Electronic Supplementary Information for

Color-Tunable Arylaminoanthraquinone Dyes through Hydrogen-Bond-Assisted Charge Transfer Interaction

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1. ORTEP drawing of 22

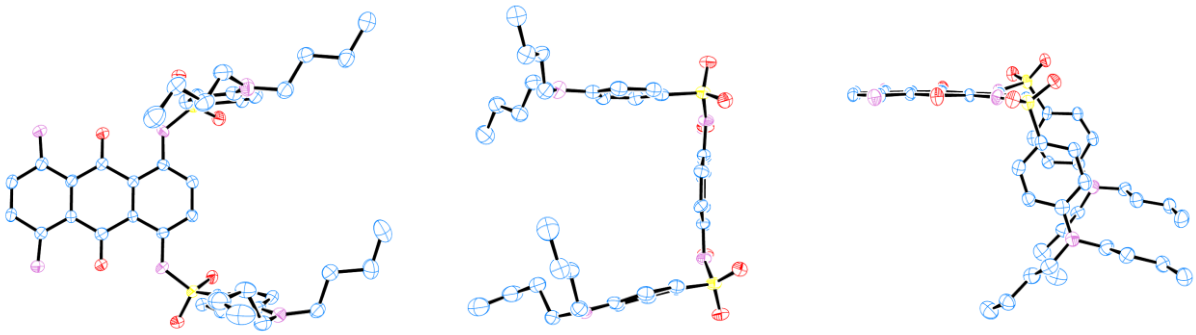
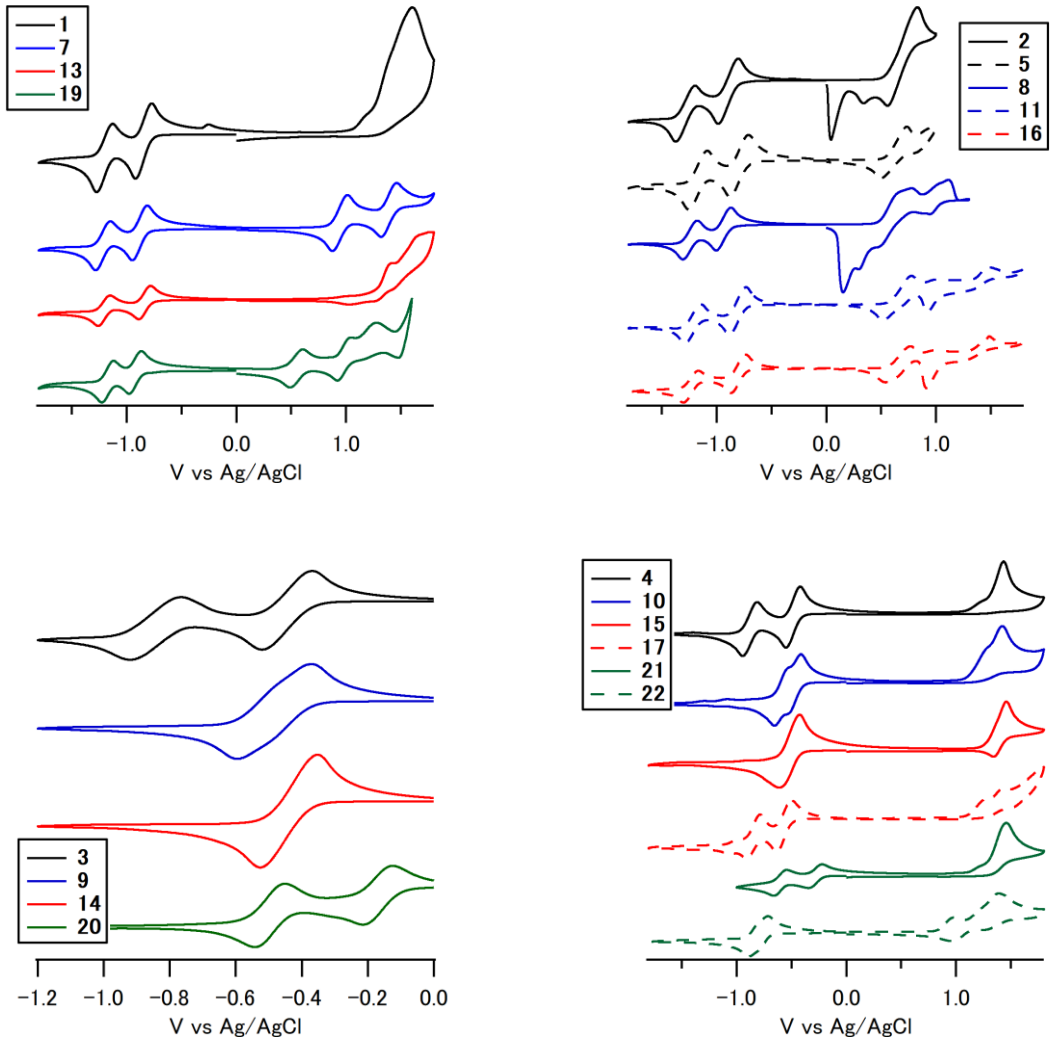


Figure S1 ORTEP drawing of **22**. Front view (left), side view (center) and top view (right). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms were omitted for clarity.

2. Cyclic voltammograms of 1-23 classified according to the substituent



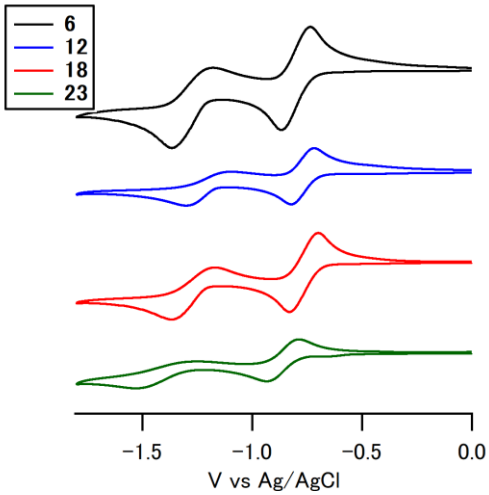


Figure S2 Cyclic voltammograms measured in CH_2Cl_2 classified according to the substituent. The color was determined according to the substitution position. Dotted line indicates monochloro-monosubstituted derivatives or diamino-disubstituted derivative.

3. HOMO and LUMO of 1-6, 11, 13-23

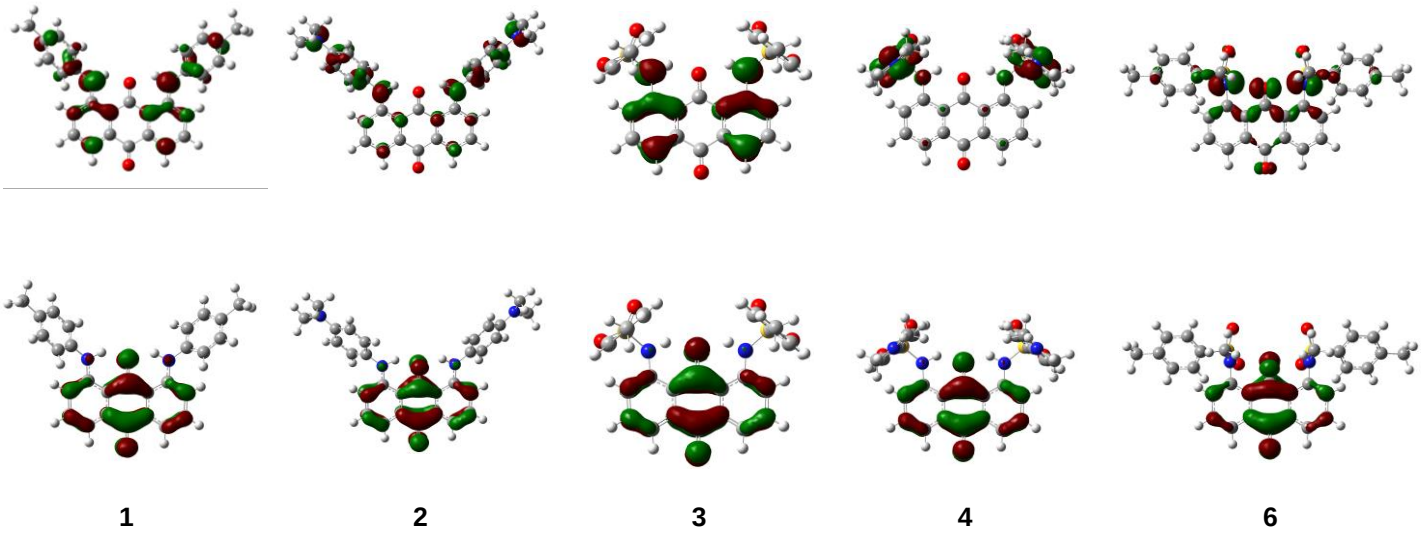


Figure S3 HOMO (top) and LUMO (bottom) of 1,8-disubstituted anthraquinones **1-4** and **6**.

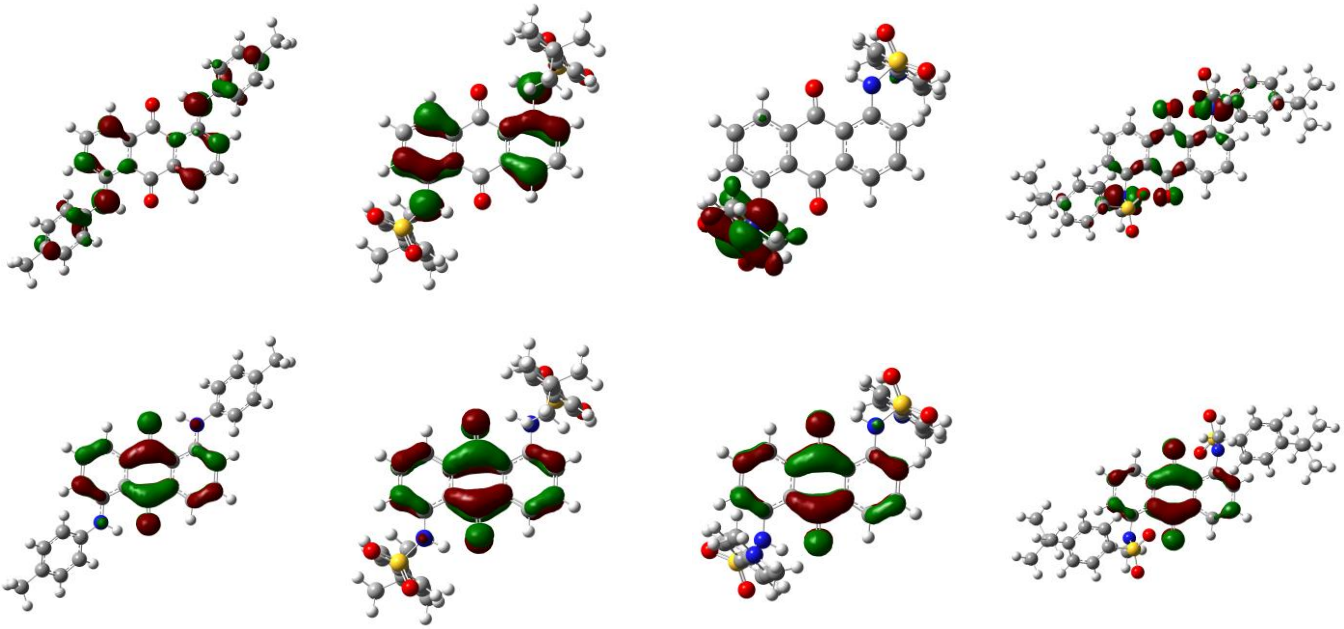


Figure S4 HOMO (top) and LUMO (bottom) of 1,5-disubstituted anthraquinones **13-15** and **18**.

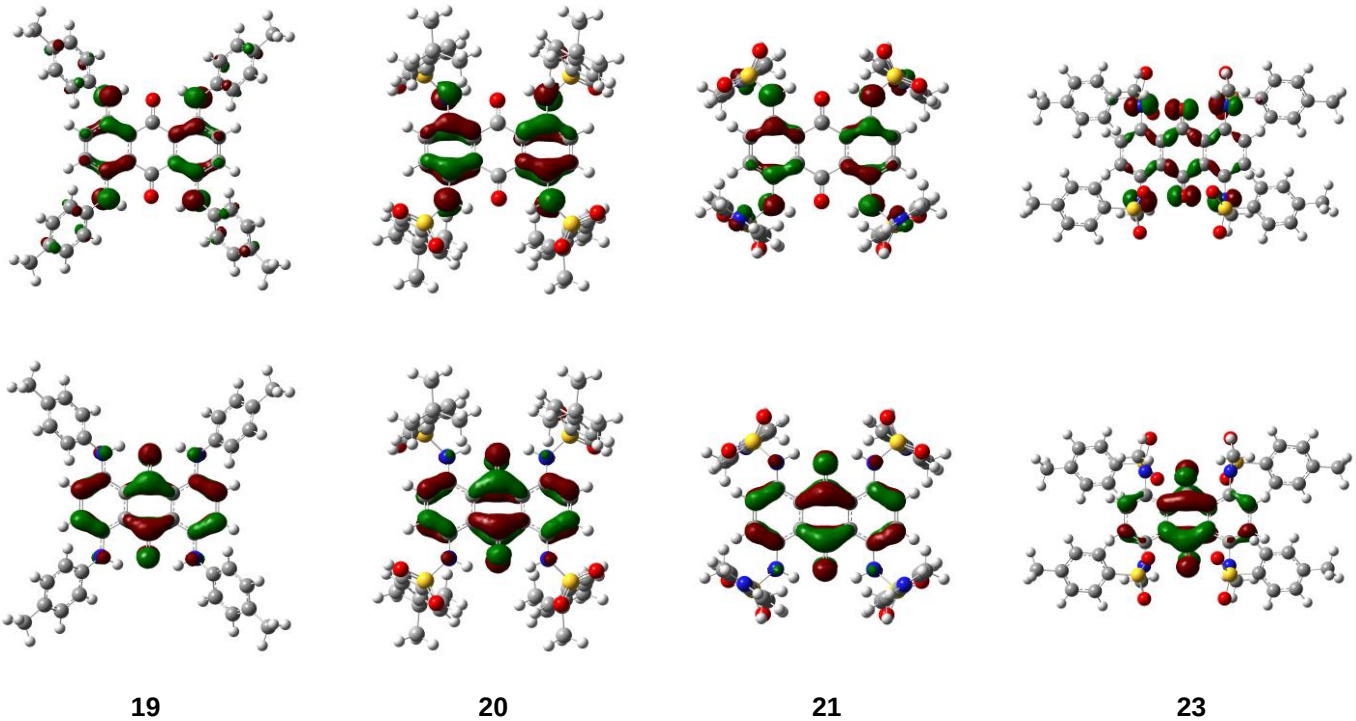
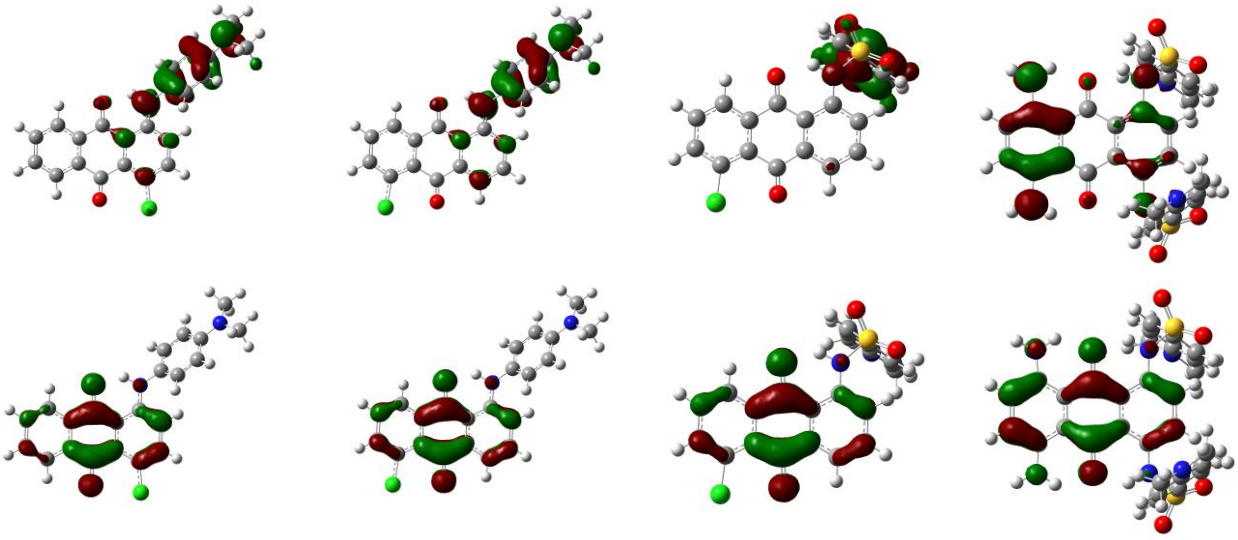


Figure S5 HOMO (top) and LUMO (bottom) of 1,4,5,8-tetrasubstituted anthraquinones **19-21** and **23**.



11 **16** **17** **20**

Figure S6 HOMO (top) and LUMO (bottom) of monochloro-monosubstituted anthraquinones **11,16,17** and diamino-disubstituted anthraquinone **20**.

4. ^{1}H and ^{13}C NMR spectra of new compounds

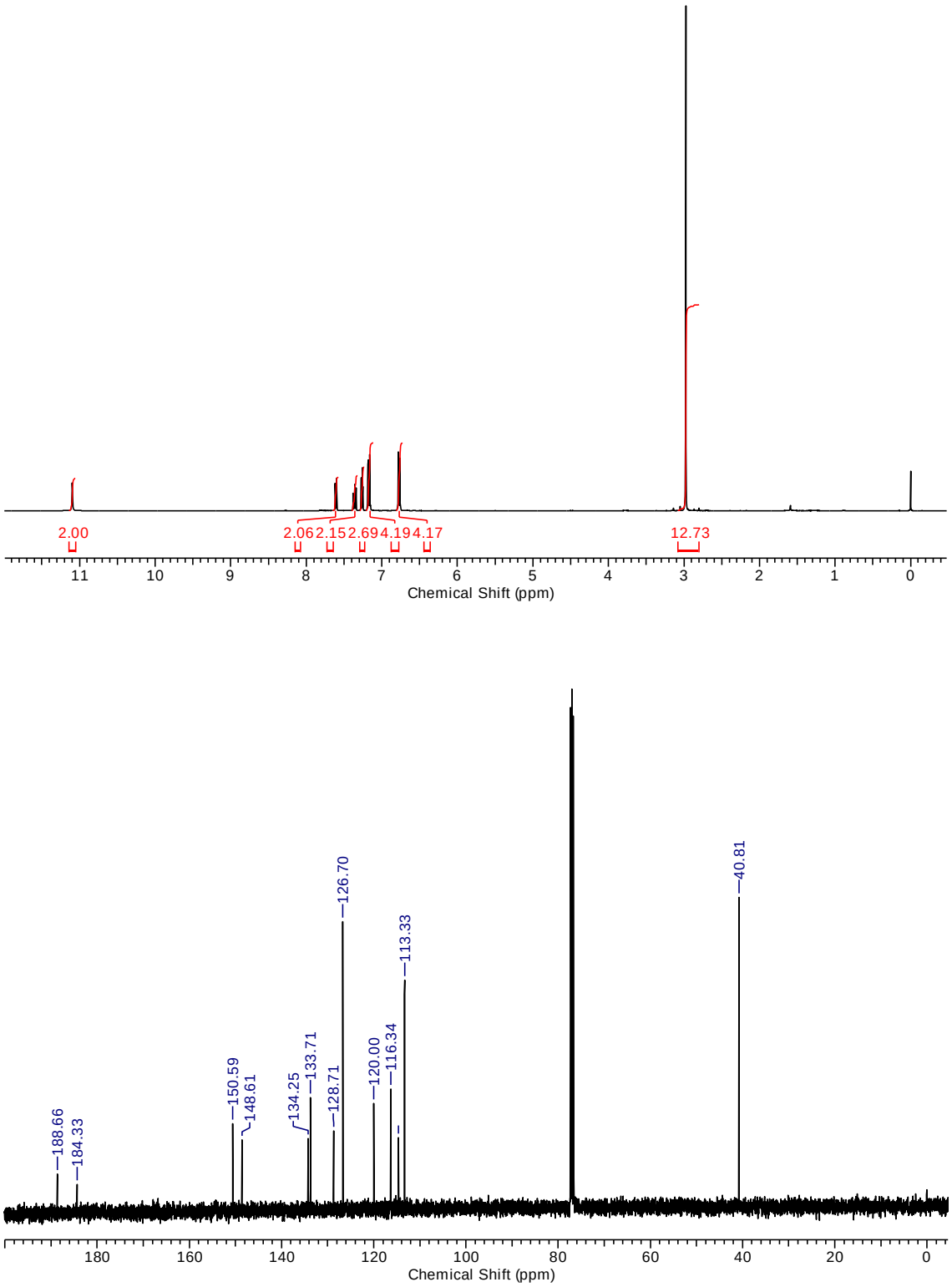


Figure S7 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2** in $CDCl_3$.

