

Supplementary Information

Untargeted metabolomic analysis of pregnant women exposure to perfluorooctanoic acid at different degrees

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Table S1. Differential metabolites between the Exp-H vs M, Exp-M vs L and Exp-H vs L groups of pregnant women's urine samples detected by GC-MS

Groups	No.	Metabolites	Formula	RT(min)	Quant mass	VIP	P-value	FC	AUC
Exp-H vs M	1	L-Tyrosine	C9H11NO3	26.14	218	2.7581	0.0268	0.2099	0.753
	2	5-Aminovaleric acid	C21H42O4	19.74	174	2.6128	0.0287	0.4477	0.687
	3	Nicotinic Acid	C6H5NO2	12.94	180	2.5681	0.0153	0.5445	0.642
	4	(-)-Catechin	C15H14O6	12.91	254	2.4157	0.0094	0.078	0.606
	5	Gluconic Acid	C6H12O7	27.11	147	2.3536	0.0228	0.1366	0.648
	6	Glycerol	C3H8O3	11.92	205	2.3252	0.028	0.2416	0.746
	7	Phenyllactic acid	C9H10O3	18.76	147	2.2475	0.0152	0.3652	0.693
	8	D-Xylose	C5H10O5	19.27	204	2.1433	0.0018	0.4649	0.711
	9	Sucrose	C12H22O11	17.48	141	1.9866	0.0362	0.6363	0.776
	10	Indoxyl Sulfate	C8H7NO4S	21.46	277	1.984	0.0013	0.4826	0.746
	11	3-(3-Hydroxyphenyl)-3-Hydroxypropionic Acid	C9H10O4	24.41	267	1.9094	0.0493	0.2988	0.63
	12	Erucic acid	C22H42O2	27.63	359	1.8356	0.0471	0.6346	0.694
	13	Ferulic Acid	C6H12N2O3	28.59	338	1.7277	0.0349	0.3699	0.629
	14	Tromethamine	C4H11NO3	17.11	306	1.6252	0.0316	0.5566	0.65

15	Ciliatine	C2H8NO3P	11.91	299	1.4445	0.0326	0.6488	0.679
16	4-Deoxyerythronic acid	C4H8O4	13.58	117	1.3444	0.0223	0.7048	0.716
17	L-Kynurenine	C10H12N2O3	25.5	209	1.0033	0.0224	0.452	0.638
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1	Pantothenic Acid	C9H17NO5	16.66	157	3.293	0.0014	5.6009	0.72
2	Dehydroabiatic acid	C20H28O2	22.87	355	2.9873	0.0271	5.2238	0.748
3	L-Cysteine	C3H7NO2S	16.48	100	2.9792	0.0291	3.8223	0.79
4	Coniferin	C16H22O8	21.18	179	2.7175	0.0028	3.2632	0.687
5	5-Aminovaleric acid	C21H42O4	19.74	174	2.7035	0.0231	2.4229	0.701
6	Catechin	C15H14O6	23.19	300	2.5157	0.0321	2.1974	0.664
7	Ciliatine	C2H8NO3P	11.91	299	2.2949	0.0161	1.6338	0.699
8	L-Threonic acid	C4H8O5	17.87	243	2.1935	0.0163	3.7129	0.628
9	Purine	C5H4N4	14	102	2.1507	0.0152	2.7839	0.66
10	Maltitol	C12H24O11	22.95	103	2.1264	0.0111	3.0789	0.63
11	Allantoin	C4H6N4O3	9.52	100	2.0042	0.0376	2.16	0.674
12	L-Tyrosine	C9H11NO3	26.14	218	1.9544	0.0398	3.7552	0.648
13	2'-Deoxyguanosine	C10H13N5O4	24.46	285	1.9462	0.013	1.7697	0.68
14	(-)-Catechin	C15H14O6	12.91	254	1.874	0.0263	5.3393	0.581

