

Electronic Supporting Information

Locked Chromophores as CD Probes for the Helical Conformation of Tetraamidic Macrocycles

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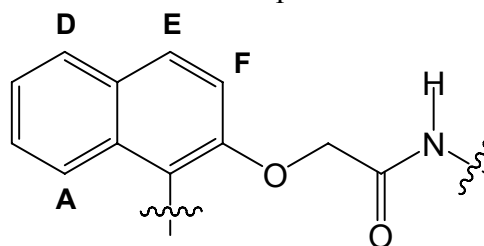
Copies of ¹H NMR and ¹³C NMR Spectra of precursors (pages S16–S29)

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Table S1. Selected ^1H NMR chemical shifts for precursors **7-9** and macrocycles **13-15**.^a



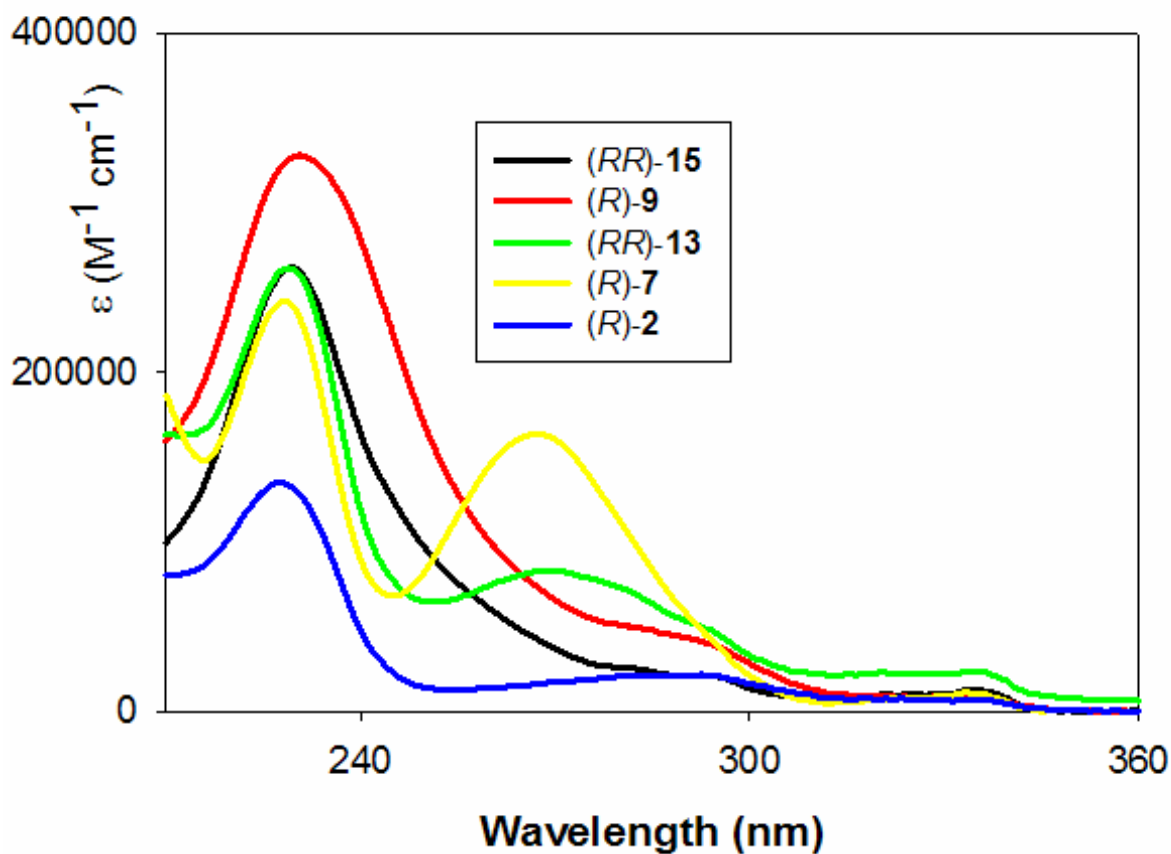
Entry	Compound	NHCO	NHCOOtBu	BINOL-E	BINOL-A	BINOL-F	BINOL-D	CH ₂	Solvent
1	2	- ^b	- ^b	7.96 (d)	- ^c	7.87 (d)	- ^c	4.26 (s)	CDCl ₃
2	7	broad	6.45 (s)	8.12 (d)	7.19 (d)	7.99 (d)	7.45 (d)	4.60 (dd)	CDCl ₃
3	7	9.25 (s)	9.08 (s)	8.12 (d)	- ^c	8.00 (d)	7.75 (d)	4.71 (dd)	DMSO- <i>d</i> ₆
4	8	broad	6.60 (s)	8.15 (d)	6.86 (d)	8.02 (d)	- ^c	4.66 (bs)	CDCl ₃
5	9	broad	6.71-6.78(d)	8.07 (d)	7.24 (d)	7.83 (d)	7.54 (d)	4.67 (s)	CDCl ₃
6	13	9.23 (s)	- ^b	8.11 (d)	6.95 (d)	7.98 (d)	7.59 (d)	4.69 (dd)	DMSO- <i>d</i> ₆
7	13	8.30 (s)	- ^b	8.08 (d)	7.10 (d)	7.55 (d)	7.90 (d)	4.57 (dd)	THF- <i>d</i> ₈
8	15	7.62 (s)	- ^b	8.02 (d)	7.25 (d)	7.78 (d)	7.76 (d)	4.80 (dd)	CDCl ₃
9	15	8.35 (s)	- ^b	7.90 (d)	7.09 (d)	7.71 (d)	7.69 (d)	4.70 (dd)	THF- <i>d</i> ₈

a) Concentrations were in the range 5-10 mM (200, 300 or 600 MHz). Peak multiplicity as follows: s singlet, bs broad singlet, d doublet, dd double doublet (AB system). b) Not applicable. c) Not clearly assigned.

Table S2. Optical rotations and Molar Optical Rotations for precursors and macrocycles.

Entry	Compound	$[\alpha]^{25}_{\text{D}}$	α_{m}
1	7	+ 2 (c=0.002, THF)	+ 3
2	8	- 3 (c=0.0017, THF)	- 3
3	9	- 39 (c=0.006, THF)	- 42
4	13	+ 247 (c=0.0008, THF)	+ 252
5	14	+ 82 (c = 0.0012, THF)	+ 75
6	15	+ 180 (c=0.001, THF)	+ 164
		+ 141 (c=0.003, CH ₂ Cl ₂)	+ 128

Figure S1. UV/Vis spectrum of macrocycles and precursors in EtOH (1.5×10^{-6} M)



Simulated UV and CD spectra. Calculation of the Electronic Circular Dichroism spectra was carried out using the TD-DFT method at the B3LYP/6-31G(d) level.¹ Rotational strength were calculated in both length and velocity representation. Since the resulting values are quite similar, errors due to basis set incompleteness are consequently small.² The simulated ECD spectra were obtained by applying a 0.4 eV Gaussian shaped line width.³ Due the molecular size, 500 transition had to be calculated in order to simulate the 400-180 nm range in the case of **15**, and 300 in the case of **13**.

Figure S2. Experimental and theoretical UV (top) and CD (bottom) spectra for macrocycles **13** (left) and **15** (right). Black traces: experimental spectra. Red traces: calculated spectra.

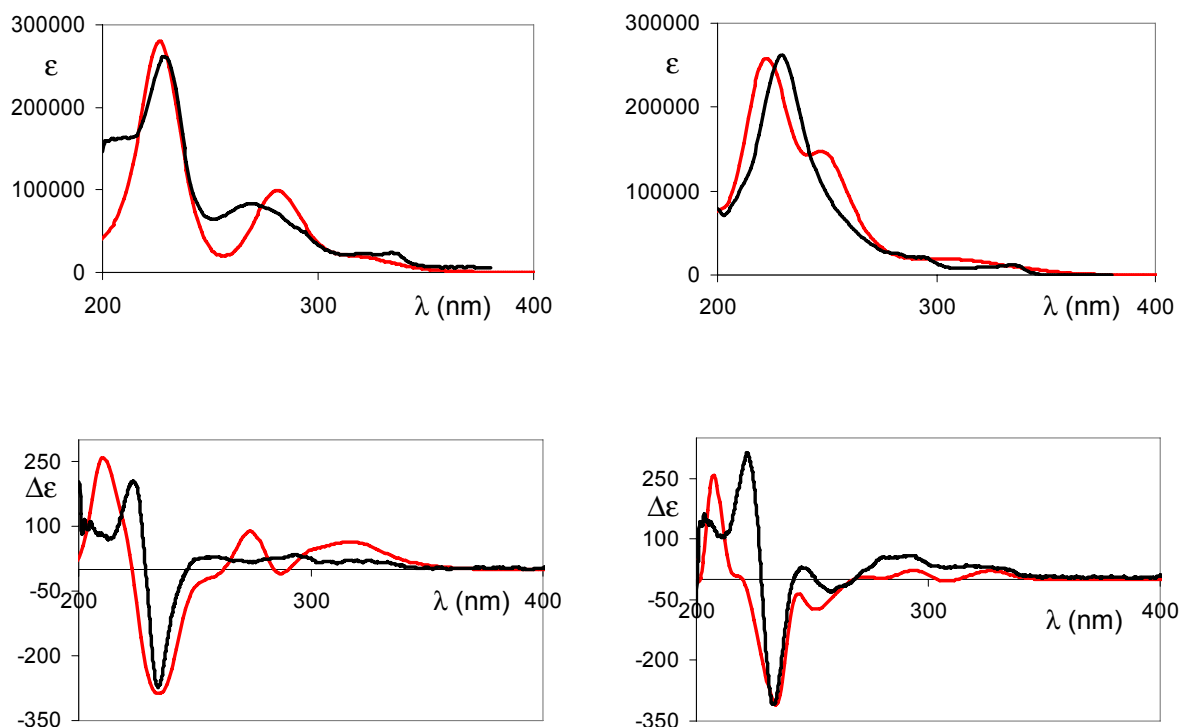
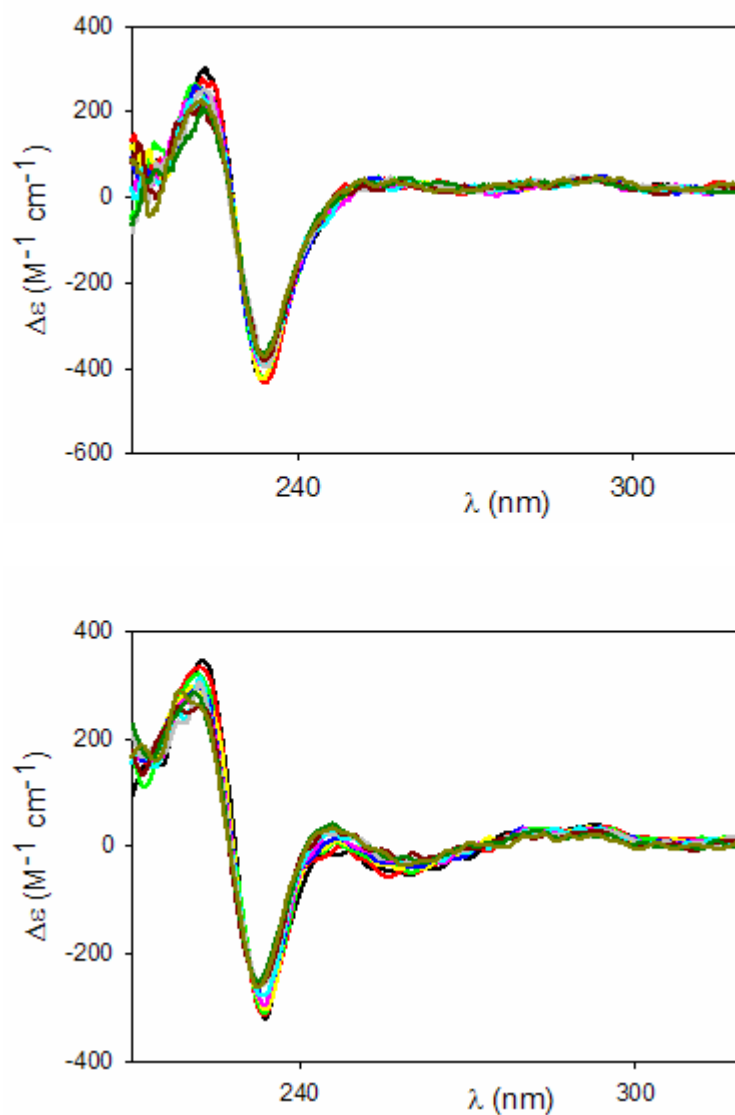
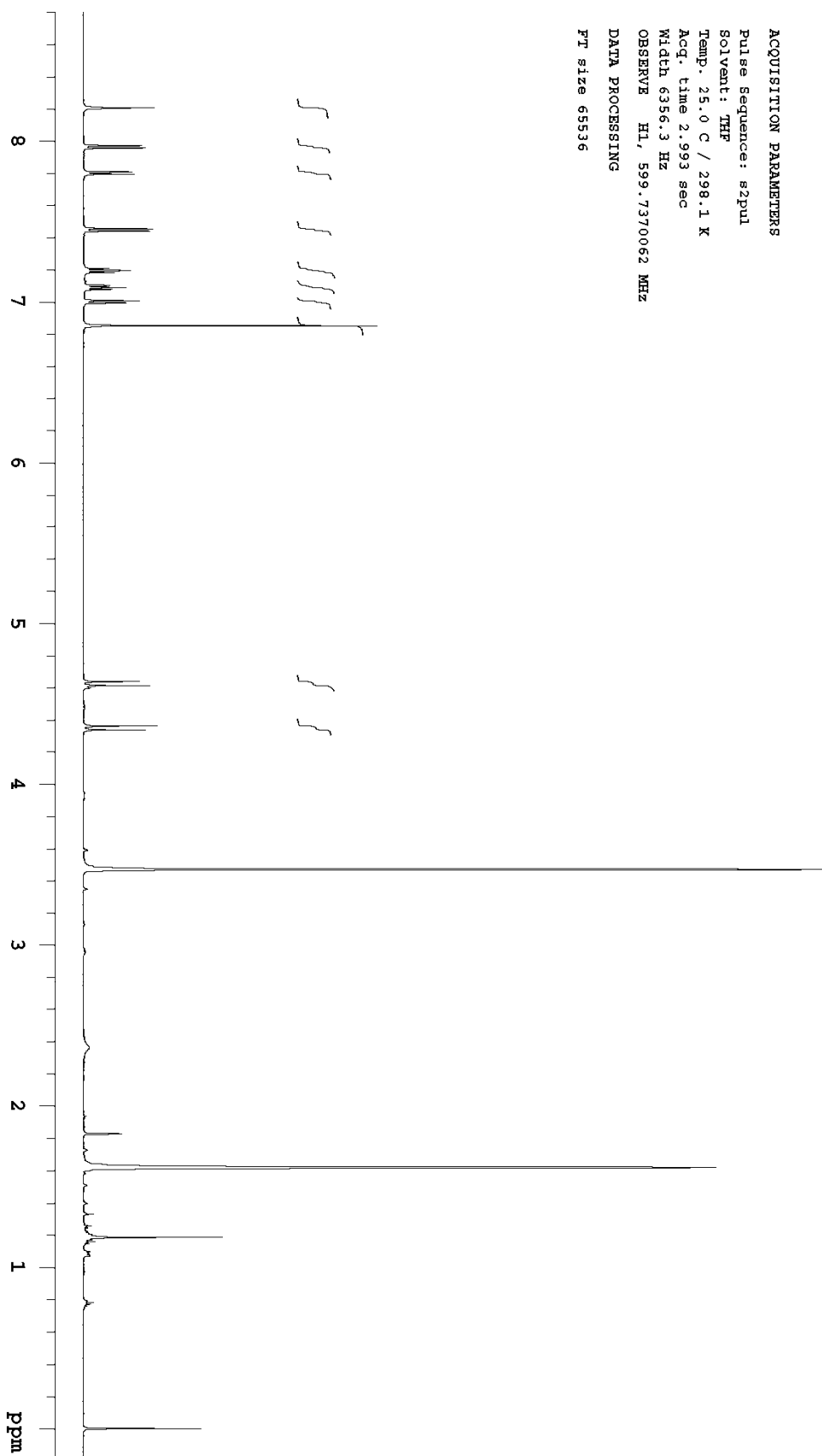