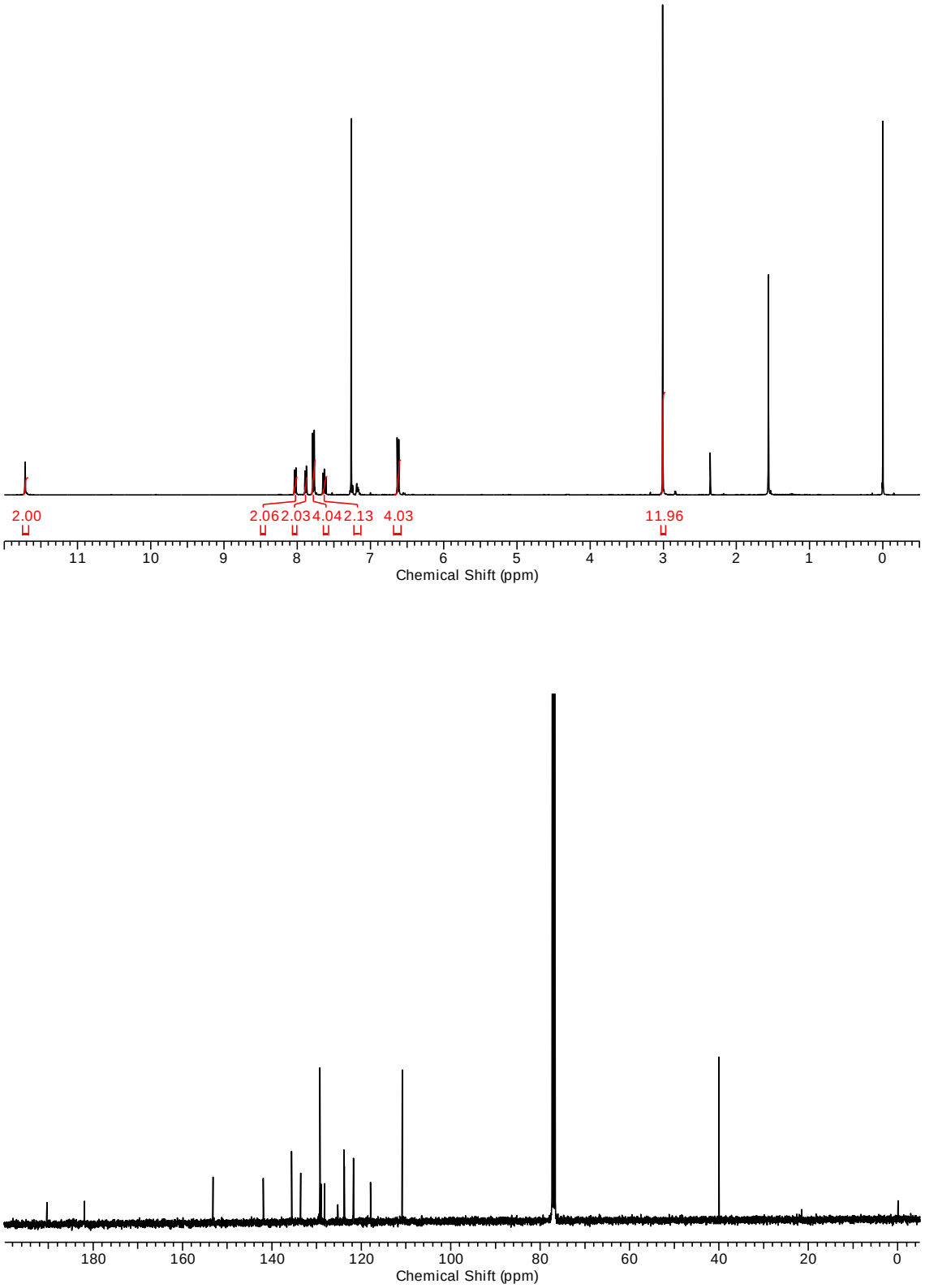


Figure S8 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4** in $CDCl_3$.

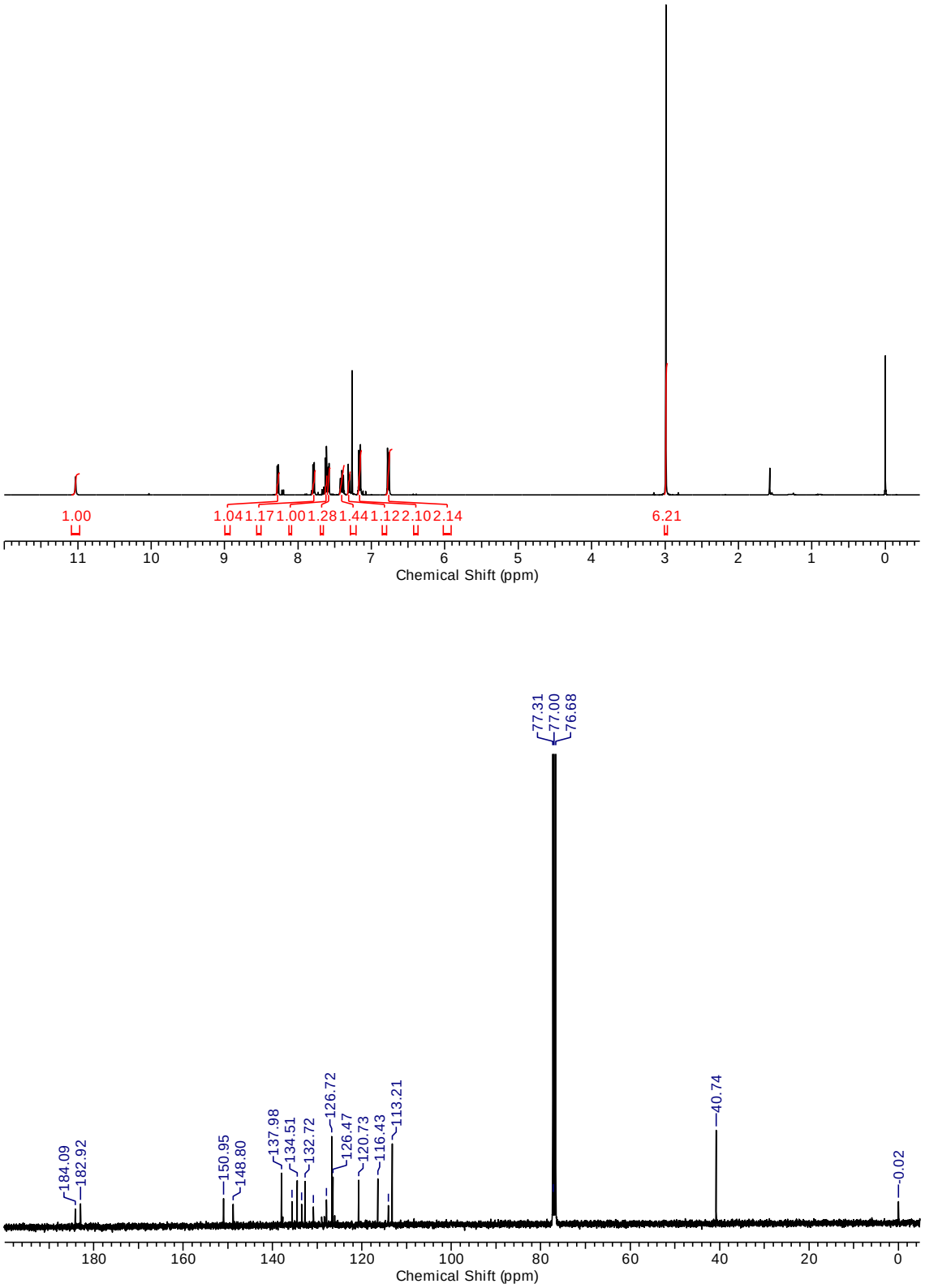


Figure S9 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **5** in $CDCl_3$.

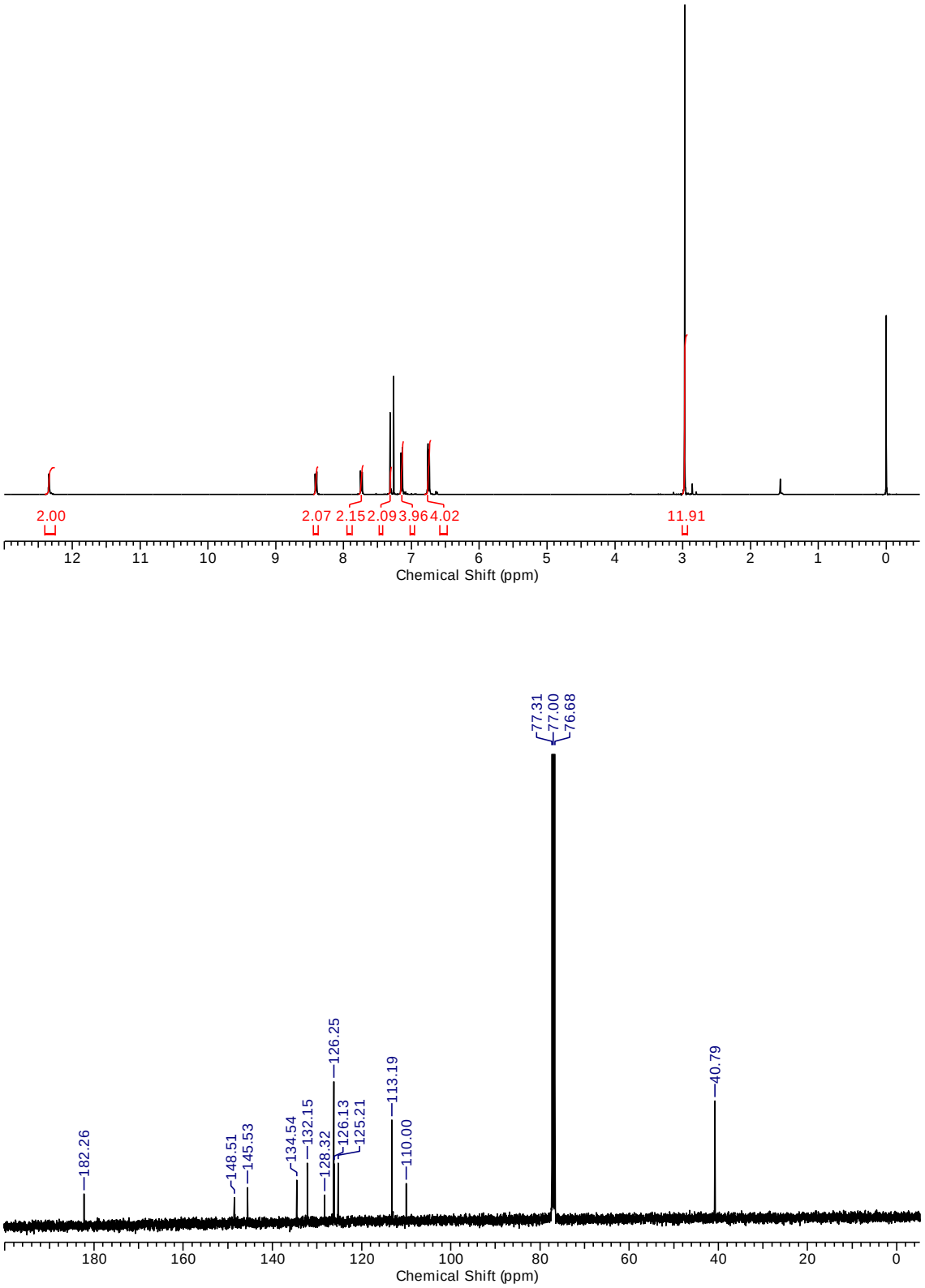


Figure S10 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **8** in $CDCl_3$.

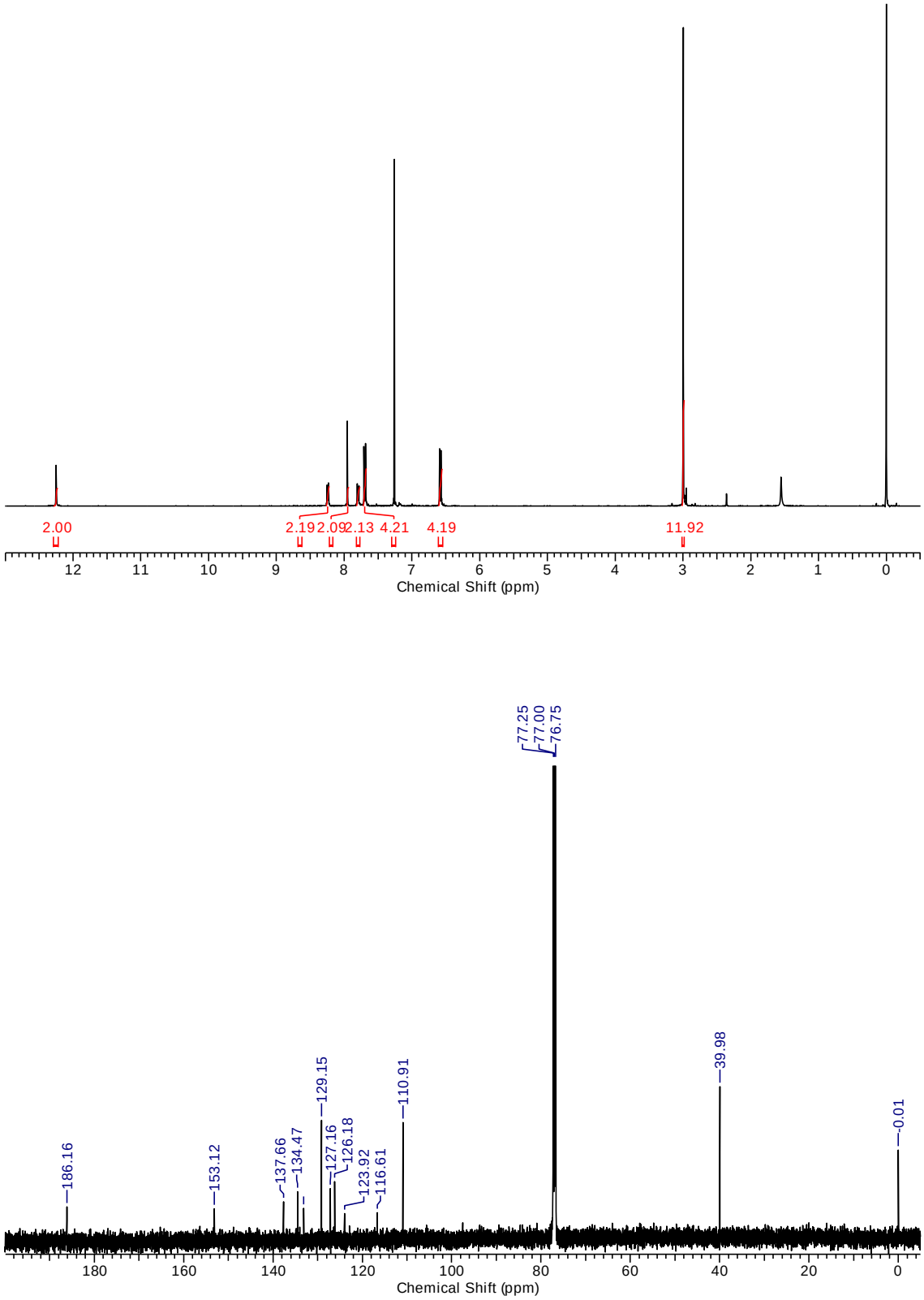


Figure S11 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **10** in $CDCl_3$.

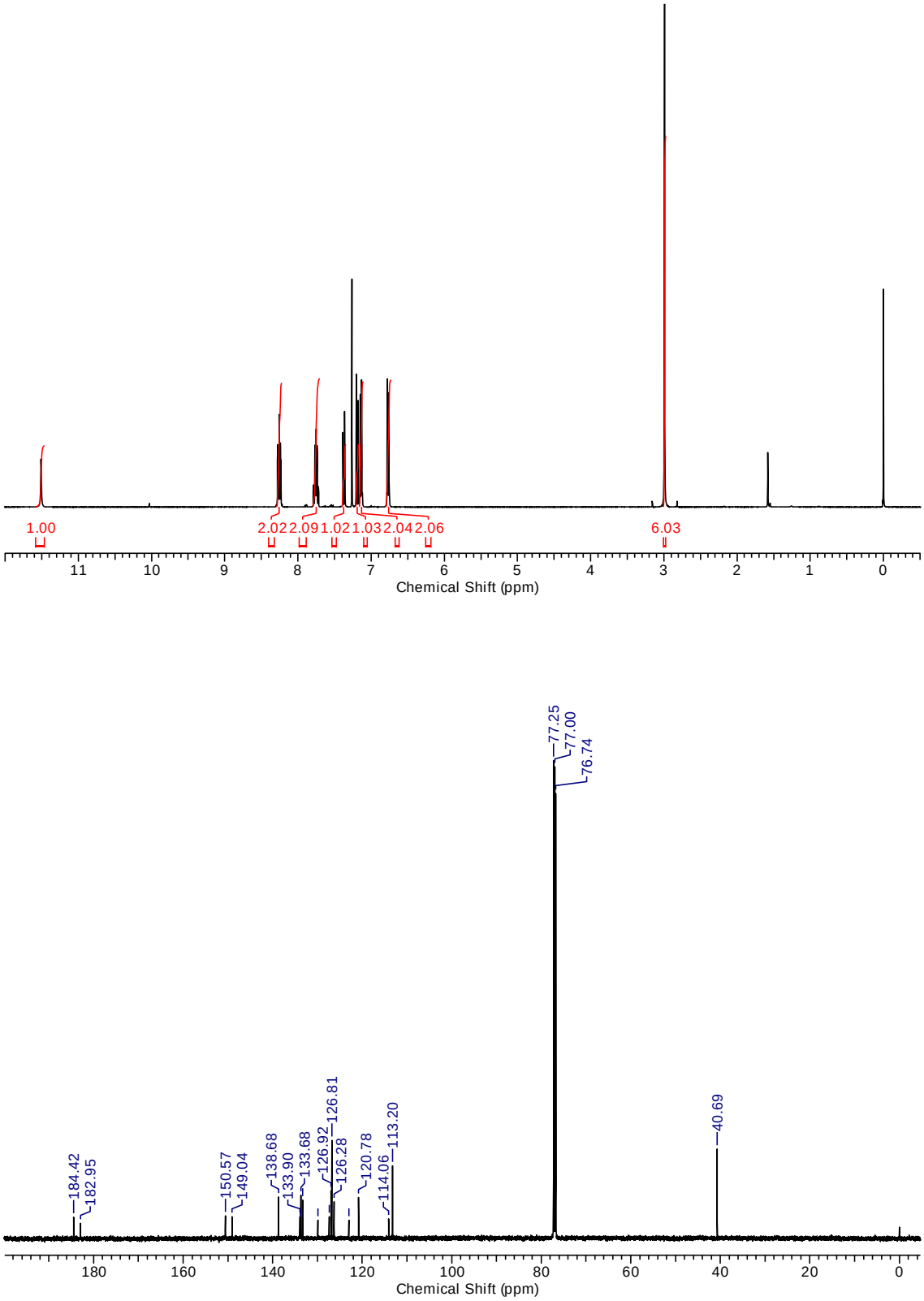


Figure S12 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **11** in $CDCl_3$.

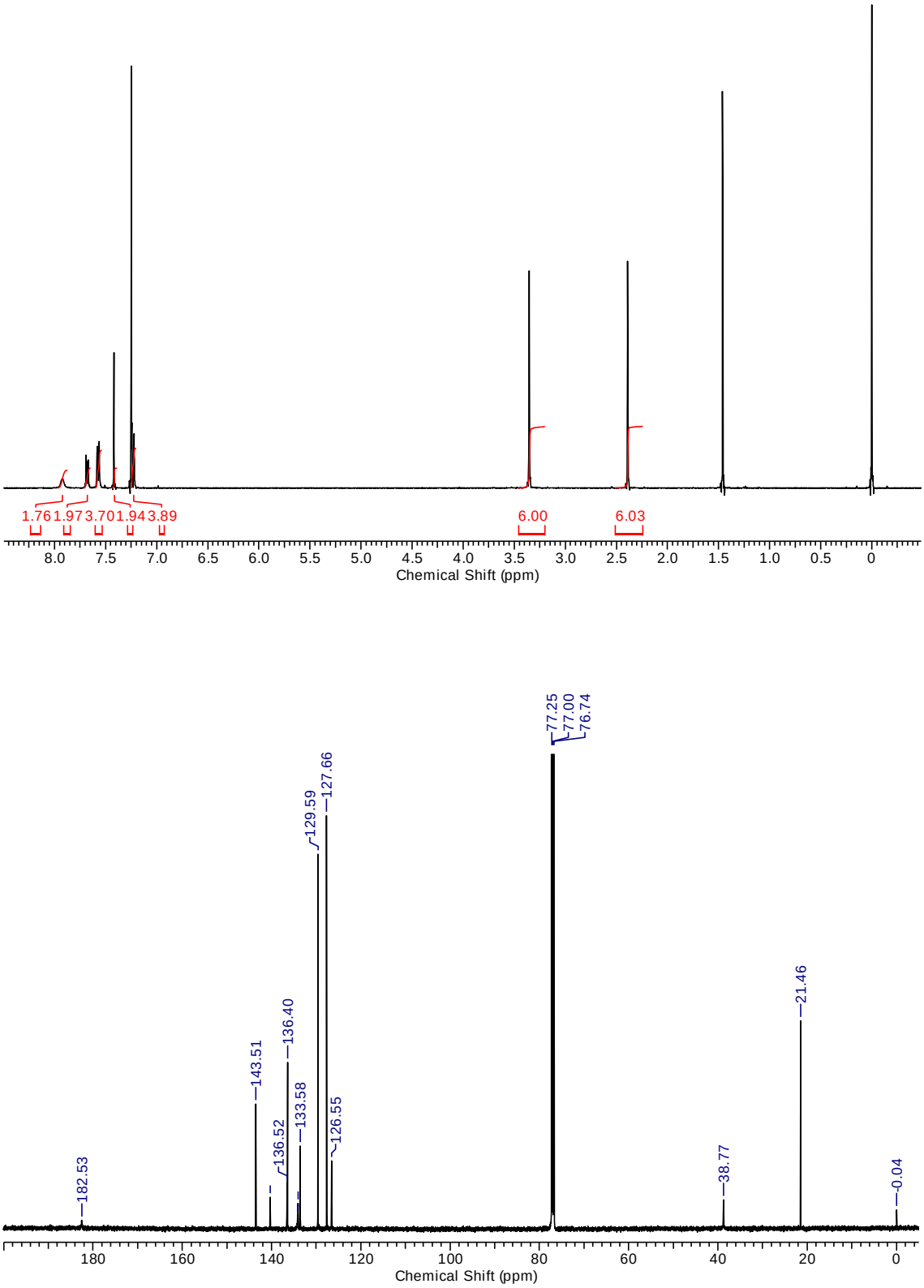


Figure S13 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **12** in $CDCl_3$ measured at 50 °C.