Exp-M vs L

	15	N-Acetylgalactosamine	C8H15NO6	28.3	103	1.6628	0.0451	1.9067	0.669
Exp-H vs L	1	Resveratrol	C14H12O3	27.48	444	4.3882	0.0266	12.9604	0.701
	2	UDP-L-arabinose	C14H22N2O16P2	21.35	166	3.6317	0.0352	0.2584	0.693
	3	L-Cysteine	C3H7NO2S	16.48	100	3.5212	0.0067	3.7221	0.841
	4	Dehydroabietic acid	C20H28O2	22.87	355	3.3255	0.0025	3.8633	0.802
	5	5-Hydroxy-3-Indoleacetic Acid	C7H8O5	30.06	290	3.2893	0.0156	0.1395	0.732
	6	Epsilon-Caprolactam	C6H11NO	7.77	102	3.0254	0.0008	2.7819	0.742
	7	L-Threo-2-pentulose	C5H10O5	20.9	137	2.45	0.0454	0.3766	0.687
	8	Catechol	C6H6O2	12.91	210	2.4494	0.0386	3.7582	0.627
	9	Ferulic Acid	C6H12N2O3	28.59	338	2.0585	0.0044	0.2797	0.657
	10	Alpha-Tocopherol	C29H50O2	25.6	198	2.0096	0.0107	3.0708	0.67
	11	m-Cresol	C7H8O	15.49	218	1.9544	0.0133	0.2166	0.628
	12	Glutamyl-Valine	C10H18N2O5	21.09	417	1.7737	0.0196	3.4014	0.608
	13	3-Hydroxyphenylacetic acid	C8H8O3	19.33	164	1.7638	0.0261	4.4952	0.663
	14	Coniferin	C16H22O8	21.18	179	1.6664	0.0316	2.6773	0.652
	15	Triacetin	C9H14O6	20.15	175	1.565	0.0383	0.5962	0.663
	16	N-Carbamylglutamate	C12H24O2	25.27	257	1.5358	0.0351	0.3462	0.602

17	Butylamine	C4H11N	8.59	174	1.4683	0.0095	1.5369	0.732
18	N-Acetylgalactosamine	C8H15NO6	28.3	103	1.4174	0.0463	1.8789	0.639
19	D-Xylose	C5H10O5	19.27	204	1.3631	0.038	0.5006	0.626
20	Orotic acid	C5H4N2O4	22.23	254	1.2784	0.043	0.2781	0.597
21	beta-Alanine	C3H7NO2	15.3	174	1.1445	0.0393	1.6617	0.634

Table S2. Differential metabolites between the Exp-H vs M, Exp-M vs L and Exp-H vs L groups of pregnant women's urine samples detected by LC-MS

Groups	No.	Metabolites	Formula	m/z	RT (min)	Ion mode	VIP	P-value	FC	AUC
Exp-H vs M	1	Allantoic acid	C4H8N4O4	175.047	0.6967	neg	1.1048	0.0043	2.3594	0.709
	2	3-Methoxy-4-hydroxyphenylethyleneglycol sulfate	C9H12O7S	263.023	7.0671	neg	1.0981	0.0264	2.1274	0.622
	3	S-sulphocysteine	C3H7NO5S2	199.969	0.6967	neg	2.3375	0.005	1.9124	0.683
	4	Adenine	C5H5N5	136.062	0.8107	pos	1.564	0.0098	1.9026	0.674
	5	Urocanic acid	C6H6N2O2	156.0771	0.9999	pos	6.5422	0.0031	1.6468	0.740
	6	Protocatechuic acid	C7H6O4	153.0192	6.7094	neg	1.1193	0.0392	1.6186	0.634
	7	N-Acetylmannosamine	C8H15NO6	222.0975	0.7644	pos	2.4757	0.0004	1.5517	0.763