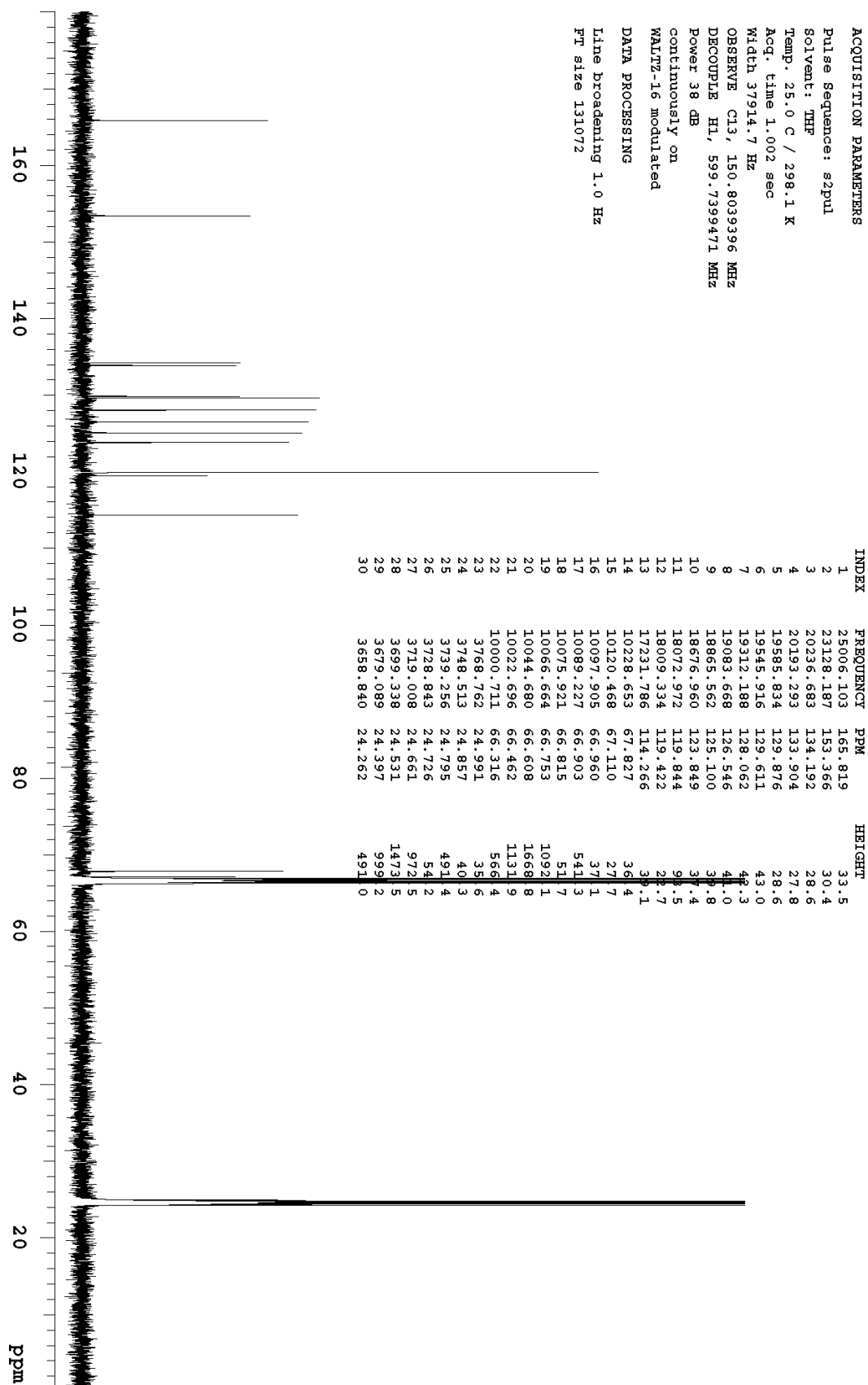
Figure S3. Variable temperature CD spectra of (*RR*)-**13** (top) and (*RR*)-**15** (bottom) in EtOH (5 to 55°C at 5°C interval).