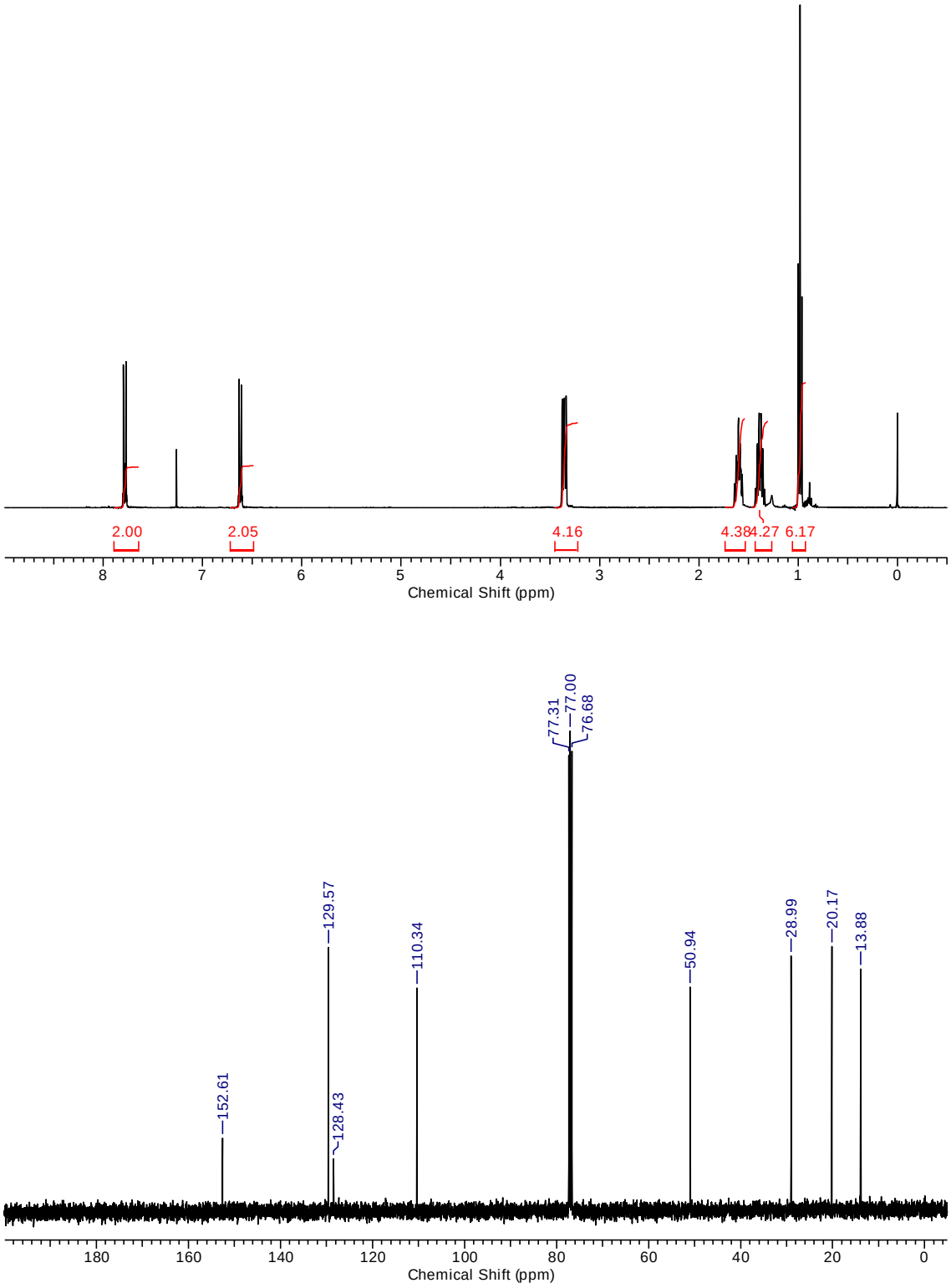


Figure S14 ^{1}H (top) and ^{13}C (bottom) NMR spectra of 4-(dibutylamino)benzenesulfonyl chloride in $CDCl_3$.

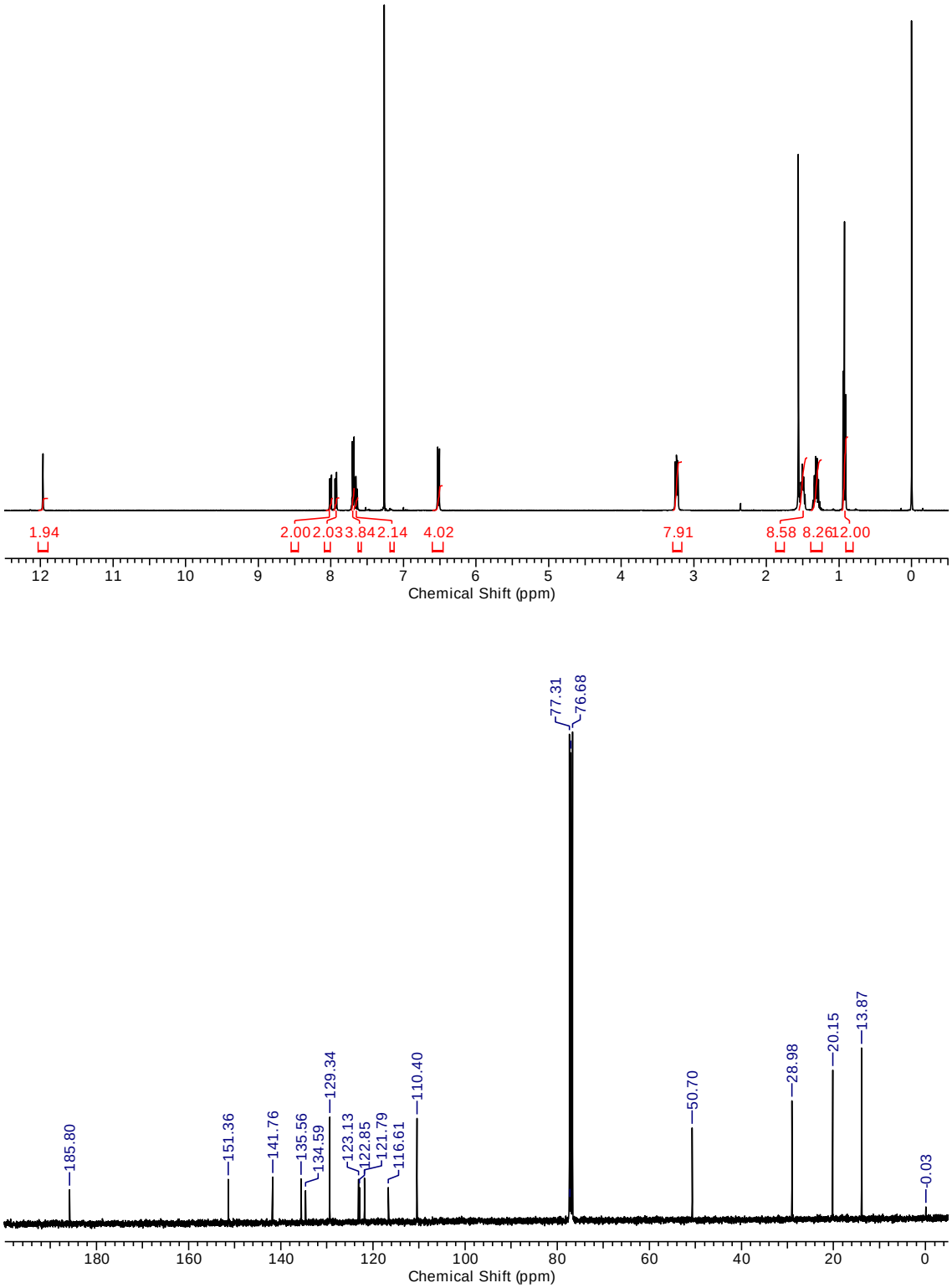


Figure S15 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **15** in $CDCl_3$.

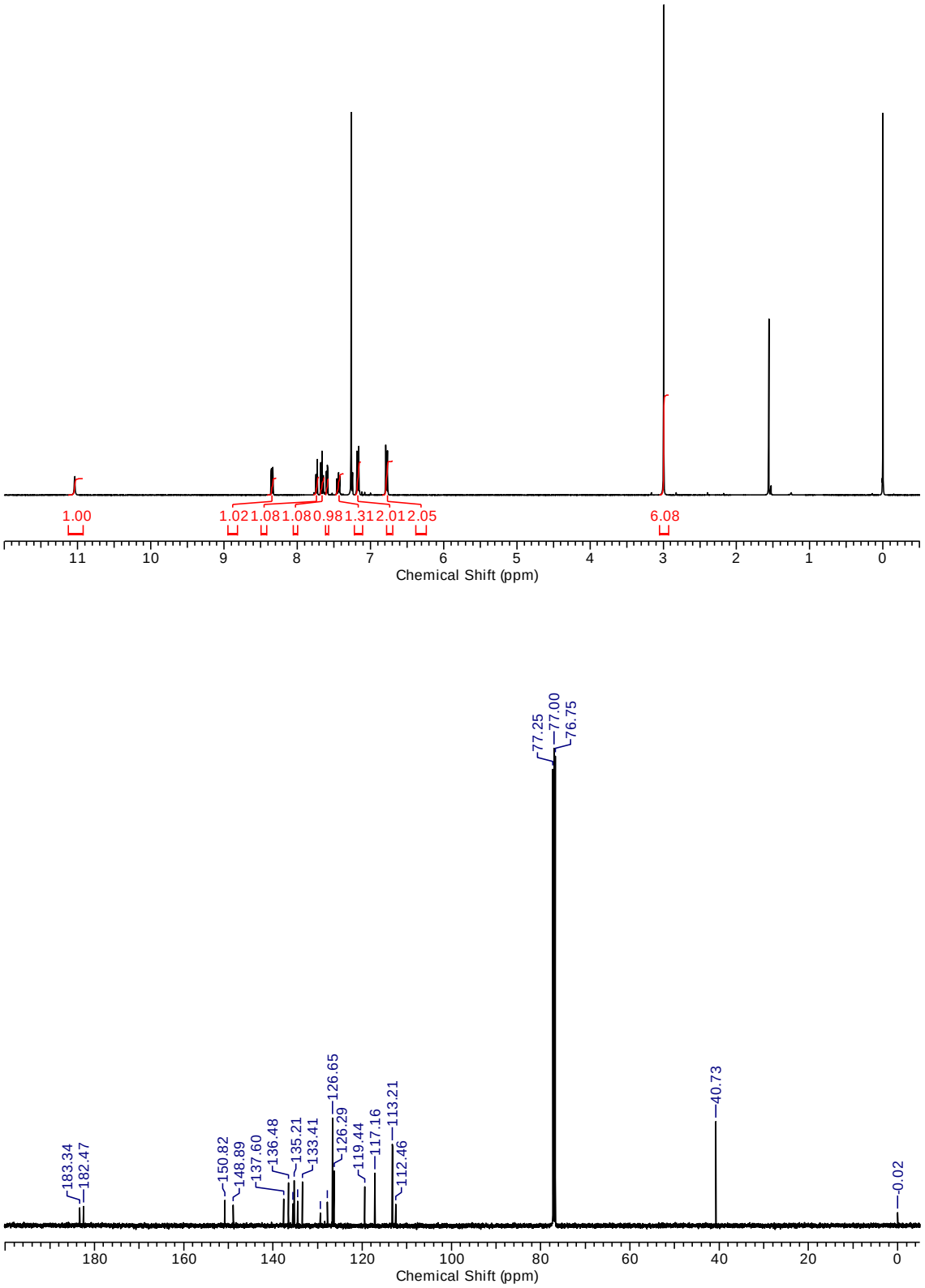


Figure S16 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **16** in $CDCl_3$.

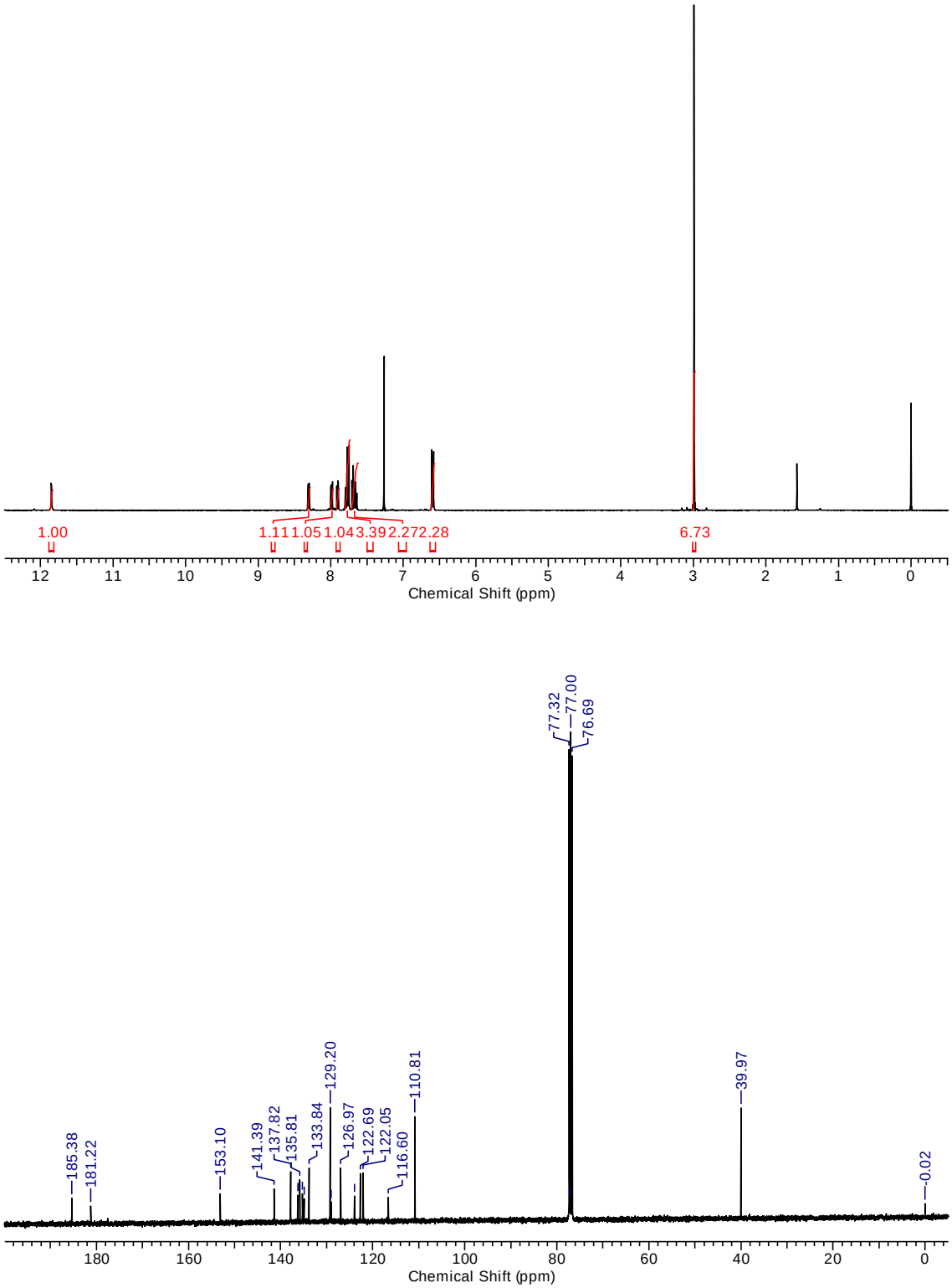


Figure S17 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **17** in $CDCl_3$.

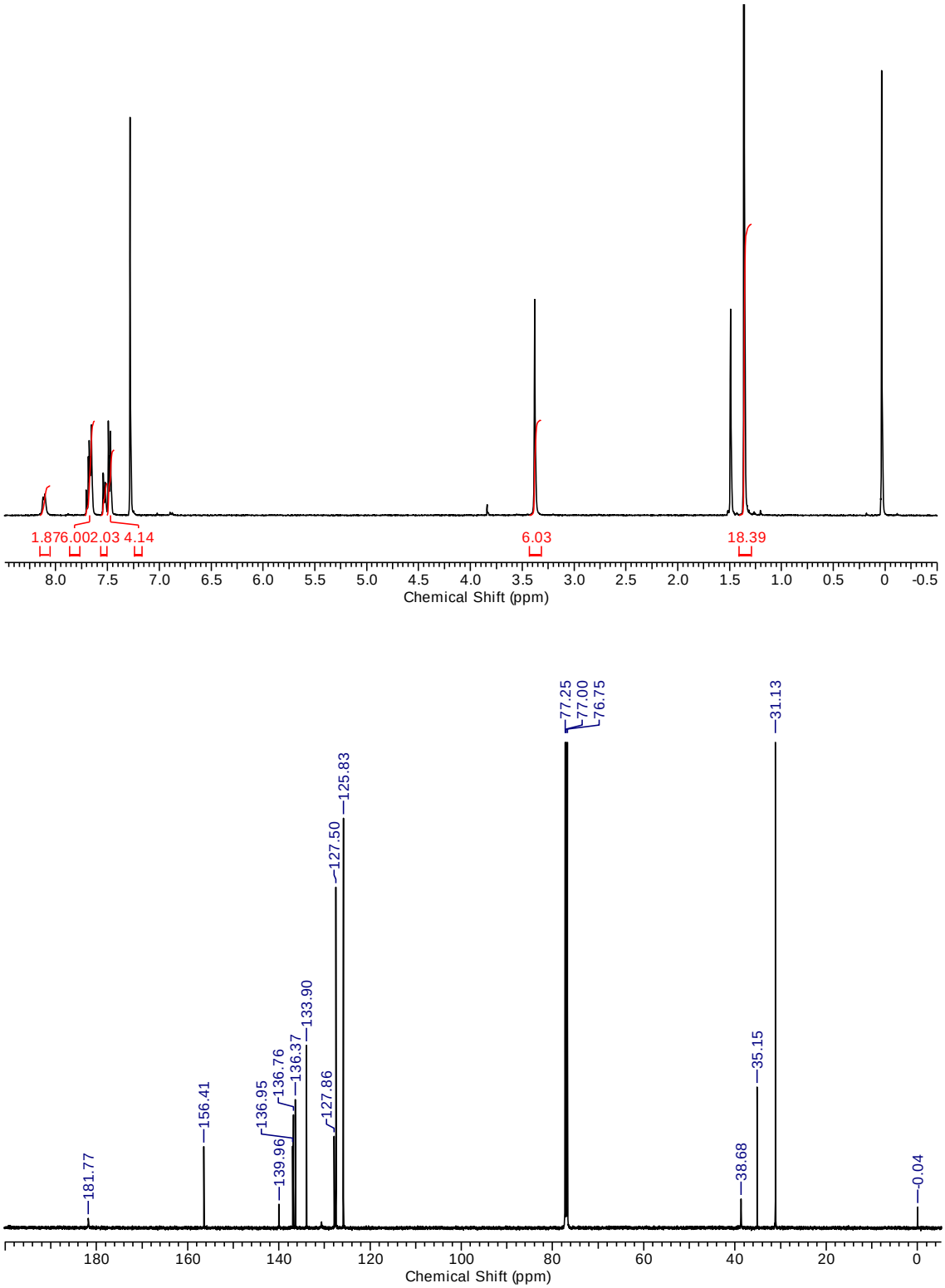


Figure S18 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **18** in $CDCl_3$ measured at 50 °C.

