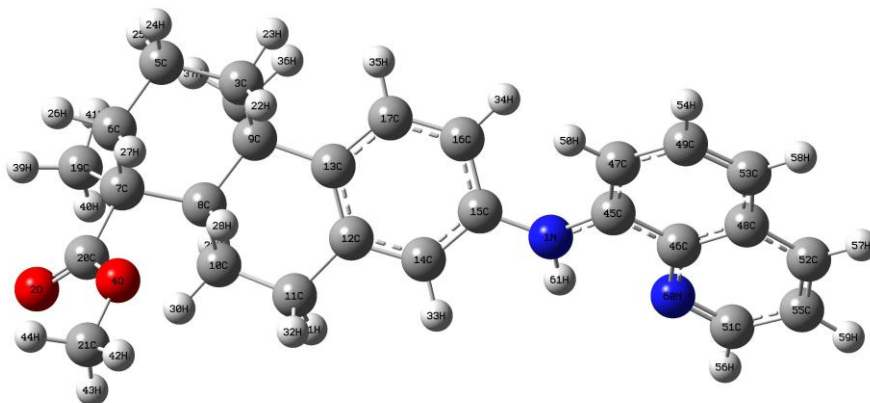
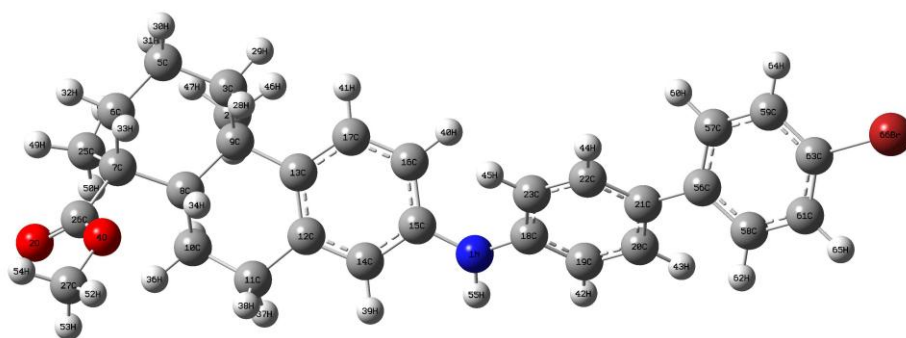