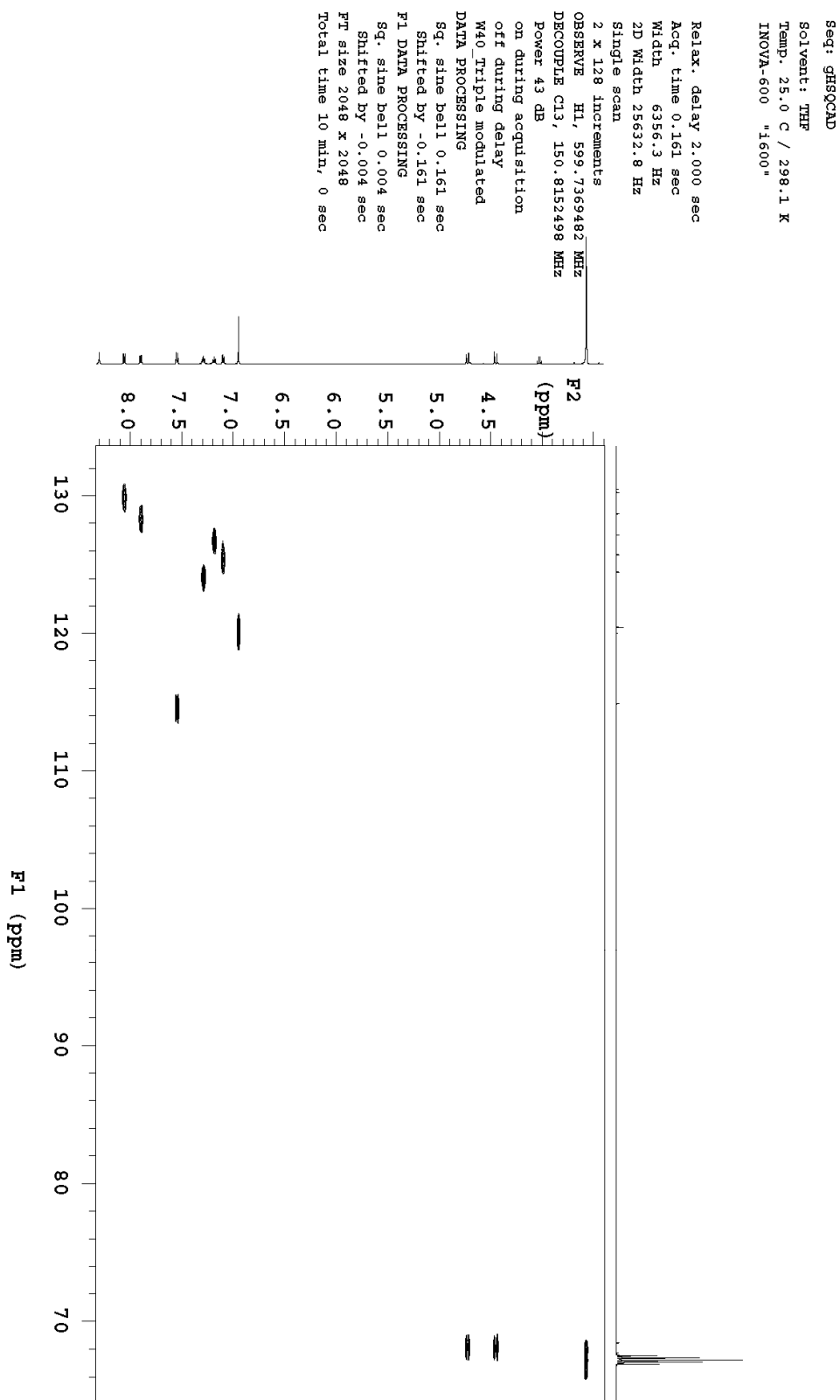
Compound 13



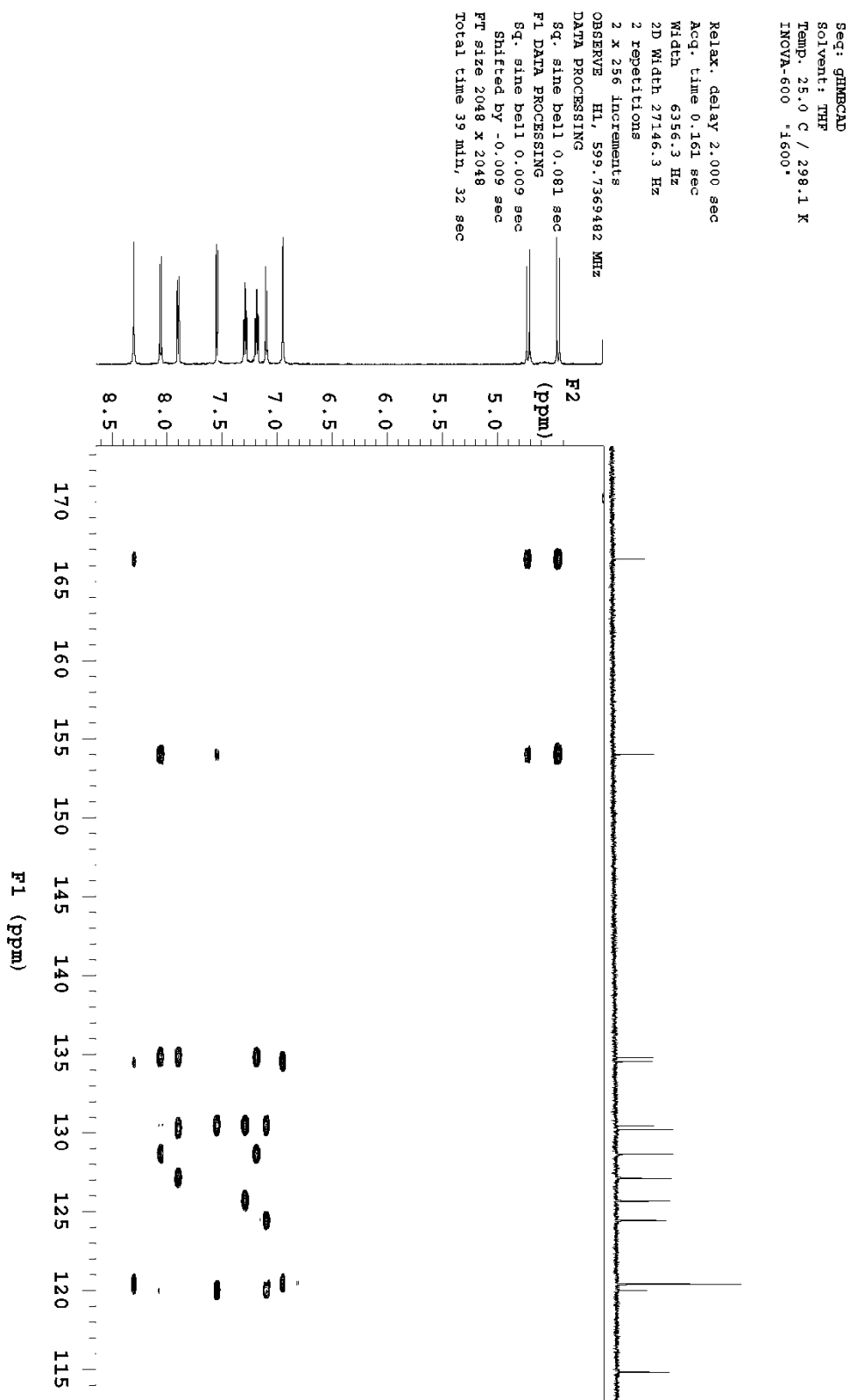
Compound 13



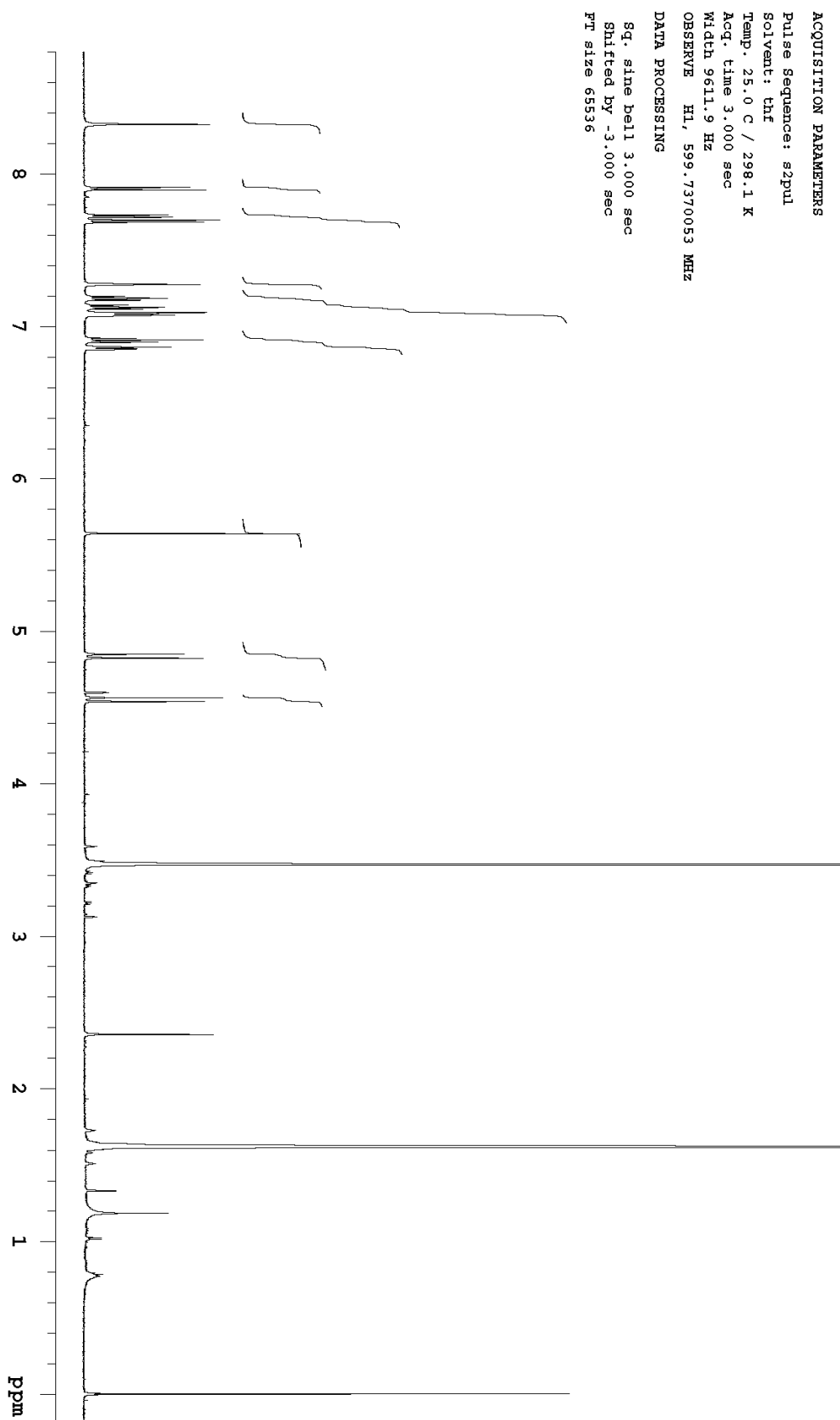
Compound **13** - HSQC spectrum



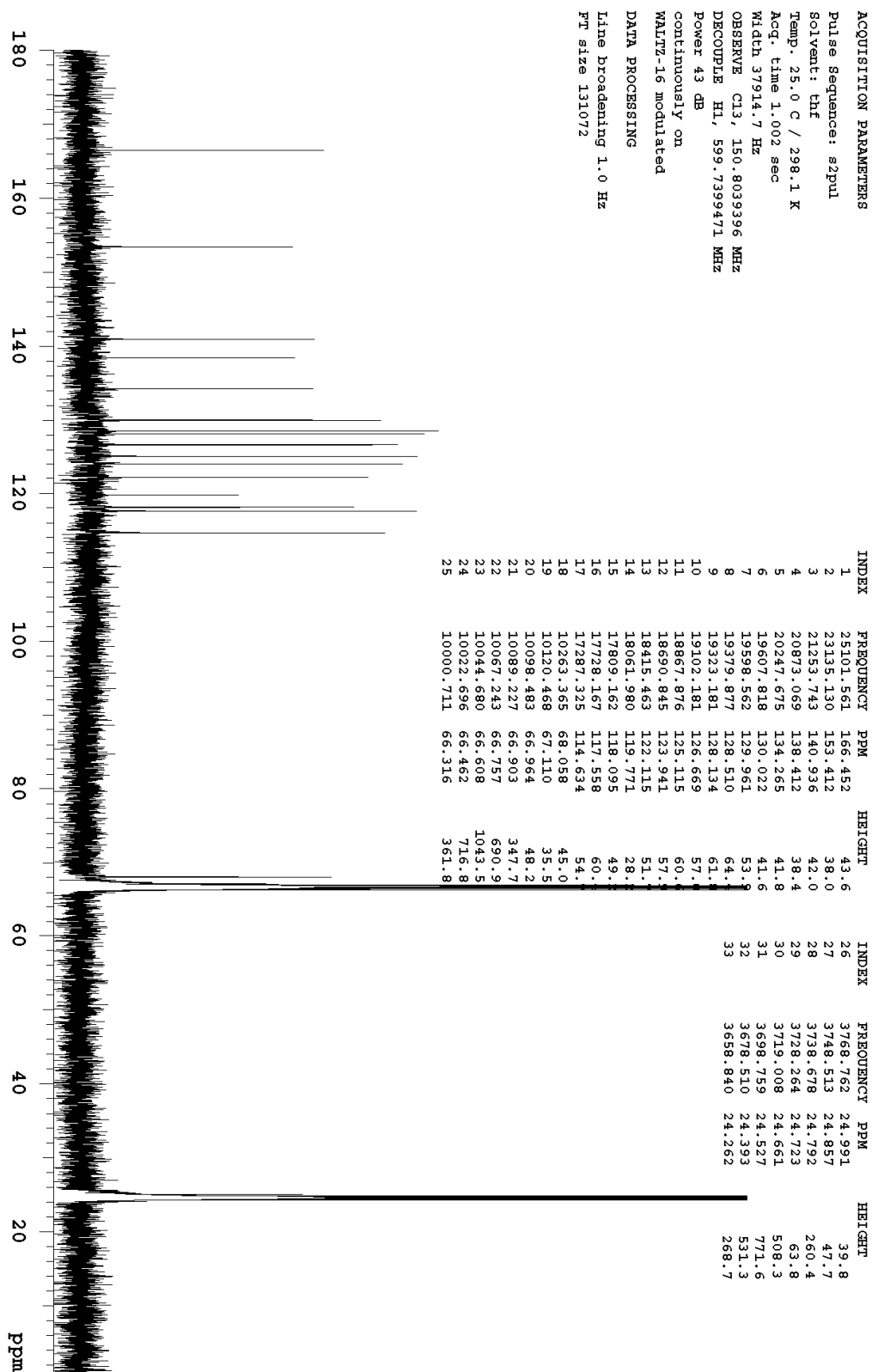
Compound 13 - HMBC spectrum



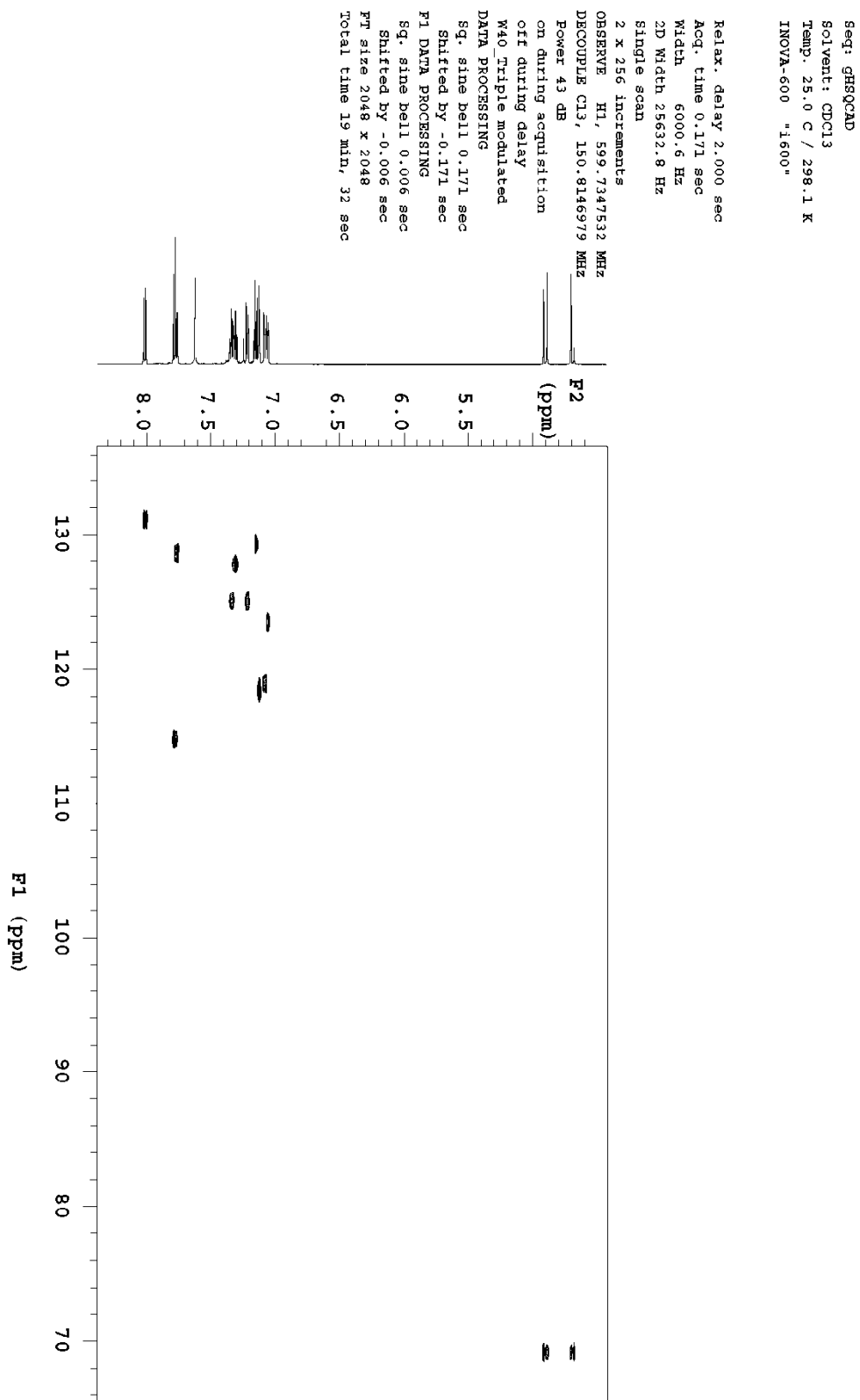
Compound 15



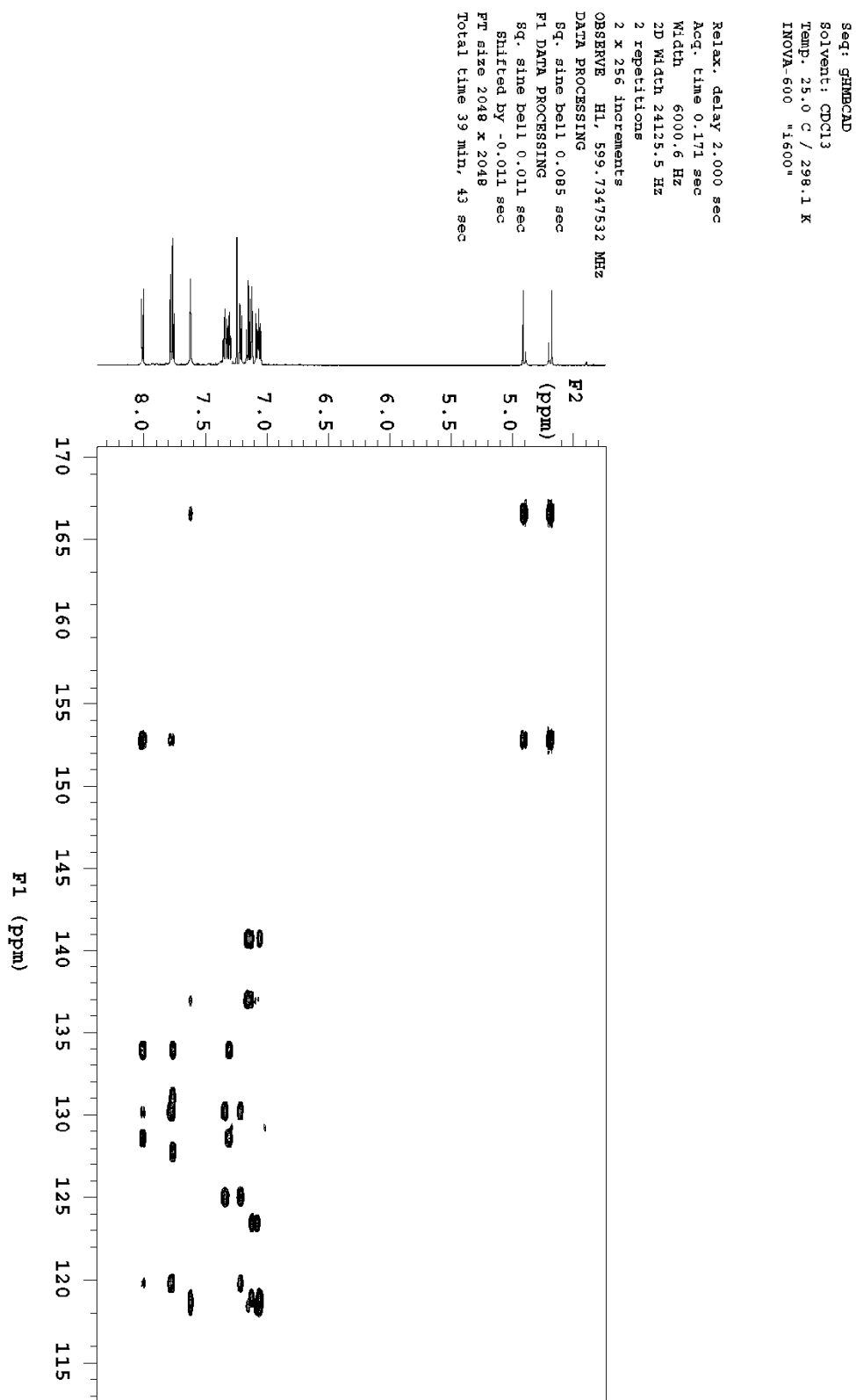
Compound 15



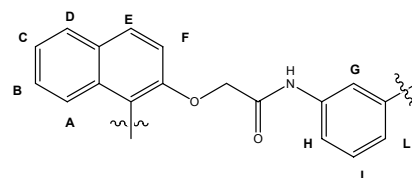
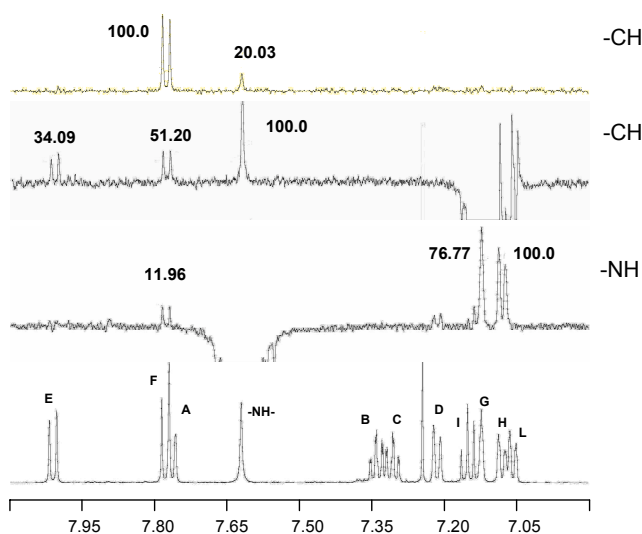
Compound **13** - HSQC spectrum



Compound 15 - HMBC spectrum

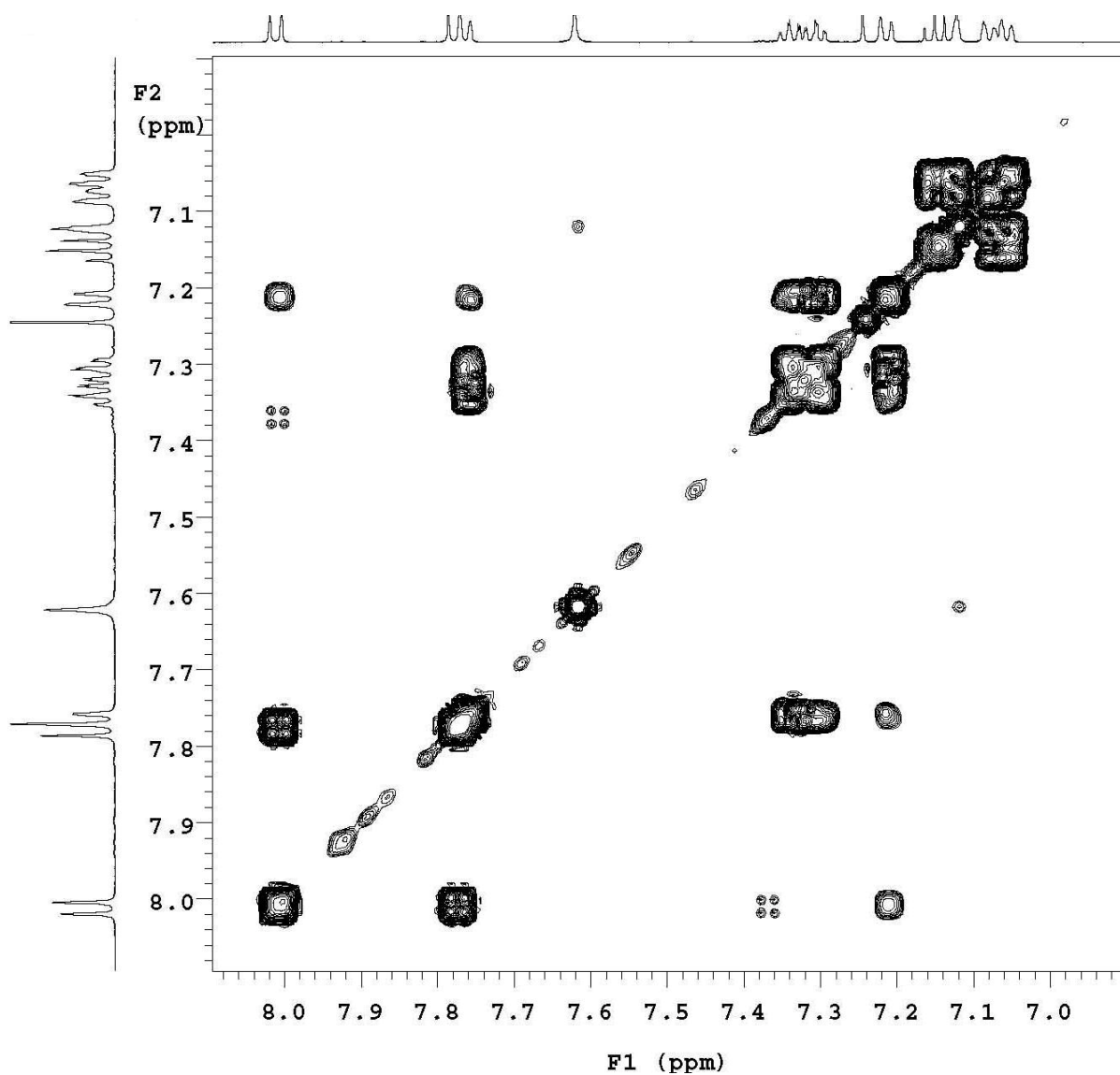


NOE traces for irradiation on selected signals of macrocycle **15** (600 MHz, CDCl₃)