8	Fumaric acid	C4H4O4	134.045	0.7644	pos	1.4485	0.0049	1.5447	0.698
9	cis-Aconitic acid	C6H6O6	175.024	1.2287	pos	2.5225	0.003	1.4852	0.718
10	Citric acid	C6H8O7	210.0611	1.2287	pos	11.4493	0.0032	1.4718	0.709
11	D-Alanyl-D-alanine	C6H12N2O3	161.0923	0.7759	pos	1.0783	0.0034	1.4561	0.714
12	N-Acetyl-L-glutamate 5-semialdehyde	C7H11NO4	191.1029	0.7526	pos	1.1636	0.0089	1.4189	0.707
13	Uric acid	C5H4N4O3	169.0359	1.1919	pos	13.4813	0.0273	1.3642	0.658
14	Oxypurinol	C5H4N4O2	153.041	1.3305	pos	4.8711	0.0096	1.3493	0.699
15	L-Glyceric acid	C3H6O4	151.026	1.3397	neg	5.7769	0.0088	1.3414	0.706
16	3-Furoic acid	C5H4O3	111.0086	1.2081	neg	3.1047	0.0093	1.339	0.688
17	5-Aminoimidazole	C3H5N3	84.0558	14.8939	pos	2.1946	0.0035	1.3338	0.728
18	Oxalic acid	C2H2O4	88.988	14.7303	neg	3.5034	0.0173	1.3299	0.703
19	Aminoacetone	C3H7NO	74.0602	0.8342	pos	2.1445	0.042	1.3235	0.668
20	Diketogulonic acid	C6H8O7	191.0195	1.2081	neg	30.6455	0.0108	1.3222	0.689
21	Glycine	C2H5NO2	76.0394	14.7771	pos	1.2957	0.0013	1.3023	0.748
22	3-Methylguanine	C6H7N5O	166.0727	1.2053	pos	7.6884	0.0002	1.3015	0.768
23	2-O-Methylcytosine	C5H7N3O	126.0664	14.8814	pos	1.8235	0.0083	1.2887	0.700

24	N6-Acetyl-L-lysine	C8H16N2O3	189.1236	0.7874	pos	1.8764	0.004	1.2825	0.709
25	Carbon monoxide	CO	72.993	14.7303	neg	1.6394	0.0358	1.2797	0.686
26	Cyanate	CHNO	88.0039	14.9045	neg	2.3737	0.0375	1.276	0.689
27	Malonic acid	C3H4O4	103.0035	14.7303	neg	1.0398	0.0416	1.273	0.680
28	Iminoaspartic acid	C4H5NO4	130.0144	14.7303	neg	1.3067	0.0464	1.2668	0.671
29	Pyrimidine	C4H4N2	81.0449	14.933	pos	2.5652	0.0112	1.2636	0.710
30	Uracil	C4H4N2O2	113.0347	0.9999	pos	1.995	0.0138	1.2412	0.670
31	L-Homoserine	C4H9NO3	120.0657	0.7874	pos	2.3794	0.0272	1.2345	0.631
32	5-Aminopentanoic acid	C5H11NO2	118.0864	0.9881	pos	3.602	0.0369	1.1794	0.713
33	N-Methylhydantoin	C4H6N2O2	115.0504	0.9999	pos	1.1566	0.0144	1.1472	0.678
34	D-Cysteine	C3H7NO2S	166.0178	0.791	neg	1.0881	0.0284	1.1377	0.669
35	Arabinonic acid	C5H10O6	165.0403	0.6967	neg	4.6472	0.0335	1.1271	0.669
36	Oxoglutaric acid	C5H6O5	191.0196	0.8385	neg	9.2877	0.0473	0.8377	0.669
37	L-Gulonolactone	C6H10O6	177.0403	0.767	neg	2.5522	0.0148	0.8223	0.672
38	2-Methyl-3-oxopropanoic acid	C4H6O3	147.0298	0.791	neg	1.4758	0.0112	0.7978	0.674
39	Hypogeic acid	C16H30O2	272.2586	13.3224	pos	1.8274	0.0109	0.7915	0.702
40	3-Methylhistidine	C7H11N3O2	170.0927	0.646	pos	4.0719	0.029	0.7876	0.702