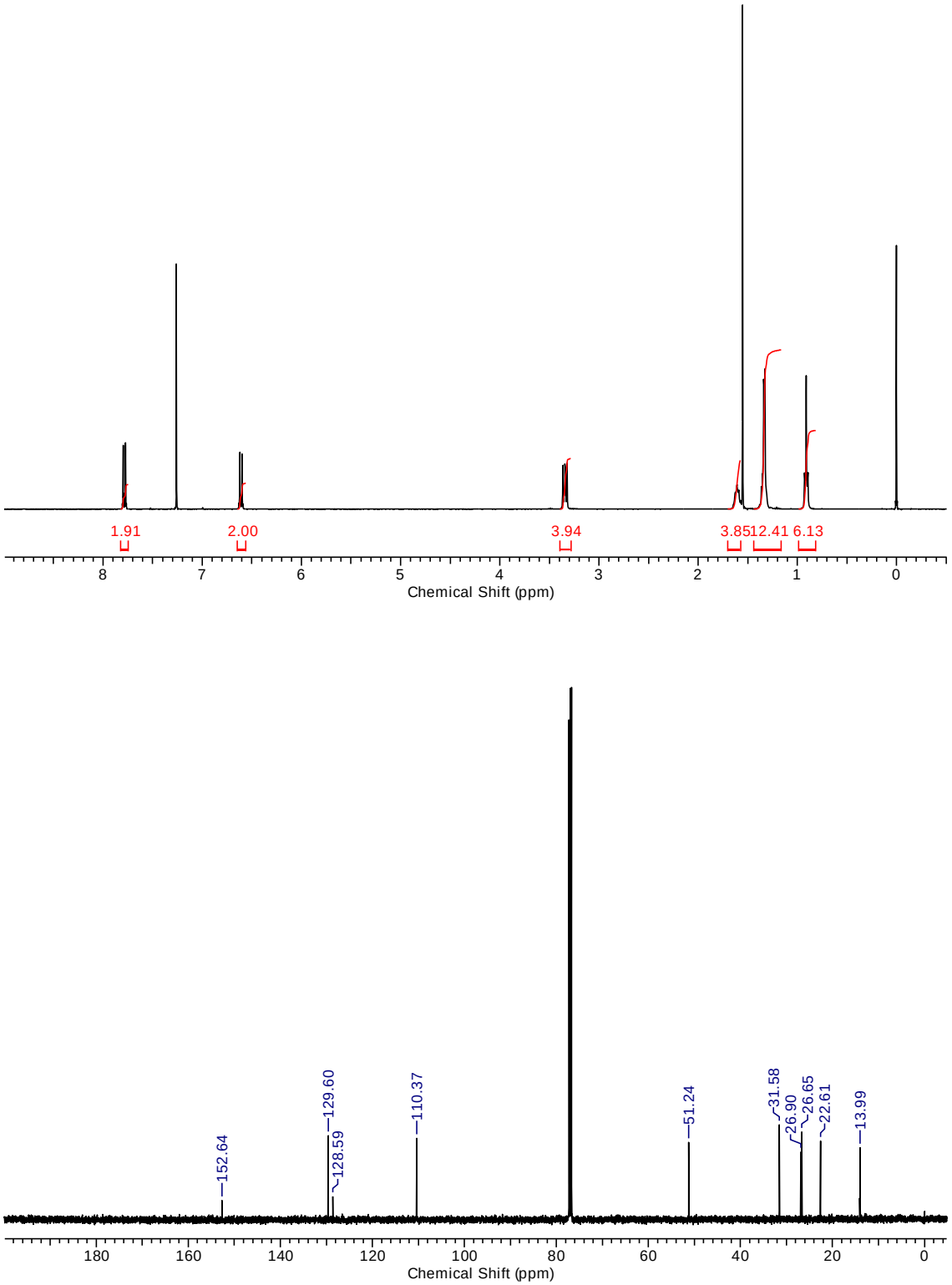


Figure S19 ^{1}H (top) and ^{13}C (bottom) NMR spectra of 4-(dihexylamino)benzenesulfonyl chloride in $CDCl_3$.

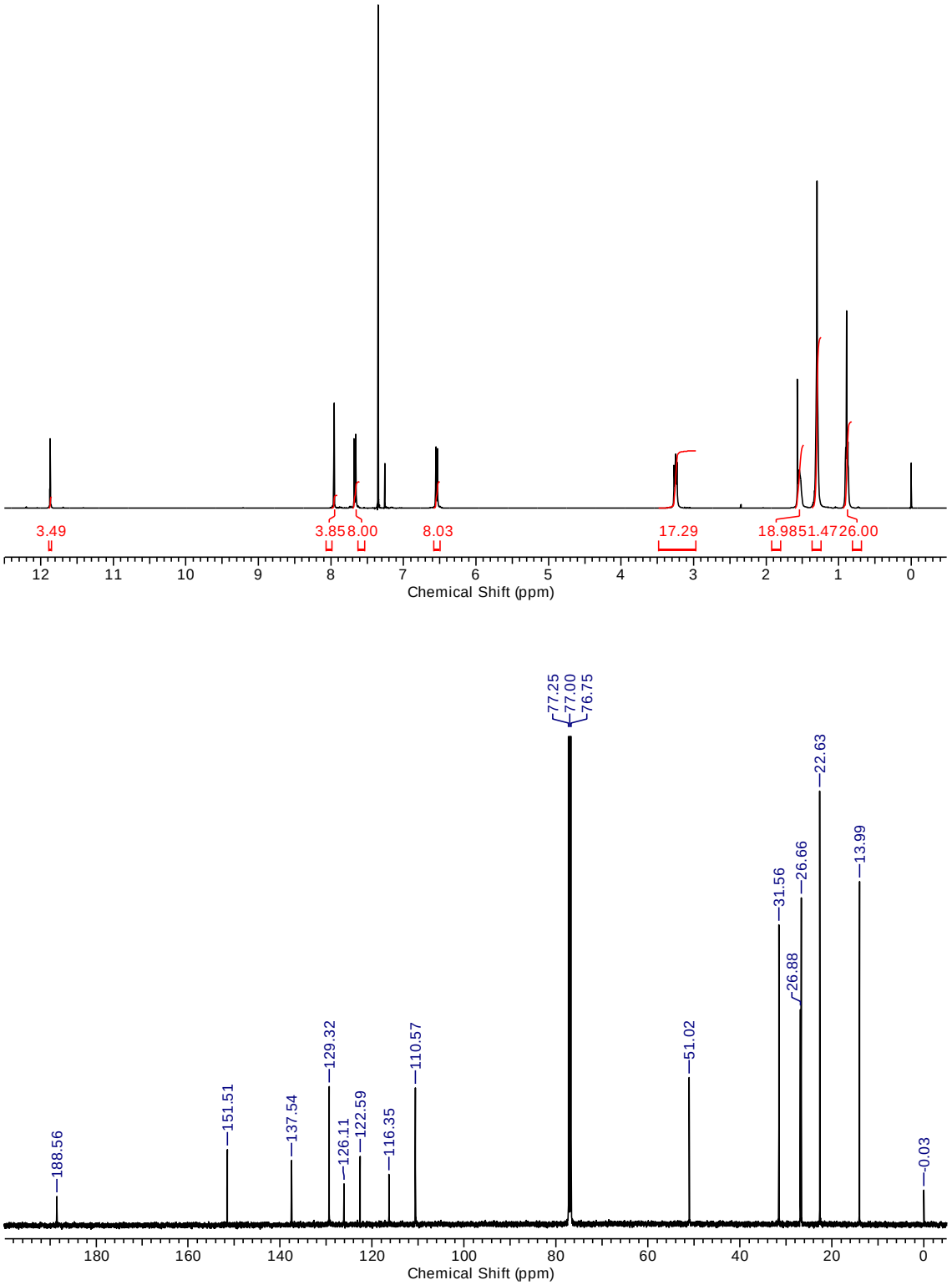


Figure S20 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **21** in $CDCl_3$.

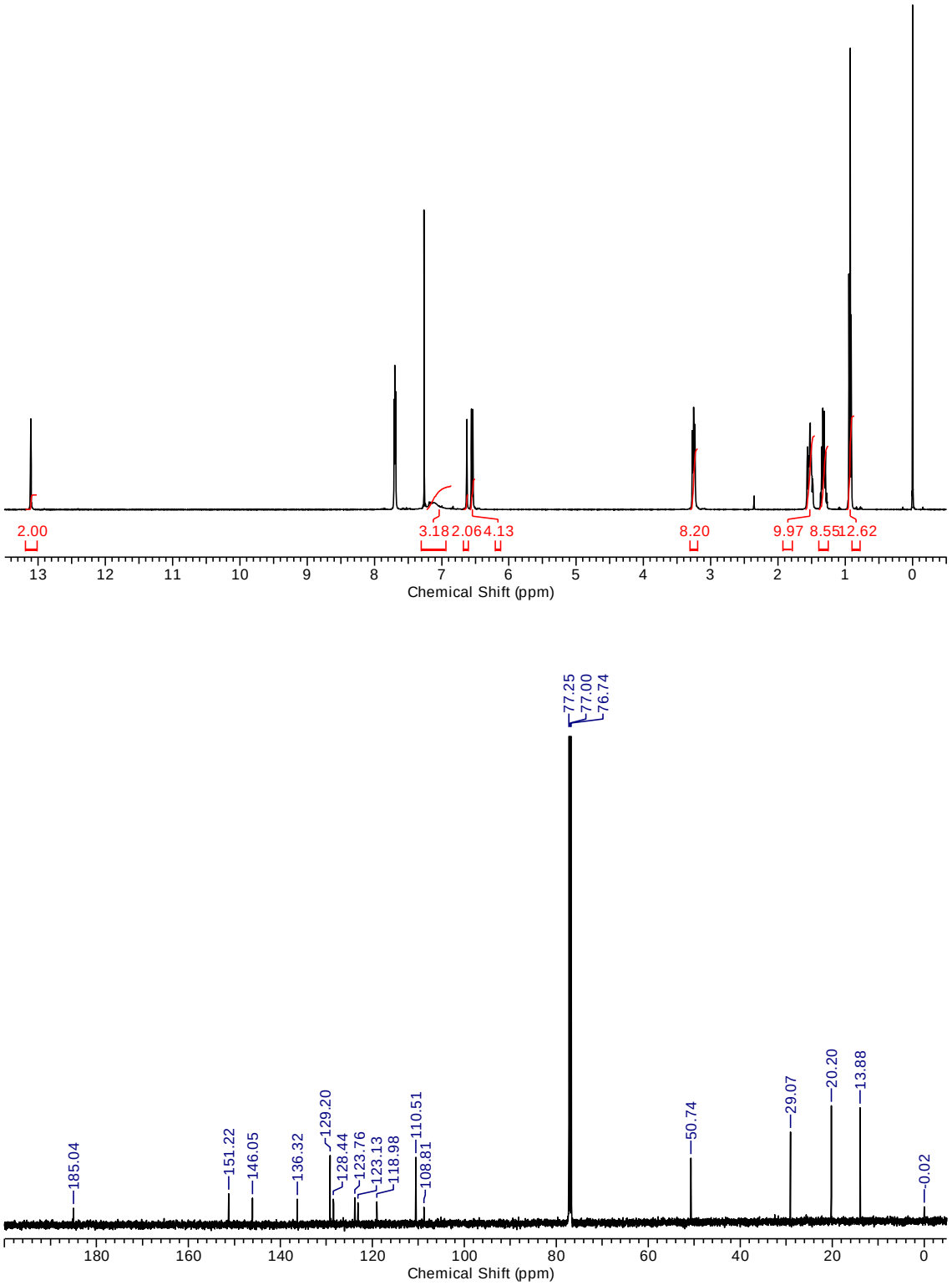


Figure S21 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **22** in $CDCl_3$.

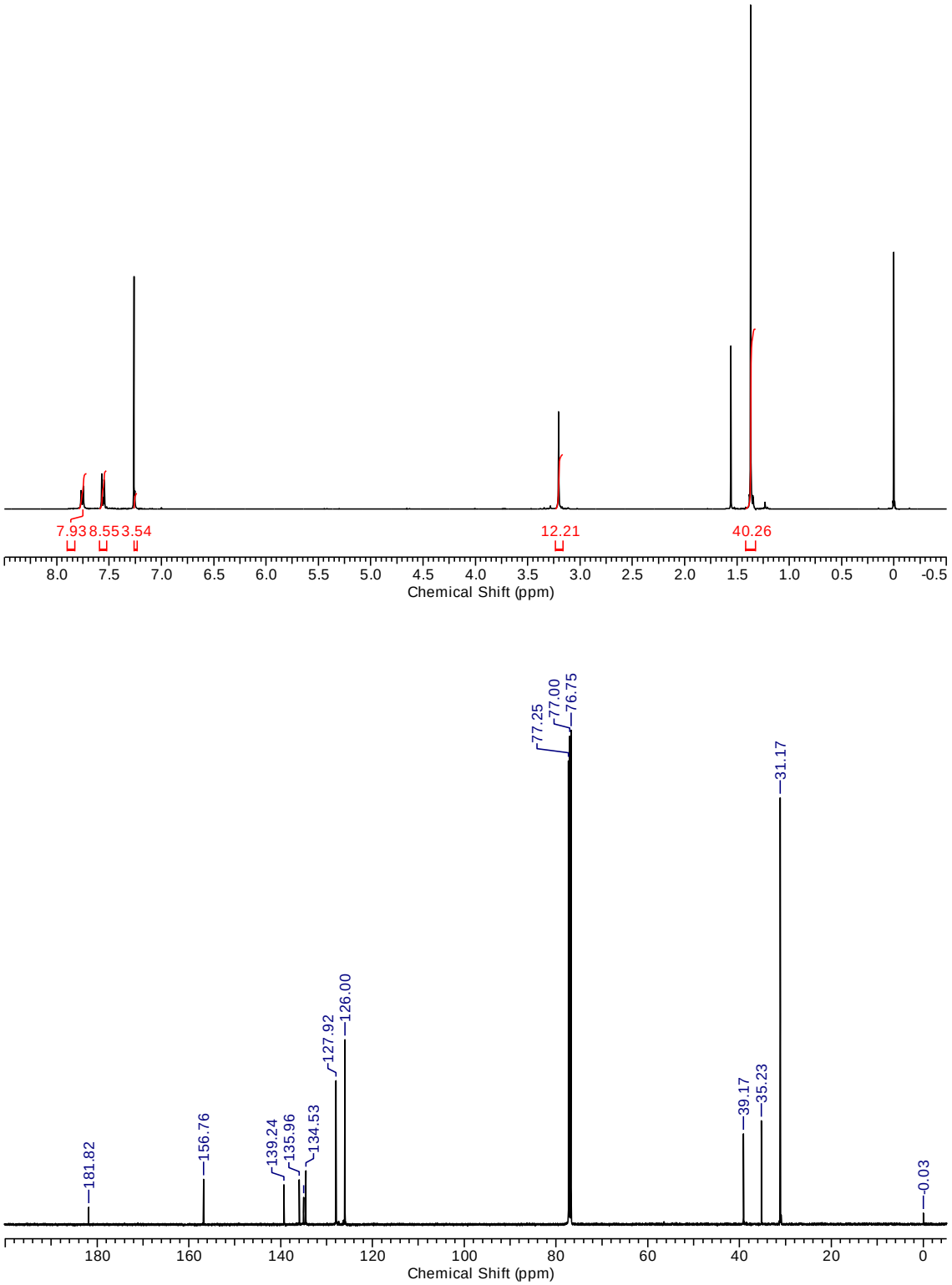
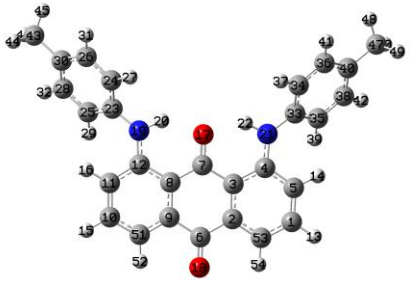


Figure S22 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **23** in $CDCl_3$ measured at 50 °C.

5. Cartesian coordinates of the optimized structures of 1-23



Cartesian coordinates of the optimized structure of **1**

E(RB3LYP) = -1340.23463628 a.u.

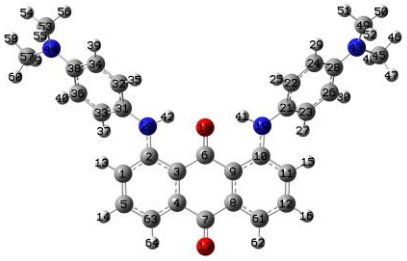
Number of imaginary frequencies: 0

Atom No.	Element	X	Y	Z
1	C	3.681494	3.124835	0.017107
2	C	1.277055	3.070207	-0.012529
3	C	1.276464	1.657479	-0.144147
4	C	2.539680	0.973540	-0.166249
5	C	3.724979	1.747621	-0.101195
6	C	-0.000005	3.834437	0.041442
7	C	-0.000029	0.932349	-0.275841
8	C	-1.276504	1.657503	-0.144138
9	C	-1.277077	3.070228	-0.012520
10	C	-3.681516	3.124875	0.017121
11	C	-3.725014	1.747662	-0.101184
12	C	-2.539719	0.973572	-0.166239
13	H	4.612209	3.684853	0.053658
14	H	4.680723	1.243036	-0.174767
15	H	-4.612226	3.684902	0.053671
16	H	-4.680761	1.243086	-0.174764
17	O	-0.000059	-0.305441	-0.507024
18	O	0.000005	5.058233	0.142424
19	N	-2.597146	-0.391992	-0.289379
20	H	-1.693379	-0.813064	-0.500537
21	N	2.597124	-0.392024	-0.289374
22	H	1.693360	-0.813115	-0.500512
23	C	-3.696068	-1.255375	-0.108584
24	C	-3.790308	-2.389263	-0.930190
25	C	-4.650667	-1.084065	0.906043
26	C	-4.815491	-3.313063	-0.749043
27	H	-3.052910	-2.537754	-1.714930
28	C	-5.681983	-2.007991	1.062800
29	H	-4.568448	-0.246400	1.590838
30	C	-5.791193	-3.136913	0.241160
31	H	-4.861923	-4.185148	-1.397639
32	H	-6.407583	-1.854848	1.858783
33	C	3.696067	-1.255379	-0.108582
34	C	3.790318	-2.389285	-0.930163
35	C	4.650687	-1.084017	0.906017
36	C	4.815528	-3.313055	-0.749014
37	H	3.052907	-2.537813	-1.714883
38	C	5.682030	-2.007912	1.062775
39	H	4.568464	-0.246332	1.590787
40	C	5.791247	-3.136855	0.241162
41	H	4.861968	-4.185155	-1.397589
42	H	6.407644	-1.854729	1.858736
43	C	-6.927778	-4.118449	0.404448
44	H	-7.780022	-3.856470	-0.237348
45	H	-6.621585	-5.135194	0.135244
46	H	-7.294342	-4.139071	1.436413
47	C	6.927862	-4.118356	0.404450
48	H	6.621709	-5.135104	0.135212
49	H	7.780113	-3.856332	-0.237319
50	H	7.294403	-4.138994	1.436424
51	C	-2.457891	3.797465	0.074519
52	H	-2.398174	4.875031	0.172503
53	C	2.457875	3.797433	0.074505
54	H	2.398168	4.875000	0.172489

Cartesian coordinates of the optimized structure of **2**

E(RB3LYP) = -1529.53098551 a.u.

Number of imaginary frequencies: 0



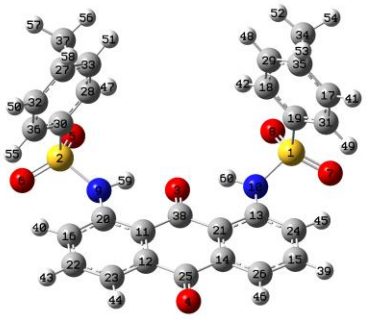
Atom No.	Element	X	Y	Z
1	C	-3.725570	2.274453	-0.115500
2	C	-2.539179	1.498872	-0.171183
3	C	-1.275318	2.184173	-0.152980
4	C	-1.276942	3.598982	-0.041942
5	C	-3.681916	3.652591	-0.017342
6	C	-0.000001	1.456208	-0.263592
7	C	0.000029	4.363924	0.003039
8	C	1.276985	3.598960	-0.041979
9	C	1.275325	2.184151	-0.152983
10	C	2.539165	1.498822	-0.171197
11	C	3.725579	2.274368	-0.115580
12	C	3.681964	3.652510	-0.017463
13	H	-4.680538	1.765879	-0.175343
14	H	-4.612755	4.213191	0.012556
15	H	4.680529	1.765757	-0.175434
16	H	4.612818	4.213088	0.012386
17	O	0.000042	5.589643	0.086895
18	O	0.000006	0.210516	-0.456749
19	N	2.599636	0.134858	-0.270248
20	N	-2.599684	0.134913	-0.270312
21	C	3.727491	-0.706920	-0.127061
22	C	3.906627	-1.762808	-1.029585
23	C	4.642169	-0.588880	0.928090
24	C	4.954161	-2.666289	-0.891584
25	H	3.214171	-1.871729	-1.860438
26	C	5.706927	-1.474185	1.061163
27	H	4.514520	0.198510	1.664836
28	C	5.887855	-2.549668	0.162499
29	H	5.045141	-3.461461	-1.621723
30	H	6.389568	-1.331696	1.890362
31	C	-3.727528	-0.706878	-0.127085
32	C	-3.906711	-1.762719	-1.029654

Atom No.	Element	X	Y	Z
33	C	-4.642148	-0.588906	0.928127
34	C	-4.954232	-2.666213	-0.891643
35	H	-3.214303	-1.871588	-1.860553
36	C	-5.706892	-1.474227	1.061213
37	H	-4.514460	0.198440	1.664913
38	C	-5.887865	-2.549660	0.162499
39	H	-5.045252	-3.461343	-1.621823
40	H	-6.389485	-1.331788	1.890458
41	H	1.692198	-0.297606	-0.437653
42	H	-1.692250	-0.297549	-0.437746
43	N	6.927583	-3.462766	0.318420
44	N	-6.927572	-3.462788	0.318423
45	C	7.988718	-3.170819	1.266320
46	H	8.705872	-3.994224	1.263392
47	H	8.531171	-2.239513	1.033437
48	H	7.592339	-3.084966	2.285055
49	C	7.212575	-4.397239	-0.756435
50	H	8.043533	-5.040253	-0.459253
51	H	6.350001	-5.045549	-0.951634
52	H	7.482908	-3.898390	-1.701820
53	C	-7.212635	-4.397151	-0.756510
54	H	-8.043521	-5.040247	-0.459307
55	H	-7.483102	-3.898208	-1.701809
56	H	-6.350045	-5.045387	-0.951877
57	C	-7.988695	-3.170887	1.266353
58	H	-8.705825	-3.994314	1.263424
59	H	-7.592297	-3.085049	2.285080
60	H	-8.531181	-2.239591	1.033504
61	C	2.458156	4.327086	0.030656
62	H	2.399116	5.406016	0.112643
63	C	-2.458091	4.327135	0.030749
64	H	-2.399022	5.406062	0.112757

Cartesian coordinates of the optimized structure of **3**

E(RB3LYP) = -2437.3643418 a.u.