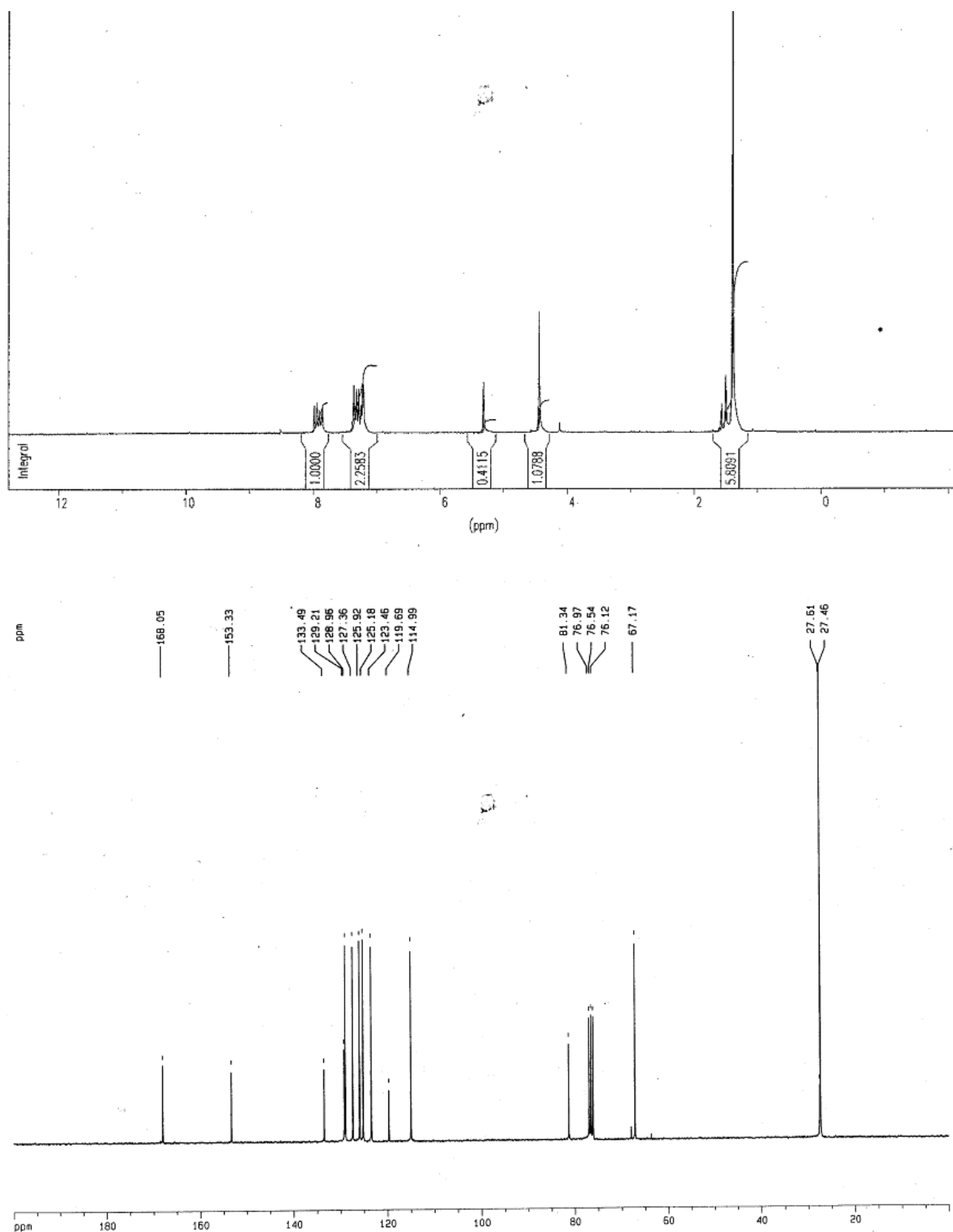


Spectra registered in CDCl₃

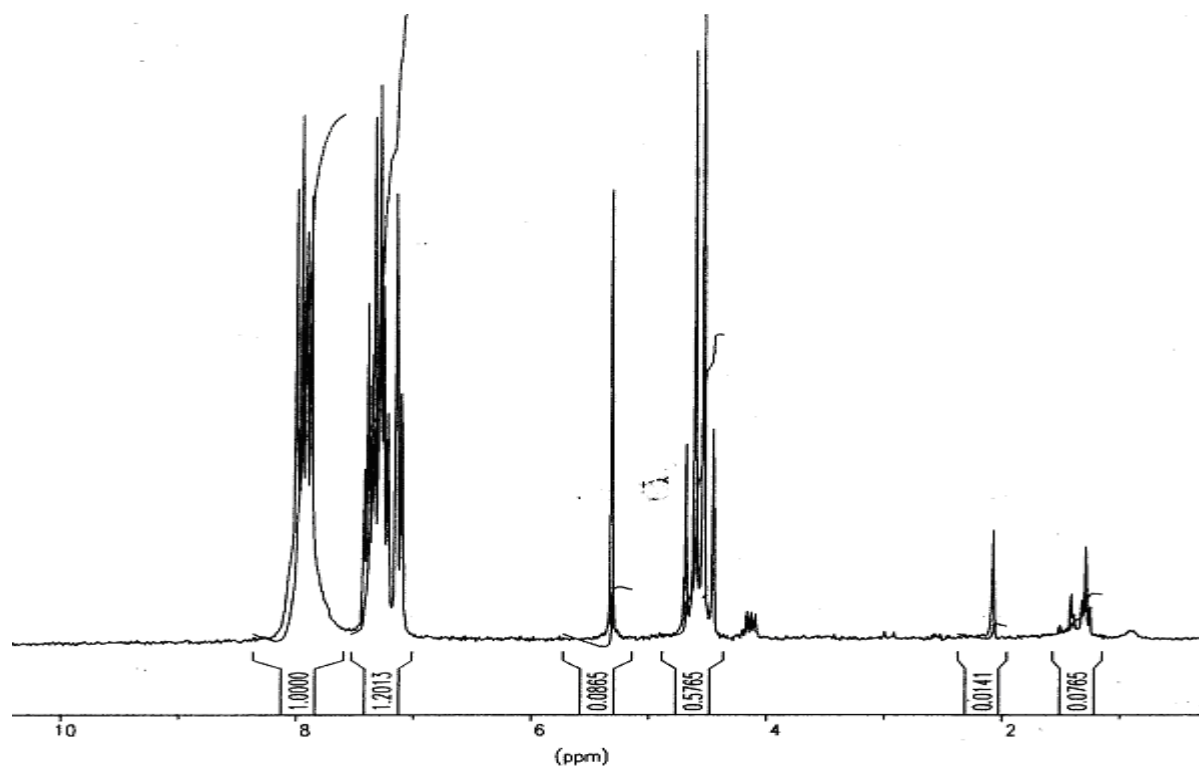
COSY spectra for macrocycle **15**.



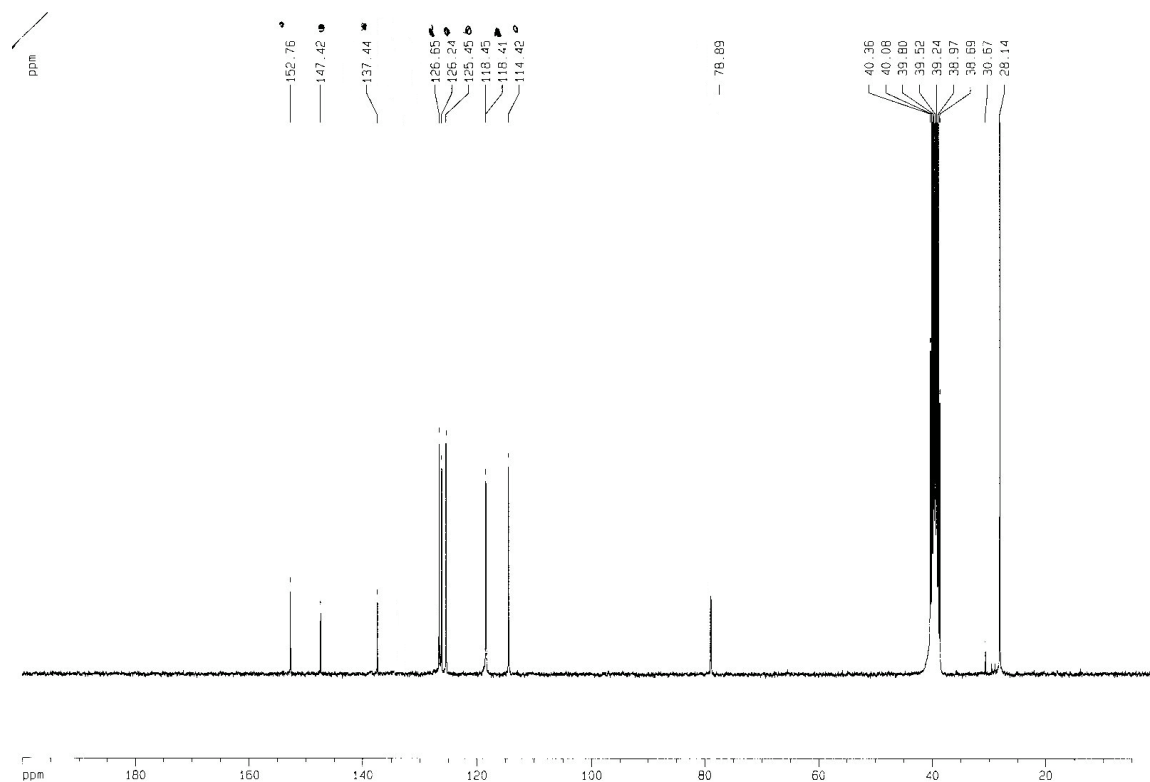
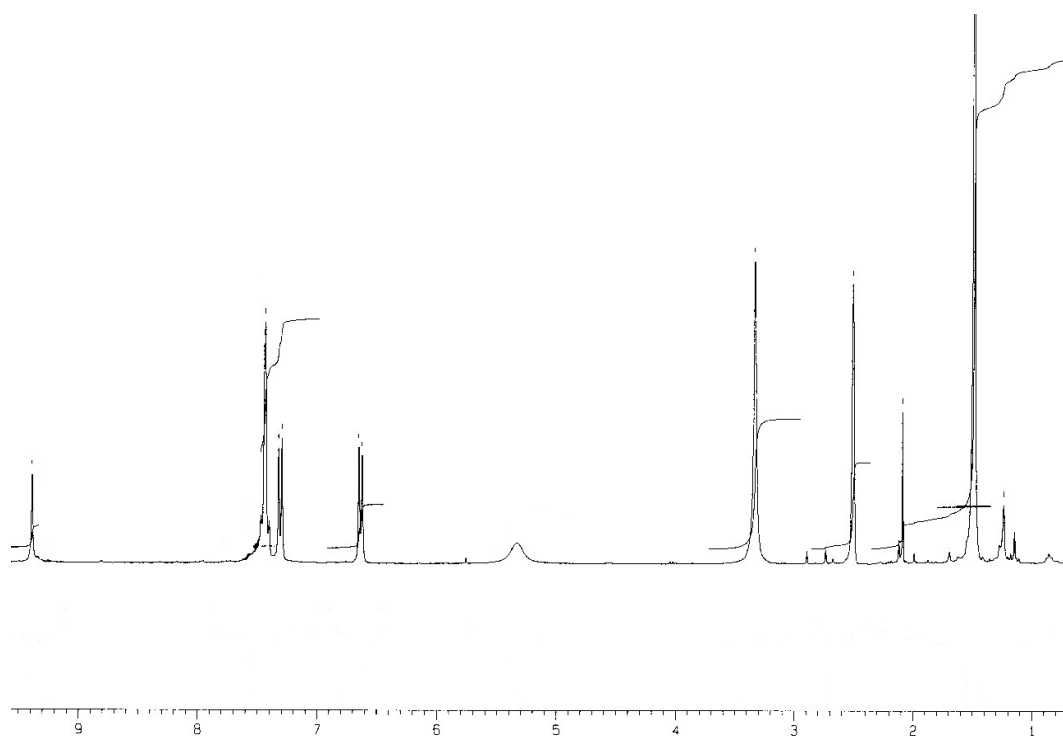
Compound 2



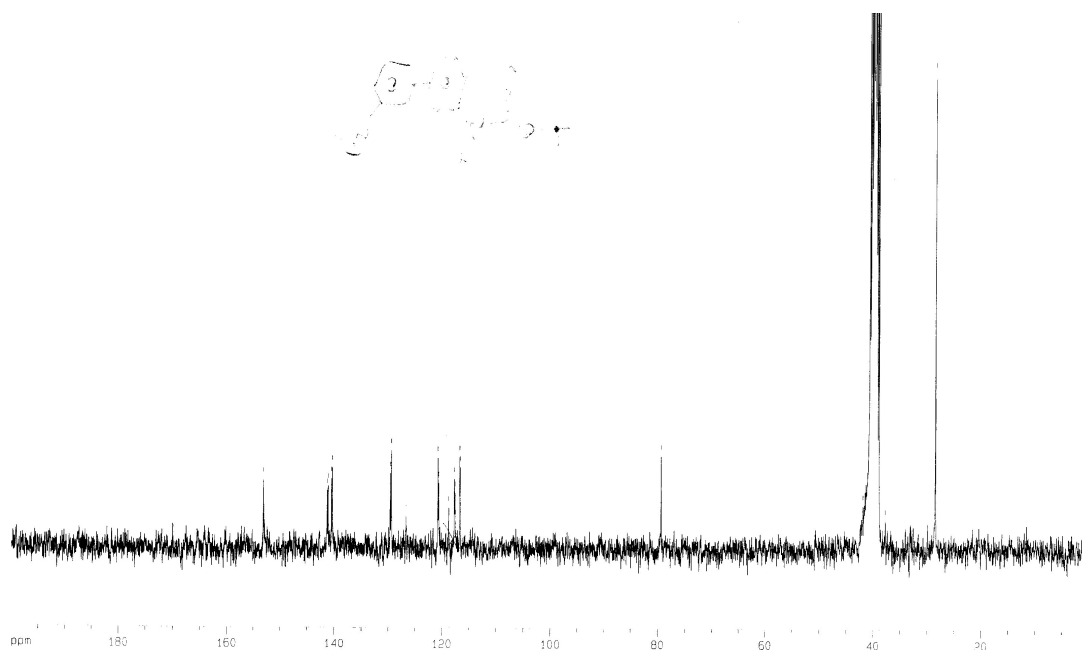
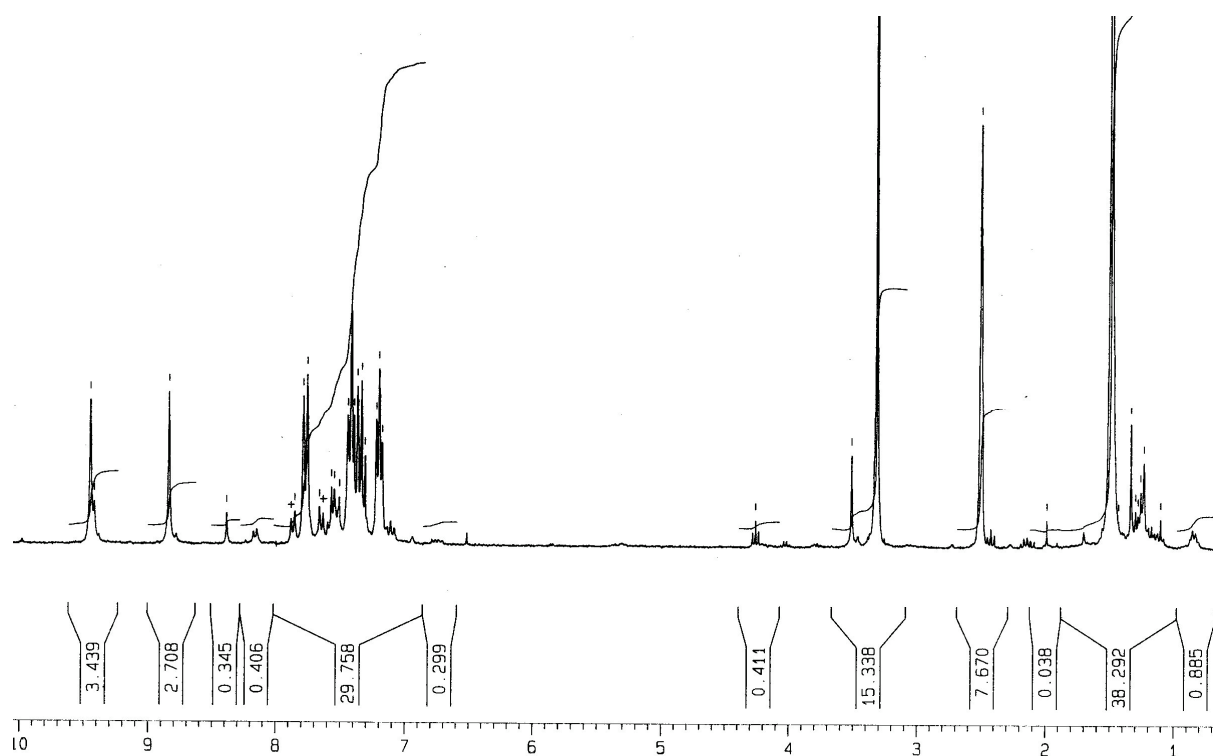
^1H NMR Compound **3**.



