated or aromatic carbon-only ring size 6	0.5717756
O00222	806	OC1CC(Cl)CCC1	0.5685875
O00222	601	N-C:C:C-N	0.568447
O00222	37	>= 1 Cl	0.5676183
O00222	368	C(~H)(~S)	0.5639264
O00222	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.5561972
O00222	704	O=C-C-C-C-C-C-C	0.5532014
O00222	502	N-C=C-[#1]	0.548355
O00222	93	>= 1 Pt	0.5480994
O00222	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.5334076
O00222	691	O-C-C-C-C-C-N	0.5273956
O00222	868	OC1C(N)CCC1	0.5261071
O00222	538	N=C-C-C	0.5243598
O00222	75	>= 1 Rh	0.5226234
O00222	256	>= 1 hetero-aromatic ring	0.5222934
O00222	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.518816
O00222	678	C-C-C=C-C	0.5175771
O00222	655	O-C-C-C:C	0.515395
O00222	490	C-C-C=C	0.5107982
O00222	837	ClC1C(Br)CCCC1	0.5090377
O00222	291	C-Si	0.5059656
O00222	807	OC1CC(Br)CCC1	0.50379
O00222	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.5030247
O00222	266	Li-C	0.4974962
O00222	696	C-C-C-C-C-C-C-C	0.4974768
O00222	803	OC1CC(O)CCC1	0.4968146
O00222	498	O-C=C-C	0.4925354
O00222	380	C(~O)(~O)	0.4838889
O00222	658	C-C-S-C-C	0.4795231
O00222	481	O-S-C:C	0.4746478
O00222	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.4726143

O00222	443	C(-C)(=O)	0.4721768
O00222	793	NC1CCC(Br)CC1	0.4664647
O00222	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.4644155
O00222	568	N#C-C-C	0.4630014
O00222	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.4603129
O00222	401	N(~O)(~O)	0.4576628
O00222	804	OC1CC(S)CCC1	0.4548765
O00222	751	Nc1cc(Br)ccc1	0.4527506
O00222	395	N(~C)(~O)	0.4510933
O00222	723	Oc1ccc(Br)cc1	0.4509302
O00222	384	C(:C)(:C)	0.4486941
O00222	470	C:C-C=C	0.4476785
O00222	825	OC1C(S)CCCC1	0.4450365
O00222	584	C:C-C=C-C	0.4417533
O00222	814	NC1CC(Br)CCC1	0.4371896
O00222	334	C(~C)(~C)(~C)(~C)	0.433012
O00222	811	SC1CC(Br)CCC1	0.4276767
O00222	90	>= 1 Re	0.4256927
O00222	765	Oc1c(Br)cccc1	0.4252385
O00222	625	O=C-C:C-O	0.4235015
O00222	424	N=P	0.4215792
O00222	463	N:C-S-[#1]	0.4204447
O00222	366	C(~H)(~O)	0.4188903
O00222	453	N(-C)(=C)	0.4130241
O00222	732	Clc1ccc(Br)cc1	0.4118685
O00222	740	Oc1cc(O)ccc1	0.4087573
O00222	36	>= 8 S	0.3996779
O00222	171	>= 5 any ring size 5	0.3936114
O00222	876	NC1C(Cl)CC1	0.3912035
O00222	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.3904159
O00222	629	S-C:C:C-N	0.3821578
O00222	540	C-N-C-[#1]	0.3781716
O00222	711	C-C(C)(C)-C-C	0.377588
O00222	33	>= 1 S	0.3771418
O00222	455	N(-O)(=O)	0.3701709
O00222	657	C-N-C:C-C	0.3652204
O00222	706	O=C-C-C-C-C(=O)-C	0.3649805
O00222	487	N-C=N-C	0.3647686
O00222	724	Sc1ccc(S)cc1	0.362299
O00222	114	>= 1 U	0.3605025
O00222	756	Cc1c(O)cccc1	0.3577561
O00222	492	N-C:O:C	0.3531691
O00222	459	S(=O)(=O)	0.3507919
O00222	537	O=C-C-O	0.3491693
O00222	737	Cc1cc(N)ccc1	0.3489996
O00222	328	C(~Br)(~C)(~C)	0.3478293
O00222	550	Cl-C-C-C	0.3476958
O00222	130	>= 1 saturated or aromatic carbon-only ring size 4	0.3475164

O00222	16	>= 4 N	0.3461353
O00222	272	B-H	0.3439823
O00222	436	C(-C)(-H)(=O)	0.3382385
O00222	661	O-C-O-C-C	0.3333718
O00222	325	As-H	0.3325065
O00222	378	C(~N)(:C)(:N)	0.3296552
O00222	235	>= 2 saturated or aromatic carbon-only ring size 8	0.3277156
O00222	456	P(-O)(=O)	0.3241189
O00222	363	C(~F)(~F)	0.3234144
O00222	482	C:N-C:C	0.3224497
O00222	103	>= 1 Pm	0.3222911
O00222	339	C(~C)(~C)(~H)(~O)	0.3200516
O00222	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.3199467
O00222	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.3060994
O00222	150	>= 2 any ring size 5	0.3038078
O00222	137	>= 2 saturated or aromatic carbon-only ring size 4	0.2996096
O00222	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.2987346
O00222	548	O-C-C:C	0.2968805
O00222	58	>= 1 Fe	0.2917385
O00222	589	C-C:C-O-C	0.2902384
O00222	457	S(-C)(=O)	0.2892599
O00222	665	N-C:C-C-C	0.2859678
O00222	602	O=C-C-N-C	0.2782726
O00222	660	C-C=C-C-C	0.2765313
O00222	61	>= 1 Cu	0.2753759
O00222	721	Oc1ccc(N)cc1	0.2748519
O00222	82	>= 1 Te	0.2743891
O00222	214	>= 1 saturated or aromatic carbon-only ring size 7	0.2708402
O00222	341	C(~C)(~C)(~O)	0.2671556
O00222	136	>= 2 any ring size 4	0.2669977
O00222	708	C-C(C)-C-C	0.2669745
O00222	77	>= 1 Ag	0.26534
O00222	399	N(~H)(:C)	0.2642196
O00222	622	O=C-O-C:C	0.2634314
O00222	612	N-C-O-C-C	0.2596976
O00222	728	Nc1ccc(N)cc1	0.2594895
O00222	451	C(-N)(=O)	0.258238
O00222	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.2579799
O00222	242	>= 1 saturated or aromatic carbon-only ring size 9	0.2579255
O00222	59	>= 1 Co	0.2549026
O00222	172	>= 5 saturated or aromatic carbon-only ring size 5	0.2499836
O00222	464	N-C-C=C	0.2489985
O00222	382	C(~O)(:C)(:C)	0.2465292
O00222	3	>= 32 H	0.2436512
O00222	675	Br-C-C-C:C	0.2358518
O00222	358	C(~C)(:N)	0.23437
O00222	593	N-C-C-C-N	0.2253893
O00222	611	N-C-C-N-C	0.2247206

O00222	729	Nc1ccc(Cl)cc1	0.2247189
O00222	539	N=C-C-[#1]	0.2172378
O00222	555	N=C-C=C	0.2143061
O00222	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.2087398
O00222	484	N-C:N:C	0.2069021
O00222	290	C-Al	0.2064908
O00222	506	C-C:N:C	0.2056111
O00222	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.2051092
O00222	468	O=S-C-N	0.203499
O00222	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.2025406
O00222	381	C(~O)(:C)	0.1910558
O00222	263	Li-H	0.1869918
O00222	834	NC1C(Cl)CCCC1	0.1841661
O00222	544	O-C:C-O	0.1789733
O00222	533	S-C:C-N	0.1699792
O00222	782	OC1CCC(O)CC1	0.1691825
O00222	526	Cl-C:C-Cl	0.1586571
O00222	819	CC1C(O)CCCC1	0.1546196
O00222	305	N-S	0.1459787
O00222	556	C=C-C-C	0.145404
O00222	848	OC1CC(Cl)CC1	0.1447162
O00222	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.1440368
O00222	841	CC1CC(S)CC1	0.1436272
O00222	317	F-S	0.1400907
O00222	54	>= 1 Ti	0.1320539
O00222	717	Cc1ccc(Cl)cc1	0.1315423
O00222	534	S-C:C-O	0.1292221
O00222	43	>= 1 Br	0.1271206
O00222	749	Nc1cc(N)ccc1	0.1257737
O00222	659	O-C-C-N-C	0.12577
O00222	595	C:C-C-C-C	0.1231271
O00222	313	O-Si	0.1156395
O00222	19	>= 2 O	0.1128122
O00222	485	N:C:C:N	0.1122046
O00222	34	>= 2 S	0.1101877
O00222	750	Nc1cc(Cl)ccc1	0.1080627
O00222	531	S-C:C-C	0.1040065
O00222	352	C(~C)(~O)	0.1023962
O00222	598	Cl-C:C:C-C	0.1008146
O00222	569	N-C-C-N	0.0999558
O00222	507	C-C-S-C	0.0995359
O00222	421	C=S	0.0995336
O00222	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.097916
O00222	432	C(-C)(-C)(=O)	0.0971842
O00222	92	>= 1 Ir	0.0968313
O00222	18	>= 1 O	0.0942191
O00222	650	O=C-N-C=O	0.0929216
O00222	357	C(~C)(:C)(:N)	0.0916998

O00222	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0861994
O00222	84	>= 1 Cs	0.0850791
O00222	651	O-C:C:C-C	0.084255
O00222	637	O-C-C-C-C	0.0832195
O00222	17	>= 8 N	0.0826273
O00222	300	N-N	0.0705802
O00222	307	N-Br	0.0693402
O00222	785	OC1CCC(Cl)CC1	0.0668843
O00222	365	C(~H)(~N)	0.0541079
O00222	348	C(~C)(~H)(~P)	0.0483121
O00222	788	SC1CCC(N)CC1	0.0482141
O00222	766	Sc1c(S)cccc1	0.0462149
O00222	585	C-C:C-N-C	0.045394
O00222	12	>= 16 C	0.0428689
O00222	473	S-C:N:C	0.0426627
O00222	308	O-H	0.0416261
O00222	857	ClC1CC(Cl)CC1	0.0407715
O00222	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0387995
O00222	833	NC1C(N)CCCC1	0.0358234
O00222	297	C-Br	0.0280429
O00222	553	O=C-C=C	0.027649
O00222	277	B-F	0.0273517
O00222	476	C-O-C=C	0.0246723
O00222	680	O-C-C-C-C-C	0.0223386
O00222	535	O=C-C-C	0.0202806
O00222	67	>= 1 Kr	0.0198478
O00222	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0171967
O00222	731	Clc1ccc(Cl)cc1	0.0170963
O00222	662	O-C-C-O-C	0.0170434
O00222	621	N-C:C:C:N	0.0167684
O00222	69	>= 1 Sr	0.0166955
O00222	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0163885
O00222	875	NC1C(N)CCC1	0.0156052
O00222	846	OC1CC(S)CC1	0.0155731
O00222	439	C(-C)(-N)(=O)	0.0152841
O00222	301	N-O	0.0142942
O00222	438	C(-C)(-N)(=N)	0.0133911
O00222	818	CC1C(C)CCCC1	0.0128504
O00222	576	N=C-C:C-[#1]	0.0128253
O00222	758	Cc1c(N)cccc1	0.0115526
O00222	505	Cl-C:C-O	0.0113929
O00222	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.0103103
O00222	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0096176
O00222	668	C-C:C-C-C	0.0095401
O00222	7	>= 2 B	0.0088789
O00222	469	S-S-C:C	0.0087878
O00222	792	NC1CCC(Cl)CC1	0.0077445
O00222	445	C(-H)(-N)(=C)	0.0068202

O00222	178	>= 1 any ring size 6	0.0065746
O00222	800	CC1CC(N)CCC1	0.0058061
O00222	73	>= 1 Mo	0.0052585
O00222	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0050177
O00222	828	OC1C(Br)CCCC1	0.0047671
O00222	616	C:C:N:N:C	0.0040547
O00222	515	N-N-C-C	0.0040398
O00222	647	O=C-N-C-N	0.0038795
O00222	346	C(~C)(~H)(~O)	0.0030615
O00222	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.0027322
O00222	588	O=C-C-C=O	0.0026
O00222	157	>= 3 any ring size 5	0.0024288
O00222	267	Li-O	0.0020235
O00222	790	SC1CCC(Br)CC1	0.0019265
O00222	835	NC1C(Br)CCCC1	0.0015592
O00222	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.0013801
O00222	342	C(~C)(~Cl)	0.0007911
O00222	856	NC1CC(Br)CC1	0.0004443
O00222	738	Cc1cc(Cl)ccc1	0.0003591
O00222	420	C=O	0.0002882
O00222	386	C(:C)(:C)(:N)	0.0002775
O00222	698	O-C-C-C-C-C-C-C	0.0001971
O00222	158	>= 3 saturated or aromatic carbon-only ring size 5	5.84E-07
O00222	829	SC1C(S)CCCC1	4.55E-08
O00222	280	B-S	-2.93E-07
O00222	99	>= 1 La	-6.93E-07
O00222	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	-1.94E-05
O00222	80	>= 1 Sn	-8.24E-05
O00222	640	C=C-C-C-C	-9.04E-05
O00222	410	P(~C)(~C)	-0.000317
O00222	821	CC1C(N)CCCC1	-0.000323
O00222	699	O-C-C-C-C-C(C)-C	-0.001473
O00222	387	C(:C)(:N)	-0.001474
O00222	81	>= 1 Sb	-0.00153
O00222	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	-0.001647
O00222	796	BrC1CCC(Br)CC1	-0.002503
O00222	50	>= 1 Mg	-0.002635
O00222	282	B-Br	-0.002695
O00222	860	CC1C(C)CCC1	-0.004182
O00222	101	>= 1 Pr	-0.004846
O00222	284	C-C	-0.004896
O00222	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	-0.005141
O00222	179	>= 1 saturated or aromatic carbon-only ring size 6	-0.005642
O00222	375	C(~N)(~N)	-0.006742
O00222	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	-0.006936
O00222	755	Cc1c(C)cccc1	-0.007034
O00222	24	>= 2 F	-0.008024
O00222	287	C-F	-0.009029

O00222	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-0.009427
O00222	543	O-C:C-N	-0.010535
O00222	763	Oc1c(N)cccc1	-0.010903
O00222	423	N=O	-0.01112
O00222	564	C=C-C=C	-0.01139
O00222	599	[#1]-C-C=C-[#1]	-0.011567
O00222	314	O-P	-0.012145
O00222	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	-0.013958
O00222	522	C-N-N-[#1]	-0.01411
O00222	718	Cc1ccc(Br)cc1	-0.014248
O00222	867	OC1C(S)CCC1	-0.014718
O00222	26	>= 1 Na	-0.015185
O00222	433	C(-C)(-Cl)(=O)	-0.015299
O00222	843	CC1CC(Cl)CC1	-0.015417
O00222	832	SC1C(Br)CCCC1	-0.016032
O00222	607	N-C-C-C:C	-0.016677
O00222	517	N-N-C-N	-0.017055
O00222	335	C(~C)(~C)(~C)(~H)	-0.020767
O00222	813	NC1CC(Cl)CCC1	-0.02095
O00222	9	>= 2 C	-0.021825
O00222	703	O-C-C-C-C-C(N)-C	-0.021841
O00222	771	Nc1c(Cl)cccc1	-0.022272
O00222	545	N-C:C-C	-0.023009
O00222	379	C(~N)(:N)	-0.023741
O00222	491	C-N:C-[#1]	-0.023794
O00222	684	O=C-C-C-C-C	-0.026818
O00222	764	Oc1c(Cl)cccc1	-0.027837
O00222	719	Oc1ccc(O)cc1	-0.034511
O00222	783	OC1CCC(S)CC1	-0.035842
O00222	642	O-C-C-C=O	-0.036945
O00222	299	N-H	-0.038234
O00222	302	N-F	-0.050017
O00222	850	SC1CC(S)CC1	-0.05096
O00222	700	O-C-C-C-C-C-O-C	-0.054412
O00222	670	Br-C:C:C-C	-0.068388
O00222	2	>= 16 H	-0.069126
O00222	32	>= 4 P	-0.079119
O00222	681	O-C-C-C-C-O	-0.081591
O00222	48	>= 4 I	-0.084118
O00222	199	>= 4 any ring size 6	-0.084541
O00222	107	>= 1 Tb	-0.087237
O00222	412	S(~C)(~C)	-0.088424
O00222	72	>= 1 Nb	-0.088957
O00222	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	-0.0904
O00222	109	>= 1 Ho	-0.092443
O00222	285	C-N	-0.093773
O00222	345	C(~C)(~H)(~N)	-0.094019
O00222	28	>= 1 Si	-0.095273

O00222	21	>= 8 O	-0.098285
O00222	689	O-C-C-C-C-C-C	-0.099121
O00222	377	C(~N)(:C)(:C)	-0.099441
O00222	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	-0.103597
O00222	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	-0.117682
O00222	746	Sc1cc(N)ccc1	-0.119243
O00222	275	B-N	-0.121791
O00222	393	N(~C)(~H)	-0.126194
O00222	646	O=C-N-C-[#1]	-0.12658
O00222	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	-0.132746
O00222	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	-0.134164
O00222	431	C(-C)(-C)(=N)	-0.135369
O00222	371	C(~H)(:C)(:C)	-0.137303
O00222	427	C(#C)(-C)	-0.138573
O00222	450	C(-N)(=N)	-0.138834
O00222	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	-0.141653
O00222	428	C(#C)(-H)	-0.143534
O00222	391	N(~C)(~C)(~C)	-0.1442
O00222	388	C(:C)(:N)(:N)	-0.145803
O00222	878	ClC1C(Cl)CCC1	-0.14749
O00222	743	Oc1cc(Cl)ccc1	-0.148258
O00222	594	C-O-C-C=C	-0.153214
O00222	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	-0.155931
O00222	260	>= 3 hetero-aromatic rings	-0.156246
O00222	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	-0.157391
O00222	283	C-H	-0.15757
O00222	727	Sc1ccc(Br)cc1	-0.159304
O00222	434	C(-C)(-H)(=C)	-0.159892
O00222	870	OC1C(Br)CCC1	-0.162556
O00222	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	-0.166603
O00222	608	C-C-C-C:C	-0.168195
O00222	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	-0.171589
O00222	688	C-C-C-C-C-C-C	-0.174308
O00222	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	-0.175259
O00222	362	C(~Cl)(:C)	-0.179326
O00222	789	SC1CCC(Cl)CC1	-0.183872
O00222	79	>= 1 In	-0.187563
O00222	360	C(~Cl)(~Cl)	-0.189702
O00222	574	O-C-C:C-C	-0.193966
O00222	547	N-C:C-N	-0.197474
O00222	836	ClC1C(Cl)CCCC1	-0.200208
O00222	682	O-C-C-C-C-N	-0.200345
O00222	47	>= 2 I	-0.211437
O00222	353	C(~C)(~S)	-0.212764
O00222	714	Cc1ccc(O)cc1	-0.213222
O00222	68	>= 1 Rb	-0.214653
O00222	730	Nc1ccc(Br)cc1	-0.219674
O00222	372	C(~H)(:C)(:N)	-0.226435

O00222	693	O=C-C-C-C-C-O	−0.226739
O00222	624	O=C-C:C-N	−0.226807
O00222	403	N(:C)(:C)	−0.229818
O00222	635	N-N-C-N-[#1]	−0.231524
O00222	122	>= 2 any ring size 3	−0.235395
O00222	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.235996
O00222	652	O-C:C:C-N	−0.240242
O00222	392	N(~C)(~C)(~H)	−0.243123
O00222	799	CC1CC(S)CCC1	−0.243693
O00222	600	N-C:C:C-C	−0.246464
O00222	575	O-C-C:C-O	−0.246738
O00222	0	>= 4 H	−0.247393
O00222	447	C(-H)(=N)	−0.254283
O00222	775	Brc1c(Br)cccc1	−0.254408
O00222	31	>= 2 P	−0.256459
O00222	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.261494
O00222	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.266167
O00222	344	C(~C)(~H)	−0.268045
O00222	143	>= 1 any ring size 5	−0.275479
O00222	398	N(~H)(~N)	−0.27794
O00222	720	Oc1ccc(S)cc1	−0.27839
O00222	877	NC1C(Br)CCC1	−0.278713
O00222	293	C-S	−0.283666
O00222	606	O-C:C-C-C	−0.292805
O00222	49	>= 1 Be	−0.293097
O00222	336	C(~C)(~C)(~C)(~N)	−0.293136
O00222	823	CC1C(Br)CCCC1	−0.294434
O00222	110	>= 1 Er	−0.306187
O00222	323	P-H	−0.31085
O00222	557	N:C-O-[#1]	−0.318654
O00222	327	C(~Br)(~C)	−0.320571
O00222	767	Sc1c(N)cccc1	−0.322144
O00222	329	C(~Br)(~H)	−0.324242
O00222	842	CC1CC(N)CC1	−0.333175
O00222	605	O=C-C-O-C	−0.334301
O00222	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.334836
O00222	880	BrC1C(Br)CCC1	−0.334902
O00222	337	C(~C)(~C)(~C)(~O)	−0.336584
O00222	795	ClC1CCC(Br)CC1	−0.337572
O00222	753	Clc1cc(Br)ccc1	−0.338665
O00222	578	C-C:C-C:C	−0.341706
O00222	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.3482
O00222	610	C-O-C-O-C	−0.35889
O00222	63	>= 1 Ga	−0.359294
O00222	757	Cc1c(S)cccc1	−0.363001
O00222	108	>= 1 Dy	−0.363339
O00222	494	O=C-C:N	−0.364378
O00222	532	S-C:C-[#1]	−0.366732

O00222	542	O-C:C-[#1]	−0.367058
O00222	666	C=C-C-O-C	−0.368012
O00222	55	>= 1 V	−0.371298
O00222	288	C-Na	−0.372204
O00222	844	CC1CC(Br)CC1	−0.373901
O00222	603	C-C:C:C-C	−0.376542
O00222	639	O-C-C-C-O	−0.376652
O00222	777	CC1CCC(O)CC1	−0.376679
O00222	326	As-As	−0.38346
O00222	71	>= 1 Zr	−0.390906
O00222	572	N:C:N:C	−0.391185
O00222	374	C(~H)(~H)(~H)	−0.393203
O00222	113	>= 1 Tc	−0.397126
O00222	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.400525
O00222	265	Li-B	−0.402789
O00222	478	S-C=N-[#1]	−0.41356
O00222	369	C(~H)(~Si)	−0.41625
O00222	111	>= 1 Tm	−0.417478
O00222	41	>= 1 K	−0.422097
O00222	503	Cl-C:C-[#1]	−0.428173
O00222	477	N-N-C:C	−0.433606
O00222	85	>= 1 Ba	−0.439759
O00222	725	Sc1ccc(N)cc1	−0.443773
O00222	430	C(-C)(-C)(=C)	−0.44488
O00222	509	Br-C:C-C	−0.449267
O00222	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.451685
O00222	633	N-C-C:C-C	−0.453645
O00222	619	O-C-C=C-C	−0.476993
O00222	416	C=C	−0.477365
O00222	70	>= 1 Y	−0.479184
O00222	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.482994
O00222	51	>= 1 Al	−0.485937
O00222	405	O(~C)(~C)	−0.488052
O00222	418	C=N	−0.493984
O00222	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.499222
O00222	446	C(-H)(=C)	−0.499649
O00222	86	>= 1 Lu	−0.505501
O00222	873	SC1C(Cl)CCC1	−0.510909
O00222	701	O-C-C-C-C-C(O)-C	−0.513814
O00222	448	C(-H)(=O)	−0.517072
O00222	521	C:N-C-[#1]	−0.517914
O00222	504	N:C:N-C	−0.519025
O00222	227	>= 1 any ring size 8	−0.521982
O00222	268	Li-F	−0.523409
O00222	454	N(-C)(=O)	−0.531377
O00222	385	C(:C)(:C)(:C)	−0.536233
O00222	38	>= 2 Cl	−0.542487
O00222	248	>= 1 any ring size 10	−0.54253

O00222	516	[#1]-C=C-[#1]	−0.543359
O00222	83	>= 1 Xe	−0.547566
O00222	735	Cc1cc(O)ccc1	−0.548014
O00222	702	O-C-C-C-C-C-N-C	−0.548196
O00222	241	>= 1 any ring size 9	−0.549846
O00222	759	Cc1c(Cl)cccc1	−0.551722
O00222	695	O=C-C-C-C-C-N	−0.553279
O00222	648	O=N-C:C-N	−0.554724
O00222	851	SC1CC(N)CC1	−0.578013
O00222	582	C-C-C-C-C	−0.579901
O00222	390	N(~C)(~C)	−0.580938
O00222	319	Al-Cl	−0.58336
O00222	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.584603
O00222	1	>= 8 H	−0.584878
O00222	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.588179
O00222	185	>= 2 any ring size 6	−0.589451
O00222	747	Sc1cc(Cl)ccc1	−0.59502
O00222	643	[#1]-C-C-N-[#1]	−0.597184
O00222	408	O(~H)(~S)	−0.606986
O00222	742	Oc1cc(N)ccc1	−0.609483
O00222	551	Cl-C-C-O	−0.612707
O00222	359	C(~C)(:N)(:N)	−0.620246
O00222	667	C=C-C-O-[#1]	−0.62067
O00222	35	>= 4 S	−0.624421
O00222	815	ClC1CC(Cl)CCC1	−0.627185
O00222	354	C(~C)(~Si)	−0.630721
O00222	407	O(~C)(~P)	−0.63307
O00222	779	CC1CCC(N)CC1	−0.633523
O00222	426	P=P	−0.637304
O00222	321	Si-Si	−0.640455
O00222	710	C-C-C(C)-C-C	−0.644342
O00222	527	C:C:N-[#1]	−0.647313
O00222	726	Sc1ccc(Cl)cc1	−0.649444
O00222	529	Cl-C-C-Cl	−0.650033
O00222	787	SC1CCC(S)CC1	−0.650073
O00222	96	>= 1 Tl	−0.650977
O00222	449	C(-N)(=C)	−0.653641
O00222	234	>= 2 any ring size 8	−0.655103
O00222	559	O-C-N-[#1]	−0.660045
O00222	383	C(~S)(:C)	−0.660442
O00222	278	B-Si	−0.660482
O00222	707	O=C-C-C-C-C(N)-C	−0.662716
O00222	772	Nc1c(Br)cccc1	−0.669168
O00222	577	C:C-N-C:C	−0.670374
O00222	676	N#C-C-C-C	−0.673573
O00222	496	N:N-C-[#1]	−0.681638
O00222	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.684497
O00222	614	C-C-O-C-C	−0.686235

O00222	88	>= 1 Ta	-0.696457
O00222	5	>= 2 Li	-0.698973
O00222	435	C(-C)(-H)(=N)	-0.704216
O00222	495	C-N-C:C	-0.709874
O00222	397	N(~C)(:C)(:C)	-0.712164
O00222	461	O-C-C=N	-0.717373
O00222	630	O-C:C-O-C	-0.719649
O00222	320	Si-H	-0.719722
O00222	104	>= 1 Sm	-0.7269
O00222	27	>= 2 Na	-0.729084
O00222	524	C-C=C-C	-0.737569
O00222	609	Cl-C-C-N-C	-0.738843
O00222	863	CC1C(N)CCC1	-0.74312
O00222	46	>= 1 I	-0.744459
O00222	349	C(~C)(~H)(~S)	-0.757
O00222	262	>= 4 hetero-aromatic rings	-0.764006
O00222	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	-0.767248
O00222	106	>= 1 Gd	-0.775615
O00222	615	N-C-C-O-C	-0.78494
O00222	452	C(-O)(=O)	-0.785131
O00222	855	NC1CC(Cl)CC1	-0.786927
O00222	697	C-C-C-C-C-C(C)-C	-0.78712
O00222	512	C-[As]-O-[#1]	-0.789492
O00222	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	-0.790087
O00222	791	NC1CCC(N)CC1	-0.793824
O00222	641	O-C-C-C=C	-0.795069
O00222	466	N#C-C=C	-0.802943
O00222	586	C-S-C-C-C	-0.803753
O00222	871	SC1C(S)CCC1	-0.813747
O00222	286	C-O	-0.814708
O00222	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	-0.819112
O00222	220	>= 2 any ring size 7	-0.82125
O00222	808	SC1CC(S)CCC1	-0.822001
O00222	324	P-P	-0.829892
O00222	10	>= 4 C	-0.830316
O00222	42	>= 2 K	-0.834023
O00222	488	N-C=N-[#1]	-0.837879
O00222	105	>= 1 Eu	-0.839331
O00222	376	C(~N)(:C)	-0.840548
O00222	830	SC1C(N)CCCC1	-0.846023
O00222	343	C(~C)(~Cl)(~H)	-0.848006
O00222	4	>= 1 Li	-0.85529
O00222	592	N-C-C-C-C	-0.859735
O00222	483	N-S-C:C	-0.894612
O00222	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	-0.896512
O00222	536	O=C-C-N	-0.906619
O00222	839	CC1CC(C)CC1	-0.914768
O00222	479	S-C-S-C	-0.917211

O00222	409	O(:C)(:C)	−0.920653
O00222	65	>= 1 As	−0.92384
O00222	259	>= 3 aromatic rings	−0.924405
O00222	355	C(~C)(:C)	−0.935195
O00222	333	C(~C)(~C)(~C)	−0.93992
O00222	356	C(~C)(:C)(:C)	−0.939929
O00222	23	>= 1 F	−0.939942
O00222	413	S(~C)(~H)	−0.941438
O00222	679	C-C-C-C-C-C	−0.941501
O00222	15	>= 2 N	−0.941545
O00222	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.957256
O00222	827	OC1C(Cl)CCCC1	−0.966329
O00222	748	Sc1cc(Br)ccc1	−0.98716
O00222	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.991668
O00222	257	>= 2 aromatic rings	−0.993328
O00222	649	O=N-C:C-O	−1.004096
O00222	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−1.005955
O00222	411	P(~O)(~O)	−1.032901
O00222	794	ClC1CCC(Cl)CC1	−1.033819
O00222	631	O-C:C-O-[#1]	−1.036746
O00222	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−1.042035
O00222	350	C(~C)(~I)	−1.063094
O00222	338	C(~C)(~C)(~H)(~N)	−1.068618
O00222	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−1.069566
O00222	417	C#C	−1.075217
O00222	552	C:C-C:C	−1.077494
O00222	402	N(~O)(:O)	−1.08188
O00222	62	>= 1 Zn	−1.107149
O00222	549	N-C-C:C	−1.149941
O00222	713	Cc1ccc(C)cc1	−1.151712
O00222	638	O-C-C-C-N	−1.158989
O00222	458	S(-O)(=O)	−1.163145
O00222	518	O=C-N-N	−1.16992
O00222	840	CC1CC(O)CC1	−1.172429
O00222	694	O=C-C-C-C-C=O	−1.172953
O00222	798	CC1CC(O)CCC1	−1.173355
O00222	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−1.199772
O00222	289	C-Mg	−1.22115
O00222	627	O=[As]-C:C:C	−1.23006
O00222	797	CC1CC(C)CCC1	−1.251798
O00222	273	B-B	−1.266846
O00222	780	CC1CCC(Cl)CC1	−1.273869
O00222	45	>= 4 Br	−1.283653
O00222	501	Cl-C:C-C	−1.288416
O00222	523	N:C:C-C	−1.292622
O00222	831	SC1C(Cl)CCCC1	−1.307085
O00222	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−1.313642
O00222	74	>= 1 Ru	−1.316544

O00222	271	Li-Cl	-1.339305
O00222	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	-1.34503
O00222	632	C-C-O-C:C	-1.347105
O00222	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	-1.357958
O00222	617	C-C-C-O-[#1]	-1.36362
O00222	634	C-C-C:C-C	-1.363753
O00222	861	CC1C(O)CCC1	-1.368125
O00222	770	Nc1c(N)cccc1	-1.377044
O00222	351	C(~C)(~N)	-1.409767
O00222	89	>= 1 W	-1.409784
O00222	866	OC1C(O)CCC1	-1.416056
O00222	541	O-C:C-C	-1.436531
O00222	709	C-C(C)-C-C-C	-1.460685
O00222	773	Clc1c(Cl)cccc1	-1.481219
O00222	741	Oc1cc(S)ccc1	-1.486498
O00222	394	N(~C)(~H)(~N)	-1.495155
O00222	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	-1.500695
O00222	636	C-N-C-N-C	-1.50725
O00222	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	-1.515455
O00222	56	>= 1 Cr	-1.52171
O00222	60	>= 1 Ni	-1.532891
O00222	623	O=C-C:C-C	-1.536214
O00222	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	-1.58734
O00222	322	Si-Cl	-1.595682
O00222	414	S(~C)(~O)	-1.615265
O00222	123	>= 2 saturated or aromatic carbon-only ring size 3	-1.644508
O00222	489	N-C-S-C	-1.644826
O00222	332	C(~C)(~C)	-1.649666
O00222	845	OC1CC(O)CC1	-1.651026
O00222	663	O-C-C-O-[#1]	-1.652625
O00222	733	Brc1ccc(Br)cc1	-1.668341
O00222	874	SC1C(Br)CCC1	-1.674354
O00222	822	CC1C(Cl)CCCC1	-1.692514
O00222	249	>= 1 saturated or aromatic carbon-only ring size 10	-1.695955
O00222	596	N=C-N-C-C	-1.711861
O00222	462	O-C-C=O	-1.72408
O00222	30	>= 1 P	-1.72795
O00222	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	-1.733004
O00222	519	N=C-N-C	-1.761803
O00222	597	O=C-C-C:C	-1.762238
O00222	91	>= 1 Os	-1.764275
O00222	565	C:C-O-C	-1.776121
O00222	315	O-K	-1.832525
O00222	422	N=N	-1.83905
O00222	826	OC1C(N)CCCC1	-1.857582
O00222	786	OC1CCC(Br)CC1	-1.886215
O00222	530	N:C-C:C	-1.895219
O00222	295	C-As	-1.924854

O00222	440	C(-C)(-O)(=O)	-1.933565
O00222	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	-1.949374
O00222	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	-1.966861
O00222	13	>= 32 C	-2.006513
O00222	493	O=C-C:C	-2.012116
O00222	653	O-C:C:C-O	-2.022678
O00222	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	-2.043284
O00222	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	-2.076022
O00222	53	>= 1 Sc	-2.092068
O00222	613	C-N-C-C-C	-2.093925
O00222	687	O=C-C-C-C=O	-2.111761
O00222	781	CC1CCC(Br)CC1	-2.150634
O00222	255	>= 1 aromatic ring	-2.183573
O00222	404	N(:C)(:C)(:C)	-2.206357
O00222	591	Cl-C-C-C-C	-2.265237
O00222	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	-2.287614
O00222	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	-2.370856
O00222	869	OC1C(Cl)CCC1	-2.510146
O00222	513	S:C:C-[#1]	-2.531531

Fingerprints（continued)

P	Q
2.844773	-4.61E-07
2.5018615	-0.00147
2.4446795	2.70E-07
2.4013688	-4.42E-07
2.3342951	-0.00066
2.2260342	-6.79E-07
2.2158176	-3.22E-07
2.2058843	6.02E-08
2.0896546	0.002465
2.0588297	0.00473
2.0426185	1.23E-06
2.0199067	0.003661
1.9769877	2.61E-07
1.9502284	-0.00131
1.9325359	0.000317
1.9203733	-0.00019
1.9009459	1.06E-06
1.8808183	-0.0007
1.868954	4.32E-07
1.8154635	-0.00187
1.7957354	-8.47E-07
1.7978401	-0.00937
1.7902238	-0.00252
1.758362	-1.29E-06
1.7468501	0.001911
1.6534935	-0.00277
1.6471402	3.29E-07
1.6485754	-0.00188
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1.5942261	-3.45E-07
1.5918986	-0.00557
1.5729681	0.003229
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1.5203293	3.44E-07
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1.4257109	-0.00158

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1.4131361	1.55E-06
1.4042842	0.004544
1.3877759	5.29E-07
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1.39011	-0.00563
1.3906873	-0.01445
1.3621553	-0.00233
1.3449457	0.002835
1.3476608	-6.13E-05
1.3223583	0.000357
1.3122117	-3.40E-07
1.3110892	0.000192
1.3102565	-0.00306
1.3068898	-0.00066
1.2978392	0.004942
1.2852984	-0.00102
1.2766772	-1.27E-06
1.2760856	-7.75E-08
1.2721113	4.03E-08
1.2374541	0.002059
1.2301593	-1.85E-07
1.2236127	-0.00172
1.2215296	1.22E-06
1.2027653	-0.00111
1.1985219	3.86E-08
1.191574	1.71E-06
1.1880707	-9.13E-07
1.1869246	9.62E-07
1.1830431	-2.26E-07
1.1776734	-0.00308
1.1587141	0.003553
1.1582824	-4.11E-05
1.1501783	-0.00062
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1.0201914	-0.00097
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0.9831407	-8.84E-07
0.981809	-0.00122
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0.9658191	0.000191
0.9631838	0.001026
0.9599132	0.000336
0.9412383	-7.26E-07
0.942176	-0.00135
0.9405783	-0.00453
0.9319911	-4.58E-05
0.9271614	1.97E-07
0.9250619	4.12E-05
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0.905709	-1.97E-07
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0.8890806	-3.48E-07
0.8860254	-2.67E-07
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0.8837352	-0.00184
0.8811385	-1.05E-06
0.8804622	-7.16E-07
0.8510693	0.003626
0.8503788	0.002909
0.8510175	-0.0026
0.8419378	0.005391
0.8500719	-0.0047
0.8450608	5.37E-07
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0.8437912	0.000321
0.8400476	1.32E-07
0.8381329	-0.00024

0.8333349 0.003077
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0.8271747 2.56E-07
0.8208127 4.60E-07
0.8108389 -0.00392
0.8059406 -1.13E-06
0.8059419 -0.0015
0.8037022 -0.00033
0.793314 3.08E-07
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0.7400152 -0.00219
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0.7001487 0.001176
0.698461 0.001747
0.6953678 -8.47E-08
0.6942736 4.63E-07
0.6895739 8.68E-08
0.687052 -0.00022
0.6863845 -9.25E-08
0.6890853 -0.00341
0.6845699 5.65E-08
0.6823716 -6.68E-08
0.6800718 -2.91E-07
0.679214 -5.02E-07
0.6760318 -0.00162
0.6718886 -0.00152
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-1.416055 -6.04E-07
-1.435476 -0.00105
-1.456594 -0.00409
-1.480841 -0.00038
-1.486497 -9.83E-07
-1.497226 0.002072
-1.500694 -7.37E-07
-1.502671 -0.00458
-1.515454 -2.25E-07
-1.521711 5.22E-07
-1.532891 1.45E-07
-1.534695 -0.00152
-1.587341 1.21E-06
-1.595683 5.01E-07
-1.616267 0.001002
-1.643156 -0.00135
-1.64484 1.33E-05
-1.647218 -0.00245
-1.651026 -5.35E-07
-1.647875 -0.00475
-1.668341 -6.49E-07
-1.674354 -5.76E-07
-1.694417 0.001904
-1.695954 -1.37E-06
-1.71367 0.001809
-1.7252 0.00112
-1.726602 -0.00135
-1.733004 1.29E-07
-1.762686 0.000882
-1.760703 -0.00154
-1.764275 1.08E-07
-1.778037 0.001916
-1.832524 -1.07E-06
-1.835276 -0.00377
-1.857683 0.000101
-1.886216 1.08E-06
-1.897215 0.001996
-1.924854 -5.17E-07

-1.93391	0.000345
-1.949374	2.43E-07
-1.96686	-8.24E-07
-2.010286	0.003773
-2.013898	0.001782
-2.023508	0.000829
-2.043285	7.74E-07
-2.075456	-0.00057
-2.092068	-6.30E-08
-2.088364	-0.00556
-2.108336	-0.00343
-2.151275	0.000641
-2.183573	-7.18E-07
-2.204973	-0.00138
-2.263895	-0.00134
-2.287037	-0.00058
-2.375502	0.004646
-2.510146	-1.60E-07
-2.532869	0.001338

Data S1. Ranking of importance of substructure features from Pubchem I

GPCR ID	Bit Posit	Bit Substructure	W
O15303	673	O=C-C=C-N	2.6351337
O15303	349	C(~C)(~H)(~S)	2.5147604
O15303	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	2.4486873
O15303	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	2.3912892
O15303	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	2.3588859
O15303	53	>= 1 Sc	2.3189502
O15303	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	2.2960694
O15303	543	O-C:C-N	2.2678064
O15303	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	2.1773673
O15303	716	Cc1ccc(N)cc1	2.083522
O15303	361	C(~Cl)(~H)	1.9632366
O15303	150	>= 2 any ring size 5	1.9141404
O15303	638	O-C-C-C-N	1.9002245
O15303	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	1.8880982
O15303	848	OC1CC(Cl)CC1	1.8751209
O15303	521	C:N-C-[#1]	1.8719108
O15303	605	O=C-C-O-C	1.8489718
O15303	107	>= 1 Tb	1.8441926
O15303	490	C-C-C=C	1.808199
O15303	657	C-N-C:C-C	1.7539899
O15303	88	>= 1 Ta	1.7026935
O15303	313	O-Si	1.6784481
O15303	552	C:C-C:C	1.6632234
O15303	419	C#N	1.6553789
O15303	400	N(~H)(:C)(:C)	1.6212327
O15303	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	1.6105596
O15303	836	ClC1C(Cl)CCCC1	1.5802455
O15303	699	O-C-C-C-C-C(C)-C	1.5480405
O15303	369	C(~H)(~Si)	1.5141571
O15303	841	CC1CC(S)CC1	1.4992981
O15303	386	C(:C)(:C)(:N)	1.4740526
O15303	749	Nc1cc(N)ccc1	1.4655239
O15303	403	N(:C)(:C)	1.4360923
O15303	78	>= 1 Cd	1.4262983
O15303	442	C(-C)(=N)	1.4222795
O15303	674	N-C-N-C:C	1.4102596
O15303	87	>= 1 Hf	1.4094275
O15303	348	C(~C)(~H)(~P)	1.3621058
O15303	345	C(~C)(~H)(~N)	1.3578475
O15303	710	C-C-C(C)-C-C	1.3556437
O15303	815	ClC1CC(Cl)CCC1	1.342548
O15303	741	Oc1cc(S)ccc1	1.3374427
O15303	822	CC1C(Cl)CCCC1	1.3323526
O15303	492	N-C:O:C	1.3083911
O15303	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	1.2922857
O15303	567	O-C-C-O	1.28156

O15303	260	>= 3 hetero-aromatic rings	1.2788609
O15303	731	Clc1ccc(Cl)cc1	1.2777343
O15303	805	OC1CC(N)CCC1	1.2698817
O15303	68	>= 1 Rb	1.2650813
O15303	108	>= 1 Dy	1.238708
O15303	565	C:C-O-C	1.234912
O15303	519	N=C-N-C	1.2181407
O15303	590	C-C:C-O-[#1]	1.1958764
O15303	113	>= 1 Tc	1.1916812
O15303	50	>= 1 Mg	1.1885592
O15303	733	Brc1ccc(Br)cc1	1.1879475
O15303	548	O-C-C:C	1.1782493
O15303	42	>= 2 K	1.1656536
O15303	407	O(~C)(~P)	1.1625391
O15303	422	N=N	1.1535387
O15303	602	O=C-C-N-C	1.150836
O15303	592	N-C-C-C-C	1.1439841
O15303	83	>= 1 Xe	1.1427253
O15303	568	N#C-C-C	1.1410314
O15303	643	[#1]-C-C-N-[#1]	1.1408124
O15303	706	O=C-C-C-C-C(=O)-C	1.1404726
O15303	562	Br-C-C=O	1.1271098
O15303	129	>= 1 any ring size 4	1.1270845
O15303	789	SC1CCC(Cl)CC1	1.1157039
O15303	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	1.1101241
O15303	792	NC1CCC(Cl)CC1	1.1031177
O15303	379	C(~N)(:N)	1.0932266
O15303	373	C(~H)(:N)	1.0874979
O15303	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	1.0773516
O15303	633	N-C-C:C-C	1.0766243
O15303	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	1.0652184
O15303	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	1.0638644
O15303	761	Oc1c(O)cccc1	1.0637117
O15303	388	C(:C)(:N)(:N)	1.0560427
O15303	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	1.0541044
O15303	637	O-C-C-C-C	1.043957
O15303	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	1.0396966
O15303	875	NC1C(N)CCC1	1.0374097
O15303	12	>= 16 C	1.0152529
O15303	474	S:C:C:N	1.0131365
O15303	524	C-C=C-C	1.0023348
O15303	401	N(~O)(~O)	1.0015734
O15303	257	>= 2 aromatic rings	0.9957315
O15303	34	>= 2 S	0.9925954
O15303	631	O-C:C-O-[#1]	0.9866918
O15303	299	N-H	0.985438
O15303	824	OC1C(O)CCCC1	0.9837954
O15303	322	Si-Cl	0.9823467

O15303	36	>= 8 S	0.9686057
O15303	717	Cc1ccc(Cl)cc1	0.9500871
O15303	539	N=C-C-[#1]	0.9476412
O15303	676	N#C-C-C-C	0.924065
O15303	488	N-C=N-[#1]	0.921197
O15303	694	O=C-C-C-C-C=O	0.9193996
O15303	591	Cl-C-C-C-C	0.9100886
O15303	528	[#1]-N-C-[#1]	0.9084564
O15303	553	O=C-C=C	0.9037606
O15303	297	C-Br	0.8970023
O15303	736	Cc1cc(S)ccc1	0.8939437
O15303	484	N-C:N:C	0.8859034
O15303	876	NC1C(Cl)CC1	0.8852567
O15303	48	>= 4 I	0.8721922
O15303	97	>= 1 Pb	0.8605572
O15303	820	CC1C(S)CCCC1	0.8564665
O15303	586	C-S-C-C-C	0.8530635
O15303	421	C=S	0.8497522
O15303	241	>= 1 any ring size 9	0.8459118
O15303	382	C(~O)(:C)(:C)	0.8382727
O15303	495	C-N-C:C	0.8318166
O15303	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.8211182
O15303	854	NC1CC(N)CC1	0.8141306
O15303	385	C(:C)(:C)(:C)	0.8069899
O15303	632	C-C-O-C:C	0.8046229
O15303	80	>= 1 Sn	0.797711
O15303	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.7930046
O15303	469	S-S-C:C	0.7923247
O15303	645	O=C-N-C-C	0.789418
O15303	29	>= 2 Si	0.7877741
O15303	512	C-[As]-O-[#1]	0.7805865
O15303	607	N-C-C-C:C	0.7792045
O15303	709	C-C(C)-C-C-C	0.7739779
O15303	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.7697181
O15303	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.7682448
O15303	411	P(~O)(~O)	0.764347
O15303	74	>= 1 Ru	0.7637766
O15303	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.7633436
O15303	476	C-O-C=C	0.7586148
O15303	151	>= 2 saturated or aromatic carbon-only ring size 5	0.7511128
O15303	90	>= 1 Re	0.7420271
O15303	516	[#1]-C=C-[#1]	0.7348352
O15303	541	O-C:C-C	0.733246
O15303	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.7303243
O15303	426	P=P	0.7298452
O15303	460	C-C-C#C	0.7298189
O15303	487	N-C=N-C	0.7273435
O15303	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.7230523

O15303	619	O-C-C=C-C	0.7209429
O15303	698	O-C-C-C-C-C-C-C	0.7209255
O15303	705	O=C-C-C-C-C(O)-C	0.7200635
O15303	597	O=C-C-C:C	0.7149338
O15303	123	>= 2 saturated or aromatic carbon-only ring size 3	0.7132088
O15303	794	ClC1CCC(Cl)CC1	0.7103073
O15303	695	O=C-C-C-C-C-N	0.6985592
O15303	227	>= 1 any ring size 8	0.6880732
O15303	819	CC1C(O)CCCC1	0.6878813
O15303	262	>= 4 hetero-aromatic rings	0.6876648
O15303	378	C(~N)(:C)(:N)	0.6823092
O15303	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.6799807
O15303	740	Oc1cc(O)ccc1	0.6724287
O15303	71	>= 1 Zr	0.6706579
O15303	279	B-P	0.6657756
O15303	768	Sc1c(Cl)cccc1	0.6638414
O15303	395	N(~C)(~O)	0.6563186
O15303	505	Cl-C:C-O	0.6542412
O15303	38	>= 2 Cl	0.6459464
O15303	873	SC1C(Cl)CCC1	0.6446154
O15303	714	Cc1ccc(O)cc1	0.6440344
O15303	412	S(~C)(~C)	0.6426115
O15303	281	B-Cl	0.6402844
O15303	850	SC1CC(S)CC1	0.6335662
O15303	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.6313026
O15303	377	C(~N)(:C)(:C)	0.629163
O15303	356	C(~C)(:C)(:C)	0.6268164
O15303	372	C(~H)(:C)(:N)	0.6244523
O15303	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.6231549
O15303	595	C:C-C-C-C	0.6207019
O15303	598	Cl-C:C:C-C	0.6191673
O15303	821	CC1C(N)CCCC1	0.6190127
O15303	323	P-H	0.6091261
O15303	830	SC1C(N)CCCC1	0.6069079
O15303	574	O-C-C:C-C	0.605392
O15303	581	O=C-C-C-O	0.6027705
O15303	572	N:C:N:C	0.6022764
O15303	266	Li-C	0.5976497
O15303	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.5896496
O15303	259	>= 3 aromatic rings	0.5854256
O15303	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.5769999
O15303	769	Sc1c(Br)cccc1	0.5762993
O15303	271	Li-Cl	0.5738978
O15303	502	N-C=C-[#1]	0.5699495
O15303	137	>= 2 saturated or aromatic carbon-only ring size 4	0.5686887
O15303	658	C-C-S-C-C	0.5670099
O15303	471	S:C:C:C	0.5629208
O15303	587	N-C:C-O-[#1]	0.5565144

O15303	65	>= 1 As	0.5558269
O15303	357	C(~C)(:C)(:N)	0.5463336
O15303	45	>= 4 Br	0.5397373
O15303	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.5356508
O15303	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.5328989
O15303	711	C-C(C)(C)-C-C	0.5292711
O15303	520	C=C-C:C	0.5235799
O15303	629	S-C:C:C-N	0.5235251
O15303	596	N=C-N-C-C	0.5201012
O15303	355	C(~C)(:C)	0.5187709
O15303	340	C(~C)(~C)(~N)	0.5172487
O15303	653	O-C:C:C-O	0.5158001
O15303	813	NC1CC(Cl)CCC1	0.5129532
O15303	563	O-C-O-C	0.5127194
O15303	503	Cl-C:C-[#1]	0.5100344
O15303	753	Clc1cc(Br)ccc1	0.5065937
O15303	846	OC1CC(S)CC1	0.4990445
O15303	307	N-Br	0.498617
O15303	305	N-S	0.4955318
O15303	66	>= 1 Se	0.4934776
O15303	517	N-N-C-N	0.4933669
O15303	786	OC1CCC(Br)CC1	0.493297
O15303	59	>= 1 Co	0.4894994
O15303	144	>= 1 saturated or aromatic carbon-only ring size 5	0.4863426
O15303	748	Sc1cc(Br)ccc1	0.4845465
O15303	538	N=C-C-C	0.4790023
O15303	797	CC1CC(C)CCC1	0.4685798
O15303	811	SC1CC(Br)CCC1	0.4651761
O15303	738	Cc1cc(Cl)ccc1	0.4628257
O15303	862	CC1C(S)CCC1	0.45556
O15303	287	C-F	0.4554035
O15303	221	>= 2 saturated or aromatic carbon-only ring size 7	0.4529287
O15303	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.4333749
O15303	618	C:C-C-C:C	0.432965
O15303	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.4271853
O15303	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.4251541
O15303	122	>= 2 any ring size 3	0.4226452
O15303	314	O-P	0.4215226
O15303	742	Oc1cc(N)ccc1	0.4206769
O15303	116	>= 1 saturated or aromatic carbon-only ring size 3	0.4204285
O15303	798	CC1CC(O)CCC1	0.4185377
O15303	425	P=O	0.4159797
O15303	727	Sc1ccc(Br)cc1	0.4089954
O15303	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.4085358
O15303	332	C(~C)(~C)	0.4084249
O15303	374	C(~H)(~H)(~H)	0.407988
O15303	849	OC1CC(Br)CC1	0.4075765
O15303	479	S-C-S-C	0.4070149

O15303	414	S(~C)(~O)	0.4066258
O15303	7	>= 2 B	0.3970746
O15303	463	N:C-S-[#1]	0.3960731
O15303	461	O-C-C=N	0.3913214
O15303	157	>= 3 any ring size 5	0.3900659
O15303	666	C=C-C-O-C	0.3867259
O15303	185	>= 2 any ring size 6	0.3839272
O15303	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.3815773
O15303	2	>= 16 H	0.3786669
O15303	387	C(:C)(:N)	0.376518
O15303	593	N-C-C-C-N	0.3477517
O15303	485	N:C:C:N	0.3437896
O15303	685	O=C-C-C-C-N	0.3390741
O15303	437	C(-C)(-N)(=C)	0.3376083
O15303	851	SC1CC(N)CC1	0.329721
O15303	843	CC1CC(Cl)CC1	0.3206406
O15303	27	>= 2 Na	0.3187935
O15303	10	>= 4 C	0.3134091
O15303	290	C-Al	0.3133377
O15303	481	O-S-C:C	0.3132312
O15303	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.312466
O15303	649	O=N-C:C-O	0.3110923
O15303	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.307999
O15303	455	N(-O)(=O)	0.3072278
O15303	559	O-C-N-[#1]	0.3066787
O15303	318	Al-H	0.3033598
O15303	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.3024298
O15303	451	C(-N)(=O)	0.300976
O15303	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.2995774
O15303	40	>= 8 Cl	0.2987719
O15303	807	OC1CC(Br)CCC1	0.2975712
O15303	656	C-C-N-C-C	0.2963594
O15303	31	>= 2 P	0.2941735
O15303	576	N=C-C:C-[#1]	0.2911789
O15303	533	S-C:C-N	0.2885465
O15303	81	>= 1 Sb	0.2817101
O15303	296	C-Se	0.2790609
O15303	696	C-C-C-C-C-C-C-C	0.2770213
O15303	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.2707409
O15303	527	C:C:N-[#1]	0.2675972
O15303	96	>= 1 Tl	0.2629094
O15303	635	N-N-C-N-[#1]	0.255565
O15303	397	N(~C)(:C)(:C)	0.2551322
O15303	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.2519614
O15303	708	C-C(C)-C-C	0.250579
O15303	362	C(~Cl)(:C)	0.2498906
O15303	86	>= 1 Lu	0.2489228
O15303	352	C(~C)(~O)	0.2472615

O15303	663	O-C-C-O-[#1]	0.2460803
O15303	704	O=C-C-C-C-C-C-C	0.2405522
O15303	827	OC1C(Cl)CCCC1	0.2279919
O15303	746	Sc1cc(N)ccc1	0.2260385
O15303	688	C-C-C-C-C-C-C	0.2257631
O15303	464	N-C-C=C	0.2238793
O15303	321	Si-Si	0.2237206
O15303	718	Cc1ccc(Br)cc1	0.2234998
O15303	268	Li-F	0.2232732
O15303	346	C(~C)(~H)(~O)	0.2202857
O15303	680	O-C-C-C-C-C	0.2197188
O15303	549	N-C-C:C	0.2161266
O15303	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.2137212
O15303	823	CC1C(Br)CCCC1	0.2107759
O15303	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.2102265
O15303	654	N-C-N-C-C	0.2082415
O15303	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.2079436
O15303	816	ClC1CC(Br)CCC1	0.2024822
O15303	831	SC1C(Cl)CCCC1	0.1993075
O15303	575	O-C-C:C-O	0.1978178
O15303	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.196871
O15303	817	BrC1CC(Br)CCC1	0.1924292
O15303	16	>= 4 N	0.1881145
O15303	681	O-C-C-C-C-O	0.1839151
O15303	35	>= 4 S	0.183237
O15303	707	O=C-C-C-C-C(N)-C	0.1826947
O15303	60	>= 1 Ni	0.1801747
O15303	845	OC1CC(O)CC1	0.1778064
O15303	441	C(-C)(=C)	0.1769782
O15303	874	SC1C(Br)CCC1	0.1766061
O15303	21	>= 8 O	0.1765861
O15303	818	CC1C(C)CCCC1	0.1765125
O15303	762	Oc1c(S)cccc1	0.1717107
O15303	609	Cl-C-C-N-C	0.1697391
O15303	420	C=O	0.1626936
O15303	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.1563537
O15303	399	N(~H)(:C)	0.1556887
O15303	264	Li-Li	0.1466644
O15303	344	C(~C)(~H)	0.143591
O15303	394	N(~C)(~H)(~N)	0.1384514
O15303	683	N-C-C-C-C-C	0.1369148
O15303	171	>= 5 any ring size 5	0.1349442
O15303	835	NC1C(Br)CCCC1	0.1340346
O15303	79	>= 1 In	0.1338816
O15303	767	Sc1c(N)cccc1	0.1330151
O15303	860	CC1C(C)CCC1	0.1210528
O15303	439	C(-C)(-N)(=O)	0.1111739
O15303	9	>= 2 C	0.1099476

O15303	25	>= 4 F	0.1092998
O15303	294	C-Cl	0.109198
O15303	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.1072296
O15303	878	ClC1C(Cl)CCC1	0.1044417
O15303	628	C-N-C-C:C	0.1043982
O15303	370	C(~H)(:C)	0.0998098
O15303	343	C(~C)(~Cl)(~H)	0.0978615
O15303	623	O=C-C:C-C	0.0954382
O15303	828	OC1C(Br)CCCC1	0.0945551
O15303	335	C(~C)(~C)(~C)(~H)	0.0923485
O15303	791	NC1CCC(N)CC1	0.0920336
O15303	23	>= 1 F	0.0849302
O15303	825	OC1C(S)CCCC1	0.0821204
O15303	601	N-C:C:C-N	0.0754603
O15303	363	C(~F)(~F)	0.0736965
O15303	444	C(-Cl)(=O)	0.0730074
O15303	393	N(~C)(~H)	0.0701366
O15303	37	>= 1 Cl	0.0692998
O15303	447	C(-H)(=N)	0.0687471
O15303	310	O-Mg	0.0685367
O15303	383	C(~S)(:C)	0.0635158
O15303	429	C(#N)(-C)	0.0620328
O15303	871	SC1C(S)CCC1	0.0594259
O15303	493	O=C-C:C	0.054639
O15303	715	Cc1ccc(S)cc1	0.0471044
O15303	840	CC1CC(O)CC1	0.0460307
O15303	812	NC1CC(N)CCC1	0.0450417
O15303	703	O-C-C-C-C-C(N)-C	0.0417038
O15303	584	C:C-C=C-C	0.039574
O15303	660	C-C=C-C-C	0.0381649
O15303	725	Sc1ccc(N)cc1	0.0376738
O15303	49	>= 1 Be	0.0366165
O15303	790	SC1CCC(Br)CC1	0.0353785
O15303	570	C:C-C-C	0.0342527
O15303	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0337847
O15303	277	B-F	0.0334633
O15303	70	>= 1 Y	0.0327375
O15303	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.0321835
O15303	3	>= 32 H	0.0320378
O15303	864	CC1C(Cl)CCC1	0.030167
O15303	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.0299178
O15303	367	C(~H)(~O)(~O)	0.0283933
O15303	677	C-C=C-C:C	0.0281771
O15303	692	O=C-C-C-C-C-C	0.0281696
O15303	747	Sc1cc(Cl)ccc1	0.0279743
O15303	63	>= 1 Ga	0.0279609
O15303	93	>= 1 Pt	0.0277701
O15303	325	As-H	0.0265888

O15303	269	Li-P	0.0265254
O15303	702	O-C-C-C-C-C-N-C	0.0251872
O15303	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.024898
O15303	780	CC1CCC(Cl)CC1	0.0240493
O15303	667	C=C-C-O-[#1]	0.0220316
O15303	594	C-O-C-C=C	0.0215373
O15303	514	O-N-C-C	0.0211002
O15303	869	OC1C(Cl)CCC1	0.0208002
O15303	409	O(:C)(:C)	0.0200991
O15303	443	C(-C)(=O)	0.019818
O15303	719	Oc1ccc(O)cc1	0.0197783
O15303	556	C=C-C-C	0.0192464
O15303	301	N-O	0.0191792
O15303	604	C-O-C-C:C	0.0186298
O15303	304	N-P	0.0179196
O15303	213	>= 1 any ring size 7	0.0167997
O15303	331	C(~Br)(:N)	0.0163801
O15303	675	Br-C-C-C:C	0.0155987
O15303	315	O-K	0.0149491
O15303	494	O=C-C:N	0.0139334
O15303	687	O=C-C-C-C=O	0.0138408
O15303	459	S(=O)(=O)	0.0136579
O15303	726	Sc1ccc(Cl)cc1	0.0134076
O15303	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0114483
O15303	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0112217
O15303	360	C(~Cl)(~Cl)	0.0109581
O15303	406	O(~C)(~H)	0.0100878
O15303	665	N-C:C-C-C	0.0100223
O15303	613	C-N-C-C-C	0.009594
O15303	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.0091369
O15303	721	Oc1ccc(N)cc1	0.009012
O15303	483	N-S-C:C	0.0083728
O15303	278	B-Si	0.006449
O15303	408	O(~H)(~S)	0.0061057
O15303	678	C-C-C=C-C	0.0058221
O15303	513	S:C:C-[#1]	0.0056596
O15303	61	>= 1 Cu	0.0047995
O15303	84	>= 1 Cs	0.0046638
O15303	11	>= 8 C	0.0044853
O15303	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0043441
O15303	67	>= 1 Kr	0.0041865
O15303	671	O=C-C=C-C	0.0041264
O15303	785	OC1CCC(Cl)CC1	0.0038812
O15303	536	O=C-C-N	0.0038785
O15303	781	CC1CCC(Br)CC1	0.0038542
O15303	588	O=C-C-C=O	0.0035132
O15303	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.0034348
O15303	526	Cl-C:C-Cl	0.0033581

O15303	457	S(-C)(=O)	0.003239
O15303	44	>= 2 Br	0.0030047
O15303	17	>= 8 N	0.002967
O15303	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.002222
O15303	92	>= 1 Ir	0.0019939
O15303	693	O=C-C-C-C-C-O	0.0017883
O15303	330	C(~Br)(:C)	0.0016121
O15303	670	Br-C:C:C-C	0.0012596
O15303	396	N(~C)(:C)	0.0011152
O15303	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0009346
O15303	867	OC1C(S)CCC1	0.0007382
O15303	857	ClC1CC(Cl)CC1	0.0006779
O15303	782	OC1CCC(O)CC1	0.0004308
O15303	75	>= 1 Rh	1.69E-06
O15303	754	Brc1cc(Br)ccc1	1.59E-06
O15303	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	1.49E-06
O15303	324	P-P	-5.12E-07
O15303	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	-1.29E-06
O15303	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	-2.02E-06
O15303	724	Sc1ccc(S)cc1	-2.22E-06
O15303	879	ClC1C(Br)CCC1	-9.83E-05
O15303	630	O-C:C-O-C	-0.000272
O15303	732	Clc1ccc(Br)cc1	-0.001048
O15303	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	-0.001071
O15303	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.001188
O15303	522	C-N-N-[#1]	-0.001315
O15303	722	Oc1ccc(Cl)cc1	-0.001336
O15303	110	>= 1 Er	-0.00134
O15303	755	Cc1c(C)cccc1	-0.001705
O15303	255	>= 1 aromatic ring	-0.002679
O15303	282	B-Br	-0.002743
O15303	557	N:C-O-[#1]	-0.00292
O15303	529	Cl-C-C-Cl	-0.003008
O15303	91	>= 1 Os	-0.003031
O15303	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	-0.003148
O15303	289	C-Mg	-0.003258
O15303	803	OC1CC(O)CCC1	-0.003375
O15303	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	-0.003473
O15303	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	-0.00349
O15303	46	>= 1 I	-0.003537
O15303	775	Brc1c(Br)cccc1	-0.004054
O15303	302	N-F	-0.004131
O15303	814	NC1CC(Br)CCC1	-0.004297
O15303	751	Nc1cc(Br)ccc1	-0.0046
O15303	256	>= 1 hetero-aromatic ring	-0.004611
O15303	404	N(:C)(:C)(:C)	-0.004641
O15303	855	NC1CC(Cl)CC1	-0.004646
O15303	470	C:C-C=C	-0.00495

O15303	544	O-C:C-O	−0.004992
O15303	870	OC1C(Br)CCC1	−0.005924
O15303	115	>= 1 any ring size 3	−0.006521
O15303	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.006925
O15303	778	CC1CCC(S)CC1	−0.00727
O15303	136	>= 2 any ring size 4	−0.007506
O15303	530	N:C-C:C	−0.007515
O15303	615	N-C-C-O-C	−0.00758
O15303	465	O=S-C-C	−0.00793
O15303	729	Nc1ccc(Cl)cc1	−0.009423
O15303	796	BrC1CCC(Br)CC1	−0.009774
O15303	57	>= 1 Mn	−0.010786
O15303	507	C-C-S-C	−0.011015
O15303	535	O=C-C-C	−0.011129
O15303	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.011539
O15303	446	C(-H)(=C)	−0.012224
O15303	809	SC1CC(N)CCC1	−0.012905
O15303	272	B-H	−0.013456
O15303	800	CC1CC(N)CCC1	−0.015259
O15303	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.015874
O15303	580	O=C-C-C-N	−0.016093
O15303	192	>= 3 any ring size 6	−0.016394
O15303	164	>= 4 any ring size 5	−0.017204
O15303	14	>= 1 N	−0.018093
O15303	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.018165
O15303	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.018772
O15303	779	CC1CCC(N)CC1	−0.019136
O15303	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.019579
O15303	220	>= 2 any ring size 7	−0.019914
O15303	518	O=C-N-N	−0.019999
O15303	770	Nc1c(N)cccc1	−0.020061
O15303	806	OC1CC(Cl)CCC1	−0.020386
O15303	43	>= 1 Br	−0.021698
O15303	566	O-C-C-N	−0.022974
O15303	402	N(~O)(:O)	−0.022982
O15303	504	N:C:N-C	−0.023357
O15303	500	C-S-C:C	−0.023636
O15303	58	>= 1 Fe	−0.024101
O15303	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.025133
O15303	308	O-H	−0.025135
O15303	274	B-C	−0.025258
O15303	558	O=N-C:C	−0.025273
O15303	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.025517
O15303	62	>= 1 Zn	−0.025713
O15303	449	C(-N)(=C)	−0.026346
O15303	655	O-C-C-C:C	−0.027471
O15303	4	>= 1 Li	−0.027906
O15303	329	C(~Br)(~H)	−0.028138