D



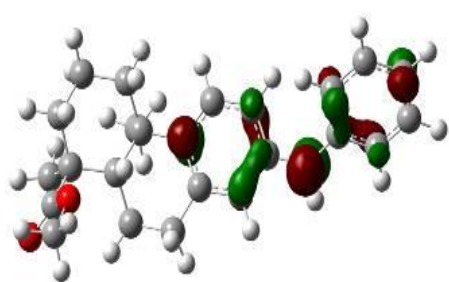
E



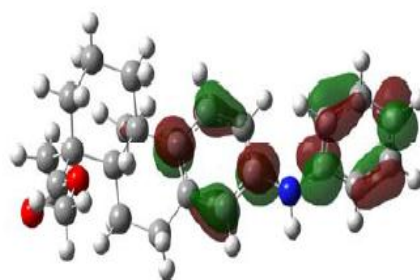
F

Fig. S1 Optimization geometry of A–F by B3LYP/6-31G*

A

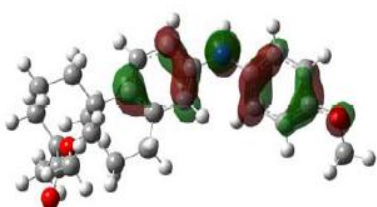


HOMO

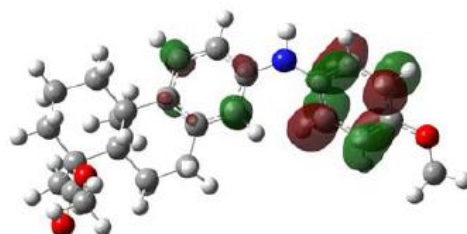


LUMO

B

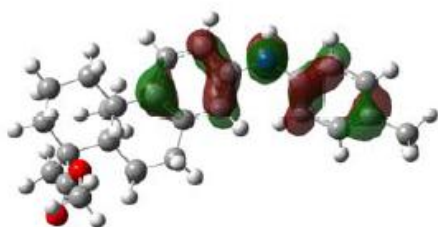


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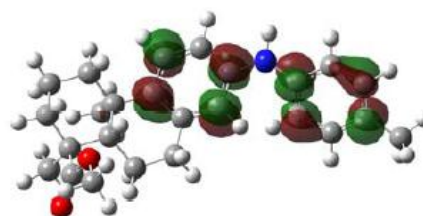


LUMO

C

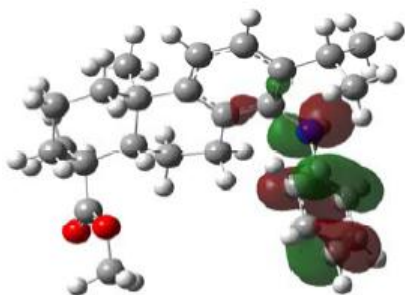


HOMO

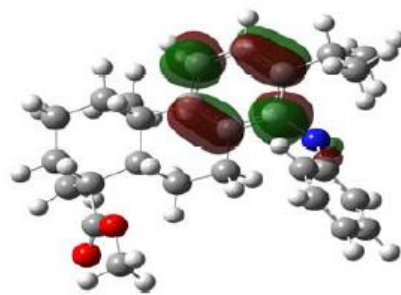


LUMO

D

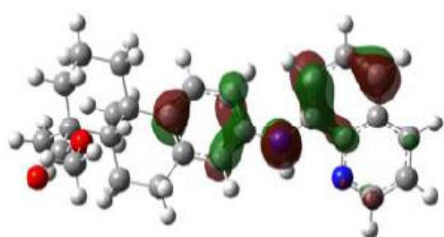


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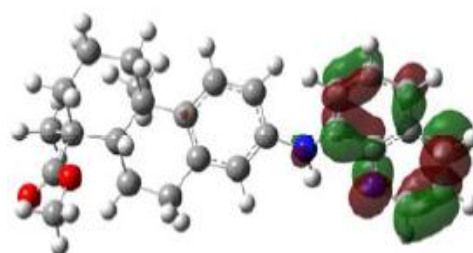


LUMO

E



HOMO

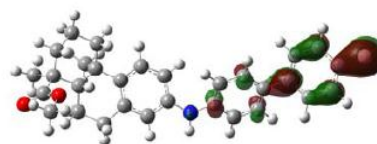


LUMO

F

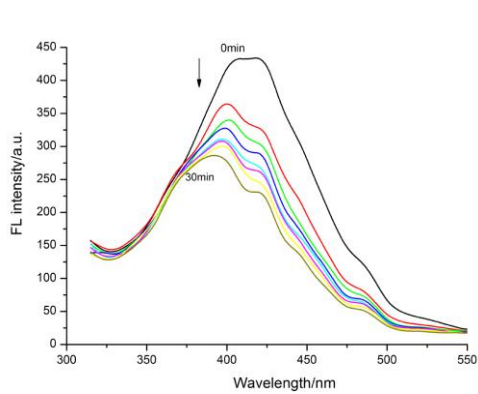


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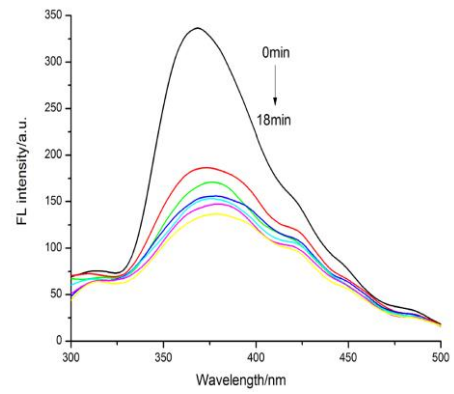