Compound 5.

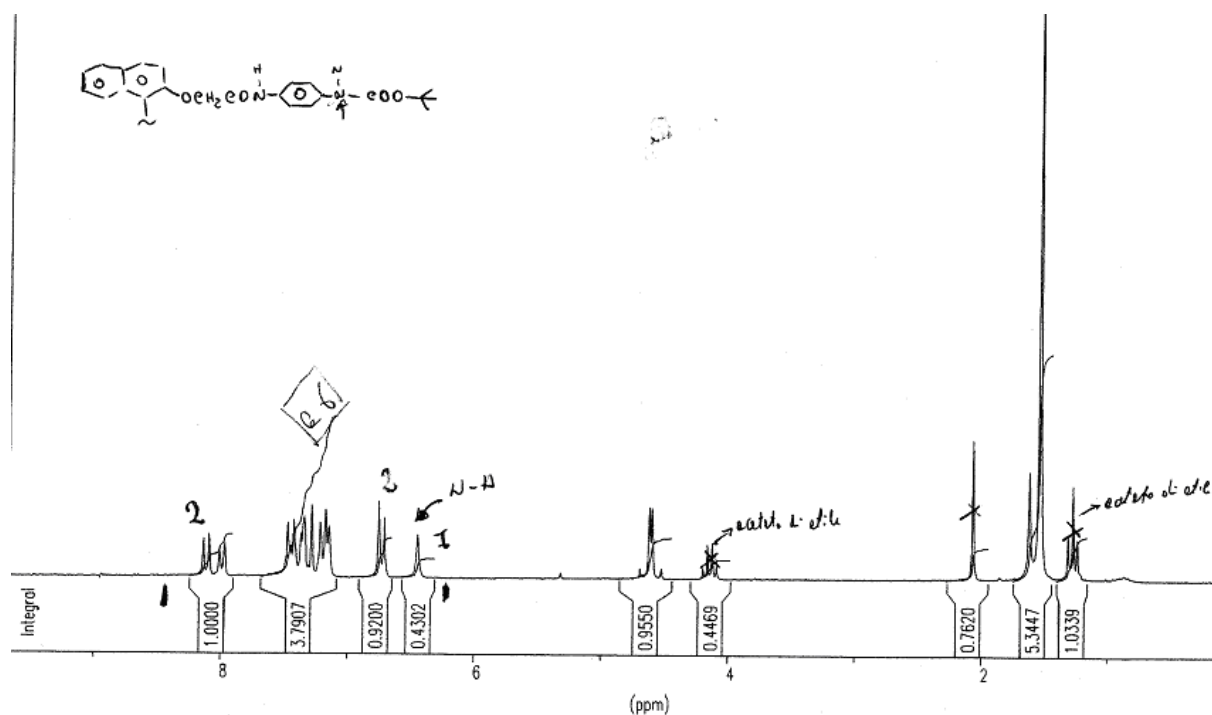


Compound 6.

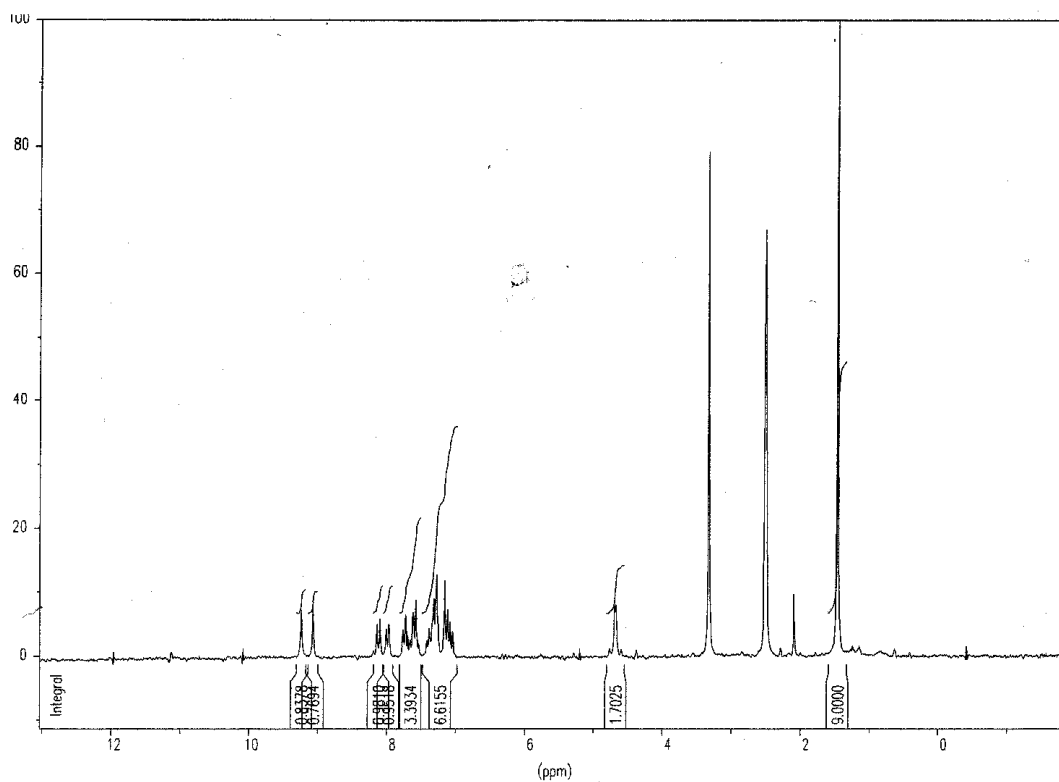


Compound 7.

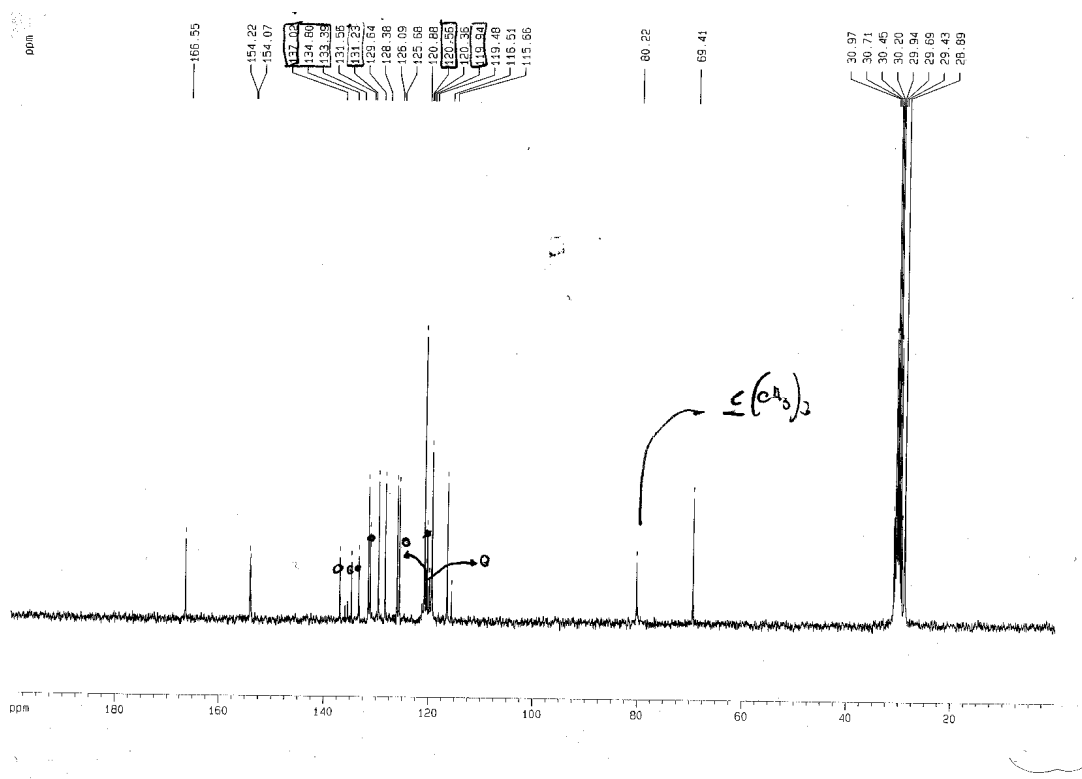
^1H NMR (200 MHz, CDCl_3)



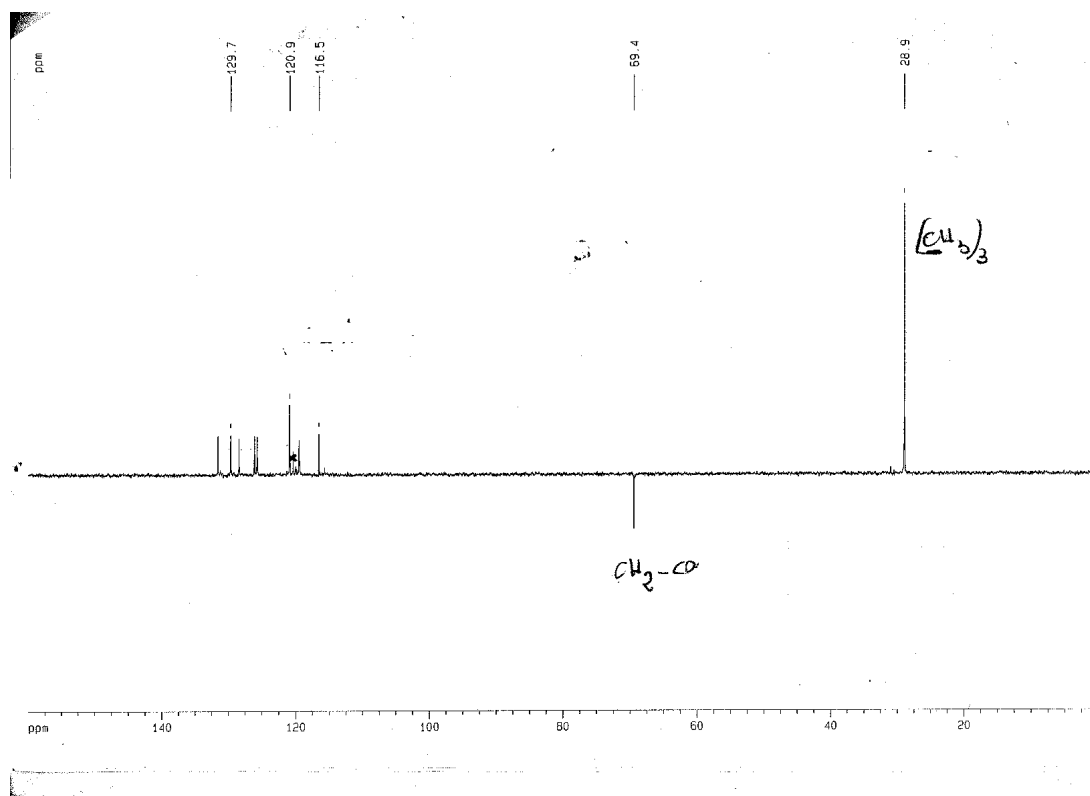
^1H NMR (200 MHz, $\text{DMSO}-d_6$)



^{13}C NMR (75 MHz, CD_3COCD_3)

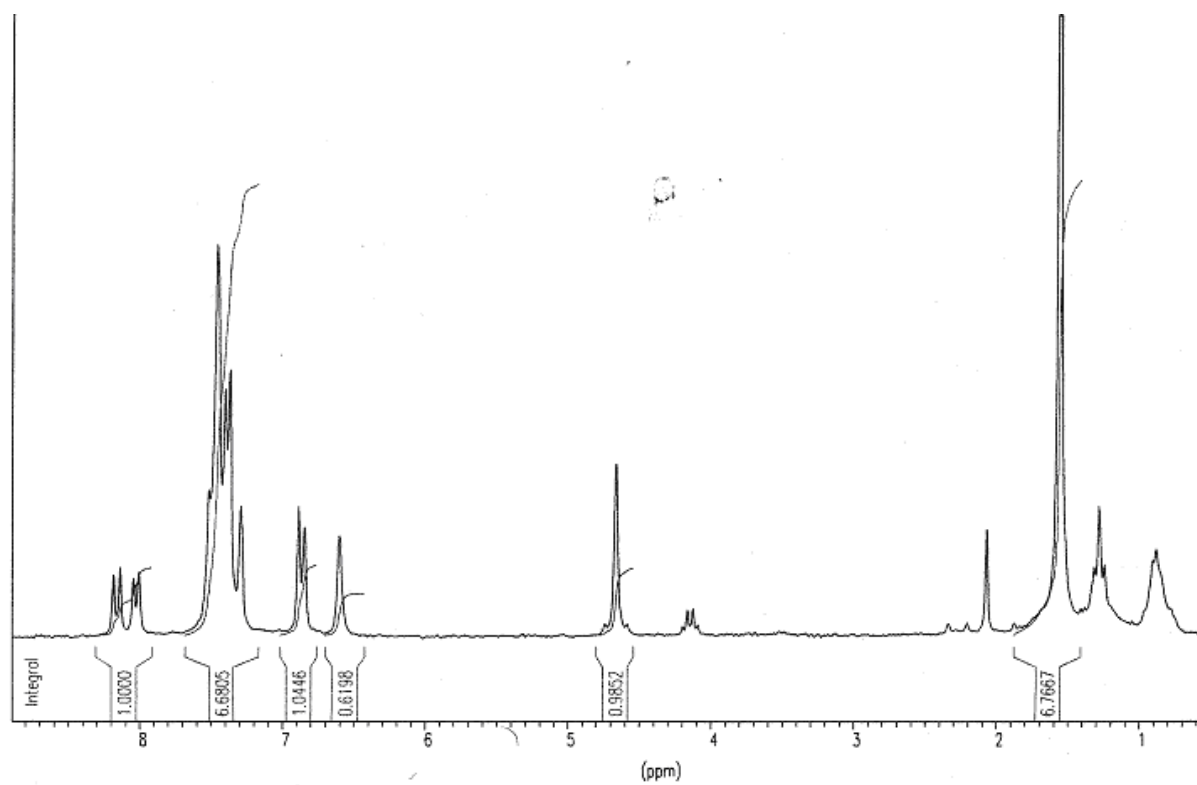


^{13}C NMR DEPT (75 MHz, CD_3COCD_3)