O15303	497	O-C:C:N	−0.029564
O15303	265	Li-B	−0.03008
O15303	491	C-N:C-[#1]	−0.030349
O15303	735	Cc1cc(O)ccc1	−0.030542
O15303	326	As-As	−0.031061
O15303	415	Si(~C)(~C)	−0.031466
O15303	416	C=C	−0.031679
O15303	143	>= 1 any ring size 5	−0.032003
O15303	298	C-I	−0.032125
O15303	477	N-N-C:C	−0.032154
O15303	103	>= 1 Pm	−0.032594
O15303	784	OC1CCC(N)CC1	−0.032666
O15303	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.032701
O15303	856	NC1CC(Br)CC1	−0.032765
O15303	720	Oc1ccc(S)cc1	−0.032805
O15303	380	C(~O)(~O)	−0.032853
O15303	276	B-O	−0.033286
O15303	499	N-C:C:N	−0.034665
O15303	700	O-C-C-C-C-C-O-C	−0.036994
O15303	5	>= 2 Li	−0.037379
O15303	626	C-O-C:C-C	−0.038352
O15303	640	C=C-C-C-C	−0.039732
O15303	178	>= 1 any ring size 6	−0.042546
O15303	480	C:S:C-C	−0.044638
O15303	341	C(~C)(~C)(~O)	−0.044725
O15303	24	>= 2 F	−0.04613
O15303	723	Oc1ccc(Br)cc1	−0.050903
O15303	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.050931
O15303	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.054705
O15303	462	O-C-C=O	−0.061071
O15303	838	BrC1C(Br)CCCC1	−0.061647
O15303	525	[As]-C:C-[#1]	−0.064965
O15303	432	C(-C)(-C)(=O)	−0.065182
O15303	639	O-C-C-C-O	−0.065252
O15303	270	Li-S	−0.066932
O15303	776	CC1CCC(C)CC1	−0.067562
O15303	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.068627
O15303	701	O-C-C-C-C-C(O)-C	−0.071861
O15303	427	C(#C)(-C)	−0.072182
O15303	288	C-Na	−0.073697
O15303	64	>= 1 Ge	−0.074378
O15303	648	O=N-C:C-N	−0.077181
O15303	6	>= 1 B	−0.084111
O15303	95	>= 1 Hg	−0.084262
O15303	306	N-Cl	−0.093456
O15303	842	CC1CC(N)CC1	−0.094656
O15303	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.095503
O15303	486	N-C:N:N	−0.095873

O15303	482	C:N-C:C	−0.09694
O15303	662	O-C-C-O-C	−0.097185
O15303	453	N(-C)(=C)	−0.097226
O15303	510	[#1]-N-N-[#1]	−0.098908
O15303	853	SC1CC(Br)CC1	−0.099462
O15303	804	OC1CC(S)CCC1	−0.105254
O15303	614	C-C-O-C-C	−0.108576
O15303	691	O-C-C-C-C-C-N	−0.110844
O15303	569	N-C-C-N	−0.114346
O15303	684	O=C-C-C-C-C	−0.120421
O15303	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.126396
O15303	498	O-C=C-C	−0.130435
O15303	366	C(~H)(~O)	−0.131114
O15303	405	O(~C)(~C)	−0.134545
O15303	478	S-C=N-[#1]	−0.13472
O15303	737	Cc1cc(N)ccc1	−0.138124
O15303	774	Clc1c(Br)cccc1	−0.138298
O15303	616	C:C:N:N:C	−0.140381
O15303	89	>= 1 W	−0.140897
O15303	744	Oc1cc(Br)ccc1	−0.144349
O15303	72	>= 1 Nb	−0.147737
O15303	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.147994
O15303	554	Br-C-C-C	−0.155473
O15303	413	S(~C)(~H)	−0.159076
O15303	651	O-C:C:C-C	−0.167079
O15303	431	C(-C)(-C)(=N)	−0.16855
O15303	22	>= 16 O	−0.178272
O15303	33	>= 1 S	−0.184909
O15303	686	O=C-C-C-C-O	−0.186949
O15303	606	O-C:C-C-C	−0.192397
O15303	773	Clc1c(Cl)cccc1	−0.195623
O15303	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.197383
O15303	551	Cl-C-C-O	−0.199735
O15303	398	N(~H)(~N)	−0.203107
O15303	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.203109
O15303	292	C-P	−0.2041
O15303	0	>= 4 H	−0.204252
O15303	612	N-C-O-C-C	−0.210473
O15303	627	O=[As]-C:C:C	−0.210968
O15303	501	Cl-C:C-C	−0.216506
O15303	365	C(~H)(~N)	−0.219457
O15303	392	N(~C)(~C)(~H)	−0.225845
O15303	371	C(~H)(:C)(:C)	−0.23383
O15303	532	S-C:C-[#1]	−0.235501
O15303	300	N-N	−0.239387
O15303	73	>= 1 Mo	−0.246535
O15303	577	C:C-N-C:C	−0.248792
O15303	30	>= 1 P	−0.248926

O15303	801	CC1CC(Cl)CCC1	−0.250393
O15303	347	C(~C)(~H)(~O)(~O)	−0.25944
O15303	859	BrC1CC(Br)CC1	−0.266114
O15303	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.273436
O15303	56	>= 1 Cr	−0.274845
O15303	668	C-C:C-C-C	−0.276366
O15303	765	Oc1c(Br)cccc1	−0.282974
O15303	844	CC1CC(Br)CC1	−0.29086
O15303	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.2922
O15303	537	O=C-C-O	−0.294194
O15303	652	O-C:C:C-N	−0.29553
O15303	728	Nc1ccc(N)cc1	−0.296714
O15303	248	>= 1 any ring size 10	−0.307302
O15303	713	Cc1ccc(C)cc1	−0.313179
O15303	8	>= 4 B	−0.31706
O15303	582	C-C-C-C-C	−0.317183
O15303	410	P(~C)(~C)	−0.317475
O15303	77	>= 1 Ag	−0.319589
O15303	28	>= 1 Si	−0.325779
O15303	642	O-C-C-C=O	−0.326232
O15303	320	Si-H	−0.328486
O15303	802	CC1CC(Br)CCC1	−0.330024
O15303	466	N#C-C=C	−0.336952
O15303	354	C(~C)(~Si)	−0.343019
O15303	55	>= 1 V	−0.343742
O15303	573	O-C-C=C	−0.352963
O15303	424	N=P	−0.356619
O15303	872	SC1C(N)CCC1	−0.358158
O15303	283	C-H	−0.358192
O15303	18	>= 1 O	−0.358579
O15303	19	>= 2 O	−0.36515
O15303	327	C(~Br)(~C)	−0.368389
O15303	863	CC1C(N)CCC1	−0.368675
O15303	808	SC1CC(S)CCC1	−0.379444
O15303	760	Cc1c(Br)cccc1	−0.380393
O15303	359	C(~C)(:N)(:N)	−0.385014
O15303	837	ClC1C(Br)CCCC1	−0.387068
O15303	109	>= 1 Ho	−0.393556
O15303	795	ClC1CCC(Br)CC1	−0.398862
O15303	847	OC1CC(N)CC1	−0.400529
O15303	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.404587
O15303	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.405457
O15303	319	Al-Cl	−0.411286
O15303	448	C(-H)(=O)	−0.411838
O15303	339	C(~C)(~C)(~H)(~O)	−0.412375
O15303	622	O=C-O-C:C	−0.412513
O15303	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.413359
O15303	599	[#1]-C-C=C-[#1]	−0.420064

O15303	273	B-B	−0.421108
O15303	99	>= 1 La	−0.429559
O15303	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.433991
O15303	98	>= 1 Bi	−0.434662
O15303	54	>= 1 Ti	−0.434851
O15303	475	S-C=N-C	−0.435665
O15303	664	C-C=C-C=C	−0.435952
O15303	690	O-C-C-C-C-C-O	−0.440984
O15303	275	B-N	−0.447988
O15303	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.450401
O15303	445	C(-H)(-N)(=C)	−0.462411
O15303	829	SC1C(S)CCCC1	−0.464978
O15303	390	N(~C)(~C)	−0.469707
O15303	636	C-N-C-N-C	−0.470428
O15303	436	C(-C)(-H)(=O)	−0.49502
O15303	206	>= 5 any ring size 6	−0.501347
O15303	353	C(~C)(~S)	−0.509115
O15303	756	Cc1c(O)cccc1	−0.509129
O15303	454	N(-C)(=O)	−0.509412
O15303	647	O=C-N-C-N	−0.509872
O15303	104	>= 1 Sm	−0.513132
O15303	625	O=C-C:C-O	−0.514059
O15303	286	C-O	−0.51704
O15303	644	C-C=N-N-C	−0.520544
O15303	672	O=C-C=C-[#1]	−0.523219
O15303	350	C(~C)(~I)	−0.524349
O15303	452	C(-O)(=O)	−0.526172
O15303	880	BrC1C(Br)CCC1	−0.528627
O15303	834	NC1C(Cl)CCCC1	−0.533407
O15303	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.533779
O15303	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.535351
O15303	438	C(-C)(-N)(=N)	−0.537189
O15303	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.545593
O15303	515	N-N-C-C	−0.549072
O15303	69	>= 1 Sr	−0.562722
O15303	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.572278
O15303	384	C(:C)(:C)	−0.573663
O15303	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.577449
O15303	542	O-C:C-[#1]	−0.578141
O15303	608	C-C-C-C:C	−0.581572
O15303	39	>= 4 Cl	−0.599889
O15303	267	Li-O	−0.604779
O15303	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.606422
O15303	364	C(~F)(:C)	−0.607451
O15303	739	Cc1cc(Br)ccc1	−0.608401
O15303	833	NC1C(N)CCCC1	−0.610047
O15303	799	CC1CC(S)CCC1	−0.610404
O15303	105	>= 1 Eu	−0.615921

O15303	826	OC1C(N)CCCC1	−0.619811
O15303	509	Br-C:C-C	−0.62083
O15303	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.633706
O15303	757	Cc1c(S)cccc1	−0.640925
O15303	333	C(~C)(~C)(~C)	−0.641617
O15303	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.646278
O15303	506	C-C:N:C	−0.649227
O15303	317	F-S	−0.650322
O15303	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.657147
O15303	391	N(~C)(~C)(~C)	−0.657594
O15303	285	C-N	−0.658968
O15303	772	Nc1c(Br)cccc1	−0.666853
O15303	199	>= 4 any ring size 6	−0.672568
O15303	102	>= 1 Nd	−0.672796
O15303	589	C-C:C-O-C	−0.673436
O15303	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.675129
O15303	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.678775
O15303	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.685417
O15303	334	C(~C)(~C)(~C)(~C)	−0.692154
O15303	434	C(-C)(-H)(=C)	−0.69379
O15303	617	C-C-C-O-[#1]	−0.695498
O15303	743	Oc1cc(Cl)ccc1	−0.696819
O15303	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.705982
O15303	450	C(-N)(=N)	−0.719168
O15303	810	SC1CC(Cl)CCC1	−0.720884
O15303	745	Sc1cc(S)ccc1	−0.721109
O15303	712	C-C(C)-C(C)-C	−0.721975
O15303	458	S(-O)(=O)	−0.722526
O15303	646	O=C-N-C-[#1]	−0.72654
O15303	600	N-C:C-C-C	−0.727276
O15303	763	Oc1c(N)cccc1	−0.730876
O15303	540	C-N-C-[#1]	−0.731627
O15303	679	C-C-C-C-C-C	−0.735954
O15303	101	>= 1 Pr	−0.737165
O15303	734	Cc1cc(C)ccc1	−0.746588
O15303	839	CC1CC(C)CC1	−0.747597
O15303	26	>= 1 Na	−0.748498
O15303	585	C-C:C-N-C	−0.753188
O15303	611	N-C-C-N-C	−0.753343
O15303	328	C(~Br)(~C)(~C)	−0.757357
O15303	473	S-C:N:C	−0.772256
O15303	311	O-Na	−0.788145
O15303	759	Cc1c(Cl)cccc1	−0.802623
O15303	564	C=C-C=C	−0.804402
O15303	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.816525
O15303	291	C-Si	−0.833909
O15303	435	C(-C)(-H)(=N)	−0.834675
O15303	280	B-S	−0.844415

O15303	661	O-C-O-C-C	−0.848929
O15303	112	>= 1 Yb	−0.859565
O15303	579	O=C-C-C-C	−0.903491
O15303	865	CC1C(Br)CCC1	−0.919411
O15303	336	C(~C)(~C)(~C)(~N)	−0.922493
O15303	758	Cc1c(N)cccc1	−0.926567
O15303	467	C=N-N-C	−0.93285
O15303	261	>= 4 aromatic rings	−0.93333
O15303	32	>= 4 P	−0.938409
O15303	284	C-C	−0.959652
O15303	531	S-C:C-C	−0.961365
O15303	534	S-C:C-O	−0.965519
O15303	752	Clc1cc(Cl)ccc1	−0.972803
O15303	94	>= 1 Au	−0.977194
O15303	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.978992
O15303	234	>= 2 any ring size 8	−0.982215
O15303	610	C-O-C-O-C	−0.988776
O15303	423	N=O	−0.994081
O15303	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.995301
O15303	868	OC1C(N)CCC1	−0.99546
O15303	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−1.004522
O15303	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−1.005836
O15303	258	>= 2 hetero-aromatic rings	−1.033935
O15303	417	C#C	−1.034572
O15303	295	C-As	−1.036891
O15303	550	Cl-C-C-C	−1.038023
O15303	368	C(~H)(~S)	−1.046203
O15303	13	>= 32 C	−1.050616
O15303	783	OC1CCC(S)CC1	−1.051054
O15303	41	>= 1 K	−1.056899
O15303	571	[#1]-C-O-[#1]	−1.059782
O15303	468	O=S-C-N	−1.077823
O15303	106	>= 1 Gd	−1.089809
O15303	316	F-P	−1.091786
O15303	418	C=N	−1.093847
O15303	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−1.094846
O15303	20	>= 4 O	−1.104197
O15303	337	C(~C)(~C)(~C)(~O)	−1.128718
O15303	433	C(-C)(-Cl)(=O)	−1.130917
O15303	697	C-C-C-C-C-C(C)-C	−1.131525
O15303	634	C-C-C:C-C	−1.131698
O15303	730	Nc1ccc(Br)cc1	−1.133885
O15303	787	SC1CCC(S)CC1	−1.138709
O15303	852	SC1CC(Cl)CC1	−1.148696
O15303	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−1.17206
O15303	456	P(-O)(=O)	−1.179123
O15303	766	Sc1c(S)cccc1	−1.181363
O15303	777	CC1CCC(O)CC1	−1.197403

O15303	578	C-C:C-C:C	-1.203553
O15303	47	>= 2 I	-1.203575
O15303	85	>= 1 Ba	-1.205118
O15303	877	NC1C(Br)CCC1	-1.214414
O15303	793	NC1CCC(Br)CC1	-1.219475
O15303	1	>= 8 H	-1.234717
O15303	51	>= 1 Al	-1.236921
O15303	583	Cl-C:C-O-C	-1.237416
O15303	764	Oc1c(Cl)cccc1	-1.259063
O15303	858	ClC1CC(Br)CC1	-1.271167
O15303	511	S=C-N-[#1]	-1.271968
O15303	82	>= 1 Te	-1.277083
O15303	496	N:N-C-[#1]	-1.280303
O15303	620	C:C-O-C-C	-1.285319
O15303	179	>= 1 saturated or aromatic carbon-only ring size 6	-1.304138
O15303	312	O-Al	-1.308138
O15303	428	C(#C)(-H)	-1.310814
O15303	111	>= 1 Tm	-1.313509
O15303	472	C:N:C-C	-1.336314
O15303	750	Nc1cc(Cl)ccc1	-1.341812
O15303	561	Cl-C-C=O	-1.343337
O15303	389	C(:N)(:N)	-1.352714
O15303	866	OC1C(O)CCC1	-1.367264
O15303	430	C(-C)(-C)(=C)	-1.392258
O15303	338	C(~C)(~C)(~H)(~N)	-1.397241
O15303	303	N-Si	-1.410013
O15303	263	Li-H	-1.420042
O15303	15	>= 2 N	-1.420653
O15303	659	O-C-C-N-C	-1.421864
O15303	52	>= 1 Ca	-1.442064
O15303	788	SC1CCC(N)CC1	-1.458149
O15303	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	-1.469418
O15303	560	N-C-N-C	-1.474278
O15303	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	-1.523273
O15303	689	O-C-C-C-C-C-C	-1.531285
O15303	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	-1.541585
O15303	523	N:C:C-C	-1.554196
O15303	624	O=C-C:C-N	-1.555081
O15303	547	N-C:C-N	-1.568079
O15303	76	>= 1 Pd	-1.583975
O15303	114	>= 1 U	-1.598769
O15303	861	CC1C(O)CCC1	-1.60501
O15303	489	N-C-S-C	-1.62083
O15303	682	O-C-C-C-C-N	-1.655074
O15303	545	N-C:C-C	-1.655433
O15303	641	O-C-C-C=C	-1.696397
O15303	376	C(~N)(:C)	-1.716191
O15303	546	N-C:C-[#1]	-1.724402

O15303	440	C(-C)(-O)(=O)	−1.727602
O15303	381	C(~O)(:C)	−1.764057
O15303	309	O-O	−1.791103
O15303	555	N=C-C=C	−1.825894
O15303	669	Cl-C:C-C=O	−1.877216
O15303	621	N-C:C:C:N	−1.910859
O15303	342	C(~C)(~Cl)	−1.922156
O15303	771	Nc1c(Cl)cccc1	−1.953252
O15303	293	C-S	−1.959341
O15303	832	SC1C(Br)CCCC1	−1.986236
O15303	375	C(~N)(~N)	−2.07628
O15303	158	>= 3 saturated or aromatic carbon-only ring size 5	−2.171817
O15303	351	C(~C)(~N)	−2.203178
O15303	603	C-C:C:C-C	−2.255916
O15303	100	>= 1 Ce	−2.258865
O15303	508	S=C-N-C	−2.266263
O15303	358	C(~C)(:N)	−2.380703
O15303	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−2.854103
O15303	650	O=C-N-C=O	−3.228136

Fingerprints（continued)

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q14832	313	O-Si	3.0142164
Q14832	309	O-O	2.7994353
Q14832	495	C-N-C:C	2.6442661
Q14832	411	P(~O)(~O)	2.5643536
Q14832	136	>= 2 any ring size 4	2.5385301
Q14832	629	S-C:C:C-N	2.3316952
Q14832	295	C-As	2.3242176
Q14832	257	>= 2 aromatic rings	2.2516422
Q14832	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	2.1945006
Q14832	476	C-O-C=C	2.0847752
Q14832	784	OC1CCC(N)CC1	2.0677364
Q14832	595	C:C-C-C-C	2.0475548
Q14832	382	C(~O)(:C)(:C)	2.0467032
Q14832	444	C(-Cl)(=O)	2.0357435
Q14832	578	C-C:C-C:C	2.0280213
Q14832	597	O=C-C-C:C	2.0260331
Q14832	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	2.0253962
Q14832	143	>= 1 any ring size 5	2.002906
Q14832	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	1.9961363
Q14832	727	Sc1ccc(Br)cc1	1.9925028
Q14832	589	C-C:C-O-C	1.9924706
Q14832	104	>= 1 Sm	1.9915971
Q14832	59	>= 1 Co	1.9789195
Q14832	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	1.9596085
Q14832	532	S-C:C-[#1]	1.9453914
Q14832	368	C(~H)(~S)	1.9400514
Q14832	355	C(~C)(:C)	1.8867636
Q14832	518	O=C-N-N	1.880183
Q14832	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	1.8485782
Q14832	680	O-C-C-C-C-C	1.8125361
Q14832	777	CC1CCC(O)CC1	1.7958891
Q14832	523	N:C:C-C	1.7953842
Q14832	399	N(~H)(:C)	1.787478
Q14832	669	Cl-C:C-C=O	1.7864518
Q14832	456	P(-O)(=O)	1.7762304
Q14832	359	C(~C)(:N)(:N)	1.7754758
Q14832	105	>= 1 Eu	1.764926
Q14832	13	>= 32 C	1.7491865
Q14832	576	N=C-C:C-[#1]	1.7061516
Q14832	441	C(-C)(=C)	1.7047094
Q14832	706	O=C-C-C-C-C(=O)-C	1.6773359
Q14832	741	Oc1cc(S)ccc1	1.6752522
Q14832	768	Sc1c(Cl)cccc1	1.6677451
Q14832	782	OC1CCC(O)CC1	1.6589806
Q14832	676	N#C-C-C-C	1.6486103
Q14832	580	O=C-C-C-N	1.6435061

Q14832	386	C(:C)(:C)(:N)	1.6214995
Q14832	94	>= 1 Au	1.62071
Q14832	530	N:C-C:C	1.6194306
Q14832	783	OC1CCC(S)CC1	1.6069172
Q14832	778	CC1CCC(S)CC1	1.6034957
Q14832	165	>= 4 saturated or aromatic carbon-only ring size 5	1.5831249
Q14832	583	Cl-C:C-O-C	1.5617132
Q14832	150	>= 2 any ring size 5	1.5381704
Q14832	619	O-C-C=C-C	1.5367673
Q14832	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	1.5353738
Q14832	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	1.5199341
Q14832	109	>= 1 Ho	1.5171169
Q14832	288	C-Na	1.494665
Q14832	803	OC1CC(O)CCC1	1.4935598
Q14832	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	1.4828949
Q14832	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	1.4652127
Q14832	618	C:C-C-C:C	1.4607919
Q14832	414	S(~C)(~O)	1.4589201
Q14832	220	>= 2 any ring size 7	1.4535704
Q14832	95	>= 1 Hg	1.4519349
Q14832	116	>= 1 saturated or aromatic carbon-only ring size 3	1.4508797
Q14832	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	1.4475878
Q14832	801	CC1CC(Cl)CCC1	1.4415842
Q14832	874	SC1C(Br)CCC1	1.440917
Q14832	853	SC1CC(Br)CC1	1.4285357
Q14832	1	>= 8 H	1.417668
Q14832	415	Si(~C)(~C)	1.4093579
Q14832	858	ClC1CC(Br)CC1	1.4038818
Q14832	462	O-C-C=O	1.3983333
Q14832	362	C(~Cl)(:C)	1.3739705
Q14832	837	ClC1C(Br)CCCC1	1.3542173
Q14832	558	O=N-C:C	1.3429101
Q14832	527	C:C:N-[#1]	1.3237706
Q14832	752	Clc1cc(Cl)ccc1	1.3211715
Q14832	791	NC1CCC(N)CC1	1.3079369
Q14832	544	O-C:C-O	1.3059881
Q14832	610	C-O-C-O-C	1.305258
Q14832	273	B-B	1.2991995
Q14832	528	[#1]-N-C-[#1]	1.2808562
Q14832	512	C-[As]-O-[#1]	1.2570727
Q14832	200	>= 4 saturated or aromatic carbon-only ring size 6	1.2567618
Q14832	793	NC1CCC(Br)CC1	1.2354132
Q14832	725	Sc1ccc(N)cc1	1.2348718
Q14832	492	N-C:O:C	1.231595
Q14832	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	1.2293878
Q14832	80	>= 1 Sn	1.2205171
Q14832	675	Br-C-C-C:C	1.2114432
Q14832	115	>= 1 any ring size 3	1.2107509

Q14832	164	>= 4 any ring size 5	1.2080329
Q14832	681	O-C-C-C-C-O	1.1976621
Q14832	563	O-C-O-C	1.1962967
Q14832	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	1.195463
Q14832	379	C(~N)(:N)	1.1904335
Q14832	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	1.1797798
Q14832	875	NC1C(N)CCC1	1.1691932
Q14832	599	[#1]-C-C=C-[#1]	1.164525
Q14832	352	C(~C)(~O)	1.1632551
Q14832	481	O-S-C:C	1.1501501
Q14832	557	N:C-O-[#1]	1.1391636
Q14832	447	C(-H)(=N)	1.1389794
Q14832	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	1.132537
Q14832	137	>= 2 saturated or aromatic carbon-only ring size 4	1.1287175
Q14832	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	1.1180923
Q14832	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	1.1157495
Q14832	344	C(~C)(~H)	1.1153805
Q14832	398	N(~H)(~N)	1.1101636
Q14832	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	1.1078808
Q14832	716	Cc1ccc(N)cc1	1.1012734
Q14832	506	C-C:N:C	1.0922434
Q14832	843	CC1CC(Cl)CC1	1.0823157
Q14832	568	N#C-C-C	1.0801014
Q14832	682	O-C-C-C-C-N	1.0645307
Q14832	84	>= 1 Cs	1.0643534
Q14832	249	>= 1 saturated or aromatic carbon-only ring size 10	1.0636703
Q14832	748	Sc1cc(Br)ccc1	1.0549624
Q14832	468	O=S-C-N	1.0526684
Q14832	497	O-C:C:N	1.0499826
Q14832	342	C(~C)(~Cl)	1.0478035
Q14832	808	SC1CC(S)CCC1	1.0473594
Q14832	40	>= 8 Cl	1.046306
Q14832	484	N-C:N:C	1.0381277
Q14832	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	1.0339622
Q14832	334	C(~C)(~C)(~C)(~C)	1.0190485
Q14832	417	C#C	1.0172952
Q14832	661	O-C-O-C-C	1.0132341
Q14832	836	ClC1C(Cl)CCCC1	1.0044006
Q14832	547	N-C:C-N	0.9936298
Q14832	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.9911699
Q14832	290	C-Al	0.9882613
Q14832	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.9877493
Q14832	422	N=N	0.9814061
Q14832	353	C(~C)(~S)	0.9761193
Q14832	833	NC1C(N)CCCC1	0.9745016
Q14832	390	N(~C)(~C)	0.9743199
Q14832	643	[#1]-C-C-N-[#1]	0.97421
Q14832	707	O=C-C-C-C-C(N)-C	0.9733373

Q14832	625	O=C-C:C-O	0.9709338
Q14832	289	C-Mg	0.9558607
Q14832	466	N#C-C=C	0.9504706
Q14832	5	>= 2 Li	0.9489967
Q14832	665	N-C:C-C-C	0.9471796
Q14832	742	Oc1cc(N)ccc1	0.9438735
Q14832	48	>= 4 I	0.9376933
Q14832	600	N-C:C:C-C	0.9203683
Q14832	861	CC1C(O)CCC1	0.9168127
Q14832	269	Li-P	0.911939
Q14832	654	N-C-N-C-C	0.9117854
Q14832	241	>= 1 any ring size 9	0.9114373
Q14832	767	Sc1c(N)cccc1	0.8987745
Q14832	672	O=C-C=C-[#1]	0.8803105
Q14832	242	>= 1 saturated or aromatic carbon-only ring size 9	0.8772664
Q14832	719	Oc1ccc(O)cc1	0.8765399
Q14832	636	C-N-C-N-C	0.8726372
Q14832	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.867072
Q14832	700	O-C-C-C-C-C-O-C	0.8664344
Q14832	11	>= 8 C	0.8551296
Q14832	38	>= 2 Cl	0.850874
Q14832	644	C-C=N-N-C	0.8501521
Q14832	806	OC1CC(Cl)CCC1	0.8479036
Q14832	865	CC1C(Br)CCC1	0.8366707
Q14832	17	>= 8 N	0.8293691
Q14832	686	O=C-C-C-C-O	0.8169663
Q14832	756	Cc1c(O)cccc1	0.8108637
Q14832	7	>= 2 B	0.8031384
Q14832	22	>= 16 O	0.799748
Q14832	77	>= 1 Ag	0.797304
Q14832	305	N-S	0.7965739
Q14832	299	N-H	0.7926532
Q14832	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.7923303
Q14832	593	N-C-C-C-N	0.784246
Q14832	23	>= 1 F	0.778762
Q14832	321	Si-Si	0.7757787
Q14832	572	N:C:N:C	0.7717294
Q14832	401	N(~O)(~O)	0.768875
Q14832	646	O=C-N-C-[#1]	0.7660906
Q14832	39	>= 4 Cl	0.7649707
Q14832	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.7639401
Q14832	499	N-C:C:N	0.7596254
Q14832	827	OC1C(Cl)CCCC1	0.7505776
Q14832	318	Al-H	0.7476743
Q14832	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.7439588
Q14832	524	C-C=C-C	0.7406933
Q14832	590	C-C:C-O-[#1]	0.7399384
Q14832	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.7398184

Q14832	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.738312
Q14832	633	N-C-C:C-C	0.7343593
Q14832	49	>= 1 Be	0.7277581
Q14832	267	Li-O	0.7181192
Q14832	588	O=C-C-C=O	0.7165161
Q14832	755	Cc1c(C)cccc1	0.7163363
Q14832	757	Cc1c(S)cccc1	0.7154093
Q14832	760	Cc1c(Br)cccc1	0.7119066
Q14832	615	N-C-C-O-C	0.7109697
Q14832	869	OC1C(Cl)CCC1	0.7062539
Q14832	402	N(~O)(:O)	0.7055752
Q14832	478	S-C=N-[#1]	0.7023413
Q14832	412	S(~C)(~C)	0.6991331
Q14832	420	C=O	0.6928691
Q14832	312	O-Al	0.6917429
Q14832	560	N-C-N-C	0.6822332
Q14832	404	N(:C)(:C)(:C)	0.6766425
Q14832	796	BrC1CCC(Br)CC1	0.6757026
Q14832	609	Cl-C-C-N-C	0.671113
Q14832	298	C-I	0.6677702
Q14832	123	>= 2 saturated or aromatic carbon-only ring size 3	0.6649874
Q14832	604	C-O-C-C:C	0.6622797
Q14832	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.6574612
Q14832	300	N-N	0.6555277
Q14832	813	NC1CC(Cl)CCC1	0.6543986
Q14832	284	C-C	0.6455253
Q14832	529	Cl-C-C-Cl	0.6420203
Q14832	101	>= 1 Pr	0.6404924
Q14832	485	N:C:C:N	0.6340186
Q14832	73	>= 1 Mo	0.6323587
Q14832	387	C(:C)(:N)	0.6316256
Q14832	46	>= 1 I	0.6310516
Q14832	345	C(~C)(~H)(~N)	0.6298096
Q14832	579	O=C-C-C-C	0.6290836
Q14832	409	O(:C)(:C)	0.624288
Q14832	526	Cl-C:C-Cl	0.6238329
Q14832	850	SC1CC(S)CC1	0.6221893
Q14832	151	>= 2 saturated or aromatic carbon-only ring size 5	0.618283
Q14832	641	O-C-C-C=C	0.6102283
Q14832	303	N-Si	0.6053673
Q14832	356	C(~C)(:C)(:C)	0.6041665
Q14832	43	>= 1 Br	0.6026152
Q14832	51	>= 1 Al	0.5873766
Q14832	805	OC1CC(N)CCC1	0.5837699
Q14832	108	>= 1 Dy	0.5708277
Q14832	227	>= 1 any ring size 8	0.5659671
Q14832	392	N(~C)(~C)(~H)	0.5632697
Q14832	25	>= 4 F	0.5601604

Q14832	369	C(~H)(~Si)	0.5597142
Q14832	705	O=C-C-C-C-C(O)-C	0.5556445
Q14832	172	>= 5 saturated or aromatic carbon-only ring size 5	0.5550255
Q14832	361	C(~Cl)(~H)	0.5523651
Q14832	830	SC1C(N)CCCC1	0.5521521
Q14832	688	C-C-C-C-C-C-C	0.5512895
Q14832	93	>= 1 Pt	0.5500445
Q14832	33	>= 1 S	0.5461212
Q14832	645	O=C-N-C-C	0.5433656
Q14832	178	>= 1 any ring size 6	0.5405629
Q14832	567	O-C-C-O	0.5386932
Q14832	389	C(:N)(:N)	0.5342492
Q14832	340	C(~C)(~C)(~N)	0.5310491
Q14832	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.5289471
Q14832	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.5245616
Q14832	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.5199045
Q14832	816	ClC1CC(Br)CCC1	0.5177985
Q14832	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.5176066
Q14832	860	CC1C(C)CCC1	0.5175283
Q14832	842	CC1CC(N)CC1	0.5162338
Q14832	370	C(~H)(:C)	0.5145813
Q14832	4	>= 1 Li	0.5132645
Q14832	322	Si-Cl	0.5126444
Q14832	185	>= 2 any ring size 6	0.509768
Q14832	280	B-S	0.5037524
Q14832	35	>= 4 S	0.4938786
Q14832	857	ClC1CC(Cl)CC1	0.4886405
Q14832	638	O-C-C-C-N	0.4856436
Q14832	856	NC1CC(Br)CC1	0.4856345
Q14832	631	O-C:C-O-[#1]	0.4824523
Q14832	377	C(~N)(:C)(:C)	0.4813842
Q14832	723	Oc1ccc(Br)cc1	0.4782789
Q14832	612	N-C-O-C-C	0.4753356
Q14832	302	N-F	0.4751833
Q14832	435	C(-C)(-H)(=N)	0.4738878
Q14832	416	C=C	0.4737102
Q14832	286	C-O	0.471792
Q14832	100	>= 1 Ce	0.471746
Q14832	571	[#1]-C-O-[#1]	0.4678949
Q14832	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.4656819
Q14832	419	C#N	0.4642895
Q14832	663	O-C-C-O-[#1]	0.4556652
Q14832	709	C-C(C)-C-C-C	0.455502
Q14832	814	NC1CC(Br)CCC1	0.4534412
Q14832	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.4529045
Q14832	112	>= 1 Yb	0.45228
Q14832	668	C-C:C-C-C	0.4512004
Q14832	575	O-C-C:C-O	0.4504171

Q14832	648	O=N-C:C-N	0.4495732
Q14832	255	>= 1 aromatic ring	0.4491173
Q14832	339	C(~C)(~C)(~H)(~O)	0.4474651
Q14832	734	Cc1cc(C)ccc1	0.4463235
Q14832	637	O-C-C-C-C	0.4444369
Q14832	849	OC1CC(Br)CC1	0.441083
Q14832	565	C:C-O-C	0.4398388
Q14832	555	N=C-C=C	0.4349098
Q14832	129	>= 1 any ring size 4	0.434429
Q14832	759	Cc1c(Cl)cccc1	0.4335265
Q14832	535	O=C-C-C	0.4319484
Q14832	31	>= 2 P	0.4292956
Q14832	745	Sc1cc(S)ccc1	0.4291764
Q14832	367	C(~H)(~O)(~O)	0.4217394
Q14832	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.4160675
Q14832	380	C(~O)(~O)	0.4137087
Q14832	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.4119093
Q14832	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.4098235
Q14832	607	N-C-C-C:C	0.4049354
Q14832	396	N(~C)(:C)	0.3957383
Q14832	729	Nc1ccc(Cl)cc1	0.3956924
Q14832	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.3952005
Q14832	662	O-C-C-O-C	0.3910588
Q14832	60	>= 1 Ni	0.3909935
Q14832	577	C:C-N-C:C	0.3872888
Q14832	357	C(~C)(:C)(:N)	0.3870526
Q14832	358	C(~C)(:N)	0.3829704
Q14832	630	O-C:C-O-C	0.3803037
Q14832	684	O=C-C-C-C-C	0.3745381
Q14832	455	N(-O)(=O)	0.3732296
Q14832	294	C-Cl	0.36932
Q14832	103	>= 1 Pm	0.3665386
Q14832	876	NC1C(Cl)CC1	0.3661036
Q14832	53	>= 1 Sc	0.3619309
Q14832	554	Br-C-C-C	0.3596216
Q14832	98	>= 1 Bi	0.3546147
Q14832	832	SC1C(Br)CCCC1	0.3502731
Q14832	58	>= 1 Fe	0.3443927
Q14832	277	B-F	0.3429536
Q14832	261	>= 4 aromatic rings	0.3279543
Q14832	373	C(~H)(:N)	0.3273789
Q14832	826	OC1C(N)CCCC1	0.326088
Q14832	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.3217095
Q14832	513	S:C:C-[#1]	0.3195077
Q14832	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.3194046
Q14832	657	C-N-C:C-C	0.3177893
Q14832	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.3081498
Q14832	699	O-C-C-C-C-C(C)-C	0.3051523

Q14832	683	N-C-C-C-C-C	0.2903021
Q14832	666	C=C-C-O-C	0.2863249
Q14832	511	S=C-N-[#1]	0.2844906
Q14832	581	O=C-C-C-O	0.279282
Q14832	471	S:C:C:C	0.269678
Q14832	493	O=C-C:C	0.2695067
Q14832	761	Oc1c(O)cccc1	0.269264
Q14832	867	OC1C(S)CCC1	0.2683363
Q14832	206	>= 5 any ring size 6	0.2675967
Q14832	751	Nc1cc(Br)ccc1	0.2669334
Q14832	617	C-C-C-O-[#1]	0.2643221
Q14832	488	N-C=N-[#1]	0.2636962
Q14832	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.2599727
Q14832	364	C(~F)(:C)	0.2563665
Q14832	509	Br-C:C-C	0.2560051
Q14832	792	NC1CCC(Cl)CC1	0.2549016
Q14832	479	S-C-S-C	0.2533389
Q14832	825	OC1C(S)CCCC1	0.2511865
Q14832	32	>= 4 P	0.2509136
Q14832	260	>= 3 hetero-aromatic rings	0.2499086
Q14832	728	Nc1ccc(N)cc1	0.2486704
Q14832	496	N:N-C-[#1]	0.2391605
Q14832	473	S-C:N:C	0.2387742
Q14832	785	OC1CCC(Cl)CC1	0.2382699
Q14832	549	N-C-C:C	0.2352651
Q14832	701	O-C-C-C-C-C(O)-C	0.2314828
Q14832	763	Oc1c(N)cccc1	0.2296031
Q14832	83	>= 1 Xe	0.222135
Q14832	385	C(:C)(:C)(:C)	0.2200997
Q14832	743	Oc1cc(Cl)ccc1	0.2188882
Q14832	812	NC1CC(N)CCC1	0.2173718
Q14832	326	As-As	0.2133156
Q14832	653	O-C:C:C-O	0.2125497
Q14832	346	C(~C)(~H)(~O)	0.2123522
Q14832	712	C-C(C)-C(C)-C	0.2079911
Q14832	351	C(~C)(~N)	0.2076273
Q14832	474	S:C:C:N	0.2075527
Q14832	24	>= 2 F	0.2068455
Q14832	92	>= 1 Ir	0.2055566
Q14832	722	Oc1ccc(Cl)cc1	0.204991
Q14832	88	>= 1 Ta	0.1892191
Q14832	651	O-C:C:C-C	0.1877305
Q14832	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.1872444
Q14832	301	N-O	0.1825781
Q14832	573	O-C-C=C	0.1794492
Q14832	395	N(~C)(~O)	0.1789869
Q14832	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.176998
Q14832	642	O-C-C-C=O	0.1732441

Q14832	824	OC1C(O)CCCC1	0.1676738
Q14832	758	Cc1c(N)cccc1	0.1648062
Q14832	703	O-C-C-C-C-C(N)-C	0.1620039
Q14832	228	>= 1 saturated or aromatic carbon-only ring size 8	0.1546947
Q14832	310	O-Mg	0.1526595
Q14832	536	O=C-C-N	0.1512502
Q14832	772	Nc1c(Br)cccc1	0.151133
Q14832	602	O=C-C-N-C	0.1475804
Q14832	47	>= 2 I	0.1460663
Q14832	771	Nc1c(Cl)cccc1	0.1398297
Q14832	606	O-C:C-C-C	0.1394306
Q14832	44	>= 2 Br	0.1285695
Q14832	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.1277678
Q14832	864	CC1C(Cl)CCC1	0.1198997
Q14832	671	O=C-C=C-C	0.1184454
Q14832	408	O(~H)(~S)	0.1149102
Q14832	691	O-C-C-C-C-C-N	0.1126469
Q14832	507	C-C-S-C	0.1088807
Q14832	96	>= 1 Tl	0.1057626
Q14832	750	Nc1cc(Cl)ccc1	0.1036668
Q14832	852	SC1CC(Cl)CC1	0.1004633
Q14832	461	O-C-C=N	0.0972068
Q14832	775	Brc1c(Br)cccc1	0.0967138
Q14832	263	Li-H	0.0962784
Q14832	405	O(~C)(~C)	0.0945412
Q14832	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0940899
Q14832	397	N(~C)(:C)(:C)	0.0934194
Q14832	34	>= 2 S	0.0914315
Q14832	86	>= 1 Lu	0.0899434
Q14832	341	C(~C)(~C)(~O)	0.0889995
Q14832	872	SC1C(N)CCC1	0.084012
Q14832	65	>= 1 As	0.0838042
Q14832	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.0783032
Q14832	690	O-C-C-C-C-C-O	0.0777194
Q14832	877	NC1C(Br)CCC1	0.0713192
Q14832	521	C:N-C-[#1]	0.0711646
Q14832	714	Cc1ccc(O)cc1	0.0695746
Q14832	489	N-C-S-C	0.0673455
Q14832	99	>= 1 La	0.066534
Q14832	542	O-C:C-[#1]	0.0653482
Q14832	347	C(~C)(~H)(~O)(~O)	0.062976
Q14832	624	O=C-C:C-N	0.0606303
Q14832	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0577956
Q14832	328	C(~Br)(~C)(~C)	0.0548655
Q14832	807	OC1CC(Br)CCC1	0.0544444
Q14832	711	C-C(C)(C)-C-C	0.054076
Q14832	56	>= 1 Cr	0.052446
Q14832	448	C(-H)(=O)	0.0521699

Q14832	354	C(~C)(~Si)	0.0500628
Q14832	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.0495738
Q14832	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0455448
Q14832	839	CC1CC(C)CC1	0.0441083
Q14832	715	Cc1ccc(S)cc1	0.0423316
Q14832	677	C-C=C-C:C	0.0395696
Q14832	564	C=C-C=C	0.0364326
Q14832	502	N-C=C-[#1]	0.0288607
Q14832	689	O-C-C-C-C-C-C	0.0238251
Q14832	569	N-C-C-N	0.0213026
Q14832	144	>= 1 saturated or aromatic carbon-only ring size 5	0.0144445
Q14832	107	>= 1 Tb	0.0124695
Q14832	268	Li-F	0.0123366
Q14832	16	>= 4 N	0.0103079
Q14832	424	N=P	0.0055917
Q14832	421	C=S	0.0050955
Q14832	0	>= 4 H	0.0031339
Q14832	787	SC1CCC(S)CC1	0.002699
Q14832	834	NC1C(Cl)CCCC1	0.0017246
Q14832	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.0016312
Q14832	601	N-C:C-C-N	0.0015782
Q14832	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0003095
Q14832	248	>= 1 any ring size 10	4.83E-05
Q14832	870	OC1C(Br)CCC1	1.20E-05
Q14832	81	>= 1 Sb	-8.44E-05
Q14832	234	>= 2 any ring size 8	-0.000125
Q14832	45	>= 4 Br	-0.000739
Q14832	291	C-Si	-0.001073
Q14832	804	OC1CC(S)CCC1	-0.002441
Q14832	802	CC1CC(Br)CCC1	-0.002833
Q14832	186	>= 2 saturated or aromatic carbon-only ring size 6	-0.003441
Q14832	519	N=C-N-C	-0.003936
Q14832	664	C-C=C-C=C	-0.005317
Q14832	730	Nc1ccc(Br)cc1	-0.011027
Q14832	584	C:C-C=C-C	-0.0115
Q14832	522	C-N-N-[#1]	-0.017759
Q14832	278	B-Si	-0.02049
Q14832	61	>= 1 Cu	-0.027153
Q14832	122	>= 2 any ring size 3	-0.028571
Q14832	343	C(~C)(~Cl)(~H)	-0.029442
Q14832	19	>= 2 O	-0.02973
Q14832	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	-0.033165
Q14832	541	O-C:C-C	-0.034003
Q14832	324	P-P	-0.034789
Q14832	293	C-S	-0.036347
Q14832	158	>= 3 saturated or aromatic carbon-only ring size 5	-0.045029
Q14832	647	O=C-N-C-N	-0.048294
Q14832	315	O-K	-0.056192

Q14832	307	N-Br	−0.056459
Q14832	67	>= 1 Kr	−0.063702
Q14832	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.068861
Q14832	640	C=C-C-C-C	−0.071651
Q14832	591	Cl-C-C-C-C	−0.079165
Q14832	570	C:C-C-C	−0.080474
Q14832	443	C(-C)(=O)	−0.088318
Q14832	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.092274
Q14832	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.097257
Q14832	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.099087
Q14832	102	>= 1 Nd	−0.09934
Q14832	639	O-C-C-C-O	−0.099944
Q14832	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.100821
Q14832	539	N=C-C-[#1]	−0.102311
Q14832	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.1098
Q14832	391	N(~C)(~C)(~C)	−0.110357
Q14832	319	Al-Cl	−0.116017
Q14832	704	O=C-C-C-C-C-C-C	−0.123023
Q14832	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.123838
Q14832	87	>= 1 Hf	−0.130883
Q14832	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.137316
Q14832	538	N=C-C-C	−0.145852
Q14832	480	C:S:C-C	−0.149345
Q14832	449	C(-N)(=C)	−0.157778
Q14832	634	C-C-C:C-C	−0.161504
Q14832	374	C(~H)(~H)(~H)	−0.163827
Q14832	546	N-C:C-[#1]	−0.169396
Q14832	192	>= 3 any ring size 6	−0.175736
Q14832	838	BrC1C(Br)CCCC1	−0.181996
Q14832	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.182142
Q14832	428	C(#C)(-H)	−0.184877
Q14832	27	>= 2 Na	−0.186594
Q14832	786	OC1CCC(Br)CC1	−0.186811
Q14832	517	N-N-C-N	−0.191732
Q14832	543	O-C:C-N	−0.194116
Q14832	608	C-C-C-C:C	−0.194584
Q14832	733	Brc1ccc(Br)cc1	−0.199365
Q14832	451	C(-N)(=O)	−0.20014
Q14832	696	C-C-C-C-C-C-C-C	−0.200911
Q14832	75	>= 1 Rh	−0.204136
Q14832	594	C-O-C-C=C	−0.205477
Q14832	835	NC1C(Br)CCCC1	−0.211318
Q14832	702	O-C-C-C-C-C-N-C	−0.221477
Q14832	304	N-P	−0.223514
Q14832	674	N-C-N-C:C	−0.223757
Q14832	766	Sc1c(S)cccc1	−0.223776
Q14832	754	Brc1cc(Br)ccc1	−0.22408
Q14832	20	>= 4 O	−0.22648

Q14832	316	F-P	−0.228483
Q14832	338	C(~C)(~C)(~H)(~N)	−0.229531
Q14832	667	C=C-C-O-[#1]	−0.230091
Q14832	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.234293
Q14832	89	>= 1 W	−0.235382
Q14832	436	C(-C)(-H)(=O)	−0.23892
Q14832	698	O-C-C-C-C-C-C-C	−0.2397
Q14832	69	>= 1 Sr	−0.240747
Q14832	828	OC1C(Br)CCCC1	−0.241567
Q14832	78	>= 1 Cd	−0.244113
Q14832	776	CC1CCC(C)CC1	−0.247464
Q14832	106	>= 1 Gd	−0.253028
Q14832	628	C-N-C-C:C	−0.256577
Q14832	452	C(-O)(=O)	−0.257651
Q14832	472	C:N:C-C	−0.260011
Q14832	10	>= 4 C	−0.261613
Q14832	297	C-Br	−0.265495
Q14832	378	C(~N)(:C)(:N)	−0.267667
Q14832	413	S(~C)(~H)	−0.269222
Q14832	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.270843
Q14832	635	N-N-C-N-[#1]	−0.272472
Q14832	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.275145
Q14832	292	C-P	−0.275976
Q14832	697	C-C-C-C-C-C(C)-C	−0.283394
Q14832	418	C=N	−0.284367
Q14832	384	C(:C)(:C)	−0.285496
Q14832	317	F-S	−0.288574
Q14832	823	CC1C(Br)CCCC1	−0.298849
Q14832	841	CC1CC(S)CC1	−0.301917
Q14832	457	S(-C)(=O)	−0.303204
Q14832	574	O-C-C:C-C	−0.31106
Q14832	516	[#1]-C=C-[#1]	−0.314976
Q14832	42	>= 2 K	−0.318305
Q14832	50	>= 1 Mg	−0.319418
Q14832	626	C-O-C:C-C	−0.321942
Q14832	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.323405
Q14832	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.326823
Q14832	693	O=C-C-C-C-C-O	−0.328502
Q14832	510	[#1]-N-N-[#1]	−0.334861
Q14832	15	>= 2 N	−0.337279
Q14832	372	C(~H)(:C)(:N)	−0.337956
Q14832	627	O=[As]-C:C:C	−0.33908
Q14832	718	Cc1ccc(Br)cc1	−0.34091
Q14832	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.347495
Q14832	279	B-P	−0.353338
Q14832	52	>= 1 Ca	−0.356719
Q14832	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.356819
Q14832	469	S-S-C:C	−0.362418

Q14832	348	C(~C)(~H)(~P)	−0.364673
Q14832	620	C:C-O-C-C	−0.366978
Q14832	797	CC1CC(C)CCC1	−0.371077
Q14832	393	N(~C)(~H)	−0.373398
Q14832	403	N(:C)(:C)	−0.377454
Q14832	63	>= 1 Ga	−0.377647
Q14832	41	>= 1 K	−0.382439
Q14832	613	C-N-C-C-C	−0.388282
Q14832	525	[As]-C:C-[#1]	−0.389096
Q14832	429	C(#N)(-C)	−0.391027
Q14832	879	ClC1C(Br)CCC1	−0.391257
Q14832	820	CC1C(S)CCCC1	−0.395082
Q14832	717	Cc1ccc(Cl)cc1	−0.395671
Q14832	311	O-Na	−0.397447
Q14832	780	CC1CCC(Cl)CC1	−0.406111
Q14832	708	C-C(C)-C-C	−0.408143
Q14832	97	>= 1 Pb	−0.408732
Q14832	845	OC1CC(O)CC1	−0.416784
Q14832	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.418995
Q14832	30	>= 1 P	−0.420441
Q14832	670	Br-C:C-C-C	−0.423097
Q14832	66	>= 1 Se	−0.424729
Q14832	720	Oc1ccc(S)cc1	−0.42572
Q14832	504	N:C:N-C	−0.429643
Q14832	673	O=C-C=C-N	−0.432692
Q14832	800	CC1CC(N)CCC1	−0.433372
Q14832	363	C(~F)(~F)	−0.438475
Q14832	817	BrC1CC(Br)CCC1	−0.441423
Q14832	467	C=N-N-C	−0.441679
Q14832	26	>= 1 Na	−0.446133
Q14832	388	C(:C)(:N)(:N)	−0.446785
Q14832	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.447999
Q14832	265	Li-B	−0.449166
Q14832	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.451619
Q14832	325	As-H	−0.45174
Q14832	327	C(~Br)(~C)	−0.456429
Q14832	111	>= 1 Tm	−0.460286
Q14832	440	C(-C)(-O)(=O)	−0.464802
Q14832	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.468719
Q14832	550	Cl-C-C-C	−0.472693
Q14832	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.476031
Q14832	371	C(~H)(:C)(:C)	−0.477494
Q14832	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.478321
Q14832	439	C(-C)(-N)(=O)	−0.48807
Q14832	213	>= 1 any ring size 7	−0.488844
Q14832	76	>= 1 Pd	−0.490229
Q14832	308	O-H	−0.491538
Q14832	8	>= 4 B	−0.491725

Q14832	79	>= 1 In	-0.491864
Q14832	873	SC1C(Cl)CCC1	-0.493218
Q14832	598	Cl-C:C:C-C	-0.494119
Q14832	829	SC1C(S)CCCC1	-0.495092
Q14832	130	>= 1 saturated or aromatic carbon-only ring size 4	-0.496456
Q14832	264	Li-Li	-0.497261
Q14832	394	N(~C)(~H)(~N)	-0.499798
Q14832	566	O-C-C-N	-0.501975
Q14832	789	SC1CCC(Cl)CC1	-0.503906
Q14832	487	N-C=N-C	-0.50521
Q14832	863	CC1C(N)CCC1	-0.506181
Q14832	2	>= 16 H	-0.516933
Q14832	74	>= 1 Ru	-0.517602
Q14832	283	C-H	-0.521516
Q14832	611	N-C-C-N-C	-0.526229
Q14832	736	Cc1cc(S)ccc1	-0.526288
Q14832	333	C(~C)(~C)(~C)	-0.530986
Q14832	454	N(-C)(=O)	-0.53263
Q14832	788	SC1CCC(N)CC1	-0.534154
Q14832	266	Li-C	-0.538136
Q14832	710	C-C-C(C)-C-C	-0.539911
Q14832	430	C(-C)(-C)(=C)	-0.540254
Q14832	605	O=C-C-O-C	-0.543921
Q14832	458	S(-O)(=O)	-0.544293
Q14832	694	O=C-C-C-C-C=O	-0.54919
Q14832	692	O=C-C-C-C-C-C	-0.549567
Q14832	652	O-C:C:C-N	-0.550737
Q14832	764	Oc1c(Cl)cccc1	-0.551622
Q14832	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.555555
Q14832	660	C-C=C-C-C	-0.559456
Q14832	737	Cc1cc(N)ccc1	-0.564098
Q14832	28	>= 1 Si	-0.584359
Q14832	810	SC1CC(Cl)CCC1	-0.586218
Q14832	855	NC1CC(Cl)CC1	-0.594463
Q14832	656	C-C-N-C-C	-0.596948
Q14832	739	Cc1cc(Br)ccc1	-0.600032
Q14832	515	N-N-C-C	-0.602236
Q14832	545	N-C:C-C	-0.61071
Q14832	822	CC1C(Cl)CCCC1	-0.614601
Q14832	445	C(-H)(-N)(=C)	-0.619298
Q14832	329	C(~Br)(~H)	-0.620456
Q14832	491	C-N:C-[#1]	-0.626163
Q14832	556	C=C-C-C	-0.626551
Q14832	383	C(~S)(:C)	-0.645432
Q14832	818	CC1C(C)CCCC1	-0.64661
Q14832	282	B-Br	-0.646796
Q14832	731	Clc1ccc(Cl)cc1	-0.649421
Q14832	774	Clc1c(Br)cccc1	-0.656552

Q14832	426	P=P	−0.661169
Q14832	559	O-C-N-[#1]	−0.663705
Q14832	878	ClC1C(Cl)CCC1	−0.665086
Q14832	501	Cl-C:C-C	−0.665347
Q14832	592	N-C-C-C-C	−0.665584
Q14832	809	SC1CC(N)CCC1	−0.675014
Q14832	274	B-C	−0.679823
Q14832	270	Li-S	−0.684124
Q14832	68	>= 1 Rb	−0.688715
Q14832	795	ClC1CCC(Br)CC1	−0.691604
Q14832	621	N-C:C:C:N	−0.693945
Q14832	799	CC1CC(S)CCC1	−0.695318
Q14832	721	Oc1ccc(N)cc1	−0.697247
Q14832	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.698984
Q14832	623	O=C-C:C-C	−0.702935
Q14832	586	C-S-C-C-C	−0.704337
Q14832	331	C(~Br)(:N)	−0.706266
Q14832	21	>= 8 O	−0.709756
Q14832	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.723345
Q14832	616	C:C:N:N:C	−0.726776
Q14832	503	Cl-C:C-[#1]	−0.728561
Q14832	846	OC1CC(S)CC1	−0.731836
Q14832	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.735271
Q14832	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.741724
Q14832	446	C(-H)(=C)	−0.747458
Q14832	762	Oc1c(S)cccc1	−0.756114
Q14832	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.772887
Q14832	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	−0.773173
Q14832	464	N-C-C=C	−0.776059
Q14832	486	N-C:N:N	−0.777678
Q14832	306	N-Cl	−0.778081
Q14832	490	C-C-C=C	−0.780755
Q14832	262	>= 4 hetero-aromatic rings	−0.786608
Q14832	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.788362
Q14832	281	B-Cl	−0.789636
Q14832	349	C(~C)(~H)(~S)	−0.80344
Q14832	287	C-F	−0.80617
Q14832	815	ClC1CC(Cl)CCC1	−0.814636
Q14832	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.822792
Q14832	29	>= 2 Si	−0.823058
Q14832	465	O=S-C-C	−0.823452
Q14832	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.825217
Q14832	695	O=C-C-C-C-C-N	−0.827285
Q14832	336	C(~C)(~C)(~C)(~N)	−0.832116
Q14832	296	C-Se	−0.834537
Q14832	749	Nc1cc(N)ccc1	−0.843277
Q14832	819	CC1C(O)CCCC1	−0.844507
Q14832	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.84751

Q14832	679	C-C-C-C-C-C	−0.847921
Q14832	505	Cl-C:C-O	−0.873169
Q14832	400	N(~H)(:C)(:C)	−0.873339
Q14832	36	>= 8 S	−0.877411
Q14832	259	>= 3 aromatic rings	−0.885887
Q14832	406	O(~C)(~H)	−0.897998
Q14832	880	BrC1C(Br)CCC1	−0.898316
Q14832	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.899578
Q14832	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.913835
Q14832	738	Cc1cc(Cl)ccc1	−0.914363
Q14832	551	Cl-C-C-O	−0.919786
Q14832	798	CC1CC(O)CCC1	−0.921276
Q14832	427	C(#C)(-C)	−0.930767
Q14832	622	O=C-O-C:C	−0.93909
Q14832	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.948654
Q14832	769	Sc1c(Br)cccc1	−0.950585
Q14832	18	>= 1 O	−0.956471
Q14832	753	Clc1cc(Br)ccc1	−0.957415
Q14832	531	S-C:C-C	−0.965033
Q14832	773	Clc1c(Cl)cccc1	−0.972619
Q14832	463	N:C-S-[#1]	−0.985019
Q14832	790	SC1CCC(Br)CC1	−0.98646
Q14832	747	Sc1cc(Cl)ccc1	−0.986597
Q14832	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.986767
Q14832	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.987281
Q14832	64	>= 1 Ge	−0.988072
Q14832	453	N(-C)(=C)	−0.992525
Q14832	658	C-C-S-C-C	−0.993257
Q14832	432	C(-C)(-C)(=O)	−1.013096
Q14832	85	>= 1 Ba	−1.021406
Q14832	434	C(-C)(-H)(=C)	−1.022263
Q14832	603	C-C:C:C-C	−1.026161
Q14832	655	O-C-C-C:C	−1.026947
Q14832	314	O-P	−1.031727
Q14832	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−1.035311
Q14832	470	C:C-C=C	−1.038386
Q14832	110	>= 1 Er	−1.038651
Q14832	735	Cc1cc(O)ccc1	−1.047379
Q14832	632	C-C-O-C:C	−1.056021
Q14832	851	SC1CC(N)CC1	−1.064179
Q14832	114	>= 1 U	−1.071075
Q14832	14	>= 1 N	−1.073566
Q14832	781	CC1CCC(Br)CC1	−1.076232
Q14832	794	ClC1CCC(Cl)CC1	−1.088555
Q14832	561	Cl-C-C=O	−1.114641
Q14832	854	NC1CC(N)CC1	−1.121036
Q14832	765	Oc1c(Br)cccc1	−1.124831
Q14832	779	CC1CCC(N)CC1	−1.135061

Q14832	821	CC1C(N)CCCC1	−1.137798
Q14832	171	>= 5 any ring size 5	−1.139284
Q14832	494	O=C-C:N	−1.147049
Q14832	365	C(~H)(~N)	−1.151205
Q14832	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−1.162586
Q14832	330	C(~Br)(:C)	−1.166127
Q14832	847	OC1CC(N)CC1	−1.174863
Q14832	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−1.181297
Q14832	407	O(~C)(~P)	−1.181553
Q14832	587	N-C:C-O-[#1]	−1.183806
Q14832	746	Sc1cc(N)ccc1	−1.185213
Q14832	437	C(-C)(-N)(=C)	−1.185305
Q14832	335	C(~C)(~C)(~C)(~H)	−1.190738
Q14832	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−1.190888
Q14832	350	C(~C)(~I)	−1.192016
Q14832	360	C(~Cl)(~Cl)	−1.192954
Q14832	442	C(-C)(=N)	−1.195
Q14832	831	SC1C(Cl)CCCC1	−1.201824
Q14832	12	>= 16 C	−1.202139
Q14832	332	C(~C)(~C)	−1.208115
Q14832	596	N=C-N-C-C	−1.219141
Q14832	744	Oc1cc(Br)ccc1	−1.223071
Q14832	433	C(-C)(-Cl)(=O)	−1.226927
Q14832	82	>= 1 Te	−1.228369
Q14832	533	S-C:C-N	−1.236487
Q14832	323	P-H	−1.24623
Q14832	54	>= 1 Ti	−1.252416
Q14832	72	>= 1 Nb	−1.253434
Q14832	685	O=C-C-C-C-N	−1.254348
Q14832	57	>= 1 Mn	−1.255719
Q14832	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−1.263559
Q14832	37	>= 1 Cl	−1.264921
Q14832	276	B-O	−1.269888
Q14832	337	C(~C)(~C)(~C)(~O)	−1.275474
Q14832	90	>= 1 Re	−1.276474
Q14832	659	O-C-C-N-C	−1.282121
Q14832	459	S(=O)(=O)	−1.290204
Q14832	500	C-S-C:C	−1.291101
Q14832	732	Clc1ccc(Br)cc1	−1.30023
Q14832	199	>= 4 any ring size 6	−1.303956
Q14832	687	O=C-C-C-C=O	−1.308603
Q14832	477	N-N-C:C	−1.310085
Q14832	553	O=C-C=C	−1.312062
Q14832	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	−1.319053
Q14832	423	N=O	−1.334957
Q14832	726	Sc1ccc(Cl)cc1	−1.342831
Q14832	55	>= 1 V	−1.345185
Q14832	71	>= 1 Zr	−1.34702

Q14832	70	>= 1 Y	-1.3634
Q14832	811	SC1CC(Br)CCC1	-1.367021
Q14832	844	CC1CC(Br)CC1	-1.373217
Q14832	258	>= 2 hetero-aromatic rings	-1.381158
Q14832	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	-1.38693
Q14832	862	CC1C(S)CCC1	-1.392554
Q14832	483	N-S-C:C	-1.397119
Q14832	438	C(-C)(-N)(=N)	-1.406874
Q14832	425	P=O	-1.434346
Q14832	650	O=C-N-C=O	-1.44399
Q14832	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	-1.449222
Q14832	534	S-C:C-O	-1.449366
Q14832	866	OC1C(O)CCC1	-1.452245
Q14832	859	BrC1CC(Br)CC1	-1.459269
Q14832	366	C(~H)(~O)	-1.459433
Q14832	740	Oc1cc(O)ccc1	-1.461348
Q14832	3	>= 32 H	-1.468446
Q14832	848	OC1CC(Cl)CC1	-1.488652
Q14832	272	B-H	-1.489908
Q14832	460	C-C-C#C	-1.496959
Q14832	381	C(~O)(:C)	-1.529695
Q14832	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-1.531438
Q14832	537	O=C-C-O	-1.536854
Q14832	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	-1.541141
Q14832	375	C(~N)(~N)	-1.563228
Q14832	514	O-N-C-C	-1.58789
Q14832	520	C=C-C:C	-1.621809
Q14832	724	Sc1ccc(S)cc1	-1.648593
Q14832	770	Nc1c(N)cccc1	-1.65557
Q14832	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	-1.660608
Q14832	376	C(~N)(:C)	-1.66706
Q14832	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	-1.678171
Q14832	508	S=C-N-C	-1.687712
Q14832	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	-1.691782
Q14832	548	O-C-C:C	-1.695761
Q14832	585	C-C:C-N-C	-1.697414
Q14832	678	C-C-C=C-C	-1.70134
Q14832	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	-1.718217
Q14832	6	>= 1 B	-1.730554
Q14832	275	B-N	-1.731307
Q14832	320	Si-H	-1.744345
Q14832	498	O-C=C-C	-1.75963
Q14832	475	S-C=N-C	-1.763459
Q14832	614	C-C-O-C-C	-1.768915
Q14832	562	Br-C-C=O	-1.771983
Q14832	9	>= 2 C	-1.786075
Q14832	256	>= 1 hetero-aromatic ring	-1.812005
Q14832	871	SC1C(S)CCC1	-1.814752

Q14832	235	>= 2 saturated or aromatic carbon-only ring size 8	-1.82207
Q14832	285	C-N	-1.829536
Q14832	649	O=N-C:C-O	-1.832495
Q14832	868	OC1C(N)CCC1	-1.868633
Q14832	582	C-C-C-C-C	-1.904177
Q14832	482	C:N-C:C	-1.912689
Q14832	840	CC1CC(O)CC1	-1.959116
Q14832	62	>= 1 Zn	-1.98516
Q14832	552	C:C-C:C	-2.096753
Q14832	450	C(-N)(=N)	-2.152406
Q14832	540	C-N-C-[#1]	-2.180085
Q14832	271	Li-Cl	-2.257439
Q14832	713	Cc1ccc(C)cc1	-2.288513
Q14832	410	P(~C)(~C)	-2.466968
Q14832	431	C(-C)(-C)(=N)	-2.495188
Q14832	91	>= 1 Os	-2.590771
Q14832	113	>= 1 Tc	-2.869064
Q14832	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	-2.992618
Q14832	157	>= 3 any ring size 5	-3.433873