41	5-Methyldeoxycytidine	C10H15N3O4	286.1044	1.458	neg	1.1866	0.0046	0.7875	0.664	
42	Xanthurenic acid	C10H7NO4	204.03	5.2503	neg	1.3774	0.0336	0.7364	0.703	
43	Pantetheine	C11H22N2O4S	279.1376	7.2629	pos	1.3604	0.0228	0.7356	0.683	
44	3-Methylglutaconic acid	C6H8O4	145.0498	2.4902	pos	1.5143	0.0134	0.7226	0.666	
45	Indoxyl	C8H7NO	134.0602	5.8716	pos	2.3774	0.0209	0.7054	0.662	
46	Indoxyl sulfate	C8H7NO4S	212.0021	6.0592	neg	22.4466	0.0051	0.6773	0.693	
47	Valerylglycine	C7H13NO3	158.0821	4.1587	neg	2.0558	0.0108	0.6735	0.713	
48	L-Octanoylcarnitine	C15H29NO4	288.2171	10.2856	pos	1.2375	0.0279	0.6551	0.660	
49	3-Methylglutaryl carnitine	C13H23NO6	290.16	4.4836	pos	2.5436	0.0122	0.6401	0.710	
50	Ubiquinone Q2	C19H26O4	336.2171	10.7973	pos	1.5449	0.0071	0.6341	0.711	
51	Decanoylcarnitine	C17H33NO4	316.2485	12.9928	pos	1.2257	0.0035	0.5478	0.691	
52	Deoxyribose 5-phosphate	C5H11O7P	213.017	0.767	neg	1.1744	0.0242	0.4739	0.672	
53	N-Acetylcadaverine	C7H16N2O	145.1338	1.1919	pos	1.483	0.0025	0.401	0.774	
54	3-Hydroxyadipic acid	C6H10O5	161.0454	4.1448	neg	1.0454	0.0427	0.2101	0.527	
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Exp-M vs L	1	Pyrophosphate	H4O7P2	176.9357	0.6613	neg	3.3039	0.0224	2.5834	0.695
	2	Phosphoric acid	H3O4P	142.9749	0.6479	neg	2.1697	0.0066	2.1526	0.711
	3	N-Acetylcadaverine	C7H16N2O	145.1338	1.1919	pos	1.0254	0.0297	1.8317	0.691

4	Putrescine	C4H12N2	89.1074	0.5609	pos	1.2903	0	1.8216	0.849
5	beta-Glycerophosphoric acid	C3H9O6P	171.0062	0.6732	neg	1.4414	0.0038	1.8188	0.737
6	Pyridine	C5H5N	80.0496	0.7759	pos	2.2658	0.0003	1.8074	0.802
7	Methylimidazole acetaldehyde	C6H8N2O	125.0711	0.9109	pos	1.6303	0.0021	1.6756	0.796
8	Creatine	C4H9N3O2	132.0769	0.7526	pos	26.8511	0.0022	1.6075	0.743
9	beta-Alanine	C3H7NO2	88.0403	0.7314	neg	1.5068	0.0103	1.5799	0.737
10	Urea	CH4N2O	78.0663	0.7053	pos	1.1322	0	1.5747	0.837
11	Palmitoylethanolamide	C18H37NO2	300.29	13.3481	pos	1.1763	0.0272	1.5603	0.686
12	Taurine	C2H7NO3S	124.0072	0.6613	neg	2.9477	0.0309	1.5121	0.648
13	Palmitic acid	C16H32O2	274.2742	13.2324	pos	10.4034	0.0001	1.4867	0.798
14	Glyceryl phosphate	C3H9O6P	217.0117	0.8385	neg	1.529	0.0006	1.4793	0.752
15	dIMP	C10H13N4O7P	331.0454	0.767	neg	1.2175	0.0048	1.4728	0.712
16	Hypogeic acid	C16H30O2	272.2586	13.3224	pos	2.4761	0.0001	1.4178	0.777
17	Glycine	C2H5NO2	76.0394	14.7771	pos	1.2966	0.0002	1.3719	0.794
18	Indoxyl	C8H7NO	134.0602	5.8716	pos	1.5285	0.0351	1.3419	0.629
19	Ureidoisobutyric acid	C5H10N2O3	145.0617	1.3001	neg	1.2989	0.0313	1.331	0.611
20	Carbon monoxide	CO	72.993	14.7303	neg	1.4465	0.0216	1.3141	0.688