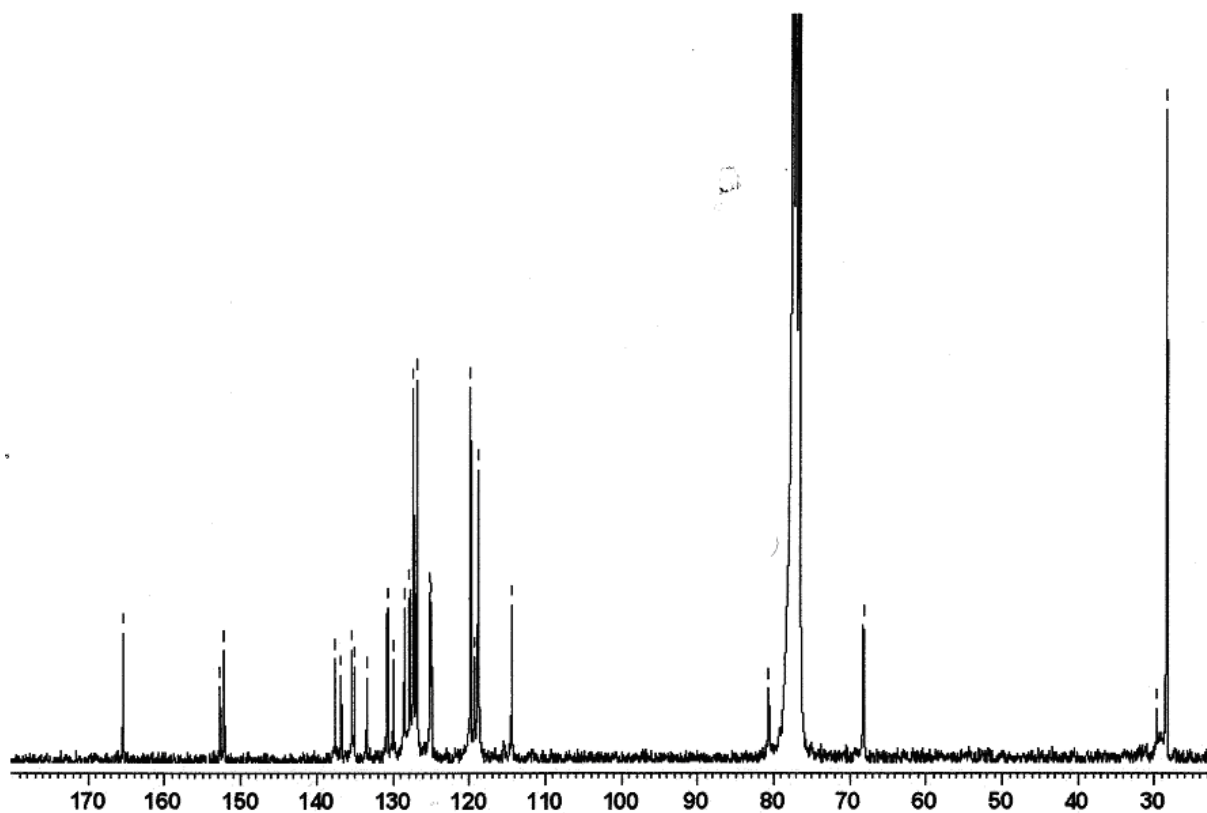


Compound **8**.

^1H NMR (200 MHz, CDCl_3)

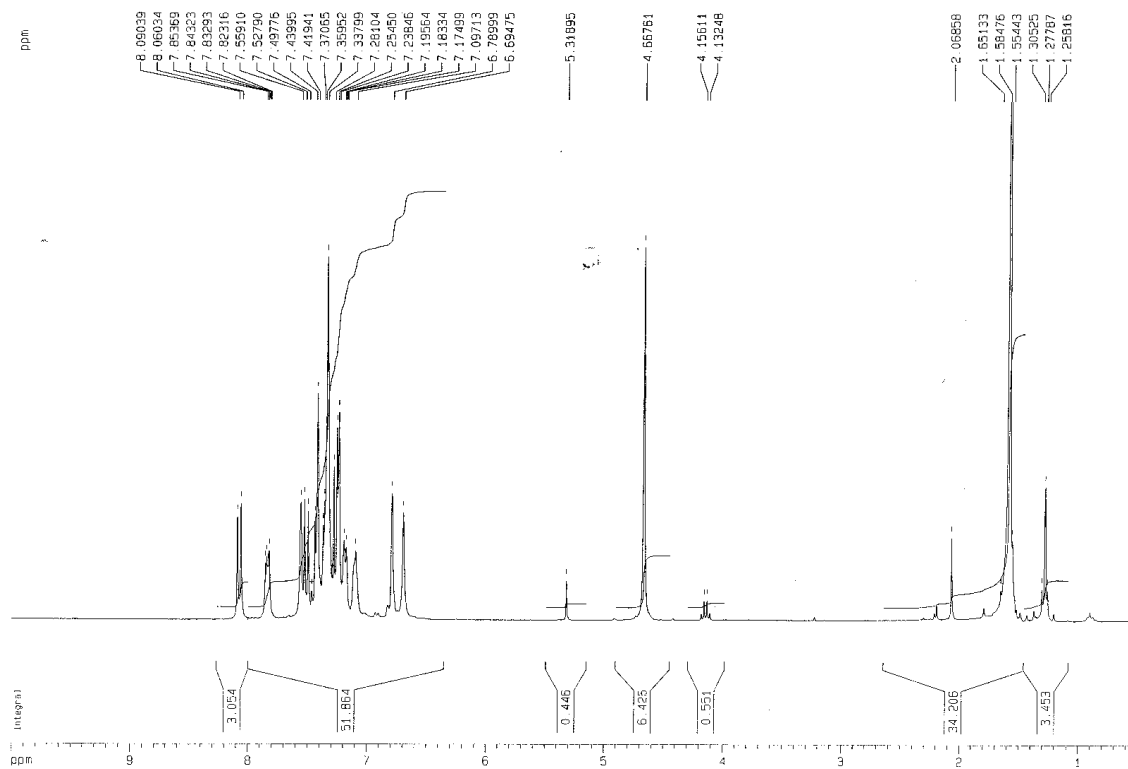


^{13}C NMR (75 MHz, CDCl_3)

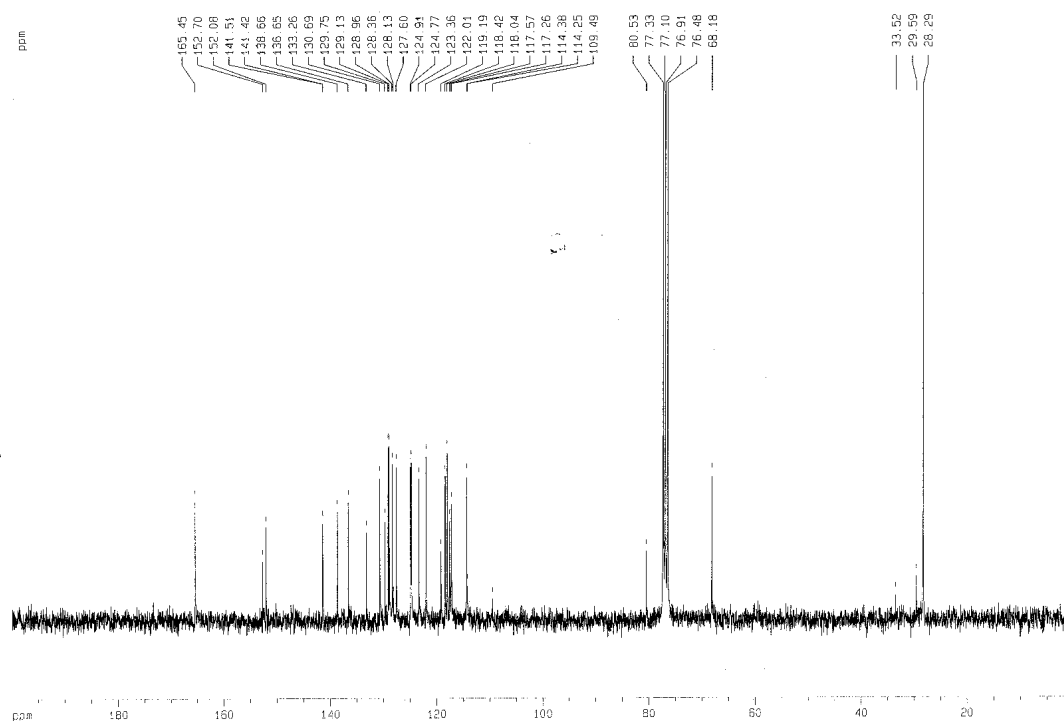


Compound 9.

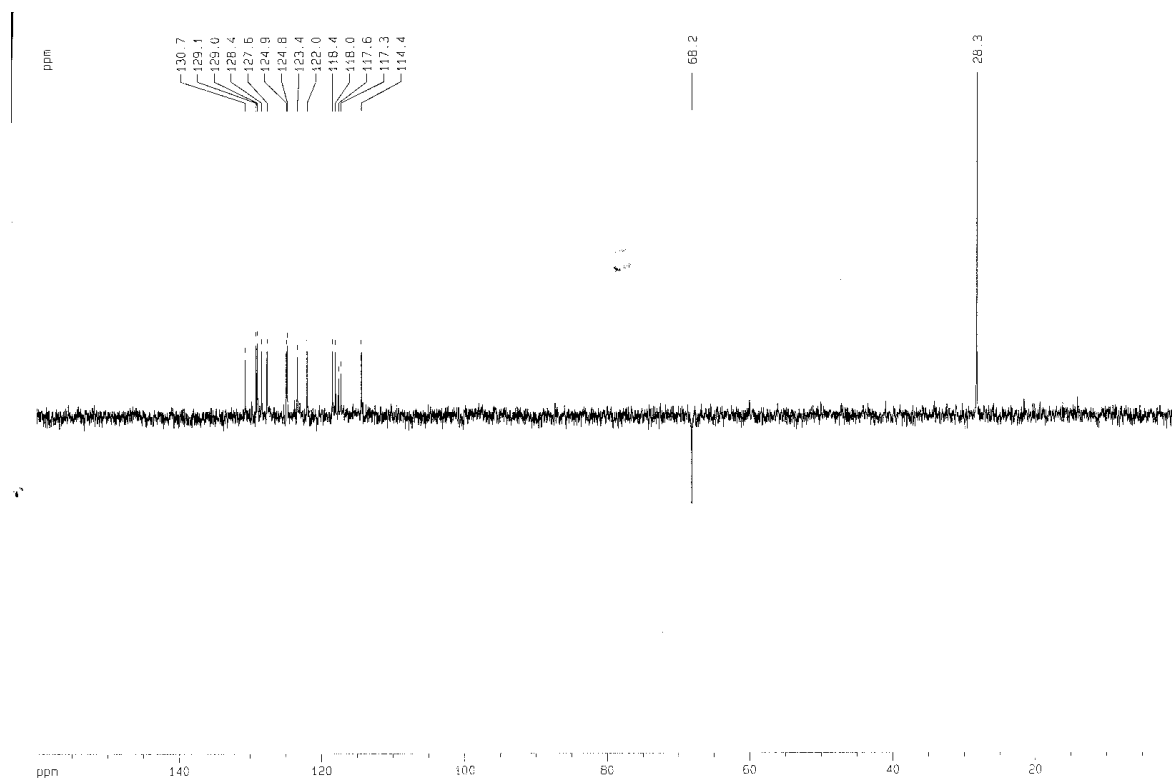
^1H NMR (200 MHz, CDCl_3)



^{13}C NMR (75 MHz, CDCl_3)

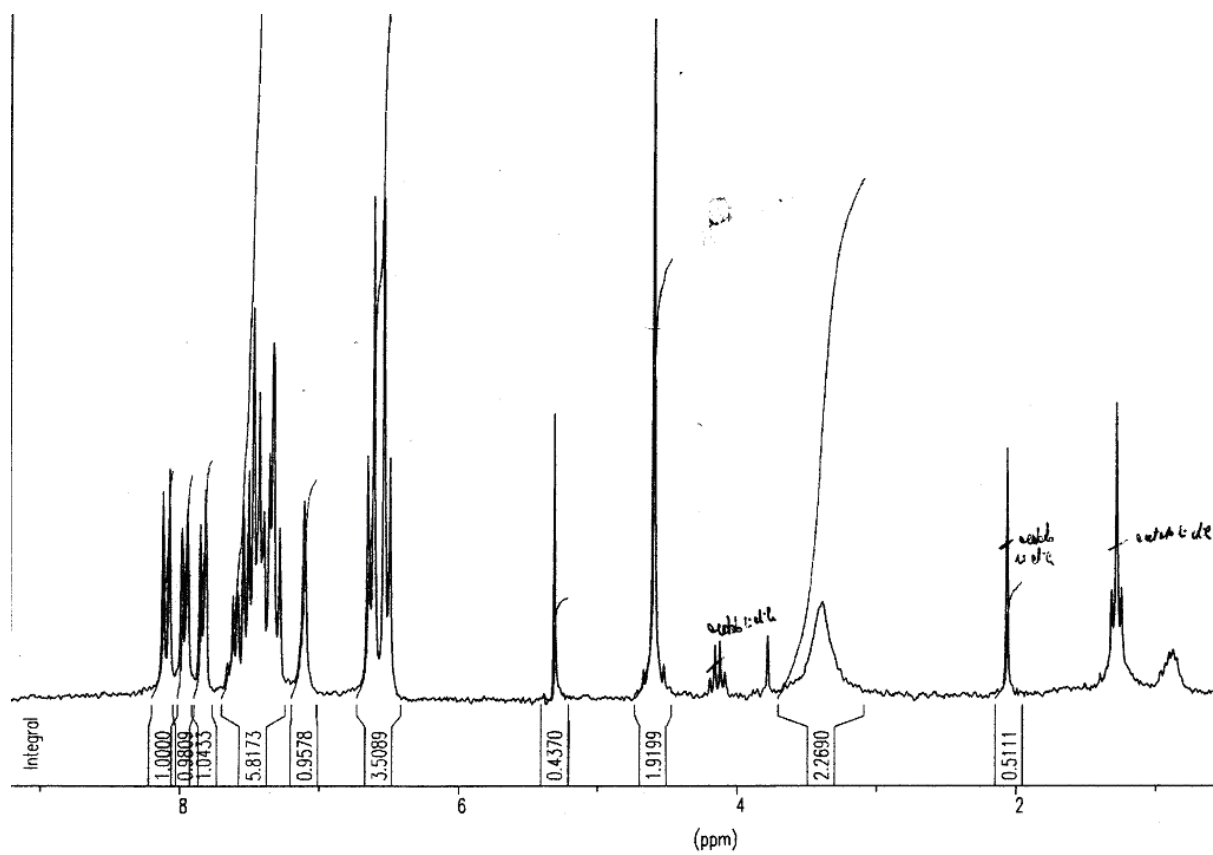


^{13}C NMR DEPT (75 MHz, CDCl_3)



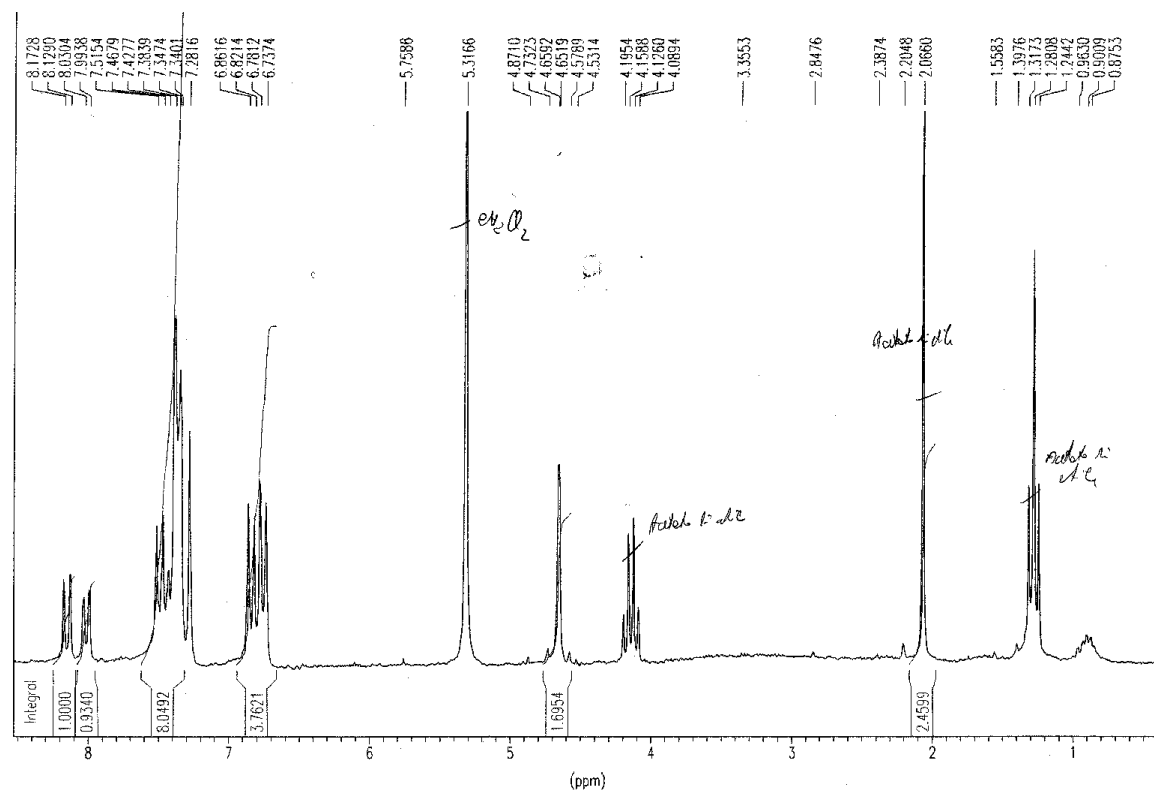
Compound **10**.