Fingerprints（continued)

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-2.172021 -0.008063
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-2.590776 5.37E-06
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-2.992627 8.86E-06
 -3.43514 0.0012677

Data S1. Ranking of importance of substructure features from Pubchem Fingerpı

GPCR ID	Bit Posit	Bit Substructure	W	P
Q96LB2	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	1.8534666	1.853467
Q96LB2	727	Sc1ccc(Br)cc1	1.6684194	1.670112
Q96LB2	805	OC1CC(N)CCC1	1.6201285	1.619213
Q96LB2	832	SC1C(Br)CCCC1	1.5030999	1.503217
Q96LB2	77	>= 1 Ag	1.4107994	1.410799
Q96LB2	400	N(~H)(:C)(:C)	1.2607731	1.255459
Q96LB2	622	O=C-O-C:C	1.2341566	1.234195
Q96LB2	228	>= 1 saturated or aromatic carbon-only ring size 8	1.2076904	1.20769
Q96LB2	50	>= 1 Mg	1.1695079	1.169508
Q96LB2	696	C-C-C-C-C-C-C-C	1.0982003	1.094378
Q96LB2	686	O=C-C-C-C-O	1.0756599	1.075094
Q96LB2	448	C(-H)(=O)	1.0231469	1.023498
Q96LB2	257	>= 2 aromatic rings	1.0005706	1.000571
Q96LB2	31	>= 2 P	0.9999289	0.999929
Q96LB2	282	B-Br	0.9363319	0.936332
Q96LB2	648	O=N-C:C-N	0.9193466	0.919712
Q96LB2	337	C(~C)(~C)(~C)(~O)	0.9094155	0.908847
Q96LB2	494	O=C-C:N	0.8901318	0.889861
Q96LB2	100	>= 1 Ce	0.8662912	0.866291
Q96LB2	845	OC1CC(O)CC1	0.8485122	0.848512
Q96LB2	298	C-I	0.8288004	0.8288
Q96LB2	542	O-C:C-[#1]	0.8160693	0.815142
Q96LB2	453	N(-C)(=C)	0.7960589	0.793604
Q96LB2	101	>= 1 Pr	0.7953153	0.795315
Q96LB2	54	>= 1 Ti	0.7907797	0.79078
Q96LB2	55	>= 1 V	0.7820428	0.782043
Q96LB2	618	C:C-C-C:C	0.7699321	0.76622
Q96LB2	633	N-C-C:C-C	0.7647459	0.764211
Q96LB2	546	N-C:C-[#1]	0.7608984	0.764483
Q96LB2	529	Cl-C-C-Cl	0.7578091	0.761895
Q96LB2	791	NC1CCC(N)CC1	0.7560422	0.756555
Q96LB2	426	P=P	0.7058371	0.705837
Q96LB2	25	>= 4 F	0.7056918	0.70544
Q96LB2	562	Br-C-C=O	0.7038791	0.703657
Q96LB2	305	N-S	0.6969514	0.698801
Q96LB2	617	C-C-C-O-[#1]	0.6921561	0.698381
Q96LB2	689	O-C-C-C-C-C-C	0.6789283	0.679294
Q96LB2	596	N=C-N-C-C	0.6365916	0.635059
Q96LB2	716	Cc1ccc(N)cc1	0.6347074	0.635212
Q96LB2	68	>= 1 Rb	0.6251126	0.625113
Q96LB2	62	>= 1 Zn	0.6137343	0.613734
Q96LB2	607	N-C-C-C:C	0.5995263	0.597375
Q96LB2	94	>= 1 Au	0.5732828	0.573283
Q96LB2	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.5521426	0.552143
Q96LB2	798	CC1CC(O)CCC1	0.5394151	0.538823
Q96LB2	702	O-C-C-C-C-C-N-C	0.5225537	0.516415

Q96LB2	761	Oc1c(O)cccc1	0.5206654	0.518226
Q96LB2	713	Cc1ccc(C)cc1	0.5138147	0.511272
Q96LB2	306	N-Cl	0.4983893	0.498389
Q96LB2	850	SC1CC(S)CC1	0.4785756	0.478576
Q96LB2	340	C(~C)(~C)(~N)	0.469839	0.469852
Q96LB2	438	C(-C)(-N)(=N)	0.4659151	0.469547
Q96LB2	513	S:C:C-[#1]	0.4638632	0.463951
Q96LB2	869	OC1C(Cl)CCC1	0.4489198	0.44892
Q96LB2	736	Cc1cc(S)ccc1	0.4438843	0.445808
Q96LB2	568	N#C-C-C	0.4353766	0.436855
Q96LB2	71	>= 1 Zr	0.4194726	0.419473
Q96LB2	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.414934	0.414163
Q96LB2	783	OC1CCC(S)CC1	0.4143472	0.414381
Q96LB2	227	>= 1 any ring size 8	0.3985673	0.398567
Q96LB2	684	O=C-C-C-C-C	0.3964578	0.397618
Q96LB2	765	Oc1c(Br)cccc1	0.3941361	0.395727
Q96LB2	554	Br-C-C-C	0.389623	0.388689
Q96LB2	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.3831418	0.387387
Q96LB2	858	ClC1CC(Br)CC1	0.3764314	0.376431
Q96LB2	30	>= 1 P	0.3735964	0.373758
Q96LB2	834	NC1C(Cl)CCCC1	0.3589554	0.357638
Q96LB2	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.345398	0.343207
Q96LB2	276	B-O	0.3428628	0.344235
Q96LB2	504	N:C:N-C	0.3388085	0.336757
Q96LB2	569	N-C-C-N	0.3104961	0.308846
Q96LB2	451	C(-N)(=O)	0.3020532	0.301024
Q96LB2	455	N(-O)(=O)	0.3008282	0.301464
Q96LB2	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.2976315	0.298464
Q96LB2	776	CC1CCC(C)CC1	0.2961227	0.292595
Q96LB2	755	Cc1c(C)cccc1	0.2922537	0.285921
Q96LB2	79	>= 1 In	0.2921098	0.29211
Q96LB2	465	O=S-C-C	0.2760398	0.274301
Q96LB2	8	>= 4 B	0.27381	0.27381
Q96LB2	812	NC1CC(N)CCC1	0.2724868	0.273836
Q96LB2	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.2719234	0.271923
Q96LB2	38	>= 2 Cl	0.2554682	0.257839
Q96LB2	511	S=C-N-[#1]	0.2439364	0.243293
Q96LB2	744	Oc1cc(Br)ccc1	0.2438834	0.243883
Q96LB2	367	C(~H)(~O)(~O)	0.2424928	0.245464
Q96LB2	585	C-C:C-N-C	0.199975	0.201745
Q96LB2	502	N-C=C-[#1]	0.1995831	0.199012
Q96LB2	703	O-C-C-C-C-C(N)-C	0.1986434	0.200564
Q96LB2	657	C-N-C:C-C	0.1980144	0.199784
Q96LB2	734	Cc1cc(C)ccc1	0.1808916	0.175937
Q96LB2	690	O-C-C-C-C-C-O	0.1795272	0.18175
Q96LB2	331	C(~Br)(:N)	0.1710225	0.171022
Q96LB2	829	SC1C(S)CCCC1	0.170818	0.170818
Q96LB2	615	N-C-C-O-C	0.1707323	0.165644

Q96LB2	665	N-C:C-C-C	0.1611068	0.1646
Q96LB2	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.1576553	0.15669
Q96LB2	277	B-F	0.153629	0.15411
Q96LB2	606	O-C:C-C-C	0.1512667	0.149277
Q96LB2	544	O-C:C-O	0.148199	0.148809
Q96LB2	558	O=N-C:C	0.1451431	0.147909
Q96LB2	11	>= 8 C	0.1418854	0.15259
Q96LB2	762	Oc1c(S)cccc1	0.1400876	0.140088
Q96LB2	630	O-C:C-O-C	0.1395356	0.144586
Q96LB2	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.1388617	0.136933
Q96LB2	405	O(~C)(~C)	0.1360596	0.134263
Q96LB2	393	N(~C)(~H)	0.134879	0.137796
Q96LB2	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.1344176	0.134418
Q96LB2	733	Brc1ccc(Br)cc1	0.134288	0.134288
Q96LB2	113	>= 1 Tc	0.1341354	0.134135
Q96LB2	76	>= 1 Pd	0.1338062	0.133806
Q96LB2	59	>= 1 Co	0.1335221	0.133522
Q96LB2	726	Sc1ccc(Cl)cc1	0.1333918	0.133754
Q96LB2	492	N-C:O:C	0.1330268	0.134024
Q96LB2	879	ClC1C(Br)CCC1	0.1323796	0.13238
Q96LB2	775	Brc1c(Br)cccc1	0.1319371	0.131937
Q96LB2	264	Li-Li	0.1311399	0.13114
Q96LB2	88	>= 1 Ta	0.1309663	0.130966
Q96LB2	752	Clc1cc(Cl)ccc1	0.1309191	0.132065
Q96LB2	610	C-O-C-O-C	0.130773	0.13373
Q96LB2	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.1298971	0.129897
Q96LB2	303	N-Si	0.129273	0.129273
Q96LB2	739	Cc1cc(Br)ccc1	0.1290374	0.131529
Q96LB2	786	OC1CCC(Br)CC1	0.1287748	0.129336
Q96LB2	692	O=C-C-C-C-C-C	0.1287489	0.128161
Q96LB2	114	>= 1 U	0.1278449	0.127845
Q96LB2	866	OC1C(O)CCC1	0.1272209	0.127221
Q96LB2	314	O-P	0.1250904	0.125252
Q96LB2	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.1231064	0.123106
Q96LB2	839	CC1CC(C)CC1	0.1223939	0.123659
Q96LB2	411	P(~O)(~O)	0.1214235	0.121585
Q96LB2	787	SC1CCC(S)CC1	0.1199124	0.119912
Q96LB2	302	N-F	0.119364	0.119364
Q96LB2	777	CC1CCC(O)CC1	0.1192589	0.118323
Q96LB2	360	C(~Cl)(~Cl)	0.1191038	0.116343
Q96LB2	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.1190454	0.119045
Q96LB2	654	N-C-N-C-C	0.1144921	0.113968
Q96LB2	530	N:C-C:C	0.1112954	0.113265
Q96LB2	330	C(~Br)(:C)	0.1089654	0.108031
Q96LB2	452	C(-O)(=O)	0.1088433	0.11007
Q96LB2	422	N=N	0.1085654	0.107485
Q96LB2	150	>= 2 any ring size 5	0.1080604	0.106491
Q96LB2	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.107579	0.106045

Q96LB2	780	CC1CCC(Cl)CC1	0.1067154	0.109337
Q96LB2	498	O-C=C-C	0.1062725	0.103221
Q96LB2	847	OC1CC(N)CC1	0.1061455	0.106145
Q96LB2	638	O-C-C-C-N	0.1060314	0.107003
Q96LB2	754	Brc1cc(Br)ccc1	0.1050088	0.106599
Q96LB2	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.1042478	0.104248
Q96LB2	853	SC1CC(Br)CC1	0.1031193	0.103119
Q96LB2	652	O-C:C:C-N	0.1030343	0.103121
Q96LB2	366	C(~H)(~O)	0.1022246	0.099405
Q96LB2	402	N(~O)(:O)	0.1018986	0.101899
Q96LB2	261	>= 4 aromatic rings	0.1017191	0.101719
Q96LB2	87	>= 1 Hf	0.1010016	0.101002
Q96LB2	466	N#C-C=C	0.1007064	0.099587
Q96LB2	576	N=C-C:C-[#1]	0.1006878	0.099056
Q96LB2	835	NC1C(Br)CCCC1	0.1002888	0.100289
Q96LB2	522	C-N-N-[#1]	0.1001309	0.102785
Q96LB2	818	CC1C(C)CCCC1	0.099842	0.094523
Q96LB2	83	>= 1 Xe	0.0997485	0.099748
Q96LB2	621	N-C:C:C:N	0.0997118	0.098298
Q96LB2	129	>= 1 any ring size 4	0.0995247	0.102199
Q96LB2	637	O-C-C-C-C	0.0983528	0.100348
Q96LB2	473	S-C:N:C	0.0976328	0.095194
Q96LB2	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.0968436	0.096844
Q96LB2	528	[#1]-N-C-[#1]	0.0959489	0.09197
Q96LB2	265	Li-B	0.0958603	0.09586
Q96LB2	842	CC1CC(N)CC1	0.0955334	0.095234
Q96LB2	781	CC1CCC(Br)CC1	0.0920283	0.090253
Q96LB2	551	Cl-C-C-O	0.0905697	0.089059
Q96LB2	875	NC1C(N)CCC1	0.0876922	0.087692
Q96LB2	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.087289	0.087289
Q96LB2	655	O-C-C-C:C	0.0859251	0.089171
Q96LB2	32	>= 4 P	0.0838302	0.08383
Q96LB2	379	C(~N)(:N)	0.0831398	0.08229
Q96LB2	2	>= 16 H	0.0830312	0.083031
Q96LB2	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0826698	0.080189
Q96LB2	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0825551	0.082555
Q96LB2	636	C-N-C-N-C	0.0816621	0.082885
Q96LB2	583	Cl-C:C-O-C	0.0814993	0.081659
Q96LB2	439	C(-C)(-N)(=O)	0.0809708	0.077907
Q96LB2	53	>= 1 Sc	0.080862	0.080862
Q96LB2	462	O-C-C=O	0.0801665	0.082123
Q96LB2	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.0796411	0.079641
Q96LB2	532	S-C:C-[#1]	0.0784005	0.079544
Q96LB2	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.0782028	0.080694
Q96LB2	286	C-O	0.0778237	0.085314
Q96LB2	74	>= 1 Ru	0.0771232	0.077123
Q96LB2	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.0766934	0.076693
Q96LB2	157	>= 3 any ring size 5	0.0757341	0.079295

Q96LB2	390	N(~C)(~C)	0.0751289	0.074785
Q96LB2	80	>= 1 Sn	0.0749718	0.074972
Q96LB2	49	>= 1 Be	0.0737639	0.073764
Q96LB2	782	OC1CCC(O)CC1	0.073409	0.074707
Q96LB2	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0720343	0.072932
Q96LB2	33	>= 1 S	0.0718505	0.070162
Q96LB2	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0700447	0.070045
Q96LB2	459	S(=O)(=O)	0.0692523	0.068919
Q96LB2	778	CC1CCC(S)CC1	0.0688643	0.063616
Q96LB2	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0665971	0.067915
Q96LB2	799	CC1CC(S)CCC1	0.0660113	0.067936
Q96LB2	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.0650186	0.065019
Q96LB2	524	C-C=C-C	0.0641095	0.071225
Q96LB2	697	C-C-C-C-C-C(C)-C	0.0623512	0.061212
Q96LB2	497	O-C:C:N	0.0612603	0.064164
Q96LB2	15	>= 2 N	0.0606409	0.069482
Q96LB2	368	C(~H)(~S)	0.0588035	0.059646
Q96LB2	844	CC1CC(Br)CC1	0.0583106	0.058311
Q96LB2	464	N-C-C=C	0.0582209	0.063829
Q96LB2	580	O=C-C-C-N	0.0574564	0.058814
Q96LB2	95	>= 1 Hg	0.0549996	0.055
Q96LB2	609	Cl-C-C-N-C	0.053767	0.055797
Q96LB2	394	N(~C)(~H)(~N)	0.0535872	0.053914
Q96LB2	766	Sc1c(S)cccc1	0.0530564	0.053057
Q96LB2	248	>= 1 any ring size 10	0.0527611	0.052761
Q96LB2	389	C(:N)(:N)	0.0515431	0.04947
Q96LB2	575	O-C-C:C-O	0.0513754	0.048576
Q96LB2	472	C:N:C-C	0.0510765	0.049358
Q96LB2	545	N-C:C-C	0.0502647	0.055424
Q96LB2	539	N=C-C-[#1]	0.0497415	0.04976
Q96LB2	784	OC1CCC(N)CC1	0.0495415	0.046294
Q96LB2	65	>= 1 As	0.0490951	0.049095
Q96LB2	13	>= 32 C	0.0474993	0.044103
Q96LB2	463	N:C-S-[#1]	0.0473395	0.047339
Q96LB2	620	C:C-O-C-C	0.046944	0.048061
Q96LB2	347	C(~C)(~H)(~O)(~O)	0.0451623	0.045162
Q96LB2	788	SC1CCC(N)CC1	0.0450889	0.046349
Q96LB2	322	Si-Cl	0.0445173	0.044517
Q96LB2	199	>= 4 any ring size 6	0.0441898	0.043539
Q96LB2	764	Oc1c(Cl)cccc1	0.0440504	0.043298
Q96LB2	3	>= 32 H	0.0438367	0.043837
Q96LB2	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.0436915	0.043692
Q96LB2	290	C-Al	0.0431451	0.043145
Q96LB2	797	CC1CC(C)CCC1	0.0427513	0.035476
Q96LB2	482	C:N-C:C	0.0427101	0.041243
Q96LB2	806	OC1CC(Cl)CCC1	0.0416108	0.041493
Q96LB2	278	B-Si	0.0411532	0.041153
Q96LB2	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.0407407	0.040993

Q96LB2	531	S-C:C-C	0.0399618	0.038255
Q96LB2	779	CC1CCC(N)CC1	0.0390788	0.039583
Q96LB2	771	Nc1c(Cl)cccc1	0.0387169	0.037399
Q96LB2	833	NC1C(N)CCCC1	0.0384376	0.035313
Q96LB2	28	>= 1 Si	0.0382064	0.038206
Q96LB2	745	Sc1cc(S)ccc1	0.037525	0.037525
Q96LB2	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0374944	0.037494
Q96LB2	658	C-C-S-C-C	0.0365477	0.033674
Q96LB2	809	SC1CC(N)CCC1	0.0365378	0.03869
Q96LB2	446	C(-H)(=C)	0.034718	0.039895
Q96LB2	714	Cc1ccc(O)cc1	0.0343189	0.032578
Q96LB2	514	O-N-C-C	0.0341276	0.034914
Q96LB2	73	>= 1 Mo	0.0340495	0.03405
Q96LB2	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0334819	0.033482
Q96LB2	371	C(~H)(:C)(:C)	0.0326491	0.031458
Q96LB2	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.0321632	0.032163
Q96LB2	822	CC1C(Cl)CCCC1	0.0314981	0.034089
Q96LB2	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0311529	0.031153
Q96LB2	856	NC1CC(Br)CC1	0.0303355	0.030336
Q96LB2	48	>= 4 I	0.0302914	0.030291
Q96LB2	651	O-C:C:C-C	0.0302732	0.028284
Q96LB2	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0298144	0.029814
Q96LB2	395	N(~C)(~O)	0.0294063	0.029655
Q96LB2	603	C-C:C:C-C	0.0285516	0.029538
Q96LB2	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.0284724	0.028472
Q96LB2	207	>= 5 saturated or aromatic carbon-only ring size 6	0.0283041	0.028304
Q96LB2	358	C(~C)(:N)	0.0282604	0.027219
Q96LB2	51	>= 1 Al	0.0272219	0.027222
Q96LB2	108	>= 1 Dy	0.0254201	0.02542
Q96LB2	527	C:C:N-[#1]	0.0245116	0.020136
Q96LB2	418	C=N	0.0243113	0.021873
Q96LB2	863	CC1C(N)CCC1	0.0242174	0.024217
Q96LB2	857	ClC1CC(Cl)CC1	0.0235465	0.023546
Q96LB2	704	O=C-C-C-C-C-C-C	0.0221077	0.020764
Q96LB2	480	C:S:C-C	0.0215413	0.019255
Q96LB2	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0215244	0.021524
Q96LB2	17	>= 8 N	0.0215074	0.02081
Q96LB2	99	>= 1 La	0.0214137	0.021414
Q96LB2	318	Al-H	0.0212973	0.021297
Q96LB2	63	>= 1 Ga	0.0212812	0.021281
Q96LB2	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0212321	0.021232
Q96LB2	309	O-O	0.021232	0.021232
Q96LB2	294	C-Cl	0.0211849	0.020619
Q96LB2	373	C(~H)(:N)	0.0207619	0.021767
Q96LB2	518	O=C-N-N	0.0196488	0.020154
Q96LB2	730	Nc1ccc(Br)cc1	0.0192578	0.019258
Q96LB2	830	SC1C(N)CCCC1	0.0184593	0.020555
Q96LB2	64	>= 1 Ge	0.0179925	0.017993

Q96LB2	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0179593	0.017959
Q96LB2	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0177377	0.017938
Q96LB2	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.0176786	0.016713
Q96LB2	102	>= 1 Nd	0.017203	0.017203
Q96LB2	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.0171835	0.017183
Q96LB2	751	Nc1cc(Br)ccc1	0.0165293	0.017632
Q96LB2	796	BrC1CCC(Br)CC1	0.0161539	0.016154
Q96LB2	748	Sc1cc(Br)ccc1	0.0161467	0.017737
Q96LB2	535	O=C-C-C	0.0161011	0.017275
Q96LB2	374	C(~H)(~H)(~H)	0.0157774	0.017822
Q96LB2	375	C(~N)(~N)	0.0151295	0.015612
Q96LB2	16	>= 4 N	0.0146401	0.01099
Q96LB2	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.0141511	0.013396
Q96LB2	613	C-N-C-C-C	0.0134996	0.012592
Q96LB2	178	>= 1 any ring size 6	0.0131191	0.013451
Q96LB2	268	Li-F	0.0130291	0.013029
Q96LB2	760	Cc1c(Br)cccc1	0.0128496	0.016542
Q96LB2	602	O=C-C-N-C	0.0126695	0.015322
Q96LB2	876	NC1C(Cl)CC1	0.0125981	0.012598
Q96LB2	143	>= 1 any ring size 5	0.0124707	0.015097
Q96LB2	7	>= 2 B	0.0124336	0.012434
Q96LB2	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0123977	0.012398
Q96LB2	263	Li-H	0.0122094	0.012209
Q96LB2	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.01186	0.01186
Q96LB2	273	B-B	0.0118119	0.011812
Q96LB2	559	O-C-N-[#1]	0.0115654	0.011477
Q96LB2	434	C(-C)(-H)(=C)	0.0115266	0.015388
Q96LB2	111	>= 1 Tm	0.0112179	0.011218
Q96LB2	664	C-C=C-C=C	0.0109201	0.014754
Q96LB2	274	B-C	0.0103514	0.011723
Q96LB2	43	>= 1 Br	0.0100333	0.009099
Q96LB2	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0098432	0.012907
Q96LB2	746	Sc1cc(N)ccc1	0.0093654	0.011517
Q96LB2	19	>= 2 O	0.0091224	0.011035
Q96LB2	598	Cl-C:C:C-C	0.0091095	0.006789
Q96LB2	671	O=C-C=C-C	0.0090193	0.008907
Q96LB2	60	>= 1 Ni	0.0088289	0.008829
Q96LB2	29	>= 2 Si	0.0086912	0.008691
Q96LB2	659	O-C-C-N-C	0.0085006	0.002194
Q96LB2	327	C(~Br)(~C)	0.0084229	0.007489
Q96LB2	519	N=C-N-C	0.008385	0.006853
Q96LB2	103	>= 1 Pm	0.0082763	0.008276
Q96LB2	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.0082529	0.008253
Q96LB2	387	C(:C)(:N)	0.0081902	0.00628
Q96LB2	256	>= 1 hetero-aromatic ring	0.00795	0.00795
Q96LB2	421	C=S	0.0077931	0.002874
Q96LB2	721	Oc1ccc(N)cc1	0.0073455	0.004098
Q96LB2	705	O=C-C-C-C-C(O)-C	0.0072086	0.010058

Q96LB2	98	>= 1 Bi	0.0069191	0.006919
Q96LB2	523	N:C:C-C	0.0067213	0.00771
Q96LB2	814	NC1CC(Br)CCC1	0.0058633	0.006966
Q96LB2	352	C(~C)(~O)	0.0055915	0.013082
Q96LB2	18	>= 1 O	0.0055631	0.009446
Q96LB2	769	Sc1c(Br)cccc1	0.0055283	0.005646
Q96LB2	461	O-C-C=N	0.0055084	0.002033
Q96LB2	476	C-O-C=C	0.0049005	0.003748
Q96LB2	5	>= 2 Li	0.0047797	0.00478
Q96LB2	626	C-O-C:C-C	0.0047592	0.006085
Q96LB2	597	O=C-C-C:C	0.0046597	0.000133
Q96LB2	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.0046242	0.004624
Q96LB2	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0046018	0.004178
Q96LB2	70	>= 1 Y	0.004578	0.004578
Q96LB2	485	N:C:C:N	0.0045527	0.000423
Q96LB2	415	Si(~C)(~C)	0.00448	0.00448
Q96LB2	329	C(~Br)(~H)	0.0042453	0.004245
Q96LB2	867	OC1C(S)CCC1	0.0041567	0.004157
Q96LB2	295	C-As	0.0039377	0.003938
Q96LB2	644	C-C=N-N-C	0.0039103	0.002013
Q96LB2	349	C(~C)(~H)(~S)	0.0038677	0.003449
Q96LB2	496	N:N-C-[#1]	0.0038286	0.001239
Q96LB2	785	OC1CCC(Cl)CC1	0.003756	0
Q96LB2	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.0037282	0.002957
Q96LB2	241	>= 1 any ring size 9	0.0037222	0.003722
Q96LB2	392	N(~C)(~C)(~H)	0.0036451	0.003962
Q96LB2	300	N-N	0.0035845	0.003667
Q96LB2	682	O-C-C-C-C-N	0.0034989	0.00193
Q96LB2	384	C(:C)(:C)	0.0034467	0.007372
Q96LB2	816	ClC1CC(Br)CCC1	0.0034313	0.003431
Q96LB2	627	O=[As]-C:C:C	0.0033622	0.003362
Q96LB2	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.0031402	0.004669
Q96LB2	624	O=C-C:C-N	0.0031131	0.001945
Q96LB2	573	O-C-C=C	0.0030732	0.004091
Q96LB2	499	N-C:C:N	0.0030328	-0.00045
Q96LB2	706	O=C-C-C-C-C(=O)-C	0.0027938	0.003452
Q96LB2	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.0027617	0.002762
Q96LB2	722	Oc1ccc(Cl)cc1	0.0027504	-0.00101
Q96LB2	339	C(~C)(~C)(~H)(~O)	0.0026992	0.004863
Q96LB2	478	S-C=N-[#1]	0.002641	0
Q96LB2	97	>= 1 Pb	0.0025583	0.002558
Q96LB2	249	>= 1 saturated or aromatic carbon-only ring size 10	0.0024462	0.002446
Q96LB2	824	OC1C(O)CCCC1	0.0024397	0
Q96LB2	846	OC1CC(S)CC1	0.0024319	0.002432
Q96LB2	639	O-C-C-C-O	0.0023457	-0.00014
Q96LB2	750	Nc1cc(Cl)ccc1	0.0023427	0
Q96LB2	862	CC1C(S)CCC1	0.0023175	0.002318
Q96LB2	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.0021168	0.002117

Q96LB2	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.0020329	0.002033
Q96LB2	44	>= 2 Br	0.001923	0.004246
Q96LB2	611	N-C-C-N-C	0.0019208	-0.00056
Q96LB2	500	C-S-C:C	0.0018975	0
Q96LB2	631	O-C:C-O-[#1]	0.001886	0
Q96LB2	567	O-C-C-O	0.0017728	0
Q96LB2	509	Br-C:C-C	0.001679	0.000745
Q96LB2	616	C:C:N:N:C	0.0015635	-0.00246
Q96LB2	1	>= 8 H	0.0015327	0.001533
Q96LB2	90	>= 1 Re	0.0015149	0.001515
Q96LB2	555	N=C-C=C	0.0015046	0
Q96LB2	804	OC1CC(S)CCC1	0.0014805	0.000832
Q96LB2	753	Clc1cc(Br)ccc1	0.0014709	0.001471
Q96LB2	89	>= 1 W	0.0013807	0.001381
Q96LB2	471	S:C:C:C	0.0013755	-0.00025
Q96LB2	105	>= 1 Eu	0.0013737	0.001374
Q96LB2	742	Oc1cc(N)ccc1	0.0013389	0.000424
Q96LB2	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0011107	0.001111
Q96LB2	599	[#1]-C-C=C-[#1]	0.0010975	0.004494
Q96LB2	768	Sc1c(Cl)cccc1	0.001092	0.000657
Q96LB2	534	S-C:C-O	0.0010894	0
Q96LB2	729	Nc1ccc(Cl)cc1	0.0010424	0
Q96LB2	792	NC1CCC(Cl)CC1	0.0010423	0
Q96LB2	517	N-N-C-N	0.0009563	0
Q96LB2	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0009033	0.000903
Q96LB2	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.000697	0.000697
Q96LB2	266	Li-C	0.0006841	0.000684
Q96LB2	625	O=C-C:C-O	0.000676	0.001088
Q96LB2	820	CC1C(S)CCCC1	0.0006608	0.002199
Q96LB2	591	Cl-C-C-C-C	0.0006296	-0.00043
Q96LB2	864	CC1C(Cl)CCC1	0.0006019	0.000602
Q96LB2	316	F-P	0.0006005	0.000601
Q96LB2	475	S-C=N-C	0.0005496	-0.00039
Q96LB2	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0004143	0.000323
Q96LB2	137	>= 2 saturated or aromatic carbon-only ring size 4	0.0003948	0.000395
Q96LB2	310	O-Mg	0.0002662	0.000266
Q96LB2	663	O-C-C-O-[#1]	0.0001973	-0.00253
Q96LB2	323	P-H	0.0001949	0.000195
Q96LB2	605	O=C-C-O-C	0.0001776	0.000972
Q96LB2	653	O-C:C:C-O	0.0001724	0
Q96LB2	319	Al-Cl	0.0001225	0.000123
Q96LB2	136	>= 2 any ring size 4	7.07E-05	7.07E-05
Q96LB2	213	>= 1 any ring size 7	6.39E-05	-0.00069
Q96LB2	362	C(~Cl)(:C)	3.56E-05	-0.00059
Q96LB2	52	>= 1 Ca	6.90E-06	6.95E-06
Q96LB2	874	SC1C(Br)CCC1	5.14E-06	5.13E-06
Q96LB2	84	>= 1 Cs	8.21E-08	0
Q96LB2	171	>= 5 any ring size 5	5.95E-08	0

Q96LB2	410	P(~C)(~C)	4.57E-08	0
Q96LB2	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	4.23E-08	0
Q96LB2	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	3.92E-08	0
Q96LB2	525	[As]-C:C-[#1]	3.90E-08	0
Q96LB2	220	>= 2 any ring size 7	3.28E-08	0
Q96LB2	289	C-Mg	2.68E-08	0
Q96LB2	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	2.57E-08	0
Q96LB2	39	>= 4 Cl	2.53E-08	0
Q96LB2	354	C(~C)(~Si)	2.29E-08	0
Q96LB2	270	Li-S	2.13E-08	0
Q96LB2	868	OC1C(N)CCC1	2.06E-08	0
Q96LB2	85	>= 1 Ba	1.86E-08	0
Q96LB2	93	>= 1 Pt	1.84E-08	0
Q96LB2	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	1.71E-08	0
Q96LB2	259	>= 3 aromatic rings	1.02E-08	0
Q96LB2	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	8.88E-09	0
Q96LB2	281	B-Cl	6.79E-09	0
Q96LB2	469	S-S-C:C	6.49E-09	0
Q96LB2	325	As-H	-3.82E-09	0
Q96LB2	106	>= 1 Gd	-4.17E-09	0
Q96LB2	841	CC1CC(S)CC1	-7.57E-09	0
Q96LB2	58	>= 1 Fe	-8.60E-09	0
Q96LB2	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	-1.34E-08	0
Q96LB2	41	>= 1 K	-1.53E-08	0
Q96LB2	854	NC1CC(N)CC1	-1.78E-08	0
Q96LB2	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	-2.10E-08	0
Q96LB2	86	>= 1 Lu	-4.66E-08	0
Q96LB2	321	Si-Si	-5.28E-08	0
Q96LB2	45	>= 4 Br	-5.94E-08	0
Q96LB2	553	O=C-C=C	-7.21E-05	0.002435
Q96LB2	813	NC1CC(Cl)CCC1	-9.04E-05	-0.00243
Q96LB2	260	>= 3 hetero-aromatic rings	-0.000129	-0.00013
Q96LB2	456	P(-O)(=O)	-0.000162	0
Q96LB2	443	C(-C)(=O)	-0.000184	0.002102
Q96LB2	503	Cl-C:C-[#1]	-0.000239	-0.0013
Q96LB2	297	C-Br	-0.0004	-0.00133
Q96LB2	57	>= 1 Mn	-0.000488	-0.00049
Q96LB2	688	C-C-C-C-C-C-C	-0.000527	0.000538
Q96LB2	520	C=C-C:C	-0.000533	0
Q96LB2	590	C-C:C-O-[#1]	-0.000638	0
Q96LB2	819	CC1C(O)CCCC1	-0.00066	0
Q96LB2	414	S(~C)(~O)	-0.000736	0.000355
Q96LB2	450	C(-N)(=N)	-0.000801	-0.00084
Q96LB2	870	OC1C(Br)CCC1	-0.000811	-0.00081
Q96LB2	801	CC1CC(Cl)CCC1	-0.000878	0
Q96LB2	311	O-Na	-0.0009	-0.0009
Q96LB2	577	C:C-N-C:C	-0.001002	-0.00306
Q96LB2	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	-0.001012	-0.00101

Q96LB2	674	N-C-N-C:C	−0.001104	−0.00147
Q96LB2	398	N(~H)(~N)	−0.001141	0.000452
Q96LB2	815	ClC1CC(Cl)CCC1	−0.001146	0
Q96LB2	386	C(:C)(:C)(:N)	−0.001209	0
Q96LB2	521	C:N-C-[#1]	−0.001245	−0.00067
Q96LB2	756	Cc1c(O)cccc1	−0.001262	−0.0006
Q96LB2	388	C(:C)(:N)(:N)	−0.001529	−0.00253
Q96LB2	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.001582	−0.00158
Q96LB2	828	OC1C(Br)CCCC1	−0.00159	0
Q96LB2	548	O-C-C:C	−0.001667	0
Q96LB2	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.001789	−0.00179
Q96LB2	711	C-C(C)(C)-C-C	−0.00179	−0.00063
Q96LB2	724	Sc1ccc(S)cc1	−0.001796	−0.0018
Q96LB2	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.001894	−0.00189
Q96LB2	407	O(~C)(~P)	−0.001896	−0.00173
Q96LB2	408	O(~H)(~S)	−0.001942	−0.00194
Q96LB2	770	Nc1c(N)cccc1	−0.00217	−0.00529
Q96LB2	491	C-N:C-[#1]	−0.002247	−0.00019
Q96LB2	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.00231	−0.00231
Q96LB2	420	C=O	−0.002362	0.002497
Q96LB2	540	C-N-C-[#1]	−0.002425	0
Q96LB2	359	C(~C)(:N)(:N)	−0.002542	0
Q96LB2	691	O-C-C-C-C-C-N	−0.002738	−0.00636
Q96LB2	710	C-C-C(C)-C-C	−0.002751	−0.00031
Q96LB2	391	N(~C)(~C)(~C)	−0.002769	0.003105
Q96LB2	679	C-C-C-C-C-C	−0.00287	−0.00096
Q96LB2	661	O-C-O-C-C	−0.002957	0
Q96LB2	709	C-C(C)-C-C-C	−0.002958	0
Q96LB2	860	CC1C(C)CCC1	−0.002962	−0.00076
Q96LB2	840	CC1CC(O)CC1	−0.003046	−0.00317
Q96LB2	695	O=C-C-C-C-C-N	−0.003088	−0.0036
Q96LB2	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.003277	−0.00275
Q96LB2	353	C(~C)(~S)	−0.003297	−0.00027
Q96LB2	873	SC1C(Cl)CCC1	−0.003319	−0.00332
Q96LB2	348	C(~C)(~H)(~P)	−0.003558	−0.00356
Q96LB2	61	>= 1 Cu	−0.003578	−0.00358
Q96LB2	793	NC1CCC(Br)CC1	−0.003686	−0.00369
Q96LB2	572	N:C:N:C	−0.003773	−0.00582
Q96LB2	681	O-C-C-C-C-O	−0.003778	0
Q96LB2	508	S=C-N-C	−0.003938	−0.00857
Q96LB2	430	C(-C)(-C)(=C)	−0.003959	0
Q96LB2	794	ClC1CCC(Cl)CC1	−0.004258	−0.00479
Q96LB2	75	>= 1 Rh	−0.00441	−0.00441
Q96LB2	693	O=C-C-C-C-C-O	−0.004456	0
Q96LB2	376	C(~N)(:C)	−0.004473	−0.00137
Q96LB2	296	C-Se	−0.004542	−0.00454
Q96LB2	406	O(~C)(~H)	−0.004619	−7.96E−05
Q96LB2	849	OC1CC(Br)CC1	−0.004629	−0.00463

Q96LB2	641	O-C-C-C=C	−0.004702	0
Q96LB2	6	>= 1 B	−0.00473	−0.00288
Q96LB2	490	C-C-C=C	−0.005034	0.000472
Q96LB2	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.005117	−0.00512
Q96LB2	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.005438	−0.00544
Q96LB2	409	O(:C)(:C)	−0.005486	−0.00291
Q96LB2	533	S-C:C-N	−0.005745	−0.00442
Q96LB2	852	SC1CC(Cl)CC1	−0.005803	−0.0058
Q96LB2	444	C(-Cl)(=O)	−0.005936	−0.00594
Q96LB2	592	N-C-C-C-C	−0.006022	−0.00135
Q96LB2	600	N-C:C:C-C	−0.006477	−0.0056
Q96LB2	341	C(~C)(~C)(~O)	−0.006705	−0.00767
Q96LB2	773	Clc1c(Cl)cccc1	−0.006876	−0.00279
Q96LB2	423	N=O	−0.007297	−0.00705
Q96LB2	612	N-C-O-C-C	−0.007321	−0.00907
Q96LB2	47	>= 2 I	−0.007519	−0.00752
Q96LB2	419	C#N	−0.007611	−0.00427
Q96LB2	872	SC1C(N)CCC1	−0.007633	−0.00763
Q96LB2	877	NC1C(Br)CCC1	−0.007925	−0.00792
Q96LB2	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.008071	−0.00807
Q96LB2	381	C(~O)(:C)	−0.008382	−0.00713
Q96LB2	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.00862	−0.00708
Q96LB2	865	CC1C(Br)CCC1	−0.008651	−0.00865
Q96LB2	537	O=C-C-O	−0.008709	−0.00675
Q96LB2	723	Oc1ccc(Br)cc1	−0.00877	−0.00821
Q96LB2	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.009045	−0.00727
Q96LB2	827	OC1C(Cl)CCCC1	−0.009126	−0.00988
Q96LB2	579	O=C-C-C-C	−0.009373	−0.00927
Q96LB2	279	B-P	−0.009562	−0.00956
Q96LB2	304	N-P	−0.009773	−0.00977
Q96LB2	401	N(~O)(~O)	−0.009777	−0.00914
Q96LB2	66	>= 1 Se	−0.009814	−0.00981
Q96LB2	313	O-Si	−0.010002	−0.01
Q96LB2	493	O=C-C:C	−0.010013	−0.0091
Q96LB2	107	>= 1 Tb	−0.010148	−0.01015
Q96LB2	382	C(~O)(:C)(:C)	−0.010442	−0.01219
Q96LB2	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.010559	−0.00954
Q96LB2	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.010923	−0.01041
Q96LB2	467	C=N-N-C	−0.011332	−0.01323
Q96LB2	424	N=P	−0.011348	−0.01135
Q96LB2	344	C(~C)(~H)	−0.011353	0
Q96LB2	115	>= 1 any ring size 3	−0.011512	−0.01025
Q96LB2	670	Br-C:C-C	−0.011542	−0.01248
Q96LB2	802	CC1CC(Br)CCC1	−0.011805	−0.00931
Q96LB2	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.012106	−0.01211
Q96LB2	346	C(~C)(~H)(~O)	−0.012327	−0.01194
Q96LB2	112	>= 1 Yb	−0.012341	−0.01234
Q96LB2	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.012361	−0.01236

Q96LB2	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.012502	−0.01018
Q96LB2	445	C(-H)(-N)(=C)	−0.012554	−0.00805
Q96LB2	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.012569	−0.01257
Q96LB2	552	C:C-C:C	−0.012679	−0.01215
Q96LB2	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.012742	−0.01239
Q96LB2	104	>= 1 Sm	−0.012858	−0.01286
Q96LB2	571	[#1]-C-O-[#1]	−0.01299	−0.01008
Q96LB2	747	Sc1cc(Cl)ccc1	−0.013118	−0.01447
Q96LB2	506	C-C:N:C	−0.013367	−0.01509
Q96LB2	487	N-C=N-C	−0.013406	−0.01042
Q96LB2	811	SC1CC(Br)CCC1	−0.01366	−0.01207
Q96LB2	441	C(-C)(=C)	−0.013737	−0.00373
Q96LB2	512	C-[As]-O-[#1]	−0.013748	−0.01375
Q96LB2	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.013827	−0.018
Q96LB2	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.014209	−0.01421
Q96LB2	594	C-O-C-C=C	−0.014212	−0.01978
Q96LB2	510	[#1]-N-N-[#1]	−0.014702	−0.0147
Q96LB2	332	C(~C)(~C)	−0.014757	−0.00251
Q96LB2	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.015058	−0.01469
Q96LB2	795	ClC1CCC(Br)CC1	−0.015161	−0.01516
Q96LB2	595	C:C-C-C-C	−0.015696	−0.01486
Q96LB2	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.015721	−0.01521
Q96LB2	645	O=C-N-C-C	−0.016917	−0.01372
Q96LB2	206	>= 5 any ring size 6	−0.017681	−0.02061
Q96LB2	293	C-S	−0.017813	−0.01808
Q96LB2	275	B-N	−0.017968	−0.01797
Q96LB2	843	CC1CC(Cl)CC1	−0.018337	−0.01834
Q96LB2	800	CC1CC(N)CCC1	−0.018529	−0.01963
Q96LB2	526	Cl-C:C-Cl	−0.018763	−0.01468
Q96LB2	515	N-N-C-C	−0.019461	−0.02057
Q96LB2	757	Cc1c(S)cccc1	−0.019534	−0.01695
Q96LB2	817	BrC1CC(Br)CCC1	−0.019672	−0.01808
Q96LB2	574	O-C-C:C-C	−0.019772	−0.01972
Q96LB2	708	C-C(C)-C-C	−0.020389	−0.01613
Q96LB2	460	C-C-C#C	−0.020742	−0.01974
Q96LB2	432	C(-C)(-C)(=O)	−0.020867	−0.01397
Q96LB2	91	>= 1 Os	−0.020916	−0.02092
Q96LB2	370	C(~H)(:C)	−0.022001	−0.02187
Q96LB2	836	ClC1C(Cl)CCCC1	−0.022114	−0.01803
Q96LB2	601	N-C:C:C-N	−0.022305	−0.01992
Q96LB2	677	C-C=C-C:C	−0.022566	−0.02158
Q96LB2	477	N-N-C:C	−0.022575	−0.02556
Q96LB2	413	S(~C)(~H)	−0.02299	−0.02299
Q96LB2	4	>= 1 Li	−0.023052	−0.02305
Q96LB2	676	N#C-C-C-C	−0.023211	−0.02407
Q96LB2	547	N-C:C-N	−0.025273	−0.02902
Q96LB2	604	C-O-C-C:C	−0.025298	−0.03011
Q96LB2	69	>= 1 Sr	−0.025513	−0.02551

Q96LB2	14	>= 1 N	−0.028035	−0.02389
Q96LB2	474	S:C:C:N	−0.02817	−0.02562
Q96LB2	342	C(~C)(~Cl)	−0.028182	−0.02875
Q96LB2	831	SC1C(Cl)CCCC1	−0.029171	−0.02961
Q96LB2	758	Cc1c(N)cccc1	−0.029184	−0.0328
Q96LB2	364	C(~F)(:C)	−0.029249	−0.02872
Q96LB2	803	OC1CC(O)CCC1	−0.029664	−0.0284
Q96LB2	790	SC1CCC(Br)CC1	−0.029742	−0.02805
Q96LB2	810	SC1CC(Cl)CCC1	−0.030326	−0.03168
Q96LB2	707	O=C-C-C-C-C(N)-C	−0.030371	−0.03312
Q96LB2	821	CC1C(N)CCCC1	−0.030646	−0.03426
Q96LB2	435	C(-C)(-H)(=N)	−0.031067	−0.02742
Q96LB2	372	C(~H)(:C)(:N)	−0.031129	−0.02764
Q96LB2	566	O-C-C-N	−0.03228	−0.03597
Q96LB2	301	N-O	−0.033428	−0.03318
Q96LB2	369	C(~H)(~Si)	−0.033962	−0.03396
Q96LB2	67	>= 1 Kr	−0.034456	−0.03446
Q96LB2	608	C-C-C-C:C	−0.034474	−0.03364
Q96LB2	363	C(~F)(~F)	−0.034507	−0.03478
Q96LB2	614	C-C-O-C-C	−0.034731	−0.03275
Q96LB2	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.03523	−0.03523
Q96LB2	483	N-S-C:C	−0.035372	−0.03648
Q96LB2	516	[#1]-C=C-[#1]	−0.035463	−0.03441
Q96LB2	486	N-C:N:N	−0.03559	−0.03444
Q96LB2	92	>= 1 Ir	−0.035976	−0.03598
Q96LB2	262	>= 4 hetero-aromatic rings	−0.037006	−0.03701
Q96LB2	774	Clc1c(Br)cccc1	−0.037988	−0.03799
Q96LB2	21	>= 8 O	−0.038059	−0.03417
Q96LB2	284	C-C	−0.038152	−0.0259
Q96LB2	81	>= 1 Sb	−0.038272	−0.03827
Q96LB2	578	C-C:C-C:C	−0.038875	−0.03789
Q96LB2	356	C(~C)(:C)(:C)	−0.039247	−0.03914
Q96LB2	855	NC1CC(Cl)CC1	−0.039402	−0.0394
Q96LB2	732	Clc1ccc(Br)cc1	−0.03982	−0.03982
Q96LB2	436	C(-C)(-H)(=O)	−0.040256	−0.03992
Q96LB2	335	C(~C)(~C)(~C)(~H)	−0.040898	−0.03399
Q96LB2	564	C=C-C=C	−0.041665	−0.03871
Q96LB2	808	SC1CC(S)CCC1	−0.041668	−0.04167
Q96LB2	56	>= 1 Cr	−0.042707	−0.04271
Q96LB2	315	O-K	−0.043613	−0.04361
Q96LB2	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.043974	−0.04397
Q96LB2	40	>= 8 Cl	−0.044005	−0.04401
Q96LB2	272	B-H	−0.044488	−0.04449
Q96LB2	581	O=C-C-C-O	−0.045069	−0.04648
Q96LB2	772	Nc1c(Br)cccc1	−0.045529	−0.04553
Q96LB2	878	ClC1C(Cl)CCC1	−0.045999	−0.046
Q96LB2	12	>= 16 C	−0.046037	−0.045
Q96LB2	593	N-C-C-C-N	−0.046691	−0.04677

Q96LB2	715	Cc1ccc(S)cc1	−0.046791	−0.05204
Q96LB2	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.047068	−0.04707
Q96LB2	454	N(-C)(=O)	−0.047872	−0.04762
Q96LB2	488	N-C=N-[#1]	−0.048151	−0.0522
Q96LB2	442	C(-C)(=N)	−0.050481	−0.05178
Q96LB2	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.050696	−0.04981
Q96LB2	308	O-H	−0.050749	−0.04484
Q96LB2	489	N-C-S-C	−0.05179	−0.05119
Q96LB2	345	C(~C)(~H)(~N)	−0.051943	−0.04678
Q96LB2	871	SC1C(S)CCC1	−0.052006	−0.05201
Q96LB2	543	O-C:C-N	−0.052132	−0.04669
Q96LB2	735	Cc1cc(O)ccc1	−0.053979	−0.05457
Q96LB2	416	C=C	−0.054532	−0.04453
Q96LB2	767	Sc1c(N)cccc1	−0.054768	−0.05297
Q96LB2	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.05762	−0.05747
Q96LB2	287	C-F	−0.057669	−0.05656
Q96LB2	565	C:C-O-C	−0.057965	−0.05664
Q96LB2	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.05919	−0.05919
Q96LB2	24	>= 2 F	−0.059398	−0.06125
Q96LB2	27	>= 2 Na	−0.059922	−0.0601
Q96LB2	859	BrC1CC(Br)CC1	−0.060267	−0.06027
Q96LB2	417	C#C	−0.062405	−0.06141
Q96LB2	725	Sc1ccc(N)cc1	−0.062705	−0.06145
Q96LB2	495	C-N-C:C	−0.067575	−0.06786
Q96LB2	743	Oc1cc(Cl)ccc1	−0.06804	−0.06816
Q96LB2	271	Li-Cl	−0.069463	−0.06946
Q96LB2	668	C-C:C-C-C	−0.070191	−0.06936
Q96LB2	848	OC1CC(Cl)CC1	−0.071679	−0.07168
Q96LB2	687	O=C-C-C-C=O	−0.072314	−0.07528
Q96LB2	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.074517	−0.07452
Q96LB2	427	C(#C)(-C)	−0.074533	−0.07354
Q96LB2	34	>= 2 S	−0.074919	−0.07298
Q96LB2	650	O=C-N-C=O	−0.076347	−0.07227
Q96LB2	449	C(-N)(=C)	−0.077112	−0.07609
Q96LB2	377	C(~N)(:C)(:C)	−0.077899	−0.07857
Q96LB2	324	P-P	−0.078554	−0.07855
Q96LB2	672	O=C-C=C-[#1]	−0.079417	−0.07679
Q96LB2	667	C=C-C-O-[#1]	−0.080426	−0.0768
Q96LB2	589	C-C:C-O-C	−0.080598	−0.07927
Q96LB2	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.080926	−0.08093
Q96LB2	789	SC1CCC(Cl)CC1	−0.081871	−0.08151
Q96LB2	635	N-N-C-N-[#1]	−0.082712	−0.08462
Q96LB2	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.084027	−0.08269
Q96LB2	431	C(-C)(-C)(=N)	−0.084278	−0.08953
Q96LB2	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.08653	−0.08743
Q96LB2	720	Oc1ccc(S)cc1	−0.086947	−0.08691
Q96LB2	807	OC1CC(Br)CCC1	−0.08934	−0.08934
Q96LB2	78	>= 1 Cd	−0.090247	−0.09025

Q96LB2	549	N-C-C:C	−0.090441	−0.08551
Q96LB2	763	Oc1c(N)cccc1	−0.092129	−0.08865
Q96LB2	299	N-H	−0.092268	−0.08853
Q96LB2	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.092378	−0.09111
Q96LB2	378	C(~N)(:C)(:N)	−0.092903	−0.09213
Q96LB2	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.093527	−0.09353
Q96LB2	646	O=C-N-C-[#1]	−0.095579	−0.09495
Q96LB2	678	C-C-C=C-C	−0.095812	−0.09191
Q96LB2	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.095821	−0.09582
Q96LB2	712	C-C(C)-C(C)-C	−0.095966	−0.09516
Q96LB2	700	O-C-C-C-C-C-O-C	−0.096037	−0.09371
Q96LB2	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.096599	−0.09702
Q96LB2	701	O-C-C-C-C-C(O)-C	−0.097746	−0.09656
Q96LB2	255	>= 1 aromatic ring	−0.097862	−0.09786
Q96LB2	383	C(~S)(:C)	−0.099223	−0.10112
Q96LB2	649	O=N-C:C-O	−0.100295	−0.09983
Q96LB2	507	C-C-S-C	−0.101639	−0.10182
Q96LB2	280	B-S	−0.103887	−0.10389
Q96LB2	122	>= 2 any ring size 3	−0.104505	−0.10492
Q96LB2	673	O=C-C=C-N	−0.105007	−0.10705
Q96LB2	343	C(~C)(~Cl)(~H)	−0.105445	−0.10545
Q96LB2	484	N-C:N:C	−0.105748	−0.10557
Q96LB2	380	C(~O)(~O)	−0.107244	−0.10557
Q96LB2	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.107929	−0.10793
Q96LB2	109	>= 1 Ho	−0.110588	−0.11059
Q96LB2	350	C(~C)(~I)	−0.11076	−0.11076
Q96LB2	365	C(~H)(~N)	−0.110766	−0.10834
Q96LB2	632	C-C-O-C:C	−0.110814	−0.1097
Q96LB2	397	N(~C)(:C)(:C)	−0.111805	−0.1079
Q96LB2	837	ClC1C(Br)CCCC1	−0.112	−0.112
Q96LB2	10	>= 4 C	−0.114537	−0.10229
Q96LB2	536	O=C-C-N	−0.11498	−0.11711
Q96LB2	505	Cl-C:C-O	−0.115101	−0.11519
Q96LB2	823	CC1C(Br)CCCC1	−0.115186	−0.11149
Q96LB2	457	S(-C)(=O)	−0.115402	−0.11431
Q96LB2	538	N=C-C-C	−0.116105	−0.11564
Q96LB2	258	>= 2 hetero-aromatic rings	−0.116829	−0.11683
Q96LB2	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.117381	−0.11923
Q96LB2	719	Oc1ccc(O)cc1	−0.117469	−0.11617
Q96LB2	312	O-Al	−0.11937	−0.11937
Q96LB2	110	>= 1 Er	−0.120046	−0.12005
Q96LB2	96	>= 1 Tl	−0.121186	−0.12119
Q96LB2	428	C(#C)(-H)	−0.121247	−0.12002
Q96LB2	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.121678	−0.12168
Q96LB2	501	Cl-C:C-C	−0.12188	−0.12251
Q96LB2	36	>= 8 S	−0.122276	−0.12228
Q96LB2	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.12237	−0.12235
Q96LB2	468	O=S-C-N	−0.123426	−0.12343

Q96LB2	741	Oc1cc(S)ccc1	−0.124065	−0.12471
Q96LB2	336	C(~C)(~C)(~C)(~N)	−0.124772	−0.12592
Q96LB2	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.12504	−0.12504
Q96LB2	9	>= 2 C	−0.126492	−0.11424
Q96LB2	355	C(~C)(:C)	−0.126987	−0.12306
Q96LB2	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.128515	−0.12851
Q96LB2	291	C-Si	−0.129156	−0.12916
Q96LB2	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.129273	−0.12927
Q96LB2	731	Clc1ccc(Cl)cc1	−0.129759	−0.13029
Q96LB2	825	OC1C(S)CCCC1	−0.129884	−0.12988
Q96LB2	23	>= 1 F	−0.130526	−0.12893
Q96LB2	328	C(~Br)(~C)(~C)	−0.13057	−0.1315
Q96LB2	550	Cl-C-C-C	−0.131119	−0.13048
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Q96LB2	72	>= 1 Nb	−0.132513	−0.13251
Q96LB2	623	O=C-C:C-C	−0.132731	−0.13381
Q96LB2	861	CC1C(O)CCC1	−0.132753	−0.13194
Q96LB2	317	F-S	−0.133354	−0.13335
Q96LB2	563	O-C-O-C	−0.133373	−0.13042
Q96LB2	82	>= 1 Te	−0.133387	−0.13339
Q96LB2	42	>= 2 K	−0.133426	−0.13343
Q96LB2	267	Li-O	−0.133571	−0.13357
Q96LB2	164	>= 4 any ring size 5	−0.133607	−0.13361
Q96LB2	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.133749	−0.13375
Q96LB2	292	C-P	−0.133861	−0.13386
Q96LB2	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.134762	−0.13394
Q96LB2	481	O-S-C:C	−0.141105	−0.14111
Q96LB2	582	C-C-C-C-C	−0.142722	−0.13686
Q96LB2	640	C=C-C-C-C	−0.148693	−0.14637
Q96LB2	333	C(~C)(~C)(~C)	−0.151199	−0.14591
Q96LB2	880	BrC1C(Br)CCC1	−0.15176	−0.15176
Q96LB2	619	O-C-C=C-C	−0.152196	−0.1528
Q96LB2	399	N(~H)(:C)	−0.157385	−0.16131
Q96LB2	351	C(~C)(~N)	−0.166144	−0.162
Q96LB2	35	>= 4 S	−0.16698	−0.16698
Q96LB2	403	N(:C)(:C)	−0.172595	−0.17431
Q96LB2	556	C=C-C-C	−0.174943	−0.16944
Q96LB2	698	O-C-C-C-C-C-C-C	−0.181311	−0.18259
Q96LB2	0	>= 4 H	−0.183656	−0.18366
Q96LB2	234	>= 2 any ring size 8	−0.185023	−0.18502
Q96LB2	642	O-C-C-C=O	−0.185598	−0.18701
Q96LB2	357	C(~C)(:C)(:N)	−0.186479	−0.19043
Q96LB2	683	N-C-C-C-C-C	−0.187369	−0.18638
Q96LB2	470	C:C-C=C	−0.191436	−0.1909
Q96LB2	447	C(-H)(=N)	−0.191446	−0.19028
Q96LB2	440	C(-C)(-O)(=O)	−0.191548	−0.18953
Q96LB2	629	S-C:C:C-N	−0.199201	−0.19478
Q96LB2	675	Br-C-C-C:C	−0.209818	−0.21075

Q96LB2	557	N:C-O-[#1]	−0.217941	−0.21632
Q96LB2	570	C:C-C-C	−0.221934	−0.22025
Q96LB2	660	C-C=C-C-C	−0.224794	−0.22089
Q96LB2	699	O-C-C-C-C-C(C)-C	−0.225069	−0.22579
Q96LB2	838	BrC1C(Br)CCCC1	−0.234435	−0.23443
Q96LB2	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.238711	−0.23871
Q96LB2	26	>= 1 Na	−0.24398	−0.24415
Q96LB2	385	C(:C)(:C)(:C)	−0.286821	−0.29032
Q96LB2	412	S(~C)(~C)	−0.287179	−0.28756
Q96LB2	458	S(-O)(=O)	−0.287197	−0.28862
Q96LB2	740	Oc1cc(O)ccc1	−0.300573	−0.2993
Q96LB2	586	C-S-C-C-C	−0.307799	−0.30852
Q96LB2	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.315927	−0.31119
Q96LB2	584	C:C-C=C-C	−0.319319	−0.31833
Q96LB2	326	As-As	−0.327949	−0.32795
Q96LB2	185	>= 2 any ring size 6	−0.328914	−0.3261
Q96LB2	541	O-C:C-C	−0.341721	−0.34178
Q96LB2	334	C(~C)(~C)(~C)(~C)	−0.354684	−0.35368
Q96LB2	283	C-H	−0.354911	−0.34356
Q96LB2	192	>= 3 any ring size 6	−0.355386	−0.35315
Q96LB2	561	Cl-C-C=O	−0.355518	−0.35256
Q96LB2	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.357875	−0.35788
Q96LB2	694	O=C-C-C-C-C=O	−0.37201	−0.36981
Q96LB2	269	Li-P	−0.389003	−0.389
Q96LB2	738	Cc1cc(Cl)ccc1	−0.422985	−0.42211
Q96LB2	429	C(#N)(-C)	−0.424449	−0.4211
Q96LB2	338	C(~C)(~C)(~H)(~N)	−0.452283	−0.44814
Q96LB2	628	C-N-C-C:C	−0.454483	−0.45311
Q96LB2	433	C(-C)(-Cl)(=O)	−0.454566	−0.45457
Q96LB2	669	Cl-C:C-C=O	−0.463693	−0.45943
Q96LB2	680	O-C-C-C-C-C	−0.468235	−0.46682
Q96LB2	285	C-N	−0.469978	−0.46583
Q96LB2	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.481112	−0.48111
Q96LB2	479	S-C-S-C	−0.49329	−0.49349
Q96LB2	643	[#1]-C-C-N-[#1]	−0.508733	−0.50426
Q96LB2	737	Cc1cc(N)ccc1	−0.511808	−0.51291
Q96LB2	851	SC1CC(N)CC1	−0.529507	−0.52951
Q96LB2	718	Cc1ccc(Br)cc1	−0.548183	−0.54996
Q96LB2	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.559056	−0.55951
Q96LB2	666	C=C-C-O-C	−0.568598	−0.57417
Q96LB2	749	Nc1cc(N)ccc1	−0.57247	−0.57112
Q96LB2	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.573782	−0.57164
Q96LB2	685	O=C-C-C-C-N	−0.614136	−0.61817
Q96LB2	288	C-Na	−0.616048	−0.61605
Q96LB2	320	Si-H	−0.625522	−0.62552
Q96LB2	396	N(~C)(:C)	−0.694425	−0.69686
Q96LB2	662	O-C-C-O-C	−0.728559	−0.72648
Q96LB2	560	N-C-N-C	−0.744267	−0.74503

Q96LB2	717	Cc1ccc(Cl)cc1	−0.751831	−0.74921
Q96LB2	647	O=C-N-C-N	−0.763605	−0.76303
Q96LB2	404	N(:C)(:C)(:C)	−0.766679	−0.76726
Q96LB2	46	>= 1 I	−0.792715	−0.79181
Q96LB2	37	>= 1 Cl	−0.827925	−0.82778
Q96LB2	728	Nc1ccc(N)cc1	−0.829811	−0.8293
Q96LB2	22	>= 16 O	−0.838534	−0.83818
Q96LB2	425	P=O	−0.840096	−0.83993
Q96LB2	826	OC1C(N)CCCC1	−0.865226	−0.86174
Q96LB2	20	>= 4 O	−0.873515	−0.86754
Q96LB2	634	C-C-C:C-C	−0.939355	−0.93852
Q96LB2	656	C-C-N-C-C	−0.942115	−0.93786
Q96LB2	759	Cc1c(Cl)cccc1	−0.944259	−0.94167
Q96LB2	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−1.117405	−1.1174
Q96LB2	587	N-C:C-O-[#1]	−1.121464	−1.11805
Q96LB2	437	C(-C)(-N)(=C)	−1.147569	−1.15066
Q96LB2	361	C(~Cl)(~H)	−1.183548	−1.18355
Q96LB2	307	N-Br	−1.210651	−1.21065
Q96LB2	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.497839	−1.49784

rints（continued)

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Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q9UPC5	510	[#1]-N-N-[#1]	1.8922712
Q9UPC5	741	Oc1cc(S)ccc1	1.8524845
Q9UPC5	723	Oc1ccc(Br)cc1	1.6556763
Q9UPC5	33	>= 1 S	1.6112593
Q9UPC5	463	N:C-S-[#1]	1.5609873
Q9UPC5	354	C(~C)(~Si)	1.5531969
Q9UPC5	727	Sc1ccc(Br)cc1	1.4576546
Q9UPC5	606	O-C:C-C-C	1.3302656
Q9UPC5	317	F-S	1.3129256
Q9UPC5	283	C-H	1.3077433
Q9UPC5	541	O-C:C-C	1.3069469
Q9UPC5	681	O-C-C-C-C-O	1.2802466
Q9UPC5	837	ClC1C(Br)CCCC1	1.2662893
Q9UPC5	297	C-Br	1.2506536
Q9UPC5	31	>= 2 P	1.2478451
Q9UPC5	612	N-C-O-C-C	1.2204832
Q9UPC5	301	N-O	1.1866183
Q9UPC5	83	>= 1 Xe	1.169027
Q9UPC5	596	N=C-N-C-C	1.1542653
Q9UPC5	834	NC1C(Cl)CCCC1	1.0969199
Q9UPC5	443	C(-C)(=O)	1.0834361
Q9UPC5	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	1.0744463
Q9UPC5	248	>= 1 any ring size 10	1.0636627
Q9UPC5	402	N(~O)(:O)	1.0064784
Q9UPC5	151	>= 2 saturated or aromatic carbon-only ring size 5	0.9881023
Q9UPC5	804	OC1CC(S)CCC1	0.9829521
Q9UPC5	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.979792
Q9UPC5	708	C-C(C)-C-C	0.9109574
Q9UPC5	502	N-C=C-[#1]	0.8958977
Q9UPC5	503	Cl-C:C-[#1]	0.8891546
Q9UPC5	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.8736445
Q9UPC5	730	Nc1ccc(Br)cc1	0.8701451
Q9UPC5	71	>= 1 Zr	0.8587556
Q9UPC5	668	C-C:C-C-C	0.856306
Q9UPC5	832	SC1C(Br)CCCC1	0.8463114
Q9UPC5	406	O(~C)(~H)	0.8429003
Q9UPC5	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.8043987
Q9UPC5	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.7784375
Q9UPC5	411	P(~O)(~O)	0.7757691
Q9UPC5	790	SC1CCC(Br)CC1	0.7475377
Q9UPC5	115	>= 1 any ring size 3	0.7456306
Q9UPC5	418	C=N	0.7419897
Q9UPC5	45	>= 4 Br	0.7350323
Q9UPC5	343	C(~C)(~Cl)(~H)	0.7218151
Q9UPC5	767	Sc1c(N)cccc1	0.7174192
Q9UPC5	480	C:S:C-C	0.6122619