Number of imaginary frequencies: 0



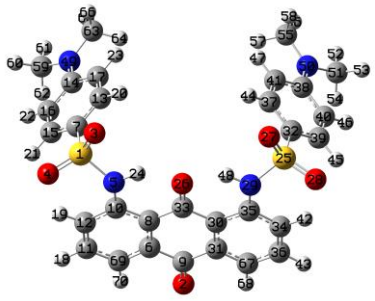
Atom No.	Element	X	Y	Z
1	S	-3.839801	0.310018	1.870099
2	S	3.837615	0.307612	1.871983
3	O	-0.001526	-0.833445	1.429284
4	O	-0.001592	-4.337014	-2.682050
5	O	3.321446	0.976680	3.063222
6	O	5.117131	-0.402755	1.869337
7	O	-5.120281	-0.398592	1.864859
8	O	-3.324647	0.977597	3.062605
9	N	2.601858	-0.791265	1.485923
10	N	-2.604994	-0.790422	1.485313
11	C	1.280381	-2.123234	-0.090179
12	C	1.275728	-3.052989	-1.159899
13	C	-2.546403	-1.685918	0.418660
14	C	-1.278871	-3.052555	-1.160228
15	C	-3.683323	-3.105313	-1.197599
16	C	3.727395	-2.206701	-0.142874
17	C	-4.809566	2.300417	-1.534825
18	C	-2.928545	2.531609	0.515469
19	C	-3.867160	1.495719	0.525866
20	C	2.543284	-1.686825	0.419380
21	C	-1.283509	-2.122770	-0.090534
22	C	3.680170	-3.106533	-1.196619
23	C	2.457569	-3.533148	-1.713741
24	C	-3.730532	-2.205447	-0.143877
25	C	-0.001578	-3.547881	-1.742934
26	C	-2.460724	-3.532330	-1.714385
27	C	3.885880	3.340762	-1.574594
28	C	2.929453	2.527567	0.512489
29	C	-2.941120	3.445290	-0.533601
30	C	3.868752	1.492246	0.526894

Atom No.	Element	X	Y	Z
31	C	-4.814415	1.375439	-0.491127
32	C	4.817893	2.296301	-1.530950
33	C	2.945095	3.440484	-0.537095
34	C	-3.899271	4.362921	-2.689883
35	C	-3.878128	3.345670	-1.574403
36	C	4.819648	1.371946	-0.486580
37	C	3.909391	4.357023	-2.690930
38	C	-0.001545	-1.641925	0.473249
39	H	-4.612420	-3.490100	-1.608775
40	H	4.677699	-1.912551	0.283604
41	H	-5.547730	2.210942	-2.327792
42	H	-2.214455	2.625783	1.327177
43	H	4.609251	-3.491595	-1.607572
44	H	2.395107	-4.241303	-2.531828
45	H	-4.680834	-1.910934	0.282353
46	H	-2.398269	-4.240525	-2.532438
47	H	2.212472	2.621880	1.321634
48	H	-2.216200	4.255648	-0.542643
49	H	-5.553628	0.583300	-0.452933
50	H	5.558986	2.206859	-2.321169
51	H	2.219675	4.250366	-0.549231
52	H	-2.885766	4.658403	-2.981878
53	H	-4.410317	3.975746	-3.576710
54	H	-4.425571	5.274873	-2.378853
55	H	5.559266	0.580345	-0.445189
56	H	2.896182	4.637342	-2.998733
57	H	4.417297	5.276987	-2.373086
58	H	4.439303	3.976304	-3.569388
59	H	1.687569	-0.498554	1.841461
60	H	-1.690623	-0.498206	1.841068

Cartesian coordinates of the optimized structure of **4**

E(RB3LYP) = -2626.66922860 a.u.

Number of imaginary frequencies: 0



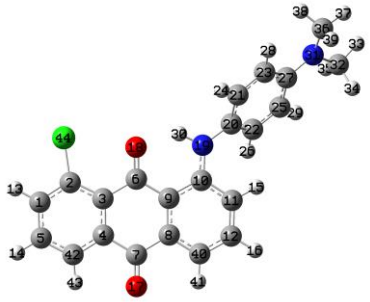
Atom No.	Element	X	Y	Z
1	S	3.886687	-0.776591	-2.076156
2	O	0.000016	-3.885639	3.623223
3	O	3.335019	-0.406051	-3.378080
4	O	5.108874	-1.573824	-1.948091
5	N	2.603321	-1.643131	-1.366534
6	C	1.276961	-3.096708	1.794119
7	C	4.092689	0.697500	-1.102422
8	C	1.281296	-2.489860	0.513035
9	C	-0.000020	-3.399486	2.496409
10	C	2.544028	-2.224633	-0.105276
11	C	3.680131	-3.178227	1.824962
12	C	3.727359	-2.596635	0.567932
13	C	3.234900	1.784509	-1.303673
14	C	4.399119	3.045065	0.434371
15	C	5.110934	0.782884	-0.149132
16	C	5.264330	1.936017	0.607543
17	C	3.384248	2.939306	-0.551983
18	H	4.608815	-3.454682	2.316631
19	H	4.676639	-2.448760	0.069743
20	H	2.464597	1.731284	-2.066527
21	H	5.799261	-0.044989	-0.020888
22	H	6.070741	1.978189	1.328931
23	H	2.714880	3.769588	-0.739953
24	H	1.693846	-1.417670	-1.777146
25	S	-3.886972	-0.776572	-2.075912
26	O	-0.000141	-1.612368	-1.276466
27	O	-3.335448	-0.406156	-3.377931
28	O	-5.109230	-1.573661	-1.947632
29	N	-2.603611	-1.643219	-1.366411
30	C	-1.281468	-2.489895	0.513102
31	C	-1.277046	-3.096739	1.794187
32	C	-4.092681	0.697609	-1.102243
33	C	-0.000106	-2.160486	-0.150756
34	C	-3.727525	-2.596727	0.568137
35	C	-2.544241	-2.224701	-0.105139

Atom No.	Element	X	Y	Z
36	C	-3.680212	-3.178312	1.825168
37	C	-3.234985	1.784616	-1.303877
38	C	-4.398586	3.045279	0.434511
39	C	-5.110634	0.783077	-0.148649
40	C	-5.263788	1.936273	0.607979
41	C	-3.384102	2.939476	-0.552233
42	H	-4.676835	-2.448867	0.070002
43	H	-4.608863	-3.454784	2.316892
44	H	-2.464970	1.731355	-2.067019
45	H	-5.798950	-0.044766	-0.020150
46	H	-6.070023	1.978517	1.329561
47	H	-2.714861	3.769775	-0.740579
48	H	-1.694147	-1.417716	-1.777031
49	N	4.542307	4.187068	1.191381
50	N	-4.541401	4.187278	1.191643
51	C	-5.638296	4.298907	2.140249
52	H	-5.568141	5.257058	2.657120
53	H	-6.620629	4.246922	1.648438
54	H	-5.593667	3.505493	2.897327
55	C	-3.705330	5.346975	0.926729
56	H	-3.963200	6.141361	1.628608
57	H	-2.641122	5.113235	1.061560
58	H	-3.843252	5.734637	-0.093123
59	C	5.638773	4.298186	2.140533
60	H	6.621264	4.245398	1.649155
61	H	5.569077	5.256560	2.657048
62	H	5.593308	3.505012	2.897839
63	C	3.705382	5.346403	0.927625
64	H	2.641415	5.112337	1.063945
65	H	3.964009	6.140973	1.629011
66	H	3.841767	5.733989	-0.092447
67	C	-2.458216	-3.427444	2.449232
68	H	-2.395548	-3.886179	3.429155
69	C	2.458175	-3.427388	2.449095
70	H	2.395574	-3.886126	3.429021

Cartesian coordinates of the optimized structure of **5**

E(RB3LYP) = -1568.73935086 a.u.

Number of imaginary frequencies: 0



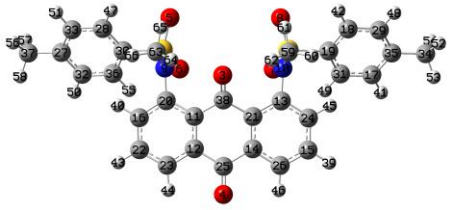
Atom No.	Element	X	Y	Z
1	C	-5.412610	-1.845713	0.292349
2	C	-4.020965	-1.813271	0.163601
3	C	-3.331435	-0.587600	0.026722
4	C	-4.113695	0.592075	0.037047
5	C	-6.155230	-0.668502	0.286138
6	C	-1.842633	-0.489375	-0.147322
7	C	-3.482767	1.940253	-0.073119
8	C	-2.001383	2.017858	-0.151494
9	C	-1.210524	0.839183	-0.170594
10	C	0.219916	0.975273	-0.232935
11	C	0.767291	2.283793	-0.303833
12	C	-0.040508	3.404148	-0.291340
13	H	-5.902249	-2.807707	0.398250
14	H	-7.236167	-0.711689	0.383615
15	H	1.841704	2.391670	-0.393305
16	H	0.415010	4.388592	-0.359713
17	O	-4.178269	2.951770	-0.082652
18	O	-1.172925	-1.524836	-0.273809
19	N	1.030908	-0.123614	-0.251667
20	C	2.441341	-0.169373	-0.129850
21	C	3.173778	-1.000914	-0.985746
22	C	3.141124	0.525849	0.865025

Atom No.	Element	X	Y	Z
23	C	4.552239	-1.131664	-0.863134
24	H	2.652747	-1.548361	-1.766948
25	C	4.522717	0.418760	0.981668
26	H	2.598234	1.151438	1.567277
27	C	5.270400	-0.423173	0.127041
28	H	5.069715	-1.785308	-1.554843
29	H	5.015750	0.984699	1.762899
30	H	0.521586	-1.003353	-0.332267
31	N	6.647504	-0.559987	0.263854
32	C	7.366658	0.349421	1.138963
33	H	8.426954	0.089274	1.130485
34	H	7.267884	1.404920	0.836553
35	H	7.015091	0.259630	2.173733
36	C	7.396577	-1.252307	-0.770742
37	H	8.452825	-1.270407	-0.495042
38	H	7.064593	-2.293041	-0.867010
39	H	7.306027	-0.773940	-1.759651
40	C	-1.432105	3.283510	-0.205662
41	H	-2.083382	4.149431	-0.191102
42	C	-5.503841	0.551980	0.160613
43	H	-6.042715	1.492746	0.157424
44	Cl	-3.244060	-3.385302	0.209156

Cartesian coordinates of the optimized structure of **6**

E(RB3LYP) = -2515.94134656 a.u.

Number of imaginary frequencies: 0



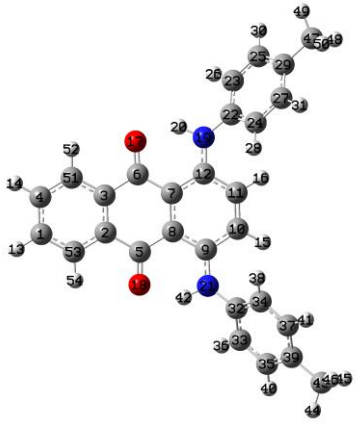
Atom No.	Element	X	Y	Z
1	S	-2.751827	-1.418072	0.079166
2	S	2.751590	-1.418108	0.079991
3	O	0.000117	0.567903	1.972344
4	O	0.000441	5.051277	-0.773200
5	O	2.417336	-2.615363	0.851430
6	O	2.046088	-1.028263	-1.139489
7	O	-2.046805	-1.028250	-1.140595
8	O	-2.417433	-2.615438	0.850370
9	N	2.582075	-0.117639	1.144218
10	N	-2.581563	-0.117730	1.143472
11	C	1.282624	1.885517	0.470806
12	C	1.277754	3.168557	-0.111779
13	C	-2.515012	1.207343	0.608491
14	C	-1.277021	3.168560	-0.112053
15	C	-3.679577	3.128258	-0.335494
16	C	3.696492	1.843725	0.211731
17	C	-6.329154	-1.056589	-1.823464
18	C	-5.363856	-2.239268	0.512278
19	C	-4.496969	-1.553763	-0.342301
20	C	2.515572	1.207383	0.609147
21	C	-1.282029	1.885492	0.470480
22	C	3.680365	3.128228	-0.334698
23	C	2.470081	3.787570	-0.503517
24	C	-3.695837	1.843734	0.210882
25	C	0.000394	3.900988	-0.349050
26	C	-2.469254	3.787595	-0.504039
27	C	7.221551	-1.730907	-0.978958
28	C	5.363625	-2.239928	0.511873
29	C	-6.717519	-2.318029	0.190749
30	C	4.496529	-1.554042	-0.342213
31	C	-4.972614	-0.965720	-1.516782
32	C	6.328273	-1.056729	-1.823871
33	C	6.717136	-2.318835	0.189829

Atom No.	Element	X	Y	Z
34	C	-8.683928	-1.852786	-1.337620
35	C	-7.222252	-1.730372	-0.978013
36	C	4.971833	-0.965746	-1.516684
37	C	8.683089	-1.853563	-1.339040
38	C	0.000229	1.340171	1.025625
39	H	-4.610330	3.603286	-0.632256
40	H	4.636116	1.313895	0.330040
41	H	-6.699106	-0.603477	-2.740298
42	H	-4.976768	-2.722855	1.403012
43	H	4.611181	3.603228	-0.631305
44	H	2.414834	4.781089	-0.935209
45	H	-4.635512	1.313957	0.329002
46	H	-2.413906	4.781124	-0.935694
47	H	4.976772	-2.723690	1.402615
48	H	-7.392232	-2.853853	0.854146
49	H	-4.280054	-0.461222	-2.181922
50	H	6.697971	-0.603403	-2.740697
51	H	7.392002	-2.854963	0.852829
52	H	-9.308319	-1.971388	-0.446173
53	H	-9.037165	-0.973961	-1.887257
54	H	-8.858997	-2.727855	-1.977426
55	H	4.279128	-0.460941	-2.181441
56	H	9.308153	-1.968129	-0.447518
57	H	8.858463	-2.731082	-1.975399
58	H	9.035266	-0.976665	-1.892391
59	C	-2.888940	-0.288256	2.564714
60	H	-3.925483	-0.009153	2.803529
61	H	-2.713267	-1.330280	2.834053
62	H	-2.195934	0.331995	3.136586
63	C	2.889144	-0.288106	2.565522
64	H	2.195671	0.331734	3.137292
65	H	2.713942	-1.330243	2.834727
66	H	3.925480	-0.008495	2.804618

Cartesian coordinates of the optimized structure of **7**

E(RB3LYP) = -1340.23491264 a.u.

Number of imaginary frequencies: 0



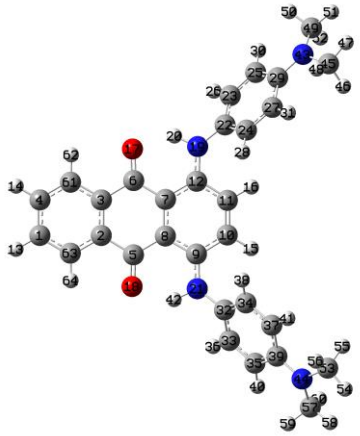
Atom No.	Element	X	Y	Z
1	C	-0.700821	6.079686	0.462865
2	C	-0.701764	3.683838	0.122234
3	C	0.701829	3.683827	0.122225
4	C	0.700928	6.079675	0.462855
5	C	-1.463033	2.425786	-0.066297
6	C	1.463074	2.425763	-0.066319
7	C	0.721681	1.163588	-0.181060
8	C	-0.721663	1.163597	-0.181057
9	C	-1.434132	-0.062740	-0.292325
10	C	-0.683367	-1.255449	-0.492931
11	C	0.683366	-1.255455	-0.492931
12	C	1.434138	-0.062753	-0.292327
13	H	-1.244041	7.011267	0.596888
14	H	1.244165	7.011248	0.596871
15	H	-1.213793	-2.179034	-0.693135
16	H	1.213787	-2.179046	-0.693128
17	O	2.708981	2.487201	-0.116899
18	O	-2.708939	2.487254	-0.116854
19	N	2.805357	-0.097467	-0.284376
20	H	3.225085	0.835080	-0.310602
21	N	-2.805351	-0.097445	-0.284389
22	C	3.661526	-1.204113	-0.134968
23	C	4.898213	-1.178221	-0.800324
24	C	3.378826	-2.291277	0.706881
25	C	5.811588	-2.214831	-0.638464
26	H	5.132816	-0.337643	-1.448178
27	C	4.296800	-3.331186	0.843578

Atom No.	Element	X	Y	Z
28	H	2.457856	-2.307132	1.280523
29	C	5.526940	-3.320528	0.175189
30	H	6.763453	-2.166836	-1.162907
31	H	4.056004	-4.160807	1.504793
32	C	-3.661540	-1.204076	-0.134975
33	C	-4.898197	-1.178189	-0.800386
34	C	-3.378901	-2.291209	0.706936
35	C	-5.811598	-2.214776	-0.638526
36	H	-5.132756	-0.337634	-1.448285
37	C	-4.296899	-3.331096	0.843634
38	H	-2.457962	-2.307053	1.280628
39	C	-5.527007	-3.320445	0.175186
40	H	-6.763439	-2.166787	-1.163014
41	H	-4.056150	-4.160692	1.504898
42	H	-3.225069	0.835106	-0.310659
43	C	-6.505869	-4.462639	0.312537
44	H	-7.541929	-4.106073	0.310495
45	H	-6.409073	-5.177126	-0.516340
46	H	-6.343349	-5.019385	1.241495
47	C	6.505774	-4.462746	0.312537
48	H	6.408999	-5.177199	-0.516370
49	H	7.541842	-4.106198	0.310551
50	H	6.343206	-5.019524	1.241467
51	C	1.398095	4.889481	0.290034
52	H	2.482215	4.863045	0.281113
53	C	-1.398008	4.889503	0.290053
54	H	-2.482129	4.863084	0.281146

Cartesian coordinates of the optimized structure of **8**

E(RB3LYP) = -1529.53116123 a.u.

Number of imaginary frequencies: 0



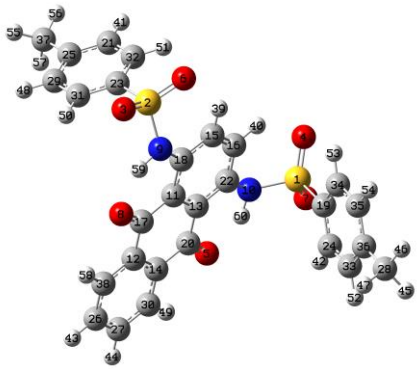
Atom No.	Element	X	Y	Z
1	C	-0.701116	6.748777	0.506634
2	C	-0.702054	4.352944	0.161021
3	C	0.702031	4.352963	0.161060
4	C	0.701022	6.748795	0.506666
5	C	-1.464074	3.095675	-0.029258
6	C	1.464083	3.095707	-0.029152
7	C	0.722592	1.838804	-0.153905
8	C	-0.722558	1.838781	-0.153935
9	C	-1.434932	0.612330	-0.273366
10	C	-0.682751	-0.582240	-0.471264
11	C	0.682891	-0.582218	-0.471248
12	C	1.435020	0.612382	-0.273331
13	H	-1.244398	7.680246	0.642323
14	H	1.244273	7.680279	0.642381
15	H	-1.215478	-1.506160	-0.665141
16	H	1.215658	-1.506124	-0.665087
17	O	2.712399	3.157404	-0.071549
18	O	-2.712391	3.157358	-0.071745
19	N	2.803143	0.574278	-0.263944
20	H	3.225909	1.506211	-0.259528
21	N	-2.803060	0.574177	-0.263988
22	C	3.647943	-0.551271	-0.153500
23	C	4.828621	-0.588367	-0.907948
24	C	3.408247	-1.610731	0.732944
25	C	5.730908	-1.638877	-0.792482
26	H	5.035862	0.219454	-1.605019
27	C	4.295367	-2.677068	0.838715
28	H	2.523821	-1.596368	1.362618
29	C	5.491089	-2.718593	0.087322
30	H	6.624733	-1.616465	-1.404241
31	H	4.056634	-3.472819	1.534127
32	C	-3.647865	-0.551363	-0.153583

Atom No.	Element	X	Y	Z
33	C	-4.828635	-0.588330	-0.907904
34	C	-3.408121	-1.610919	0.732735
35	C	-5.730949	-1.638815	-0.792459
36	H	-5.035925	0.219583	-1.604856
37	C	-4.295270	-2.677236	0.838487
38	H	-2.523657	-1.596638	1.362354
39	C	-5.491055	-2.718648	0.087195
40	H	-6.624850	-1.616302	-1.404101
41	H	-4.056527	-3.473065	1.533810
42	H	-3.225863	1.506086	-0.259801
43	N	6.400392	-3.765387	0.220743
44	N	-6.400298	-3.765457	0.220579
45	C	6.000943	-4.957474	0.948190
46	H	5.126698	-5.461562	0.503619
47	H	6.833808	-5.663562	0.960415
48	H	5.759085	-4.718364	1.990492
49	C	7.478441	-3.889788	-0.745095
50	H	8.125881	-3.005214	-0.726426
51	H	8.095562	-4.751125	-0.481293
52	H	7.118643	-4.025840	-1.778447
53	C	-6.001021	-4.957348	0.948408
54	H	-6.833811	-5.663522	0.960485
55	H	-5.126590	-5.461447	0.504222
56	H	-5.759490	-4.718012	1.990748
57	C	-7.478734	-3.889635	-0.744843
58	H	-8.095578	-4.751206	-0.481170
59	H	-8.126348	-3.005190	-0.725562
60	H	-7.119317	-4.025184	-1.778386
61	C	1.397708	5.559032	0.331796
62	H	2.481873	5.531697	0.323229
63	C	-1.397766	5.558997	0.331728
64	H	-2.481930	5.531641	0.323103

Cartesian coordinates of the optimized structure of **9**

E(RB3LYP) = -2437.36582586 a.u.