LUMO

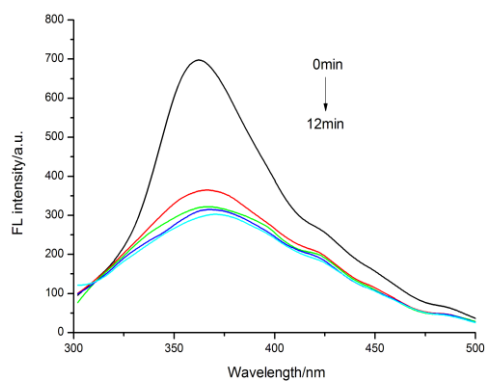
Fig. S2 Molecular orbital surfaces of A–F



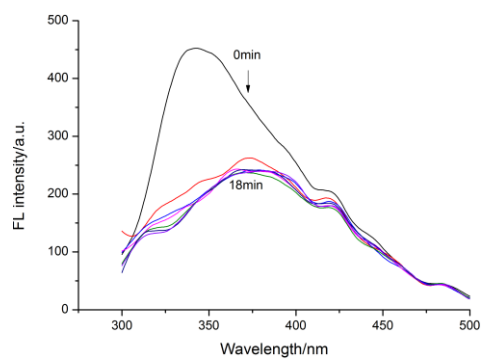
A



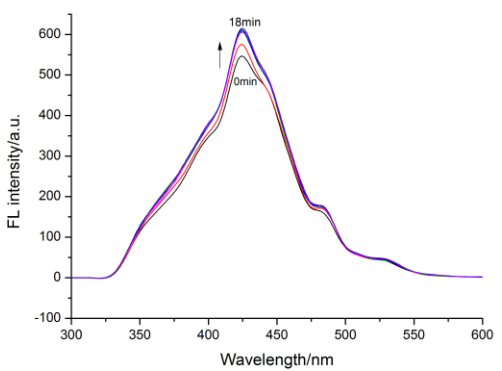
B



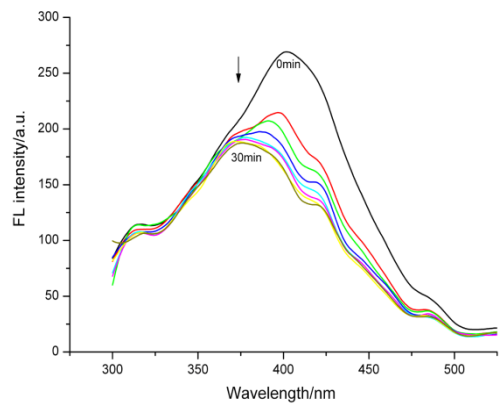
C



D

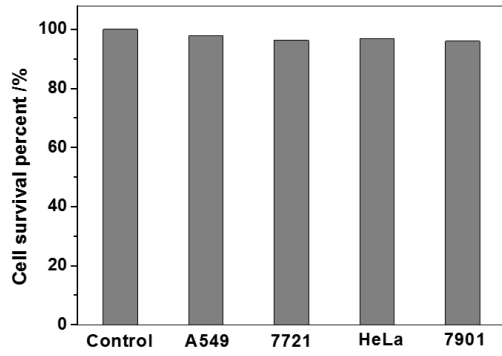


E

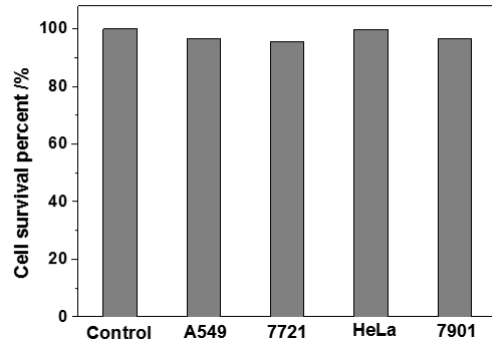


F

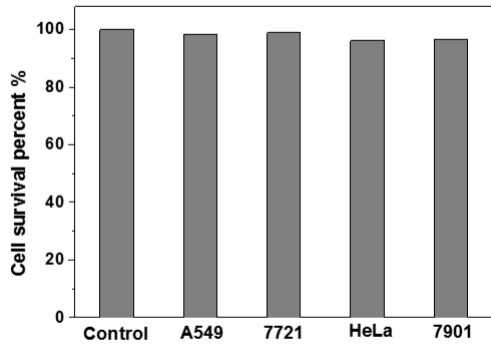
Fig. S3 Fluorescent emission spectra of **A–F** by UV irradiation