21	Galactaric acid	C6H10O8	209.0301	0.6967	neg	3.6103	0.0242	1.3137	0.676
22	Pyrroline hydroxycarboxylic acid	C5H7NO3	130.0501	6.3923	pos	2.9515	0.0006	1.3097	0.728
23	Oxalic acid	C2H2O4	88.988	14.7303	neg	2.4999	0.031	1.2916	0.678
24	Lactaldehyde	C3H6O2	119.0348	0.8385	neg	6.29	0.0002	1.2878	0.789
25	Iminoaspartic acid	C4H5NO4	130.0144	14.7303	neg	1.0953	0.0359	1.285	0.664
26	N-Acetylserine	C5H9NO4	146.0457	0.9444	neg	1.7327	0.0187	1.2626	0.658
27	L-Histidine	C6H9N3O2	156.0771	0.646	pos	5.2193	0.031	1.2554	0.648
28	5-Aminopentanoic acid	C5H11NO2	118.0864	0.9881	pos	4.7227	0.0056	1.2436	0.747
29	2,4-dihydroxybutanoic acid	C4H8O4	119.0348	0.997	neg	4.0679	0.0037	1.2196	0.711
30	Arachidic acid	C20H40O2	330.3369	13.8031	pos	2.8295	0.0432	1.2157	0.661
31	Pyrimidine	C4H4N2	81.0449	14.933	pos	1.6367	0.0449	1.1977	0.658
32	Nicotinuric acid	C8H8N2O3	179.0461	5.4009	neg	1.8779	0.0472	1.1948	0.651
33	Homocysteinesulfinic acid	C4H9NO4S	166.0177	0.8921	neg	1.0865	0.0205	1.1484	0.652
34	2-Hydroxyethanesulfonate	C2H6O4S	124.9912	0.7198	neg	3.0976	0.0265	1.133	0.653
35	5-Methylthioribose	C6H12O4S	181.0532	0.9759	pos	2.231	0.0325	1.1165	0.666
36	Erythritol	C4H10O4	167.0559	0.7198	neg	1.1426	0.0114	0.8163	0.700
37	cis-Aconitic acid	C6H6O6	175.024	1.2287	pos	1.616	0.0141	0.7812	0.687