^1H NMR (200 MHz, CDCl_3)



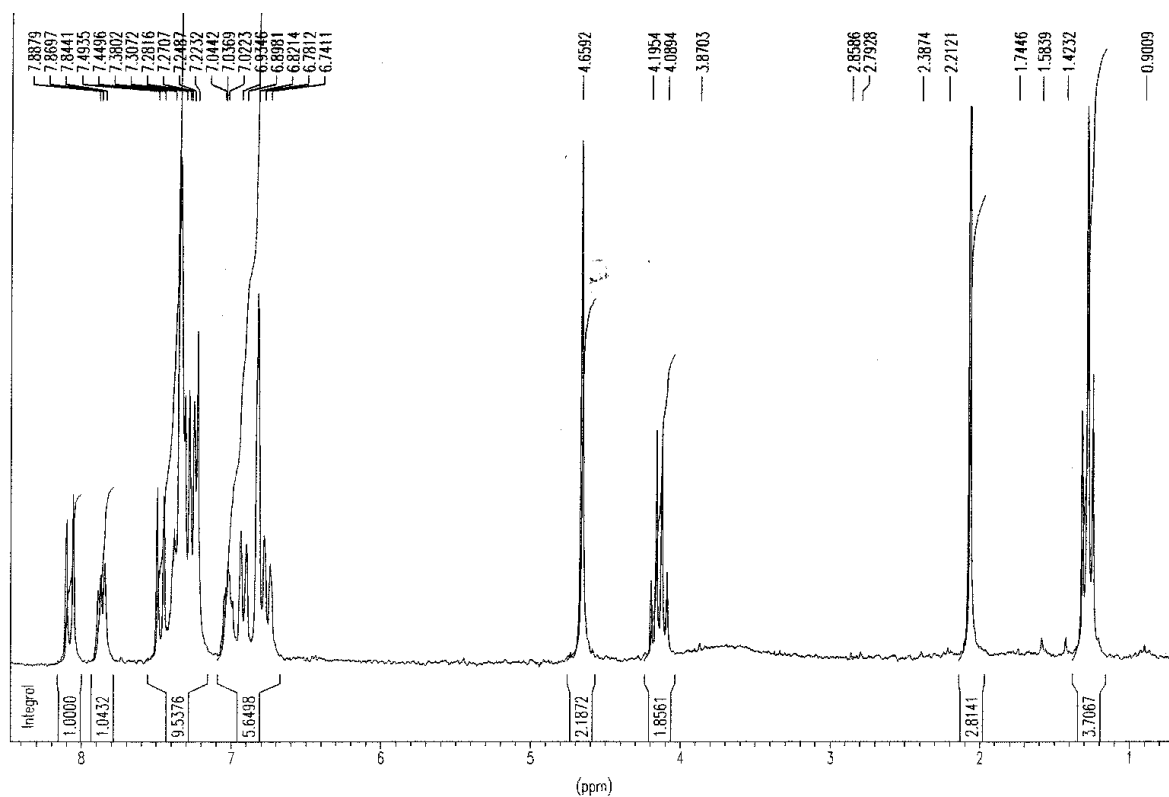
Compound 11.

^1H NMR (200 MHz, CDCl_3)

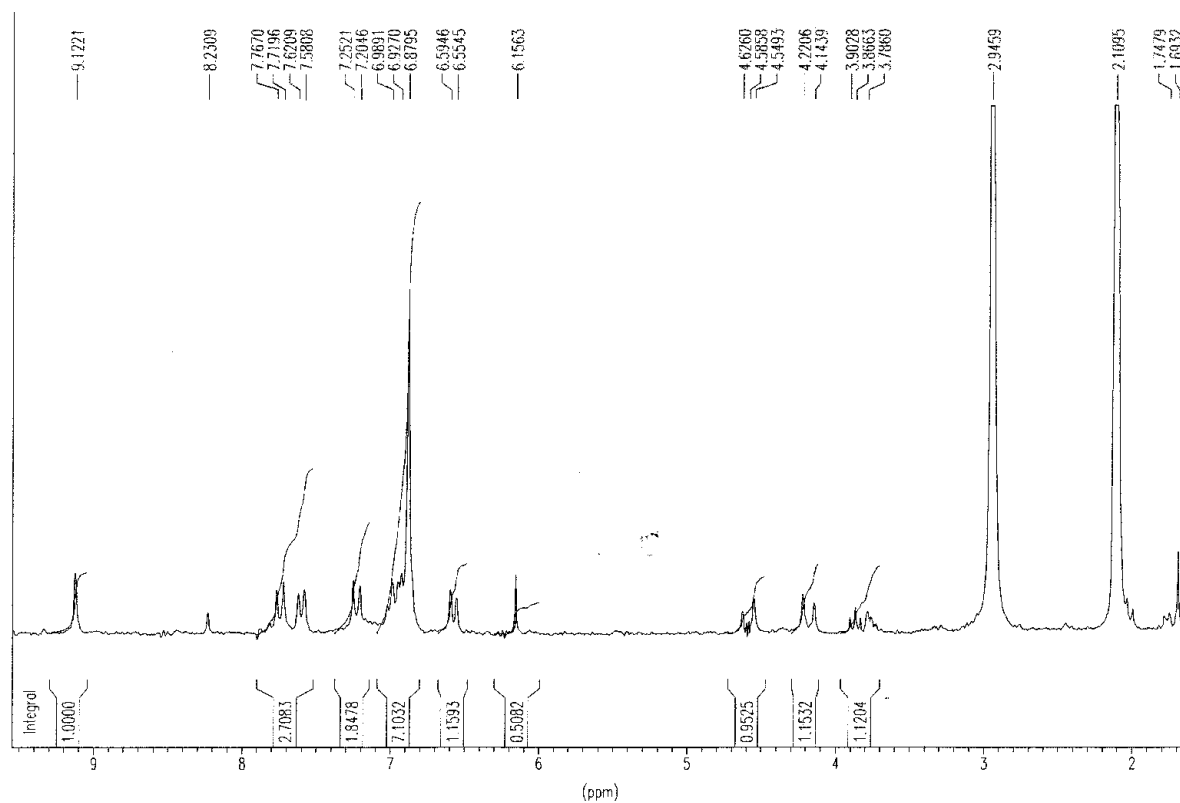


Compound 12.

^1H NMR (200 MHz, CDCl_3)

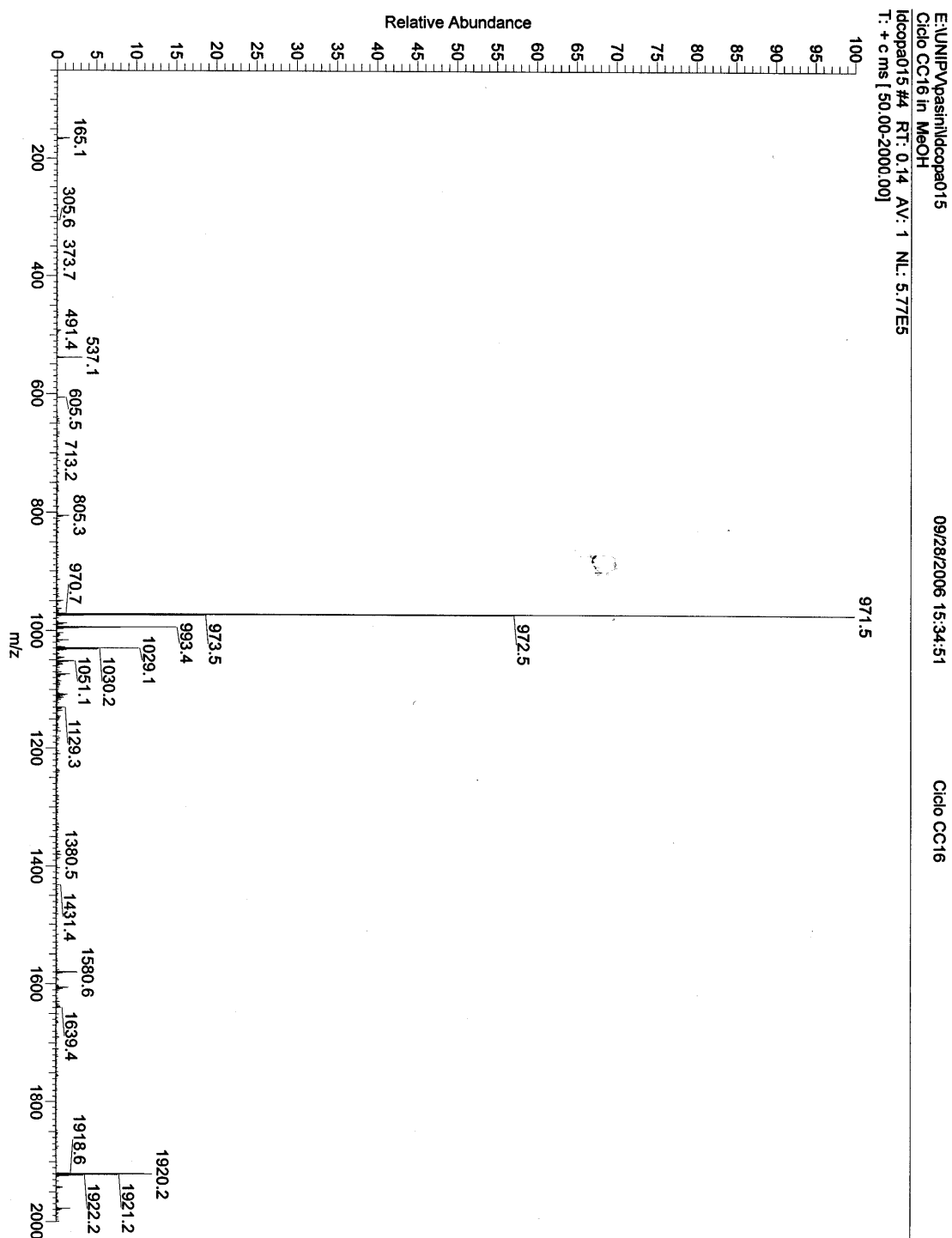


Compound **14**.

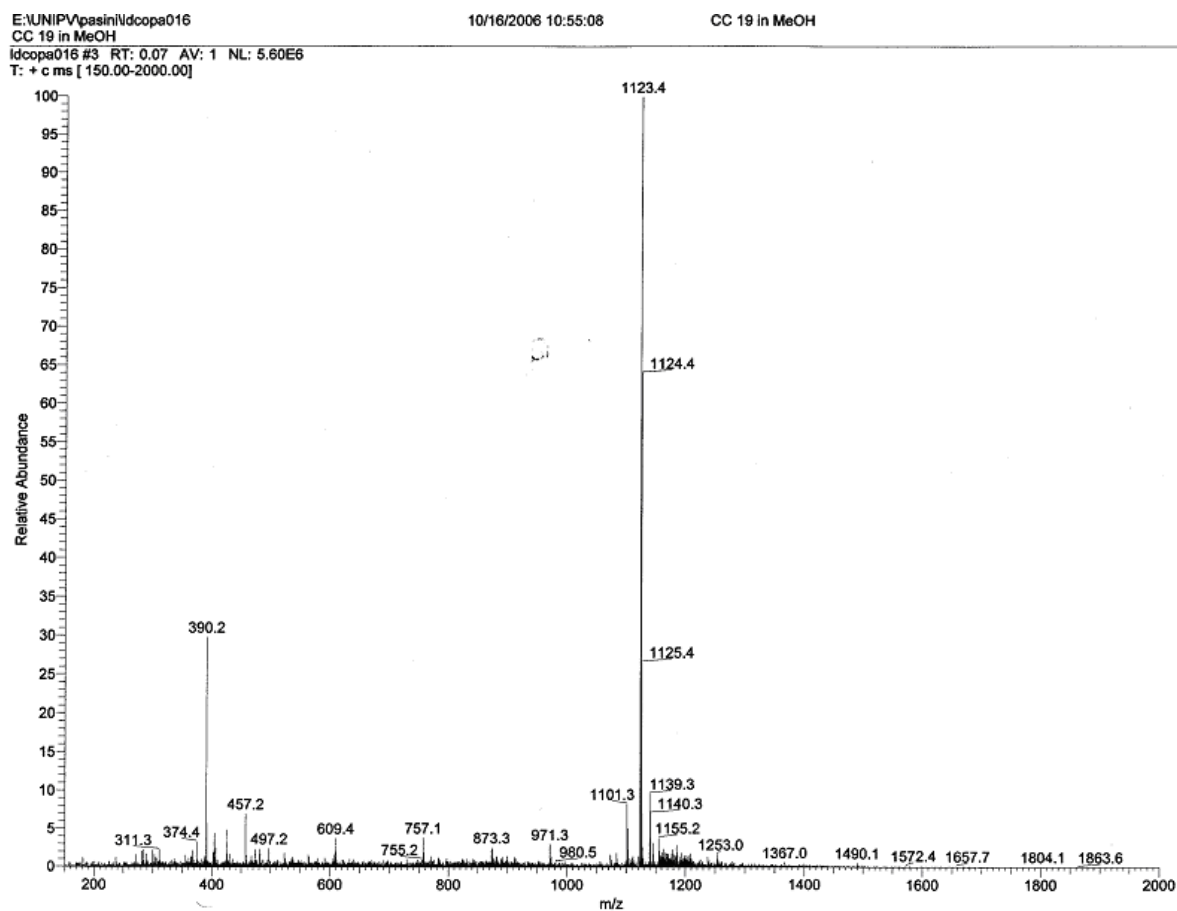


Mass Spectra (ESI)

Compound 13.