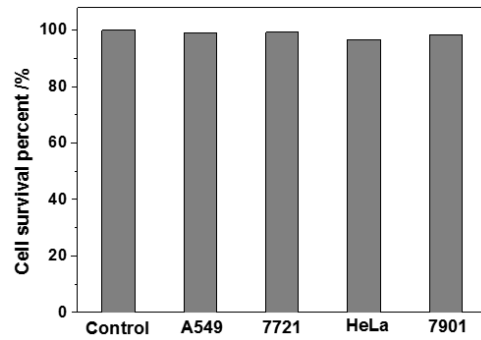
A



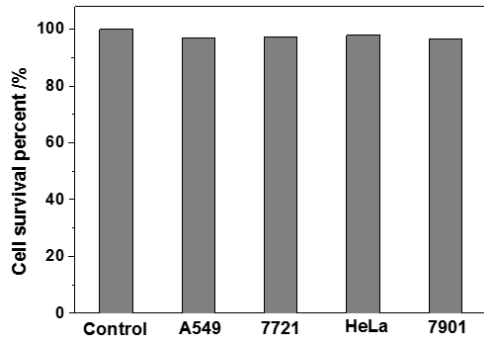
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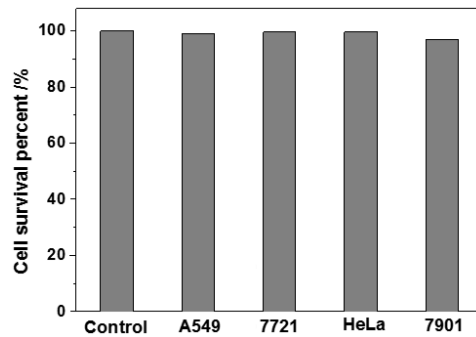
C



D



E



F

Fig. S4 Survival percent of cells incubated with A–F for 24h

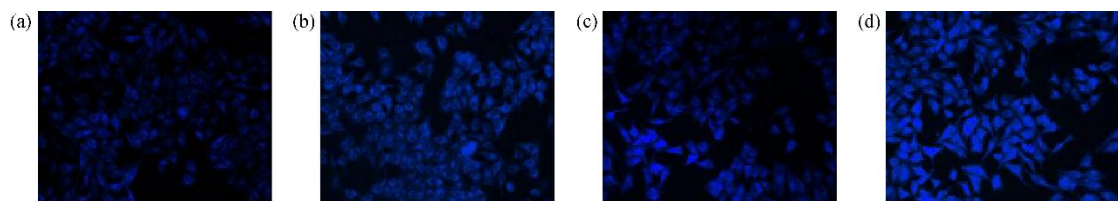


Fig. S5 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound A

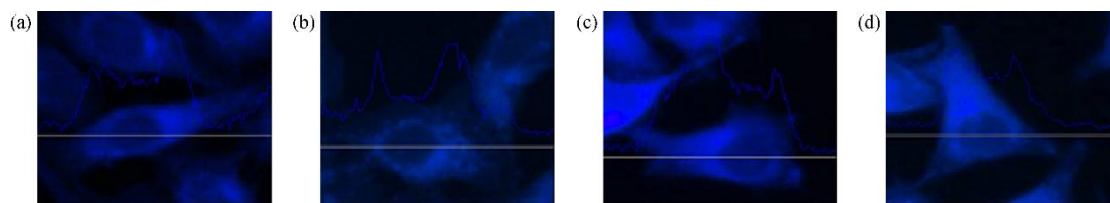


Fig. S6 Fluorescence distribution of cytoplasm and nuclear in compound **A** treated HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells

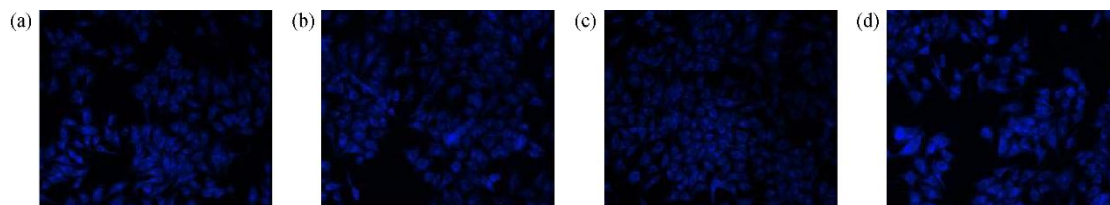


Fig. S7 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound **B**

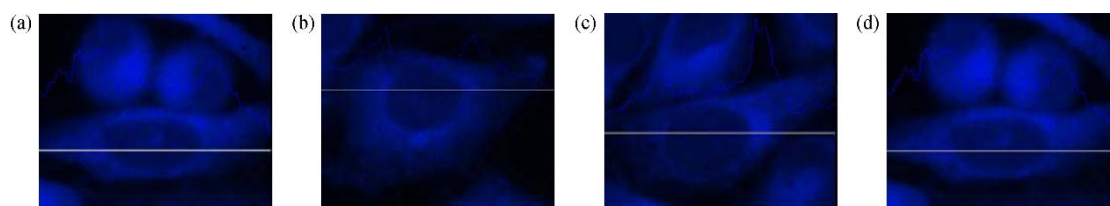


Fig. S8 Fluorescence distribution of cytoplasm and nuclear in compound **B** treated HeLa (a), 7721(b), 7901 (c), and A549 (d) cells

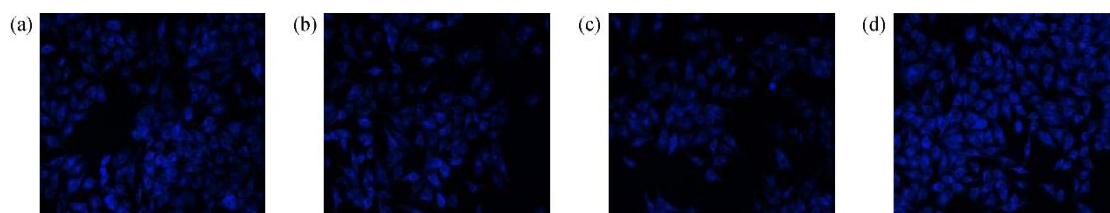


Fig. S9 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound **C**

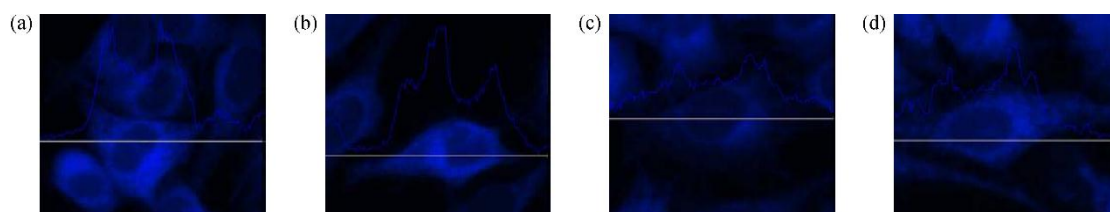


Fig. S10 Fluorescence distribution of cytoplasm and nuclear in compound **C** treated HeLa (a), 7721 (b), 7901(c), and A549 (d) cells