Q9UPC5	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.5937187
Q9UPC5	654	N-C-N-C-C	0.5895
Q9UPC5	6	>= 1 B	0.5818517
Q9UPC5	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.5642035
Q9UPC5	878	ClC1C(Cl)CCC1	0.5539454
Q9UPC5	328	C(~Br)(~C)(~C)	0.5399692
Q9UPC5	494	O=C-C:N	0.5201577
Q9UPC5	803	OC1CC(O)CCC1	0.5155403
Q9UPC5	533	S-C:C-N	0.5088637
Q9UPC5	306	N-Cl	0.4973848
Q9UPC5	46	>= 1 I	0.4462737
Q9UPC5	466	N#C-C=C	0.4460245
Q9UPC5	695	O=C-C-C-C-C-N	0.4296843
Q9UPC5	777	CC1CCC(O)CC1	0.4255222
Q9UPC5	610	C-O-C-O-C	0.4154228
Q9UPC5	422	N=N	0.4007457
Q9UPC5	473	S-C:N:C	0.373797
Q9UPC5	570	C:C-C-C	0.3635413
Q9UPC5	18	>= 1 O	0.3621202
Q9UPC5	567	O-C-C-O	0.3614277
Q9UPC5	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.3484204
Q9UPC5	601	N-C:C:C-N	0.3479733
Q9UPC5	30	>= 1 P	0.3443849
Q9UPC5	602	O=C-C-N-C	0.314725
Q9UPC5	575	O-C-C:C-O	0.3059473
Q9UPC5	852	SC1CC(Cl)CC1	0.3011655
Q9UPC5	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.2985308
Q9UPC5	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.2922245
Q9UPC5	57	>= 1 Mn	0.2752496
Q9UPC5	827	OC1C(Cl)CCCC1	0.2581604
Q9UPC5	386	C(:C)(:C)(:N)	0.2559608
Q9UPC5	583	Cl-C:C-O-C	0.2509912
Q9UPC5	600	N-C:C:C-C	0.2436602
Q9UPC5	488	N-C=N-[#1]	0.2423474
Q9UPC5	362	C(~Cl)(:C)	0.2336442
Q9UPC5	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.2297013
Q9UPC5	281	B-Cl	0.2246713
Q9UPC5	799	CC1CC(S)CCC1	0.2141332
Q9UPC5	273	B-B	0.209725
Q9UPC5	320	Si-H	0.2021044
Q9UPC5	733	Brc1ccc(Br)cc1	0.2014832
Q9UPC5	754	Brc1cc(Br)ccc1	0.2002647
Q9UPC5	772	Nc1c(Br)cccc1	0.1949796
Q9UPC5	717	Cc1ccc(Cl)cc1	0.1945146
Q9UPC5	28	>= 1 Si	0.1902517
Q9UPC5	648	O=N-C:C-N	0.1877834
Q9UPC5	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.1834245
Q9UPC5	822	CC1C(Cl)CCCC1	0.1829045

Q9UPC5	652	O-C:C:C-N	0.1812989
Q9UPC5	409	O(:C)(:C)	0.1760663
Q9UPC5	836	ClC1C(Cl)CCCC1	0.1725815
Q9UPC5	672	O=C-C=C-[#1]	0.1694931
Q9UPC5	387	C(:C)(:N)	0.1655598
Q9UPC5	38	>= 2 Cl	0.165431
Q9UPC5	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.1648983
Q9UPC5	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.1591573
Q9UPC5	17	>= 8 N	0.1548865
Q9UPC5	665	N-C:C-C-C	0.1483525
Q9UPC5	629	S-C:C:C-N	0.1471877
Q9UPC5	405	O(~C)(~C)	0.1413427
Q9UPC5	73	>= 1 Mo	0.1380058
Q9UPC5	569	N-C-C-N	0.1344744
Q9UPC5	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.1344412
Q9UPC5	707	O=C-C-C-C-C(N)-C	0.1342149
Q9UPC5	234	>= 2 any ring size 8	0.1342075
Q9UPC5	875	NC1C(N)CCC1	0.1339816
Q9UPC5	760	Cc1c(Br)cccc1	0.1337525
Q9UPC5	27	>= 2 Na	0.1336914
Q9UPC5	551	Cl-C-C-O	0.1335964
Q9UPC5	164	>= 4 any ring size 5	0.1335816
Q9UPC5	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.1333659
Q9UPC5	242	>= 1 saturated or aromatic carbon-only ring size 9	0.1332965
Q9UPC5	7	>= 2 B	0.1332498
Q9UPC5	72	>= 1 Nb	0.1330869
Q9UPC5	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.1330495
Q9UPC5	818	CC1C(C)CCCC1	0.1327118
Q9UPC5	858	ClC1CC(Br)CC1	0.1321629
Q9UPC5	544	O-C:C-O	0.1319667
Q9UPC5	199	>= 4 any ring size 6	0.1319173
Q9UPC5	171	>= 5 any ring size 5	0.131576
Q9UPC5	787	SC1CCC(S)CC1	0.1305877
Q9UPC5	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	0.1302483
Q9UPC5	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.1298372
Q9UPC5	358	C(~C)(:N)	0.1292707
Q9UPC5	664	C-C=C-C=C	0.1290192
Q9UPC5	555	N=C-C=C	0.1288725
Q9UPC5	102	>= 1 Nd	0.1281652
Q9UPC5	60	>= 1 Ni	0.127653
Q9UPC5	263	Li-H	0.1276254
Q9UPC5	206	>= 5 any ring size 6	0.1267315
Q9UPC5	8	>= 4 B	0.1266303
Q9UPC5	314	O-P	0.1256789
Q9UPC5	831	SC1C(Cl)CCCC1	0.125324
Q9UPC5	266	Li-C	0.1249906
Q9UPC5	361	C(~Cl)(~H)	0.1249444
Q9UPC5	625	O=C-C:C-O	0.1243616

Q9UPC5	761	Oc1c(O)cccc1	0.1240584
Q9UPC5	41	>= 1 K	0.1237067
Q9UPC5	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.1222003
Q9UPC5	25	>= 4 F	0.1220063
Q9UPC5	43	>= 1 Br	0.120936
Q9UPC5	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.1202542
Q9UPC5	638	O-C-C-C-N	0.1201581
Q9UPC5	506	C-C:N:C	0.1199092
Q9UPC5	67	>= 1 Kr	0.1196407
Q9UPC5	775	Brc1c(Br)cccc1	0.1193746
Q9UPC5	806	OC1CC(Cl)CCC1	0.1168664
Q9UPC5	781	CC1CCC(Br)CC1	0.1167852
Q9UPC5	744	Oc1cc(Br)ccc1	0.1165079
Q9UPC5	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.1157639
Q9UPC5	572	N:C:N:C	0.1150032
Q9UPC5	588	O=C-C-C=O	0.1148594
Q9UPC5	345	C(~C)(~H)(~N)	0.1145338
Q9UPC5	54	>= 1 Ti	0.1144586
Q9UPC5	747	Sc1cc(Cl)ccc1	0.1144031
Q9UPC5	722	Oc1ccc(Cl)cc1	0.113557
Q9UPC5	325	As-H	0.112573
Q9UPC5	103	>= 1 Pm	0.1107857
Q9UPC5	666	C=C-C-O-C	0.1104268
Q9UPC5	355	C(~C)(:C)	0.1103814
Q9UPC5	525	[As]-C:C-[#1]	0.1102498
Q9UPC5	848	OC1CC(Cl)CC1	0.1094319
Q9UPC5	675	Br-C-C-C:C	0.1092467
Q9UPC5	585	C-C:C-N-C	0.1078416
Q9UPC5	731	Clc1ccc(Cl)cc1	0.1077974
Q9UPC5	577	C:C-N-C:C	0.1073916
Q9UPC5	22	>= 16 O	0.1070461
Q9UPC5	332	C(~C)(~C)	0.1067544
Q9UPC5	472	C:N:C-C	0.1055601
Q9UPC5	550	Cl-C-C-C	0.1052151
Q9UPC5	660	C-C=C-C-C	0.1051999
Q9UPC5	710	C-C-C(C)-C-C	0.104786
Q9UPC5	363	C(~F)(~F)	0.1030457
Q9UPC5	5	>= 2 Li	0.1028528
Q9UPC5	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.1014592
Q9UPC5	700	O-C-C-C-C-C-O-C	0.0999741
Q9UPC5	36	>= 8 S	0.099417
Q9UPC5	597	O=C-C-C:C	0.0993757
Q9UPC5	109	>= 1 Ho	0.097285
Q9UPC5	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.0958336
Q9UPC5	493	O=C-C:C	0.0957516
Q9UPC5	200	>= 4 saturated or aromatic carbon-only ring size 6	0.0948076
Q9UPC5	410	P(~C)(~C)	0.094627
Q9UPC5	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0939226

Q9UPC5	498	O-C=C-C	0.0916501
Q9UPC5	495	C-N-C:C	0.0906666
Q9UPC5	782	OC1CCC(O)CC1	0.0884204
Q9UPC5	676	N#C-C-C-C	0.0869642
Q9UPC5	647	O=C-N-C-N	0.0848117
Q9UPC5	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0842224
Q9UPC5	582	C-C-C-C-C	0.0841131
Q9UPC5	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.0837657
Q9UPC5	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.0814077
Q9UPC5	643	[#1]-C-C-N-[#1]	0.0804078
Q9UPC5	749	Nc1cc(N)ccc1	0.0803203
Q9UPC5	819	CC1C(O)CCCC1	0.0772759
Q9UPC5	766	Sc1c(S)cccc1	0.0770649
Q9UPC5	499	N-C:C:N	0.0762454
Q9UPC5	449	C(-N)(=C)	0.0740457
Q9UPC5	110	>= 1 Er	0.0734804
Q9UPC5	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0731269
Q9UPC5	318	Al-H	0.073027
Q9UPC5	599	[#1]-C-C=C-[#1]	0.0719545
Q9UPC5	753	Clc1cc(Br)ccc1	0.0716673
Q9UPC5	78	>= 1 Cd	0.0699789
Q9UPC5	770	Nc1c(N)cccc1	0.0675798
Q9UPC5	714	Cc1ccc(O)cc1	0.0670828
Q9UPC5	51	>= 1 Al	0.0669196
Q9UPC5	851	SC1CC(N)CC1	0.0665531
Q9UPC5	259	>= 3 aromatic rings	0.0662179
Q9UPC5	300	N-N	0.0658201
Q9UPC5	876	NC1C(Cl)CC1	0.064578
Q9UPC5	417	C#C	0.064175
Q9UPC5	129	>= 1 any ring size 4	0.0637353
Q9UPC5	593	N-C-C-C-N	0.0630247
Q9UPC5	520	C=C-C:C	0.0604008
Q9UPC5	346	C(~C)(~H)(~O)	0.0599153
Q9UPC5	704	O=C-C-C-C-C-C-C	0.0581043
Q9UPC5	59	>= 1 Co	0.0564873
Q9UPC5	546	N-C:C-[#1]	0.0536877
Q9UPC5	123	>= 2 saturated or aromatic carbon-only ring size 3	0.0518579
Q9UPC5	694	O=C-C-C-C-C=O	0.0496966
Q9UPC5	359	C(~C)(:N)(:N)	0.0476145
Q9UPC5	543	O-C:C-N	0.0472667
Q9UPC5	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0464959
Q9UPC5	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0464886
Q9UPC5	530	N:C-C:C	0.0464238
Q9UPC5	276	B-O	0.0464222
Q9UPC5	436	C(-C)(-H)(=O)	0.0461214
Q9UPC5	701	O-C-C-C-C-C(O)-C	0.0460442
Q9UPC5	563	O-C-O-C	0.0455985
Q9UPC5	609	Cl-C-C-N-C	0.0444732

Q9UPC5	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.0444519
Q9UPC5	798	CC1CC(O)CCC1	0.04435
Q9UPC5	735	Cc1cc(O)ccc1	0.0433678
Q9UPC5	87	>= 1 Hf	0.0433161
Q9UPC5	144	>= 1 saturated or aromatic carbon-only ring size 5	0.0433019
Q9UPC5	548	O-C-C:C	0.0432385
Q9UPC5	106	>= 1 Gd	0.0430209
Q9UPC5	453	N(-C)(=C)	0.0429997
Q9UPC5	287	C-F	0.0420429
Q9UPC5	844	CC1CC(Br)CC1	0.0419997
Q9UPC5	0	>= 4 H	0.0419581
Q9UPC5	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.0414575
Q9UPC5	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.0412538
Q9UPC5	757	Cc1c(S)cccc1	0.0409971
Q9UPC5	375	C(~N)(~N)	0.0406757
Q9UPC5	855	NC1CC(Cl)CC1	0.040383
Q9UPC5	869	OC1C(Cl)CCC1	0.0390572
Q9UPC5	268	Li-F	0.0383516
Q9UPC5	487	N-C=N-C	0.0383356
Q9UPC5	264	Li-Li	0.0374867
Q9UPC5	308	O-H	0.0368586
Q9UPC5	56	>= 1 Cr	0.036646
Q9UPC5	392	N(~C)(~C)(~H)	0.0353433
Q9UPC5	789	SC1CCC(Cl)CC1	0.0345468
Q9UPC5	656	C-C-N-C-C	0.0345059
Q9UPC5	349	C(~C)(~H)(~S)	0.0342975
Q9UPC5	485	N:C:C:N	0.0342427
Q9UPC5	516	[#1]-C=C-[#1]	0.0340836
Q9UPC5	711	C-C(C)(C)-C-C	0.0335606
Q9UPC5	438	C(-C)(-N)(=N)	0.0334169
Q9UPC5	319	Al-Cl	0.033346
Q9UPC5	751	Nc1cc(Br)ccc1	0.0323714
Q9UPC5	568	N#C-C-C	0.031481
Q9UPC5	615	N-C-C-O-C	0.0314042
Q9UPC5	671	O=C-C=C-C	0.0312978
Q9UPC5	573	O-C-C=C	0.0308457
Q9UPC5	699	O-C-C-C-C-C(C)-C	0.0296806
Q9UPC5	313	O-Si	0.0295782
Q9UPC5	456	P(-O)(=O)	0.0285739
Q9UPC5	524	C-C=C-C	0.0281365
Q9UPC5	515	N-N-C-C	0.0279572
Q9UPC5	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.0276933
Q9UPC5	446	C(-H)(=C)	0.0271602
Q9UPC5	637	O-C-C-C-C	0.0264727
Q9UPC5	673	O=C-C=C-N	0.0262653
Q9UPC5	61	>= 1 Cu	0.0259094
Q9UPC5	678	C-C-C=C-C	0.0257254
Q9UPC5	414	S(~C)(~O)	0.0257101

Q9UPC5	348	C(~C)(~H)(~P)	0.0256385
Q9UPC5	416	C=C	0.0252956
Q9UPC5	451	C(-N)(=O)	0.0247637
Q9UPC5	861	CC1C(O)CCC1	0.024639
Q9UPC5	640	C=C-C-C-C	0.024067
Q9UPC5	284	C-C	0.0237939
Q9UPC5	865	CC1C(Br)CCC1	0.0227923
Q9UPC5	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.0226312
Q9UPC5	312	O-Al	0.022125
Q9UPC5	628	C-N-C-C:C	0.0214297
Q9UPC5	227	>= 1 any ring size 8	0.0209655
Q9UPC5	584	C:C-C=C-C	0.0209403
Q9UPC5	79	>= 1 In	0.0206179
Q9UPC5	77	>= 1 Ag	0.0205755
Q9UPC5	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0205599
Q9UPC5	547	N-C:C-N	0.0203514
Q9UPC5	496	N:N-C-[#1]	0.0194843
Q9UPC5	857	ClC1CC(Cl)CC1	0.0194676
Q9UPC5	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0193571
Q9UPC5	756	Cc1c(O)cccc1	0.0184468
Q9UPC5	86	>= 1 Lu	0.0181511
Q9UPC5	339	C(~C)(~C)(~H)(~O)	0.0178351
Q9UPC5	611	N-C-C-N-C	0.017551
Q9UPC5	262	>= 4 hetero-aromatic rings	0.016967
Q9UPC5	728	Nc1ccc(N)cc1	0.0169454
Q9UPC5	475	S-C=N-C	0.0166708
Q9UPC5	91	>= 1 Os	0.0162151
Q9UPC5	685	O=C-C-C-C-N	0.0160443
Q9UPC5	759	Cc1c(Cl)cccc1	0.0153409
Q9UPC5	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0149307
Q9UPC5	794	ClC1CCC(Cl)CC1	0.0148539
Q9UPC5	501	Cl-C:C-C	0.0147326
Q9UPC5	489	N-C-S-C	0.0140645
Q9UPC5	645	O=C-N-C-C	0.0138745
Q9UPC5	101	>= 1 Pr	0.0135681
Q9UPC5	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.0134823
Q9UPC5	737	Cc1cc(N)ccc1	0.0134313
Q9UPC5	527	C:C:N-[#1]	0.0132726
Q9UPC5	823	CC1C(Br)CCCC1	0.0132525
Q9UPC5	797	CC1CC(C)CCC1	0.0130685
Q9UPC5	122	>= 2 any ring size 3	0.0130004
Q9UPC5	326	As-As	0.0128922
Q9UPC5	868	OC1C(N)CCC1	0.0110512
Q9UPC5	864	CC1C(Cl)CCC1	0.0105841
Q9UPC5	632	C-C-O-C:C	0.0104192
Q9UPC5	329	C(~Br)(~H)	0.0103986
Q9UPC5	55	>= 1 V	0.0102854
Q9UPC5	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.0100563

Q9UPC5	393	N(~C)(~H)	0.0096495
Q9UPC5	302	N-F	0.0095758
Q9UPC5	540	C-N-C-[#1]	0.0095621
Q9UPC5	684	O=C-C-C-C-C	0.0095437
Q9UPC5	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.0094902
Q9UPC5	743	Oc1cc(Cl)ccc1	0.0091486
Q9UPC5	53	>= 1 Sc	0.0085946
Q9UPC5	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0079958
Q9UPC5	35	>= 4 S	0.0079236
Q9UPC5	642	O-C-C-C=O	0.0078292
Q9UPC5	801	CC1CC(Cl)CCC1	0.0076913
Q9UPC5	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	0.0072383
Q9UPC5	785	OC1CCC(Cl)CC1	0.00708
Q9UPC5	553	O=C-C=C	0.0070734
Q9UPC5	58	>= 1 Fe	0.0070225
Q9UPC5	316	F-P	0.0065372
Q9UPC5	705	O=C-C-C-C-C(O)-C	0.0065307
Q9UPC5	344	C(~C)(~H)	0.0064731
Q9UPC5	24	>= 2 F	0.0063893
Q9UPC5	829	SC1C(S)CCCC1	0.0060065
Q9UPC5	428	C(#C)(-H)	0.0059932
Q9UPC5	39	>= 4 Cl	0.0056998
Q9UPC5	70	>= 1 Y	0.0056695
Q9UPC5	739	Cc1cc(Br)ccc1	0.0056534
Q9UPC5	644	C-C=N-N-C	0.0055839
Q9UPC5	291	C-Si	0.0053981
Q9UPC5	16	>= 4 N	0.0053943
Q9UPC5	286	C-O	0.0053772
Q9UPC5	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0052889
Q9UPC5	13	>= 32 C	0.0050942
Q9UPC5	383	C(~S)(:C)	0.0048983
Q9UPC5	476	C-O-C=C	0.0048162
Q9UPC5	586	C-S-C-C-C	0.0047186
Q9UPC5	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0044166
Q9UPC5	157	>= 3 any ring size 5	0.0043563
Q9UPC5	327	C(~Br)(~C)	0.0043271
Q9UPC5	4	>= 1 Li	0.0042714
Q9UPC5	158	>= 3 saturated or aromatic carbon-only ring size 5	0.0040503
Q9UPC5	450	C(-N)(=N)	0.0037489
Q9UPC5	249	>= 1 saturated or aromatic carbon-only ring size 10	0.0035056
Q9UPC5	824	OC1C(O)CCCC1	0.0032978
Q9UPC5	426	P=P	0.0032416
Q9UPC5	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0030911
Q9UPC5	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.0030079
Q9UPC5	634	C-C-C:C-C	0.0028966
Q9UPC5	725	Sc1ccc(N)cc1	0.0028897
Q9UPC5	788	SC1CCC(N)CC1	0.0028896
Q9UPC5	256	>= 1 hetero-aromatic ring	0.0028809

Q9UPC5	461	O-C-C=N	0.002823
Q9UPC5	598	Cl-C:C:C-C	0.0027629
Q9UPC5	403	N(:C)(:C)	0.0027091
Q9UPC5	873	SC1C(Cl)CCC1	0.0027002
Q9UPC5	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0025934
Q9UPC5	114	>= 1 U	0.0024859
Q9UPC5	342	C(~C)(~Cl)	0.0024385
Q9UPC5	641	O-C-C-C=C	0.0022998
Q9UPC5	398	N(~H)(~N)	0.0020874
Q9UPC5	404	N(:C)(:C)(:C)	0.0020807
Q9UPC5	729	Nc1ccc(Cl)cc1	0.0020607
Q9UPC5	843	CC1CC(Cl)CC1	0.0020589
Q9UPC5	518	O=C-N-N	0.0020434
Q9UPC5	860	CC1C(C)CCC1	0.002026
Q9UPC5	391	N(~C)(~C)(~C)	0.0019192
Q9UPC5	850	SC1CC(S)CC1	0.0018825
Q9UPC5	667	C=C-C-O-[#1]	0.001881
Q9UPC5	536	O=C-C-N	0.0018232
Q9UPC5	394	N(~C)(~H)(~N)	0.0017991
Q9UPC5	220	>= 2 any ring size 7	0.0017025
Q9UPC5	687	O=C-C-C-C=O	0.0015654
Q9UPC5	594	C-O-C-C=C	0.0015483
Q9UPC5	813	NC1CC(Cl)CCC1	0.0014931
Q9UPC5	381	C(~O)(:C)	0.0014445
Q9UPC5	677	C-C=C-C:C	0.0014208
Q9UPC5	336	C(~C)(~C)(~C)(~N)	0.0013899
Q9UPC5	719	Oc1ccc(O)cc1	0.0013403
Q9UPC5	521	C:N-C-[#1]	0.0012996
Q9UPC5	830	SC1C(N)CCCC1	0.0011161
Q9UPC5	706	O=C-C-C-C-C(=O)-C	0.001079
Q9UPC5	479	S-C-S-C	0.0010635
Q9UPC5	828	OC1C(Br)CCCC1	0.0007707
Q9UPC5	352	C(~C)(~O)	0.0007219
Q9UPC5	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	0.000393
Q9UPC5	517	N-N-C-N	0.0003618
Q9UPC5	514	O-N-C-C	0.0003585
Q9UPC5	307	N-Br	0.0001807
Q9UPC5	486	N-C:N:N	9.52E-05
Q9UPC5	566	O-C-C-N	7.91E-05
Q9UPC5	709	C-C(C)-C-C-C	7.27E-05
Q9UPC5	880	BrC1C(Br)CCC1	4.41E-05
Q9UPC5	47	>= 2 I	1.28E-05
Q9UPC5	2	>= 16 H	7.40E-08
Q9UPC5	724	Sc1ccc(S)cc1	2.04E-08
Q9UPC5	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	1.04E-08
Q9UPC5	107	>= 1 Tb	8.46E-09
Q9UPC5	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	7.56E-09
Q9UPC5	261	>= 4 aromatic rings	6.73E-09

Q9UPC5	269	Li-P	1.07E-09
Q9UPC5	66	>= 1 Se	-8.47E-09
Q9UPC5	260	>= 3 hetero-aromatic rings	-1.01E-08
Q9UPC5	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	-1.18E-08
Q9UPC5	292	C-P	-2.34E-08
Q9UPC5	48	>= 4 I	-2.70E-08
Q9UPC5	137	>= 2 saturated or aromatic carbon-only ring size 4	-5.41E-08
Q9UPC5	89	>= 1 W	-5.92E-08
Q9UPC5	433	C(-C)(-Cl)(=O)	-7.88E-08
Q9UPC5	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	-9.20E-08
Q9UPC5	104	>= 1 Sm	-9.51E-08
Q9UPC5	29	>= 2 Si	-9.96E-08
Q9UPC5	853	SC1CC(Br)CC1	-1.35E-07
Q9UPC5	613	C-N-C-C-C	-1.53E-05
Q9UPC5	42	>= 2 K	-4.32E-05
Q9UPC5	866	OC1C(O)CCC1	-8.80E-05
Q9UPC5	374	C(~H)(~H)(~H)	-0.000145
Q9UPC5	522	C-N-N-[#1]	-0.000147
Q9UPC5	97	>= 1 Pb	-0.000158
Q9UPC5	624	O=C-C:C-N	-0.000272
Q9UPC5	784	OC1CCC(N)CC1	-0.000402
Q9UPC5	63	>= 1 Ga	-0.000471
Q9UPC5	491	C-N:C-[#1]	-0.000488
Q9UPC5	435	C(-C)(-H)(=N)	-0.000551
Q9UPC5	655	O-C-C-C:C	-0.000593
Q9UPC5	769	Sc1c(Br)cccc1	-0.0006
Q9UPC5	779	CC1CCC(N)CC1	-0.000672
Q9UPC5	289	C-Mg	-0.000736
Q9UPC5	372	C(~H)(:C)(:N)	-0.000942
Q9UPC5	165	>= 4 saturated or aromatic carbon-only ring size 5	-0.000944
Q9UPC5	780	CC1CCC(Cl)CC1	-0.000983
Q9UPC5	69	>= 1 Sr	-0.00107
Q9UPC5	635	N-N-C-N-[#1]	-0.001106
Q9UPC5	814	NC1CC(Br)CCC1	-0.001333
Q9UPC5	616	C:C:N:N:C	-0.001351
Q9UPC5	793	NC1CCC(Br)CC1	-0.00145
Q9UPC5	258	>= 2 hetero-aromatic rings	-0.001468
Q9UPC5	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	-0.001651
Q9UPC5	454	N(-C)(=O)	-0.00185
Q9UPC5	565	C:C-O-C	-0.001891
Q9UPC5	835	NC1C(Br)CCCC1	-0.001892
Q9UPC5	812	NC1CC(N)CCC1	-0.0019
Q9UPC5	470	C:C-C=C	-0.002183
Q9UPC5	315	O-K	-0.002217
Q9UPC5	786	OC1CCC(Br)CC1	-0.002243
Q9UPC5	452	C(-O)(=O)	-0.002408
Q9UPC5	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	-0.00244
Q9UPC5	742	Oc1cc(N)ccc1	-0.002628

Q9UPC5	802	CC1CC(Br)CCC1	−0.002637
Q9UPC5	213	>= 1 any ring size 7	−0.002754
Q9UPC5	337	C(~C)(~C)(~C)(~O)	−0.002763
Q9UPC5	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	−0.002867
Q9UPC5	556	C=C-C-C	−0.002868
Q9UPC5	434	C(-C)(-H)(=C)	−0.002893
Q9UPC5	774	Clc1c(Br)cccc1	−0.00293
Q9UPC5	631	O-C:C-O-[#1]	−0.002941
Q9UPC5	321	Si-Si	−0.003017
Q9UPC5	576	N=C-C:C-[#1]	−0.003035
Q9UPC5	715	Cc1ccc(S)cc1	−0.00308
Q9UPC5	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.003081
Q9UPC5	833	NC1C(N)CCCC1	−0.003167
Q9UPC5	432	C(-C)(-C)(=O)	−0.003504
Q9UPC5	492	N-C:O:C	−0.00357
Q9UPC5	587	N-C:C-O-[#1]	−0.00359
Q9UPC5	440	C(-C)(-O)(=O)	−0.003636
Q9UPC5	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.003703
Q9UPC5	698	O-C-C-C-C-C-C-C	−0.003743
Q9UPC5	298	C-I	−0.003842
Q9UPC5	571	[#1]-C-O-[#1]	−0.004106
Q9UPC5	809	SC1CC(N)CCC1	−0.004142
Q9UPC5	75	>= 1 Rh	−0.004175
Q9UPC5	143	>= 1 any ring size 5	−0.004217
Q9UPC5	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.004268
Q9UPC5	178	>= 1 any ring size 6	−0.004642
Q9UPC5	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.004678
Q9UPC5	96	>= 1 Tl	−0.004693
Q9UPC5	34	>= 2 S	−0.004774
Q9UPC5	11	>= 8 C	−0.004836
Q9UPC5	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.004857
Q9UPC5	335	C(~C)(~C)(~C)(~H)	−0.004964
Q9UPC5	290	C-Al	−0.005015
Q9UPC5	304	N-P	−0.005139
Q9UPC5	420	C=O	−0.005141
Q9UPC5	574	O-C-C:C-C	−0.005256
Q9UPC5	539	N=C-C-[#1]	−0.005298
Q9UPC5	696	C-C-C-C-C-C-C-C	−0.005303
Q9UPC5	444	C(-Cl)(=O)	−0.00553
Q9UPC5	52	>= 1 Ca	−0.005636
Q9UPC5	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.005979
Q9UPC5	369	C(~H)(~Si)	−0.006038
Q9UPC5	408	O(~H)(~S)	−0.006304
Q9UPC5	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.006323
Q9UPC5	15	>= 2 N	−0.00635
Q9UPC5	838	BrC1C(Br)CCCC1	−0.006565
Q9UPC5	44	>= 2 Br	−0.006581
Q9UPC5	19	>= 2 O	−0.006795

Q9UPC5	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	−0.00697
Q9UPC5	481	O-S-C:C	−0.007174
Q9UPC5	734	Cc1cc(C)ccc1	−0.007288
Q9UPC5	112	>= 1 Yb	−0.007329
Q9UPC5	605	O=C-C-O-C	−0.007337
Q9UPC5	758	Cc1c(N)cccc1	−0.007667
Q9UPC5	136	>= 2 any ring size 4	−0.007821
Q9UPC5	792	NC1CCC(Cl)CC1	−0.007943
Q9UPC5	88	>= 1 Ta	−0.007979
Q9UPC5	842	CC1CC(N)CC1	−0.008044
Q9UPC5	646	O=C-N-C-[#1]	−0.008118
Q9UPC5	867	OC1C(S)CCC1	−0.008309
Q9UPC5	282	B-Br	−0.008358
Q9UPC5	534	S-C:C-O	−0.008516
Q9UPC5	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.008523
Q9UPC5	513	S:C:C-[#1]	−0.008645
Q9UPC5	65	>= 1 As	−0.00865
Q9UPC5	847	OC1CC(N)CC1	−0.009
Q9UPC5	689	O-C-C-C-C-C-C	−0.009037
Q9UPC5	324	P-P	−0.009321
Q9UPC5	507	C-C-S-C	−0.009384
Q9UPC5	407	O(~C)(~P)	−0.009586
Q9UPC5	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.00972
Q9UPC5	474	S:C:C:N	−0.009878
Q9UPC5	670	Br-C:C:C-C	−0.00993
Q9UPC5	150	>= 2 any ring size 5	−0.010168
Q9UPC5	825	OC1C(S)CCCC1	−0.010309
Q9UPC5	270	Li-S	−0.010349
Q9UPC5	526	Cl-C:C-Cl	−0.010655
Q9UPC5	581	O=C-C-C-O	−0.011536
Q9UPC5	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.011786
Q9UPC5	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.012094
Q9UPC5	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.012285
Q9UPC5	713	Cc1ccc(C)cc1	−0.012618
Q9UPC5	662	O-C-C-O-C	−0.012911
Q9UPC5	697	C-C-C-C-C-C(C)-C	−0.013102
Q9UPC5	552	C:C-C:C	−0.013155
Q9UPC5	839	CC1CC(C)CC1	−0.013342
Q9UPC5	820	CC1C(S)CCCC1	−0.013705
Q9UPC5	378	C(~N)(:C)(:N)	−0.014086
Q9UPC5	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.01436
Q9UPC5	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.01468
Q9UPC5	763	Oc1c(N)cccc1	−0.015036
Q9UPC5	650	O=C-N-C=O	−0.015497
Q9UPC5	682	O-C-C-C-C-N	−0.016193
Q9UPC5	389	C(:N)(:N)	−0.016276
Q9UPC5	364	C(~F)(:C)	−0.016752
Q9UPC5	294	C-Cl	−0.017338

Q9UPC5	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.017389
Q9UPC5	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.01761
Q9UPC5	366	C(~H)(~O)	−0.01786
Q9UPC5	691	O-C-C-C-C-C-N	−0.018073
Q9UPC5	512	C-[As]-O-[#1]	−0.018691
Q9UPC5	26	>= 1 Na	−0.018964
Q9UPC5	557	N:C-O-[#1]	−0.019826
Q9UPC5	396	N(~C)(:C)	−0.019886
Q9UPC5	365	C(~H)(~N)	−0.019905
Q9UPC5	752	Clc1cc(Cl)ccc1	−0.020079
Q9UPC5	674	N-C-N-C:C	−0.020088
Q9UPC5	278	B-Si	−0.020147
Q9UPC5	23	>= 1 F	−0.020159
Q9UPC5	532	S-C:C-[#1]	−0.020246
Q9UPC5	862	CC1C(S)CCC1	−0.020788
Q9UPC5	471	S:C:C:C	−0.020878
Q9UPC5	771	Nc1c(Cl)cccc1	−0.020939
Q9UPC5	288	C-Na	−0.020983
Q9UPC5	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.021012
Q9UPC5	90	>= 1 Re	−0.021047
Q9UPC5	111	>= 1 Tm	−0.021158
Q9UPC5	509	Br-C:C-C	−0.021364
Q9UPC5	380	C(~O)(~O)	−0.021396
Q9UPC5	368	C(~H)(~S)	−0.021412
Q9UPC5	397	N(~C)(:C)(:C)	−0.021454
Q9UPC5	702	O-C-C-C-C-C-N-C	−0.021726
Q9UPC5	595	C:C-C-C-C	−0.022491
Q9UPC5	10	>= 4 C	−0.022578
Q9UPC5	659	O-C-C-N-C	−0.022754
Q9UPC5	653	O-C:C:C-O	−0.022794
Q9UPC5	549	N-C-C:C	−0.023928
Q9UPC5	460	C-C-C#C	−0.024452
Q9UPC5	390	N(~C)(~C)	−0.024721
Q9UPC5	465	O=S-C-C	−0.025853
Q9UPC5	716	Cc1ccc(N)cc1	−0.025945
Q9UPC5	856	NC1CC(Br)CC1	−0.025955
Q9UPC5	50	>= 1 Mg	−0.026461
Q9UPC5	636	C-N-C-N-C	−0.026649
Q9UPC5	413	S(~C)(~H)	−0.026716
Q9UPC5	686	O=C-C-C-C-O	−0.027242
Q9UPC5	1	>= 8 H	−0.027399
Q9UPC5	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.027505
Q9UPC5	663	O-C-C-O-[#1]	−0.027629
Q9UPC5	580	O=C-C-C-N	−0.028337
Q9UPC5	738	Cc1cc(Cl)ccc1	−0.02865
Q9UPC5	579	O=C-C-C-C	−0.029255
Q9UPC5	113	>= 1 Tc	−0.029281
Q9UPC5	558	O=N-C:C	−0.029742

Q9UPC5	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.029972
Q9UPC5	718	Cc1ccc(Br)cc1	−0.030071
Q9UPC5	745	Sc1cc(S)ccc1	−0.030732
Q9UPC5	257	>= 2 aromatic rings	−0.030756
Q9UPC5	840	CC1CC(O)CC1	−0.030891
Q9UPC5	619	O-C-C=C-C	−0.031483
Q9UPC5	657	C-N-C:C-C	−0.03178
Q9UPC5	3	>= 32 H	−0.032097
Q9UPC5	334	C(~C)(~C)(~C)(~C)	−0.033312
Q9UPC5	796	BrC1CCC(Br)CC1	−0.03449
Q9UPC5	185	>= 2 any ring size 6	−0.035381
Q9UPC5	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.036866
Q9UPC5	617	C-C-C-O-[#1]	−0.037076
Q9UPC5	661	O-C-O-C-C	−0.03754
Q9UPC5	811	SC1CC(Br)CCC1	−0.038118
Q9UPC5	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.038518
Q9UPC5	562	Br-C-C=O	−0.039426
Q9UPC5	538	N=C-C-C	−0.039794
Q9UPC5	401	N(~O)(~O)	−0.039957
Q9UPC5	484	N-C:N:C	−0.040019
Q9UPC5	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.040392
Q9UPC5	877	NC1C(Br)CCC1	−0.040598
Q9UPC5	849	OC1CC(Br)CC1	−0.041118
Q9UPC5	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.041626
Q9UPC5	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.042194
Q9UPC5	537	O=C-C-O	−0.042302
Q9UPC5	859	BrC1CC(Br)CC1	−0.042323
Q9UPC5	458	S(-O)(=O)	−0.044535
Q9UPC5	776	CC1CCC(C)CC1	−0.044609
Q9UPC5	630	O-C:C-O-C	−0.044733
Q9UPC5	863	CC1C(N)CCC1	−0.044888
Q9UPC5	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.045757
Q9UPC5	651	O-C:C:C-C	−0.046902
Q9UPC5	528	[#1]-N-C-[#1]	−0.047265
Q9UPC5	400	N(~H)(:C)(:C)	−0.047774
Q9UPC5	303	N-Si	−0.048224
Q9UPC5	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.048966
Q9UPC5	377	C(~N)(:C)(:C)	−0.049365
Q9UPC5	505	Cl-C:C-O	−0.050188
Q9UPC5	447	C(-H)(=N)	−0.051192
Q9UPC5	633	N-C-C:C-C	−0.052282
Q9UPC5	305	N-S	−0.052868
Q9UPC5	778	CC1CCC(S)CC1	−0.056056
Q9UPC5	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.057357
Q9UPC5	95	>= 1 Hg	−0.057383
Q9UPC5	590	C-C:C-O-[#1]	−0.058846
Q9UPC5	589	C-C:C-O-C	−0.059067
Q9UPC5	592	N-C-C-C-C	−0.059931

Q9UPC5	265	Li-B	−0.060514
Q9UPC5	459	S(=O)(=O)	−0.060726
Q9UPC5	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.067406
Q9UPC5	267	Li-O	−0.067854
Q9UPC5	373	C(~H)(:N)	−0.068529
Q9UPC5	692	O=C-C-C-C-C-C	−0.070797
Q9UPC5	712	C-C(C)-C(C)-C	−0.070933
Q9UPC5	367	C(~H)(~O)(~O)	−0.073878
Q9UPC5	310	O-Mg	−0.074067
Q9UPC5	457	S(-C)(=O)	−0.0741
Q9UPC5	427	C(#C)(-C)	−0.074611
Q9UPC5	773	Clc1c(Cl)cccc1	−0.076765
Q9UPC5	554	Br-C-C-C	−0.077451
Q9UPC5	441	C(-C)(=C)	−0.077625
Q9UPC5	721	Oc1ccc(N)cc1	−0.078069
Q9UPC5	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.079645
Q9UPC5	85	>= 1 Ba	−0.083261
Q9UPC5	20	>= 4 O	−0.085042
Q9UPC5	469	S-S-C:C	−0.086749
Q9UPC5	559	O-C-N-[#1]	−0.087577
Q9UPC5	80	>= 1 Sn	−0.087765
Q9UPC5	545	N-C:C-C	−0.088161
Q9UPC5	295	C-As	−0.088441
Q9UPC5	815	ClC1CC(Cl)CCC1	−0.089132
Q9UPC5	430	C(-C)(-C)(=C)	−0.089435
Q9UPC5	424	N=P	−0.0897
Q9UPC5	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.090479
Q9UPC5	21	>= 8 O	−0.090946
Q9UPC5	279	B-P	−0.091989
Q9UPC5	40	>= 8 Cl	−0.094418
Q9UPC5	720	Oc1ccc(S)cc1	−0.094677
Q9UPC5	768	Sc1c(Cl)cccc1	−0.094779
Q9UPC5	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.095569
Q9UPC5	748	Sc1cc(Br)ccc1	−0.095673
Q9UPC5	455	N(-O)(=O)	−0.096784
Q9UPC5	331	C(~Br)(:N)	−0.09694
Q9UPC5	255	>= 1 aromatic ring	−0.097329
Q9UPC5	309	O-O	−0.097838
Q9UPC5	500	C-S-C:C	−0.099054
Q9UPC5	669	Cl-C:C-C=O	−0.099072
Q9UPC5	535	O=C-C-C	−0.100214
Q9UPC5	845	OC1CC(O)CC1	−0.100285
Q9UPC5	385	C(:C)(:C)(:C)	−0.102051
Q9UPC5	750	Nc1cc(Cl)ccc1	−0.102822
Q9UPC5	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.103308
Q9UPC5	388	C(:C)(:N)(:N)	−0.10354
Q9UPC5	821	CC1C(N)CCCC1	−0.105254
Q9UPC5	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.105619

Q9UPC5	415	Si(~C)(~C)	−0.10571
Q9UPC5	340	C(~C)(~C)(~N)	−0.107353
Q9UPC5	338	C(~C)(~C)(~H)(~N)	−0.108617
Q9UPC5	497	O-C:C:N	−0.108974
Q9UPC5	755	Cc1c(C)cccc1	−0.110319
Q9UPC5	658	C-C-S-C-C	−0.113068
Q9UPC5	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.115053
Q9UPC5	94	>= 1 Au	−0.115618
Q9UPC5	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.11744
Q9UPC5	561	Cl-C-C=O	−0.117939
Q9UPC5	14	>= 1 N	−0.119137
Q9UPC5	874	SC1C(Br)CCC1	−0.119806
Q9UPC5	442	C(-C)(=N)	−0.120855
Q9UPC5	511	S=C-N-[#1]	−0.121069
Q9UPC5	578	C-C:C-C:C	−0.121363
Q9UPC5	531	S-C:C-C	−0.121883
Q9UPC5	384	C(:C)(:C)	−0.122182
Q9UPC5	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.122199
Q9UPC5	351	C(~C)(~N)	−0.123435
Q9UPC5	221	>= 2 saturated or aromatic carbon-only ring size 7	−0.123869
Q9UPC5	68	>= 1 Rb	−0.124438
Q9UPC5	807	OC1CC(Br)CCC1	−0.124766
Q9UPC5	680	O-C-C-C-C-C	−0.124923
Q9UPC5	350	C(~C)(~I)	−0.124981
Q9UPC5	356	C(~C)(:C)(:C)	−0.12581
Q9UPC5	805	OC1CC(N)CCC1	−0.125813
Q9UPC5	519	N=C-N-C	−0.125906
Q9UPC5	299	N-H	−0.125997
Q9UPC5	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.126146
Q9UPC5	275	B-N	−0.127238
Q9UPC5	542	O-C:C-[#1]	−0.127251
Q9UPC5	795	ClC1CCC(Br)CC1	−0.127257
Q9UPC5	504	N:C:N-C	−0.127258
Q9UPC5	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.127472
Q9UPC5	468	O=S-C-N	−0.127558
Q9UPC5	49	>= 1 Be	−0.128254
Q9UPC5	732	Clc1ccc(Br)cc1	−0.129005
Q9UPC5	82	>= 1 Te	−0.129193
Q9UPC5	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.129972
Q9UPC5	627	O=[As]-C:C:C	−0.130458
Q9UPC5	846	OC1CC(S)CC1	−0.130508
Q9UPC5	323	P-H	−0.130641
Q9UPC5	870	OC1C(Br)CCC1	−0.131625
Q9UPC5	62	>= 1 Zn	−0.131721
Q9UPC5	370	C(~H)(:C)	−0.13316
Q9UPC5	603	C-C:C:C-C	−0.133211
Q9UPC5	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.133387
Q9UPC5	649	O=N-C:C-O	−0.133457

Q9UPC5	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.133604
Q9UPC5	618	C:C-C-C:C	−0.133668
Q9UPC5	92	>= 1 Ir	−0.13367
Q9UPC5	9	>= 2 C	−0.134098
Q9UPC5	810	SC1CC(Cl)CCC1	−0.13414
Q9UPC5	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.134304
Q9UPC5	423	N=O	−0.134754
Q9UPC5	621	N-C:C:C:N	−0.141898
Q9UPC5	100	>= 1 Ce	−0.142851
Q9UPC5	614	C-C-O-C-C	−0.148362
Q9UPC5	477	N-N-C:C	−0.150132
Q9UPC5	690	O-C-C-C-C-C-O	−0.150618
Q9UPC5	448	C(-H)(=O)	−0.158572
Q9UPC5	523	N:C:C-C	−0.168676
Q9UPC5	464	N-C-C=C	−0.169149
Q9UPC5	490	C-C-C=C	−0.171729
Q9UPC5	462	O-C-C=O	−0.173541
Q9UPC5	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.175584
Q9UPC5	683	N-C-C-C-C-C	−0.178932
Q9UPC5	192	>= 3 any ring size 6	−0.178969
Q9UPC5	623	O=C-C:C-C	−0.179307
Q9UPC5	419	C#N	−0.179683
Q9UPC5	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.201044
Q9UPC5	529	Cl-C-C-Cl	−0.211455
Q9UPC5	277	B-F	−0.213783
Q9UPC5	736	Cc1cc(S)ccc1	−0.217869
Q9UPC5	808	SC1CC(S)CCC1	−0.235782
Q9UPC5	81	>= 1 Sb	−0.250507
Q9UPC5	274	B-C	−0.258011
Q9UPC5	395	N(~C)(~O)	−0.25978
Q9UPC5	679	C-C-C-C-C-C	−0.27559
Q9UPC5	478	S-C=N-[#1]	−0.277123
Q9UPC5	371	C(~H)(:C)(:C)	−0.277746
Q9UPC5	703	O-C-C-C-C-C(N)-C	−0.281523
Q9UPC5	437	C(-C)(-N)(=C)	−0.288445
Q9UPC5	826	OC1C(N)CCCC1	−0.289247
Q9UPC5	421	C=S	−0.290291
Q9UPC5	591	Cl-C-C-C-C	−0.291883
Q9UPC5	293	C-S	−0.292135
Q9UPC5	604	C-O-C-C:C	−0.300143
Q9UPC5	879	ClC1C(Br)CCC1	−0.301224
Q9UPC5	74	>= 1 Ru	−0.303337
Q9UPC5	399	N(~H)(:C)	−0.304414
Q9UPC5	84	>= 1 Cs	−0.321195
Q9UPC5	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.32883
Q9UPC5	425	P=O	−0.333421
Q9UPC5	854	NC1CC(N)CC1	−0.336804
Q9UPC5	746	Sc1cc(N)ccc1	−0.342207

Q9UPC5	439	C(-C)(-N)(=O)	−0.343411
Q9UPC5	626	C-O-C:C-C	−0.352804
Q9UPC5	841	CC1CC(S)CC1	−0.363518
Q9UPC5	272	B-H	−0.365553
Q9UPC5	800	CC1CC(N)CCC1	−0.366342
Q9UPC5	412	S(~C)(~C)	−0.370951
Q9UPC5	783	OC1CCC(S)CC1	−0.381447
Q9UPC5	467	C=N-N-C	−0.38231
Q9UPC5	564	C=C-C=C	−0.385604
Q9UPC5	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.400121
Q9UPC5	445	C(-H)(-N)(=C)	−0.403474
Q9UPC5	93	>= 1 Pt	−0.414116
Q9UPC5	508	S=C-N-C	−0.420255
Q9UPC5	483	N-S-C:C	−0.430124
Q9UPC5	791	NC1CCC(N)CC1	−0.448512
Q9UPC5	693	O=C-C-C-C-C-O	−0.451644
Q9UPC5	76	>= 1 Pd	−0.456944
Q9UPC5	726	Sc1ccc(Cl)cc1	−0.457773
Q9UPC5	817	BrC1CC(Br)CCC1	−0.458125
Q9UPC5	376	C(~N)(:C)	−0.468175
Q9UPC5	620	C:C-O-C-C	−0.469496
Q9UPC5	99	>= 1 La	−0.51212
Q9UPC5	816	ClC1CC(Br)CCC1	−0.523987
Q9UPC5	330	C(~Br)(:C)	−0.530057
Q9UPC5	285	C-N	−0.546951
Q9UPC5	429	C(#N)(-C)	−0.559945
Q9UPC5	560	N-C-N-C	−0.565603
Q9UPC5	360	C(~Cl)(~Cl)	−0.598928
Q9UPC5	311	O-Na	−0.60238
Q9UPC5	764	Oc1c(Cl)cccc1	−0.614371
Q9UPC5	271	Li-Cl	−0.614402
Q9UPC5	482	C:N-C:C	−0.631372
Q9UPC5	379	C(~N)(:N)	−0.675133
Q9UPC5	608	C-C-C-C:C	−0.692187
Q9UPC5	431	C(-C)(-C)(=N)	−0.692442
Q9UPC5	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.703976
Q9UPC5	740	Oc1cc(O)ccc1	−0.706016
Q9UPC5	353	C(~C)(~S)	−0.707949
Q9UPC5	322	Si-Cl	−0.727204
Q9UPC5	382	C(~O)(:C)(:C)	−0.727814
Q9UPC5	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	−0.779586
Q9UPC5	64	>= 1 Ge	−0.786292
Q9UPC5	32	>= 4 P	−0.870105
Q9UPC5	333	C(~C)(~C)(~C)	−0.897318
Q9UPC5	280	B-S	−0.899811
Q9UPC5	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.910006
Q9UPC5	762	Oc1c(S)cccc1	−0.970858
Q9UPC5	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.986133

Q9UPC5	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.99883
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Q9UPC5	688	C-C-C-C-C-C-C	−1.040332
Q9UPC5	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−1.072736
Q9UPC5	37	>= 1 Cl	−1.105509
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Q9UPC5	357	C(~C)(:C)(:N)	−1.239602
Q9UPC5	98	>= 1 Bi	−1.24283
Q9UPC5	241	>= 1 any ring size 9	−1.27586
Q9UPC5	607	N-C-C-C:C	−1.27817
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Q9UPC5	622	O=C-O-C:C	−1.385464
Q9UPC5	765	Oc1c(Br)cccc1	−1.434903
Q9UPC5	872	SC1C(N)CCC1	−1.45574
Q9UPC5	639	O-C-C-C-O	−1.518554
Q9UPC5	105	>= 1 Eu	−1.597902
Q9UPC5	296	C-Se	−1.653507
Q9UPC5	108	>= 1 Dy	−1.695352
Q9UPC5	12	>= 16 C	−2.030696

Fingerprints（continued)

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-1.695352	-6.67E-08
-2.031125	0.0004294

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q7Z601	704	O=C-C-C-C-C-C-C	1.7685628
Q7Z601	94	>= 1 Au	1.5212337
Q7Z601	213	>= 1 any ring size 7	1.2180903
Q7Z601	850	SC1CC(S)CC1	1.1529133
Q7Z601	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	1.0907711
Q7Z601	614	C-C-O-C-C	1.0632977
Q7Z601	4	>= 1 Li	0.9766151
Q7Z601	164	>= 4 any ring size 5	0.9394016
Q7Z601	116	>= 1 saturated or aromatic carbon-only ring size 3	0.875632
Q7Z601	321	Si-Si	0.8602104
Q7Z601	712	C-C(C)-C(C)-C	0.8141521
Q7Z601	836	ClC1C(Cl)CCCC1	0.7713521
Q7Z601	529	Cl-C-C-Cl	0.7520161
Q7Z601	761	Oc1c(O)cccc1	0.7414144
Q7Z601	325	As-H	0.7203321
Q7Z601	421	C=S	0.7139913
Q7Z601	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.7135194
Q7Z601	666	C=C-C-O-C	0.6930788
Q7Z601	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.6776723
Q7Z601	553	O=C-C=C	0.6768501
Q7Z601	328	C(~Br)(~C)(~C)	0.6728761
Q7Z601	798	CC1CC(O)CCC1	0.6689951
Q7Z601	428	C(#C)(-H)	0.666235
Q7Z601	654	N-C-N-C-C	0.6651907
Q7Z601	143	>= 1 any ring size 5	0.5878816
Q7Z601	57	>= 1 Mn	0.5754149
Q7Z601	495	C-N-C:C	0.5448419
Q7Z601	106	>= 1 Gd	0.5290642
Q7Z601	816	ClC1CC(Br)CCC1	0.4956464
Q7Z601	536	O=C-C-N	0.4719131
Q7Z601	56	>= 1 Cr	0.4655535
Q7Z601	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.458295
Q7Z601	760	Cc1c(Br)cccc1	0.4427582
Q7Z601	855	NC1CC(Cl)CC1	0.4420579
Q7Z601	595	C:C-C-C-C	0.4366244
Q7Z601	368	C(~H)(~S)	0.4347248
Q7Z601	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.4300877
Q7Z601	24	>= 2 F	0.4295779
Q7Z601	15	>= 2 N	0.4253976
Q7Z601	471	S:C:C:C	0.4075842
Q7Z601	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.4054334
Q7Z601	511	S=C-N-[#1]	0.3982682
Q7Z601	300	N-N	0.366332
Q7Z601	728	Nc1ccc(N)cc1	0.3650195
Q7Z601	308	O-H	0.3591392
Q7Z601	658	C-C-S-C-C	0.3217567

Q7Z601	271	Li-Cl	0.3177161
Q7Z601	67	>= 1 Kr	0.3142335
Q7Z601	398	N(~H)(~N)	0.28874
Q7Z601	519	N=C-N-C	0.2832707
Q7Z601	611	N-C-C-N-C	0.2745099
Q7Z601	484	N-C:N:C	0.2726696
Q7Z601	369	C(~H)(~Si)	0.2633508
Q7Z601	533	S-C:C-N	0.2524425
Q7Z601	490	C-C-C=C	0.2483109
Q7Z601	73	>= 1 Mo	0.2272968
Q7Z601	679	C-C-C-C-C-C	0.2187668
Q7Z601	303	N-Si	0.216579
Q7Z601	674	N-C-N-C:C	0.2132835
Q7Z601	378	C(~N)(:C)(:N)	0.2111419
Q7Z601	686	O=C-C-C-C-O	0.2098996
Q7Z601	596	N=C-N-C-C	0.2086813
Q7Z601	667	C=C-C-O-[#1]	0.2048968
Q7Z601	21	>= 8 O	0.2029162
Q7Z601	296	C-Se	0.2022742
Q7Z601	542	O-C:C-[#1]	0.200043
Q7Z601	621	N-C:C:C:N	0.1961873
Q7Z601	53	>= 1 Sc	0.1922073
Q7Z601	485	N:C:C:N	0.1744081
Q7Z601	290	C-Al	0.1698096
Q7Z601	635	N-N-C-N-[#1]	0.1600469
Q7Z601	41	>= 1 K	0.1557333
Q7Z601	516	[#1]-C=C-[#1]	0.1524156
Q7Z601	737	Cc1cc(N)ccc1	0.1487841
Q7Z601	179	>= 1 saturated or aromatic carbon-only ring size 6	0.1380411
Q7Z601	634	C-C-C:C-C	0.1368938
Q7Z601	329	C(~Br)(~H)	0.1352046
Q7Z601	97	>= 1 Pb	0.135077
Q7Z601	878	ClC1C(Cl)CCC1	0.1350689
Q7Z601	687	O=C-C-C-C=O	0.1348271
Q7Z601	727	Sc1ccc(Br)cc1	0.1345278
Q7Z601	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.1342609
Q7Z601	715	Cc1ccc(S)cc1	0.1341441
Q7Z601	249	>= 1 saturated or aromatic carbon-only ring size 10	0.1337283
Q7Z601	207	>= 5 saturated or aromatic carbon-only ring size 6	0.13328
Q7Z601	463	N:C-S-[#1]	0.1332599
Q7Z601	310	O-Mg	0.132218
Q7Z601	50	>= 1 Mg	0.1314232
Q7Z601	423	N=O	0.1308169
Q7Z601	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.1307522
Q7Z601	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.1292078
Q7Z601	101	>= 1 Pr	0.1290425
Q7Z601	69	>= 1 Sr	0.1286825
Q7Z601	280	B-S	0.1272111

Q7Z601	610	C-O-C-O-C	0.1271436
Q7Z601	701	O-C-C-C-C-C(O)-C	0.1267833
Q7Z601	675	Br-C-C-C:C	0.1261393
Q7Z601	601	N-C:C:C-N	0.1256233
Q7Z601	547	N-C:C-N	0.1253332
Q7Z601	312	O-Al	0.1245665
Q7Z601	846	OC1CC(S)CC1	0.1244751
Q7Z601	694	O=C-C-C-C-C=O	0.1239283
Q7Z601	64	>= 1 Ge	0.1236634
Q7Z601	642	O-C-C-C=O	0.1222618
Q7Z601	862	CC1C(S)CCC1	0.1218563
Q7Z601	494	O=C-C:N	0.121802
Q7Z601	109	>= 1 Ho	0.1193074
Q7Z601	690	O-C-C-C-C-C-O	0.1190447
Q7Z601	483	N-S-C:C	0.118384
Q7Z601	100	>= 1 Ce	0.1167309
Q7Z601	399	N(~H)(:C)	0.1159696
Q7Z601	799	CC1CC(S)CCC1	0.1154497
Q7Z601	49	>= 1 Be	0.1145874
Q7Z601	269	Li-P	0.1139966
Q7Z601	409	O(:C)(:C)	0.1138421
Q7Z601	740	Oc1cc(O)ccc1	0.1134836
Q7Z601	871	SC1C(S)CCC1	0.1128893
Q7Z601	639	O-C-C-C-O	0.1107165
Q7Z601	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.11033
Q7Z601	859	BrC1CC(Br)CC1	0.1090102
Q7Z601	651	O-C:C:C-C	0.1084408
Q7Z601	700	O-C-C-C-C-C-O-C	0.1065687
Q7Z601	302	N-F	0.1050694
Q7Z601	62	>= 1 Zn	0.1049199
Q7Z601	66	>= 1 Se	0.1043489
Q7Z601	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.104179
Q7Z601	72	>= 1 Nb	0.1032799
Q7Z601	655	O-C-C-C:C	0.1025467
Q7Z601	524	C-C=C-C	0.101293
Q7Z601	58	>= 1 Fe	0.1010437
Q7Z601	765	Oc1c(Br)cccc1	0.0997728
Q7Z601	342	C(~C)(~Cl)	0.0987442
Q7Z601	807	OC1CC(Br)CCC1	0.0986415
Q7Z601	730	Nc1ccc(Br)cc1	0.0976205
Q7Z601	38	>= 2 Cl	0.0964146
Q7Z601	282	B-Br	0.0963127
Q7Z601	808	SC1CC(S)CCC1	0.0956519
Q7Z601	318	Al-H	0.0956407
Q7Z601	640	C=C-C-C-C	0.0947043
Q7Z601	815	ClC1CC(Cl)CCC1	0.0935848
Q7Z601	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0926686
Q7Z601	441	C(-C)(=C)	0.0923819

Q7Z601	123	>= 2 saturated or aromatic carbon-only ring size 3	0.0904454
Q7Z601	576	N=C-C:C-[#1]	0.0904427
Q7Z601	527	C:C:N-[#1]	0.0902617
Q7Z601	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.0900393
Q7Z601	781	CC1CCC(Br)CC1	0.0899403
Q7Z601	710	C-C-C(C)-C-C	0.0899106
Q7Z601	13	>= 32 C	0.0885655
Q7Z601	835	NC1C(Br)CCCC1	0.0866657
Q7Z601	744	Oc1cc(Br)ccc1	0.0861599
Q7Z601	345	C(~C)(~H)(~N)	0.0835126
Q7Z601	633	N-C-C:C-C	0.0826802
Q7Z601	270	Li-S	0.0814251
Q7Z601	357	C(~C)(:C)(:N)	0.0807278
Q7Z601	413	S(~C)(~H)	0.0803587
Q7Z601	418	C=N	0.0799117
Q7Z601	479	S-C-S-C	0.0794741
Q7Z601	111	>= 1 Tm	0.0794006
Q7Z601	19	>= 2 O	0.078525
Q7Z601	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0774214
Q7Z601	447	C(-H)(=N)	0.0771903
Q7Z601	400	N(~H)(:C)(:C)	0.0767529
Q7Z601	395	N(~C)(~O)	0.0763521
Q7Z601	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	0.0750843
Q7Z601	158	>= 3 saturated or aromatic carbon-only ring size 5	0.0745819
Q7Z601	561	Cl-C-C=O	0.0741967
Q7Z601	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0741097
Q7Z601	749	Nc1cc(N)ccc1	0.0737844
Q7Z601	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0714824
Q7Z601	144	>= 1 saturated or aromatic carbon-only ring size 5	0.0706165
Q7Z601	115	>= 1 any ring size 3	0.0688551
Q7Z601	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.067566
Q7Z601	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.0674784
Q7Z601	294	C-Cl	0.0669394
Q7Z601	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0641698
Q7Z601	841	CC1CC(S)CC1	0.0639984
Q7Z601	699	O-C-C-C-C-C(C)-C	0.0639248
Q7Z601	5	>= 2 Li	0.0635781
Q7Z601	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.06191
Q7Z601	99	>= 1 La	0.061855
Q7Z601	460	C-C-C#C	0.0596339
Q7Z601	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	0.0589148
Q7Z601	842	CC1CC(N)CC1	0.0586997
Q7Z601	594	C-O-C-C=C	0.0578059
Q7Z601	608	C-C-C-C:C	0.0576025
Q7Z601	565	C:C-O-C	0.0573002
Q7Z601	371	C(~H)(:C)(:C)	0.0571264
Q7Z601	431	C(-C)(-C)(=N)	0.0566992
Q7Z601	383	C(~S)(:C)	0.0563958

Q7Z601	645	O=C-N-C-C	0.0548511
Q7Z601	804	OC1CC(S)CCC1	0.0544097
Q7Z601	559	O-C-N-[#1]	0.0541144
Q7Z601	372	C(~H)(:C)(:N)	0.0540532
Q7Z601	28	>= 1 Si	0.0536321
Q7Z601	739	Cc1cc(Br)ccc1	0.0536294
Q7Z601	458	S(-O)(=O)	0.0533798
Q7Z601	17	>= 8 N	0.0530154
Q7Z601	435	C(-C)(-H)(=N)	0.0528504
Q7Z601	650	O=C-N-C=O	0.0525024
Q7Z601	385	C(:C)(:C)(:C)	0.05221
Q7Z601	46	>= 1 I	0.0502355
Q7Z601	497	O-C:C:N	0.0495709
Q7Z601	791	NC1CCC(N)CC1	0.0490162
Q7Z601	734	Cc1cc(C)ccc1	0.0488768
Q7Z601	864	CC1C(Cl)CCC1	0.046603
Q7Z601	786	OC1CCC(Br)CC1	0.0461869
Q7Z601	425	P=O	0.0456784
Q7Z601	779	CC1CCC(N)CC1	0.0456201
Q7Z601	695	O=C-C-C-C-C-N	0.0450576
Q7Z601	860	CC1C(C)CCC1	0.0449371
Q7Z601	84	>= 1 Cs	0.0448924
Q7Z601	61	>= 1 Cu	0.0446168
Q7Z601	86	>= 1 Lu	0.0444152
Q7Z601	130	>= 1 saturated or aromatic carbon-only ring size 4	0.0439369
Q7Z601	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.0438172
Q7Z601	278	B-Si	0.0436202
Q7Z601	114	>= 1 U	0.0435958
Q7Z601	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.0429988
Q7Z601	102	>= 1 Nd	0.0429861
Q7Z601	720	Oc1ccc(S)cc1	0.0427886
Q7Z601	743	Oc1cc(Cl)ccc1	0.0425679
Q7Z601	336	C(~C)(~C)(~C)(~N)	0.0425528
Q7Z601	822	CC1C(Cl)CCCC1	0.0424786
Q7Z601	768	Sc1c(Cl)cccc1	0.0424074
Q7Z601	879	ClC1C(Br)CCC1	0.0422665
Q7Z601	185	>= 2 any ring size 6	0.0422406
Q7Z601	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	0.041811
Q7Z601	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.0417881
Q7Z601	652	O-C:C:C-N	0.0415637
Q7Z601	436	C(-C)(-H)(=O)	0.0414597
Q7Z601	830	SC1C(N)CCCC1	0.0406154
Q7Z601	825	OC1C(S)CCCC1	0.0394692
Q7Z601	505	Cl-C:C-O	0.0393981
Q7Z601	199	>= 4 any ring size 6	0.0376111
Q7Z601	673	O=C-C=C-N	0.0372342
Q7Z601	386	C(:C)(:C)(:N)	0.0360853
Q7Z601	31	>= 2 P	0.0360036

Q7Z601	517	N-N-C-N	0.0358168
Q7Z601	504	N:C:N-C	0.0357506
Q7Z601	104	>= 1 Sm	0.0349767
Q7Z601	821	CC1C(N)CCCC1	0.0345017
Q7Z601	678	C-C-C=C-C	0.034143
Q7Z601	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.0340797
Q7Z601	507	C-C-S-C	0.0330464
Q7Z601	284	C-C	0.0329452
Q7Z601	45	>= 4 Br	0.032817
Q7Z601	745	Sc1cc(S)ccc1	0.0325414
Q7Z601	643	[#1]-C-C-N-[#1]	0.0318982
Q7Z601	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.0312659
Q7Z601	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.030426
Q7Z601	87	>= 1 Hf	0.0304089
Q7Z601	703	O-C-C-C-C-C(N)-C	0.0301585
Q7Z601	390	N(~C)(~C)	0.0290845
Q7Z601	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.0290482
Q7Z601	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.0285068
Q7Z601	292	C-P	0.0283454
Q7Z601	619	O-C-C=C-C	0.0279689
Q7Z601	474	S:C:C:N	0.0272458
Q7Z601	718	Cc1ccc(Br)cc1	0.0264614
Q7Z601	373	C(~H)(:N)	0.0259587
Q7Z601	577	C:C-N-C:C	0.0257063
Q7Z601	627	O=[As]-C:C:C	0.0255298
Q7Z601	659	O-C-C-N-C	0.0250423
Q7Z601	579	O=C-C-C-C	0.0240729
Q7Z601	707	O=C-C-C-C-C(N)-C	0.0228151
Q7Z601	774	Clc1c(Br)cccc1	0.0220074
Q7Z601	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.021942
Q7Z601	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0218218
Q7Z601	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.0217736
Q7Z601	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.021241
Q7Z601	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.021208
Q7Z601	525	[As]-C:C-[#1]	0.0210891
Q7Z601	257	>= 2 aromatic rings	0.0209796
Q7Z601	813	NC1CC(Cl)CCC1	0.0208609
Q7Z601	466	N#C-C=C	0.0204989
Q7Z601	832	SC1C(Br)CCCC1	0.0202035
Q7Z601	285	C-N	0.0201281
Q7Z601	756	Cc1c(O)cccc1	0.0190253
Q7Z601	22	>= 16 O	0.018886
Q7Z601	755	Cc1c(C)cccc1	0.0187618
Q7Z601	824	OC1C(O)CCCC1	0.0185393
Q7Z601	326	As-As	0.0184653
Q7Z601	746	Sc1cc(N)ccc1	0.0183091
Q7Z601	301	N-O	0.018172
Q7Z601	796	BrC1CCC(Br)CC1	0.0178302