Number of imaginary frequencies: 0



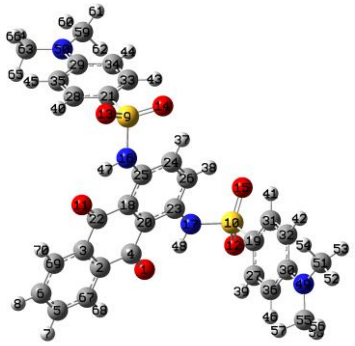
Atom No.	Element	X	Y	Z
1	S	-3.342205	-1.526368	-2.005691
2	S	3.339433	-1.533019	2.002978
3	O	4.161644	-1.018258	3.095132
4	O	-2.744575	-2.862143	-2.051508
5	O	-2.009446	2.220223	-1.804454
6	O	2.740697	-2.868420	2.044922
7	O	-4.164896	-1.008211	-3.095879
8	O	2.010788	2.215081	1.807501
9	N	2.090244	-0.382587	1.888108
10	N	-2.092073	-0.377172	-1.888926
11	C	0.540943	0.881965	0.472760
12	C	0.529356	3.436159	0.463831
13	C	-0.540910	0.883350	-0.472053
14	C	-0.525587	3.437500	-0.460001
15	C	0.507563	-1.555106	0.459718
16	C	-0.510592	-1.553780	-0.462614
17	C	1.094992	2.162555	0.971616
18	C	1.066741	-0.349523	0.939358
19	C	-4.265490	-1.390661	-0.475687
20	C	-1.093339	2.165345	-0.969057
21	C	4.795663	-2.200442	-1.727590
22	C	-1.068314	-0.346790	-0.940397
23	C	4.264167	-1.394121	0.474138
24	C	-5.159299	-0.327661	-0.313034
25	C	5.691872	-1.141631	-1.919118
26	C	0.530113	5.854452	0.465232
27	C	-0.522379	5.855791	-0.458914
28	C	-6.445084	-0.991121	3.218498
29	C	5.865961	-0.216160	-0.877095
30	C	-1.048274	4.653263	-0.920366

Atom No.	Element	X	Y	Z
31	C	5.160719	-0.332746	0.316041
32	C	4.078972	-2.335121	-0.538418
33	C	-5.863494	-0.213791	0.880979
34	C	-4.081997	-2.335894	0.533213
35	C	-4.797655	-2.203935	1.723315
36	C	-5.691096	-1.143625	1.919401
37	C	6.447071	-0.986115	-3.217156
38	C	1.054015	4.650589	0.925468
39	H	0.893390	-2.494264	0.836110
40	H	-0.897563	-2.491896	-0.840432
41	H	4.659053	-2.935960	-2.516191
42	H	-5.311343	0.384831	-1.117486
43	H	0.939032	6.794697	0.824338
44	H	-0.929746	6.797074	-0.817062
45	H	-7.487052	-0.701098	3.044270
46	H	-6.442197	-1.920591	3.795648
47	H	-5.992911	-0.211648	3.845579
48	H	6.570210	0.602896	-1.000970
49	H	-1.861694	4.628968	-1.637046
50	H	5.314007	0.376298	1.123288
51	H	3.403478	-3.169580	-0.386540
52	H	-6.565586	0.606580	1.008361
53	H	-3.408555	-3.171353	0.377781
54	H	-4.662375	-2.942755	2.509052
55	H	7.489315	-0.698133	-3.041214
56	H	6.443316	-1.913755	-3.797245
57	H	5.996477	-0.204050	-3.842143
58	H	1.867363	4.624226	1.642156
59	H	2.399428	0.549578	2.186331
60	H	-2.400409	0.555776	-2.185555

Cartesian coordinates of the optimized structure of **10**

E(RB3LYP) = -2626.67121233 a.u.

Number of imaginary frequencies: 0



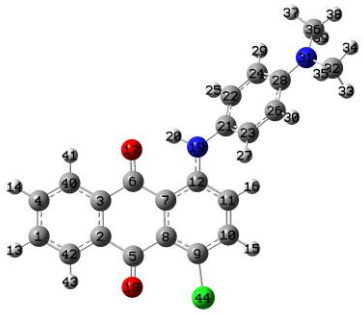
Atom No.	Element	X	Y	Z
1	O	-1.709567	2.560166	-2.094372
2	C	-0.450874	3.777626	-0.536642
3	C	0.450913	3.777550	0.536982
4	C	-0.930087	2.504304	-1.129045
5	C	-0.450752	6.196188	-0.535734
6	C	0.450856	6.196112	0.536362
7	H	-0.800377	7.137057	-0.951656
8	H	0.800506	7.136922	0.952396
9	S	2.863861	-1.248558	2.632458
10	S	-2.864011	-1.248149	-2.632661
11	O	1.709608	2.559872	2.094539
12	O	-3.506200	-0.686472	-3.820032
13	O	3.505969	-0.687081	3.819967
14	O	2.157424	-2.532277	2.669174
15	O	-2.157584	-2.531865	-2.669634
16	N	1.741751	-0.034443	2.212108
17	N	-1.741861	-0.034111	-2.212194
18	C	0.456202	1.225875	0.555849
19	C	-4.048345	-1.313431	-1.309223
20	C	-0.456218	1.225955	-0.555825
21	C	4.048287	-1.313637	1.309091
22	C	0.930108	2.504143	1.129219
23	C	-0.894544	-0.004595	-1.109000
24	C	0.422862	-1.211010	0.540294
25	C	0.894498	-0.004757	1.108868
26	C	-0.422900	-1.210931	-0.540611
27	C	-5.038336	-0.328654	-1.214426
28	C	5.038198	-0.328766	1.214430
29	C	5.918808	-1.388164	-0.802508
30	C	-5.918675	-1.388232	0.802536
31	C	-3.994682	-2.339762	-0.362205
32	C	-4.913639	-2.379992	0.676532
33	C	3.994788	-2.339914	0.362007
34	C	4.913833	-2.380005	-0.676658
35	C	5.958358	-0.363206	0.178964

Atom No.	Element	X	Y	Z
36	C	-5.958408	-0.363235	-0.178885
37	H	0.734583	-2.150250	0.979384
38	H	-0.734638	-2.150106	-0.979827
39	H	-5.096687	0.455109	-1.963192
40	H	5.096416	0.454969	1.963238
41	H	-3.245641	-3.118559	-0.453910
42	H	-4.852223	-3.192750	1.389403
43	H	3.245795	-3.118770	0.453602
44	H	4.852530	-3.192714	-1.389595
45	H	6.718643	0.406727	0.135362
46	H	-6.718769	0.406619	-0.135185
47	H	2.023901	0.894163	2.544064
48	H	-2.024044	0.894549	-2.543969
49	N	-6.827245	-1.420858	1.835554
50	N	6.827494	-1.420686	-1.835425
51	C	-6.779017	-2.494589	2.815115
52	H	-7.564957	-2.339701	3.555521
53	H	-6.937501	-3.478952	2.352607
54	H	-5.816806	-2.517031	3.344120
55	C	-7.867602	-0.408969	1.927619
56	H	-8.477695	-0.603046	2.810858
57	H	-7.444650	0.600185	2.024598
58	H	-8.528843	-0.418738	1.049694
59	C	6.779280	-2.494233	-2.815186
60	H	7.565380	-2.339336	-3.555420
61	H	6.937560	-3.478684	-2.352804
62	H	5.817156	-2.516476	-3.344367
63	C	7.867597	-0.408538	-1.927523
64	H	8.477855	-0.602602	-2.810650
65	H	7.444416	0.600504	-2.024699
66	H	8.528727	-0.418027	-1.049517
67	C	-0.899355	4.993062	-1.070770
68	H	-1.594265	4.966915	-1.902854
69	C	0.899428	4.992910	1.071253
70	H	1.594340	4.966646	1.903332

Cartesian coordinates of the optimized structure of **11**

E(RB3LYP) = -1568.73908622 a.u.

Number of imaginary frequencies: 0



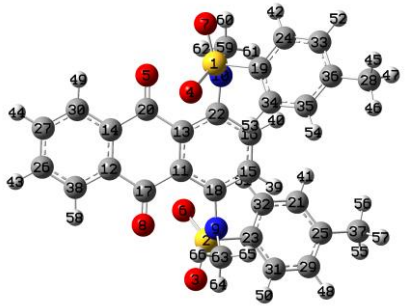
Atom No.	Element	X	Y	Z
1	C	5.909513	-2.313814	0.300028
2	C	4.149104	-0.666394	0.111396
3	C	3.193225	-1.689681	0.079316
4	C	4.953706	-3.337591	0.267572
5	C	3.749902	0.765343	0.027984
6	C	1.747278	-1.377902	-0.042761
7	C	1.316285	0.027696	-0.100742
8	C	2.286822	1.089049	-0.092021
9	C	1.844019	2.412223	-0.188779
10	C	0.470636	2.693667	-0.306398
11	C	-0.467513	1.692623	-0.299221
12	C	-0.084473	0.332455	-0.177618
13	H	6.964833	-2.557878	0.385894
14	H	5.267767	-4.376046	0.328811
15	H	0.159600	3.727699	-0.412017
16	H	-1.516880	1.937251	-0.410231
17	O	0.944862	-2.328890	-0.096007
18	O	4.613807	1.632168	0.063665
19	N	-1.028901	-0.651143	-0.167518
20	H	-0.636613	-1.593482	-0.192918
21	C	-2.436438	-0.502637	-0.079734
22	C	-3.256130	-1.233111	-0.948256

Atom No.	Element	X	Y	Z
23	C	-3.055123	0.289009	0.896598
24	C	-4.641754	-1.175584	-0.854596
25	H	-2.797343	-1.851201	-1.715562
26	C	-4.440428	0.370699	0.984556
27	H	-2.446216	0.840718	1.606871
28	C	-5.277223	-0.370159	0.118281
29	H	-5.229219	-1.757410	-1.554341
30	H	-4.869313	1.003946	1.751673
31	N	-6.661040	-0.319828	0.228403
32	C	-7.270076	0.676018	1.093153
33	H	-7.017313	1.708069	0.800898
34	H	-8.355524	0.566501	1.054695
35	H	-6.961903	0.534597	2.136308
36	C	-7.480031	-0.935469	-0.801440
37	H	-7.278209	-2.011053	-0.873369
38	H	-8.532952	-0.816738	-0.538655
39	H	-7.321465	-0.492485	-1.798089
40	C	3.602178	-3.028168	0.156839
41	H	2.843822	-3.802716	0.128010
42	C	5.509070	-0.984105	0.221873
43	H	6.227179	-0.171541	0.243730
44	Cl	2.877922	3.828079	-0.194432

Cartesian coordinates of the optimized structure of **12**

E(RB3LYP) = -1568.73908622 a.u.

Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z
1	S	3.902684	0.230832	-0.448976
2	S	-3.902816	0.231067	0.448748
3	O	-4.950253	0.599458	1.403088
4	O	3.530578	1.080487	0.684792
5	O	1.968497	2.591975	-1.826979
6	O	-3.530604	1.080574	-0.685090
7	O	4.950049	0.599080	-1.403453
8	O	-1.968484	2.592211	1.826841
9	N	-2.498366	-0.046946	1.338678
10	N	2.498164	-0.047271	-1.338750
11	C	-0.599128	1.276765	0.377930
12	C	-0.546751	3.844682	0.438376
13	C	0.599076	1.276699	-0.377988
14	C	0.547102	3.844621	-0.438325
15	C	-0.619558	-1.151870	0.316463
16	C	0.619336	-1.151934	-0.316324
17	C	-1.130678	2.571767	0.934947
18	C	-1.234620	0.045978	0.678939
19	C	4.351731	-1.371675	0.231569
20	C	1.130764	2.571640	-0.935005
21	C	-4.190415	-3.014980	-1.982491
22	C	1.234465	0.045840	-0.678931
23	C	-4.351824	-1.371520	-0.231621
24	C	5.183305	-2.222830	-0.501786
25	C	-5.013581	-3.891410	-1.264591
26	C	-0.545835	6.261470	0.438569
27	C	0.546630	6.261408	-0.438310
28	C	5.377654	-5.250174	1.814673
29	C	-5.506019	-3.472469	-0.018380
30	C	1.090416	5.058457	-0.877552
31	C	-5.183389	-2.222606	0.501824
32	C	-3.856898	-1.757712	-1.477495
33	C	5.505972	-3.472623	0.018560

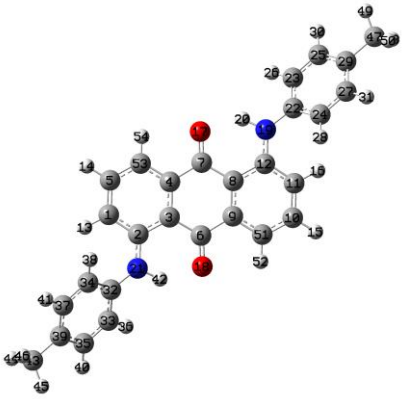
Atom No.	Element	X	Y	Z
34	C	3.856831	-1.757733	1.477495
35	C	4.190386	-3.014935	1.982636
36	C	5.013568	-3.891426	1.264831
37	C	-5.377551	-5.250265	-1.814243
38	C	-1.089846	5.058581	0.877702
39	H	-1.121549	-2.085320	0.550986
40	H	1.121269	-2.085432	-0.550784
41	H	-3.812003	-3.314197	-2.956815
42	H	5.586969	-1.895264	-1.453983
43	H	-0.970777	7.202616	0.776305
44	H	0.971747	7.202505	-0.775963
45	H	6.464327	-5.359692	1.915007
46	H	4.932296	-5.417374	2.799999
47	H	5.034430	-6.053219	1.150684
48	H	-6.159973	-4.131949	0.547648
49	H	1.935737	5.031362	-1.556574
50	H	-5.587079	-1.894941	1.453976
51	H	-3.239366	-1.072853	-2.048509
52	H	6.159924	-4.132160	-0.547405
53	H	3.239290	-1.072823	2.048437
54	H	3.811993	-3.314049	2.956999
55	H	-6.464252	-5.360218	-1.913761
56	H	-4.932854	-5.417237	-2.799906
57	H	-5.033498	-6.053213	-1.150560
58	H	-1.935176	5.031584	1.556717
59	C	2.538140	-0.211256	-2.793683
60	H	3.577577	-0.174898	-3.119856
61	H	2.095560	-1.171671	-3.085043
62	H	2.001836	0.612711	-3.272197
63	C	-2.538470	-0.210937	2.793589
64	H	-3.577865	-0.173539	3.119781
65	H	-2.096800	-1.171758	3.085021
66	H	-2.001382	0.612533	3.272079

Cartesian coordinates of the optimized structure of **13**

(Terminal *tert*-butyl groups were replaced with methyl groups.)

E(RB3LYP) = -1340.23723443 a.u.

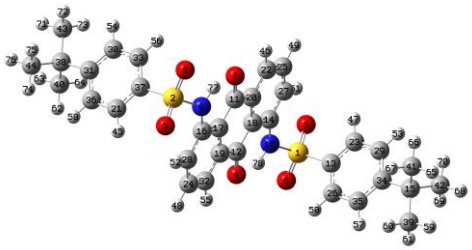
Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z
1	C	-3.190363	2.031576	-0.268568
2	C	-2.834174	0.660637	-0.237204
3	C	-1.441152	0.319725	-0.281475
4	C	-0.476224	1.359553	-0.303171
5	C	-2.221678	3.018334	-0.300880
6	C	-0.991686	-1.073628	-0.325485
7	C	0.991700	1.073544	-0.325436
8	C	1.441160	-0.319806	-0.281474
9	C	0.476238	-1.359635	-0.303206
10	C	2.221706	-3.018402	-0.300961
11	C	3.190385	-2.031637	-0.268625
12	C	2.834181	-0.660702	-0.237215
13	H	-4.238633	2.302814	-0.296018
14	H	-2.528753	4.060496	-0.333097
15	H	2.528790	-4.060560	-0.333212
16	H	4.238656	-2.302864	-0.296089
17	O	1.784166	2.031258	-0.379529
18	O	-1.784136	-2.031356	-0.379553
19	N	3.780596	0.329907	-0.209462
20	H	3.386662	1.262496	-0.344760
21	N	-3.780618	-0.329943	-0.209481
22	C	5.165910	0.233633	0.029737
23	C	6.017621	1.115347	-0.654683
24	C	5.725886	-0.637688	0.976081
25	C	7.386906	1.111596	-0.408647
26	H	5.594248	1.801544	-1.383625
27	C	7.102264	-0.642517	1.197472

Atom No.	Element	X	Y	Z
28	H	5.084037	-1.286914	1.562174
29	C	7.961631	0.224034	0.511794
30	H	8.023264	1.808152	-0.950206
31	H	7.513014	-1.325194	1.938139
32	C	-5.165929	-0.233620	0.029719
33	C	-6.017678	-1.115273	-0.654731
34	C	-5.725865	0.637694	0.976092
35	C	-7.386964	-1.111471	-0.408690
36	H	-5.594336	-1.801465	-1.383695
37	C	-7.102241	0.642576	1.197487
38	H	-5.083985	1.286873	1.562204
39	C	-7.961647	-0.223915	0.511780
40	H	-8.023353	-1.807982	-0.950271
41	H	-7.512960	1.325245	1.938179
42	H	-3.386717	-1.262543	-0.344810
43	C	-9.454290	-0.195422	0.742417
44	H	-9.969068	0.390760	-0.030918
45	H	-9.883764	-1.203317	0.721186
46	H	-9.700968	0.254871	1.709664
47	C	9.454275	0.195613	0.742428
48	H	9.969119	-0.390226	-0.031121
49	H	9.883644	1.203561	0.721573
50	H	9.700994	-0.255010	1.709511
51	C	0.860548	-2.695369	-0.305084
52	H	0.093656	-3.460093	-0.323188
53	C	-0.860523	2.695290	-0.305017
54	H	-0.093625	3.460008	-0.323097

Cartesian coordinates of the optimized structure of **14**



E(RB3LYP) = -2673.24185913 a.u.

Number of imaginary frequencies: 0

Atom No.	Element	X	Y	Z
1	S	4.526451	-2.923566	0.429243
2	S	-4.527321	2.923812	-0.428959
3	O	4.750985	-3.729265	-0.772115
4	O	1.347899	-1.073002	2.080642
5	O	-4.752324	3.729261	0.772479
6	O	4.716193	-3.462751	1.773222
7	O	-1.348252	1.074259	-2.080303
8	O	-4.717193	3.463077	-1.772887
9	N	-2.904824	2.417282	-0.441662
10	N	2.904203	-2.416304	0.442028
11	C	-0.753207	0.594814	-1.104196
12	C	0.752767	-0.593662	1.104533
13	C	5.495880	-1.424885	0.276412
14	C	2.190157	-1.813608	-0.592378
15	C	7.789990	2.252706	-0.109998
16	C	-2.190753	1.814561	0.592723
17	C	-1.115960	0.928776	0.284669
18	C	1.115447	-0.927715	-0.284326
19	C	-0.378250	0.352139	1.347757
20	C	0.377749	-0.351062	-1.347416
21	C	-5.999870	1.039209	0.967413
22	C	0.694634	-0.632854	-2.673390
23	C	5.999658	-1.039758	-0.967507
24	C	-1.744352	1.508401	2.959582
25	C	1.743695	-1.507511	-2.959235
26	C	5.728261	-0.645673	1.409270
27	C	2.478322	-2.099060	-1.942247
28	C	-2.479001	2.099922	1.942592
29	C	6.730230	0.140836	-1.065792
30	C	-6.462358	-0.533667	-1.288991
31	C	-6.976240	-0.957215	-0.053346
32	C	-0.695196	0.633859	2.673733
33	C	-5.727901	0.645435	-1.409351
34	C	6.977114	0.956296	0.052936
35	C	6.463245	0.533077	1.288699
36	C	-6.729917	-0.141728	1.065485
37	C	-5.496070	1.424666	-0.276393
38	C	-7.788564	-2.253997	0.109354
39	C	7.963606	3.007744	1.221480

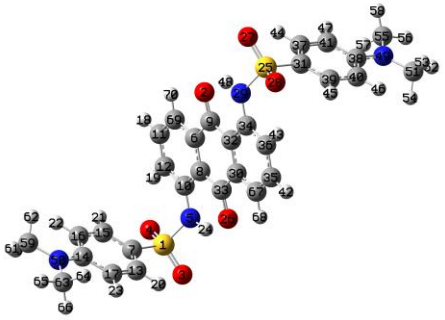
Atom No.	Element	X	Y	Z
40	C	-7.061617	-3.189488	1.105251
41	C	7.063333	3.188408	-1.105907
42	C	9.196436	1.910660	-0.657466
43	C	-7.961706	-3.008975	-1.222219
44	C	-9.195219	-1.912615	0.656705
45	H	-5.839923	1.667477	1.836561
46	H	0.110668	-0.168649	-3.459071
47	H	5.839292	-1.668023	-1.836580
48	H	-1.984406	1.744868	3.992485
49	H	1.983694	-1.744042	-3.992135
50	H	5.353147	-0.964450	2.376504
51	H	3.265733	-2.805921	-2.170353
52	H	-3.266507	2.806680	2.170693
53	H	7.120463	0.425245	-2.038342
54	H	-6.635138	-1.121641	-2.182799
55	H	-0.111208	0.169681	3.459413
56	H	-5.352775	0.964456	-2.376499
57	H	6.636444	1.121041	2.182432
58	H	-7.120187	-0.426387	2.037947
59	H	8.546405	3.919673	1.052200
60	H	7.001209	3.307641	1.651406
61	H	8.500613	2.407817	1.964961
62	H	-6.951582	-2.729917	2.092981
63	H	-7.628194	-4.119562	1.232220
64	H	-6.060480	-3.448641	0.742715
65	H	7.630282	4.118237	-1.233012
66	H	6.953014	2.728795	-2.093587
67	H	6.062338	3.448006	-0.743301
68	H	9.786020	2.826802	-0.781396
69	H	9.736262	1.250146	0.030388
70	H	9.148145	1.412656	-1.631409
71	H	-8.544127	-3.921174	-1.053097
72	H	-8.498888	-2.409205	-1.965699
73	H	-6.999131	-3.308413	-1.652069
74	H	-9.147250	-1.414697	1.630708
75	H	-9.735252	-1.252256	-0.031135
76	H	-9.784426	-2.829020	0.780478
77	H	-2.585211	2.144947	-1.378019
78	H	2.584704	-2.143812	1.378388

Cartesian coordinates of the optimized structure of **15**

(Terminal butyl groups were replaced with methyl groups.)