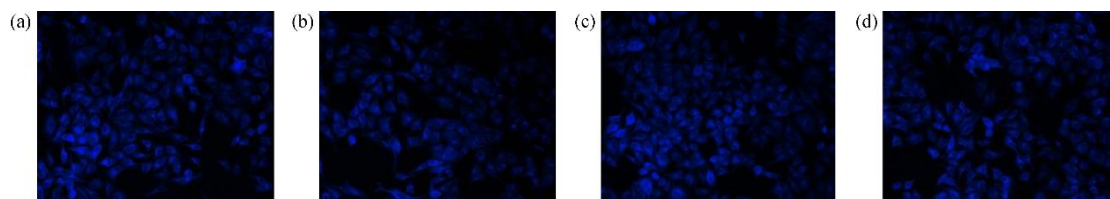


Fig. S11 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound **D**

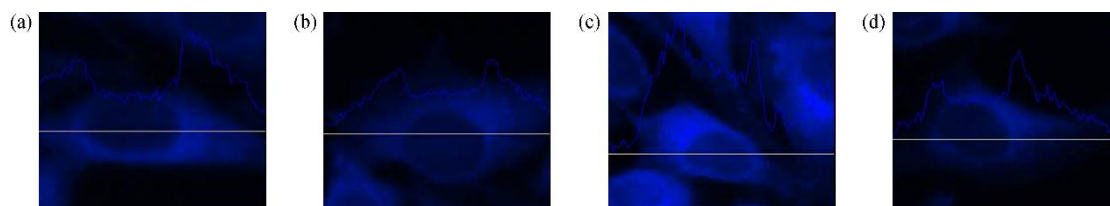


Fig. S12 Fluorescence distribution of cytoplasm and nuclear in compound **D** treated HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells

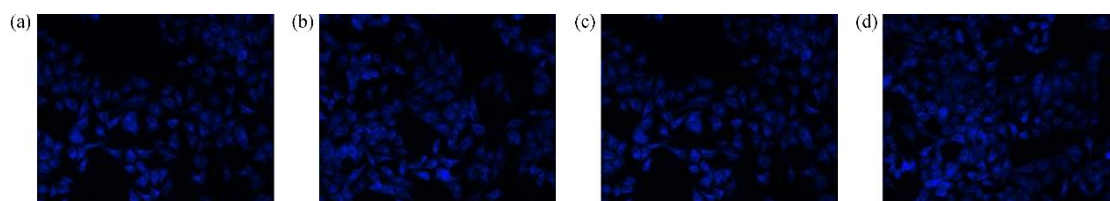


Fig. S13 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound **E**

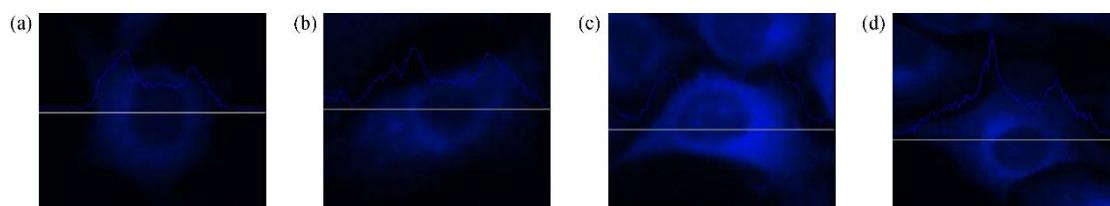


Fig. S14 Fluorescence distribution of cytoplasm and nuclear in compound **E** treated HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells

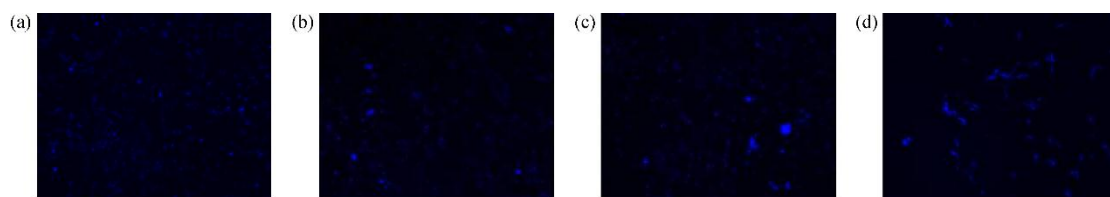


Fig. S15 Microscope fluorescence images of HeLa (a), 7721 (b), 7901 (c), and A549 (d) cells imaged after 4 h of treatment with compound **F**