38	N-alpha-Acetyl-L-arginine	C8H16N4O3	217.1298	0.9999	pos	1.5952	0.0056	0.7695	0.709	
39	N2-Succinyl-L-ornithine	C9H16N2O5	233.1134	1.2656	pos	1.0964	0.0135	0.7032	0.686	
40	Prostaglandin D2	C20H32O5	397.223	13.8165	neg	1.1367	0.0039	0.6605	0.750	
41	2-Aminobenzoic acid	C7H7NO2	138.0552	0.7526	pos	5.8693	0.0181	0.6524	0.712	
42	Norepinephrine sulfate	C8H11NO6S	250.0382	1.3569	pos	3.8164	0.0022	0.5927	0.720	
43	Cystathionine ketimine	C7H9NO4S	248.0233	1.2339	neg	2.1725	0.0003	0.5923	0.763	
44	Ribitol	C5H12O5	197.0665	0.7198	neg	3.1444	0.0423	0.5888	0.732	
45	Sulfolithocholylglycine	C26H43NO7S	512.2686	14.3371	neg	4.0449	0.0093	0.5559	0.688	
46	Taurolithocholic acid 3-sulfate	C26H45NO8S2	280.6219	14.4056	neg	2.0783	0.0073	0.5253	0.727	
47	Allantoic acid	C4H8N4O4	175.047	0.6967	neg	1.0892	0.013	0.4767	0.706	
48	Thiamine pyrophosphate	C12H19N4O7P2S+	424.0375	4.5003	neg	2.0328	0.0197	0.4437	0.616	
49	Gentisic acid	C7H6O4	153.0192	5.5378	neg	1.5932	0.0069	0.4352	0.663	
50	Thromboxane B2	C20H34O6	415.2337	13.4619	neg	1.1361	0.013	0.0586	0.784	
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Exp-H vs L	1	Homovanillin	C9H10O3	211.0611	5.0862	neg	2.1509	0.012	2.1528	0.656
	2	Adenine	C5H5N5	136.062	0.8107	pos	1.3218	0.0032	2.0275	0.673
	3	L-Cystine	C6H12N2O4S2	241.0314	0.658	pos	1.3906	0.0106	1.9048	0.677
	4	L-Serine	C3H7NO3	104.0352	0.6358	neg	1.1138	0.0082	1.8871	0.692

5	Putrescine	C4H12N2	89.1074	0.5609	pos	1.0386	0	1.8303	0.894
6	Glycine	C2H5NO2	76.0394	14.7771	pos	1.7069	0	1.7866	0.917
7	dIMP	C10H13N4O7P	331.0454	0.767	neg	1.4447	0.0003	1.7621	0.754
8	L-2-Amino-3-oxobutanoate	C4H7NO3	116.0352	0.9845	neg	1.2695	0.0022	1.7253	0.716
9	Oxalic acid	C2H2O4	88.988	14.7303	neg	4.3772	0	1.7177	0.831
10	Carbon monoxide	CO	72.993	14.7303	neg	2.2507	0	1.6816	0.829
11	Malonic acid	C3H4O4	103.0035	14.7303	neg	1.47	0	1.6807	0.828
12	S-sulphocysteine	C3H7NO5S2	199.969	0.6967	neg	1.2973	0.0432	1.6801	0.682
13	Fumaric acid	C4H4O4	134.045	0.7644	pos	1.0755	0.0016	1.6569	0.718
14	Aminoacetone	C3H7NO	74.0602	0.8342	pos	2.4046	0.0005	1.6507	0.751
15	Iminoaspartic acid	C4H5NO4	130.0144	14.7303	neg	1.7711	0.0001	1.6278	0.808
16	Taurine	C2H7NO3S	124.0072	0.6613	neg	2.5027	0.0105	1.6264	0.710
17	Palmitoylethanolamide	C18H37NO2	300.29	13.3481	pos	1.1363	0.0004	1.6033	0.749
18	N-Acetylmannosamine	C8H15NO6	222.0975	0.7644	pos	1.7421	0.0001	1.596	0.806
19	Creatine	C4H9N3O2	132.0769	0.7526	pos	13.5427	0.0175	1.5566	0.688
20	Cyanate	CHNO	88.0039	14.9045	neg	2.9241	0.0003	1.5562	0.790
21	1-Methylhistamine	C6H11N3	126.1028	0.585	pos	1.05	0.0002	1.5415	0.786