Q7Z601	660	C-C=C-C-C	0.0175688
Q7Z601	863	CC1C(N)CCC1	0.0175561
Q7Z601	262	>= 4 hetero-aromatic rings	0.0173095
Q7Z601	676	N#C-C-C-C	0.0166536
Q7Z601	362	C(~Cl)(:C)	0.016322
Q7Z601	77	>= 1 Ag	0.0162742
Q7Z601	70	>= 1 Y	0.0157319
Q7Z601	574	O-C-C:C-C	0.0153611
Q7Z601	110	>= 1 Er	0.0151255
Q7Z601	470	C:C-C=C	0.0150412
Q7Z601	584	C:C-C=C-C	0.0148406
Q7Z601	560	N-C-N-C	0.0135758
Q7Z601	427	C(#C)(-C)	0.0128051
Q7Z601	374	C(~H)(~H)(~H)	0.0126536
Q7Z601	543	O-C:C-N	0.0120633
Q7Z601	324	P-P	0.0119171
Q7Z601	36	>= 8 S	0.0119025
Q7Z601	381	C(~O)(:C)	0.0118945
Q7Z601	500	C-S-C:C	0.0118729
Q7Z601	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.0114126
Q7Z601	499	N-C:C:N	0.0113944
Q7Z601	583	Cl-C:C-O-C	0.0113423
Q7Z601	872	SC1C(N)CCC1	0.011121
Q7Z601	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.0110656
Q7Z601	537	O=C-C-O	0.0107898
Q7Z601	360	C(~Cl)(~Cl)	0.0104364
Q7Z601	298	C-I	0.0104054
Q7Z601	235	>= 2 saturated or aromatic carbon-only ring size 8	0.0097281
Q7Z601	404	N(:C)(:C)(:C)	0.0096424
Q7Z601	566	O-C-C-N	0.0096051
Q7Z601	291	C-Si	0.009366
Q7Z601	766	Sc1c(S)cccc1	0.0092822
Q7Z601	437	C(-C)(-N)(=C)	0.0092613
Q7Z601	480	C:S:C-C	0.0090278
Q7Z601	548	O-C-C:C	0.0085966
Q7Z601	293	C-S	0.0084385
Q7Z601	382	C(~O)(:C)(:C)	0.0083592
Q7Z601	508	S=C-N-C	0.0083285
Q7Z601	268	Li-F	0.0082734
Q7Z601	299	N-H	0.0082266
Q7Z601	723	Oc1ccc(Br)cc1	0.0082027
Q7Z601	530	N:C-C:C	0.0079728
Q7Z601	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.0079374
Q7Z601	59	>= 1 Co	0.007589
Q7Z601	346	C(~C)(~H)(~O)	0.0075308
Q7Z601	613	C-N-C-C-C	0.0073111
Q7Z601	89	>= 1 W	0.0071257
Q7Z601	90	>= 1 Re	0.0065552

Q7Z601	9	>= 2 C	0.0064734
Q7Z601	541	O-C:C-C	0.0064588
Q7Z601	819	CC1C(O)CCCC1	0.0064493
Q7Z601	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0063023
Q7Z601	785	OC1CCC(Cl)CC1	0.0062495
Q7Z601	375	C(~N)(~N)	0.0061483
Q7Z601	663	O-C-C-O-[#1]	0.0060607
Q7Z601	467	C=N-N-C	0.0055838
Q7Z601	455	N(-O)(=O)	0.0054888
Q7Z601	623	O=C-C:C-C	0.0054401
Q7Z601	637	O-C-C-C-C	0.0053941
Q7Z601	713	Cc1ccc(C)cc1	0.0053843
Q7Z601	0	>= 4 H	0.0051879
Q7Z601	870	OC1C(Br)CCC1	0.005027
Q7Z601	445	C(-H)(-N)(=C)	0.004836
Q7Z601	665	N-C:C-C-C	0.0046115
Q7Z601	567	O-C-C-O	0.0046057
Q7Z601	492	N-C:O:C	0.0043015
Q7Z601	397	N(~C)(:C)(:C)	0.0042909
Q7Z601	865	CC1C(Br)CCC1	0.0042834
Q7Z601	417	C#C	0.0042107
Q7Z601	731	Clc1ccc(Cl)cc1	0.0042009
Q7Z601	677	C-C=C-C:C	0.0041197
Q7Z601	444	C(-Cl)(=O)	0.004013
Q7Z601	332	C(~C)(~C)	0.0038419
Q7Z601	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0037248
Q7Z601	867	OC1C(S)CCC1	0.0037079
Q7Z601	295	C-As	0.0037029
Q7Z601	573	O-C-C=C	0.0034052
Q7Z601	834	NC1C(Cl)CCCC1	0.0032957
Q7Z601	592	N-C-C-C-C	0.0032941
Q7Z601	664	C-C=C-C=C	0.0032645
Q7Z601	107	>= 1 Tb	0.0031233
Q7Z601	496	N:N-C-[#1]	0.0031191
Q7Z601	81	>= 1 Sb	0.0030636
Q7Z601	264	Li-Li	0.0030621
Q7Z601	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0030044
Q7Z601	432	C(-C)(-C)(=O)	0.0029843
Q7Z601	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0029801
Q7Z601	3	>= 32 H	0.0029729
Q7Z601	414	S(~C)(~O)	0.0029371
Q7Z601	510	[#1]-N-N-[#1]	0.0029028
Q7Z601	571	[#1]-C-O-[#1]	0.0028795
Q7Z601	512	C-[As]-O-[#1]	0.0028392
Q7Z601	540	C-N-C-[#1]	0.0028319
Q7Z601	392	N(~C)(~C)(~H)	0.0027723
Q7Z601	688	C-C-C-C-C-C-C	0.0027573
Q7Z601	681	O-C-C-C-C-O	0.0026929

Q7Z601	856	NC1CC(Br)CC1	0.0026049
Q7Z601	7	>= 2 B	0.0025941
Q7Z601	422	N=N	0.0024984
Q7Z601	578	C-C:C-C:C	0.0024816
Q7Z601	27	>= 2 Na	0.0024678
Q7Z601	136	>= 2 any ring size 4	0.0024096
Q7Z601	810	SC1CC(Cl)CCC1	0.002291
Q7Z601	649	O=N-C:C-O	0.0022644
Q7Z601	406	O(~C)(~H)	0.0021451
Q7Z601	65	>= 1 As	0.0021354
Q7Z601	526	Cl-C:C-Cl	0.0020979
Q7Z601	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	0.0020955
Q7Z601	10	>= 4 C	0.0020686
Q7Z601	305	N-S	0.0019815
Q7Z601	443	C(-C)(=O)	0.0019553
Q7Z601	416	C=C	0.001854
Q7Z601	48	>= 4 I	0.0017742
Q7Z601	741	Oc1cc(S)ccc1	0.0015474
Q7Z601	353	C(~C)(~S)	0.0015107
Q7Z601	748	Sc1cc(Br)ccc1	0.0014682
Q7Z601	478	S-C=N-[#1]	0.0014307
Q7Z601	283	C-H	0.0012628
Q7Z601	387	C(:C)(:N)	0.0012082
Q7Z601	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.0011415
Q7Z601	725	Sc1ccc(N)cc1	0.0011166
Q7Z601	770	Nc1c(N)cccc1	0.0011063
Q7Z601	277	B-F	0.0009065
Q7Z601	644	C-C=N-N-C	0.00089
Q7Z601	773	Clc1c(Cl)cccc1	0.0007879
Q7Z601	647	O=C-N-C-N	0.0007366
Q7Z601	314	O-P	0.0007252
Q7Z601	778	CC1CCC(S)CC1	0.0006736
Q7Z601	350	C(~C)(~I)	0.0006299
Q7Z601	454	N(-C)(=O)	0.0006204
Q7Z601	14	>= 1 N	0.0005983
Q7Z601	599	[#1]-C-C=C-[#1]	0.0005224
Q7Z601	801	CC1CC(Cl)CCC1	0.0005158
Q7Z601	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.0004973
Q7Z601	464	N-C-C=C	0.0004293
Q7Z601	648	O=N-C:C-N	0.0002865
Q7Z601	669	Cl-C:C-C=O	0.0002824
Q7Z601	563	O-C-O-C	0.0002371
Q7Z601	848	OC1CC(Cl)CC1	0.000167
Q7Z601	330	C(~Br)(:C)	0.0001291
Q7Z601	327	C(~Br)(~C)	0.0001291
Q7Z601	670	Br-C:C-C-C	0.0001291
Q7Z601	287	C-F	0.0001254
Q7Z601	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0001191

Q7Z601	349	C(~C)(~H)(~S)	8.90E-06
Q7Z601	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	3.93E-06
Q7Z601	279	B-P	4.45E-08
Q7Z601	241	>= 1 any ring size 9	2.41E-08
Q7Z601	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	2.40E-08
Q7Z601	8	>= 4 B	2.39E-08
Q7Z601	311	O-Na	2.30E-08
Q7Z601	793	NC1CCC(Br)CC1	2.26E-08
Q7Z601	172	>= 5 saturated or aromatic carbon-only ring size 5	1.69E-08
Q7Z601	410	P(~C)(~C)	1.13E-08
Q7Z601	108	>= 1 Dy	1.04E-08
Q7Z601	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	9.39E-09
Q7Z601	2	>= 16 H	7.95E-09
Q7Z601	47	>= 2 I	4.08E-09
Q7Z601	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	3.00E-09
Q7Z601	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	2.97E-09
Q7Z601	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	2.52E-09
Q7Z601	289	C-Mg	-4.09E-10
Q7Z601	112	>= 1 Yb	-8.19E-10
Q7Z601	98	>= 1 Bi	-1.15E-09
Q7Z601	260	>= 3 hetero-aromatic rings	-2.35E-09
Q7Z601	55	>= 1 V	-2.44E-09
Q7Z601	869	OC1C(Cl)CCC1	-3.59E-09
Q7Z601	469	S-S-C:C	-7.67E-09
Q7Z601	68	>= 1 Rb	-9.08E-09
Q7Z601	113	>= 1 Tc	-1.69E-08
Q7Z601	415	Si(~C)(~C)	-1.93E-08
Q7Z601	306	N-Cl	-1.96E-08
Q7Z601	29	>= 2 Si	-1.98E-08
Q7Z601	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	-2.15E-08
Q7Z601	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	-2.55E-08
Q7Z601	880	BrC1C(Br)CCC1	-3.93E-08
Q7Z601	80	>= 1 Sn	-5.53E-08
Q7Z601	420	C=O	-1.20E-05
Q7Z601	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	-2.02E-05
Q7Z601	481	O-S-C:C	-4.74E-05
Q7Z601	767	Sc1c(N)cccc1	-5.80E-05
Q7Z601	281	B-Cl	-7.18E-05
Q7Z601	74	>= 1 Ru	-0.00013
Q7Z601	340	C(~C)(~C)(~N)	-0.000133
Q7Z601	20	>= 4 O	-0.000172
Q7Z601	662	O-C-C-O-C	-0.000219
Q7Z601	334	C(~C)(~C)(~C)(~C)	-0.000245
Q7Z601	706	O=C-C-C-C-C(=O)-C	-0.000322
Q7Z601	501	Cl-C:C-C	-0.000415
Q7Z601	751	Nc1cc(Br)ccc1	-0.000425
Q7Z601	814	NC1CC(Br)CCC1	-0.000425
Q7Z601	602	O=C-C-N-C	-0.000429

Q7Z601	631	O-C:C-O-[#1]	−0.00057
Q7Z601	401	N(~O)(~O)	−0.000625
Q7Z601	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.000685
Q7Z601	607	N-C-C-C:C	−0.000834
Q7Z601	827	OC1C(Cl)CCCC1	−0.000896
Q7Z601	705	O=C-C-C-C-C(O)-C	−0.000986
Q7Z601	37	>= 1 Cl	−0.001055
Q7Z601	818	CC1C(C)CCCC1	−0.001072
Q7Z601	448	C(-H)(=O)	−0.001119
Q7Z601	629	S-C:C:C-N	−0.001148
Q7Z601	852	SC1CC(Cl)CC1	−0.00115
Q7Z601	472	C:N:C-C	−0.001214
Q7Z601	248	>= 1 any ring size 10	−0.001239
Q7Z601	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.001288
Q7Z601	304	N-P	−0.001289
Q7Z601	258	>= 2 hetero-aromatic rings	−0.001328
Q7Z601	771	Nc1c(Cl)cccc1	−0.001378
Q7Z601	23	>= 1 F	−0.001391
Q7Z601	535	O=C-C-C	−0.001396
Q7Z601	624	O=C-C:C-N	−0.001424
Q7Z601	552	C:C-C:C	−0.001486
Q7Z601	794	ClC1CCC(Cl)CC1	−0.001539
Q7Z601	489	N-C-S-C	−0.00159
Q7Z601	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.001721
Q7Z601	805	OC1CC(N)CCC1	−0.001733
Q7Z601	803	OC1CC(O)CCC1	−0.001737
Q7Z601	522	C-N-N-[#1]	−0.001863
Q7Z601	192	>= 3 any ring size 6	−0.00191
Q7Z601	783	OC1CCC(S)CC1	−0.001981
Q7Z601	509	Br-C:C-C	−0.001991
Q7Z601	227	>= 1 any ring size 8	−0.002022
Q7Z601	809	SC1CC(N)CCC1	−0.00208
Q7Z601	570	C:C-C-C	−0.002113
Q7Z601	590	C-C:C-O-[#1]	−0.002142
Q7Z601	498	O-C=C-C	−0.002169
Q7Z601	593	N-C-C-C-N	−0.002213
Q7Z601	585	C-C:C-N-C	−0.002257
Q7Z601	632	C-C-O-C:C	−0.002366
Q7Z601	724	Sc1ccc(S)cc1	−0.002486
Q7Z601	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.002639
Q7Z601	764	Oc1c(Cl)cccc1	−0.002664
Q7Z601	736	Cc1cc(S)ccc1	−0.002678
Q7Z601	370	C(~H)(:C)	−0.002699
Q7Z601	307	N-Br	−0.002814
Q7Z601	538	N=C-C-C	−0.002989
Q7Z601	337	C(~C)(~C)(~C)(~O)	−0.003122
Q7Z601	626	C-O-C:C-C	−0.003236
Q7Z601	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.003394

Q7Z601	391	N(~C)(~C)(~C)	−0.003487
Q7Z601	355	C(~C)(:C)	−0.003522
Q7Z601	657	C-N-C:C-C	−0.003591
Q7Z601	682	O-C-C-C-C-N	−0.003709
Q7Z601	829	SC1C(S)CCCC1	−0.003967
Q7Z601	545	N-C:C-C	−0.004014
Q7Z601	721	Oc1ccc(N)cc1	−0.004064
Q7Z601	722	Oc1ccc(Cl)cc1	−0.004068
Q7Z601	503	Cl-C:C-[#1]	−0.004239
Q7Z601	777	CC1CCC(O)CC1	−0.004331
Q7Z601	598	Cl-C:C:C-C	−0.004343
Q7Z601	811	SC1CC(Br)CCC1	−0.004511
Q7Z601	317	F-S	−0.004727
Q7Z601	732	Clc1ccc(Br)cc1	−0.004903
Q7Z601	442	C(-C)(=N)	−0.004911
Q7Z601	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.004919
Q7Z601	518	O=C-N-N	−0.00492
Q7Z601	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.004957
Q7Z601	18	>= 1 O	−0.004997
Q7Z601	43	>= 1 Br	−0.005
Q7Z601	380	C(~O)(~O)	−0.005117
Q7Z601	557	N:C-O-[#1]	−0.005142
Q7Z601	6	>= 1 B	−0.005297
Q7Z601	275	B-N	−0.005299
Q7Z601	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.005369
Q7Z601	857	ClC1CC(Cl)CC1	−0.005382
Q7Z601	75	>= 1 Rh	−0.005525
Q7Z601	475	S-C=N-C	−0.005606
Q7Z601	861	CC1C(O)CCC1	−0.005983
Q7Z601	671	O=C-C=C-C	−0.00617
Q7Z601	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.006478
Q7Z601	354	C(~C)(~Si)	−0.006702
Q7Z601	683	N-C-C-C-C-C	−0.006734
Q7Z601	356	C(~C)(:C)(:C)	−0.006744
Q7Z601	429	C(#N)(-C)	−0.006809
Q7Z601	506	C-C:N:C	−0.006905
Q7Z601	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.006961
Q7Z601	684	O=C-C-C-C-C	−0.006971
Q7Z601	790	SC1CCC(Br)CC1	−0.007119
Q7Z601	93	>= 1 Pt	−0.007153
Q7Z601	685	O=C-C-C-C-N	−0.00731
Q7Z601	554	Br-C-C-C	−0.007478
Q7Z601	513	S:C:C-[#1]	−0.007666
Q7Z601	858	ClC1CC(Br)CC1	−0.007682
Q7Z601	680	O-C-C-C-C-C	−0.007697
Q7Z601	532	S-C:C-[#1]	−0.007882
Q7Z601	364	C(~F)(:C)	−0.007915
Q7Z601	837	ClC1C(Br)CCCC1	−0.007955

Q7Z601	539	N=C-C-[#1]	−0.007999
Q7Z601	591	Cl-C-C-C-C	−0.008277
Q7Z601	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.008312
Q7Z601	693	O=C-C-C-C-C-O	−0.008673
Q7Z601	394	N(~C)(~H)(~N)	−0.008846
Q7Z601	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.008907
Q7Z601	272	B-H	−0.008946
Q7Z601	40	>= 8 Cl	−0.009222
Q7Z601	389	C(:N)(:N)	−0.009309
Q7Z601	361	C(~Cl)(~H)	−0.009519
Q7Z601	763	Oc1c(N)cccc1	−0.009546
Q7Z601	459	S(=O)(=O)	−0.010209
Q7Z601	348	C(~C)(~H)(~P)	−0.010213
Q7Z601	735	Cc1cc(O)ccc1	−0.010428
Q7Z601	589	C-C:C-O-C	−0.010544
Q7Z601	616	C:C:N:N:C	−0.010694
Q7Z601	523	N:C:C-C	−0.010734
Q7Z601	612	N-C-O-C-C	−0.010734
Q7Z601	265	Li-B	−0.010821
Q7Z601	34	>= 2 S	−0.010846
Q7Z601	477	N-N-C:C	−0.011112
Q7Z601	122	>= 2 any ring size 3	−0.01113
Q7Z601	44	>= 2 Br	−0.011156
Q7Z601	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.011173
Q7Z601	316	F-P	−0.011425
Q7Z601	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.011664
Q7Z601	656	C-C-N-C-C	−0.012021
Q7Z601	320	Si-H	−0.012163
Q7Z601	405	O(~C)(~C)	−0.012284
Q7Z601	672	O=C-C=C-[#1]	−0.012295
Q7Z601	367	C(~H)(~O)(~O)	−0.012345
Q7Z601	347	C(~C)(~H)(~O)(~O)	−0.012481
Q7Z601	462	O-C-C=O	−0.013029
Q7Z601	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.013135
Q7Z601	439	C(-C)(-N)(=O)	−0.013282
Q7Z601	91	>= 1 Os	−0.013821
Q7Z601	286	C-O	−0.014337
Q7Z601	274	B-C	−0.014569
Q7Z601	606	O-C:C-C-C	−0.015259
Q7Z601	840	CC1CC(O)CC1	−0.015532
Q7Z601	54	>= 1 Ti	−0.016799
Q7Z601	344	C(~C)(~H)	−0.016872
Q7Z601	575	O-C-C:C-O	−0.016988
Q7Z601	366	C(~H)(~O)	−0.017163
Q7Z601	775	Brc1c(Br)cccc1	−0.017199
Q7Z601	784	OC1CCC(N)CC1	−0.017213
Q7Z601	866	OC1C(O)CCC1	−0.017697
Q7Z601	531	S-C:C-C	−0.017921

Q7Z601	641	O-C-C-C=C	−0.01795
Q7Z601	515	N-N-C-C	−0.017982
Q7Z601	323	P-H	−0.018159
Q7Z601	259	>= 3 aromatic rings	−0.018215
Q7Z601	726	Sc1ccc(Cl)cc1	−0.018228
Q7Z601	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.018335
Q7Z601	52	>= 1 Ca	−0.01837
Q7Z601	206	>= 5 any ring size 6	−0.019406
Q7Z601	408	O(~H)(~S)	−0.019627
Q7Z601	452	C(-O)(=O)	−0.019892
Q7Z601	757	Cc1c(S)cccc1	−0.0203
Q7Z601	615	N-C-C-O-C	−0.020413
Q7Z601	568	N#C-C-C	−0.020694
Q7Z601	620	C:C-O-C-C	−0.020845
Q7Z601	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.020913
Q7Z601	352	C(~C)(~O)	−0.021147
Q7Z601	384	C(:C)(:C)	−0.021295
Q7Z601	873	SC1C(Cl)CCC1	−0.02159
Q7Z601	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−0.021761
Q7Z601	171	>= 5 any ring size 5	−0.021858
Q7Z601	105	>= 1 Eu	−0.021891
Q7Z601	719	Oc1ccc(O)cc1	−0.021998
Q7Z601	461	O-C-C=N	−0.022276
Q7Z601	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.022349
Q7Z601	1	>= 8 H	−0.022607
Q7Z601	157	>= 3 any ring size 5	−0.023381
Q7Z601	438	C(-C)(-N)(=N)	−0.02347
Q7Z601	622	O=C-O-C:C	−0.023626
Q7Z601	617	C-C-C-O-[#1]	−0.024316
Q7Z601	702	O-C-C-C-C-C-N-C	−0.024646
Q7Z601	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.024716
Q7Z601	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.024998
Q7Z601	750	Nc1cc(Cl)ccc1	−0.025649
Q7Z601	502	N-C=C-[#1]	−0.025664
Q7Z601	605	O=C-C-O-C	−0.026398
Q7Z601	709	C-C(C)-C-C-C	−0.026902
Q7Z601	343	C(~C)(~Cl)(~H)	−0.027379
Q7Z601	465	O=S-C-C	−0.02785
Q7Z601	550	Cl-C-C-C	−0.028527
Q7Z601	797	CC1CC(C)CCC1	−0.028665
Q7Z601	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.02895
Q7Z601	95	>= 1 Hg	−0.029933
Q7Z601	838	BrC1C(Br)CCCC1	−0.030692
Q7Z601	580	O=C-C-C-N	−0.030756
Q7Z601	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.031805
Q7Z601	341	C(~C)(~C)(~O)	−0.031886
Q7Z601	823	CC1C(Br)CCCC1	−0.031887
Q7Z601	26	>= 1 Na	−0.032896

Q7Z601	716	Cc1ccc(N)cc1	−0.033038
Q7Z601	276	B-O	−0.033588
Q7Z601	638	O-C-C-C-N	−0.033638
Q7Z601	877	NC1C(Br)CCC1	−0.03401
Q7Z601	339	C(~C)(~C)(~H)(~O)	−0.035329
Q7Z601	546	N-C:C-[#1]	−0.036274
Q7Z601	698	O-C-C-C-C-C-C-C	−0.036606
Q7Z601	16	>= 4 N	−0.037236
Q7Z601	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.03851
Q7Z601	711	C-C(C)(C)-C-C	−0.03867
Q7Z601	795	ClC1CCC(Br)CC1	−0.039281
Q7Z601	33	>= 1 S	−0.039587
Q7Z601	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.039639
Q7Z601	753	Clc1cc(Br)ccc1	−0.040836
Q7Z601	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.040845
Q7Z601	769	Sc1c(Br)cccc1	−0.040915
Q7Z601	875	NC1C(N)CCC1	−0.041431
Q7Z601	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.042003
Q7Z601	569	N-C-C-N	−0.04241
Q7Z601	653	O-C:C:C-O	−0.042653
Q7Z601	25	>= 4 F	−0.042743
Q7Z601	319	Al-Cl	−0.043684
Q7Z601	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.044192
Q7Z601	782	OC1CCC(O)CC1	−0.044325
Q7Z601	628	C-N-C-C:C	−0.044414
Q7Z601	772	Nc1c(Br)cccc1	−0.044557
Q7Z601	273	B-B	−0.04472
Q7Z601	806	OC1CC(Cl)CCC1	−0.045814
Q7Z601	358	C(~C)(:N)	−0.046782
Q7Z601	482	C:N-C:C	−0.046805
Q7Z601	333	C(~C)(~C)(~C)	−0.047756
Q7Z601	572	N:C:N:C	−0.048538
Q7Z601	220	>= 2 any ring size 7	−0.049839
Q7Z601	618	C:C-C-C:C	−0.049867
Q7Z601	597	O=C-C-C:C	−0.049867
Q7Z601	178	>= 1 any ring size 6	−0.05124
Q7Z601	668	C-C:C-C-C	−0.053216
Q7Z601	71	>= 1 Zr	−0.054187
Q7Z601	762	Oc1c(S)cccc1	−0.055783
Q7Z601	697	C-C-C-C-C-C-C(C)-C	−0.056534
Q7Z601	800	CC1CC(N)CCC1	−0.057492
Q7Z601	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.057819
Q7Z601	636	C-N-C-N-C	−0.058244
Q7Z601	433	C(-C)(-Cl)(=O)	−0.05862
Q7Z601	661	O-C-O-C-C	−0.058784
Q7Z601	363	C(~F)(~F)	−0.058806
Q7Z601	582	C-C-C-C-C	−0.06021
Q7Z601	430	C(-C)(-C)(=C)	−0.060473

Q7Z601	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.062319
Q7Z601	549	N-C-C:C	−0.062799
Q7Z601	826	OC1C(N)CCCC1	−0.063743
Q7Z601	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.064842
Q7Z601	586	C-S-C-C-C	−0.065057
Q7Z601	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	−0.066132
Q7Z601	96	>= 1 Tl	−0.066971
Q7Z601	603	C-C:C:C-C	−0.067011
Q7Z601	780	CC1CCC(Cl)CC1	−0.067516
Q7Z601	491	C-N:C-[#1]	−0.070161
Q7Z601	714	Cc1ccc(O)cc1	−0.071947
Q7Z601	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.075561
Q7Z601	407	O(~C)(~P)	−0.076283
Q7Z601	558	O=N-C:C	−0.080023
Q7Z601	514	O-N-C-C	−0.0802
Q7Z601	393	N(~C)(~H)	−0.080735
Q7Z601	802	CC1CC(Br)CCC1	−0.081891
Q7Z601	876	NC1C(Cl)CC1	−0.082526
Q7Z601	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.085163
Q7Z601	42	>= 2 K	−0.085646
Q7Z601	322	Si-Cl	−0.086226
Q7Z601	450	C(-N)(=N)	−0.088509
Q7Z601	833	NC1C(N)CCCC1	−0.090655
Q7Z601	587	N-C:C-O-[#1]	−0.092055
Q7Z601	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.092591
Q7Z601	820	CC1C(S)CCCC1	−0.093166
Q7Z601	534	S-C:C-O	−0.093486
Q7Z601	853	SC1CC(Br)CC1	−0.094575
Q7Z601	78	>= 1 Cd	−0.09993
Q7Z601	376	C(~N)(:C)	−0.102313
Q7Z601	717	Cc1ccc(Cl)cc1	−0.104759
Q7Z601	831	SC1C(Cl)CCCC1	−0.104861
Q7Z601	453	N(-C)(=C)	−0.105561
Q7Z601	828	OC1C(Br)CCCC1	−0.107176
Q7Z601	83	>= 1 Xe	−0.107374
Q7Z601	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.111482
Q7Z601	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−0.111628
Q7Z601	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.112211
Q7Z601	255	>= 1 aromatic ring	−0.113979
Q7Z601	609	Cl-C-C-N-C	−0.116215
Q7Z601	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.117668
Q7Z601	315	O-K	−0.118363
Q7Z601	468	O=S-C-N	−0.11927
Q7Z601	788	SC1CCC(N)CC1	−0.121114
Q7Z601	843	CC1CC(Cl)CC1	−0.121693
Q7Z601	556	C=C-C-C	−0.12251
Q7Z601	85	>= 1 Ba	−0.123088
Q7Z601	742	Oc1cc(N)ccc1	−0.124096

Q7Z601	261	>= 4 aromatic rings	−0.125882
Q7Z601	402	N(~O)(:O)	−0.127608
Q7Z601	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.127801
Q7Z601	426	P=P	−0.12882
Q7Z601	562	Br-C-C=O	−0.129226
Q7Z601	60	>= 1 Ni	−0.129358
Q7Z601	729	Nc1ccc(Cl)cc1	−0.129925
Q7Z601	335	C(~C)(~C)(~C)(~H)	−0.130061
Q7Z601	30	>= 1 P	−0.130155
Q7Z601	544	O-C:C-O	−0.130409
Q7Z601	388	C(:C)(:N)(:N)	−0.130554
Q7Z601	92	>= 1 Ir	−0.131535
Q7Z601	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	−0.131957
Q7Z601	331	C(~Br)(:N)	−0.13302
Q7Z601	847	OC1CC(N)CC1	−0.133215
Q7Z601	377	C(~N)(:C)(:C)	−0.133291
Q7Z601	733	Brc1ccc(Br)cc1	−0.133522
Q7Z601	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.133807
Q7Z601	851	SC1CC(N)CC1	−0.134086
Q7Z601	266	Li-C	−0.134417
Q7Z601	839	CC1CC(C)CC1	−0.134509
Q7Z601	868	OC1C(N)CCC1	−0.134563
Q7Z601	76	>= 1 Pd	−0.134983
Q7Z601	288	C-Na	−0.135399
Q7Z601	551	Cl-C-C-O	−0.136416
Q7Z601	419	C#N	−0.13843
Q7Z601	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.138831
Q7Z601	451	C(-N)(=O)	−0.141473
Q7Z601	457	S(-C)(=O)	−0.143432
Q7Z601	12	>= 16 C	−0.146702
Q7Z601	488	N-C=N-[#1]	−0.152737
Q7Z601	424	N=P	−0.153688
Q7Z601	521	C:N-C-[#1]	−0.156936
Q7Z601	708	C-C(C)-C-C	−0.157963
Q7Z601	776	CC1CCC(C)CC1	−0.159076
Q7Z601	35	>= 4 S	−0.160743
Q7Z601	351	C(~C)(~N)	−0.164612
Q7Z601	359	C(~C)(:N)(:N)	−0.16783
Q7Z601	689	O-C-C-C-C-C-C	−0.175629
Q7Z601	150	>= 2 any ring size 5	−0.20145
Q7Z601	338	C(~C)(~C)(~H)(~N)	−0.21672
Q7Z601	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.22247
Q7Z601	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.23079
Q7Z601	103	>= 1 Pm	−0.231653
Q7Z601	267	Li-O	−0.231762
Q7Z601	812	NC1CC(N)CCC1	−0.242303
Q7Z601	555	N=C-C=C	−0.252675
Q7Z601	691	O-C-C-C-C-C-N	−0.254872

Q7Z601	738	Cc1cc(Cl)ccc1	−0.259082
Q7Z601	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.264456
Q7Z601	446	C(-H)(=C)	−0.278881
Q7Z601	129	>= 1 any ring size 4	−0.280198
Q7Z601	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.301986
Q7Z601	434	C(-C)(-H)(=C)	−0.304136
Q7Z601	692	O=C-C-C-C-C-C	−0.307238
Q7Z601	486	N-C:N:N	−0.307899
Q7Z601	759	Cc1c(Cl)cccc1	−0.320365
Q7Z601	787	SC1CCC(S)CC1	−0.325936
Q7Z601	411	P(~O)(~O)	−0.33923
Q7Z601	256	>= 1 hetero-aromatic ring	−0.343643
Q7Z601	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.356708
Q7Z601	440	C(-C)(-O)(=O)	−0.366099
Q7Z601	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.380323
Q7Z601	365	C(~H)(~N)	−0.387683
Q7Z601	313	O-Si	−0.392958
Q7Z601	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−0.401619
Q7Z601	752	Clc1cc(Cl)ccc1	−0.405061
Q7Z601	32	>= 4 P	−0.407317
Q7Z601	456	P(-O)(=O)	−0.426301
Q7Z601	51	>= 1 Al	−0.428716
Q7Z601	263	Li-H	−0.448431
Q7Z601	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.455686
Q7Z601	646	O=C-N-C-[#1]	−0.465026
Q7Z601	39	>= 4 Cl	−0.474017
Q7Z601	297	C-Br	−0.487489
Q7Z601	487	N-C=N-C	−0.501036
Q7Z601	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.525367
Q7Z601	476	C-O-C=C	−0.52668
Q7Z601	600	N-C:C:C-C	−0.528234
Q7Z601	403	N(:C)(:C)	−0.532854
Q7Z601	564	C=C-C=C	−0.537317
Q7Z601	11	>= 8 C	−0.569735
Q7Z601	845	OC1CC(O)CC1	−0.581779
Q7Z601	234	>= 2 any ring size 8	−0.587146
Q7Z601	528	[#1]-N-C-[#1]	−0.607863
Q7Z601	309	O-O	−0.628616
Q7Z601	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.643297
Q7Z601	396	N(~C)(:C)	−0.653403
Q7Z601	625	O=C-C:C-O	−0.654878
Q7Z601	817	BrC1CC(Br)CCC1	−0.668575
Q7Z601	588	O=C-C-C=O	−0.691753
Q7Z601	137	>= 2 saturated or aromatic carbon-only ring size 4	−0.706334
Q7Z601	79	>= 1 In	−0.747376
Q7Z601	412	S(~C)(~C)	−0.768469
Q7Z601	473	S-C:N:C	−0.779275
Q7Z601	758	Cc1c(N)cccc1	−0.779644

Q7Z601	379	C(~N)(:N)	-0.79019
Q7Z601	581	O=C-C-C-O	-0.796252
Q7Z601	449	C(-N)(=C)	-0.806744
Q7Z601	82	>= 1 Te	-0.839512
Q7Z601	630	O-C:C-O-C	-0.926424
Q7Z601	792	NC1CCC(Cl)CC1	-0.943061
Q7Z601	63	>= 1 Ga	-0.966939
Q7Z601	874	SC1C(Br)CCC1	-0.980502
Q7Z601	844	CC1CC(Br)CC1	-0.985266
Q7Z601	520	C=C-C:C	-0.994318
Q7Z601	696	C-C-C-C-C-C-C-C	-1.006103
Q7Z601	604	C-O-C-C:C	-1.01812
Q7Z601	493	O=C-C:C	-1.085464
Q7Z601	854	NC1CC(N)CC1	-1.15503
Q7Z601	849	OC1CC(Br)CC1	-1.182751
Q7Z601	747	Sc1cc(Cl)ccc1	-1.391392
Q7Z601	88	>= 1 Ta	-1.415427
Q7Z601	789	SC1CCC(Cl)CC1	-1.657311
Q7Z601	754	Brc1cc(Br)ccc1	-2.083552

Fingerprints（continued)

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1.2178533	0.000237
1.1529133	-1.48E-08
1.0907711	-4.78E-09
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0.9766151	-4.27E-08
0.9394016	-1.78E-08
0.8707934	0.004839
0.8602104	6.55E-09
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0.7708528	0.000499
0.7520827	-6.66E-05
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0.7203321	-1.69E-08
0.7091093	0.004882
0.7135194	1.53E-08
0.689426	0.003653
0.6776723	-1.02E-08
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0.672747	0.000129
0.6664889	0.002506
0.6665615	-0.00033
0.6654162	-0.00023
0.5813414	0.00654
0.5754149	-2.04E-08
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0.5290642	-7.00E-09
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0.4655535	-1.15E-09
0.458295	2.38E-10
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0.4420579	3.58E-08
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0.4293172	0.000261
0.4288	-0.0034
0.4078889	-0.0003
0.4026367	0.002797
0.3976517	0.000617
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0.358128	0.001011
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0.256861	-0.00442
0.2479496	0.000361
0.2272968	1.29E-08
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0.201935	0.009207
0.2069386	0.002961
0.2066726	0.002009
0.2092958	-0.0044
0.2040396	-0.00112
0.2022741	3.64E-08
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0.1912179	0.004969
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0.1517376	0.000678
0.1509276	-0.00214
0.1352615	0.00278
0.136228	0.000666
0.1352046	8.97E-09
0.135077	8.38E-09
0.1350689	-9.53E-10
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0.13328	3.95E-09
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0.1314232	2.48E-08
0.1314997	-0.00068
0.1307522	5.53E-09
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0.0770349	-0.00068
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0.0745819	-1.19E-08
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0.0523192	-0.00011
0.0506232	-0.00039
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0.0412846	-0.00067
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0.0033285	0.005699
0.0067697	0.001827
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0.0106404	-0.00228
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0.0063659	-0.00088
0.007055	-0.00161
0.0061341	-0.00074
0.0089047	-0.00352
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0.0036292	-0.00073
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0	-0.00226
0	-0.00237
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-0.002807	0.000129
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-0.005222	7.98E-05
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-0.006702	7.76E-09
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-0.018479 -0.00237
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-0.043466 -0.00095
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-0.046673 -0.00108
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-0.113979 2.22E-08
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-0.129816 -0.00059
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-0.133522 1.30E-08
-0.133807 5.12E-08
-0.134086 -2.81E-08
-0.134417 -1.27E-08
-0.13548 0.000971
-0.134563 -2.07E-08
-0.134983 -9.61E-09
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-0.132666 -0.00616
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-0.211991 -0.00473
-0.22247 -1.78E-08
-0.221523 -0.00927
-0.231653 6.84E-09
-0.231762 -5.63E-09
-0.236012 -0.00629
-0.254339 0.001664
-0.250991 -0.00388

-0.259598	0.000516
-0.264422	-3.42E-05
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-0.280599	0.000401
-0.301986	-6.16E-09
-0.305851	0.001715
-0.301282	-0.00596
-0.311932	0.004033
-0.321436	0.001071
-0.325936	-4.23E-08
-0.339955	0.000725
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-0.355308	-0.0014
-0.361993	-0.00411
-0.380483	0.00016
-0.387354	-0.00033
-0.392958	-2.66E-08
-0.401711	9.23E-05
-0.405182	0.000121
-0.407317	9.68E-10
-0.427026	0.000725
-0.428716	-3.10E-08
-0.448431	9.68E-09
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-0.474017	2.73E-08
-0.487618	0.000129
-0.501307	0.000271
-0.525367	-8.86E-09
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-0.531641	-0.00121
-0.539043	0.001726
-0.570836	0.001101
-0.581779	8.68E-09
-0.587146	-2.33E-08
-0.600347	-0.00752
-0.628616	3.19E-09
-0.643297	-2.11E-08
-0.652122	-0.00128
-0.656529	0.001651
-0.668695	0.000119
-0.692278	0.000524
-0.706334	2.06E-08
-0.747376	9.73E-09
-0.769446	0.000978
-0.780569	0.001294
-0.777531	-0.00211

-0.79106	0.00087
-0.797772	0.001519
-0.803381	-0.00336
-0.839512	-2.34E-08
-0.92611	-0.00031
-0.943084	2.36E-05
-0.966939	-5.40E-09
-0.980502	-2.93E-08
-0.985266	-1.84E-08
-0.995043	0.000725
-0.999658	-0.00644
-1.021537	0.003417
-1.083954	-0.00151
-1.15503	-1.07E-08
-1.182751	-1.95E-08
-1.391181	-0.00021
-1.415427	-6.74E-09
-1.657752	0.000441
-2.083671	0.000119

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
P32249	609	Cl-C-C-N-C	2.3064895
P32249	667	C=C-C-O-[#1]	1.5959676
P32249	397	N(~C)(:C)(:C)	1.3258002
P32249	261	>= 4 aromatic rings	1.3107773
P32249	468	O=S-C-N	1.2418162
P32249	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	1.1929648
P32249	422	N=N	1.116928
P32249	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	1.0843972
P32249	538	N=C-C-C	1.0701348
P32249	756	Cc1c(O)cccc1	1.0237503
P32249	859	BrC1CC(Br)CC1	1.0047546
P32249	475	S-C=N-C	0.9416382
P32249	752	Clc1cc(Cl)ccc1	0.9206623
P32249	714	Cc1ccc(O)cc1	0.8975347
P32249	351	C(~C)(~N)	0.8726076
P32249	273	B-B	0.8498807
P32249	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.8420588
P32249	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.8415254
P32249	801	CC1CC(Cl)CCC1	0.8352898
P32249	298	C-I	0.7797441
P32249	373	C(~H)(:N)	0.7749295
P32249	337	C(~C)(~C)(~C)(~O)	0.7526218
P32249	864	CC1C(Cl)CCC1	0.7286298
P32249	857	ClC1CC(Cl)CC1	0.6753508
P32249	459	S(=O)(=O)	0.6518383
P32249	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.6434955
P32249	612	N-C-O-C-C	0.637064
P32249	36	>= 8 S	0.6197779
P32249	786	OC1CCC(Br)CC1	0.6110205
P32249	19	>= 2 O	0.6045855
P32249	359	C(~C)(:N)(:N)	0.6024213
P32249	670	Br-C:C:C-C	0.590041
P32249	185	>= 2 any ring size 6	0.5676108
P32249	709	C-C(C)-C-C-C	0.5585613
P32249	641	O-C-C-C=C	0.555479
P32249	581	O=C-C-C-O	0.5520332
P32249	750	Nc1cc(Cl)ccc1	0.5508174
P32249	728	Nc1ccc(N)cc1	0.5376835
P32249	564	C=C-C=C	0.5328202
P32249	27	>= 2 Na	0.4989394
P32249	501	Cl-C:C-C	0.4904947
P32249	672	O=C-C=C-[#1]	0.4901832
P32249	267	Li-O	0.4896285
P32249	868	OC1C(N)CCC1	0.4787392

P32249	28	>= 1 Si	0.4656028
P32249	449	C(-N)(=C)	0.4576138
P32249	853	SC1CC(Br)CC1	0.452314
P32249	577	C:C-N-C:C	0.439486
P32249	25	>= 4 F	0.4384488
P32249	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	0.4254412
P32249	51	>= 1 Al	0.3977401
P32249	467	C=N-N-C	0.3946179
P32249	528	[#1]-N-C-[#1]	0.3617629
P32249	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.3531795
P32249	484	N-C:N:C	0.35182
P32249	12	>= 16 C	0.3505064
P32249	507	C-C-S-C	0.3372
P32249	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.3177702
P32249	800	CC1CC(N)CCC1	0.3176724
P32249	607	N-C-C-C:C	0.3171081
P32249	720	Oc1ccc(S)cc1	0.31308
P32249	49	>= 1 Be	0.3116498
P32249	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.3109425
P32249	865	CC1C(Br)CCC1	0.3088933
P32249	407	O(~C)(~P)	0.3070951
P32249	418	C=N	0.2927759
P32249	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	0.2855397
P32249	4	>= 1 Li	0.2835455
P32249	646	O=C-N-C-[#1]	0.2781643
P32249	199	>= 4 any ring size 6	0.273283
P32249	342	C(~C)(~Cl)	0.2710868
P32249	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.2680606
P32249	70	>= 1 Y	0.2579724
P32249	850	SC1CC(S)CC1	0.2572228
P32249	464	N-C-C=C	0.2571911
P32249	789	SC1CCC(Cl)CC1	0.2435118
P32249	410	P(~C)(~C)	0.2431187
P32249	810	SC1CC(Cl)CCC1	0.2320235
P32249	258	>= 2 hetero-aromatic rings	0.2309873
P32249	265	Li-B	0.226681
P32249	834	NC1C(Cl)CCCC1	0.2232097
P32249	72	>= 1 Nb	0.2177331
P32249	747	Sc1cc(Cl)ccc1	0.2175988
P32249	563	O-C-O-C	0.2166513
P32249	178	>= 1 any ring size 6	0.2148825
P32249	385	C(:C)(:C)(:C)	0.2108768
P32249	860	CC1C(C)CCC1	0.2074053
P32249	486	N-C:N:N	0.203889
P32249	574	O-C-C:C-C	0.202554
P32249	778	CC1CCC(S)CC1	0.197664

P32249	248	>= 1 any ring size 10	0.1941782
P32249	374	C(~H)(~H)(~H)	0.1899854
P32249	643	[#1]-C-C-N-[#1]	0.1833825
P32249	463	N:C-S-[#1]	0.1773987
P32249	722	Oc1ccc(Cl)cc1	0.1764392
P32249	832	SC1C(Br)CCCC1	0.1736341
P32249	584	C:C-C=C-C	0.1726037
P32249	558	O=N-C:C	0.1724582
P32249	523	N:C:C-C	0.1713321
P32249	595	C:C-C-C-C	0.1682591
P32249	619	O-C-C=C-C	0.1665818
P32249	645	O=C-N-C-C	0.1573131
P32249	371	C(~H)(:C)(:C)	0.1559513
P32249	255	>= 1 aromatic ring	0.153385
P32249	381	C(~O)(:C)	0.1509334
P32249	257	>= 2 aromatic rings	0.1504297
P32249	80	>= 1 Sn	0.1475646
P32249	726	Sc1ccc(Cl)cc1	0.1473665
P32249	220	>= 2 any ring size 7	0.1471746
P32249	808	SC1CC(S)CCC1	0.145503
P32249	774	Clc1c(Br)cccc1	0.1453467
P32249	451	C(-N)(=O)	0.1380204
P32249	346	C(~C)(~H)(~O)	0.1351835
P32249	353	C(~C)(~S)	0.1344809
P32249	723	Oc1ccc(Br)cc1	0.1344458
P32249	268	Li-F	0.1337693
P32249	719	Oc1ccc(O)cc1	0.1337468
P32249	687	O=C-C-C-C=O	0.1336463
P32249	53	>= 1 Sc	0.1332848
P32249	852	SC1CC(Cl)CC1	0.1332018
P32249	741	Oc1cc(S)ccc1	0.1326454
P32249	816	ClC1CC(Br)CCC1	0.1322697
P32249	112	>= 1 Yb	0.1319771
P32249	64	>= 1 Ge	0.1318104
P32249	136	>= 2 any ring size 4	0.1315083
P32249	52	>= 1 Ca	0.1313277
P32249	875	NC1C(N)CCC1	0.1311705
P32249	436	C(-C)(-H)(=O)	0.1310557
P32249	697	C-C-C-C-C-C(C)-C	0.1295739
P32249	673	O=C-C=C-N	0.1286563
P32249	482	C:N-C:C	0.1281069
P32249	755	Cc1c(C)cccc1	0.1280854
P32249	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.1276149
P32249	430	C(-C)(-C)(=C)	0.1269445
P32249	498	O-C=C-C	0.1250164
P32249	601	N-C:C:C-N	0.1243107

P32249	270	Li-S	0.1234174
P32249	547	N-C:C-N	0.122976
P32249	105	>= 1 Eu	0.1229074
P32249	213	>= 1 any ring size 7	0.1224438
P32249	100	>= 1 Ce	0.1221421
P32249	343	C(~C)(~Cl)(~H)	0.1215867
P32249	880	BrC1C(Br)CCC1	0.1214688
P32249	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.1208912
P32249	157	>= 3 any ring size 5	0.1188808
P32249	544	O-C:C-O	0.1185231
P32249	441	C(-C)(=C)	0.11787
P32249	293	C-S	0.1165169
P32249	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.116165
P32249	280	B-S	0.1159618
P32249	514	O-N-C-C	0.1158417
P32249	316	F-P	0.1156542
P32249	440	C(-C)(-O)(=O)	0.1155284
P32249	698	O-C-C-C-C-C-C-C	0.1152572
P32249	377	C(~N)(:C)(:C)	0.1147159
P32249	428	C(#C)(-H)	0.1119288
P32249	376	C(~N)(:C)	0.1112346
P32249	806	OC1CC(Cl)CCC1	0.1095416
P32249	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.1094281
P32249	590	C-C:C-O-[#1]	0.1093611
P32249	685	O=C-C-C-C-N	0.1093237
P32249	93	>= 1 Pt	0.1088376
P32249	398	N(~H)(~N)	0.1085005
P32249	473	S-C:N:C	0.1069681
P32249	545	N-C:C-C	0.103746
P32249	82	>= 1 Te	0.1025942
P32249	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	0.1015894
P32249	485	N:C:C:N	0.1010842
P32249	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.1010331
P32249	552	C:C-C:C	0.1008406
P32249	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.0955014
P32249	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.0954307
P32249	335	C(~C)(~C)(~C)(~H)	0.0938119
P32249	297	C-Br	0.0937581
P32249	776	CC1CCC(C)CC1	0.0936815
P32249	762	Oc1c(S)cccc1	0.0936281
P32249	634	C-C-C:C-C	0.0926015
P32249	42	>= 2 K	0.0914029
P32249	707	O=C-C-C-C-C(N)-C	0.091004
P32249	695	O=C-C-C-C-C-N	0.0897484
P32249	38	>= 2 Cl	0.0893798
P32249	772	Nc1c(Br)cccc1	0.0879059

P32249	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.0875731
P32249	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0873427
P32249	320	Si-H	0.0857613
P32249	6	>= 1 B	0.0839175
P32249	24	>= 2 F	0.0815379
P32249	761	Oc1c(O)cccc1	0.0802962
P32249	107	>= 1 Tb	0.0799618
P32249	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.0790716
P32249	844	CC1CC(Br)CC1	0.0782687
P32249	497	O-C:C:N	0.0781397
P32249	753	Clc1cc(Br)ccc1	0.07786
P32249	530	N:C-C:C	0.0760943
P32249	435	C(-C)(-H)(=N)	0.0757309
P32249	506	C-C:N:C	0.0756295
P32249	662	O-C-C-O-C	0.0745249
P32249	651	O-C:C:C-C	0.0729171
P32249	781	CC1CCC(Br)CC1	0.0725335
P32249	839	CC1CC(C)CC1	0.0721565
P32249	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.0721066
P32249	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	0.0720115
P32249	773	Clc1c(Cl)cccc1	0.068802
P32249	393	N(~C)(~H)	0.0678812
P32249	794	ClC1CCC(Cl)CC1	0.0669958
P32249	813	NC1CC(Cl)CCC1	0.066445
P32249	165	>= 4 saturated or aromatic carbon-only ring size 5	0.0662226
P32249	18	>= 1 O	0.0657835
P32249	712	C-C(C)-C(C)-C	0.0648101
P32249	822	CC1C(Cl)CCCC1	0.064418
P32249	826	OC1C(N)CCCC1	0.0637018
P32249	553	O=C-C=C	0.0634167
P32249	479	S-C-S-C	0.0633188
P32249	647	O=C-N-C-N	0.0630143
P32249	694	O=C-C-C-C-C=O	0.0620749
P32249	438	C(-C)(-N)(=N)	0.0618247
P32249	470	C:C-C=C	0.0612521
P32249	517	N-N-C-N	0.0603375
P32249	684	O=C-C-C-C-C	0.0595333
P32249	616	C:C:N:N:C	0.0590282
P32249	355	C(~C)(:C)	0.0553089
P32249	731	Clc1ccc(Cl)cc1	0.0532002
P32249	817	BrC1CC(Br)CCC1	0.0531251
P32249	636	C-N-C-N-C	0.0507906
P32249	322	Si-Cl	0.049594
P32249	757	Cc1c(S)cccc1	0.0494992
P32249	858	ClC1CC(Br)CC1	0.0490579
P32249	548	O-C-C:C	0.0488438

P32249	611	N-C-C-N-C	0.0483229
P32249	423	N=O	0.0479151
P32249	409	O(:C)(:C)	0.0474433
P32249	833	NC1C(N)CCCC1	0.0472678
P32249	26	>= 1 Na	0.0459721
P32249	492	N-C:O:C	0.0457771
P32249	411	P(~O)(~O)	0.0441028
P32249	71	>= 1 Zr	0.0439688
P32249	302	N-F	0.0432297
P32249	587	N-C:C-O-[#1]	0.042676
P32249	474	S:C:C:N	0.0426009
P32249	648	O=N-C:C-N	0.0421067
P32249	288	C-Na	0.0416805
P32249	172	>= 5 saturated or aromatic carbon-only ring size 5	0.0415703
P32249	878	ClC1C(Cl)CCC1	0.0413789
P32249	782	OC1CCC(O)CC1	0.0412479
P32249	109	>= 1 Ho	0.0411205
P32249	95	>= 1 Hg	0.0410261
P32249	708	C-C(C)-C-C	0.0408978
P32249	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0408725
P32249	521	C:N-C-[#1]	0.0408547
P32249	150	>= 2 any ring size 5	0.0403027
P32249	873	SC1C(Cl)CCC1	0.0402784
P32249	403	N(:C)(:C)	0.0399243
P32249	35	>= 4 S	0.0398386
P32249	256	>= 1 hetero-aromatic ring	0.0395235
P32249	400	N(~H)(:C)(:C)	0.0394127
P32249	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.0389502
P32249	784	OC1CCC(N)CC1	0.0388541
P32249	751	Nc1cc(Br)ccc1	0.0386565
P32249	638	O-C-C-C-N	0.0386075
P32249	537	O=C-C-O	0.0384773
P32249	10	>= 4 C	0.0381889
P32249	158	>= 3 saturated or aromatic carbon-only ring size 5	0.0374928
P32249	311	O-Na	0.0367262
P32249	313	O-Si	0.0364013
P32249	527	C:C:N-[#1]	0.0362311
P32249	431	C(-C)(-C)(=N)	0.0360081
P32249	554	Br-C-C-C	0.0355963
P32249	725	Sc1ccc(N)cc1	0.0340218
P32249	715	Cc1ccc(S)cc1	0.033945
P32249	114	>= 1 U	0.0337277
P32249	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.0321517
P32249	494	O=C-C:N	0.0309164
P32249	369	C(~H)(~Si)	0.0301633
P32249	713	Cc1ccc(C)cc1	0.0298783

P32249	241	>= 1 any ring size 9	0.0292971
P32249	664	C-C=C-C=C	0.0292246
P32249	690	O-C-C-C-C-C-O	0.0289854
P32249	737	Cc1cc(N)ccc1	0.0286902
P32249	323	P-H	0.0285977
P32249	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.0277506
P32249	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0275888
P32249	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.0274588
P32249	437	C(-C)(-N)(=C)	0.0270976
P32249	681	O-C-C-C-C-O	0.0267958
P32249	652	O-C:C:C-N	0.0266056
P32249	711	C-C(C)(C)-C-C	0.0263995
P32249	339	C(~C)(~C)(~H)(~O)	0.0263858
P32249	378	C(~N)(:C)(:N)	0.0262679
P32249	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.025577
P32249	626	C-O-C:C-C	0.0255213
P32249	234	>= 2 any ring size 8	0.0249539
P32249	760	Cc1c(Br)cccc1	0.0247338
P32249	471	S:C:C:C	0.023723
P32249	345	C(~C)(~H)(~N)	0.0229403
P32249	505	Cl-C:C-O	0.0224316
P32249	621	N-C:C:C:N	0.0219441
P32249	271	Li-Cl	0.0217635
P32249	692	O=C-C-C-C-C-C	0.0212439
P32249	291	C-Si	0.021073
P32249	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.0210489
P32249	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0209701
P32249	455	N(-O)(=O)	0.0205599
P32249	477	N-N-C:C	0.0202219
P32249	304	N-P	0.0201463
P32249	835	NC1C(Br)CCCC1	0.0198934
P32249	704	O=C-C-C-C-C-C-C	0.0190641
P32249	631	O-C:C-O-[#1]	0.0188344
P32249	310	O-Mg	0.0187984
P32249	491	C-N:C-[#1]	0.0187194
P32249	665	N-C:C-C-C	0.0182259
P32249	488	N-C=N-[#1]	0.0180663
P32249	562	Br-C-C=O	0.0175517
P32249	702	O-C-C-C-C-C-N-C	0.0174579
P32249	88	>= 1 Ta	0.0174413
P32249	413	S(~C)(~H)	0.0173083
P32249	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	0.0167529
P32249	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	0.0159125
P32249	104	>= 1 Sm	0.0151797
P32249	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.0148369
P32249	718	Cc1ccc(Br)cc1	0.0146664

P32249	394	N(~C)(~H)(~N)	0.0145451
P32249	263	Li-H	0.0142104
P32249	703	O-C-C-C-C-C(N)-C	0.0137229
P32249	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	0.0136394
P32249	47	>= 2 I	0.0134411
P32249	576	N=C-C:C-[#1]	0.0131914
P32249	78	>= 1 Cd	0.0131111
P32249	349	C(~C)(~H)(~S)	0.0131095
P32249	333	C(~C)(~C)(~C)	0.0129159
P32249	593	N-C-C-C-N	0.0128829
P32249	613	C-N-C-C-C	0.0128451
P32249	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.0128323
P32249	179	>= 1 saturated or aromatic carbon-only ring size 6	0.0124799
P32249	730	Nc1ccc(Br)cc1	0.0122814
P32249	77	>= 1 Ag	0.0122171
P32249	417	C#C	0.0117506
P32249	511	S=C-N-[#1]	0.0114959
P32249	434	C(-C)(-H)(=C)	0.0113239
P32249	797	CC1CC(C)CCC1	0.0110308
P32249	13	>= 32 C	0.0108719
P32249	787	SC1CCC(S)CC1	0.01082
P32249	614	C-C-O-C-C	0.0107166
P32249	285	C-N	0.0107089
P32249	566	O-C-C-N	0.0105803
P32249	276	B-O	0.0104843
P32249	541	O-C:C-C	0.0103499
P32249	653	O-C:C:C-O	0.0101776
P32249	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.0099384
P32249	732	Clc1ccc(Br)cc1	0.0095699
P32249	582	C-C-C-C-C	0.0095456
P32249	650	O=C-N-C=O	0.0094178
P32249	738	Cc1cc(Cl)ccc1	0.0093489
P32249	41	>= 1 K	0.0086304
P32249	838	BrC1C(Br)CCCC1	0.0080724
P32249	627	O=[As]-C:C:C	0.0078326
P32249	759	Cc1c(Cl)cccc1	0.007648
P32249	569	N-C-C-N	0.0075957
P32249	43	>= 1 Br	0.0074416
P32249	367	C(~H)(~O)(~O)	0.0073478
P32249	743	Oc1cc(Cl)ccc1	0.007315
P32249	186	>= 2 saturated or aromatic carbon-only ring size 6	0.0072684
P32249	543	O-C:C-N	0.0071017
P32249	671	O=C-C=C-C	0.0069738
P32249	568	N#C-C-C	0.0067263
P32249	809	SC1CC(N)CCC1	0.006301
P32249	620	C:C-O-C-C	0.0062913

P32249	330	C(~Br)(:C)	0.0062541
P32249	427	C(#C)(-C)	0.0061654
P32249	526	Cl-C:C-Cl	0.0060676
P32249	565	C:C-O-C	0.0060512
P32249	453	N(-C)(=C)	0.005828
P32249	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0057494
P32249	534	S-C:C-O	0.0056905
P32249	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0053565
P32249	454	N(-C)(=O)	0.0052735
P32249	836	ClC1C(Cl)CCCC1	0.0052715
P32249	62	>= 1 Zn	0.0051998
P32249	499	N-C:C:N	0.0051227
P32249	640	C=C-C-C-C	0.0049175
P32249	674	N-C-N-C:C	0.0048969
P32249	446	C(-H)(=C)	0.0045026
P32249	618	C:C-C-C:C	0.0044763
P32249	622	O=C-O-C:C	0.0044465
P32249	44	>= 2 Br	0.004156
P32249	828	OC1C(Br)CCCC1	0.0038029
P32249	460	C-C-C#C	0.0037916
P32249	352	C(~C)(~O)	0.0037591
P32249	783	OC1CCC(S)CC1	0.0037544
P32249	429	C(#N)(-C)	0.0037299
P32249	469	S-S-C:C	0.0036672
P32249	758	Cc1c(N)cccc1	0.0036051
P32249	678	C-C-C=C-C	0.003572
P32249	550	Cl-C-C-C	0.0034073
P32249	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.003385
P32249	319	Al-Cl	0.0031107
P32249	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0030682
P32249	490	C-C-C=C	0.0029816
P32249	414	S(~C)(~O)	0.0029725
P32249	871	SC1C(S)CCC1	0.0027841
P32249	278	B-Si	0.002627
P32249	831	SC1C(Cl)CCCC1	0.002243
P32249	368	C(~H)(~S)	0.0020547
P32249	688	C-C-C-C-C-C-C	0.0020483
P32249	849	OC1CC(Br)CC1	0.0019667
P32249	785	OC1CCC(Cl)CC1	0.0017802
P32249	677	C-C=C-C:C	0.001621
P32249	327	C(~Br)(~C)	0.0015557
P32249	46	>= 1 I	0.0014413
P32249	600	N-C:C:C-C	0.0014328
P32249	391	N(~C)(~C)(~C)	0.0014225
P32249	129	>= 1 any ring size 4	0.0013745
P32249	122	>= 2 any ring size 3	0.001328

P32249	404	N(:C)(:C)(:C)	0.0012115
P32249	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.0010447
P32249	382	C(~O)(:C)(:C)	0.0009886
P32249	539	N=C-C-[#1]	0.0009486
P32249	17	>= 8 N	0.0009133
P32249	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.0009097
P32249	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.0008647
P32249	283	C-H	0.0007979
P32249	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	0.0006968
P32249	515	N-N-C-C	0.0006781
P32249	289	C-Mg	0.0006208
P32249	412	S(~C)(~C)	0.0006159
P32249	401	N(~O)(~O)	0.000601
P32249	799	CC1CC(S)CCC1	0.0005996
P32249	583	Cl-C:C-O-C	0.0005707
P32249	512	C-[As]-O-[#1]	0.000561
P32249	130	>= 1 saturated or aromatic carbon-only ring size 4	0.000537
P32249	676	N#C-C-C-C	0.0004941
P32249	356	C(~C)(:C)(:C)	0.0004807
P32249	872	SC1C(N)CCC1	0.0004637
P32249	84	>= 1 Cs	0.0003558
P32249	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0003374
P32249	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.0003304
P32249	450	C(-N)(=N)	0.0002708
P32249	706	O=C-C-C-C-C(=O)-C	0.0002169
P32249	754	Brc1cc(Br)ccc1	0.0001631
P32249	765	Oc1c(Br)cccc1	0.0001631
P32249	555	N=C-C=C	0.0001311
P32249	847	OC1CC(N)CC1	3.42E-05
P32249	350	C(~C)(~I)	3.09E-05
P32249	101	>= 1 Pr	2.63E-05
P32249	326	As-As	2.27E-05
P32249	415	Si(~C)(~C)	9.92E-09
P32249	266	Li-C	8.35E-09
P32249	1	>= 8 H	5.63E-09
P32249	264	Li-Li	5.23E-09
P32249	481	O-S-C:C	3.65E-09
P32249	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	2.73E-09
P32249	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	1.85E-09
P32249	766	Sc1c(S)cccc1	2.88E-10
P32249	292	C-P	1.49E-10
P32249	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	-3.17E-10
P32249	262	>= 4 hetero-aromatic rings	-4.35E-10
P32249	85	>= 1 Ba	-8.56E-10
P32249	863	CC1C(N)CCC1	-2.34E-09
P32249	200	>= 4 saturated or aromatic carbon-only ring size 6	-3.27E-09

P32249	309	O-O	-4.24E-09
P32249	296	C-Se	-4.51E-09
P32249	525	[As]-C:C-[#1]	-6.77E-09
P32249	318	Al-H	-7.51E-09
P32249	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-8.83E-09
P32249	846	OC1CC(S)CC1	-1.06E-08
P32249	745	Sc1cc(S)ccc1	-1.11E-08
P32249	65	>= 1 As	-1.44E-08
P32249	870	OC1C(Br)CCC1	-1.47E-08
P32249	290	C-Al	-1.55E-08
P32249	228	>= 1 saturated or aromatic carbon-only ring size 8	-1.56E-08
P32249	848	OC1CC(Cl)CC1	-1.74E-08
P32249	137	>= 2 saturated or aromatic carbon-only ring size 4	-1.83E-08
P32249	279	B-P	-6.04E-06
P32249	466	N#C-C=C	-1.35E-05
P32249	729	Nc1ccc(Cl)cc1	-4.18E-05
P32249	746	Sc1cc(N)ccc1	-5.97E-05
P32249	845	OC1CC(O)CC1	-6.04E-05
P32249	769	Sc1c(Br)cccc1	-9.80E-05
P32249	604	C-O-C-C:C	-0.000132
P32249	489	N-C-S-C	-0.000149
P32249	842	CC1CC(N)CC1	-0.000169
P32249	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	-0.000199
P32249	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	-0.000242
P32249	867	OC1C(S)CCC1	-0.000302
P32249	764	Oc1c(Cl)cccc1	-0.000306
P32249	742	Oc1cc(N)ccc1	-0.000352
P32249	358	C(~C)(:N)	-0.000444
P32249	843	CC1CC(Cl)CC1	-0.000457
P32249	519	N=C-N-C	-0.000458
P32249	693	O=C-C-C-C-C-O	-0.000492
P32249	419	C#N	-0.000508
P32249	476	C-O-C=C	-0.000531
P32249	567	O-C-C-O	-0.000552
P32249	221	>= 2 saturated or aromatic carbon-only ring size 7	-0.000613
P32249	540	C-N-C-[#1]	-0.000656
P32249	649	O=N-C:C-O	-0.000671
P32249	9	>= 2 C	-0.000681
P32249	388	C(:C)(:N)(:N)	-0.000777
P32249	472	C:N:C-C	-0.000785
P32249	841	CC1CC(S)CC1	-0.000804
P32249	336	C(~C)(~C)(~C)(~N)	-0.000856
P32249	504	N:C:N-C	-0.000873
P32249	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	-0.001009
P32249	610	C-O-C-O-C	-0.001081
P32249	683	N-C-C-C-C-C	-0.001166