E(RB3LYP) = -2626.67311205 a.u.

Number of imaginary frequencies: 0



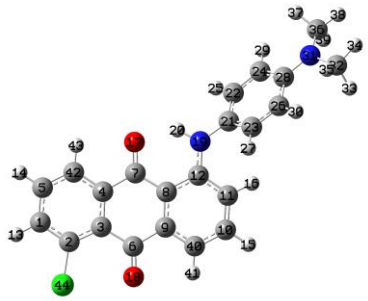
Atom No.	Element	X	Y	Z
1	S	-4.742260	-2.690698	0.415592
2	O	1.349485	0.856586	-2.208223
3	O	-4.950742	-3.230329	1.758003
4	O	-5.067276	-3.457859	-0.789443
5	N	-3.065811	-2.365865	0.398433
6	C	-0.448108	-0.457366	-1.438527
7	C	-5.552937	-1.112974	0.301888
8	C	-1.205987	-0.977965	-0.360465
9	C	0.731520	0.433751	-1.219828
10	C	-2.329571	-1.809581	-0.645618
11	C	-1.889845	-1.561982	-3.021203
12	C	-2.646042	-2.097179	-1.989292
13	C	-5.690526	-0.323058	1.448795
14	C	-6.786904	1.419027	0.134390
15	C	-6.036743	-0.650135	-0.924981
16	C	-6.646235	0.593681	-1.009767
17	C	-6.297867	0.919969	1.369808
18	H	-2.151678	-1.800018	-4.048557
19	H	-3.475185	-2.761329	-2.197735
20	H	-5.336847	-0.692734	2.406020
21	H	-5.954744	-1.276245	-1.806686
22	H	-7.022997	0.921101	-1.970761
23	H	-6.400636	1.504492	2.275584
24	H	-2.717934	-2.105153	1.327227
25	S	4.599036	2.648245	-0.587600
26	O	-1.416267	-1.084870	2.008879
27	O	4.818180	3.082646	-1.966091
28	O	4.808097	3.546575	0.550916
29	N	2.959100	2.180485	-0.602742
30	C	0.355260	0.263014	1.237850
31	C	5.529587	1.162908	-0.292926
32	C	1.111257	0.785176	0.159260
33	C	-0.814246	-0.641725	1.019885
34	C	2.223181	1.633574	0.442868
35	C	1.774793	1.398436	2.818068

Atom No.	Element	X	Y	Z
36	C	2.528625	1.936107	1.786038
37	C	5.695390	0.232975	-1.325787
38	C	6.975621	-1.216754	0.165495
39	C	6.092287	0.916703	0.962037
40	C	6.806281	-0.251342	1.189622
41	C	6.404841	-0.936159	-1.103783
42	H	2.028983	1.647551	3.844721
43	H	3.344650	2.615914	1.995539
44	H	5.280932	0.433943	-2.308813
45	H	5.986556	1.652377	1.751718
46	H	7.239762	-0.409765	2.169233
47	H	6.524588	-1.633002	-1.923946
48	H	2.638800	1.893344	-1.533501
49	N	7.671921	-2.382264	0.391146
50	N	-7.381457	2.657821	0.052446
51	C	8.288026	-2.624453	1.685918
52	H	8.782144	-3.596802	1.670875
53	H	9.042246	-1.863415	1.931545
54	H	7.542166	-2.637960	2.491947
55	C	7.863171	-3.340482	-0.686171
56	H	8.414864	-4.201118	-0.305481
57	H	6.903807	-3.703039	-1.078511
58	H	8.434718	-2.912966	-1.522250
59	C	-7.919753	3.126551	-1.214506
60	H	-8.721515	2.474018	-1.588860
61	H	-8.333795	4.126656	-1.079183
62	H	-7.140584	3.186350	-1.985969
63	C	-7.562319	3.461975	1.250719
64	H	-6.601834	3.692971	1.730098
65	H	-8.035986	4.406452	0.979448
66	H	-8.201991	2.960884	1.991185
67	C	0.689418	0.560879	2.555849
68	H	0.090980	0.137650	3.353704
69	C	-0.791520	-0.742225	-2.757196
70	H	-0.189879	-0.322217	-3.554406

Cartesian coordinates of the optimized structure of **16**

E(RB3LYP) = -1568.74061805 a.u.

Number of imaginary frequencies: 0



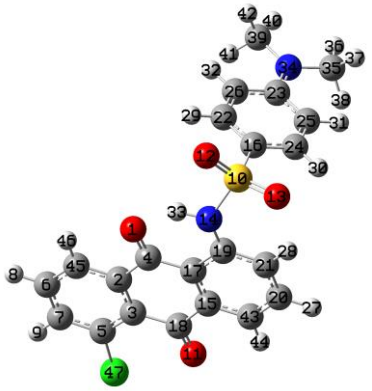
Atom	Element	X	Y	Z
1	C	5.657922	-1.826626	0.297263
2	C	5.244164	-0.499533	0.159827
3	C	3.876396	-0.173590	0.037987
4	C	2.944973	-1.239696	0.060451
5	C	4.721653	-2.856618	0.313958
6	C	3.367680	1.223502	-0.117620
7	C	1.467143	-1.015889	-0.061027
8	C	0.963960	0.348405	-0.162080
9	C	1.884266	1.428528	-0.205105
10	C	0.072028	2.998911	-0.430872
11	C	-0.854310	1.975216	-0.382285
12	C	-0.444335	0.625392	-0.230483
13	H	6.717731	-2.037660	0.389816
14	H	5.054697	-3.885094	0.420615
15	H	-0.274539	4.021359	-0.557198
16	H	-1.910918	2.192511	-0.482954
17	O	0.723407	-2.013751	-0.070485
18	O	4.117597	2.189249	-0.171451
19	N	-1.351765	-0.393317	-0.179418
20	H	-0.924710	-1.319881	-0.184358
21	C	-2.762141	-0.305397	-0.079572
22	C	-3.554733	-1.134754	-0.882459

Atom	Element	X	Y	Z
23	C	-3.409411	0.523719	0.845709
24	C	-4.940524	-1.137245	-0.774591
25	H	-3.074584	-1.783307	-1.610699
26	C	-4.796321	0.544282	0.945830
27	H	-2.822430	1.153507	1.507448
28	C	-5.604974	-0.295803	0.146643
29	H	-5.505400	-1.795008	-1.424001
30	H	-5.247240	1.209899	1.671808
31	N	-6.989835	-0.305214	0.272734
32	C	-7.637335	0.731513	1.057976
33	H	-7.444377	1.745974	0.672307
34	H	-8.715922	0.562661	1.051087
35	H	-7.306663	0.698315	2.102963
36	C	-7.786029	-1.015802	-0.713108
37	H	-7.532991	-2.082621	-0.726311
38	H	-8.841495	-0.933546	-0.446110
39	H	-7.656693	-0.622996	-1.734931
40	C	1.445145	2.739464	-0.331040
41	H	2.179376	3.535474	-0.360614
42	C	3.368047	-2.564420	0.194828
43	H	2.614644	-3.343254	0.202845
44	Cl	6.530300	0.689886	0.155834

Cartesian coordinates of the optimized structure of **17**

E(RB3LYP) = -2117.30947670 a.u.

Number of imaginary frequencies: 0



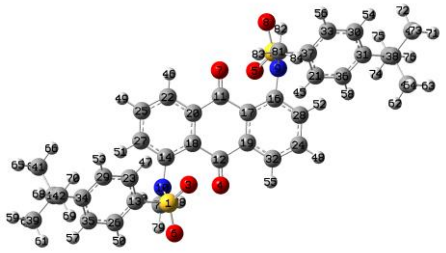
Atom No.	Element	X	Y	Z
1	O	1.097533	-0.925523	-2.094278
2	C	3.010595	0.094541	-1.179376
3	C	3.793252	0.444138	-0.052637
4	C	1.717047	-0.651815	-1.056066
5	C	4.997609	1.141521	-0.285801
6	C	4.607824	1.116837	-2.674585
7	C	5.395684	1.472427	-1.583901
8	H	4.928463	1.378371	-3.678805
9	H	6.327878	2.008809	-1.724040
10	S	-2.435245	-2.361189	-0.717368
11	O	3.927500	0.340345	2.325393
12	O	-2.635858	-2.711580	-2.122197
13	O	-2.812588	-3.266000	0.371057
14	N	-0.750601	-2.106522	-0.637612
15	C	2.009083	-0.681830	1.413727
16	C	-3.188237	-0.781661	-0.405052
17	C	1.235332	-1.029305	0.279211
18	C	3.307712	0.062241	1.308252
19	C	0.006251	-1.732948	0.466986
20	C	0.383685	-1.707302	2.865200
21	C	-0.393177	-2.071806	1.775866
22	C	-3.217488	0.183810	-1.417977
23	C	-4.360324	1.739789	0.077843
24	C	-3.750881	-0.498634	0.842379

Atom No.	Element	X	Y	Z
25	C	-4.330004	0.739590	1.081923
26	C	-3.792555	1.422429	-1.183936
27	H	0.055926	-1.982719	3.863919
28	H	-1.301446	-2.644422	1.913128
29	H	-2.805944	-0.043455	-2.396414
30	H	-3.754329	-1.258995	1.615563
31	H	-4.769285	0.925789	2.053988
32	H	-3.810619	2.145749	-1.989640
33	H	-0.353807	-1.815737	-1.536433
34	N	-4.925277	2.972441	0.314710
35	C	-5.552129	3.252485	1.596791
36	H	-5.932735	4.274795	1.593556
37	H	-6.394423	2.575940	1.800318
38	H	-4.835389	3.162829	2.423888
39	C	-4.994867	3.961175	-0.749649
40	H	-5.459276	4.869707	-0.363867
41	H	-3.995503	4.225639	-1.119659
42	H	-5.592620	3.608666	-1.602362
43	C	1.582616	-1.012729	2.695923
44	H	2.201391	-0.728579	3.538792
45	C	3.417155	0.428012	-2.473613
46	H	2.783968	0.134478	-3.302556
47	Cl	6.087355	1.649236	0.985881

Cartesian coordinates of the optimized structure of **18**

E(RB3LYP) = -2751.8185173 a.u.

Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z
1	S	-4.284243	1.878759	-0.318031
2	S	4.284380	-1.829799	0.411457
3	O	-3.512131	1.337292	-1.439372
4	O	-1.081074	2.482747	0.355759
5	O	3.587897	-1.241578	1.558105
6	O	-4.573379	3.307603	-0.176219
7	O	1.075283	-2.428591	-0.073988
8	O	4.527809	-3.268740	0.287668
9	N	3.467072	-1.346404	-0.987040
10	N	-3.527518	1.388550	1.110323
11	C	0.624383	-1.295565	0.034594
12	C	-0.652090	1.347493	0.195133
13	C	-5.861849	1.016146	-0.322870
14	C	-2.746070	0.190745	1.088692
15	C	-9.661379	-1.113821	-0.327439
16	C	2.688803	-0.147000	-0.937681
17	C	1.361385	-0.088660	-0.441886
18	C	-1.404860	0.136010	0.632455
19	C	0.709694	1.160986	-0.407515
20	C	-0.750585	-1.112001	0.608933
21	C	6.071735	0.229706	0.916697
22	C	-1.391007	-2.266449	1.076146
23	C	-5.981600	-0.209913	-0.980657
24	C	2.626423	2.240784	-1.407962
25	C	-2.691215	-2.197268	1.556960
26	C	-6.958099	1.574884	0.331517
27	C	-3.365529	-0.975447	1.546208
28	C	3.296426	1.016745	-1.417003
29	C	-7.204966	-0.873905	-0.965438
30	C	8.158746	-0.976536	-0.482934
31	C	8.378747	0.278375	0.104656
32	C	1.340257	2.313738	-0.891297
33	C	6.926503	-1.623753	-0.385005
34	C	-8.328921	-0.343772	-0.306722

Atom No.	Element	X	Y	Z
43	C	10.766970	0.237334	-0.812635
44	C	10.295594	1.213835	1.441791
45	H	5.263867	0.681872	1.481844
46	H	-0.845082	-3.202473	1.041743
47	H	-5.130686	-0.621887	-1.512186
48	H	3.114521	3.131338	-1.793508
49	H	-3.187882	-3.089721	1.926842
50	H	-6.866427	2.542682	0.813512
51	H	-4.392348	-0.905518	1.891163
52	H	4.310988	0.942418	-1.795511
53	H	-7.282793	-1.822176	-1.489366
54	H	8.955864	-1.474398	-1.023002
55	H	0.797663	3.251082	-0.843135
56	H	6.783175	-2.604712	-0.825973
57	H	-9.016087	1.351395	0.846007
58	H	7.440402	1.822470	1.293312
59	H	-11.693238	-0.979791	0.419632
60	H	-10.506672	-0.261812	1.515113
61	H	-10.993522	0.596691	0.038043
62	H	8.818916	3.021872	-0.082074
63	H	10.468137	2.934785	-0.715810
64	H	9.116979	2.286110	-1.664712
65	H	-10.398025	-3.074744	0.290223
66	H	-8.710063	-3.101227	-0.238289
67	H	-9.126860	-2.428924	1.345676
68	H	-11.080628	-1.829439	-1.825617
69	H	-10.295184	-0.298883	-2.261959
70	H	-9.406217	-1.822964	-2.398960
71	H	11.703052	0.805089	-0.854324
72	H	10.994658	-0.739345	-0.370936
73	H	10.431325	0.078212	-1.843780
74	H	9.619978	1.800261	2.073047
75	H	10.462201	0.249812	1.935495
76	H	11.254929	1.743440	1.397586

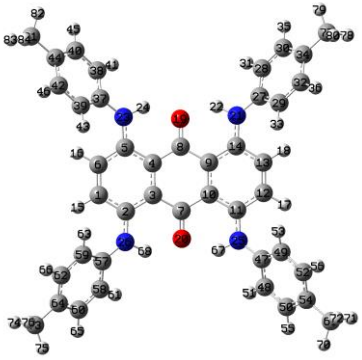
35	C	-8.176016	0.893832	0.336231	77	C	-3.410805	2.296701	2.254930
36	C	7.308564	0.859514	0.808460	78	H	-2.381831	2.653326	2.356012
37	C	5.883315	-1.013295	0.308450	79	H	-4.056585	3.158135	2.084780
38	C	9.727272	1.014996	0.016187	80	H	-3.724596	1.780601	3.169587
39	C	-10.770689	-0.390145	0.459140	81	C	3.278488	-2.273359	-2.106564
40	C	9.515429	2.395927	-0.649550	82	H	3.934292	-3.132248	-1.963898
41	C	-9.457002	-2.512078	0.303797	83	H	2.246062	-2.633274	-2.139193
42	C	-10.134646	-1.275628	-1.791895	84	H	3.534976	-1.771243	-3.046336

Cartesian coordinates of the optimized structure of **19**

(Terminal *tert*-butyl groups were replaced with methyl groups.)

E(RB3LYP) = -1991.68566348 a.u.

Number of imaginary frequencies: 0



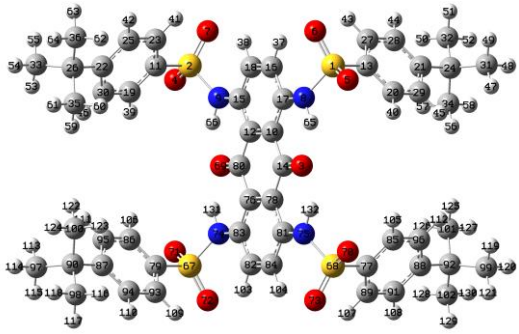
Atom No.	Element	X	Y	Z	Atom No.	Element	X	Y	Z
1	C	-3.702472	-0.684856	-0.510489	43	H	-4.358264	2.414071	1.453166
2	C	-2.498748	-1.433761	-0.547688	44	C	-5.568827	5.515397	0.688414
3	C	-1.270382	-0.717654	-0.651085	45	H	-4.734526	6.787837	-0.838809
4	C	-1.270442	0.717575	-0.651093	46	H	-6.101268	4.006431	2.129857
5	C	-2.498873	1.433578	-0.547718	47	C	3.584480	-3.657250	-0.136947
6	C	-3.702531	0.684569	-0.510505	48	C	3.701601	-4.912986	-0.756514
7	C	0.000052	-1.441391	-0.763927	49	C	4.461507	-3.351791	0.917202
8	C	-0.000065	1.441419	-0.763904	50	C	4.670194	-5.821814	-0.342582
9	C	1.270369	0.717678	-0.651083	51	H	3.025747	-5.166533	-1.569311
10	C	1.270428	-0.717549	-0.651110	52	C	5.437806	-4.266092	1.307486
11	C	2.498859	-1.433555	-0.547757	53	H	4.358309	-2.413992	1.453059
12	C	3.702519	-0.684551	-0.510572	54	C	5.568777	-5.515385	0.688429
13	C	3.702462	0.684876	-0.510541	55	H	4.734387	-6.787887	-0.838696
14	C	2.498739	1.433782	-0.547698	56	H	6.101295	-4.006358	2.129777
15	H	-4.647359	-1.215185	-0.530907	57	C	-3.584202	-3.657528	-0.136838
16	H	-4.647465	1.214813	-0.530943	58	C	-3.701283	-4.913252	-0.756429
17	H	4.647450	-1.214799	-0.531048	59	C	-4.461210	-3.352131	0.917348
18	H	4.647349	1.215204	-0.530980	60	C	-4.669824	-5.822134	-0.342483
19	O	-0.000114	2.695083	-0.935074	61	H	-3.025445	-5.166752	-1.569254
20	O	0.000102	-2.695051	-0.935123	62	C	-5.437454	-4.266481	1.307644
21	N	2.544925	2.809294	-0.552967	63	H	-4.358030	-2.414335	1.453215

22	H	1.650088	3.232804	-0.799350	64	C	-5.568385	-5.515770	0.688561
23	N	-2.545170	2.809082	-0.553051	65	H	-4.733991	-6.788199	-0.838616
24	H	-1.650350	3.232644	-0.799420	66	H	-6.100928	-4.006798	2.129963
25	N	2.545152	-2.809061	-0.553092	67	H	1.650339	-3.232620	-0.799484
26	N	-2.544927	-2.809271	-0.552979	68	H	-1.650092	-3.232769	-0.799394
27	C	3.584226	3.657525	-0.136823	69	C	6.648003	-6.487724	1.102992
28	C	3.701362	4.913233	-0.756436	70	H	6.324486	-7.526263	0.972563
29	C	4.461208	3.352111	0.917377	71	H	7.560458	-6.355916	0.505282
30	C	4.669929	5.822088	-0.342494	72	H	6.927548	-6.352046	2.153440
31	H	3.025544	5.166738	-1.569277	73	C	-6.647560	-6.488157	1.103143
32	C	5.437482	4.266433	1.307670	74	H	-7.560201	-6.356063	0.505780
33	H	4.357994	2.414323	1.453252	75	H	-6.324172	-7.526677	0.972252
34	C	5.568464	5.515706	0.688569	76	H	-6.926753	-6.352817	2.153730
35	H	4.734139	6.788140	-0.838643	77	C	6.647669	6.488062	1.103151
36	H	6.100939	4.006738	2.129998	78	H	7.560195	6.356146	0.505575
37	C	-3.584516	3.657268	-0.136926	79	H	6.324199	7.526594	0.972556
38	C	-3.701689	4.912964	-0.756561	80	H	6.927077	6.352502	2.153652
39	C	-4.461500	3.351841	0.917265	81	C	-6.648060	6.487733	1.102968
40	C	-4.670289	5.821792	-0.342645	82	H	-6.324645	7.526270	0.972280
41	H	-3.025867	5.166477	-1.569396	83	H	-7.560606	6.355734	0.505436
42	C	-5.437811	4.266139	1.307532	84	H	-6.927423	6.352239	2.153488

Cartesian coordinates of the optimized structure of **20**

E(RB3LYP) = -4657.69514443 a.u.

Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z	Atom No.	Element	X	Y	Z
1	S	2.706436	3.774376	2.786221	67	S	-2.707041	-3.768188	-2.785029
2	S	-2.703416	3.774135	-2.788940	68	S	2.703961	-3.767880	2.787625
3	O	1.526499	0.003866	2.227805	69	O	-1.526814	0.003188	-2.227691
4	O	-3.259145	3.239571	-4.029371	70	O	3.263102	-3.231889	4.025917
5	O	3.260575	3.240511	4.027659	71	O	-3.264703	-3.232857	-4.024269
6	O	2.031948	5.072554	2.731493	72	O	-2.030239	-5.065331	-2.734273
7	O	-2.027897	5.071855	-2.736033	73	O	2.026298	-5.064641	2.738568
8	N	1.605498	2.566055	2.313956	74	N	-1.607234	-2.558884	-2.312798

9	N	-1.602896	2.565413	-2.316649	75	N	1.604453	-2.558271	2.315411
10	C	0.418172	1.285603	0.580736	76	C	-0.418492	-1.278431	-0.580600
11	C	-3.987595	3.773413	-1.540689	77	C	3.985391	-3.771661	1.536576
12	C	-0.416818	1.285427	-0.582142	78	C	0.416921	-1.278258	0.581960
13	C	3.991874	3.771531	1.539261	79	C	-3.989680	-3.770078	-1.535210
14	C	0.829352	0.003759	1.183475	80	C	-0.829532	0.003384	-1.183446
15	C	-0.822612	2.518688	-1.163335	81	C	0.823195	-2.511509	1.162819
16	C	0.390703	3.722247	0.563459	82	C	-0.391032	-3.715060	-0.563342
17	C	0.825391	2.519065	1.160556	83	C	-0.826091	-2.511879	-1.160171
18	C	-0.386262	3.722038	-0.567799	84	C	0.386654	-3.714855	0.567412
19	C	-4.970618	2.779670	-1.574270	85	C	4.968898	-2.778213	1.564682
20	C	4.974364	2.777346	1.575064	86	C	-4.972808	-2.776323	-1.565472
21	C	6.011679	3.741217	-0.418319	87	C	-6.005296	-3.747632	0.426817
22	C	-6.005384	3.746469	0.419026	88	C	5.999103	-3.752285	-0.427444
23	C	-4.004184	4.754935	-0.552904	89	C	3.999569	-4.756587	0.552152
24	C	7.132807	3.691417	-1.471191	90	C	-7.124195	-3.701882	1.482252
25	C	-5.009220	4.732386	0.416523	91	C	5.002582	-4.737801	-0.419458
26	C	-7.125453	3.698396	1.473116	92	C	7.117010	-3.708119	-1.484007
27	C	4.009973	4.751856	0.550315	93	C	-4.005160	-4.753818	-0.549623
28	C	5.015999	4.727626	-0.418039	94	C	-5.009111	-4.733503	0.420983
29	C	5.966761	2.771963	0.602505	95	C	-5.963087	-2.774833	-0.590759
30	C	-5.962000	2.775958	-0.600673	96	C	5.958221	-2.778246	0.589003
31	C	8.504985	3.808253	-0.764802	97	C	-8.497840	-3.816805	0.778410
32	C	7.022869	4.832326	-2.499854	98	C	-7.011674	-4.846277	2.506747
33	C	-8.498318	3.814905	0.768009	99	C	8.491296	-3.822596	-0.781344
34	C	7.058590	2.345910	-2.232574	100	C	-7.048820	-2.358990	2.248122
35	C	-7.050968	2.353797	2.236076	101	C	7.041283	-2.366129	-2.251423
36	C	-7.014028	4.840510	2.500273	102	C	7.003200	-4.853700	-2.507027
37	H	0.673927	4.662354	1.019337	103	H	-0.674368	-4.655186	-1.019111
38	H	-0.668260	4.661925	-1.024899	104	H	0.668893	-4.654771	1.024304
39	H	-4.966884	2.035622	-2.364442	105	H	4.967095	-2.031404	2.352252
40	H	4.969461	2.034271	2.366147	106	H	-4.969996	-2.030482	-2.353956
41	H	-3.255608	5.539338	-0.554066	107	H	3.250690	-5.540684	0.557549
42	H	-5.006502	5.507684	1.173537	108	H	4.997937	-5.515694	-1.173791
43	H	3.261797	5.536639	0.549795	109	H	-3.256571	-5.538200	-0.553382
44	H	5.014469	5.502016	-1.175986	110	H	-5.005492	-5.510497	1.176250
45	H	6.728392	1.999337	0.646057	111	H	-6.725188	-2.002446	-0.629913
46	H	-6.724042	2.003644	-0.642458	112	H	6.720616	-2.006069	0.626446
47	H	8.671447	2.994070	-0.051854	113	H	-8.666176	-3.000230	0.068644
48	H	9.313650	3.773091	-1.504428	114	H	-9.304919	-3.784507	1.519900
49	H	8.586258	4.754109	-0.217670	115	H	-8.579934	-4.760803	0.228198
50	H	6.080879	4.790691	-3.058179	116	H	-6.068553	-4.806178	3.063266
51	H	7.100265	5.817970	-2.027286	117	H	-7.089686	-5.830317	2.030950
52	H	7.839036	4.751492	-3.225971	118	H	-7.826377	-4.768207	3.234797
53	H	-8.665842	2.999928	0.056218	119	H	8.660551	-3.005224	-0.072713
54	H	-9.306226	3.780940	1.508519	120	H	9.297673	-3.791410	-1.523644

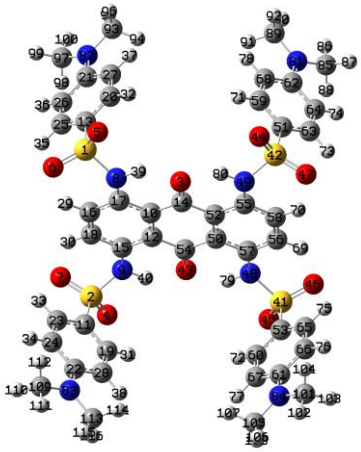
55	H	-8.579802	4.760133	0.219825	121	H	8.573648	-4.765961	-0.230087
56	H	7.175582	1.488299	-1.561362	122	H	-7.167570	-1.499067	1.580195
57	H	6.098436	2.238441	-2.749588	123	H	-6.087601	-2.252982	2.763456
58	H	7.856276	2.292277	-2.982817	124	H	-7.844919	-2.308272	3.000250
59	H	-7.168978	1.495393	1.566064	125	H	7.160891	-1.505420	-1.584666
60	H	-6.090326	2.246605	2.752243	126	H	6.079613	-2.260487	-2.765990
61	H	-7.847908	2.301406	2.987200	127	H	7.836696	-2.316545	-3.004351
62	H	-6.071504	4.799168	3.057714	128	H	6.059565	-4.814004	-3.062700
63	H	-7.091503	5.825606	2.026576	129	H	7.081407	-5.837191	-2.030132
64	H	-7.829511	4.760868	3.227285	130	H	7.817237	-4.776694	-3.235933
65	H	1.848331	1.645056	2.689430	131	H	-1.850428	-1.638039	-2.688375
66	H	-1.846793	1.644314	-2.691156	132	H	1.848555	-1.637339	2.690144

Cartesian coordinates of the optimized structure of **21**

(Terminal hexyl groups were replaced with methyl groups.)

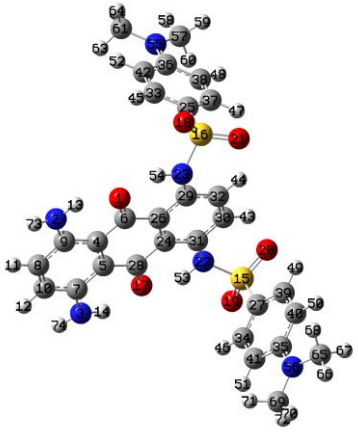
E(RB3LYP) = -4564.55737465 a.u.

Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z	Atom No.	Element	X	Y	Z
1	S	2.790619	3.806904	2.680474	59	C	5.022924	-2.985967	1.269045
2	S	-2.801901	3.798949	-2.680764	60	C	-5.012851	-2.997896	-1.268656
3	O	1.648682	0.002474	2.140353	61	C	-5.866458	-4.119913	0.726188
4	O	-3.455482	3.232725	-3.859683	62	C	5.879249	-4.107281	-0.725037
5	O	3.445782	3.243023	3.859640	63	C	3.906880	-4.963480	0.432342
6	O	2.046907	5.068554	2.738392	64	C	4.833827	-5.055586	-0.595931
7	O	-2.060918	5.062167	-2.739422	65	C	-3.892540	-4.972647	-0.431123
8	N	1.710796	2.565344	2.233719	66	C	-4.819110	-5.066126	0.597374
9	N	-1.719573	2.560090	-2.232728	67	C	-5.941571	-3.086201	-0.243753
10	C	0.443648	1.281797	0.560641	68	C	5.952027	-3.072902	0.244373
11	C	-3.991415	3.926714	-1.365442	69	H	-0.707155	-4.658251	-0.991654
12	C	-0.447992	1.280447	-0.560136	70	H	0.722456	-4.656143	0.990736
13	C	3.979480	3.936241	1.364697	71	H	5.107289	-2.198023	2.010897
14	C	0.891055	0.001331	1.138293	72	H	-5.098989	-2.210511	-2.010902
15	C	-0.883069	2.512858	-1.122184	73	H	3.127578	-5.711439	0.527852

16	C	0.408054	3.717717	0.547272	74	H	4.746900	-5.876403	-1.296830
17	C	0.874622	2.515489	1.122974	75	H	-3.111668	-5.718994	-0.526409
18	C	-0.420471	3.716487	-0.546189	76	H	-4.730362	-5.886407	1.298674
19	C	-5.022683	2.986024	-1.269013	77	H	-6.737276	-2.352709	-0.201714
20	C	5.012797	2.997760	1.268793	78	H	6.746266	-2.337837	0.202089
21	C	5.866347	4.119613	-0.726170	79	H	-1.992491	-1.647667	-2.588358
22	C	-5.879332	4.107747	0.724698	80	H	1.998342	-1.641615	2.587864
23	C	-3.906982	4.963910	-0.432736	81	N	6.794770	-4.190185	-1.749773
24	C	-4.834004	5.056140	0.595460	82	N	6.781451	4.203773	-1.751182
25	C	3.892448	4.972428	0.431115	83	N	-6.795023	4.190854	1.749248
26	C	4.818985	5.065821	-0.597418	84	N	-6.781580	-4.204133	1.751178
27	C	5.941485	3.085981	0.243855	85	C	6.722817	-5.284489	-2.705138
28	C	-5.951857	3.073072	-0.244419	86	H	7.512475	-5.163824	-3.447988
29	H	0.707017	4.658241	0.991899	87	H	6.856436	-6.262980	-2.222186
30	H	-0.722522	4.656145	-0.990542	88	H	5.761251	-5.293521	-3.234843
31	H	-5.106873	2.197856	-2.010648	89	C	7.891558	-3.239673	-1.828796
32	H	5.098958	2.210444	2.011108	90	H	8.497842	-3.465421	-2.707157
33	H	-3.127746	5.711925	-0.528358	91	H	7.525914	-2.208617	-1.928350
34	H	-4.747187	5.877094	1.296213	92	H	8.543473	-3.286540	-0.944682
35	H	3.111567	5.718774	0.526341	93	C	7.880497	3.255821	-1.829562
36	H	4.730184	5.886016	-1.298812	94	H	7.517292	2.223819	-1.928140
37	H	6.737192	2.352489	0.201859	95	H	8.486062	3.482215	-2.708253
38	H	-6.745957	2.337865	-0.201962	96	H	8.532474	3.305019	-0.945618
39	H	1.992421	1.647664	2.588537	97	C	6.707239	5.297541	-2.706995
40	H	-1.998274	1.641618	-2.587795	98	H	5.745469	5.304615	-3.236348
41	S	-2.790644	-3.806928	-2.680349	99	H	6.839295	6.276498	-2.224544
42	S	2.802084	-3.798894	2.680706	100	H	7.496841	5.177925	-3.450074
43	O	-1.648710	-0.002482	-2.140202	101	C	-6.707400	-5.297970	2.706913
44	O	3.455731	-3.232693	3.859600	102	H	-7.496855	-5.178257	3.450134
45	O	-3.445797	-3.243024	-3.859511	103	H	-6.839687	-6.276893	2.224449
46	O	-2.046885	-5.068548	-2.738305	104	H	-5.745547	-5.305209	3.236105
47	O	2.061194	-5.062167	2.739350	105	C	-7.880762	-3.256328	1.829443
48	N	-1.710900	-2.565343	-2.233505	106	H	-8.486393	-3.482807	2.708067
49	N	1.719624	-2.560094	2.232829	107	H	-7.517705	-2.224278	1.928061
50	C	-0.443686	-1.281802	-0.560480	108	H	-8.532639	-3.305609	0.945428
51	C	3.991514	-3.926517	1.365292	109	C	-6.722878	5.284986	2.704792
52	C	0.447980	-1.280453	0.560275	110	H	-6.855745	6.263555	2.221823
53	C	-3.979534	-3.936370	-1.364608	111	H	-7.512999	5.164736	3.447214
54	C	-0.891073	-0.001335	-1.138148	112	H	-5.761557	5.293503	3.234981
55	C	0.883064	-2.512860	1.122318	113	C	-7.891025	3.239512	1.829083
56	C	-0.408151	-3.717724	-0.547064	114	H	-7.524600	2.208808	1.929527
57	C	-0.874697	-2.515496	-1.122785	115	H	-8.497549	3.465557	2.707201
58	C	0.420410	-3.716490	0.546369	116	H	-8.542924	3.285136	0.944904



Cartesian coordinates of the optimized structure of **22**

(Terminal hexyl groups were replaced with methyl groups.)

E(RB3LYP) = -2737.38886137 a.u.

Number of imaginary frequencies: 0

Atom No.	Element	X	Y	Z
1	O	1.717009	2.251980	2.098124
2	N	1.867166	4.827102	2.079242
3	N	-1.862606	4.828661	-2.078658
4	C	0.471708	3.507947	0.543212
5	C	-0.468423	3.508327	-0.542531
6	C	0.924430	2.243559	1.119359
7	C	-0.940314	4.735881	-1.077841
8	C	0.453341	5.945279	0.513318
9	C	0.944561	4.735088	1.078568
10	C	-0.448239	5.945664	-0.512443
11	H	0.814517	6.889076	0.915581
12	H	-0.808709	6.889768	-0.914620
13	H	2.104520	3.968604	2.563371
14	H	-2.101090	3.970401	-2.562627
15	S	-2.869715	-1.507601	-2.609041
16	S	2.869187	-1.509590	2.609249
17	O	-1.715000	2.253390	-2.097253
18	O	3.542216	-0.947783	3.781277
19	O	-3.542081	-0.945136	-3.781132
20	O	-2.191273	-2.806445	-2.661573
21	O	2.190290	-2.808205	2.661600
22	N	-1.719081	-0.314506	-2.233339
23	N	1.718775	-0.315940	2.234433
24	C	-0.449350	0.960036	-0.556521
25	C	4.020482	-1.555717	1.252815
26	C	0.450281	0.959667	0.557410
27	C	-4.021566	-1.553781	-1.253083
28	C	-0.922260	2.244319	-1.118610
29	C	0.880650	-0.275244	1.116870
30	C	-0.416252	-1.476444	-0.547342
31	C	-0.880886	-0.274549	-1.115847
32	C	0.414873	-1.476765	0.548522
33	C	4.999149	-0.562417	1.138324
34	C	-4.999902	-0.560150	-1.138611
35	C	-5.834679	-1.595632	0.909684
36	C	5.832666	-1.597414	-0.910729
37	C	3.949781	-2.574217	0.298954

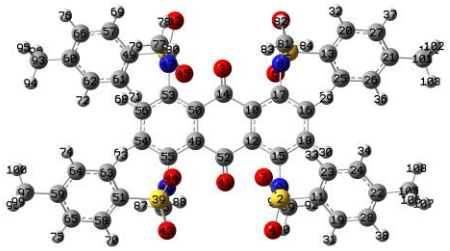
Atom No.	Element	X	Y	Z
38	C	4.840384	-2.598505	-0.765112
39	C	-3.951677	-2.572693	-0.299604
40	C	-4.842730	-2.597054	0.764084
41	C	-5.892887	-0.578853	-0.078657
42	C	5.891684	-0.581049	0.077988
43	H	-0.721437	-2.415359	-0.991945
44	H	0.719215	-2.415900	0.993247
45	H	5.071161	0.215746	1.891690
46	H	-5.071302	0.218337	-1.891701
47	H	3.209702	-3.359660	0.404744
48	H	4.765531	-3.405838	-1.482930
49	H	-3.211885	-3.358403	-0.405413
50	H	-4.768516	-3.404722	1.481592
51	H	-6.645722	0.197614	-0.021278
52	H	6.644803	0.195143	0.020614
53	H	-2.005681	0.616413	-2.554499
54	H	2.006219	0.614769	2.555438
55	N	6.711985	-1.612940	-1.970793
56	N	-6.714457	-1.611232	1.969365
57	C	6.656279	-2.688532	-2.947347
58	H	7.416066	-2.518467	-3.711533
59	H	6.847133	-3.670167	-2.490481
60	H	5.679357	-2.729673	-3.447192
61	C	7.752037	-0.602575	-2.072757
62	H	8.333364	-0.778042	-2.979143
63	H	7.328543	0.408968	-2.134963
64	H	8.441032	-0.631201	-1.216320
65	C	-6.659412	-2.687079	2.945675
66	H	-7.419353	-2.516927	3.709687
67	H	-6.850480	-3.668540	2.488524
68	H	-5.682646	-2.728682	3.445788
69	C	-7.754206	-0.600545	2.071241
70	H	-8.336162	-0.776305	2.977165
71	H	-7.330407	0.410826	2.134250
72	H	-8.442672	-0.628481	1.214361
73	H	1.995561	5.717079	2.536762
74	H	-1.991117	5.718933	-2.535541

Cartesian coordinates of the optimized structure of **23**

(Terminal hexyl groups were replaced with methyl groups.)

E(RB3LYP) = -2737.38886137 a.u.

Number of imaginary frequencies: 0



Atom No.	Element	X	Y	Z
1	S	2.755151	3.910807	0.085900
2	S	2.755077	-3.910869	-0.085981
3	O	0.000002	1.884399	1.847799
4	O	2.407974	-5.104068	-0.857707
5	O	2.408029	5.104056	0.857546
6	O	2.075605	3.532062	-1.152113
7	O	2.075499	-3.532236	1.152050
8	N	2.557005	2.603225	1.135950
9	N	2.556882	-2.603238	-1.135982
10	C	1.292317	0.625056	0.324876
11	C	4.509779	-4.038976	0.294944
12	C	1.292318	-0.625097	-0.324780
13	C	4.509855	4.038936	-0.295019
14	C	0.000009	1.156549	0.867133
15	C	2.517863	-1.285093	-0.583046
16	C	3.714471	0.640252	0.274283
17	C	2.517882	1.285081	0.583045
18	C	3.714469	-0.640196	-0.274495
19	C	5.358109	-4.727017	-0.576237
20	C	5.358062	4.727366	0.575980
21	C	7.250948	4.198941	-0.863287
22	C	7.250875	-4.198789	0.863265
23	C	5.012165	-3.439099	1.452124
24	C	6.376378	-3.521940	1.725410
25	C	5.012360	3.438751	-1.451981
26	C	6.376581	3.521690	-1.725243
27	C	6.719603	4.798098	0.287820
28	C	6.719660	-4.797645	-0.288053
29	H	4.652975	1.148142	0.471275
30	H	4.652978	-1.148009	-0.471651
31	H	4.950645	-5.218831	-1.453268
32	H	4.950504	5.219412	1.452837
33	H	4.334456	-2.932456	2.130721
34	H	6.767224	-3.060050	2.629096
35	H	4.334740	2.931795	-2.130432
36	H	6.767519	3.059574	-2.628774

Atom No.	Element	X	Y	Z
55	C	-2.517799	-1.285212	-0.582878
56	C	-3.714444	0.640201	0.274245
57	C	-5.358074	4.727317	0.575680
58	C	-5.357905	-4.727435	-0.575636
59	C	-7.250937	-4.198770	0.863357
60	C	-7.250967	4.198969	-0.863607
61	C	-5.012380	3.438816	-1.452352
62	C	-6.376600	3.521771	-1.725607
63	C	-5.012379	-3.438661	1.452252
64	C	-6.376647	-3.521499	1.725350
65	C	-6.719479	-4.798061	-0.287645
66	C	-6.719618	4.798063	0.287530
67	H	-4.652915	-1.148189	-0.471431
68	H	-4.652963	1.148077	0.471196
69	H	-4.950513	5.219318	1.452562
70	H	-4.950253	-5.219571	-1.452399
71	H	-4.334762	2.931901	-2.130836
72	H	-6.767539	3.059710	-2.629165
73	H	-4.334829	-2.931675	2.130751
74	H	-6.767675	-3.059263	2.628778
75	H	-7.379491	-5.336811	-0.963384
76	H	-7.379679	5.336777	0.963246
77	C	-2.842884	2.760595	2.562992
78	H	-2.644938	3.795902	2.842546
79	H	-3.880800	2.497424	2.813860
80	H	-2.153688	2.119571	3.116024
81	C	2.842746	2.760399	2.563258
82	H	2.644889	3.795709	2.842862
83	H	2.153417	2.119415	3.116176
84	H	3.880604	2.497091	2.814220
85	C	-2.842879	-2.760920	-2.562772
86	H	-2.644123	-3.796039	-2.842452
87	H	-3.881062	-2.498592	-2.813440
88	H	-2.154336	-2.119279	-3.115903
89	C	2.842898	-2.760402	-2.563233
90	H	2.644254	-3.795495	-2.843086

37	H	7.379667	5.336851	0.963504	91	H	2.154238	-2.118744	-3.116200
38	H	7.379824	-5.336067	-0.963900	92	H	3.881032	-2.497898	-2.813919
39	S	-2.755013	-3.910865	-0.085293	93	C	-8.721646	4.313433	-1.187362
40	S	-2.755164	3.910781	0.085552	94	H	-9.081033	3.437779	-1.738028
41	O	0.000010	-1.884234	-1.847882	95	H	-9.325684	4.417705	-0.280155
42	O	-2.408007	5.104088	0.857090	96	H	-8.918570	5.194011	-1.813105
43	O	-2.407737	-5.104229	-0.856683	97	C	-8.721648	-4.313219	1.186968
44	O	-2.075616	-3.531885	1.152731	98	H	-9.325749	-4.416294	0.279667
45	O	-2.075640	3.531932	-1.152441	99	H	-8.918791	-5.194508	1.811656
46	N	-2.556781	-2.603458	-1.135572	100	H	-9.080792	-3.438135	1.738684
47	N	-2.557002	2.603289	1.135725	101	C	8.721627	4.313396	-1.187045
48	C	-1.292268	-0.625148	-0.324711	102	H	9.325689	4.417428	-0.279824
49	C	-4.509871	4.038930	-0.295353	103	H	9.080957	3.437850	-1.737918
50	C	-1.292292	0.625049	0.324858	104	H	8.918588	5.194110	-1.812585
51	C	-4.509761	-4.038967	0.295414	105	C	8.721529	-4.313161	1.187162
52	C	0.000024	-1.156546	-0.867098	106	H	8.918123	-5.192524	1.814729
53	C	-2.517871	1.285088	0.582944	107	H	9.325525	-4.419531	0.280185
54	C	-3.714415	-0.640315	-0.274381	108	H	9.081260	-3.436530	1.736057