22	5-Aminoimidazole	C3H5N3	84.0558	14.8939	pos	2.128	0.0001	1.5383	0.804
23	Pyrimidine	C4H4N2	81.0449	14.933	pos	2.8781	0	1.5133	0.808
24	2-O-Methylcytosine	C5H7N3O	126.0664	14.8814	pos	1.8617	0.0001	1.5056	0.792
25	Carbon Dioxide	CO2	88.988	2.8131	neg	2.4318	0.0008	1.5032	0.753
26	Uric acid	C5H4N4O3	169.0359	1.1919	pos	9.8995	0.0031	1.5011	0.704
27	4-Hydroxybenzoic acid	C7H6O3	137.0243	5.6748	neg	1.266	0.0058	1.4896	0.671
28	Imidazolone	C3H4N2O	83.025	14.9841	neg	3.4271	0.001	1.4791	0.749
29	5-Aminopentanoic acid	C5H11NO2	118.0864	0.9881	pos	6.2706	0	1.4668	0.869
30	Ureidoisobutyric acid	C5H10N2O3	145.0617	1.3001	neg	1.2382	0.0031	1.4452	0.682
31	3-Aminopropionaldehyde	C3H7NO	74.0602	14.7638	pos	1.3279	0.0003	1.419	0.769
32	L-Homoserine	C4H9NO3	120.0657	0.7874	pos	2.3615	0.004	1.4049	0.754
33	Aminoadipic acid	C6H11NO4	162.0763	0.7759	pos	3.2345	0.0007	1.4018	0.748
34	Thymine	C5H6N2O2	125.0355	14.9436	neg	1.8925	0.0065	1.387	0.717
35	L-Glyceric acid	C3H6O4	151.026	1.3397	neg	3.8401	0.0013	1.3787	0.730
36	4-Imidazolone-5-propionic acid	C6H8N2O3	155.0461	14.9841	neg	1.3651	0.0078	1.375	0.713
37	Oxypurinol	C5H4N4O2	153.041	1.3305	pos	3.1403	0.001	1.3672	0.730
38	L-Valine	C5H11NO2	118.0864	0.6932	pos	3.6967	0.008	1.3607	0.704

39	Imidazole-4-acetaldehyde	C5H6N2O	109.0406	14.9841	neg	1.5054	0.0202	1.3271	0.688
40	l-Glutamic-gamma-semialdehyde	C5H9NO3	132.0657	1.3174	pos	1.0896	0.0136	1.3152	0.669
41	L-Histidine	C6H9N3O2	156.0771	0.646	pos	4.0695	0.0078	1.3082	0.679
42	Arachidic acid	C20H40O2	330.3369	13.8031	pos	2.9707	0.0068	1.302	0.708
43	Uracil	C4H4N2O2	113.0347	0.9999	pos	1.8823	0.0075	1.2973	0.712
44	Stearic acid	C18H36O2	302.3056	13.5954	pos	2.9882	0.0227	1.2913	0.644
45	Palmitic acid	C16H32O2	274.2742	13.2324	pos	5.2567	0.0149	1.2905	0.677
46	alpha-CEHC	C16H22O4	279.1593	14.0339	pos	4.7484	0.0125	1.2903	0.708
47	Homocysteinesulfinic acid	C4H9NO4S	166.0177	0.8921	neg	1.117	0.0022	1.2901	0.706
48	N-Acetyls erine	C5H9NO4	146.0457	0.9444	neg	1.102	0.0141	1.2645	0.672
49	Palmitaldehyde	C16H32O	258.2794	13.6084	pos	1.1289	0.0459	1.2632	0.641
50	Myristic acid	C14H28O2	246.243	11.7814	pos	1.2904	0.049	1.2607	0.650
51	3-Furoic acid	C5H4O3	111.0086	1.2081	neg	1.4943	0.0188	1.2502	0.660
52	N-Methylhydantoin	C4H6N2O2	115.0504	0.9999	pos	1.8196	0.0011	1.2493	0.762
53	Pyrroline hydroxycarboxylic acid	C5H7NO3	130.0501	6.3923	pos	2.2635	0.0054	1.2454	0.699
54	3-Methylguanine	C6H7N5O	166.0727	1.2053	pos	4.1446	0.0034	1.2314	0.713
55	Lactaldehyde	C3H6O2	119.0348	0.8385	neg	3.8549	0.0046	1.2283	0.704