P32249	642	O-C-C-C=O	−0.001231
P32249	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−0.00135
P32249	370	C(~H)(:C)	−0.00136
P32249	33	>= 1 S	−0.001601
P32249	827	OC1C(Cl)CCCC1	−0.001802
P32249	16	>= 4 N	−0.00186
P32249	390	N(~C)(~C)	−0.002258
P32249	54	>= 1 Ti	−0.002285
P32249	663	O-C-C-O-[#1]	−0.002334
P32249	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.002353
P32249	465	O=S-C-C	−0.002693
P32249	585	C-C:C-N-C	−0.002824
P32249	724	Sc1ccc(S)cc1	−0.002894
P32249	637	O-C-C-C-C	−0.003163
P32249	286	C-O	−0.00317
P32249	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.00322
P32249	503	Cl-C:C-[#1]	−0.003293
P32249	357	C(~C)(:C)(:N)	−0.003349
P32249	94	>= 1 Au	−0.003433
P32249	639	O-C-C-C-O	−0.003543
P32249	775	Brc1c(Br)cccc1	−0.003589
P32249	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.003599
P32249	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.003679
P32249	851	SC1CC(N)CC1	−0.003949
P32249	392	N(~C)(~C)(~H)	−0.004203
P32249	734	Cc1cc(C)ccc1	−0.004236
P32249	312	O-Al	−0.004412
P32249	559	O-C-N-[#1]	−0.004485
P32249	366	C(~H)(~O)	−0.004513
P32249	360	C(~Cl)(~Cl)	−0.004529
P32249	32	>= 4 P	−0.004626
P32249	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.004686
P32249	379	C(~N)(:N)	−0.004756
P32249	877	NC1C(Br)CCC1	−0.004822
P32249	710	C-C-C(C)-C-C	−0.005092
P32249	862	CC1C(S)CCC1	−0.005206
P32249	624	O=C-C:C-N	−0.005389
P32249	14	>= 1 N	−0.005684
P32249	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.005976
P32249	89	>= 1 W	−0.006036
P32249	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.006186
P32249	31	>= 2 P	−0.006537
P32249	284	C-C	−0.006936
P32249	110	>= 1 Er	−0.007105
P32249	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.007359
P32249	56	>= 1 Cr	−0.007453

P32249	586	C-S-C-C-C	−0.007592
P32249	657	C-N-C:C-C	−0.007674
P32249	432	C(-C)(-C)(=O)	−0.007715
P32249	389	C(:N)(:N)	−0.007717
P32249	73	>= 1 Mo	−0.007784
P32249	272	B-H	−0.00789
P32249	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.008234
P32249	445	C(-H)(-N)(=C)	−0.008299
P32249	242	>= 1 saturated or aromatic carbon-only ring size 9	−0.008314
P32249	699	O-C-C-C-C-C(C)-C	−0.00847
P32249	420	C=O	−0.008763
P32249	45	>= 4 Br	−0.008779
P32249	20	>= 4 O	−0.008997
P32249	395	N(~C)(~O)	−0.009223
P32249	103	>= 1 Pm	−0.010874
P32249	143	>= 1 any ring size 5	−0.010906
P32249	876	NC1C(Cl)CC1	−0.011046
P32249	736	Cc1cc(S)ccc1	−0.011282
P32249	86	>= 1 Lu	−0.011756
P32249	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	−0.011927
P32249	260	>= 3 hetero-aromatic rings	−0.011991
P32249	733	Brc1ccc(Br)cc1	−0.012092
P32249	632	C-C-O-C:C	−0.012292
P32249	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.012452
P32249	452	C(-O)(=O)	−0.013263
P32249	97	>= 1 Pb	−0.013403
P32249	500	C-S-C:C	−0.013541
P32249	113	>= 1 Tc	−0.014414
P32249	448	C(-H)(=O)	−0.014474
P32249	608	C-C-C-C:C	−0.014487
P32249	749	Nc1cc(N)ccc1	−0.014696
P32249	74	>= 1 Ru	−0.01473
P32249	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.014746
P32249	348	C(~C)(~H)(~P)	−0.015608
P32249	63	>= 1 Ga	−0.015669
P32249	329	C(~Br)(~H)	−0.015879
P32249	561	Cl-C-C=O	−0.016036
P32249	55	>= 1 V	−0.016403
P32249	615	N-C-C-O-C	−0.016828
P32249	805	OC1CC(N)CCC1	−0.017391
P32249	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.01808
P32249	591	Cl-C-C-C-C	−0.018286
P32249	7	>= 2 B	−0.018975
P32249	748	Sc1cc(Br)ccc1	−0.01908
P32249	315	O-K	−0.019683
P32249	363	C(~F)(~F)	−0.019729

P32249	384	C(:C)(:C)	−0.01987
P32249	372	C(~H)(:C)(:N)	−0.020246
P32249	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.02076
P32249	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.020785
P32249	164	>= 4 any ring size 5	−0.020884
P32249	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.02093
P32249	866	OC1C(O)CCC1	−0.021134
P32249	840	CC1CC(O)CC1	−0.021199
P32249	300	N-N	−0.021763
P32249	628	C-N-C-C:C	−0.022042
P32249	281	B-Cl	−0.023278
P32249	462	O-C-C=O	−0.023429
P32249	332	C(~C)(~C)	−0.023506
P32249	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.023964
P32249	68	>= 1 Rb	−0.024084
P32249	659	O-C-C-N-C	−0.024091
P32249	580	O=C-C-C-N	−0.024383
P32249	0	>= 4 H	−0.024464
P32249	98	>= 1 Bi	−0.024549
P32249	546	N-C:C-[#1]	−0.024926
P32249	740	Oc1cc(O)ccc1	−0.025683
P32249	575	O-C-C:C-O	−0.026015
P32249	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.026711
P32249	325	As-H	−0.027041
P32249	39	>= 4 Cl	−0.027796
P32249	102	>= 1 Nd	−0.027957
P32249	542	O-C:C-[#1]	−0.028077
P32249	5	>= 2 Li	−0.028581
P32249	717	Cc1ccc(Cl)cc1	−0.028798
P32249	598	Cl-C:C:C-C	−0.028909
P32249	811	SC1CC(Br)CCC1	−0.030694
P32249	206	>= 5 any ring size 6	−0.030917
P32249	705	O=C-C-C-C-C(O)-C	−0.031059
P32249	535	O=C-C-C	−0.031544
P32249	364	C(~F)(:C)	−0.031688
P32249	666	C=C-C-O-C	−0.031767
P32249	457	S(-C)(=O)	−0.033992
P32249	81	>= 1 Sb	−0.034356
P32249	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.034691
P32249	820	CC1C(S)CCCC1	−0.034771
P32249	92	>= 1 Ir	−0.035406
P32249	171	>= 5 any ring size 5	−0.035804
P32249	549	N-C-C:C	−0.036199
P32249	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.036429
P32249	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.036587
P32249	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.036589

P32249	874	SC1C(Br)CCC1	−0.038149
P32249	295	C-As	−0.03831
P32249	287	C-F	−0.039577
P32249	496	N:N-C-[#1]	−0.04021
P32249	442	C(-C)(=N)	−0.041042
P32249	855	NC1CC(Cl)CC1	−0.041185
P32249	301	N-O	−0.041191
P32249	21	>= 8 O	−0.042324
P32249	823	CC1C(Br)CCCC1	−0.042554
P32249	536	O=C-C-N	−0.042674
P32249	560	N-C-N-C	−0.042765
P32249	767	Sc1c(N)cccc1	−0.042931
P32249	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.043062
P32249	520	C=C-C:C	−0.043331
P32249	829	SC1C(S)CCCC1	−0.043459
P32249	90	>= 1 Re	−0.043818
P32249	48	>= 4 I	−0.044071
P32249	321	Si-Si	−0.044485
P32249	661	O-C-O-C-C	−0.044635
P32249	589	C-C:C-O-C	−0.044736
P32249	324	P-P	−0.045882
P32249	76	>= 1 Pd	−0.046049
P32249	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.046241
P32249	15	>= 2 N	−0.047676
P32249	96	>= 1 Tl	−0.0479
P32249	192	>= 3 any ring size 6	−0.047972
P32249	338	C(~C)(~C)(~H)(~N)	−0.049777
P32249	812	NC1CC(N)CCC1	−0.050899
P32249	655	O-C-C-C:C	−0.052644
P32249	75	>= 1 Rh	−0.053178
P32249	354	C(~C)(~Si)	−0.055342
P32249	57	>= 1 Mn	−0.055454
P32249	421	C=S	−0.055917
P32249	770	Nc1c(N)cccc1	−0.056136
P32249	818	CC1C(C)CCCC1	−0.056175
P32249	700	O-C-C-C-C-C-O-C	−0.056202
P32249	691	O-C-C-C-C-C-N	−0.05699
P32249	115	>= 1 any ring size 3	−0.057071
P32249	779	CC1CCC(N)CC1	−0.05718
P32249	788	SC1CCC(N)CC1	−0.058797
P32249	819	CC1C(O)CCCC1	−0.059799
P32249	660	C-C=C-C-C	−0.060042
P32249	383	C(~S)(:C)	−0.060609
P32249	605	O=C-C-O-C	−0.064725
P32249	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.065191
P32249	739	Cc1cc(Br)ccc1	−0.065674

P32249	588	O=C-C-C=O	−0.066839
P32249	341	C(~C)(~C)(~O)	−0.069027
P32249	573	O-C-C=C	−0.070989
P32249	478	S-C=N-[#1]	−0.073429
P32249	533	S-C:C-N	−0.073474
P32249	334	C(~C)(~C)(~C)(~C)	−0.073777
P32249	803	OC1CC(O)CCC1	−0.074021
P32249	495	C-N-C:C	−0.074516
P32249	493	O=C-C:C	−0.074546
P32249	804	OC1CC(S)CCC1	−0.075545
P32249	796	BrC1CCC(Br)CC1	−0.07714
P32249	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.07792
P32249	510	[#1]-N-N-[#1]	−0.078182
P32249	425	P=O	−0.07882
P32249	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.078945
P32249	87	>= 1 Hf	−0.080541
P32249	456	P(-O)(=O)	−0.08113
P32249	815	ClC1CC(Cl)CCC1	−0.081653
P32249	518	O=C-N-N	−0.084078
P32249	34	>= 2 S	−0.085736
P32249	556	C=C-C-C	−0.085743
P32249	375	C(~N)(~N)	−0.086689
P32249	814	NC1CC(Br)CCC1	−0.087168
P32249	570	C:C-C-C	−0.087847
P32249	303	N-Si	−0.09132
P32249	869	OC1C(Cl)CCC1	−0.091633
P32249	635	N-N-C-N-[#1]	−0.091933
P32249	2	>= 16 H	−0.093652
P32249	656	C-C-N-C-C	−0.096322
P32249	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	−0.096669
P32249	578	C-C:C-C:C	−0.097193
P32249	387	C(:C)(:N)	−0.097454
P32249	347	C(~C)(~H)(~O)(~O)	−0.097745
P32249	682	O-C-C-C-C-N	−0.098212
P32249	768	Sc1c(Cl)cccc1	−0.100147
P32249	617	C-C-C-O-[#1]	−0.101566
P32249	606	O-C:C-C-C	−0.101637
P32249	830	SC1C(N)CCCC1	−0.102488
P32249	30	>= 1 P	−0.102969
P32249	60	>= 1 Ni	−0.103629
P32249	727	Sc1ccc(Br)cc1	−0.103785
P32249	861	CC1C(O)CCC1	−0.103797
P32249	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.104196
P32249	824	OC1C(O)CCCC1	−0.105291
P32249	793	NC1CCC(Br)CC1	−0.105852
P32249	780	CC1CCC(Cl)CC1	−0.106652

P32249	59	>= 1 Co	−0.11125
P32249	406	O(~C)(~H)	−0.112165
P32249	61	>= 1 Cu	−0.112868
P32249	40	>= 8 Cl	−0.114251
P32249	317	F-S	−0.115503
P32249	502	N-C=C-[#1]	−0.116004
P32249	644	C-C=N-N-C	−0.11654
P32249	99	>= 1 La	−0.116885
P32249	791	NC1CCC(N)CC1	−0.117286
P32249	29	>= 2 Si	−0.117932
P32249	675	Br-C-C-C:C	−0.118223
P32249	579	O=C-C-C-C	−0.119131
P32249	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−0.119213
P32249	23	>= 1 F	−0.119244
P32249	461	O-C-C=N	−0.119541
P32249	361	C(~Cl)(~H)	−0.120267
P32249	444	C(-Cl)(=O)	−0.121285
P32249	111	>= 1 Tm	−0.122709
P32249	299	N-H	−0.122752
P32249	508	S=C-N-C	−0.122966
P32249	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.124048
P32249	630	O-C:C-O-C	−0.1248
P32249	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.125166
P32249	307	N-Br	−0.125255
P32249	447	C(-H)(=N)	−0.125514
P32249	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.126792
P32249	513	S:C:C-[#1]	−0.126801
P32249	402	N(~O)(:O)	−0.127175
P32249	633	N-C-C:C-C	−0.127426
P32249	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.128763
P32249	91	>= 1 Os	−0.12955
P32249	602	O=C-C-N-C	−0.129932
P32249	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.130095
P32249	654	N-C-N-C-C	−0.131816
P32249	22	>= 16 O	−0.132076
P32249	328	C(~Br)(~C)(~C)	−0.132371
P32249	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.132534
P32249	792	NC1CCC(Cl)CC1	−0.132535
P32249	408	O(~H)(~S)	−0.133232
P32249	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.133332
P32249	66	>= 1 Se	−0.133454
P32249	856	NC1CC(Br)CC1	−0.133472
P32249	399	N(~H)(:C)	−0.133595
P32249	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.133927
P32249	426	P=P	−0.134058
P32249	396	N(~C)(:C)	−0.134066

P32249	879	ClC1C(Br)CCC1	−0.134997
P32249	821	CC1C(N)CCCC1	−0.135511
P32249	689	O-C-C-C-C-C-C	−0.138797
P32249	344	C(~C)(~H)	−0.138995
P32249	509	Br-C:C-C	−0.146052
P32249	680	O-C-C-C-C-C	−0.14657
P32249	668	C-C:C-C-C	−0.148675
P32249	716	Cc1ccc(N)cc1	−0.159903
P32249	532	S-C:C-[#1]	−0.161156
P32249	439	C(-C)(-N)(=O)	−0.164895
P32249	790	SC1CCC(Br)CC1	−0.165601
P32249	8	>= 4 B	−0.167527
P32249	701	O-C-C-C-C-C(O)-C	−0.175181
P32249	798	CC1CC(O)CCC1	−0.179467
P32249	480	C:S:C-C	−0.182102
P32249	405	O(~C)(~C)	−0.184369
P32249	362	C(~Cl)(:C)	−0.188022
P32249	623	O=C-C:C-C	−0.189054
P32249	529	Cl-C-C-Cl	−0.203305
P32249	572	N:C:N:C	−0.207586
P32249	365	C(~H)(~N)	−0.213756
P32249	735	Cc1cc(O)ccc1	−0.214622
P32249	837	ClC1C(Br)CCCC1	−0.218215
P32249	380	C(~O)(~O)	−0.220015
P32249	825	OC1C(S)CCCC1	−0.226966
P32249	269	Li-P	−0.227967
P32249	487	N-C=N-C	−0.234862
P32249	599	[#1]-C-C=C-[#1]	−0.238521
P32249	763	Oc1c(N)cccc1	−0.243949
P32249	308	O-H	−0.24461
P32249	69	>= 1 Sr	−0.246114
P32249	458	S(-O)(=O)	−0.24789
P32249	807	OC1CC(Br)CCC1	−0.256195
P32249	58	>= 1 Fe	−0.262007
P32249	227	>= 1 any ring size 8	−0.263785
P32249	108	>= 1 Dy	−0.267532
P32249	424	N=P	−0.280626
P32249	106	>= 1 Gd	−0.303072
P32249	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.314962
P32249	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.329955
P32249	524	C-C=C-C	−0.336782
P32249	522	C-N-N-[#1]	−0.338026
P32249	795	ClC1CCC(Br)CC1	−0.34213
P32249	282	B-Br	−0.348714
P32249	37	>= 1 Cl	−0.353005
P32249	483	N-S-C:C	−0.361055

P32249	571	[#1]-C-O-[#1]	−0.363679
P32249	744	Oc1cc(Br)ccc1	−0.368122
P32249	551	Cl-C-C-O	−0.37862
P32249	386	C(:C)(:C)(:N)	−0.38683
P32249	771	Nc1c(Cl)cccc1	−0.388174
P32249	592	N-C-C-C-C	−0.407011
P32249	67	>= 1 Kr	−0.414153
P32249	658	C-C-S-C-C	−0.432873
P32249	294	C-Cl	−0.474924
P32249	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	−0.491267
P32249	340	C(~C)(~C)(~N)	−0.491367
P32249	594	C-O-C-C=C	−0.499674
P32249	516	[#1]-C=C-[#1]	−0.501149
P32249	274	B-C	−0.506381
P32249	443	C(-C)(=O)	−0.507483
P32249	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.510685
P32249	11	>= 8 C	−0.528529
P32249	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.538846
P32249	305	N-S	−0.543138
P32249	597	O=C-C-C:C	−0.545212
P32249	79	>= 1 In	−0.555682
P32249	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.569946
P32249	277	B-F	−0.576332
P32249	83	>= 1 Xe	−0.584695
P32249	416	C=C	−0.595465
P32249	557	N:C-O-[#1]	−0.605924
P32249	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−0.606117
P32249	3	>= 32 H	−0.641239
P32249	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.669696
P32249	275	B-N	−0.75794
P32249	854	NC1CC(N)CC1	−0.768379
P32249	50	>= 1 Mg	−0.776404
P32249	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.778102
P32249	629	S-C:C:C-N	−0.82504
P32249	686	O=C-C-C-C-O	−0.926771
P32249	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.934618
P32249	625	O=C-C:C-O	−0.959002
P32249	802	CC1CC(Br)CCC1	−0.986327
P32249	596	N=C-N-C-C	−1.002592
P32249	531	S-C:C-C	−1.005544
P32249	696	C-C-C-C-C-C-C-C	−1.021385
P32249	306	N-Cl	−1.0728
P32249	721	Oc1ccc(N)cc1	−1.122495
P32249	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−1.157654
P32249	314	O-P	−1.162635
P32249	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	−1.167391

P32249	603	C-C:C:C-C	−1.172508
P32249	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−1.20495
P32249	259	>= 3 aromatic rings	−1.273533
P32249	777	CC1CCC(O)CC1	−1.274501
P32249	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	−1.291554
P32249	679	C-C-C-C-C-C	−1.310057
P32249	669	Cl-C:C-C=O	−1.476062
P32249	331	C(~Br)(:N)	−1.558632
P32249	433	C(-C)(-Cl)(=O)	−2.251619

Fingerprints（continued)

P	Q
2.304738	0.001751
1.593495	0.002473
1.324647	0.001153
1.310777	-3.42E-09
1.241746	7.00E-05
1.193234	-0.00027
1.119265	-0.00234
1.084397	1.71E-08
1.069833	0.000302
1.022942	0.000808
1.004755	-9.12E-09
0.94105	0.000588
0.920408	0.000254
0.899353	-0.00182
0.872183	0.000425
0.849881	-9.42E-09
0.841245	0.000814
0.841525	3.49E-09
0.832116	0.003174
0.779744	-1.92E-09
0.776018	-0.00109
0.75118	0.001442
0.72863	1.51E-10
0.675351	4.30E-09
0.652921	-0.00108
0.643616	-0.00012
0.636283	0.000781
0.619778	-4.45E-09
0.610984	3.68E-05
0.605882	-0.0013
0.605992	-0.00357
0.590949	-0.00091
0.566042	0.001569
0.558089	0.000472
0.559072	-0.00359
0.553264	-0.00123
0.550234	0.000584
0.537359	0.000324
0.530174	0.002646
0.498588	0.000352
0.493169	-0.00267
0.48866	0.001523
0.489628	-1.25E-08
0.478739	1.10E-08

0.465603	-1.81E-08
0.456478	0.001136
0.452314	-9.86E-09
0.439485	9.36E-07
0.437725	0.000724
0.425441	-9.50E-09
0.39774	4.95E-09
0.39378	0.000838
0.362866	-0.0011
0.35318	-8.43E-09
0.351813	7.44E-06
0.347441	0.003065
0.338077	-0.00088
0.318521	-0.00075
0.31738	0.000292
0.316835	0.000273
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-0.10365 -0.00013
-0.1029 -0.00089
-0.1042 7.47E-09
-0.10381 -0.00148
-0.10585 -5.18E-09
-0.10527 -0.00138

-0.11125 -2.29E-09
-0.11069 -0.00147
-0.11287 1.62E-08
-0.11425 4.09E-09
-0.1155 -7.73E-09
-0.11706 0.00106
-0.11738 0.000838
-0.11688 3.89E-09
-0.11761 0.000324
-0.11793 -1.14E-08
-0.11732 -0.00091
-0.11817 -0.00096
-0.11921 9.99E-09
-0.11939 0.000148
-0.12212 0.00258
-0.12027 -1.33E-09
-0.12128 -4.72E-09
-0.12271 -7.27E-09
-0.12042 -0.00233
-0.12158 -0.00139
-0.12405 -1.39E-08
-0.12714 0.002343
-0.12515 -1.30E-05
-0.12526 5.94E-09
-0.12439 -0.00113
-0.12679 -9.96E-10
-0.12521 -0.00159
-0.12717 -9.63E-09
-0.12493 -0.0025
-0.12912 0.000359
-0.12955 -3.13E-09
-0.13404 0.004112
-0.1301 6.90E-09
-0.13189 7.55E-05
-0.13222 0.000142
-0.13146 -0.00091
-0.13253 -5.22E-09
-0.13249 -4.18E-05
-0.13323 -8.05E-09
-0.13333 1.31E-08
-0.13345 -9.23E-09
-0.13347 1.30E-09
-0.13142 -0.00217
-0.1337 -0.00023
-0.13406 -6.17E-09
-0.13304 -0.00103

-0.135	2.33E-10
-0.13415	-0.00136
-0.13448	-0.00432
-0.13716	-0.00183
-0.14514	-0.00091
-0.14283	-0.00374
-0.15009	0.001415
-0.16027	0.000364
-0.15675	-0.0044
-0.16413	-0.00076
-0.16547	-0.00013
-0.16753	2.65E-09
-0.17619	0.001011
-0.17933	-0.00014
-0.18187	-0.00024
-0.18287	-0.0015
-0.18535	-0.00267
-0.18634	-0.00272
-0.20444	0.001136
-0.20656	-0.00103
-0.2115	-0.00226
-0.21448	-0.00014
-0.21821	1.88E-08
-0.21754	-0.00248
-0.22697	-3.58E-09
-0.22797	-1.13E-08
-0.23574	0.000875
-0.23942	0.000901
-0.24454	0.000595
-0.24297	-0.00164
-0.24611	8.80E-09
-0.2481	0.000215
-0.2562	1.78E-08
-0.26201	1.87E-08
-0.26378	-3.13E-09
-0.26753	9.11E-10
-0.28063	1.47E-09
-0.30307	1.89E-08
-0.31521	0.000246
-0.32996	-5.88E-09
-0.34031	0.003528
-0.33617	-0.00186
-0.34213	-5.97E-09
-0.34871	8.28E-09
-0.35044	-0.00256
-0.35762	-0.00343

-0.36182	-0.00186
-0.36812	1.65E-08
-0.37766	-0.00096
-0.3866	-0.00023
-0.38807	-0.0001
-0.40691	-0.0001
-0.41415	-4.38E-09
-0.43122	-0.00166
-0.47258	-0.00234
-0.49188	0.000611
-0.49421	0.002843
-0.49918	-0.0005
-0.50399	0.002838
-0.50622	-0.00016
-0.50568	-0.0018
-0.51069	7.62E-09
-0.52655	-0.00198
-0.53885	-1.38E-08
-0.5434	0.000261
-0.54612	0.000907
-0.55568	-5.14E-09
-0.56995	1.34E-09
-0.57714	0.000807
-0.58469	9.31E-09
-0.59784	0.002371
-0.60541	-0.00051
-0.60643	0.000315
-0.64124	-1.40E-09
-0.6697	6.21E-09
-0.75794	-8.06E-09
-0.76838	-2.04E-08
-0.7764	1.85E-08
-0.77975	0.001651
-0.82513	9.21E-05
-0.92658	-0.00019
-0.93462	2.16E-09
-0.96035	0.001345
-0.98548	-0.00084
-1.00213	-0.00046
-1.00261	-0.00293
-1.01693	-0.00445
-1.0728	3.94E-09
-1.12124	-0.00125
-1.15765	1.22E-08
-1.16286	0.000227
-1.1668	-0.00059

-1.17392	0.001415
-1.20495	5.98E-09
-1.27353	-3.04E-09
-1.27296	-0.00154
-1.29155	-6.40E-09
-1.31159	0.001536
-1.473	-0.00306
-1.55863	8.81E-09
-2.25162	5.56E-09

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q9GZN0	25	>= 4 F	2.0740621
Q9GZN0	321	Si-Si	1.9598438
Q9GZN0	685	O=C-C-C-C-N	1.8169603
Q9GZN0	575	O-C-C:C-O	1.654634
Q9GZN0	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	1.5882625
Q9GZN0	462	O-C-C=O	1.5632576
Q9GZN0	266	Li-C	1.5136008
Q9GZN0	846	OC1CC(S)CC1	1.4736291
Q9GZN0	494	O=C-C:N	1.4634089
Q9GZN0	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	1.4470487
Q9GZN0	72	>= 1 Nb	1.4450889
Q9GZN0	596	N=C-N-C-C	1.3744553
Q9GZN0	96	>= 1 Tl	1.3377562
Q9GZN0	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	1.2556676
Q9GZN0	866	OC1C(O)CCC1	1.2369585
Q9GZN0	371	C(~H)(:C)(:C)	1.2245009
Q9GZN0	263	Li-H	1.2175246
Q9GZN0	18	>= 1 O	1.2050657
Q9GZN0	666	C=C-C-O-C	1.1136655
Q9GZN0	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	1.0866657
Q9GZN0	278	B-Si	1.0707285
Q9GZN0	522	C-N-N-[#1]	1.0311421
Q9GZN0	407	O(~C)(~P)	0.9849219
Q9GZN0	495	C-N-C:C	0.975033
Q9GZN0	114	>= 1 U	0.9090115
Q9GZN0	398	N(~H)(~N)	0.8726913
Q9GZN0	93	>= 1 Pt	0.8636456
Q9GZN0	269	Li-P	0.8578843
Q9GZN0	400	N(~H)(:C)(:C)	0.8301497
Q9GZN0	36	>= 8 S	0.810876
Q9GZN0	795	ClC1CCC(Br)CC1	0.7648376
Q9GZN0	618	C:C-C-C:C	0.7572308
Q9GZN0	445	C(-H)(-N)(=C)	0.7196113
Q9GZN0	384	C(:C)(:C)	0.6928912
Q9GZN0	87	>= 1 Hf	0.6267379
Q9GZN0	716	Cc1ccc(N)cc1	0.6074934
Q9GZN0	39	>= 4 Cl	0.5959597
Q9GZN0	431	C(-C)(-C)(=N)	0.5871747
Q9GZN0	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.5855094
Q9GZN0	129	>= 1 any ring size 4	0.5712953
Q9GZN0	722	Oc1ccc(Cl)cc1	0.5578245
Q9GZN0	689	O-C-C-C-C-C-C	0.5462644
Q9GZN0	419	C#N	0.5136607
Q9GZN0	363	C(~F)(~F)	0.5129621

Q9GZN0	368	C(~H)(~S)	0.4853172
Q9GZN0	595	C:C-C-C-C	0.4720875
Q9GZN0	387	C(:C)(:N)	0.4677091
Q9GZN0	779	CC1CCC(N)CC1	0.4674258
Q9GZN0	823	CC1C(Br)CCCC1	0.4381299
Q9GZN0	179	>= 1 saturated or aromatic carbon-only ring size 6	0.4330269
Q9GZN0	853	SC1CC(Br)CC1	0.4288002
Q9GZN0	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.4177206
Q9GZN0	192	>= 3 any ring size 6	0.4172624
Q9GZN0	88	>= 1 Ta	0.4126772
Q9GZN0	811	SC1CC(Br)CCC1	0.4087792
Q9GZN0	638	O-C-C-C-N	0.3981423
Q9GZN0	702	O-C-C-C-C-C-N-C	0.3818652
Q9GZN0	452	C(-O)(=O)	0.3747327
Q9GZN0	273	B-B	0.3735081
Q9GZN0	386	C(:C)(:C)(:N)	0.3724484
Q9GZN0	646	O=C-N-C-[#1]	0.3703197
Q9GZN0	735	Cc1cc(O)ccc1	0.360831
Q9GZN0	773	Clc1c(Cl)cccc1	0.3601916
Q9GZN0	714	Cc1ccc(O)cc1	0.3564867
Q9GZN0	71	>= 1 Zr	0.3488883
Q9GZN0	497	O-C:C:N	0.3355689
Q9GZN0	185	>= 2 any ring size 6	0.3335257
Q9GZN0	346	C(~C)(~H)(~O)	0.3273197
Q9GZN0	123	>= 2 saturated or aromatic carbon-only ring size 3	0.3226111
Q9GZN0	373	C(~H)(:N)	0.3208066
Q9GZN0	578	C-C:C-C:C	0.3202336
Q9GZN0	122	>= 2 any ring size 3	0.3126645
Q9GZN0	440	C(-C)(-O)(=O)	0.3007218
Q9GZN0	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	0.2995174
Q9GZN0	463	N:C-S-[#1]	0.292089
Q9GZN0	471	S:C:C:C	0.2699914
Q9GZN0	523	N:C:C-C	0.267372
Q9GZN0	396	N(~C)(:C)	0.2508572
Q9GZN0	7	>= 2 B	0.2503096
Q9GZN0	693	O=C-C-C-C-C-O	0.2481289
Q9GZN0	687	O=C-C-C-C=O	0.2448697
Q9GZN0	409	O(:C)(:C)	0.2429076
Q9GZN0	680	O-C-C-C-C-C	0.2413408
Q9GZN0	380	C(~O)(~O)	0.2408543
Q9GZN0	634	C-C-C:C-C	0.2253932
Q9GZN0	130	>= 1 saturated or aromatic carbon-only ring size 4	0.2234471
Q9GZN0	454	N(-C)(=O)	0.2195421
Q9GZN0	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.2170084
Q9GZN0	694	O=C-C-C-C-C=O	0.2153933
Q9GZN0	334	C(~C)(~C)(~C)(~C)	0.2105574

Q9GZN0	777	CC1CCC(O)CC1	0.2056469
Q9GZN0	199	>= 4 any ring size 6	0.1952739
Q9GZN0	675	Br-C-C-C:C	0.1947023
Q9GZN0	788	SC1CCC(N)CC1	0.1758293
Q9GZN0	30	>= 1 P	0.1672135
Q9GZN0	467	C=N-N-C	0.1670991
Q9GZN0	248	>= 1 any ring size 10	0.1515151
Q9GZN0	55	>= 1 V	0.1477322
Q9GZN0	581	O=C-C-C-O	0.1457322
Q9GZN0	632	C-C-O-C:C	0.1390782
Q9GZN0	599	[#1]-C-C=C-[#1]	0.1347947
Q9GZN0	315	O-K	0.1346915
Q9GZN0	631	O-C:C-O-[#1]	0.1343893
Q9GZN0	105	>= 1 Eu	0.1342659
Q9GZN0	109	>= 1 Ho	0.1335872
Q9GZN0	583	Cl-C:C-O-C	0.1334975
Q9GZN0	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.1334288
Q9GZN0	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	0.1333761
Q9GZN0	98	>= 1 Bi	0.1327747
Q9GZN0	627	O=[As]-C:C:C	0.1325006
Q9GZN0	76	>= 1 Pd	0.1316199
Q9GZN0	841	CC1CC(S)CC1	0.1315979
Q9GZN0	51	>= 1 Al	0.1309794
Q9GZN0	95	>= 1 Hg	0.1302252
Q9GZN0	852	SC1CC(Cl)CC1	0.1297011
Q9GZN0	298	C-I	0.1284155
Q9GZN0	728	Nc1ccc(N)cc1	0.1283331
Q9GZN0	814	NC1CC(Br)CCC1	0.1281694
Q9GZN0	715	Cc1ccc(S)cc1	0.1278308
Q9GZN0	290	C-Al	0.1277348
Q9GZN0	725	Sc1ccc(N)cc1	0.127433
Q9GZN0	765	Oc1c(Br)cccc1	0.1266198
Q9GZN0	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.1265059
Q9GZN0	772	Nc1c(Br)cccc1	0.1261131
Q9GZN0	774	Clc1c(Br)cccc1	0.1254587
Q9GZN0	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.1251647
Q9GZN0	32	>= 4 P	0.1250325
Q9GZN0	559	O-C-N-[#1]	0.1244825
Q9GZN0	329	C(~Br)(~H)	0.1237214
Q9GZN0	515	N-N-C-C	0.1234929
Q9GZN0	158	>= 3 saturated or aromatic carbon-only ring size 5	0.122443
Q9GZN0	65	>= 1 As	0.1224402
Q9GZN0	292	C-P	0.122161
Q9GZN0	678	C-C-C=C-C	0.1215269
Q9GZN0	831	SC1C(Cl)CCCC1	0.119995
Q9GZN0	864	CC1C(Cl)CCC1	0.1189138

Q9GZN0	791	NC1CCC(N)CC1	0.1180596
Q9GZN0	660	C-C=C-C-C	0.1167045
Q9GZN0	164	>= 4 any ring size 5	0.1166827
Q9GZN0	15	>= 2 N	0.1158102
Q9GZN0	345	C(~C)(~H)(~N)	0.1154054
Q9GZN0	860	CC1C(C)CCC1	0.1150168
Q9GZN0	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.1149696
Q9GZN0	768	Sc1c(Cl)cccc1	0.114341
Q9GZN0	847	OC1CC(N)CC1	0.1130975
Q9GZN0	417	C#C	0.113051
Q9GZN0	102	>= 1 Nd	0.1122476
Q9GZN0	108	>= 1 Dy	0.1116546
Q9GZN0	756	Cc1c(O)cccc1	0.1111388
Q9GZN0	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	0.111121
Q9GZN0	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.1111083
Q9GZN0	771	Nc1c(Cl)cccc1	0.1108724
Q9GZN0	107	>= 1 Tb	0.1096146
Q9GZN0	35	>= 4 S	0.1052198
Q9GZN0	695	O=C-C-C-C-C-N	0.1038053
Q9GZN0	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.0993012
Q9GZN0	365	C(~H)(~N)	0.0991794
Q9GZN0	585	C-C:C-N-C	0.0986983
Q9GZN0	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	0.0984036
Q9GZN0	614	C-C-O-C-C	0.0976138
Q9GZN0	651	O-C:C:C-C	0.0967768
Q9GZN0	551	Cl-C-C-O	0.0964021
Q9GZN0	427	C(#C)(-C)	0.0960866
Q9GZN0	616	C:C:N:N:C	0.0960802
Q9GZN0	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0947516
Q9GZN0	872	SC1C(N)CCC1	0.0946247
Q9GZN0	723	Oc1ccc(Br)cc1	0.0938985
Q9GZN0	817	BrC1CC(Br)CCC1	0.092426
Q9GZN0	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0902945
Q9GZN0	540	C-N-C-[#1]	0.0896979
Q9GZN0	513	S:C:C-[#1]	0.0829983
Q9GZN0	519	N=C-N-C	0.082651
Q9GZN0	381	C(~O)(:C)	0.0797756
Q9GZN0	839	CC1CC(C)CC1	0.0797637
Q9GZN0	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0790874
Q9GZN0	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0786924
Q9GZN0	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0774426
Q9GZN0	441	C(-C)(=C)	0.0770993
Q9GZN0	418	C=N	0.0764556
Q9GZN0	241	>= 1 any ring size 9	0.0753926
Q9GZN0	567	O-C-C-O	0.075296
Q9GZN0	593	N-C-C-C-N	0.0746469

Q9GZN0	828	OC1C(Br)CCCC1	0.0741974
Q9GZN0	612	N-C-O-C-C	0.0722725
Q9GZN0	643	[#1]-C-C-N-[#1]	0.0696311
Q9GZN0	521	C:N-C-[#1]	0.069568
Q9GZN0	857	ClC1CC(Cl)CC1	0.0678657
Q9GZN0	242	>= 1 saturated or aromatic carbon-only ring size 9	0.067555
Q9GZN0	782	OC1CCC(O)CC1	0.0653355
Q9GZN0	67	>= 1 Kr	0.0620595
Q9GZN0	633	N-C-C:C-C	0.0616422
Q9GZN0	664	C-C=C-C=C	0.0614327
Q9GZN0	802	CC1CC(Br)CCC1	0.0611829
Q9GZN0	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0601967
Q9GZN0	460	C-C-C#C	0.0598697
Q9GZN0	257	>= 2 aromatic rings	0.0593484
Q9GZN0	615	N-C-C-O-C	0.0589115
Q9GZN0	274	B-C	0.0581831
Q9GZN0	336	C(~C)(~C)(~C)(~N)	0.057716
Q9GZN0	8	>= 4 B	0.0570552
Q9GZN0	17	>= 8 N	0.056879
Q9GZN0	798	CC1CC(O)CCC1	0.056598
Q9GZN0	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	0.0564808
Q9GZN0	438	C(-C)(-N)(=N)	0.0555053
Q9GZN0	832	SC1C(Br)CCCC1	0.0546153
Q9GZN0	472	C:N:C-C	0.0538823
Q9GZN0	761	Oc1c(O)cccc1	0.0530703
Q9GZN0	227	>= 1 any ring size 8	0.0522286
Q9GZN0	69	>= 1 Sr	0.052119
Q9GZN0	637	O-C-C-C-C	0.0519458
Q9GZN0	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.0516953
Q9GZN0	412	S(~C)(~C)	0.0506465
Q9GZN0	12	>= 16 C	0.0500144
Q9GZN0	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0492601
Q9GZN0	502	N-C=C-[#1]	0.049045
Q9GZN0	27	>= 2 Na	0.0487742
Q9GZN0	115	>= 1 any ring size 3	0.0486717
Q9GZN0	447	C(-H)(=N)	0.0484834
Q9GZN0	341	C(~C)(~C)(~O)	0.0472175
Q9GZN0	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	0.0470235
Q9GZN0	738	Cc1cc(Cl)ccc1	0.0457812
Q9GZN0	61	>= 1 Cu	0.0446079
Q9GZN0	113	>= 1 Tc	0.0444659
Q9GZN0	851	SC1CC(N)CC1	0.0441761
Q9GZN0	478	S-C=N-[#1]	0.0437125
Q9GZN0	92	>= 1 Ir	0.0432842
Q9GZN0	299	N-H	0.0432355
Q9GZN0	367	C(~H)(~O)(~O)	0.0430363

Q9GZN0	296	C-Se	0.0428647
Q9GZN0	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.0425932
Q9GZN0	444	C(-Cl)(=O)	0.0424253
Q9GZN0	100	>= 1 Ce	0.0421278
Q9GZN0	281	B-Cl	0.0421055
Q9GZN0	213	>= 1 any ring size 7	0.042046
Q9GZN0	271	Li-Cl	0.0414763
Q9GZN0	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0413027
Q9GZN0	57	>= 1 Mn	0.0408898
Q9GZN0	577	C:C-N-C:C	0.0404372
Q9GZN0	550	Cl-C-C-C	0.0402902
Q9GZN0	867	OC1C(S)CCC1	0.0402366
Q9GZN0	378	C(~N)(:C)(:N)	0.0387088
Q9GZN0	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.0380984
Q9GZN0	681	O-C-C-C-C-O	0.0380815
Q9GZN0	842	CC1CC(N)CC1	0.038065
Q9GZN0	757	Cc1c(S)cccc1	0.0375297
Q9GZN0	784	OC1CCC(N)CC1	0.0371629
Q9GZN0	425	P=O	0.0359466
Q9GZN0	85	>= 1 Ba	0.0352724
Q9GZN0	506	C-C:N:C	0.0338386
Q9GZN0	517	N-N-C-N	0.0337374
Q9GZN0	356	C(~C)(:C)(:C)	0.0337185
Q9GZN0	330	C(~Br)(:C)	0.0335444
Q9GZN0	317	F-S	0.0332418
Q9GZN0	355	C(~C)(:C)	0.0328494
Q9GZN0	532	S-C:C-[#1]	0.0324677
Q9GZN0	701	O-C-C-C-C-C(O)-C	0.0313256
Q9GZN0	4	>= 1 Li	0.0311906
Q9GZN0	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0292564
Q9GZN0	813	NC1CC(Cl)CCC1	0.02811
Q9GZN0	143	>= 1 any ring size 5	0.0280524
Q9GZN0	747	Sc1cc(Cl)ccc1	0.0277055
Q9GZN0	422	N=N	0.0272433
Q9GZN0	624	O=C-C:C-N	0.0268755
Q9GZN0	408	O(~H)(~S)	0.0256326
Q9GZN0	255	>= 1 aromatic ring	0.0251983
Q9GZN0	309	O-O	0.0246953
Q9GZN0	684	O=C-C-C-C-C	0.0246245
Q9GZN0	283	C-H	0.0245406
Q9GZN0	653	O-C:C:C-O	0.0244621
Q9GZN0	639	O-C-C-C-O	0.0238063
Q9GZN0	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.0237469
Q9GZN0	228	>= 1 saturated or aromatic carbon-only ring size 8	0.0234666
Q9GZN0	607	N-C-C-C:C	0.023368
Q9GZN0	555	N=C-C=C	0.0232681

Q9GZN0	537	O=C-C-O	0.0228045
Q9GZN0	311	O-Na	0.022506
Q9GZN0	41	>= 1 K	0.0221883
Q9GZN0	717	Cc1ccc(Cl)cc1	0.0220689
Q9GZN0	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.0216291
Q9GZN0	206	>= 5 any ring size 6	0.0215552
Q9GZN0	288	C-Na	0.0215056
Q9GZN0	833	NC1C(N)CCCC1	0.0213159
Q9GZN0	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.0213063
Q9GZN0	752	Clc1cc(Cl)ccc1	0.0211084
Q9GZN0	270	Li-S	0.0210711
Q9GZN0	235	>= 2 saturated or aromatic carbon-only ring size 8	0.0209312
Q9GZN0	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	0.02092
Q9GZN0	770	Nc1c(N)cccc1	0.020288
Q9GZN0	799	CC1CC(S)CCC1	0.0198438
Q9GZN0	372	C(~H)(:C)(:N)	0.0195969
Q9GZN0	34	>= 2 S	0.0192486
Q9GZN0	488	N-C=N-[#1]	0.0188212
Q9GZN0	878	ClC1C(Cl)CCC1	0.0181274
Q9GZN0	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0177849
Q9GZN0	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0176635
Q9GZN0	749	Nc1cc(N)ccc1	0.0173197
Q9GZN0	625	O=C-C:C-O	0.0170654
Q9GZN0	531	S-C:C-C	0.0168318
Q9GZN0	261	>= 4 aromatic rings	0.0160311
Q9GZN0	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.0160116
Q9GZN0	801	CC1CC(Cl)CCC1	0.0143267
Q9GZN0	810	SC1CC(Cl)CCC1	0.0132507
Q9GZN0	99	>= 1 La	0.0130673
Q9GZN0	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	0.0127087
Q9GZN0	319	Al-Cl	0.0126684
Q9GZN0	691	O-C-C-C-C-C-N	0.0125942
Q9GZN0	704	O=C-C-C-C-C-C-C	0.0123995
Q9GZN0	78	>= 1 Cd	0.0122825
Q9GZN0	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	0.0120392
Q9GZN0	819	CC1C(O)CCCC1	0.0119063
Q9GZN0	683	N-C-C-C-C-C	0.011532
Q9GZN0	696	C-C-C-C-C-C-C-C	0.0112671
Q9GZN0	571	[#1]-C-O-[#1]	0.011264
Q9GZN0	708	C-C(C)-C-C	0.0106301
Q9GZN0	443	C(-C)(=O)	0.010471
Q9GZN0	528	[#1]-N-C-[#1]	0.0098634
Q9GZN0	741	Oc1cc(S)ccc1	0.0096999
Q9GZN0	669	Cl-C:C-C=O	0.0095215
Q9GZN0	709	C-C(C)-C-C-C	0.0085812
Q9GZN0	620	C:C-O-C-C	0.0083906

Q9GZN0	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	0.0082452
Q9GZN0	586	C-S-C-C-C	0.0081575
Q9GZN0	33	>= 1 S	0.0081108
Q9GZN0	448	C(-H)(=O)	0.0080068
Q9GZN0	785	OC1CCC(Cl)CC1	0.0079457
Q9GZN0	343	C(~C)(~Cl)(~H)	0.0075849
Q9GZN0	318	Al-H	0.0074445
Q9GZN0	171	>= 5 any ring size 5	0.0073878
Q9GZN0	60	>= 1 Ni	0.0071853
Q9GZN0	70	>= 1 Y	0.0068327
Q9GZN0	403	N(:C)(:C)	0.0065994
Q9GZN0	647	O=C-N-C-N	0.0065928
Q9GZN0	565	C:C-O-C	0.006573
Q9GZN0	455	N(-O)(=O)	0.0063032
Q9GZN0	86	>= 1 Lu	0.0062813
Q9GZN0	668	C-C:C-C-C	0.0062334
Q9GZN0	804	OC1CC(S)CCC1	0.0062192
Q9GZN0	500	C-S-C:C	0.0061774
Q9GZN0	644	C-C=N-N-C	0.0061353
Q9GZN0	358	C(~C)(:N)	0.0060533
Q9GZN0	335	C(~C)(~C)(~C)(~H)	0.0058003
Q9GZN0	432	C(-C)(-C)(=O)	0.0057804
Q9GZN0	360	C(~Cl)(~Cl)	0.0054357
Q9GZN0	479	S-C-S-C	0.0052484
Q9GZN0	812	NC1CC(N)CCC1	0.0051961
Q9GZN0	354	C(~C)(~Si)	0.0050594
Q9GZN0	530	N:C-C:C	0.0049041
Q9GZN0	493	O=C-C:C	0.004883
Q9GZN0	552	C:C-C:C	0.0046835
Q9GZN0	470	C:C-C=C	0.0046834
Q9GZN0	308	O-H	0.0045659
Q9GZN0	302	N-F	0.0045524
Q9GZN0	665	N-C:C-C-C	0.0044828
Q9GZN0	705	O=C-C-C-C-C(O)-C	0.0043679
Q9GZN0	509	Br-C:C-C	0.0043557
Q9GZN0	50	>= 1 Mg	0.0043223
Q9GZN0	465	O=S-C-C	0.0040758
Q9GZN0	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.0040668
Q9GZN0	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	0.0038343
Q9GZN0	73	>= 1 Mo	0.0037628
Q9GZN0	446	C(-H)(=C)	0.003629
Q9GZN0	745	Sc1cc(S)ccc1	0.0034057
Q9GZN0	397	N(~C)(:C)(:C)	0.0032702
Q9GZN0	310	O-Mg	0.0032552
Q9GZN0	856	NC1CC(Br)CC1	0.0031484
Q9GZN0	401	N(~O)(~O)	0.0031363

Q9GZN0	483	N-S-C:C	0.0028472
Q9GZN0	726	Sc1ccc(Cl)cc1	0.0021428
Q9GZN0	794	ClC1CCC(Cl)CC1	0.0021353
Q9GZN0	848	OC1CC(Cl)CC1	0.0018499
Q9GZN0	353	C(~C)(~S)	0.0018229
Q9GZN0	564	C=C-C=C	0.0017299
Q9GZN0	306	N-Cl	0.0017092
Q9GZN0	796	BrC1CCC(Br)CC1	0.0016281
Q9GZN0	730	Nc1ccc(Br)cc1	0.0016089
Q9GZN0	661	O-C-O-C-C	0.0015086
Q9GZN0	406	O(~C)(~H)	0.001386
Q9GZN0	498	O-C=C-C	0.0013738
Q9GZN0	340	C(~C)(~C)(~N)	0.0012664
Q9GZN0	609	Cl-C-C-N-C	0.0012439
Q9GZN0	645	O=C-N-C-C	0.0010812
Q9GZN0	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.0009449
Q9GZN0	663	O-C-C-O-[#1]	0.0008329
Q9GZN0	43	>= 1 Br	0.0008091
Q9GZN0	327	C(~Br)(~C)	0.0008089
Q9GZN0	825	OC1C(S)CCCC1	0.0007631
Q9GZN0	838	BrC1C(Br)CCCC1	0.0007102
Q9GZN0	536	O=C-C-N	0.0006766
Q9GZN0	534	S-C:C-O	0.0006726
Q9GZN0	344	C(~C)(~H)	0.0005354
Q9GZN0	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0004529
Q9GZN0	563	O-C-O-C	0.0004509
Q9GZN0	481	O-S-C:C	0.0004502
Q9GZN0	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	0.0003679
Q9GZN0	303	N-Si	0.0003449
Q9GZN0	621	N-C:C:C:N	0.0002753
Q9GZN0	561	Cl-C-C=O	0.0002503
Q9GZN0	670	Br-C:C:C-C	9.02E-05
Q9GZN0	47	>= 2 I	2.96E-05
Q9GZN0	807	OC1CC(Br)CCC1	5.08E-07
Q9GZN0	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	3.85E-07
Q9GZN0	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	1.95E-07
Q9GZN0	29	>= 2 Si	9.15E-08
Q9GZN0	249	>= 1 saturated or aromatic carbon-only ring size 10	5.70E-08
Q9GZN0	79	>= 1 In	4.92E-08
Q9GZN0	837	ClC1C(Br)CCCC1	-2.56E-08
Q9GZN0	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	-2.95E-08
Q9GZN0	80	>= 1 Sn	-5.84E-08
Q9GZN0	56	>= 1 Cr	-8.40E-08
Q9GZN0	258	>= 2 hetero-aromatic rings	-1.08E-07
Q9GZN0	775	Brc1c(Br)cccc1	-1.18E-07
Q9GZN0	28	>= 1 Si	-1.25E-07

Q9GZN0	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	-1.27E-07
Q9GZN0	75	>= 1 Rh	-1.30E-07
Q9GZN0	268	Li-F	-1.73E-07
Q9GZN0	200	>= 4 saturated or aromatic carbon-only ring size 6	-2.01E-07
Q9GZN0	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	-3.02E-07
Q9GZN0	186	>= 2 saturated or aromatic carbon-only ring size 6	-1.65E-05
Q9GZN0	861	CC1C(O)CCC1	-2.59E-05
Q9GZN0	137	>= 2 saturated or aromatic carbon-only ring size 4	-7.12E-05
Q9GZN0	348	C(~C)(~H)(~P)	-8.33E-05
Q9GZN0	699	O-C-C-C-C-C(C)-C	-9.95E-05
Q9GZN0	780	CC1CCC(Cl)CC1	-0.000177
Q9GZN0	112	>= 1 Yb	-0.000258
Q9GZN0	442	C(-C)(=N)	-0.00027
Q9GZN0	394	N(~C)(~H)(~N)	-0.000317
Q9GZN0	732	Clc1ccc(Br)cc1	-0.000322
Q9GZN0	736	Cc1cc(S)ccc1	-0.000495
Q9GZN0	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	-0.000545
Q9GZN0	843	CC1CC(Cl)CC1	-0.000568
Q9GZN0	456	P(-O)(=O)	-0.000642
Q9GZN0	628	C-N-C-C:C	-0.000724
Q9GZN0	89	>= 1 W	-0.000772
Q9GZN0	220	>= 2 any ring size 7	-0.000844
Q9GZN0	849	OC1CC(Br)CC1	-0.000868
Q9GZN0	291	C-Si	-0.000877
Q9GZN0	325	As-H	-0.000881
Q9GZN0	313	O-Si	-0.000982
Q9GZN0	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	-0.001133
Q9GZN0	81	>= 1 Sb	-0.00117
Q9GZN0	554	Br-C-C-C	-0.001237
Q9GZN0	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	-0.001273
Q9GZN0	295	C-As	-0.001316
Q9GZN0	742	Oc1cc(N)ccc1	-0.001459
Q9GZN0	314	O-P	-0.001583
Q9GZN0	820	CC1C(S)CCCC1	-0.001656
Q9GZN0	764	Oc1c(Cl)cccc1	-0.001789
Q9GZN0	413	S(~C)(~H)	-0.00181
Q9GZN0	556	C=C-C-C	-0.002025
Q9GZN0	111	>= 1 Tm	-0.002083
Q9GZN0	48	>= 4 I	-0.00226
Q9GZN0	320	Si-H	-0.002277
Q9GZN0	482	C:N-C:C	-0.002286
Q9GZN0	436	C(-C)(-H)(=O)	-0.002346
Q9GZN0	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	-0.002613
Q9GZN0	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	-0.002638
Q9GZN0	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	-0.002673
Q9GZN0	719	Oc1ccc(O)cc1	-0.002737

Q9GZN0	480	C:S:C-C	−0.002892
Q9GZN0	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.003018
Q9GZN0	570	C:C-C-C	−0.003096
Q9GZN0	547	N-C:C-N	−0.003172
Q9GZN0	827	OC1C(Cl)CCCC1	−0.003216
Q9GZN0	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−0.003656
Q9GZN0	45	>= 4 Br	−0.004004
Q9GZN0	490	C-C-C=C	−0.004087
Q9GZN0	608	C-C-C-C:C	−0.004145
Q9GZN0	727	Sc1ccc(Br)cc1	−0.00432
Q9GZN0	53	>= 1 Sc	−0.004358
Q9GZN0	673	O=C-C=C-N	−0.004406
Q9GZN0	763	Oc1c(N)cccc1	−0.004432
Q9GZN0	830	SC1C(N)CCCC1	−0.004475
Q9GZN0	505	Cl-C:C-O	−0.004512
Q9GZN0	297	C-Br	−0.004695
Q9GZN0	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.004826
Q9GZN0	1	>= 8 H	−0.005053
Q9GZN0	873	SC1C(Cl)CCC1	−0.005055
Q9GZN0	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	−0.005174
Q9GZN0	349	C(~C)(~H)(~S)	−0.005212
Q9GZN0	739	Cc1cc(Br)ccc1	−0.005285
Q9GZN0	64	>= 1 Ge	−0.005303
Q9GZN0	42	>= 2 K	−0.005337
Q9GZN0	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	−0.005396
Q9GZN0	826	OC1C(N)CCCC1	−0.005474
Q9GZN0	484	N-C:N:C	−0.005529
Q9GZN0	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	−0.005537
Q9GZN0	751	Nc1cc(Br)ccc1	−0.005538
Q9GZN0	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	−0.005951
Q9GZN0	404	N(:C)(:C)(:C)	−0.006134
Q9GZN0	602	O=C-C-N-C	−0.006229
Q9GZN0	379	C(~N)(:N)	−0.006253
Q9GZN0	450	C(-N)(=N)	−0.00627
Q9GZN0	815	ClC1CC(Cl)CCC1	−0.006273
Q9GZN0	809	SC1CC(N)CCC1	−0.006344
Q9GZN0	507	C-C-S-C	−0.006364
Q9GZN0	473	S-C:N:C	−0.006378
Q9GZN0	428	C(#C)(-H)	−0.00649
Q9GZN0	516	[#1]-C=C-[#1]	−0.006655
Q9GZN0	572	N:C:N:C	−0.006748
Q9GZN0	392	N(~C)(~C)(~H)	−0.006756
Q9GZN0	603	C-C:C:C-C	−0.006975
Q9GZN0	376	C(~N)(:C)	−0.007374
Q9GZN0	104	>= 1 Sm	−0.007405
Q9GZN0	655	O-C-C-C:C	−0.007924

Q9GZN0	411	P(~O)(~O)	−0.008113
Q9GZN0	520	C=C-C:C	−0.008257
Q9GZN0	14	>= 1 N	−0.00826
Q9GZN0	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.008287
Q9GZN0	97	>= 1 Pb	−0.008292
Q9GZN0	875	NC1C(N)CCC1	−0.008432
Q9GZN0	636	C-N-C-N-C	−0.008476
Q9GZN0	301	N-O	−0.009409
Q9GZN0	512	C-[As]-O-[#1]	−0.010023
Q9GZN0	613	C-N-C-C-C	−0.011073
Q9GZN0	66	>= 1 Se	−0.011241
Q9GZN0	656	C-C-N-C-C	−0.01146
Q9GZN0	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.011597
Q9GZN0	591	Cl-C-C-C-C	−0.011851
Q9GZN0	382	C(~O)(:C)(:C)	−0.011952
Q9GZN0	676	N#C-C-C-C	−0.012144
Q9GZN0	304	N-P	−0.012392
Q9GZN0	786	OC1CCC(Br)CC1	−0.012495
Q9GZN0	529	Cl-C-C-Cl	−0.012623
Q9GZN0	466	N#C-C=C	−0.012662
Q9GZN0	748	Sc1cc(Br)ccc1	−0.012785
Q9GZN0	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.012903
Q9GZN0	469	S-S-C:C	−0.012908
Q9GZN0	560	N-C-N-C	−0.012955
Q9GZN0	150	>= 2 any ring size 5	−0.013112
Q9GZN0	703	O-C-C-C-C-C(N)-C	−0.013446
Q9GZN0	712	C-C(C)-C(C)-C	−0.013963
Q9GZN0	59	>= 1 Co	−0.014364
Q9GZN0	44	>= 2 Br	−0.014434
Q9GZN0	789	SC1CCC(Cl)CC1	−0.014973
Q9GZN0	692	O=C-C-C-C-C-C	−0.015056
Q9GZN0	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	−0.015168
Q9GZN0	721	Oc1ccc(N)cc1	−0.015714
Q9GZN0	369	C(~H)(~Si)	−0.016535
Q9GZN0	508	S=C-N-C	−0.016561
Q9GZN0	272	B-H	−0.01687
Q9GZN0	74	>= 1 Ru	−0.016919
Q9GZN0	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.016928
Q9GZN0	165	>= 4 saturated or aromatic carbon-only ring size 5	−0.017895
Q9GZN0	729	Nc1ccc(Cl)cc1	−0.018053
Q9GZN0	339	C(~C)(~C)(~H)(~O)	−0.018401
Q9GZN0	524	C-C=C-C	−0.018436
Q9GZN0	207	>= 5 saturated or aromatic carbon-only ring size 6	−0.018478
Q9GZN0	527	C:C:N-[#1]	−0.01856
Q9GZN0	677	C-C=C-C:C	−0.018952
Q9GZN0	824	OC1C(O)CCCC1	−0.019083

Q9GZN0	503	Cl-C:C-[#1]	−0.019208
Q9GZN0	347	C(~C)(~H)(~O)(~O)	−0.019435
Q9GZN0	52	>= 1 Ca	−0.019841
Q9GZN0	598	Cl-C:C:C-C	−0.020336
Q9GZN0	518	O=C-N-N	−0.020497
Q9GZN0	68	>= 1 Rb	−0.020725
Q9GZN0	548	O-C-C:C	−0.020824
Q9GZN0	279	B-P	−0.021073
Q9GZN0	753	Clc1cc(Br)ccc1	−0.021097
Q9GZN0	803	OC1CC(O)CCC1	−0.021177
Q9GZN0	370	C(~H)(:C)	−0.021189
Q9GZN0	316	F-P	−0.021735
Q9GZN0	816	ClC1CC(Br)CCC1	−0.021814
Q9GZN0	46	>= 1 I	−0.021921
Q9GZN0	700	O-C-C-C-C-C-O-C	−0.022108
Q9GZN0	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.022972
Q9GZN0	0	>= 4 H	−0.023023
Q9GZN0	659	O-C-C-N-C	−0.023655
Q9GZN0	275	B-N	−0.023847
Q9GZN0	499	N-C:C:N	−0.024413
Q9GZN0	305	N-S	−0.024429
Q9GZN0	880	BrC1C(Br)CCC1	−0.024472
Q9GZN0	718	Cc1ccc(Br)cc1	−0.025461
Q9GZN0	282	B-Br	−0.026435
Q9GZN0	758	Cc1c(N)cccc1	−0.026597
Q9GZN0	337	C(~C)(~C)(~C)(~O)	−0.026902
Q9GZN0	762	Oc1c(S)cccc1	−0.027203
Q9GZN0	324	P-P	−0.029032
Q9GZN0	580	O=C-C-C-N	−0.029033
Q9GZN0	464	N-C-C=C	−0.029891
Q9GZN0	657	C-N-C:C-C	−0.030564
Q9GZN0	415	Si(~C)(~C)	−0.030686
Q9GZN0	110	>= 1 Er	−0.032089
Q9GZN0	674	N-C-N-C:C	−0.032119
Q9GZN0	579	O=C-C-C-C	−0.03216
Q9GZN0	697	C-C-C-C-C-C(C)-C	−0.032848
Q9GZN0	9	>= 2 C	−0.034277
Q9GZN0	710	C-C-C(C)-C-C	−0.034625
Q9GZN0	492	N-C:O:C	−0.034736
Q9GZN0	594	C-O-C-C=C	−0.035534
Q9GZN0	790	SC1CCC(Br)CC1	−0.036518
Q9GZN0	865	CC1C(Br)CCC1	−0.036965
Q9GZN0	760	Cc1c(Br)cccc1	−0.037009
Q9GZN0	606	O-C:C-C-C	−0.037136
Q9GZN0	626	C-O-C:C-C	−0.038504
Q9GZN0	783	OC1CCC(S)CC1	−0.038736

Q9GZN0	37	>= 1 Cl	−0.039305
Q9GZN0	3	>= 32 H	−0.039511
Q9GZN0	544	O-C:C-O	−0.039602
Q9GZN0	10	>= 4 C	−0.039732
Q9GZN0	642	O-C-C-C=O	−0.03982
Q9GZN0	829	SC1C(S)CCCC1	−0.040303
Q9GZN0	234	>= 2 any ring size 8	−0.040313
Q9GZN0	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.040579
Q9GZN0	40	>= 8 Cl	−0.041135
Q9GZN0	256	>= 1 hetero-aromatic ring	−0.041286
Q9GZN0	787	SC1CCC(S)CC1	−0.041353
Q9GZN0	402	N(~O)(:O)	−0.041509
Q9GZN0	526	Cl-C:C-Cl	−0.042414
Q9GZN0	94	>= 1 Au	−0.04251
Q9GZN0	879	ClC1C(Br)CCC1	−0.042524
Q9GZN0	510	[#1]-N-N-[#1]	−0.042665
Q9GZN0	352	C(~C)(~O)	−0.042967
Q9GZN0	332	C(~C)(~C)	−0.043324
Q9GZN0	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	−0.043427
Q9GZN0	276	B-O	−0.043681
Q9GZN0	876	NC1C(Cl)CC1	−0.043732
Q9GZN0	157	>= 3 any ring size 5	−0.043974
Q9GZN0	420	C=O	−0.04489
Q9GZN0	285	C-N	−0.045529
Q9GZN0	740	Oc1cc(O)ccc1	−0.046482
Q9GZN0	855	NC1CC(Cl)CC1	−0.047995
Q9GZN0	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.04812
Q9GZN0	326	As-As	−0.049047
Q9GZN0	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	−0.05277
Q9GZN0	487	N-C=N-C	−0.053142
Q9GZN0	286	C-O	−0.05364
Q9GZN0	713	Cc1ccc(C)cc1	−0.05449
Q9GZN0	767	Sc1c(N)cccc1	−0.055732
Q9GZN0	871	SC1C(S)CCC1	−0.05597
Q9GZN0	658	C-C-S-C-C	−0.057016
Q9GZN0	416	C=C	−0.057914
Q9GZN0	541	O-C:C-C	−0.057917
Q9GZN0	136	>= 2 any ring size 4	−0.058402
Q9GZN0	476	C-O-C=C	−0.059373
Q9GZN0	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.060946
Q9GZN0	778	CC1CCC(S)CC1	−0.060999
Q9GZN0	362	C(~Cl)(:C)	−0.061351
Q9GZN0	262	>= 4 hetero-aromatic rings	−0.061363
Q9GZN0	359	C(~C)(:N)(:N)	−0.062585
Q9GZN0	357	C(~C)(:C)(:N)	−0.063266
Q9GZN0	822	CC1C(Cl)CCCC1	−0.064504

Q9GZN0	590	C-C:C-O-[#1]	−0.065218
Q9GZN0	265	Li-B	−0.065891
Q9GZN0	366	C(~H)(~O)	−0.066467
Q9GZN0	383	C(~S)(:C)	−0.066616
Q9GZN0	862	CC1C(S)CCC1	−0.066804
Q9GZN0	83	>= 1 Xe	−0.067201
Q9GZN0	672	O=C-C=C-[#1]	−0.067444
Q9GZN0	11	>= 8 C	−0.067608
Q9GZN0	686	O=C-C-C-C-O	−0.069013
Q9GZN0	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.070493
Q9GZN0	840	CC1CC(O)CC1	−0.072465
Q9GZN0	458	S(-O)(=O)	−0.072708
Q9GZN0	605	O=C-C-O-C	−0.076108
Q9GZN0	844	CC1CC(Br)CC1	−0.076414
Q9GZN0	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.077148
Q9GZN0	49	>= 1 Be	−0.077554
Q9GZN0	103	>= 1 Pm	−0.077991
Q9GZN0	805	OC1CC(N)CCC1	−0.078013
Q9GZN0	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.078473
Q9GZN0	649	O=N-C:C-O	−0.079444
Q9GZN0	863	CC1C(N)CCC1	−0.079653
Q9GZN0	16	>= 4 N	−0.080819
Q9GZN0	2	>= 16 H	−0.081336
Q9GZN0	617	C-C-C-O-[#1]	−0.081466
Q9GZN0	58	>= 1 Fe	−0.081625
Q9GZN0	264	Li-Li	−0.082259
Q9GZN0	434	C(-C)(-H)(=C)	−0.083567
Q9GZN0	623	O=C-C:C-C	−0.084075
Q9GZN0	850	SC1CC(S)CC1	−0.085264
Q9GZN0	766	Sc1c(S)cccc1	−0.086117
Q9GZN0	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	−0.088494
Q9GZN0	539	N=C-C-[#1]	−0.08904
Q9GZN0	300	N-N	−0.089279
Q9GZN0	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.090662
Q9GZN0	106	>= 1 Gd	−0.093146
Q9GZN0	307	N-Br	−0.094898
Q9GZN0	558	O=N-C:C	−0.096633
Q9GZN0	610	C-O-C-O-C	−0.097233
Q9GZN0	38	>= 2 Cl	−0.097692
Q9GZN0	584	C:C-C=C-C	−0.098208
Q9GZN0	793	NC1CCC(Br)CC1	−0.099582
Q9GZN0	706	O=C-C-C-C-C(=O)-C	−0.100337
Q9GZN0	459	S(=O)(=O)	−0.100347
Q9GZN0	845	OC1CC(O)CC1	−0.100383
Q9GZN0	22	>= 16 O	−0.103121
Q9GZN0	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.103169