Table S1 Bond lengths (Å), bond angles (°) and torsion angles (°) of **A–F**

	A	B	C	D	E	F
Bond lengths/Å						
N–C15	1.399	1.396	1.398	N–C14 1.438	1.399	1.401
N–C18	1.398	1.404	1.399	1.397	N–C45 1.378	1.393
N–H	1.010	1.009	1.009	1.012	1.015	1.010
C15–C14	1.400	1.400	1.399	1.407	1.400	1.399
C14–C12	1.398	1.401	1.401	1.418	1.397	1.398
C12–C13	1.409	1.408	1.408	1.409	1.410	1.409
C13–C17	1.404	1.405	1.405	1.401	1.403	1.404
C17–C16	1.390	1.387	1.387	1.388	1.390	1.389
C16–C15	1.404	1.406	1.405	1.400	1.404	1.403
C18–C19	1.407	1.400	1.405	1.406	C45–C46 1.445	1.407
C19–C20	1.391	1.397	1.393	1.394	C46–C48 1.428	1.388
C20–C21	1.396	1.397	1.400	1.395	C45–C47 1.391	1.406
C21–C22	1.395	1.401	1.400	1.397	C47–C49 1.411	1.404
C22–C23	1.394	1.387	1.391	1.391	C46–N 1.359	1.390
C23–C18	1.406	1.407	1.405	1.408	N–C51 1.319	1.406
C21–O		1.369	C21–C28 1.510	C15–C57 1.528	C49–C53 1.377	C21–C56 1.481
O–C57		1.416		C57–C56 1.540	C52–C55 1.376	C56–C58 1.406
Bond angles/°						
C15–N–C18	129.7	129.4	129.8	C14–N–C18 123.8	C15–N–C45 130.9	129.7
C15–N–H	115.0	115.0	114.9	C14–N–H 115.1	117.0	115.0
C14–C15–N	118.7	123.6	123.5	C15–C14–N 119.0	118.2	118.7
C16–C15–N	123.3	118.6	118.6	C12–C14–N 119.1	123.8	123.2
N–C18–C23	123.0	118.8	118.5	119.5	N–C45–C47 126.1	123.4

	A	B	C	D	E	F
N-C18-C19	118.3	123.0	123.2	121.9	N-C45-C46 115.5	118.5
C14-C15-C16	117.8	117.6	117.7	116.9	117.8	117.9
C12-C14-C15	122.4	121.8	121.8	121.8	122.4	122.3
C12-C13-C17	117.1	117.0	117.1	117.7	117.2	117.2
C13-C17-C16	123.0	122.5	122.4	121.7	122.9	122.9
C17-C16-C15	119.7	120.3	120.3	121.7	119.7	119.6
C18-C19-C20	120.7	121.0	120.2	120.2	C45-C46-C48 119.9	121.0
C19-C20-C21	120.5	120.3	122.0	121.1	C48-C53-C49 119.1	121.5
C20-C21-C22	118.8	119.0	117.1	118.7	C46-N-C51 118.5	117.0
C21-C22-C23	121.1	120.4	121.5	120.7	N-C51-C55 123.4	122.0
Torsion angles/°						
C16-C15-N-C18	25.1	-164.5	-157.9	C15-C14-N-C18 111.5	C16-C15-N-C45 27.7	27.7
C14-C15-N-C18	-157.8	17.2	24.4	C12-C15-N-C18 -70.0	C14-C15-N-C45 -155.4	-155.4
C15-N-C18-C19	-158.0	33.4	24.8	C14-N-C18-C19 -20.5	C15-N-C45-C47 12.4	-161.0
C15-N-C18-C23	24.5	-149.6	-158.2	161.8	C15-N-C45-C46 -170.1	21.3