56	Behenic acid	C22H44O2	358.3681	13.9185	pos	2.3232	0.0254	1.2236	0.687
57	N6-Acetyl-L-lysine	C8H16N2O3	189.1236	0.7874	pos	1.3244	0.0397	1.2183	0.688
58	D-Cysteine	C3H7NO2S	166.0178	0.791	neg	1.1983	0.002	1.2103	0.721
59	L-Aspartic acid	C4H7NO4	132.0301	0.7552	neg	1.3983	0.0142	1.2015	0.664
60	Glycolic acid	C2H4O3	75.0087	0.779	neg	1.2753	0.0304	1.1867	0.660
61	2-Hydroxyethanesulfonate	C2H6O4S	124.9912	0.7198	neg	2.3075	0.0343	1.1833	0.629
62	5-Methylthioribose	C6H12O4S	181.0532	0.9759	pos	2.0487	0.0024	1.1792	0.729
63	3-Hydroxyvaleric acid	C5H10O3	117.0556	3.2669	neg	1.9236	0.0427	1.1607	0.640
64	3-Butyn-1-al	C4H4O	86.0601	2.2096	pos	1.327	0.0086	1.1576	0.712
65	Pyrrole-2-carboxylic acid	C5H5NO2	129.066	0.7403	pos	2.2727	0.0071	1.1519	0.684
66	2-Methylglutaconic acid	C6H8O4	189.0403	1.4995	neg	1.6816	0.0208	0.8558	0.651
67	(N-acetylneuraminosyl (alpha2-6)lactosamine)	C25H42N2O19	673.2311	0.791	neg	1.5999	0.0006	0.8238	0.747
68	Homo-L-arginine	C7H16N4O2	189.1349	0.7168	pos	3.2111	0.0006	0.7799	0.746
69	Erythritol	C4H10O4	167.0559	0.7198	neg	1.2131	0.0004	0.7625	0.751
70	Threonolactone	C10H22O4Si2	307.1034	4.9649	neg	1.1622	0.0361	0.7369	0.668
71	N4-Acetylcytidine	C11H15N3O6	286.1036	4.2826	pos	1.7764	0.0274	0.7087	0.692

72	N-alpha-Acetyl-L-arginine	C8H16N4O3	217.1298	0.9999	pos	2.4544	0	0.6581	0.807
73	glycochenodeoxycholate-3-sulfate	C26H43NO8S	528.2635	13.3658	neg	2.4626	0.0236	0.6397	0.707
74	Deoxycholic acid 3-glucuronide	C30H48O10	567.3176	12.9553	neg	2.1267	0.0028	0.6231	0.728
75	Prostaglandin D2	C20H32O5	397.223	13.8165	neg	1.3022	0.0002	0.6141	0.773
76	N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfooxy)cholan-24-yl]-Glycine	C26H43NO8S	528.2636	13.2429	neg	2.2274	0.0009	0.6031	0.741
77	S-(2-carboxypropyl)-Cysteamine	C6H13NO2S	164.0742	2.1827	pos	2.1788	0.0049	0.6028	0.719
78	Cystathionine ketimine	C7H9NO4S	248.0233	1.2339	neg	1.5437	0.0009	0.5992	0.730
79	Sulfolithocholylglycine	C26H43NO7S	512.2686	14.3371	neg	2.5991	0.0176	0.5801	0.677
80	Ubiquinone Q2	C19H26O4	336.2171	10.7973	pos	1.4766	0.0013	0.5492	0.719
81	Norepinephrine sulfate	C8H11NO6S	250.0382	1.3569	pos	3.1655	0.0004	0.5262	0.757
82	Carnosol	C20H26O4	375.1812	10.2921	neg	1.1046	0.008	0.5089	0.716
83	Ribitol	C5H12O5	197.0665	0.7198	neg	2.9854	0.0132	0.5035	0.823
84	Decanoylcarnitine	C17H33NO4	316.2485	12.9928	pos	1.2857	0.0001	0.423	0.751