Q9GZN0	361	C(~Cl)(~H)	−0.103644
Q9GZN0	328	C(~Br)(~C)(~C)	−0.105666
Q9GZN0	19	>= 2 O	−0.10699
Q9GZN0	707	O=C-C-C-C-C(N)-C	−0.107231
Q9GZN0	391	N(~C)(~C)(~C)	−0.10908
Q9GZN0	652	O-C:C:C-N	−0.110108
Q9GZN0	671	O=C-C=C-C	−0.110158
Q9GZN0	26	>= 1 Na	−0.111099
Q9GZN0	566	O-C-C-N	−0.111358
Q9GZN0	90	>= 1 Re	−0.111504
Q9GZN0	525	[As]-C:C-[#1]	−0.111629
Q9GZN0	858	ClC1CC(Br)CC1	−0.111839
Q9GZN0	485	N:C:C:N	−0.113082
Q9GZN0	542	O-C:C-[#1]	−0.114
Q9GZN0	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	−0.114906
Q9GZN0	504	N:C:N-C	−0.115022
Q9GZN0	259	>= 3 aromatic rings	−0.118164
Q9GZN0	731	Clc1ccc(Cl)cc1	−0.118914
Q9GZN0	331	C(~Br)(:N)	−0.119335
Q9GZN0	84	>= 1 Cs	−0.119993
Q9GZN0	433	C(-C)(-Cl)(=O)	−0.12115
Q9GZN0	54	>= 1 Ti	−0.121918
Q9GZN0	806	OC1CC(Cl)CCC1	−0.122031
Q9GZN0	781	CC1CCC(Br)CC1	−0.122336
Q9GZN0	733	Brc1ccc(Br)cc1	−0.124243
Q9GZN0	423	N=O	−0.124565
Q9GZN0	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	−0.124568
Q9GZN0	439	C(-C)(-N)(=O)	−0.124752
Q9GZN0	280	B-S	−0.127011
Q9GZN0	836	ClC1C(Cl)CCCC1	−0.127101
Q9GZN0	776	CC1CCC(C)CC1	−0.127638
Q9GZN0	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.127997
Q9GZN0	468	O=S-C-N	−0.129172
Q9GZN0	746	Sc1cc(N)ccc1	−0.129288
Q9GZN0	750	Nc1cc(Cl)ccc1	−0.129393
Q9GZN0	62	>= 1 Zn	−0.129807
Q9GZN0	754	Brc1cc(Br)ccc1	−0.129941
Q9GZN0	289	C-Mg	−0.130166
Q9GZN0	496	N:N-C-[#1]	−0.130747
Q9GZN0	859	BrC1CC(Br)CC1	−0.131182
Q9GZN0	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	−0.131186
Q9GZN0	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.132097
Q9GZN0	486	N-C:N:N	−0.132441
Q9GZN0	711	C-C(C)(C)-C-C	−0.132928
Q9GZN0	854	NC1CC(N)CC1	−0.133172
Q9GZN0	557	N:C-O-[#1]	−0.133207

Q9GZN0	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.13353
Q9GZN0	82	>= 1 Te	−0.133607
Q9GZN0	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.133729
Q9GZN0	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.133867
Q9GZN0	426	P=P	−0.133972
Q9GZN0	333	C(~C)(~C)(~C)	−0.136115
Q9GZN0	543	O-C:C-N	−0.138804
Q9GZN0	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.141677
Q9GZN0	724	Sc1ccc(S)cc1	−0.142896
Q9GZN0	312	O-Al	−0.143042
Q9GZN0	393	N(~C)(~H)	−0.143724
Q9GZN0	759	Cc1c(Cl)cccc1	−0.146199
Q9GZN0	589	C-C:C-O-C	−0.147175
Q9GZN0	501	Cl-C:C-C	−0.149961
Q9GZN0	421	C=S	−0.150435
Q9GZN0	679	C-C-C-C-C-C	−0.153891
Q9GZN0	597	O=C-C-C:C	−0.15432
Q9GZN0	410	P(~C)(~C)	−0.154627
Q9GZN0	351	C(~C)(~N)	−0.155612
Q9GZN0	545	N-C:C-C	−0.156433
Q9GZN0	284	C-C	−0.15983
Q9GZN0	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.16225
Q9GZN0	611	N-C-C-N-C	−0.164081
Q9GZN0	619	O-C-C=C-C	−0.164425
Q9GZN0	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.166073
Q9GZN0	654	N-C-N-C-C	−0.167552
Q9GZN0	682	O-C-C-C-C-N	−0.167595
Q9GZN0	178	>= 1 any ring size 6	−0.169187
Q9GZN0	744	Oc1cc(Br)ccc1	−0.170019
Q9GZN0	667	C=C-C-O-[#1]	−0.171907
Q9GZN0	461	O-C-C=N	−0.174375
Q9GZN0	601	N-C:C:C-N	−0.17747
Q9GZN0	743	Oc1cc(Cl)ccc1	−0.178167
Q9GZN0	13	>= 32 C	−0.183453
Q9GZN0	24	>= 2 F	−0.18492
Q9GZN0	342	C(~C)(~Cl)	−0.185502
Q9GZN0	437	C(-C)(-N)(=C)	−0.186438
Q9GZN0	91	>= 1 Os	−0.188001
Q9GZN0	453	N(-C)(=C)	−0.190721
Q9GZN0	797	CC1CC(C)CCC1	−0.190857
Q9GZN0	588	O=C-C-C=O	−0.191378
Q9GZN0	630	O-C:C-O-C	−0.191904
Q9GZN0	546	N-C:C-[#1]	−0.19464
Q9GZN0	477	N-N-C:C	−0.197801
Q9GZN0	604	C-O-C-C:C	−0.199698
Q9GZN0	576	N=C-C:C-[#1]	−0.201923

Q9GZN0	635	N-N-C-N-[#1]	−0.202358
Q9GZN0	648	O=N-C:C-N	−0.203449
Q9GZN0	553	O=C-C=C	−0.20582
Q9GZN0	475	S-C=N-C	−0.205846
Q9GZN0	641	O-C-C-C=C	−0.209343
Q9GZN0	6	>= 1 B	−0.216135
Q9GZN0	877	NC1C(Br)CCC1	−0.221988
Q9GZN0	821	CC1C(N)CCCC1	−0.226675
Q9GZN0	769	Sc1c(Br)cccc1	−0.230453
Q9GZN0	385	C(:C)(:C)(:C)	−0.232058
Q9GZN0	834	NC1C(Cl)CCCC1	−0.236136
Q9GZN0	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	−0.238054
Q9GZN0	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.23978
Q9GZN0	600	N-C:C-C-C	−0.242263
Q9GZN0	574	O-C-C:C-C	−0.242881
Q9GZN0	374	C(~H)(~H)(~H)	−0.247398
Q9GZN0	533	S-C:C-N	−0.256671
Q9GZN0	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.270516
Q9GZN0	23	>= 1 F	−0.27378
Q9GZN0	388	C(:C)(:N)(:N)	−0.282081
Q9GZN0	414	S(~C)(~O)	−0.283595
Q9GZN0	364	C(~F)(:C)	−0.293894
Q9GZN0	870	OC1C(Br)CCC1	−0.295042
Q9GZN0	535	O=C-C-C	−0.295289
Q9GZN0	755	Cc1c(C)cccc1	−0.295741
Q9GZN0	573	O-C-C=C	−0.314854
Q9GZN0	457	S(-C)(=O)	−0.320202
Q9GZN0	818	CC1C(C)CCCC1	−0.334762
Q9GZN0	31	>= 2 P	−0.336027
Q9GZN0	287	C-F	−0.34412
Q9GZN0	491	C-N:C-[#1]	−0.354018
Q9GZN0	737	Cc1cc(N)ccc1	−0.361459
Q9GZN0	395	N(~C)(~O)	−0.396184
Q9GZN0	792	NC1CCC(Cl)CC1	−0.412057
Q9GZN0	267	Li-O	−0.415665
Q9GZN0	474	S:C:C:N	−0.416554
Q9GZN0	874	SC1C(Br)CCC1	−0.42098
Q9GZN0	587	N-C:C-O-[#1]	−0.423856
Q9GZN0	562	Br-C-C=O	−0.424891
Q9GZN0	293	C-S	−0.430482
Q9GZN0	511	S=C-N-[#1]	−0.446803
Q9GZN0	869	OC1C(Cl)CCC1	−0.45575
Q9GZN0	435	C(-C)(-H)(=N)	−0.461711
Q9GZN0	277	B-F	−0.462023
Q9GZN0	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.473409
Q9GZN0	592	N-C-C-C-C	−0.477554

Q9GZN0	389	C(:N)(:N)	−0.485046
Q9GZN0	429	C(#N)(-C)	−0.495976
Q9GZN0	800	CC1CC(N)CCC1	−0.504962
Q9GZN0	430	C(-C)(-C)(=C)	−0.518651
Q9GZN0	424	N=P	−0.528523
Q9GZN0	549	N-C-C:C	−0.568424
Q9GZN0	390	N(~C)(~C)	−0.577209
Q9GZN0	734	Cc1cc(C)ccc1	−0.585842
Q9GZN0	323	P-H	−0.601752
Q9GZN0	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.602982
Q9GZN0	489	N-C-S-C	−0.60394
Q9GZN0	322	Si-Cl	−0.607687
Q9GZN0	569	N-C-C-N	−0.624122
Q9GZN0	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.628188
Q9GZN0	451	C(-N)(=O)	−0.62944
Q9GZN0	449	C(-N)(=C)	−0.654015
Q9GZN0	698	O-C-C-C-C-C-C-C	−0.654995
Q9GZN0	690	O-C-C-C-C-C-O	−0.655137
Q9GZN0	514	O-N-C-C	−0.655997
Q9GZN0	629	S-C:C:C-N	−0.681949
Q9GZN0	350	C(~C)(~I)	−0.695697
Q9GZN0	582	C-C-C-C-C	−0.719117
Q9GZN0	399	N(~H)(:C)	−0.723681
Q9GZN0	622	O=C-O-C:C	−0.724555
Q9GZN0	405	O(~C)(~C)	−0.727656
Q9GZN0	377	C(~N)(:C)(:C)	−0.734117
Q9GZN0	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	−0.737537
Q9GZN0	650	O=C-N-C=O	−0.755135
Q9GZN0	21	>= 8 O	−0.755812
Q9GZN0	338	C(~C)(~C)(~H)(~N)	−0.756443
Q9GZN0	568	N#C-C-C	−0.764802
Q9GZN0	808	SC1CC(S)CCC1	−0.78367
Q9GZN0	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.784073
Q9GZN0	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	−0.785155
Q9GZN0	868	OC1C(N)CCC1	−0.816487
Q9GZN0	294	C-Cl	−0.886378
Q9GZN0	640	C=C-C-C-C	−0.908614
Q9GZN0	101	>= 1 Pr	−0.915126
Q9GZN0	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.935862
Q9GZN0	63	>= 1 Ga	−0.944795
Q9GZN0	835	NC1C(Br)CCCC1	−0.965742
Q9GZN0	5	>= 2 Li	−1.018482
Q9GZN0	662	O-C-C-O-C	−1.039429
Q9GZN0	77	>= 1 Ag	−1.040582
Q9GZN0	375	C(~N)(~N)	−1.056617
Q9GZN0	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−1.062463

Q9GZN0	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−1.102928
Q9GZN0	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	−1.144725
Q9GZN0	688	C-C-C-C-C-C-C	−1.213073
Q9GZN0	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−1.292478
Q9GZN0	720	Oc1ccc(S)cc1	−1.371066
Q9GZN0	538	N=C-C-C	−1.438168
Q9GZN0	20	>= 4 O	−1.541175
Q9GZN0	260	>= 3 hetero-aromatic rings	−1.711943
Q9GZN0	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−3.243403

Fingerprints（continued)

P	Q
2.0668399	0.0072223
1.9598433	5.16E-07
1.8097985	0.0071618
1.6562303	-0.001596
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-3.243403 -1.43E-07

Data S1. Ranking of importance of substructure features from Pubchem F

GPCR ID	Bit Posit	Bit Substructure	W
Q9HC97	105	>= 1 Eu	2.0456211
Q9HC97	55	>= 1 V	1.4466614
Q9HC97	81	>= 1 Sb	1.3376895
Q9HC97	76	>= 1 Pd	1.2002132
Q9HC97	426	P=P	1.1869253
Q9HC97	851	SC1CC(N)CC1	1.1085605
Q9HC97	107	>= 1 Tb	1.0203086
Q9HC97	570	C:C-C-C	1.0110128
Q9HC97	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	1.0022889
Q9HC97	837	ClC1C(Br)CCCC1	0.9161011
Q9HC97	723	Oc1ccc(Br)cc1	0.7553191
Q9HC97	38	>= 2 Cl	0.7456881
Q9HC97	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.7274727
Q9HC97	242	>= 1 saturated or aromatic carbon-only ring size 9	0.696407
Q9HC97	165	>= 4 saturated or aromatic carbon-only ring size 5	0.6763158
Q9HC97	51	>= 1 Al	0.6279756
Q9HC97	781	CC1CCC(Br)CC1	0.6211061
Q9HC97	92	>= 1 Ir	0.6162188
Q9HC97	100	>= 1 Ce	0.6020752
Q9HC97	591	Cl-C-C-C-C	0.5675983
Q9HC97	548	O-C-C:C	0.5577487
Q9HC97	589	C-C:C-O-C	0.5443795
Q9HC97	541	O-C:C-C	0.5375493
Q9HC97	352	C(~C)(~O)	0.5016753
Q9HC97	693	O=C-C-C-C-C-O	0.490297
Q9HC97	257	>= 2 aromatic rings	0.4860288
Q9HC97	836	ClC1C(Cl)CCCC1	0.4638182
Q9HC97	876	NC1C(Cl)CC1	0.4345246
Q9HC97	701	O-C-C-C-C-C(O)-C	0.4173798
Q9HC97	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	0.4161013
Q9HC97	819	CC1C(O)CCCC1	0.4124745
Q9HC97	11	>= 8 C	0.4099356
Q9HC97	495	C-N-C:C	0.3929358
Q9HC97	681	O-C-C-C-C-O	0.3813323
Q9HC97	653	O-C:C:C-O	0.3811714
Q9HC97	850	SC1CC(S)CC1	0.3795584
Q9HC97	722	Oc1ccc(Cl)cc1	0.3719662
Q9HC97	266	Li-C	0.3529334
Q9HC97	12	>= 16 C	0.3513787
Q9HC97	364	C(~F)(:C)	0.3446151
Q9HC97	45	>= 4 Br	0.3154779
Q9HC97	659	O-C-C-N-C	0.3113955
Q9HC97	523	N:C:C-C	0.3094976
Q9HC97	662	O-C-C-O-C	0.296907

Q9HC97	506	C-C:N:C	0.2959221
Q9HC97	692	O=C-C-C-C-C-C	0.2926905
Q9HC97	489	N-C-S-C	0.2895334
Q9HC97	706	O=C-C-C-C-C(=O)-C	0.2876817
Q9HC97	669	Cl-C:C-C=O	0.280811
Q9HC97	32	>= 4 P	0.2804159
Q9HC97	609	Cl-C-C-N-C	0.2791461
Q9HC97	312	O-Al	0.2746529
Q9HC97	798	CC1CC(O)CCC1	0.2733964
Q9HC97	407	O(~C)(~P)	0.2725609
Q9HC97	455	N(-O)(=O)	0.2695703
Q9HC97	472	C:N:C-C	0.2640128
Q9HC97	760	Cc1c(Br)cccc1	0.2616919
Q9HC97	4	>= 1 Li	0.2606259
Q9HC97	620	C:C-O-C-C	0.2479738
Q9HC97	379	C(~N)(:N)	0.247379
Q9HC97	457	S(-C)(=O)	0.2380474
Q9HC97	631	O-C:C-O-[#1]	0.2253922
Q9HC97	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	0.2225386
Q9HC97	823	CC1C(Br)CCCC1	0.2171476
Q9HC97	336	C(~C)(~C)(~C)(~N)	0.2154177
Q9HC97	452	C(-O)(=O)	0.2144026
Q9HC97	780	CC1CCC(Cl)CC1	0.2133131
Q9HC97	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	0.2129662
Q9HC97	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.2120156
Q9HC97	484	N-C:N:C	0.2095445
Q9HC97	786	OC1CCC(Br)CC1	0.2025796
Q9HC97	683	N-C-C-C-C-C	0.1996469
Q9HC97	327	C(~Br)(~C)	0.1915206
Q9HC97	807	OC1CC(Br)CCC1	0.1843953
Q9HC97	560	N-C-N-C	0.1818591
Q9HC97	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.1773472
Q9HC97	366	C(~H)(~O)	0.1683503
Q9HC97	755	Cc1c(C)cccc1	0.1661957
Q9HC97	270	Li-S	0.1620653
Q9HC97	714	Cc1ccc(O)cc1	0.1620107
Q9HC97	341	C(~C)(~C)(~O)	0.1613038
Q9HC97	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	0.1610193
Q9HC97	20	>= 4 O	0.161002
Q9HC97	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	0.1607195
Q9HC97	856	NC1CC(Br)CC1	0.160201
Q9HC97	775	Brc1c(Br)cccc1	0.1601023
Q9HC97	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	0.1598174
Q9HC97	413	S(~C)(~H)	0.1595861
Q9HC97	46	>= 1 I	0.159436
Q9HC97	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	0.1592926

Q9HC97	380	C(~O)(~O)	0.1589836
Q9HC97	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.1586947
Q9HC97	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	0.1582175
Q9HC97	627	O=[As]-C:C:C	0.1581716
Q9HC97	84	>= 1 Cs	0.1580653
Q9HC97	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	0.1550746
Q9HC97	879	ClC1C(Br)CCC1	0.154608
Q9HC97	326	As-As	0.1543667
Q9HC97	102	>= 1 Nd	0.1536629
Q9HC97	478	S-C=N-[#1]	0.1533528
Q9HC97	779	CC1CCC(N)CC1	0.1531034
Q9HC97	63	>= 1 Ga	0.1529418
Q9HC97	311	O-Na	0.152578
Q9HC97	164	>= 4 any ring size 5	0.152512
Q9HC97	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.1522123
Q9HC97	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	0.1520041
Q9HC97	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	0.1518616
Q9HC97	13	>= 32 C	0.1516643
Q9HC97	421	C=S	0.148889
Q9HC97	110	>= 1 Er	0.1475238
Q9HC97	72	>= 1 Nb	0.1471175
Q9HC97	439	C(-C)(-N)(=O)	0.144158
Q9HC97	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.1440995
Q9HC97	446	C(-H)(=C)	0.143283
Q9HC97	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.1424977
Q9HC97	527	C:C:N-[#1]	0.1405807
Q9HC97	552	C:C-C:C	0.140426
Q9HC97	810	SC1CC(Cl)CCC1	0.1402891
Q9HC97	772	Nc1c(Br)cccc1	0.136975
Q9HC97	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.1368334
Q9HC97	870	OC1C(Br)CCC1	0.1327883
Q9HC97	530	N:C-C:C	0.1327865
Q9HC97	743	Oc1cc(Cl)ccc1	0.1303479
Q9HC97	658	C-C-S-C-C	0.1283127
Q9HC97	249	>= 1 saturated or aromatic carbon-only ring size 10	0.1282635
Q9HC97	291	C-Si	0.1282591
Q9HC97	7	>= 2 B	0.1259285
Q9HC97	64	>= 1 Ge	0.125924
Q9HC97	15	>= 2 N	0.1259007
Q9HC97	2	>= 16 H	0.1229502
Q9HC97	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	0.1227259
Q9HC97	104	>= 1 Sm	0.1226504
Q9HC97	418	C=N	0.1219689
Q9HC97	818	CC1C(C)CCCC1	0.1217377
Q9HC97	649	O=N-C:C-O	0.1191122
Q9HC97	583	Cl-C:C-O-C	0.1189949

Q9HC97	596	N=C-N-C-C	0.1188056
Q9HC97	488	N-C=N-[#1]	0.1162987
Q9HC97	621	N-C:C:C:N	0.1158059
Q9HC97	832	SC1C(Br)CCCC1	0.1157509
Q9HC97	642	O-C-C-C=O	0.1157405
Q9HC97	553	O=C-C=C	0.1117627
Q9HC97	393	N(~C)(~H)	0.1114392
Q9HC97	685	O=C-C-C-C-N	0.1108034
Q9HC97	47	>= 2 I	0.1088326
Q9HC97	814	NC1CC(Br)CCC1	0.1087195
Q9HC97	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	0.1083245
Q9HC97	611	N-C-C-N-C	0.1074289
Q9HC97	801	CC1CC(Cl)CCC1	0.1061821
Q9HC97	599	[#1]-C-C=C-[#1]	0.1055368
Q9HC97	738	Cc1cc(Cl)ccc1	0.1050625
Q9HC97	601	N-C:C:C-N	0.1049307
Q9HC97	23	>= 1 F	0.1046341
Q9HC97	713	Cc1ccc(C)cc1	0.1042059
Q9HC97	705	O=C-C-C-C-C(O)-C	0.1027807
Q9HC97	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	0.1022795
Q9HC97	838	BrC1C(Br)CCCC1	0.1022469
Q9HC97	350	C(~C)(~I)	0.0996712
Q9HC97	448	C(-H)(=O)	0.0987043
Q9HC97	716	Cc1ccc(N)cc1	0.0973306
Q9HC97	399	N(~H)(:C)	0.0959701
Q9HC97	750	Nc1cc(Cl)ccc1	0.0958079
Q9HC97	831	SC1C(Cl)CCCC1	0.0957044
Q9HC97	276	B-O	0.0948008
Q9HC97	434	C(-C)(-H)(=C)	0.0916878
Q9HC97	815	ClC1CC(Cl)CCC1	0.0894767
Q9HC97	402	N(~O)(:O)	0.0892701
Q9HC97	708	C-C(C)-C-C	0.0886654
Q9HC97	756	Cc1c(O)cccc1	0.0883984
Q9HC97	436	C(-C)(-H)(=O)	0.0880321
Q9HC97	458	S(-O)(=O)	0.0855719
Q9HC97	25	>= 4 F	0.0845809
Q9HC97	471	S:C:C:C	0.0836779
Q9HC97	715	Cc1ccc(S)cc1	0.0820649
Q9HC97	785	OC1CCC(Cl)CC1	0.0817353
Q9HC97	33	>= 1 S	0.0805808
Q9HC97	435	C(-C)(-H)(=N)	0.0800759
Q9HC97	294	C-Cl	0.0797996
Q9HC97	65	>= 1 As	0.0790229
Q9HC97	383	C(~S)(:C)	0.0788905
Q9HC97	617	C-C-C-O-[#1]	0.0759762
Q9HC97	517	N-N-C-N	0.0755974

Q9HC97	137	>= 2 saturated or aromatic carbon-only ring size 4	0.0739291
Q9HC97	806	OC1CC(Cl)CCC1	0.0723778
Q9HC97	575	O-C-C:C-O	0.0721715
Q9HC97	319	Al-Cl	0.0721621
Q9HC97	678	C-C-C=C-C	0.0714153
Q9HC97	430	C(-C)(-C)(=C)	0.0702807
Q9HC97	606	O-C:C-C-C	0.0702307
Q9HC97	287	C-F	0.0689721
Q9HC97	415	Si(~C)(~C)	0.0688224
Q9HC97	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	0.0683551
Q9HC97	691	O-C-C-C-C-C-N	0.0683312
Q9HC97	370	C(~H)(:C)	0.0677693
Q9HC97	404	N(:C)(:C)(:C)	0.0630356
Q9HC97	338	C(~C)(~C)(~H)(~N)	0.0624585
Q9HC97	597	O=C-C-C:C	0.0618116
Q9HC97	178	>= 1 any ring size 6	0.0617766
Q9HC97	567	O-C-C-O	0.0613816
Q9HC97	771	Nc1c(Cl)cccc1	0.0608585
Q9HC97	717	Cc1ccc(Cl)cc1	0.0598367
Q9HC97	425	P=O	0.0596952
Q9HC97	712	C-C(C)-C(C)-C	0.0584183
Q9HC97	442	C(-C)(=N)	0.0583687
Q9HC97	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	0.0575885
Q9HC97	667	C=C-C-O-[#1]	0.0575722
Q9HC97	438	C(-C)(-N)(=N)	0.0574669
Q9HC97	374	C(~H)(~H)(~H)	0.0572995
Q9HC97	769	Sc1c(Br)cccc1	0.0571936
Q9HC97	834	NC1C(Cl)CCCC1	0.0566794
Q9HC97	654	N-C-N-C-C	0.0563794
Q9HC97	639	O-C-C-C-O	0.0563688
Q9HC97	682	O-C-C-C-C-N	0.0549422
Q9HC97	94	>= 1 Au	0.054461
Q9HC97	652	O-C:C-C-N	0.0542978
Q9HC97	635	N-N-C-N-[#1]	0.0529309
Q9HC97	411	P(~O)(~O)	0.0524247
Q9HC97	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	0.0524112
Q9HC97	487	N-C=N-C	0.052227
Q9HC97	103	>= 1 Pm	0.0520124
Q9HC97	629	S-C:C-C-N	0.0513328
Q9HC97	813	NC1CC(Cl)CCC1	0.0505143
Q9HC97	221	>= 2 saturated or aromatic carbon-only ring size 7	0.0504643
Q9HC97	77	>= 1 Ag	0.049954
Q9HC97	511	S=C-N-[#1]	0.0494913
Q9HC97	532	S-C:C-[#1]	0.049272
Q9HC97	585	C-C:C-N-C	0.0491044
Q9HC97	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.0487914

Q9HC97	863	CC1C(N)CCC1	0.0485939
Q9HC97	262	>= 4 hetero-aromatic rings	0.0484332
Q9HC97	333	C(~C)(~C)(~C)	0.0479984
Q9HC97	345	C(~C)(~H)(~N)	0.0477873
Q9HC97	787	SC1CCC(S)CC1	0.0473976
Q9HC97	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.0470653
Q9HC97	437	C(-C)(-N)(=C)	0.0465877
Q9HC97	101	>= 1 Pr	0.0460891
Q9HC97	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.0459895
Q9HC97	592	N-C-C-C-C	0.0454479
Q9HC97	397	N(~C)(:C)(:C)	0.0449728
Q9HC97	433	C(-C)(-Cl)(=O)	0.0449159
Q9HC97	630	O-C:C-O-C	0.0448237
Q9HC97	504	N:C:N-C	0.0447159
Q9HC97	875	NC1C(N)CCC1	0.0446875
Q9HC97	492	N-C:O:C	0.0445614
Q9HC97	869	OC1C(Cl)CCC1	0.0441211
Q9HC97	451	C(-N)(=O)	0.0438703
Q9HC97	710	C-C-C(C)-C-C	0.043823
Q9HC97	604	C-O-C-C:C	0.0435665
Q9HC97	812	NC1CC(N)CCC1	0.0432492
Q9HC97	645	O=C-N-C-C	0.0428579
Q9HC97	874	SC1C(Br)CCC1	0.0422554
Q9HC97	854	NC1CC(N)CC1	0.0417513
Q9HC97	293	C-S	0.0399979
Q9HC97	580	O=C-C-C-N	0.039698
Q9HC97	622	O=C-O-C:C	0.0390403
Q9HC97	827	OC1C(Cl)CCCC1	0.0385579
Q9HC97	509	Br-C:C-C	0.0380047
Q9HC97	510	[#1]-N-N-[#1]	0.0376692
Q9HC97	676	N#C-C-C-C	0.0373713
Q9HC97	445	C(-H)(-N)(=C)	0.0371848
Q9HC97	759	Cc1c(Cl)cccc1	0.0365359
Q9HC97	767	Sc1c(N)cccc1	0.036434
Q9HC97	784	OC1CCC(N)CC1	0.0355693
Q9HC97	562	Br-C-C=O	0.0355342
Q9HC97	8	>= 4 B	0.0354456
Q9HC97	833	NC1C(N)CCCC1	0.0352135
Q9HC97	313	O-Si	0.0351459
Q9HC97	35	>= 4 S	0.0351201
Q9HC97	640	C=C-C-C-C	0.0350717
Q9HC97	29	>= 2 Si	0.0348747
Q9HC97	515	N-N-C-C	0.0341927
Q9HC97	758	Cc1c(N)cccc1	0.0332336
Q9HC97	721	Oc1ccc(N)cc1	0.0331035
Q9HC97	526	Cl-C:C-Cl	0.0326826

Q9HC97	376	C(~N)(:C)	0.0322701
Q9HC97	389	C(:N)(:N)	0.0322035
Q9HC97	59	>= 1 Co	0.0318985
Q9HC97	278	B-Si	0.031791
Q9HC97	618	C:C-C-C:C	0.0313839
Q9HC97	702	O-C-C-C-C-C-N-C	0.0313211
Q9HC97	657	C-N-C:C-C	0.0311882
Q9HC97	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	0.0310611
Q9HC97	21	>= 8 O	0.0307938
Q9HC97	565	C:C-O-C	0.030702
Q9HC97	802	CC1CC(Br)CCC1	0.030462
Q9HC97	638	O-C-C-C-N	0.0301787
Q9HC97	406	O(~C)(~H)	0.0297635
Q9HC97	123	>= 2 saturated or aromatic carbon-only ring size 3	0.0292985
Q9HC97	612	N-C-O-C-C	0.0291742
Q9HC97	747	Sc1cc(Cl)ccc1	0.0287394
Q9HC97	514	O-N-C-C	0.0282044
Q9HC97	641	O-C-C-C=C	0.0275914
Q9HC97	480	C:S:C-C	0.0274405
Q9HC97	323	P-H	0.0272765
Q9HC97	67	>= 1 Kr	0.0271933
Q9HC97	533	S-C:C-N	0.0270692
Q9HC97	829	SC1C(S)CCCC1	0.0268456
Q9HC97	16	>= 4 N	0.026567
Q9HC97	96	>= 1 Tl	0.0260123
Q9HC97	277	B-F	0.0259545
Q9HC97	307	N-Br	0.0257196
Q9HC97	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	0.0253244
Q9HC97	732	Clc1ccc(Br)cc1	0.0252907
Q9HC97	502	N-C=C-[#1]	0.0252545
Q9HC97	793	NC1CCC(Br)CC1	0.0241666
Q9HC97	637	O-C-C-C-C	0.0239697
Q9HC97	746	Sc1cc(N)ccc1	0.0237825
Q9HC97	736	Cc1cc(S)ccc1	0.0237234
Q9HC97	412	S(~C)(~C)	0.0236948
Q9HC97	794	ClC1CCC(Cl)CC1	0.0236685
Q9HC97	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.0233028
Q9HC97	279	B-P	0.0230051
Q9HC97	675	Br-C-C-C:C	0.0228823
Q9HC97	499	N-C:C:N	0.0226468
Q9HC97	579	O=C-C-C-C	0.0223224
Q9HC97	835	NC1C(Br)CCCC1	0.0218457
Q9HC97	581	O=C-C-C-O	0.0216521
Q9HC97	308	O-H	0.0215449
Q9HC97	696	C-C-C-C-C-C-C-C	0.0215241
Q9HC97	5	>= 2 Li	0.0208673

Q9HC97	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.0204365
Q9HC97	1	>= 8 H	0.0203584
Q9HC97	299	N-H	0.0199918
Q9HC97	358	C(~C)(:N)	0.0199616
Q9HC97	355	C(~C)(:C)	0.0199309
Q9HC97	768	Sc1c(Cl)cccc1	0.0196157
Q9HC97	650	O=C-N-C=O	0.0195309
Q9HC97	282	B-Br	0.0194823
Q9HC97	849	OC1CC(Br)CC1	0.0193997
Q9HC97	68	>= 1 Rb	0.0188659
Q9HC97	648	O=N-C:C-N	0.0187177
Q9HC97	71	>= 1 Zr	0.0186535
Q9HC97	403	N(:C)(:C)	0.0178472
Q9HC97	375	C(~N)(~N)	0.0173401
Q9HC97	494	O=C-C:N	0.0170552
Q9HC97	429	C(#N)(-C)	0.0165192
Q9HC97	600	N-C:C:C-C	0.016342
Q9HC97	328	C(~Br)(~C)(~C)	0.0163177
Q9HC97	43	>= 1 Br	0.0162231
Q9HC97	356	C(~C)(:C)(:C)	0.0155681
Q9HC97	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	0.0154578
Q9HC97	485	N:C:C:N	0.0153836
Q9HC97	193	>= 3 saturated or aromatic carbon-only ring size 6	0.0153162
Q9HC97	467	C=N-N-C	0.0152057
Q9HC97	269	Li-P	0.0149327
Q9HC97	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.0138715
Q9HC97	261	>= 4 aromatic rings	0.0133645
Q9HC97	440	C(-C)(-O)(=O)	0.0132008
Q9HC97	330	C(~Br)(:C)	0.0131656
Q9HC97	41	>= 1 K	0.0127631
Q9HC97	878	ClC1C(Cl)CCC1	0.0126728
Q9HC97	459	S(=O)(=O)	0.0126063
Q9HC97	422	N=N	0.0123395
Q9HC97	556	C=C-C-C	0.0122808
Q9HC97	703	O-C-C-C-C-C(N)-C	0.0121783
Q9HC97	409	O(:C)(:C)	0.0120912
Q9HC97	805	OC1CC(N)CCC1	0.0120298
Q9HC97	840	CC1CC(O)CC1	0.0118141
Q9HC97	255	>= 1 aromatic ring	0.011807
Q9HC97	861	CC1C(O)CCC1	0.0114549
Q9HC97	505	Cl-C:C-O	0.0113097
Q9HC97	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	0.0112911
Q9HC97	668	C-C:C-C-C	0.0111274
Q9HC97	381	C(~O)(:C)	0.0108668
Q9HC97	419	C#N	0.0102986
Q9HC97	280	B-S	0.0101577

Q9HC97	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.0100498
Q9HC97	501	Cl-C:C-C	0.0096815
Q9HC97	568	N#C-C-C	0.0096642
Q9HC97	365	C(~H)(~N)	0.0096127
Q9HC97	220	>= 2 any ring size 7	0.0092753
Q9HC97	587	N-C:C-O-[#1]	0.0091851
Q9HC97	660	C-C=C-C-C	0.0091109
Q9HC97	584	C:C-C=C-C	0.0089144
Q9HC97	357	C(~C)(:C)(:N)	0.0086741
Q9HC97	288	C-Na	0.008393
Q9HC97	520	C=C-C:C	0.0083125
Q9HC97	360	C(~Cl)(~Cl)	0.0075322
Q9HC97	561	Cl-C-C=O	0.0073258
Q9HC97	150	>= 2 any ring size 5	0.0072349
Q9HC97	674	N-C-N-C:C	0.007153
Q9HC97	359	C(~C)(:N)(:N)	0.0070297
Q9HC97	274	B-C	0.0069327
Q9HC97	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	0.0069153
Q9HC97	783	OC1CCC(S)CC1	0.0060797
Q9HC97	633	N-C-C:C-C	0.0060786
Q9HC97	709	C-C(C)-C-C-C	0.0057869
Q9HC97	129	>= 1 any ring size 4	0.0056605
Q9HC97	114	>= 1 U	0.0056596
Q9HC97	521	C:N-C-[#1]	0.0055367
Q9HC97	734	Cc1cc(C)ccc1	0.0052788
Q9HC97	877	NC1C(Br)CCC1	0.0050597
Q9HC97	296	C-Se	0.004559
Q9HC97	466	N#C-C=C	0.004536
Q9HC97	49	>= 1 Be	0.0044994
Q9HC97	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.0042703
Q9HC97	99	>= 1 La	0.0041944
Q9HC97	803	OC1CC(O)CCC1	0.004083
Q9HC97	595	C:C-C-C-C	0.003912
Q9HC97	862	CC1C(S)CCC1	0.0038796
Q9HC97	664	C-C=C-C=C	0.0038225
Q9HC97	799	CC1CC(S)CCC1	0.0035873
Q9HC97	559	O-C-N-[#1]	0.0034208
Q9HC97	58	>= 1 Fe	0.0031449
Q9HC97	537	O=C-C-O	0.0029848
Q9HC97	273	B-B	0.0029177
Q9HC97	268	Li-F	0.0028417
Q9HC97	830	SC1C(N)CCCC1	0.0023688
Q9HC97	73	>= 1 Mo	0.0020839
Q9HC97	347	C(~C)(~H)(~O)(~O)	0.0018481
Q9HC97	334	C(~C)(~C)(~C)(~C)	0.0017477
Q9HC97	808	SC1CC(S)CCC1	0.0016949

Q9HC97	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.001559
Q9HC97	671	O=C-C=C-C	0.0015038
Q9HC97	699	O-C-C-C-C-C(C)-C	0.0013439
Q9HC97	578	C-C:C-C:C	0.0013096
Q9HC97	846	OC1CC(S)CC1	0.0012808
Q9HC97	753	Clc1cc(Br)ccc1	0.001272
Q9HC97	306	N-Cl	0.0012089
Q9HC97	462	O-C-C=O	0.0011701
Q9HC97	496	N:N-C-[#1]	0.0008412
Q9HC97	844	CC1CC(Br)CC1	0.0006903
Q9HC97	394	N(~C)(~H)(~N)	0.0004533
Q9HC97	111	>= 1 Tm	0.0003957
Q9HC97	607	N-C-C-C:C	0.0003741
Q9HC97	470	C:C-C=C	0.0002772
Q9HC97	199	>= 4 any ring size 6	0.0001779
Q9HC97	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	0.0001377
Q9HC97	36	>= 8 S	0.0001178
Q9HC97	113	>= 1 Tc	1.21E-06
Q9HC97	86	>= 1 Lu	1.09E-06
Q9HC97	57	>= 1 Mn	8.97E-07
Q9HC97	39	>= 4 Cl	7.65E-07
Q9HC97	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	5.19E-07
Q9HC97	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	3.76E-07
Q9HC97	304	N-P	2.96E-07
Q9HC97	816	ClC1CC(Br)CCC1	2.75E-07
Q9HC97	171	>= 5 any ring size 5	1.18E-07
Q9HC97	424	N=P	4.36E-09
Q9HC97	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	-1.08E-07
Q9HC97	112	>= 1 Yb	-1.30E-07
Q9HC97	52	>= 1 Ca	-1.91E-07
Q9HC97	82	>= 1 Te	-3.46E-07
Q9HC97	207	>= 5 saturated or aromatic carbon-only ring size 6	-4.70E-07
Q9HC97	318	Al-H	-6.44E-07
Q9HC97	50	>= 1 Mg	-6.53E-07
Q9HC97	53	>= 1 Sc	-6.72E-07
Q9HC97	322	Si-Cl	-8.04E-07
Q9HC97	31	>= 2 P	-1.02E-06
Q9HC97	98	>= 1 Bi	-1.15E-06
Q9HC97	74	>= 1 Ru	-2.02E-06
Q9HC97	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	-3.47E-05
Q9HC97	90	>= 1 Re	-4.80E-05
Q9HC97	88	>= 1 Ta	-0.000188
Q9HC97	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	-0.000192
Q9HC97	22	>= 16 O	-0.000242
Q9HC97	880	BrC1C(Br)CCC1	-0.000349
Q9HC97	130	>= 1 saturated or aromatic carbon-only ring size 4	-0.000356

Q9HC97	454	N(-C)(=O)	-0.00045
Q9HC97	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	-0.001048
Q9HC97	483	N-S-C:C	-0.001088
Q9HC97	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	-0.001145
Q9HC97	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	-0.001187
Q9HC97	348	C(~C)(~H)(~P)	-0.001305
Q9HC97	842	CC1CC(N)CC1	-0.001944
Q9HC97	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	-0.002048
Q9HC97	677	C-C=C-C:C	-0.002238
Q9HC97	871	SC1C(S)CCC1	-0.002495
Q9HC97	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	-0.002564
Q9HC97	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	-0.002664
Q9HC97	853	SC1CC(Br)CC1	-0.002871
Q9HC97	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	-0.00296
Q9HC97	401	N(~O)(~O)	-0.003082
Q9HC97	754	Brc1cc(Br)ccc1	-0.003122
Q9HC97	62	>= 1 Zn	-0.003196
Q9HC97	85	>= 1 Ba	-0.003871
Q9HC97	563	O-C-O-C	-0.004077
Q9HC97	564	C=C-C=C	-0.004117
Q9HC97	689	O-C-C-C-C-C-C	-0.004455
Q9HC97	493	O=C-C:C	-0.00449
Q9HC97	30	>= 1 P	-0.00487
Q9HC97	825	OC1C(S)CCCC1	-0.004893
Q9HC97	694	O=C-C-C-C-C=O	-0.005214
Q9HC97	777	CC1CCC(O)CC1	-0.005401
Q9HC97	264	Li-Li	-0.005539
Q9HC97	737	Cc1cc(N)ccc1	-0.005591
Q9HC97	475	S-C=N-C	-0.005734
Q9HC97	748	Sc1cc(Br)ccc1	-0.005786
Q9HC97	800	CC1CC(N)CCC1	-0.005798
Q9HC97	447	C(-H)(=N)	-0.006085
Q9HC97	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	-0.006498
Q9HC97	873	SC1C(Cl)CCC1	-0.006906
Q9HC97	339	C(~C)(~C)(~H)(~O)	-0.007984
Q9HC97	300	N-N	-0.00805
Q9HC97	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	-0.008259
Q9HC97	672	O=C-C=C-[#1]	-0.008315
Q9HC97	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	-0.008746
Q9HC97	275	B-N	-0.008944
Q9HC97	19	>= 2 O	-0.009047
Q9HC97	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	-0.009293
Q9HC97	372	C(~H)(:C)(:N)	-0.009772
Q9HC97	423	N=O	-0.00985
Q9HC97	680	O-C-C-C-C-C	-0.010046
Q9HC97	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	-0.010072

Q9HC97	546	N-C:C-[#1]	−0.010111
Q9HC97	259	>= 3 aromatic rings	−0.010312
Q9HC97	745	Sc1cc(S)ccc1	−0.010458
Q9HC97	655	O-C-C-C:C	−0.011056
Q9HC97	817	BrC1CC(Br)CCC1	−0.011888
Q9HC97	704	O=C-C-C-C-C-C-C	−0.012345
Q9HC97	687	O=C-C-C-C=O	−0.012555
Q9HC97	408	O(~H)(~S)	−0.012649
Q9HC97	679	C-C-C-C-C-C	−0.013096
Q9HC97	791	NC1CCC(N)CC1	−0.013531
Q9HC97	616	C:C:N:N:C	−0.013586
Q9HC97	267	Li-O	−0.013642
Q9HC97	241	>= 1 any ring size 9	−0.014081
Q9HC97	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.014546
Q9HC97	481	O-S-C:C	−0.014562
Q9HC97	534	S-C:C-O	−0.01482
Q9HC97	3	>= 32 H	−0.014847
Q9HC97	822	CC1C(Cl)CCCC1	−0.015566
Q9HC97	555	N=C-C=C	−0.015724
Q9HC97	37	>= 1 Cl	−0.016128
Q9HC97	75	>= 1 Rh	−0.016567
Q9HC97	773	Clc1c(Cl)cccc1	−0.016982
Q9HC97	865	CC1C(Br)CCC1	−0.017014
Q9HC97	368	C(~H)(~S)	−0.017095
Q9HC97	809	SC1CC(N)CCC1	−0.017597
Q9HC97	848	OC1CC(Cl)CC1	−0.017916
Q9HC97	109	>= 1 Ho	−0.018039
Q9HC97	486	N-C:N:N	−0.018175
Q9HC97	256	>= 1 hetero-aromatic ring	−0.018545
Q9HC97	387	C(:C)(:N)	−0.018564
Q9HC97	69	>= 1 Sr	−0.018907
Q9HC97	673	O=C-C=C-N	−0.019262
Q9HC97	821	CC1C(N)CCCC1	−0.019292
Q9HC97	719	Oc1ccc(O)cc1	−0.019412
Q9HC97	718	Cc1ccc(Br)cc1	−0.020152
Q9HC97	302	N-F	−0.020164
Q9HC97	26	>= 1 Na	−0.020386
Q9HC97	317	F-S	−0.02067
Q9HC97	206	>= 5 any ring size 6	−0.020673
Q9HC97	656	C-C-N-C-C	−0.02101
Q9HC97	569	N-C-C-N	−0.021444
Q9HC97	468	O=S-C-N	−0.021495
Q9HC97	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	−0.021958
Q9HC97	739	Cc1cc(Br)ccc1	−0.022139
Q9HC97	367	C(~H)(~O)(~O)	−0.02242
Q9HC97	450	C(-N)(=N)	−0.022573

Q9HC97	386	C(:C)(:C)(:N)	−0.022708
Q9HC97	70	>= 1 Y	−0.023088
Q9HC97	143	>= 1 any ring size 5	−0.023398
Q9HC97	342	C(~C)(~Cl)	−0.023488
Q9HC97	213	>= 1 any ring size 7	−0.023498
Q9HC97	263	Li-H	−0.023693
Q9HC97	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.02451
Q9HC97	80	>= 1 Sn	−0.024599
Q9HC97	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.025234
Q9HC97	301	N-O	−0.025291
Q9HC97	405	O(~C)(~C)	−0.025383
Q9HC97	0	>= 4 H	−0.025536
Q9HC97	724	Sc1ccc(S)cc1	−0.02554
Q9HC97	665	N-C:C-C-C	−0.025907
Q9HC97	295	C-As	−0.025911
Q9HC97	820	CC1C(S)CCCC1	−0.02783
Q9HC97	281	B-Cl	−0.027885
Q9HC97	449	C(-N)(=C)	−0.027929
Q9HC97	136	>= 2 any ring size 4	−0.028475
Q9HC97	797	CC1CC(C)CCC1	−0.029003
Q9HC97	214	>= 1 saturated or aromatic carbon-only ring size 7	−0.029248
Q9HC97	531	S-C:C-C	−0.030813
Q9HC97	469	S-S-C:C	−0.031583
Q9HC97	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	−0.031668
Q9HC97	545	N-C:C-C	−0.032411
Q9HC97	508	S=C-N-C	−0.032475
Q9HC97	588	O=C-C-C=O	−0.032732
Q9HC97	519	N=C-N-C	−0.032935
Q9HC97	544	O-C:C-O	−0.033267
Q9HC97	619	O-C-C=C-C	−0.033723
Q9HC97	513	S:C:C-[#1]	−0.036144
Q9HC97	503	Cl-C:C-[#1]	−0.036191
Q9HC97	661	O-C-O-C-C	−0.036355
Q9HC97	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.037171
Q9HC97	593	N-C-C-C-N	−0.038189
Q9HC97	522	C-N-N-[#1]	−0.038419
Q9HC97	292	C-P	−0.038932
Q9HC97	543	O-C:C-N	−0.039005
Q9HC97	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	−0.039158
Q9HC97	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	−0.039167
Q9HC97	644	C-C=N-N-C	−0.039287
Q9HC97	740	Oc1cc(O)ccc1	−0.039295
Q9HC97	61	>= 1 Cu	−0.039343
Q9HC97	826	OC1C(N)CCCC1	−0.039467
Q9HC97	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.039578
Q9HC97	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	−0.03968

Q9HC97	711	C-C(C)(C)-C-C	−0.040019
Q9HC97	864	CC1C(Cl)CCC1	−0.040323
Q9HC97	34	>= 2 S	−0.040903
Q9HC97	390	N(~C)(~C)	−0.04114
Q9HC97	839	CC1CC(C)CC1	−0.041207
Q9HC97	763	Oc1c(N)cccc1	−0.041487
Q9HC97	395	N(~C)(~O)	−0.042027
Q9HC97	398	N(~H)(~N)	−0.042463
Q9HC97	260	>= 3 hetero-aromatic rings	−0.042801
Q9HC97	227	>= 1 any ring size 8	−0.042879
Q9HC97	576	N=C-C:C-[#1]	−0.044113
Q9HC97	751	Nc1cc(Br)ccc1	−0.044144
Q9HC97	525	[As]-C:C-[#1]	−0.045054
Q9HC97	697	C-C-C-C-C-C(C)-C	−0.045247
Q9HC97	766	Sc1c(S)cccc1	−0.046019
Q9HC97	605	O=C-C-O-C	−0.046185
Q9HC97	586	C-S-C-C-C	−0.046257
Q9HC97	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	−0.046671
Q9HC97	377	C(~N)(:C)(:C)	−0.046784
Q9HC97	535	O=C-C-C	−0.04708
Q9HC97	602	O=C-C-N-C	−0.047343
Q9HC97	384	C(:C)(:C)	−0.049044
Q9HC97	727	Sc1ccc(Br)cc1	−0.049099
Q9HC97	83	>= 1 Xe	−0.049812
Q9HC97	845	OC1CC(O)CC1	−0.050021
Q9HC97	453	N(-C)(=C)	−0.050283
Q9HC97	742	Oc1cc(N)ccc1	−0.050362
Q9HC97	6	>= 1 B	−0.050534
Q9HC97	524	C-C=C-C	−0.050606
Q9HC97	868	OC1C(N)CCC1	−0.051171
Q9HC97	417	C#C	−0.051361
Q9HC97	234	>= 2 any ring size 8	−0.051407
Q9HC97	303	N-Si	−0.051461
Q9HC97	528	[#1]-N-C-[#1]	−0.051679
Q9HC97	108	>= 1 Dy	−0.05199
Q9HC97	48	>= 4 I	−0.052501
Q9HC97	540	C-N-C-[#1]	−0.052545
Q9HC97	354	C(~C)(~Si)	−0.052578
Q9HC97	122	>= 2 any ring size 3	−0.052789
Q9HC97	151	>= 2 saturated or aromatic carbon-only ring size 5	−0.053936
Q9HC97	392	N(~C)(~C)(~H)	−0.054515
Q9HC97	337	C(~C)(~C)(~C)(~O)	−0.055214
Q9HC97	632	C-C-O-C:C	−0.055806
Q9HC97	373	C(~H)(:N)	−0.055831
Q9HC97	385	C(:C)(:C)(:C)	−0.056383
Q9HC97	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.057206

Q9HC97	144	>= 1 saturated or aromatic carbon-only ring size 5	−0.057598
Q9HC97	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.057726
Q9HC97	663	O-C-C-O-[#1]	−0.058923
Q9HC97	860	CC1C(C)CCC1	−0.058987
Q9HC97	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	−0.05916
Q9HC97	538	N=C-C-C	−0.059648
Q9HC97	473	S-C:N:C	−0.059701
Q9HC97	463	N:C-S-[#1]	−0.059714
Q9HC97	516	[#1]-C=C-[#1]	−0.05995
Q9HC97	248	>= 1 any ring size 10	−0.060772
Q9HC97	464	N-C-C=C	−0.060776
Q9HC97	789	SC1CCC(Cl)CC1	−0.061026
Q9HC97	735	Cc1cc(O)ccc1	−0.061665
Q9HC97	643	[#1]-C-C-N-[#1]	−0.061738
Q9HC97	284	C-C	−0.063204
Q9HC97	363	C(~F)(~F)	−0.063428
Q9HC97	476	C-O-C=C	−0.063697
Q9HC97	491	C-N:C-[#1]	−0.06453
Q9HC97	843	CC1CC(Cl)CC1	−0.064866
Q9HC97	776	CC1CCC(C)CC1	−0.065694
Q9HC97	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.066452
Q9HC97	443	C(-C)(=O)	−0.067311
Q9HC97	185	>= 2 any ring size 6	−0.067337
Q9HC97	536	O=C-C-N	−0.068712
Q9HC97	414	S(~C)(~O)	−0.068912
Q9HC97	614	C-C-O-C-C	−0.069089
Q9HC97	66	>= 1 Se	−0.069431
Q9HC97	551	Cl-C-C-O	−0.070621
Q9HC97	298	C-I	−0.072054
Q9HC97	314	O-P	−0.073274
Q9HC97	14	>= 1 N	−0.073356
Q9HC97	670	Br-C:C:C-C	−0.073874
Q9HC97	539	N=C-C-[#1]	−0.074529
Q9HC97	811	SC1CC(Br)CCC1	−0.074962
Q9HC97	428	C(#C)(-H)	−0.075235
Q9HC97	762	Oc1c(S)cccc1	−0.075421
Q9HC97	634	C-C-C:C-C	−0.077165
Q9HC97	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	−0.077215
Q9HC97	40	>= 8 Cl	−0.077347
Q9HC97	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.078955
Q9HC97	474	S:C:C:N	−0.078957
Q9HC97	725	Sc1ccc(N)cc1	−0.080221
Q9HC97	594	C-O-C-C=C	−0.080299
Q9HC97	479	S-C-S-C	−0.080367
Q9HC97	192	>= 3 any ring size 6	−0.080957
Q9HC97	477	N-N-C:C	−0.081263

Q9HC97	688	C-C-C-C-C-C-C	−0.081988
Q9HC97	349	C(~C)(~H)(~S)	−0.082761
Q9HC97	54	>= 1 Ti	−0.083273
Q9HC97	636	C-N-C-N-C	−0.083766
Q9HC97	741	Oc1cc(S)ccc1	−0.084239
Q9HC97	547	N-C:C-N	−0.084938
Q9HC97	729	Nc1ccc(Cl)cc1	−0.085913
Q9HC97	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.086192
Q9HC97	792	NC1CCC(Cl)CC1	−0.086569
Q9HC97	9	>= 2 C	−0.087101
Q9HC97	574	O-C-C:C-C	−0.087895
Q9HC97	87	>= 1 Hf	−0.088776
Q9HC97	549	N-C-C:C	−0.089055
Q9HC97	388	C(:C)(:N)(:N)	−0.090602
Q9HC97	859	BrC1CC(Br)CC1	−0.091541
Q9HC97	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	−0.091576
Q9HC97	695	O=C-C-C-C-C-N	−0.092448
Q9HC97	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	−0.09332
Q9HC97	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	−0.094043
Q9HC97	391	N(~C)(~C)(~C)	−0.095242
Q9HC97	613	C-N-C-C-C	−0.095294
Q9HC97	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	−0.095351
Q9HC97	427	C(#C)(-C)	−0.097403
Q9HC97	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	−0.098101
Q9HC97	782	OC1CCC(O)CC1	−0.100818
Q9HC97	91	>= 1 Os	−0.103574
Q9HC97	749	Nc1cc(N)ccc1	−0.104335
Q9HC97	628	C-N-C-C:C	−0.104367
Q9HC97	361	C(~Cl)(~H)	−0.105418
Q9HC97	93	>= 1 Pt	−0.105439
Q9HC97	610	C-O-C-O-C	−0.106449
Q9HC97	857	ClC1CC(Cl)CC1	−0.108363
Q9HC97	686	O=C-C-C-C-O	−0.111086
Q9HC97	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	−0.112904
Q9HC97	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	−0.113955
Q9HC97	321	Si-Si	−0.11487
Q9HC97	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	−0.115921
Q9HC97	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	−0.117181
Q9HC97	157	>= 3 any ring size 5	−0.117508
Q9HC97	324	P-P	−0.119163
Q9HC97	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−0.119219
Q9HC97	286	C-O	−0.119822
Q9HC97	554	Br-C-C-C	−0.120133
Q9HC97	498	O-C=C-C	−0.12047
Q9HC97	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	−0.121153
Q9HC97	56	>= 1 Cr	−0.121763

Q9HC97	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.122098
Q9HC97	320	Si-H	−0.122496
Q9HC97	557	N:C-O-[#1]	−0.122984
Q9HC97	10	>= 4 C	−0.123274
Q9HC97	852	SC1CC(Cl)CC1	−0.124213
Q9HC97	651	O-C:C:C-C	−0.124692
Q9HC97	788	SC1CCC(N)CC1	−0.12759
Q9HC97	456	P(-O)(=O)	−0.128159
Q9HC97	431	C(-C)(-C)(=N)	−0.12873
Q9HC97	726	Sc1ccc(Cl)cc1	−0.130429
Q9HC97	309	O-O	−0.130973
Q9HC97	378	C(~N)(:C)(:N)	−0.130985
Q9HC97	362	C(~Cl)(:C)	−0.131154
Q9HC97	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.132429
Q9HC97	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−0.132578
Q9HC97	778	CC1CCC(S)CC1	−0.132582
Q9HC97	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	−0.133152
Q9HC97	497	O-C:C:N	−0.134428
Q9HC97	346	C(~C)(~H)(~O)	−0.134501
Q9HC97	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	−0.134949
Q9HC97	106	>= 1 Gd	−0.135466
Q9HC97	420	C=O	−0.137264
Q9HC97	558	O=N-C:C	−0.138054
Q9HC97	289	C-Mg	−0.141306
Q9HC97	432	C(-C)(-C)(=O)	−0.142383
Q9HC97	490	C-C-C=C	−0.143632
Q9HC97	78	>= 1 Cd	−0.143636
Q9HC97	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	−0.143778
Q9HC97	624	O=C-C:C-N	−0.145931
Q9HC97	271	Li-Cl	−0.148005
Q9HC97	27	>= 2 Na	−0.148251
Q9HC97	566	O-C-C-N	−0.14939
Q9HC97	733	Brc1ccc(Br)cc1	−0.150187
Q9HC97	744	Oc1cc(Br)ccc1	−0.152087
Q9HC97	310	O-Mg	−0.152192
Q9HC97	340	C(~C)(~C)(~N)	−0.153167
Q9HC97	335	C(~C)(~C)(~C)(~H)	−0.153256
Q9HC97	858	ClC1CC(Br)CC1	−0.153753
Q9HC97	855	NC1CC(Cl)CC1	−0.154932
Q9HC97	369	C(~H)(~Si)	−0.155539
Q9HC97	400	N(~H)(:C)(:C)	−0.155768
Q9HC97	17	>= 8 N	−0.155863
Q9HC97	95	>= 1 Hg	−0.156047
Q9HC97	577	C:C-N-C:C	−0.15616
Q9HC97	315	O-K	−0.156633
Q9HC97	60	>= 1 Ni	−0.157055

Q9HC97	730	Nc1ccc(Br)cc1	−0.158311
Q9HC97	329	C(~Br)(~H)	−0.158384
Q9HC97	79	>= 1 In	−0.158681
Q9HC97	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	−0.158762
Q9HC97	752	Clc1cc(Cl)ccc1	−0.15887
Q9HC97	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.158878
Q9HC97	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	−0.159133
Q9HC97	444	C(-Cl)(=O)	−0.159208
Q9HC97	410	P(~C)(~C)	−0.15988
Q9HC97	731	Clc1ccc(Cl)cc1	−0.160155
Q9HC97	265	Li-B	−0.160437
Q9HC97	228	>= 1 saturated or aromatic carbon-only ring size 8	−0.160552
Q9HC97	97	>= 1 Pb	−0.160949
Q9HC97	518	O=C-N-N	−0.163843
Q9HC97	500	C-S-C:C	−0.165667
Q9HC97	297	C-Br	−0.167304
Q9HC97	550	Cl-C-C-C	−0.167732
Q9HC97	700	O-C-C-C-C-C-O-C	−0.170873
Q9HC97	866	OC1C(O)CCC1	−0.171019
Q9HC97	351	C(~C)(~N)	−0.174203
Q9HC97	382	C(~O)(:C)(:C)	−0.175577
Q9HC97	371	C(~H)(:C)(:C)	−0.177469
Q9HC97	647	O=C-N-C-N	−0.180611
Q9HC97	720	Oc1ccc(S)cc1	−0.180939
Q9HC97	757	Cc1c(S)cccc1	−0.181528
Q9HC97	460	C-C-C#C	−0.182014
Q9HC97	646	O=C-N-C-[#1]	−0.184495
Q9HC97	615	N-C-C-O-C	−0.191883
Q9HC97	761	Oc1c(O)cccc1	−0.196173
Q9HC97	258	>= 2 hetero-aromatic rings	−0.197998
Q9HC97	24	>= 2 F	−0.202568
Q9HC97	598	Cl-C:C:C-C	−0.206526
Q9HC97	684	O=C-C-C-C-C	−0.209287
Q9HC97	325	As-H	−0.210293
Q9HC97	824	OC1C(O)CCCC1	−0.215344
Q9HC97	707	O=C-C-C-C-C(N)-C	−0.222445
Q9HC97	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.229689
Q9HC97	396	N(~C)(:C)	−0.230039
Q9HC97	507	C-C-S-C	−0.234384
Q9HC97	44	>= 2 Br	−0.250267
Q9HC97	305	N-S	−0.251541
Q9HC97	18	>= 1 O	−0.253545
Q9HC97	285	C-N	−0.262198
Q9HC97	623	O=C-C:C-C	−0.266102
Q9HC97	770	Nc1c(N)cccc1	−0.268728
Q9HC97	728	Nc1ccc(N)cc1	−0.270214

Q9HC97	666	C=C-C-O-C	−0.282893
Q9HC97	764	Oc1c(Cl)cccc1	−0.283376
Q9HC97	571	[#1]-C-O-[#1]	−0.28909
Q9HC97	186	>= 2 saturated or aromatic carbon-only ring size 6	−0.2935
Q9HC97	416	C=C	−0.295714
Q9HC97	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.29727
Q9HC97	625	O=C-C:C-O	−0.30596
Q9HC97	804	OC1CC(S)CCC1	−0.311169
Q9HC97	828	OC1C(Br)CCCC1	−0.34616
Q9HC97	573	O-C-C=C	−0.346927
Q9HC97	465	O=S-C-C	−0.348083
Q9HC97	790	SC1CCC(Br)CC1	−0.348228
Q9HC97	872	SC1C(N)CCC1	−0.349398
Q9HC97	582	C-C-C-C-C	−0.350299
Q9HC97	847	OC1CC(N)CC1	−0.357843
Q9HC97	774	Clc1c(Br)cccc1	−0.364229
Q9HC97	283	C-H	−0.366296
Q9HC97	331	C(~Br)(:N)	−0.368741
Q9HC97	353	C(~C)(~S)	−0.375495
Q9HC97	626	C-O-C:C-C	−0.384676
Q9HC97	441	C(-C)(=C)	−0.384823
Q9HC97	867	OC1C(S)CCC1	−0.396096
Q9HC97	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	−0.399666
Q9HC97	89	>= 1 W	−0.413284
Q9HC97	115	>= 1 any ring size 3	−0.421373
Q9HC97	608	C-C-C-C:C	−0.424063
Q9HC97	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	−0.43116
Q9HC97	461	O-C-C=N	−0.440627
Q9HC97	765	Oc1c(Br)cccc1	−0.455069
Q9HC97	698	O-C-C-C-C-C-C-C	−0.469938
Q9HC97	542	O-C:C-[#1]	−0.486465
Q9HC97	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	−0.493932
Q9HC97	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	−0.495263
Q9HC97	482	C:N-C:C	−0.536878
Q9HC97	512	C-[As]-O-[#1]	−0.554475
Q9HC97	290	C-Al	−0.570124
Q9HC97	590	C-C:C-O-[#1]	−0.645293
Q9HC97	795	ClC1CCC(Br)CC1	−0.645869
Q9HC97	796	BrC1CCC(Br)CC1	−0.668657
Q9HC97	42	>= 2 K	−0.678795
Q9HC97	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.698488
Q9HC97	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.699207
Q9HC97	235	>= 2 saturated or aromatic carbon-only ring size 8	−0.706538
Q9HC97	332	C(~C)(~C)	−0.803413
Q9HC97	343	C(~C)(~Cl)(~H)	−0.827604
Q9HC97	316	F-P	−0.848489

Q9HC97	572	N:C:N:C	−0.859853
Q9HC97	690	O-C-C-C-C-C-O	−0.869677
Q9HC97	603	C-C:C:C-C	−1.005327
Q9HC97	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	−1.079704
Q9HC97	529	Cl-C-C-Cl	−1.104732
Q9HC97	28	>= 1 Si	−1.233049
Q9HC97	841	CC1CC(S)CC1	−1.387434
Q9HC97	344	C(~C)(~H)	−1.49909
Q9HC97	272	B-H	−1.616266

Fingerprints（continued)

P	Q
2.045619	1.80E-06
1.446662	-4.19E-07
1.337689	8.20E-07
1.200212	1.07E-06
1.186925	5.13E-07
1.108559	1.56E-06
1.020308	8.32E-07
1.015777	-0.00476
1.002289	-3.59E-07
0.9161	1.47E-06
0.755762	-0.00044
0.731207	0.014481
0.727472	9.38E-07
0.696406	1.06E-06
0.676315	8.57E-07
0.627975	1.66E-07
0.640329	-0.01922
0.616218	1.30E-06
0.602074	1.42E-06
0.582634	-0.01504
0.542742	0.015006
0.555197	-0.01082
0.523348	0.014201
0.517158	-0.01548
0.437772	0.052525
0.486029	-4.84E-07
0.480145	-0.01633
0.434525	-4.81E-09
0.343205	0.074174
0.4161	1.19E-06
0.31818	0.094294
0.413613	-0.00368
0.346548	0.046388
0.357394	0.023938
0.352288	0.028884
0.379558	-1.14E-07
0.313835	0.058131
0.352933	6.06E-07
0.324467	0.026912
0.279803	0.064812
0.315477	1.06E-06
0.285503	0.025892
0.28413	0.025368
0.252636	0.044271

0.286751	0.009171
0.305407	-0.01272
0.228061	0.061472
0.233813	0.053869
0.227281	0.05353
0.280415	6.94E-07
0.206959	0.072187
0.274653	-3.83E-08
0.270281	0.003115
0.274422	-0.00186
0.268186	0.001384
0.254841	0.009172
0.259952	0.00174
0.260625	6.37E-07
0.239455	0.008519
0.211879	0.0355
0.224136	0.013912
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-0.02056 -0.09053
 -0.1129 3.94E-07
-0.13101 0.017053
-0.11487 2.12E-07
-0.11592 9.42E-07
-0.11718 -1.40E-06
-0.10227 -0.01524
-0.11916 1.13E-06
-0.11922 1.09E-06
-0.10434 -0.01548
-0.13636 0.016225
-0.10578 -0.01469
-0.06987 -0.05128
-0.12176 7.50E-07

-0.1221	-6.34E-07
-0.1225	8.05E-07
-0.12279	-0.0002
-0.06558	-0.05769
-0.12421	-1.17E-06
-0.14164	0.01695
-0.02904	-0.09855
-0.1263	-0.00186
-0.06937	-0.05936
-0.06941	-0.06102
-0.13097	-2.27E-07
-0.08008	-0.0509
-0.12817	-0.00299
-0.13243	8.54E-07
-0.13258	7.26E-07
-0.12506	-0.00752
-0.13315	-8.22E-07
-0.13437	-6.11E-05
-0.06978	-0.06472
-0.09311	-0.04183
-0.13547	2.84E-07
-0.07449	-0.06277
-0.06435	-0.0737
-0.14131	-5.86E-07
-0.14614	0.00376
-0.11983	-0.0238
-0.14364	-5.69E-07
-0.14378	-1.23E-07
-0.10732	-0.03862
-0.14801	7.45E-07
-0.14825	-1.83E-07
-0.10323	-0.04616
-0.15019	1.77E-06
-0.15209	-1.38E-07
-0.15219	4.45E-07
-0.08739	-0.06577
-0.103	-0.05026
-0.15375	-2.48E-07
-0.15493	1.44E-06
-0.15554	5.32E-07
-0.15055	-0.00521
-0.15149	-0.00437
-0.15605	-7.99E-07
-0.07652	-0.07964
-0.15663	4.03E-08
-0.15706	6.89E-07

-0.15831	7.15E-07
-0.15838	-8.00E-07
-0.15868	7.32E-08
-0.15876	3.42E-07
-0.16842	0.009553
-0.15888	2.24E-07
-0.15913	6.72E-07
-0.15921	2.08E-06
-0.15988	1.35E-06
-0.16016	5.35E-07
-0.16044	4.13E-07
-0.16055	1.08E-06
-0.16095	-3.40E-07
-0.17657	0.012725
-0.17609	0.01042
-0.18353	0.016224
-0.15736	-0.01037
-0.15606	-0.01481
-0.17102	6.13E-07
-0.14623	-0.02798
-0.08831	-0.08727
-0.14368	-0.03379
-0.18192	0.001313
-0.18843	0.007494
-0.15642	-0.02511
-0.13449	-0.04752
-0.08879	-0.09571
-0.19202	0.000134
-0.19422	-0.00196
-0.198	-9.71E-08
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-0.19887	-0.00766
-0.11331	-0.09597
-0.21029	5.33E-07
-0.21339	-0.00196
-0.15715	-0.0653
-0.16919	-0.0605
-0.20829	-0.02175
-0.20664	-0.02774
-0.2365	-0.01376
-0.24843	-0.00311
-0.22193	-0.03161
-0.23422	-0.02797
-0.24488	-0.02123
-0.25269	-0.01604
-0.25668	-0.01353

-0.25376 -0.02913
-0.29585 0.012471
-0.26903 -0.02006
-0.30994 0.016445
-0.23935 -0.05636
-0.24111 -0.05616
-0.28487 -0.02109
-0.27214 -0.03903
-0.34284 -0.00332
-0.32262 -0.02431
-0.32301 -0.02507
-0.35593 0.007707
-0.3494 4.39E-07
-0.33498 -0.01531
-0.35784 -1.23E-06
-0.36423 -1.61E-06
-0.29807 -0.06823
-0.36874 -5.96E-07
-0.31656 -0.05894
-0.37386 -0.01082
-0.32846 -0.05636
-0.3961 2.48E-07
-0.39967 -6.14E-08
-0.41328 -3.48E-07
-0.36088 -0.0605
-0.43434 0.010272
-0.40351 -0.02765
-0.37892 -0.06171
-0.45175 -0.00331
-0.36541 -0.10453
-0.42975 -0.05671
-0.49393 1.88E-07
-0.49526 -6.68E-07
-0.47468 -0.0622
-0.55448 9.01E-07
-0.57012 -6.06E-07
-0.56796 -0.07734
-0.64587 -1.38E-06
-0.66866 3.04E-07
-0.67879 -1.49E-06
-0.69849 -5.56E-07
-0.69921 3.21E-07
-0.70654 -7.41E-07
-0.74572 -0.05769
-0.8276 2.82E-07
-0.84849 -5.78E-07

-0.89664 0.036791
-0.94617 0.076496
-1.00124 -0.00409
-1.05804 -0.02166
-1.11325 0.008516
-1.23305 -1.58E-06
-1.38743 -3.16E-06
-1.43086 -0.06823
-1.61626 -1.35E-06

Data S1. Ranking of importance of substructure features from Pubchem

GPCR ID	Bit Posit	Bit Substructure	W
Q9NQS5	693	O=C-C-C-C-C-O	4.9339691
Q9NQS5	378	C(~N)(:C)(:N)	2.7472332
Q9NQS5	205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6	2.2825485
Q9NQS5	386	C(:C)(:C)(:N)	2.2577574
Q9NQS5	635	N-N-C-N-[#1]	2.0481184
Q9NQS5	438	C(-C)(-N)(=N)	2.0287062
Q9NQS5	653	O-C:C:C-O	1.9516303
Q9NQS5	768	Sc1c(Cl)cccc1	1.9361849
Q9NQS5	20	>= 4 O	1.8992335
Q9NQS5	577	C:C-N-C:C	1.8969498
Q9NQS5	199	>= 4 any ring size 6	1.8429046
Q9NQS5	867	OC1C(S)CCC1	1.6857257
Q9NQS5	776	CC1CCC(C)CC1	1.5590976
Q9NQS5	782	OC1CCC(O)CC1	1.5515378
Q9NQS5	711	C-C(C)(C)-C-C	1.5121381
Q9NQS5	335	C(~C)(~C)(~C)(~H)	1.3608397
Q9NQS5	568	N#C-C-C	1.3146601
Q9NQS5	840	CC1CC(O)CC1	1.2922062
Q9NQS5	654	N-C-N-C-C	1.2911148
Q9NQS5	719	Oc1ccc(O)cc1	1.2881824
Q9NQS5	43	>= 1 Br	1.2696062
Q9NQS5	144	>= 1 saturated or aromatic carbon-only ring size 5	1.1045521
Q9NQS5	401	N(~O)(~O)	1.052971
Q9NQS5	689	O-C-C-C-C-C-C	0.9863992
Q9NQS5	703	O-C-C-C-C-C(N)-C	0.9547445
Q9NQS5	615	N-C-C-O-C	0.9509003
Q9NQS5	660	C-C=C-C-C	0.9395956
Q9NQS5	329	C(~Br)(~H)	0.9299891
Q9NQS5	691	O-C-C-C-C-C-N	0.8769666
Q9NQS5	557	N:C-O-[#1]	0.8694044
Q9NQS5	204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6	0.8674899
Q9NQS5	616	C:C:N:N:C	0.8566926
Q9NQS5	680	O-C-C-C-C-C	0.8295772
Q9NQS5	1	>= 8 H	0.8117307
Q9NQS5	334	C(~C)(~C)(~C)(~C)	0.8052937
Q9NQS5	308	O-H	0.7886132
Q9NQS5	866	OC1C(O)CCC1	0.7767408
Q9NQS5	514	O-N-C-C	0.7760761
Q9NQS5	628	C-N-C-C:C	0.7696247
Q9NQS5	233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8	0.7599002
Q9NQS5	655	O-C-C-C:C	0.7539519
Q9NQS5	377	C(~N)(:C)(:C)	0.7157467
Q9NQS5	311	O-Na	0.6896926
Q9NQS5	203	>= 4 unsaturated non-aromatic carbon-only ring size 6	0.6872501

Q9NQS5	862	CC1C(S)CCC1	0.6839759
Q9NQS5	4	>= 1 Li	0.6797503
Q9NQS5	149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	0.6744932
Q9NQS5	87	>= 1 Hf	0.6689065
Q9NQS5	631	O-C:C-O-[#1]	0.6586569
Q9NQS5	611	N-C-C-N-C	0.6544044
Q9NQS5	564	C=C-C=C	0.6447982
Q9NQS5	696	C-C-C-C-C-C-C-C	0.6360356
Q9NQS5	270	Li-S	0.6307149
Q9NQS5	672	O=C-C=C-[#1]	0.6208043
Q9NQS5	803	OC1CC(O)CCC1	0.6186209
Q9NQS5	726	Sc1ccc(Cl)cc1	0.6107221
Q9NQS5	575	O-C-C:C-O	0.5885089
Q9NQS5	89	>= 1 W	0.5883214
Q9NQS5	695	O=C-C-C-C-C-N	0.5830604
Q9NQS5	501	Cl-C:C-C	0.5790598
Q9NQS5	147	>= 1 unsaturated non-aromatic carbon-only ring size 5	0.5484853
Q9NQS5	393	N(~C)(~H)	0.5422827
Q9NQS5	626	C-O-C:C-C	0.5301265
Q9NQS5	569	N-C-C-N	0.5290078
Q9NQS5	469	S-S-C:C	0.5196693
Q9NQS5	320	Si-H	0.5174842
Q9NQS5	584	C:C-C=C-C	0.4950489
Q9NQS5	688	C-C-C-C-C-C-C	0.4894069
Q9NQS5	196	>= 3 unsaturated non-aromatic carbon-only ring size 6	0.4803019
Q9NQS5	558	O=N-C:C	0.4798939
Q9NQS5	834	NC1C(Cl)CCCC1	0.4797715
Q9NQS5	572	N:C:N:C	0.4689628
Q9NQS5	176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	0.4618215
Q9NQS5	774	Clc1c(Br)cccc1	0.4560612
Q9NQS5	713	Cc1ccc(C)cc1	0.454157
Q9NQS5	778	CC1CCC(S)CC1	0.4512139
Q9NQS5	685	O=C-C-C-C-N	0.4329909
Q9NQS5	294	C-Cl	0.4329253
Q9NQS5	189	>= 2 unsaturated non-aromatic carbon-only ring size 6	0.4315298
Q9NQS5	566	O-C-C-N	0.4240289
Q9NQS5	206	>= 5 any ring size 6	0.4167313
Q9NQS5	574	O-C-C:C-C	0.4144494
Q9NQS5	449	C(-N)(=C)	0.401708
Q9NQS5	573	O-C-C=C	0.3988315
Q9NQS5	542	O-C:C-[#1]	0.3908523
Q9NQS5	197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6	0.383056
Q9NQS5	779	CC1CCC(N)CC1	0.3744311
Q9NQS5	432	C(-C)(-C)(=O)	0.3720807
Q9NQS5	786	OC1CCC(Br)CC1	0.3706621
Q9NQS5	392	N(~C)(~C)(~H)	0.3622082

Q9NQS5	31	>= 2 P	0.3583051
Q9NQS5	478	S-C=N-[#1]	0.358054
Q9NQS5	548	O-C-C:C	0.3571221
Q9NQS5	247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9	0.3543408
Q9NQS5	537	O=C-C-O	0.3525943
Q9NQS5	327	C(~Br)(~C)	0.3469624
Q9NQS5	455	N(-O)(=O)	0.3465673
Q9NQS5	322	Si-Cl	0.3386181
Q9NQS5	318	Al-H	0.3261964
Q9NQS5	182	>= 1 unsaturated non-aromatic carbon-only ring size 6	0.3149931
Q9NQS5	671	O=C-C=C-C	0.3136486
Q9NQS5	740	Oc1cc(O)ccc1	0.3131201
Q9NQS5	580	O=C-C-C-N	0.3118434
Q9NQS5	461	O-C-C=N	0.3111968
Q9NQS5	48	>= 4 I	0.3054376
Q9NQS5	824	OC1C(O)CCCC1	0.3032853
Q9NQS5	581	O=C-C-C-O	0.3027262
Q9NQS5	647	O=C-N-C-N	0.3019734
Q9NQS5	701	O-C-C-C-C-C(O)-C	0.292834
Q9NQS5	221	>= 2 saturated or aromatic carbon-only ring size 7	0.2919641
Q9NQS5	433	C(-C)(-Cl)(=O)	0.2894882
Q9NQS5	773	Clc1c(Cl)cccc1	0.2838303
Q9NQS5	735	Cc1cc(O)ccc1	0.2800566
Q9NQS5	571	[#1]-C-O-[#1]	0.2788814
Q9NQS5	761	Oc1c(O)cccc1	0.27605
Q9NQS5	229	>= 1 saturated or aromatic nitrogen-containing ring size 8	0.268555
Q9NQS5	32	>= 4 P	0.2677536
Q9NQS5	536	O=C-C-N	0.2614515
Q9NQS5	843	CC1CC(Cl)CC1	0.2574978
Q9NQS5	541	O-C:C-C	0.2540968
Q9NQS5	477	N-N-C:C	0.2531258
Q9NQS5	496	N:N-C-[#1]	0.2499202
Q9NQS5	72	>= 1 Nb	0.2496896
Q9NQS5	25	>= 4 F	0.2419514
Q9NQS5	590	C-C:C-O-[#1]	0.237445
Q9NQS5	281	B-Cl	0.2364918
Q9NQS5	340	C(~C)(~C)(~N)	0.2148169
Q9NQS5	716	Cc1ccc(N)cc1	0.2096982
Q9NQS5	795	ClC1CCC(Br)CC1	0.2064363
Q9NQS5	357	C(~C)(:C)(:N)	0.1951131
Q9NQS5	30	>= 1 P	0.1890176
Q9NQS5	652	O-C:C:C-N	0.1854435
Q9NQS5	638	O-C-C-C-N	0.1842138
Q9NQS5	567	O-C-C-O	0.1823621
Q9NQS5	667	C=C-C-O-[#1]	0.1783558
Q9NQS5	651	O-C:C:C-C	0.1759896

Q9NQS5	431	C(-C)(-C)(=N)	0.1749716
Q9NQS5	11	>= 8 C	0.1725825
Q9NQS5	827	OC1C(Cl)CCCC1	0.1686759
Q9NQS5	712	C-C(C)-C(C)-C	0.1644231
Q9NQS5	190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6	0.1637355
Q9NQS5	535	O=C-C-C	0.1616394
Q9NQS5	192	>= 3 any ring size 6	0.1596124
Q9NQS5	397	N(~C)(:C)(:C)	0.1573472
Q9NQS5	539	N=C-C-[#1]	0.1557836
Q9NQS5	531	S-C:C-C	0.1540106
Q9NQS5	418	C=N	0.1473428
Q9NQS5	684	O=C-C-C-C-C	0.1464544
Q9NQS5	409	O(:C)(:C)	0.1431959
Q9NQS5	612	N-C-O-C-C	0.1403717
Q9NQS5	646	O=C-N-C-[#1]	0.1395983
Q9NQS5	173	>= 5 saturated or aromatic nitrogen-containing ring size 5	0.139084
Q9NQS5	785	OC1CCC(Cl)CC1	0.1388041
Q9NQS5	625	O=C-C:C-O	0.1373559
Q9NQS5	702	O-C-C-C-C-C-N-C	0.1361556
Q9NQS5	57	>= 1 Mn	0.1340788
Q9NQS5	670	Br-C:C:C-C	0.1338507
Q9NQS5	361	C(~Cl)(~H)	0.1332314
Q9NQS5	525	[As]-C:C-[#1]	0.1330892
Q9NQS5	58	>= 1 Fe	0.1329264
Q9NQS5	744	Oc1cc(Br)ccc1	0.1329123
Q9NQS5	66	>= 1 Se	0.1324832
Q9NQS5	456	P(-O)(=O)	0.1319739
Q9NQS5	875	NC1C(N)CCC1	0.1301905
Q9NQS5	128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	0.1286903
Q9NQS5	872	SC1C(N)CCC1	0.1280251
Q9NQS5	234	>= 2 any ring size 8	0.1277108
Q9NQS5	211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6	0.127581
Q9NQS5	46	>= 1 I	0.1271458
Q9NQS5	230	>= 1 saturated or aromatic heteroatom-containing ring size 8	0.1269463
Q9NQS5	463	N:C-S-[#1]	0.1267875
Q9NQS5	509	Br-C:C-C	0.1263802
Q9NQS5	227	>= 1 any ring size 8	0.1261239
Q9NQS5	614	C-C-O-C-C	0.1260972
Q9NQS5	208	>= 5 saturated or aromatic nitrogen-containing ring size 6	0.1259401
Q9NQS5	648	O=N-C:C-N	0.1243999
Q9NQS5	743	Oc1cc(Cl)ccc1	0.123912
Q9NQS5	559	O-C-N-[#1]	0.123797
Q9NQS5	661	O-C-O-C-C	0.1235565
Q9NQS5	228	>= 1 saturated or aromatic carbon-only ring size 8	0.1235048
Q9NQS5	212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6	0.1228184
Q9NQS5	309	O-O	0.122534

Q9NQS5	114	>= 1 U	0.1220646
Q9NQS5	836	ClC1C(Cl)CCCC1	0.121778
Q9NQS5	266	Li-C	0.1189729
Q9NQS5	394	N(~C)(~H)(~N)	0.1183652
Q9NQS5	288	C-Na	0.117872
Q9NQS5	742	Oc1cc(N)ccc1	0.1172586
Q9NQS5	181	>= 1 saturated or aromatic heteroatom-containing ring size 6	0.1165608
Q9NQS5	600	N-C:C:C-C	0.1162513
Q9NQS5	835	NC1C(Br)CCCC1	0.1155911
Q9NQS5	594	C-O-C-C=C	0.1149015
Q9NQS5	156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	0.1139177
Q9NQS5	117	>= 1 saturated or aromatic nitrogen-containing ring size 3	0.113896
Q9NQS5	505	Cl-C:C-O	0.1135381
Q9NQS5	565	C:C-O-C	0.1134334
Q9NQS5	151	>= 2 saturated or aromatic carbon-only ring size 5	0.1129291
Q9NQS5	828	OC1C(Br)CCCC1	0.1113299
Q9NQS5	388	C(:C)(:N)(:N)	0.1113216
Q9NQS5	2	>= 16 H	0.1104195
Q9NQS5	642	O-C-C-C=O	0.1094905
Q9NQS5	267	Li-O	0.1083108
Q9NQS5	248	>= 1 any ring size 10	0.1076345
Q9NQS5	100	>= 1 Ce	0.1076263
Q9NQS5	363	C(~F)(~F)	0.107284
Q9NQS5	847	OC1CC(N)CC1	0.1055094
Q9NQS5	538	N=C-C-C	0.105491
Q9NQS5	51	>= 1 Al	0.1054842
Q9NQS5	166	>= 4 saturated or aromatic nitrogen-containing ring size 5	0.1050579
Q9NQS5	841	CC1CC(S)CC1	0.1049059
Q9NQS5	178	>= 1 any ring size 6	0.1044976
Q9NQS5	637	O-C-C-C-C	0.1012876
Q9NQS5	498	O-C=C-C	0.1009518
Q9NQS5	63	>= 1 Ga	0.1002815
Q9NQS5	112	>= 1 Yb	0.0997784
Q9NQS5	223	>= 2 saturated or aromatic heteroatom-containing ring size 7	0.0959322
Q9NQS5	602	O=C-C-N-C	0.0959024
Q9NQS5	342	C(~C)(~Cl)	0.0954586
Q9NQS5	764	Oc1c(Cl)cccc1	0.0948199
Q9NQS5	444	C(-Cl)(=O)	0.0948089
Q9NQS5	139	>= 2 saturated or aromatic heteroatom-containing ring size 4	0.0914729
Q9NQS5	601	N-C:C:C-N	0.0912088
Q9NQS5	414	S(~C)(~O)	0.0906005
Q9NQS5	54	>= 1 Ti	0.0877623
Q9NQS5	285	C-N	0.0865317
Q9NQS5	810	SC1CC(Cl)CCC1	0.08617
Q9NQS5	37	>= 1 Cl	0.0836732
Q9NQS5	91	>= 1 Os	0.0830461

Q9NQS5	837	ClC1C(Br)CCCC1	0.08304
Q9NQS5	337	C(~C)(~C)(~C)(~O)	0.0828787
Q9NQS5	341	C(~C)(~C)(~O)	0.079444
Q9NQS5	816	ClC1CC(Br)CCC1	0.0793262
Q9NQS5	801	CC1CC(Cl)CCC1	0.0747581
Q9NQS5	399	N(~H)(:C)	0.0731707
Q9NQS5	529	Cl-C-C-Cl	0.0729907
Q9NQS5	448	C(-H)(=O)	0.0729779
Q9NQS5	27	>= 2 Na	0.0710461
Q9NQS5	747	Sc1cc(Cl)ccc1	0.0710345
Q9NQS5	170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	0.0702216
Q9NQS5	527	C:C:N-[#1]	0.0697033
Q9NQS5	820	CC1C(S)CCCC1	0.0696711
Q9NQS5	666	C=C-C-O-C	0.0688144
Q9NQS5	265	Li-B	0.068
Q9NQS5	36	>= 8 S	0.0675748
Q9NQS5	806	OC1CC(Cl)CCC1	0.0675674
Q9NQS5	715	Cc1ccc(S)cc1	0.0658635
Q9NQS5	598	Cl-C:C:C-C	0.0658127
Q9NQS5	850	SC1CC(S)CC1	0.0649771
Q9NQS5	499	N-C:C:N	0.0644311
Q9NQS5	295	C-As	0.0601359
Q9NQS5	390	N(~C)(~C)	0.0590068
Q9NQS5	561	Cl-C-C=O	0.0585465
Q9NQS5	437	C(-C)(-N)(=C)	0.0574527
Q9NQS5	143	>= 1 any ring size 5	0.0555793
Q9NQS5	346	C(~C)(~H)(~O)	0.0519731
Q9NQS5	366	C(~H)(~O)	0.051355
Q9NQS5	503	Cl-C:C-[#1]	0.0508209
Q9NQS5	339	C(~C)(~C)(~H)(~O)	0.0484012
Q9NQS5	644	C-C=N-N-C	0.0478
Q9NQS5	849	OC1CC(Br)CC1	0.0473131
Q9NQS5	280	B-S	0.047121
Q9NQS5	481	O-S-C:C	0.0450033
Q9NQS5	656	C-C-N-C-C	0.0444134
Q9NQS5	8	>= 4 B	0.0439783
Q9NQS5	120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	0.0439104
Q9NQS5	102	>= 1 Nd	0.0435891
Q9NQS5	765	Oc1c(Br)cccc1	0.0435258
Q9NQS5	138	>= 2 saturated or aromatic nitrogen-containing ring size 4	0.0430678
Q9NQS5	665	N-C:C-C-C	0.0426709
Q9NQS5	679	C-C-C-C-C-C	0.0424037
Q9NQS5	82	>= 1 Te	0.0423204
Q9NQS5	423	N=O	0.0422527
Q9NQS5	592	N-C-C-C-C	0.0421791
Q9NQS5	105	>= 1 Eu	0.041668

Q9NQS5	530	N:C-C:C	0.0414859
Q9NQS5	255	>= 1 aromatic ring	0.0409387
Q9NQS5	607	N-C-C-C:C	0.0406245
Q9NQS5	347	C(~C)(~H)(~O)(~O)	0.0397258
Q9NQS5	244	>= 1 saturated or aromatic heteroatom-containing ring size 9	0.039606
Q9NQS5	141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	0.0395203
Q9NQS5	627	O=[As]-C:C:C	0.0388273
Q9NQS5	502	N-C=C-[#1]	0.0383152
Q9NQS5	310	O-Mg	0.0380626
Q9NQS5	219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7	0.0376245
Q9NQS5	315	O-K	0.0374566
Q9NQS5	474	S:C:C:N	0.0368385
Q9NQS5	858	ClC1CC(Br)CC1	0.0361207
Q9NQS5	159	>= 3 saturated or aromatic nitrogen-containing ring size 5	0.0354754
Q9NQS5	246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9	0.0352373
Q9NQS5	395	N(~C)(~O)	0.033532
Q9NQS5	751	Nc1cc(Br)ccc1	0.0325867
Q9NQS5	201	>= 4 saturated or aromatic nitrogen-containing ring size 6	0.0306846
Q9NQS5	28	>= 1 Si	0.0304011
Q9NQS5	150	>= 2 any ring size 5	0.030367
Q9NQS5	187	>= 2 saturated or aromatic nitrogen-containing ring size 6	0.0302647
Q9NQS5	305	N-S	0.0299815
Q9NQS5	802	CC1CC(Br)CCC1	0.0297021
Q9NQS5	268	Li-F	0.0296684
Q9NQS5	14	>= 1 N	0.0292821
Q9NQS5	709	C-C(C)-C-C-C	0.027636
Q9NQS5	485	N:C:C:N	0.0275201
Q9NQS5	44	>= 2 Br	0.0274866
Q9NQS5	547	N-C:C-N	0.0272347
Q9NQS5	239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8	0.0270342
Q9NQS5	632	C-C-O-C:C	0.0262867
Q9NQS5	738	Cc1cc(Cl)ccc1	0.0258734
Q9NQS5	161	>= 3 unsaturated non-aromatic carbon-only ring size 5	0.0258661
Q9NQS5	29	>= 2 Si	0.0258587
Q9NQS5	699	O-C-C-C-C-C(C)-C	0.0251382
Q9NQS5	633	N-C-C:C-C	0.0242787
Q9NQS5	272	B-H	0.0235398
Q9NQS5	436	C(-C)(-H)(=O)	0.0218286
Q9NQS5	618	C:C-C-C:C	0.0212441
Q9NQS5	111	>= 1 Tm	0.0211725
Q9NQS5	132	>= 1 saturated or aromatic heteroatom-containing ring size 4	0.0209682
Q9NQS5	163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	0.0208251
Q9NQS5	69	>= 1 Sr	0.0206778
Q9NQS5	846	OC1CC(S)CC1	0.0200741
Q9NQS5	825	OC1C(S)CCCC1	0.0197837
Q9NQS5	218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7	0.0190952

Q9NQS5	877	NC1C(Br)CCC1	0.0190553
Q9NQS5	252	>= 1 unsaturated non-aromatic carbon-only ring size 10	0.0188048
Q9NQS5	19	>= 2 O	0.018797
Q9NQS5	18	>= 1 O	0.0186374
Q9NQS5	844	CC1CC(Br)CC1	0.0185697
Q9NQS5	480	C:S:C-C	0.0185295
Q9NQS5	241	>= 1 any ring size 9	0.0184785
Q9NQS5	576	N=C-C:C-[#1]	0.0184754
Q9NQS5	421	C=S	0.0177061
Q9NQS5	623	O=C-C:C-C	0.017623
Q9NQS5	191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6	0.0175715
Q9NQS5	755	Cc1c(C)cccc1	0.0168753
Q9NQS5	683	N-C-C-C-C-C	0.0168092
Q9NQS5	606	O-C:C-C-C	0.0155507
Q9NQS5	323	P-H	0.0154521
Q9NQS5	383	C(~S)(:C)	0.0150791
Q9NQS5	518	O=C-N-N	0.0147487
Q9NQS5	845	OC1CC(O)CC1	0.013739
Q9NQS5	224	>= 2 unsaturated non-aromatic carbon-only ring size 7	0.013164
Q9NQS5	604	C-O-C-C:C	0.0131531
Q9NQS5	226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7	0.0126634
Q9NQS5	791	NC1CCC(N)CC1	0.0121947
Q9NQS5	610	C-O-C-O-C	0.0121893
Q9NQS5	586	C-S-C-C-C	0.011876
Q9NQS5	175	>= 5 unsaturated non-aromatic carbon-only ring size 5	0.0118398
Q9NQS5	721	Oc1ccc(N)cc1	0.0109397
Q9NQS5	240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8	0.0109191
Q9NQS5	303	N-Si	0.0107761
Q9NQS5	296	C-Se	0.010681
Q9NQS5	6	>= 1 B	0.0106439
Q9NQS5	722	Oc1ccc(Cl)cc1	0.0105725
Q9NQS5	387	C(:C)(:N)	0.0097266
Q9NQS5	214	>= 1 saturated or aromatic carbon-only ring size 7	0.0093789
Q9NQS5	817	BrC1CC(Br)CCC1	0.0092316
Q9NQS5	727	Sc1ccc(Br)cc1	0.0089688
Q9NQS5	470	C:C-C=C	0.0088084
Q9NQS5	24	>= 2 F	0.0086969
Q9NQS5	462	O-C-C=O	0.0082318
Q9NQS5	369	C(~H)(~Si)	0.0082017
Q9NQS5	468	O=S-C-N	0.0076146
Q9NQS5	724	Sc1ccc(S)cc1	0.0074186
Q9NQS5	669	Cl-C:C-C=O	0.0072772
Q9NQS5	869	OC1C(Cl)CCC1	0.006642
Q9NQS5	532	S-C:C-[#1]	0.0065271
Q9NQS5	588	O=C-C-C=O	0.0060652
Q9NQS5	772	Nc1c(Br)cccc1	0.0058219

Q9NQS5	276	B-O	0.0058037
Q9NQS5	358	C(~C)(:N)	0.0057194
Q9NQS5	284	C-C	0.0056872
Q9NQS5	157	>= 3 any ring size 5	0.0056224
Q9NQS5	375	C(~N)(~N)	0.0053553
Q9NQS5	98	>= 1 Bi	0.0053171
Q9NQS5	35	>= 4 S	0.0050754
Q9NQS5	202	>= 4 saturated or aromatic heteroatom-containing ring size 6	0.0050381
Q9NQS5	215	>= 1 saturated or aromatic nitrogen-containing ring size 7	0.0050366
Q9NQS5	823	CC1C(Br)CCCC1	0.005009
Q9NQS5	804	OC1CC(S)CCC1	0.00482
Q9NQS5	256	>= 1 hetero-aromatic ring	0.0047005
Q9NQS5	769	Sc1c(Br)cccc1	0.0046986
Q9NQS5	9	>= 2 C	0.0045874
Q9NQS5	404	N(:C)(:C)(:C)	0.004477
Q9NQS5	763	Oc1c(N)cccc1	0.0044145
Q9NQS5	38	>= 2 Cl	0.0037199
Q9NQS5	291	C-Si	0.0036966
Q9NQS5	93	>= 1 Pt	0.0035152
Q9NQS5	526	Cl-C:C-Cl	0.0034866
Q9NQS5	723	Oc1ccc(Br)cc1	0.003409
Q9NQS5	274	B-C	0.0032593
Q9NQS5	622	O=C-O-C:C	0.0032188
Q9NQS5	831	SC1C(Cl)CCCC1	0.003118
Q9NQS5	826	OC1C(N)CCCC1	0.0029956
Q9NQS5	279	B-P	0.0028713
Q9NQS5	101	>= 1 Pr	0.0028001
Q9NQS5	731	Clc1ccc(Cl)cc1	0.0024572
Q9NQS5	815	ClC1CC(Cl)CCC1	0.002354
Q9NQS5	235	>= 2 saturated or aromatic carbon-only ring size 8	0.0020319
Q9NQS5	60	>= 1 Ni	0.0019498
Q9NQS5	664	C-C=C-C=C	0.0018575
Q9NQS5	578	C-C:C-C:C	0.0017529
Q9NQS5	434	C(-C)(-H)(=C)	0.001661
Q9NQS5	107	>= 1 Tb	0.001606
Q9NQS5	860	CC1C(C)CCC1	0.0014699
Q9NQS5	408	O(~H)(~S)	0.0014329
Q9NQS5	325	As-H	0.0013429
Q9NQS5	328	C(~Br)(~C)(~C)	0.0012008
Q9NQS5	736	Cc1cc(S)ccc1	0.0011363
Q9NQS5	603	C-C:C:C-C	0.0011055
Q9NQS5	771	Nc1c(Cl)cccc1	0.0010851
Q9NQS5	350	C(~C)(~I)	0.0010529
Q9NQS5	243	>= 1 saturated or aromatic nitrogen-containing ring size 9	0.0009148
Q9NQS5	238	>= 2 unsaturated non-aromatic carbon-only ring size 8	0.0008004
Q9NQS5	675	Br-C-C-C:C	0.0007901

Q9NQS5	263	Li-H	0.0007204
Q9NQS5	425	P=O	0.0005564
Q9NQS5	352	C(~C)(~O)	0.0005368
Q9NQS5	750	Nc1cc(Cl)ccc1	0.0003112
Q9NQS5	634	C-C-C:C-C	0.0001725
Q9NQS5	207	>= 5 saturated or aromatic carbon-only ring size 6	0.0001072
Q9NQS5	231	>= 1 unsaturated non-aromatic carbon-only ring size 8	5.08E-05
Q9NQS5	76	>= 1 Pd	3.72E-05
Q9NQS5	136	>= 2 any ring size 4	2.88E-05
Q9NQS5	262	>= 4 hetero-aromatic rings	2.73E-05
Q9NQS5	195	>= 3 saturated or aromatic heteroatom-containing ring size 6	2.72E-05
Q9NQS5	110	>= 1 Er	2.32E-05
Q9NQS5	52	>= 1 Ca	2.28E-05
Q9NQS5	348	C(~C)(~H)(~P)	2.01E-05
Q9NQS5	321	Si-Si	1.42E-05
Q9NQS5	275	B-N	1.08E-05
Q9NQS5	137	>= 2 saturated or aromatic carbon-only ring size 4	9.86E-06
Q9NQS5	39	>= 4 Cl	-8.68E-07
Q9NQS5	413	S(~C)(~H)	-1.26E-05
Q9NQS5	5	>= 2 Li	-1.86E-05
Q9NQS5	50	>= 1 Mg	-2.52E-05
Q9NQS5	79	>= 1 In	-3.78E-05
Q9NQS5	629	S-C:C:C-N	-0.000157
Q9NQS5	668	C-C:C-C-C	-0.000157
Q9NQS5	298	C-I	-0.000224
Q9NQS5	725	Sc1ccc(N)cc1	-0.000231
Q9NQS5	186	>= 2 saturated or aromatic carbon-only ring size 6	-0.000303
Q9NQS5	520	C=C-C:C	-0.000328
Q9NQS5	718	Cc1ccc(Br)cc1	-0.000405
Q9NQS5	242	>= 1 saturated or aromatic carbon-only ring size 9	-0.000591
Q9NQS5	458	S(-O)(=O)	-0.000663
Q9NQS5	106	>= 1 Gd	-0.00077
Q9NQS5	749	Nc1cc(N)ccc1	-0.001052
Q9NQS5	402	N(~O)(:O)	-0.001082
Q9NQS5	165	>= 4 saturated or aromatic carbon-only ring size 5	-0.001271
Q9NQS5	109	>= 1 Ho	-0.001295
Q9NQS5	879	ClC1C(Br)CCC1	-0.001402
Q9NQS5	379	C(~N)(:N)	-0.001429
Q9NQS5	209	>= 5 saturated or aromatic heteroatom-containing ring size 6	-0.001448
Q9NQS5	451	C(-N)(=O)	-0.001508
Q9NQS5	808	SC1CC(S)CCC1	-0.001525
Q9NQS5	312	O-Al	-0.001554
Q9NQS5	812	NC1CC(N)CCC1	-0.001586
Q9NQS5	134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	-0.001877
Q9NQS5	790	SC1CCC(Br)CC1	-0.001953
Q9NQS5	56	>= 1 Cr	-0.002066

Q9NQS5	490	C-C-C=C	−0.002184
Q9NQS5	426	P=P	−0.002457
Q9NQS5	775	Brc1c(Br)cccc1	−0.002551
Q9NQS5	184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	−0.002554
Q9NQS5	833	NC1C(N)CCCC1	−0.00278
Q9NQS5	512	C-[As]-O-[#1]	−0.002889
Q9NQS5	510	[#1]-N-N-[#1]	−0.003149
Q9NQS5	508	S=C-N-C	−0.003154
Q9NQS5	22	>= 16 O	−0.003402
Q9NQS5	545	N-C:C-C	−0.00356
Q9NQS5	854	NC1CC(N)CC1	−0.003589
Q9NQS5	108	>= 1 Dy	−0.003754
Q9NQS5	61	>= 1 Cu	−0.003766
Q9NQS5	687	O=C-C-C-C=O	−0.003821
Q9NQS5	251	>= 1 saturated or aromatic heteroatom-containing ring size 10	−0.004065
Q9NQS5	523	N:C:C-C	−0.004114
Q9NQS5	855	NC1CC(Cl)CC1	−0.004474
Q9NQS5	407	O(~C)(~P)	−0.004693
Q9NQS5	593	N-C-C-C-N	−0.004934
Q9NQS5	122	>= 2 any ring size 3	−0.005011
Q9NQS5	550	Cl-C-C-C	−0.005055
Q9NQS5	442	C(-C)(=N)	−0.005213
Q9NQS5	370	C(~H)(:C)	−0.005269
Q9NQS5	464	N-C-C=C	−0.005374
Q9NQS5	261	>= 4 aromatic rings	−0.005386
Q9NQS5	260	>= 3 hetero-aromatic rings	−0.005546
Q9NQS5	483	N-S-C:C	−0.005552
Q9NQS5	813	NC1CC(Cl)CCC1	−0.005575
Q9NQS5	257	>= 2 aromatic rings	−0.005746
Q9NQS5	868	OC1C(N)CCC1	−0.005994
Q9NQS5	416	C=C	−0.006108
Q9NQS5	319	Al-Cl	−0.006145
Q9NQS5	686	O=C-C-C-C-O	−0.006315
Q9NQS5	608	C-C-C-C:C	−0.006685
Q9NQS5	64	>= 1 Ge	−0.006729
Q9NQS5	533	S-C:C-N	−0.006729
Q9NQS5	396	N(~C)(:C)	−0.006925
Q9NQS5	424	N=P	−0.007053
Q9NQS5	119	>= 1 unsaturated non-aromatic carbon-only ring size 3	−0.007159
Q9NQS5	549	N-C-C:C	−0.007438
Q9NQS5	70	>= 1 Y	−0.007633
Q9NQS5	113	>= 1 Tc	−0.007898
Q9NQS5	210	>= 5 unsaturated non-aromatic carbon-only ring size 6	−0.007982
Q9NQS5	34	>= 2 S	−0.008049
Q9NQS5	748	Sc1cc(Br)ccc1	−0.008113
Q9NQS5	585	C-C:C-N-C	−0.008234

Q9NQS5	583	Cl-C:C-O-C	−0.008277
Q9NQS5	546	N-C:C-[#1]	−0.008643
Q9NQS5	167	>= 4 saturated or aromatic heteroatom-containing ring size 5	−0.008688
Q9NQS5	75	>= 1 Rh	−0.009121
Q9NQS5	86	>= 1 Lu	−0.009121
Q9NQS5	832	SC1C(Br)CCCC1	−0.009312
Q9NQS5	595	C:C-C-C-C	−0.009988
Q9NQS5	746	Sc1cc(N)ccc1	−0.010043
Q9NQS5	55	>= 1 V	−0.010154
Q9NQS5	613	C-N-C-C-C	−0.010407
Q9NQS5	216	>= 1 saturated or aromatic heteroatom-containing ring size 7	−0.010552
Q9NQS5	124	>= 2 saturated or aromatic nitrogen-containing ring size 3	−0.010562
Q9NQS5	269	Li-P	−0.010795
Q9NQS5	814	NC1CC(Br)CCC1	−0.011153
Q9NQS5	554	Br-C-C-C	−0.011296
Q9NQS5	74	>= 1 Ru	−0.011334
Q9NQS5	430	C(-C)(-C)(=C)	−0.011417
Q9NQS5	570	C:C-C-C	−0.011514
Q9NQS5	253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10	−0.011584
Q9NQS5	677	C-C=C-C:C	−0.012062
Q9NQS5	657	C-N-C:C-C	−0.012427
Q9NQS5	174	>= 5 saturated or aromatic heteroatom-containing ring size 5	−0.012584
Q9NQS5	640	C=C-C-C-C	−0.012799
Q9NQS5	168	>= 4 unsaturated non-aromatic carbon-only ring size 5	−0.014405
Q9NQS5	770	Nc1c(N)cccc1	−0.014513
Q9NQS5	829	SC1C(S)CCCC1	−0.015078
Q9NQS5	185	>= 2 any ring size 6	−0.015592
Q9NQS5	154	>= 2 unsaturated non-aromatic carbon-only ring size 5	−0.015786
Q9NQS5	599	[#1]-C-C=C-[#1]	−0.017082
Q9NQS5	314	O-P	−0.017362
Q9NQS5	454	N(-C)(=O)	−0.017709
Q9NQS5	155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	−0.017933
Q9NQS5	809	SC1CC(N)CCC1	−0.018343
Q9NQS5	85	>= 1 Ba	−0.018596
Q9NQS5	249	>= 1 saturated or aromatic carbon-only ring size 10	−0.01923
Q9NQS5	123	>= 2 saturated or aromatic carbon-only ring size 3	−0.019397
Q9NQS5	591	Cl-C-C-C-C	−0.020221
Q9NQS5	142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	−0.020229
Q9NQS5	88	>= 1 Ta	−0.020305
Q9NQS5	62	>= 1 Zn	−0.020345
Q9NQS5	94	>= 1 Au	−0.021124
Q9NQS5	674	N-C-N-C:C	−0.021239
Q9NQS5	853	SC1CC(Br)CC1	−0.022327
Q9NQS5	519	N=C-N-C	−0.022354
Q9NQS5	504	N:C:N-C	−0.022597
Q9NQS5	446	C(-H)(=C)	−0.022599

Q9NQS5	283	C-H	−0.022811
Q9NQS5	317	F-S	−0.024031
Q9NQS5	411	P(~O)(~O)	−0.024181
Q9NQS5	842	CC1CC(N)CC1	−0.024429
Q9NQS5	441	C(-C)(=C)	−0.024693
Q9NQS5	560	N-C-N-C	−0.024756
Q9NQS5	500	C-S-C:C	−0.025292
Q9NQS5	104	>= 1 Sm	−0.025713
Q9NQS5	472	C:N:C-C	−0.025813
Q9NQS5	516	[#1]-C=C-[#1]	−0.026038
Q9NQS5	148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	−0.026695
Q9NQS5	299	N-H	−0.02692
Q9NQS5	760	Cc1c(Br)cccc1	−0.027152
Q9NQS5	286	C-O	−0.02773
Q9NQS5	739	Cc1cc(Br)ccc1	−0.02828
Q9NQS5	41	>= 1 K	−0.028443
Q9NQS5	78	>= 1 Cd	−0.02882
Q9NQS5	636	C-N-C-N-C	−0.029035
Q9NQS5	878	ClC1C(Cl)CCC1	−0.02999
Q9NQS5	292	C-P	−0.03019
Q9NQS5	410	P(~C)(~C)	−0.030342
Q9NQS5	313	O-Si	−0.030412
Q9NQS5	473	S-C:N:C	−0.031537
Q9NQS5	403	N(:C)(:C)	−0.032861
Q9NQS5	271	Li-Cl	−0.032946
Q9NQS5	863	CC1C(N)CCC1	−0.033595
Q9NQS5	254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10	−0.034739
Q9NQS5	405	O(~C)(~C)	−0.034999
Q9NQS5	534	S-C:C-O	−0.035632
Q9NQS5	389	C(:N)(:N)	−0.036487
Q9NQS5	400	N(~H)(:C)(:C)	−0.036896
Q9NQS5	133	>= 1 unsaturated non-aromatic carbon-only ring size 4	−0.037948
Q9NQS5	511	S=C-N-[#1]	−0.038306
Q9NQS5	865	CC1C(Br)CCC1	−0.038498
Q9NQS5	799	CC1CC(S)CCC1	−0.038618
Q9NQS5	278	B-Si	−0.039303
Q9NQS5	222	>= 2 saturated or aromatic nitrogen-containing ring size 7	−0.039353
Q9NQS5	482	C:N-C:C	−0.039791
Q9NQS5	870	OC1C(Br)CCC1	−0.039962
Q9NQS5	720	Oc1ccc(S)cc1	−0.040429
Q9NQS5	15	>= 2 N	−0.04049
Q9NQS5	330	C(~Br)(:C)	−0.040523
Q9NQS5	830	SC1C(N)CCCC1	−0.04434
Q9NQS5	471	S:C:C:C	−0.045845
Q9NQS5	794	ClC1CCC(Cl)CC1	−0.048086
Q9NQS5	290	C-Al	−0.048185

Q9NQS5	717	Cc1ccc(Cl)cc1	−0.048678
Q9NQS5	788	SC1CCC(N)CC1	−0.049091
Q9NQS5	53	>= 1 Sc	−0.050435
Q9NQS5	780	CC1CCC(Cl)CC1	−0.051876
Q9NQS5	544	O-C:C-O	−0.052166
Q9NQS5	450	C(-N)(=N)	−0.056498
Q9NQS5	259	>= 3 aromatic rings	−0.057067
Q9NQS5	540	C-N-C-[#1]	−0.057522
Q9NQS5	179	>= 1 saturated or aromatic carbon-only ring size 6	−0.057666
Q9NQS5	784	OC1CCC(N)CC1	−0.058662
Q9NQS5	304	N-P	−0.058971
Q9NQS5	852	SC1CC(Cl)CC1	−0.05917
Q9NQS5	193	>= 3 saturated or aromatic carbon-only ring size 6	−0.059459
Q9NQS5	528	[#1]-N-C-[#1]	−0.061907
Q9NQS5	757	Cc1c(S)cccc1	−0.062838
Q9NQS5	77	>= 1 Ag	−0.063487
Q9NQS5	171	>= 5 any ring size 5	−0.066952
Q9NQS5	355	C(~C)(:C)	−0.067759
Q9NQS5	741	Oc1cc(S)ccc1	−0.068188
Q9NQS5	465	O=S-C-C	−0.069268
Q9NQS5	353	C(~C)(~S)	−0.069493
Q9NQS5	391	N(~C)(~C)(~C)	−0.069674
Q9NQS5	217	>= 1 unsaturated non-aromatic carbon-only ring size 7	−0.072761
Q9NQS5	459	S(=O)(=O)	−0.075032
Q9NQS5	332	C(~C)(~C)	−0.075166
Q9NQS5	324	P-P	−0.075865
Q9NQS5	521	C:N-C-[#1]	−0.075865
Q9NQS5	524	C-C=C-C	−0.076892
Q9NQS5	140	>= 2 unsaturated non-aromatic carbon-only ring size 4	−0.076963
Q9NQS5	297	C-Br	−0.078025
Q9NQS5	620	C:C-O-C-C	−0.079695
Q9NQS5	630	O-C:C-O-C	−0.080467
Q9NQS5	0	>= 4 H	−0.08104
Q9NQS5	589	C-C:C-O-C	−0.08138
Q9NQS5	597	O=C-C-C:C	−0.083273
Q9NQS5	300	N-N	−0.08385
Q9NQS5	65	>= 1 As	−0.084641
Q9NQS5	492	N-C:O:C	−0.087117
Q9NQS5	365	C(~H)(~N)	−0.0872
Q9NQS5	49	>= 1 Be	−0.087687
Q9NQS5	818	CC1C(C)CCCC1	−0.090158
Q9NQS5	857	ClC1CC(Cl)CC1	−0.092537
Q9NQS5	17	>= 8 N	−0.093246
Q9NQS5	752	Clc1cc(Cl)ccc1	−0.093725
Q9NQS5	658	C-C-S-C-C	−0.094517
Q9NQS5	343	C(~C)(~Cl)(~H)	−0.094737

Q9NQS5	587	N-C:C-O-[#1]	−0.095426
Q9NQS5	258	>= 2 hetero-aromatic rings	−0.095704
Q9NQS5	873	SC1C(Cl)CCC1	−0.09609
Q9NQS5	851	SC1CC(N)CC1	−0.096906
Q9NQS5	10	>= 4 C	−0.098614
Q9NQS5	555	N=C-C=C	−0.102372
Q9NQS5	486	N-C:N:N	−0.102535
Q9NQS5	506	C-C:N:C	−0.103532
Q9NQS5	419	C#N	−0.104996
Q9NQS5	838	BrC1C(Br)CCCC1	−0.105113
Q9NQS5	236	>= 2 saturated or aromatic nitrogen-containing ring size 8	−0.105196
Q9NQS5	489	N-C-S-C	−0.105618
Q9NQS5	871	SC1C(S)CCC1	−0.107058
Q9NQS5	556	C=C-C-C	−0.10716
Q9NQS5	792	NC1CCC(Cl)CC1	−0.109145
Q9NQS5	326	As-As	−0.109319
Q9NQS5	805	OC1CC(N)CCC1	−0.109697
Q9NQS5	194	>= 3 saturated or aromatic nitrogen-containing ring size 6	−0.109992
Q9NQS5	152	>= 2 saturated or aromatic nitrogen-containing ring size 5	−0.111487
Q9NQS5	700	O-C-C-C-C-C-O-C	−0.1115
Q9NQS5	624	O=C-C:C-N	−0.112091
Q9NQS5	183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	−0.112309
Q9NQS5	811	SC1CC(Br)CCC1	−0.113507
Q9NQS5	237	>= 2 saturated or aromatic heteroatom-containing ring size 8	−0.115165
Q9NQS5	26	>= 1 Na	−0.115755
Q9NQS5	131	>= 1 saturated or aromatic nitrogen-containing ring size 4	−0.117579
Q9NQS5	422	N=N	−0.117728
Q9NQS5	33	>= 1 S	−0.118112
Q9NQS5	200	>= 4 saturated or aromatic carbon-only ring size 6	−0.118787
Q9NQS5	220	>= 2 any ring size 7	−0.119678
Q9NQS5	753	Clc1cc(Br)ccc1	−0.119899
Q9NQS5	293	C-S	−0.120199
Q9NQS5	783	OC1CCC(S)CC1	−0.121399
Q9NQS5	553	O=C-C=C	−0.121626
Q9NQS5	177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	−0.122694
Q9NQS5	429	C(#N)(-C)	−0.123241
Q9NQS5	273	B-B	−0.124025
Q9NQS5	3	>= 32 H	−0.124199
Q9NQS5	880	BrC1C(Br)CCC1	−0.124306
Q9NQS5	475	S-C=N-C	−0.124578
Q9NQS5	97	>= 1 Pb	−0.125596
Q9NQS5	83	>= 1 Xe	−0.12611
Q9NQS5	673	O=C-C=C-N	−0.126778
Q9NQS5	848	OC1CC(Cl)CC1	−0.127864
Q9NQS5	126	>= 2 unsaturated non-aromatic carbon-only ring size 3	−0.12823
Q9NQS5	164	>= 4 any ring size 5	−0.129015

Q9NQS5	495	C-N-C:C	−0.129077
Q9NQS5	732	Clc1ccc(Br)cc1	−0.129254
Q9NQS5	84	>= 1 Cs	−0.129749
Q9NQS5	728	Nc1ccc(N)cc1	−0.130774
Q9NQS5	338	C(~C)(~C)(~H)(~N)	−0.130976
Q9NQS5	767	Sc1c(N)cccc1	−0.131397
Q9NQS5	376	C(~N)(:C)	−0.131569
Q9NQS5	125	>= 2 saturated or aromatic heteroatom-containing ring size 3	−0.131719
Q9NQS5	116	>= 1 saturated or aromatic carbon-only ring size 3	−0.131861
Q9NQS5	781	CC1CCC(Br)CC1	−0.132132
Q9NQS5	95	>= 1 Hg	−0.132719
Q9NQS5	766	Sc1c(S)cccc1	−0.132732
Q9NQS5	127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	−0.1329
Q9NQS5	68	>= 1 Rb	−0.132962
Q9NQS5	733	Brc1ccc(Br)cc1	−0.133048
Q9NQS5	874	SC1C(Br)CCC1	−0.133212
Q9NQS5	729	Nc1ccc(Cl)cc1	−0.133324
Q9NQS5	7	>= 2 B	−0.133369
Q9NQS5	861	CC1C(O)CCC1	−0.135084
Q9NQS5	789	SC1CCC(Cl)CC1	−0.135348
Q9NQS5	494	O=C-C:N	−0.135892
Q9NQS5	118	>= 1 saturated or aromatic heteroatom-containing ring size 3	−0.138874
Q9NQS5	115	>= 1 any ring size 3	−0.140524
Q9NQS5	681	O-C-C-C-C-O	−0.14808
Q9NQS5	453	N(-C)(=C)	−0.150534
Q9NQS5	351	C(~C)(~N)	−0.150784
Q9NQS5	67	>= 1 Kr	−0.151084
Q9NQS5	621	N-C:C:C:N	−0.152409
Q9NQS5	543	O-C:C-N	−0.153101
Q9NQS5	710	C-C-C(C)-C-C	−0.153141
Q9NQS5	487	N-C=N-C	−0.154095
Q9NQS5	796	BrC1CCC(Br)CC1	−0.154614
Q9NQS5	797	CC1CC(C)CCC1	−0.156248
Q9NQS5	704	O=C-C-C-C-C-C-C	−0.15669
Q9NQS5	362	C(~Cl)(:C)	−0.157945
Q9NQS5	439	C(-C)(-N)(=O)	−0.166774
Q9NQS5	121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	−0.167002
Q9NQS5	460	C-C-C#C	−0.169371
Q9NQS5	427	C(#C)(-C)	−0.173766
Q9NQS5	676	N#C-C-C-C	−0.175798
Q9NQS5	734	Cc1cc(C)ccc1	−0.175903
Q9NQS5	349	C(~C)(~H)(~S)	−0.176459
Q9NQS5	301	N-O	−0.18586
Q9NQS5	398	N(~H)(~N)	−0.189111
Q9NQS5	282	B-Br	−0.193258
Q9NQS5	81	>= 1 Sb	−0.196884

Q9NQS5	447	C(-H)(=N)	−0.197844
Q9NQS5	417	C#C	−0.201519
Q9NQS5	798	CC1CC(O)CCC1	−0.208196
Q9NQS5	551	Cl-C-C-O	−0.214887
Q9NQS5	364	C(~F)(:C)	−0.218163
Q9NQS5	706	O=C-C-C-C-C(=O)-C	−0.226339
Q9NQS5	609	Cl-C-C-N-C	−0.227415
Q9NQS5	331	C(~Br)(:N)	−0.228405
Q9NQS5	479	S-C-S-C	−0.229587
Q9NQS5	491	C-N:C-[#1]	−0.235765
Q9NQS5	507	C-C-S-C	−0.240394
Q9NQS5	705	O=C-C-C-C-C(O)-C	−0.24045
Q9NQS5	694	O=C-C-C-C-C=O	−0.240863
Q9NQS5	515	N-N-C-C	−0.244682
Q9NQS5	162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	−0.251556
Q9NQS5	372	C(~H)(:C)(:N)	−0.252386
Q9NQS5	457	S(-C)(=O)	−0.25796
Q9NQS5	345	C(~C)(~H)(~N)	−0.259349
Q9NQS5	420	C=O	−0.261036
Q9NQS5	807	OC1CC(Br)CCC1	−0.280526
Q9NQS5	92	>= 1 Ir	−0.281399
Q9NQS5	690	O-C-C-C-C-C-O	−0.284671
Q9NQS5	864	CC1C(Cl)CCC1	−0.291735
Q9NQS5	876	NC1C(Cl)CC1	−0.293143
Q9NQS5	659	O-C-C-N-C	−0.297327
Q9NQS5	367	C(~H)(~O)(~O)	−0.29809
Q9NQS5	452	C(-O)(=O)	−0.301264
Q9NQS5	443	C(-C)(=O)	−0.308252
Q9NQS5	250	>= 1 saturated or aromatic nitrogen-containing ring size 10	−0.312224
Q9NQS5	13	>= 32 C	−0.316904
Q9NQS5	368	C(~H)(~S)	−0.317481
Q9NQS5	708	C-C(C)-C-C	−0.318376
Q9NQS5	232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8	−0.320894
Q9NQS5	289	C-Mg	−0.325502
Q9NQS5	745	Sc1cc(S)ccc1	−0.330599
Q9NQS5	371	C(~H)(:C)(:C)	−0.334214
Q9NQS5	172	>= 5 saturated or aromatic carbon-only ring size 5	−0.341506
Q9NQS5	707	O=C-C-C-C-C(N)-C	−0.341555
Q9NQS5	316	F-P	−0.344288
Q9NQS5	582	C-C-C-C-C	−0.345862
Q9NQS5	415	Si(~C)(~C)	−0.347213
Q9NQS5	380	C(~O)(~O)	−0.353243
Q9NQS5	777	CC1CCC(O)CC1	−0.353467
Q9NQS5	225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7	−0.358293
Q9NQS5	497	O-C:C:N	−0.360805
Q9NQS5	787	SC1CCC(S)CC1	−0.3625

Q9NQS5	662	O-C-C-O-C	−0.364102
Q9NQS5	160	>= 3 saturated or aromatic heteroatom-containing ring size 5	−0.365913
Q9NQS5	47	>= 2 I	−0.365972
Q9NQS5	71	>= 1 Zr	−0.393771
Q9NQS5	135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	−0.40209
Q9NQS5	42	>= 2 K	−0.405495
Q9NQS5	384	C(:C)(:C)	−0.409551
Q9NQS5	793	NC1CCC(Br)CC1	−0.418356
Q9NQS5	373	C(~H)(:N)	−0.420574
Q9NQS5	435	C(-C)(-H)(=N)	−0.431139
Q9NQS5	730	Nc1ccc(Br)cc1	−0.434045
Q9NQS5	406	O(~C)(~H)	−0.437453
Q9NQS5	649	O=N-C:C-O	−0.457522
Q9NQS5	596	N=C-N-C-C	−0.461343
Q9NQS5	307	N-Br	−0.469967
Q9NQS5	374	C(~H)(~H)(~H)	−0.470502
Q9NQS5	605	O=C-C-O-C	−0.477468
Q9NQS5	287	C-F	−0.48626
Q9NQS5	476	C-O-C=C	−0.493989
Q9NQS5	180	>= 1 saturated or aromatic nitrogen-containing ring size 6	−0.497011
Q9NQS5	563	O-C-O-C	−0.500617
Q9NQS5	440	C(-C)(-O)(=O)	−0.50344
Q9NQS5	356	C(~C)(:C)(:C)	−0.529502
Q9NQS5	412	S(~C)(~C)	−0.534953
Q9NQS5	488	N-C=N-[#1]	−0.542399
Q9NQS5	467	C=N-N-C	−0.544281
Q9NQS5	99	>= 1 La	−0.544988
Q9NQS5	513	S:C:C-[#1]	−0.550051
Q9NQS5	103	>= 1 Pm	−0.562054
Q9NQS5	198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6	−0.580597
Q9NQS5	264	Li-Li	−0.58451
Q9NQS5	381	C(~O)(:C)	−0.599587
Q9NQS5	619	O-C-C=C-C	−0.611263
Q9NQS5	129	>= 1 any ring size 4	−0.611826
Q9NQS5	158	>= 3 saturated or aromatic carbon-only ring size 5	−0.616373
Q9NQS5	756	Cc1c(O)cccc1	−0.617376
Q9NQS5	277	B-F	−0.620354
Q9NQS5	856	NC1CC(Br)CC1	−0.624596
Q9NQS5	682	O-C-C-C-C-N	−0.645146
Q9NQS5	385	C(:C)(:C)(:C)	−0.646543
Q9NQS5	306	N-Cl	−0.652814
Q9NQS5	153	>= 2 saturated or aromatic heteroatom-containing ring size 5	−0.654812
Q9NQS5	552	C:C-C:C	−0.65786
Q9NQS5	21	>= 8 O	−0.665781
Q9NQS5	382	C(~O)(:C)(:C)	−0.674886
Q9NQS5	73	>= 1 Mo	−0.703401

Q9NQS5	579	O=C-C-C-C	−0.72908
Q9NQS5	617	C-C-C-O-[#1]	−0.730475
Q9NQS5	493	O=C-C:C	−0.732944
Q9NQS5	737	Cc1cc(N)ccc1	−0.741009
Q9NQS5	445	C(-H)(-N)(=C)	−0.744585
Q9NQS5	692	O=C-C-C-C-C-C	−0.749351
Q9NQS5	678	C-C-C=C-C	−0.755671
Q9NQS5	758	Cc1c(N)cccc1	−0.779003
Q9NQS5	517	N-N-C-N	−0.779872
Q9NQS5	213	>= 1 any ring size 7	−0.782152
Q9NQS5	643	[#1]-C-C-N-[#1]	−0.833774
Q9NQS5	130	>= 1 saturated or aromatic carbon-only ring size 4	−0.859485
Q9NQS5	302	N-F	−0.862452
Q9NQS5	698	O-C-C-C-C-C-C-C	−0.867185
Q9NQS5	714	Cc1ccc(O)cc1	−0.86784
Q9NQS5	754	Brc1cc(Br)ccc1	−0.890727
Q9NQS5	59	>= 1 Co	−0.897961
Q9NQS5	354	C(~C)(~Si)	−0.926706
Q9NQS5	641	O-C-C-C=C	−0.946033
Q9NQS5	146	>= 1 saturated or aromatic heteroatom-containing ring size 5	−0.949001
Q9NQS5	80	>= 1 Sn	−0.968695
Q9NQS5	245	>= 1 unsaturated non-aromatic carbon-only ring size 9	−1.006167
Q9NQS5	333	C(~C)(~C)(~C)	−1.026642
Q9NQS5	859	BrC1CC(Br)CC1	−1.033614
Q9NQS5	188	>= 2 saturated or aromatic heteroatom-containing ring size 6	−1.039889
Q9NQS5	360	C(~Cl)(~Cl)	−1.062394
Q9NQS5	484	N-C:N:C	−1.066555
Q9NQS5	16	>= 4 N	−1.068956
Q9NQS5	762	Oc1c(S)cccc1	−1.088663
Q9NQS5	40	>= 8 Cl	−1.128678
Q9NQS5	562	Br-C-C=O	−1.142028
Q9NQS5	839	CC1CC(C)CC1	−1.158984
Q9NQS5	822	CC1C(Cl)CCCC1	−1.168317
Q9NQS5	697	C-C-C-C-C-C(C)-C	−1.178015
Q9NQS5	522	C-N-N-[#1]	−1.189691
Q9NQS5	428	C(#C)(-H)	−1.190427
Q9NQS5	650	O=C-N-C=O	−1.240671
Q9NQS5	169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	−1.255963
Q9NQS5	90	>= 1 Re	−1.270218
Q9NQS5	23	>= 1 F	−1.278575
Q9NQS5	663	O-C-C-O-[#1]	−1.300271
Q9NQS5	821	CC1C(N)CCCC1	−1.385976
Q9NQS5	819	CC1C(O)CCCC1	−1.453946
Q9NQS5	96	>= 1 Tl	−1.476328
Q9NQS5	336	C(~C)(~C)(~C)(~N)	−1.565024
Q9NQS5	359	C(~C)(:N)(:N)	−1.615093

Q9NQS5	145	>= 1 saturated or aromatic nitrogen-containing ring size 5	−1.644117
Q9NQS5	645	O=C-N-C-C	−1.64493
Q9NQS5	12	>= 16 C	−1.663418
Q9NQS5	344	C(~C)(~H)	−1.975312
Q9NQS5	759	Cc1c(Cl)cccc1	−2.017141
Q9NQS5	800	CC1CC(N)CCC1	−2.089555
Q9NQS5	639	O-C-C-C-O	−2.154135
Q9NQS5	45	>= 4 Br	−2.279043
Q9NQS5	466	N#C-C=C	−2.456301

Fingerprints（continued)

P	Q
4.0698061	0.864163
2.4667376	0.2804956
1.6443046	0.6382439
1.7629042	0.4948533
1.4533677	0.5947507
1.8843174	0.1443888
1.7514346	0.2001957
1.9313106	0.0048743
1.6351868	0.2640466
1.8449156	0.0520341
1.5149721	0.3279325
1.6856959	2.99E-05
1.2771331	0.2819645
1.2911556	0.2603821
1.2747552	0.2373829
1.1574281	0.2034116
1.1001747	0.2144854
1.2935672	-0.001361
1.3219865	-0.030872
1.0278062	0.2603762
1.2688101	0.0007961
0.9277329	0.1768192
0.8006641	0.2523069
0.9014822	0.084917
0.6376504	0.3170941
0.7640875	0.1868128
0.9384841	0.0011115
0.929976	1.32E-05
0.6747339	0.2022327
0.7803778	0.0890266
0.5791393	0.2883506
0.8020184	0.0546743
0.7526303	0.0769469
0.8116953	3.54E-05
0.7327596	0.072534
0.78211	0.0065032
0.7767106	3.02E-05
0.7463518	0.0297243
0.7823293	-0.012705
0.7598297	7.05E-05
0.4386257	0.3153262
0.3573276	0.3584191
0.689689	3.62E-06
0.6994259	-0.012176

0.6839248	5.12E-05
0.6797533	-2.95E-06
0.4314731	0.2430201
0.668878	2.84E-05
0.6580382	0.0006187
0.3841174	0.270287
0.6454199	-0.000622
0.379896	0.2561395
0.6306926	2.22E-05
0.4831196	0.1376846
0.4179067	0.2007142
0.6128129	-0.002091
0.3920203	0.1964886
0.5883105	1.10E-05
0.2753016	0.3077588
0.593704	-0.014644
0.5529441	-0.004459
0.3354288	0.2068539
0.5036489	0.0264777
0.2626181	0.2663897
0.5196521	1.73E-05
0.5174832	9.80E-07
0.4932814	0.0017675
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