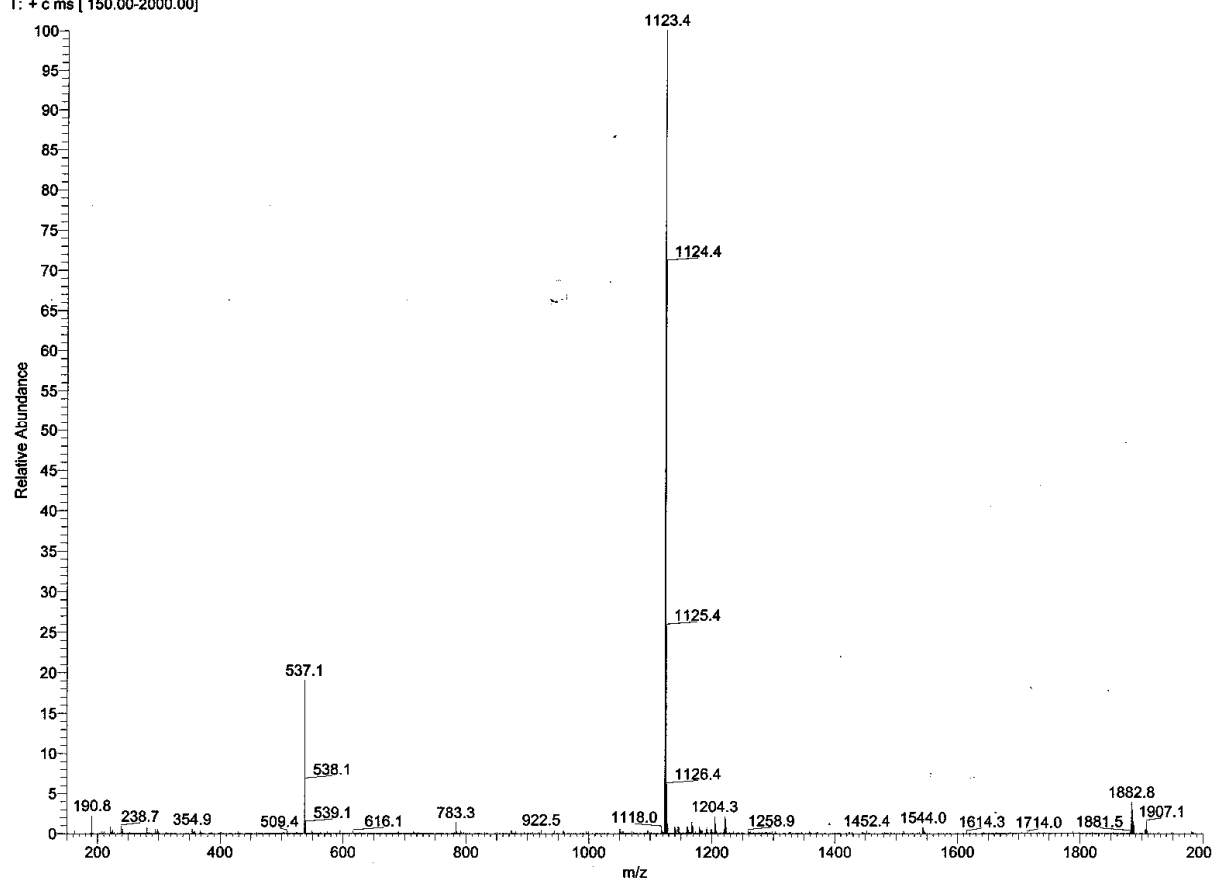
Compound **14**.



Compound 15.

CH₂Cl₂, MeOH

Idcopa025 #3-11 RT: 0.06-0.30 AV: 9 NL: 2.64E6
T: + c ms [150.00-2000.00]



Compound 13, global minimum

Method: B3LYP/6-31G(d)

SCF Done: E(RB+HF-LYP) = -3133.75808938 A.U. after 1 cycles
Convrg = 0.3981D-08 -V/T = 2.0095
S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.534734	1.208018	-2.023889
2	6	0	9.954539	2.019337	-0.996015
3	6	0	9.198736	2.086251	0.199458
4	6	0	8.049439	1.343154	0.349313
5	6	0	7.585079	0.489335	-0.692925
6	6	0	8.350575	0.431508	-1.905909
7	6	0	6.387132	-0.284805	-0.572413
8	6	0	7.899588	-0.401534	-2.958676
9	6	0	6.747335	-1.141503	-2.837191
10	6	0	5.987208	-1.076912	-1.642973
11	6	0	7.158107	-1.786343	1.862047
12	6	0	7.527093	-2.483678	2.990659
13	6	0	6.737167	-2.428699	4.163548
14	6	0	5.584567	-1.678124	4.177887
15	6	0	5.172639	-0.949192	3.030035
16	6	0	5.976752	-0.993439	1.842459
17	6	0	3.973740	-0.189450	3.024086
18	6	0	5.567605	-0.257265	0.679294
19	6	0	4.383439	0.464798	0.731809
20	6	0	3.583392	0.498634	1.900428
21	8	0	4.846003	-1.817555	-1.471757
22	8	0	3.908125	1.117699	-0.395308
23	6	0	2.701801	-2.653902	-2.268963
24	8	0	2.000083	-3.168921	-3.129823
25	6	0	-1.360680	-2.639012	-0.540072
26	6	0	-0.123324	-2.660578	-1.174438
27	6	0	1.033566	-2.374852	-0.434619
28	6	0	0.918042	-2.110237	0.937215
29	6	0	-1.479856	-2.334715	0.822231
30	8	0	-2.417185	-2.209582	3.647758
31	6	0	-3.160287	-2.176779	2.674695
32	6	0	-4.526526	0.747494	2.685021
33	6	0	-5.226114	-0.023199	1.721382
34	6	0	-5.841840	0.575822	0.628382
35	6	0	-5.788577	1.998193	0.488868
36	6	0	-5.098494	2.782415	1.472825
37	6	0	-4.473533	2.117143	2.556368
38	6	0	-5.049074	4.195784	1.331614
39	6	0	-5.651282	4.820468	0.264972
40	6	0	-6.331032	4.049884	-0.709947
41	6	0	-6.398702	2.679385	-0.603176
42	6	0	-6.535165	-0.270847	-0.391186
43	6	0	-5.812182	-0.811708	-1.445274
44	8	0	-4.450161	-0.580450	-1.458413
45	6	0	-4.684330	-2.082110	2.856977

46	8	0	-5.341795	-1.393427	1.798519
47	6	0	-7.939410	-0.531474	-0.309334
48	6	0	-8.745712	-0.017665	0.744941
49	6	0	-10.096869	-0.276259	0.794170
50	6	0	-10.720084	-1.062648	-0.205145
51	6	0	-9.970905	-1.575142	-1.238292
52	6	0	-8.574148	-1.327369	-1.320177
53	6	0	-7.785941	-1.846460	-2.377068
54	6	0	-6.434762	-1.601587	-2.442897
55	6	0	-2.410508	0.115774	-2.619824
56	6	0	1.276009	2.811299	-0.102711
57	6	0	0.143053	2.661647	0.710156
58	6	0	-0.984558	1.995625	0.246622
59	6	0	-1.006296	1.446814	-1.043275
60	6	0	0.122419	1.594966	-1.863451
61	6	0	1.240934	2.280937	-1.396996
62	7	0	2.363168	3.559484	0.416993
63	7	0	2.318894	-2.305939	-1.008959
64	7	0	-2.176168	0.771244	-1.448150
65	7	0	-2.783452	-2.255769	1.365529
66	8	0	-1.660221	0.054953	-3.584587
67	6	0	-3.771215	-0.583106	-2.713457
68	6	0	3.727880	3.543818	0.222056
69	8	0	4.421807	4.425863	0.712557
70	6	0	4.394979	2.441774	-0.609774
71	6	0	4.159154	-2.324883	-2.609166
72	1	0	10.102789	1.149099	-2.949516
73	1	0	10.860093	2.610734	-1.097842
74	1	0	9.528761	2.732789	1.007970
75	1	0	7.482361	1.405302	1.272003
76	1	0	8.482350	-0.455334	-3.874935
77	1	0	6.429580	-1.785036	-3.649756
78	1	0	7.770530	-1.838755	0.968391
79	1	0	8.433230	-3.083433	2.980822
80	1	0	7.041256	-2.982667	5.047348
81	1	0	4.965400	-1.633064	5.070751
82	1	0	3.362930	-0.161953	3.923246
83	1	0	2.658743	1.064998	1.875849
84	1	0	-2.255462	-2.859134	-1.118152
85	1	0	-0.045297	-2.883757	-2.229360
86	1	0	1.811665	-1.900701	1.519406
87	1	0	-4.018938	0.269805	3.514593
88	1	0	-3.941099	2.705671	3.299658
89	1	0	-4.522421	4.775113	2.086544
90	1	0	-5.607374	5.901355	0.165904
91	1	0	-6.804881	4.547945	-1.551563
92	1	0	-6.925555	2.100435	-1.354351
93	1	0	-5.111924	-3.089820	2.844991
94	1	0	-4.888147	-1.638631	3.835727
95	1	0	-8.278411	0.585653	1.516191
96	1	0	-10.692655	0.126041	1.609138
97	1	0	-11.787358	-1.258551	-0.151914
98	1	0	-10.437198	-2.180763	-2.011966
99	1	0	-8.263660	-2.452587	-3.142755
100	1	0	-5.846174	-2.021161	-3.251304
101	1	0	-1.851717	1.894547	0.894765
102	1	0	0.109845	1.184400	-2.863261
103	1	0	2.085648	2.406589	-2.063473
104	1	0	3.049293	-1.893702	-0.439024

105	1	0	-2.922457	0.706735	-0.765161
106	1	0	-4.366778	-0.065716	-3.475856
107	1	0	-3.579818	-1.603660	-3.064920
108	1	0	4.251333	2.649328	-1.675597
109	1	0	5.463357	2.514821	-0.391364
110	1	0	4.631522	-3.240328	-2.986468
111	1	0	4.142715	-1.586815	-3.420375
112	1	0	-3.536825	-2.174396	0.691200
113	6	0	-0.320450	-2.086916	1.568913
114	1	0	-0.396581	-1.878668	2.627227
115	1	0	2.110423	4.306749	1.055093
116	1	0	0.147476	3.071418	1.717440

Compound 15, global minimum

Method: B3LYP/6-31G(d)

SCF Done: E(RB+HF-LYP) = -3595.87754802 A.U. after 10 cycles

Convg = 0.5451D-08 -V/T = 2.0095

S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.806310	0.688753	5.212580
2	6	0	-3.712955	0.048560	6.024967
3	6	0	-4.756364	-0.714099	5.448760
4	6	0	-4.866835	-0.832657	4.081273
5	6	0	-3.941849	-0.192901	3.209167
6	6	0	-2.895745	0.594284	3.797597
7	6	0	-4.042596	-0.291106	1.778292
8	6	0	-1.976691	1.268098	2.952158
9	6	0	-2.098428	1.193025	1.586737
10	6	0	-3.141040	0.430602	1.010099
11	6	0	-3.866908	-3.244334	1.856994
12	6	0	-3.781372	-4.618477	1.907512
13	6	0	-4.789131	-5.429990	1.333869
14	6	0	-5.861747	-4.837807	0.708831
15	6	0	-5.976385	-3.424229	0.629974
16	6	0	-4.967302	-2.594346	1.224009
17	6	0	-7.064060	-2.803893	-0.032347
18	6	0	-5.074405	-1.165926	1.138333
19	6	0	-6.139898	-0.612131	0.431009
20	6	0	-7.146046	-1.437460	-0.135958
21	8	0	-3.275123	0.499685	-0.369056
22	8	0	-6.188755	0.747270	0.341936
23	6	0	-3.697240	-0.778024	-2.347541
24	8	0	-4.723910	-0.131811	-2.498730
25	6	0	-3.069510	3.993914	-0.986498
26	6	0	-4.455013	4.086596	-1.177190
27	6	0	-5.020737	5.317232	-1.546621
28	6	0	-4.182707	6.419576	-1.715432
29	6	0	-2.806181	6.328531	-1.519867

30	6	0	-2.230224	5.103161	-1.144959
31	6	0	-0.754328	-3.565557	-5.182362
32	6	0	-1.892801	-2.826295	-4.877275
33	6	0	-2.172000	-2.473255	-3.546116
34	6	0	-1.304666	-2.907622	-2.537924
35	6	0	-0.133364	-3.615750	-2.846487
36	6	0	0.138246	-3.946526	-4.180366
37	8	0	4.784055	-3.318454	-3.263165
38	6	0	5.141373	-3.069640	-2.119799
39	6	0	8.059541	-0.011848	-1.294414
40	6	0	6.938704	-0.479427	-0.561606
41	6	0	6.188199	0.371519	0.233537
42	6	0	6.548171	1.758842	0.290368
43	6	0	7.664248	2.237991	-0.471820
44	6	0	8.406332	1.315773	-1.253744
45	6	0	8.001866	3.616913	-0.424570
46	6	0	7.272707	4.499445	0.338597
47	6	0	6.171170	4.031171	1.094150
48	6	0	5.818793	2.698866	1.072332
49	6	0	5.010573	-0.129079	1.008003
50	6	0	3.750263	-0.130549	0.421719
51	8	0	3.692562	0.289901	-0.891013
52	6	0	6.523999	-2.451277	-1.875295
53	8	0	6.611252	-1.820984	-0.593131
54	6	0	5.148345	-0.561140	2.364519
55	6	0	6.409241	-0.600323	3.024986
56	6	0	6.511961	-1.024372	4.330431
57	6	0	5.363369	-1.431429	5.052488
58	6	0	4.129469	-1.405309	4.445861
59	6	0	3.987037	-0.974813	3.098784
60	6	0	2.725050	-0.934112	2.456902
61	6	0	2.599157	-0.524136	1.149921
62	6	0	1.420492	1.160522	-1.397545
63	6	0	-0.023534	6.039965	-0.366867
64	6	0	-0.770212	4.972949	-0.892347
65	6	0	-0.117957	3.757537	-1.155761
66	6	0	1.243924	3.602896	-0.873189
67	6	0	1.980035	4.678233	-0.355538
68	6	0	1.339101	5.889890	-0.112228
69	6	0	2.183329	-3.631279	-1.939271
70	6	0	0.825490	-3.927141	-1.752448
71	6	0	0.390806	-4.412490	-0.509126
72	6	0	1.304997	-4.580809	0.530280
73	6	0	2.646430	-4.247184	0.358677
74	6	0	3.088804	-3.759207	-0.878378
75	7	0	-5.205705	2.913938	-0.965646
76	7	0	-3.333085	-1.703139	-3.309956
77	7	0	1.933488	2.390245	-1.110672
78	7	0	4.429715	-3.323490	-0.981607
79	8	0	0.230667	0.887313	-1.529392
80	6	0	2.487713	0.082292	-1.624012
81	6	0	-6.562664	2.777083	-0.932403
82	8	0	-7.385986	3.655122	-1.162348
83	6	0	-7.034975	1.349837	-0.637781
84	6	0	-2.801097	-0.609290	-1.122159
85	1	0	-2.006440	1.287960	5.641723
86	1	0	-3.636114	0.132392	7.105619
87	1	0	-5.479822	-1.208030	6.091919
88	1	0	-5.676109	-1.413591	3.652989

89	1	0	-1.178866	1.855187	3.400382
90	1	0	-1.405223	1.701464	0.924189
91	1	0	-3.087193	-2.640719	2.308348
92	1	0	-2.931938	-5.085196	2.399968
93	1	0	-4.710771	-6.512308	1.385888
94	1	0	-6.641867	-5.445780	0.256131
95	1	0	-7.841036	-3.427354	-0.468106
96	1	0	-7.989058	-0.986594	-0.645946
97	1	0	-2.653395	3.040451	-0.680964
98	1	0	-6.089238	5.393092	-1.690309
99	1	0	-4.618952	7.369696	-2.013133
100	1	0	-2.176921	7.198534	-1.682317
101	1	0	-0.554004	-3.833170	-6.216119
102	1	0	-2.561969	-2.501621	-5.670548
103	1	0	-1.501545	-2.679667	-1.500487
104	1	0	1.034138	-4.507899	-4.427282
105	1	0	8.646712	-0.716834	-1.874725
106	1	0	9.265230	1.672267	-1.816821
107	1	0	8.852035	3.963353	-1.007616
108	1	0	7.540663	5.551834	0.366679
109	1	0	5.604407	4.727755	1.706487
110	1	0	4.980870	2.349853	1.666843
111	1	0	7.281186	-3.242933	-1.939721
112	1	0	6.697834	-1.740814	-2.686718
113	1	0	7.296038	-0.291179	2.481650
114	1	0	7.484976	-1.046977	4.813860
115	1	0	5.461247	-1.761965	6.082736
116	1	0	3.239210	-1.713357	4.989415
117	1	0	1.839630	-1.231017	3.013186
118	1	0	1.617411	-0.496094	0.691813
119	1	0	-0.515318	6.977941	-0.129353
120	1	0	-0.660567	2.931305	-1.590604
121	1	0	3.040247	4.560537	-0.141392
122	1	0	1.906503	6.721473	0.297005
123	1	0	2.532493	-3.252867	-2.890393
124	1	0	-0.655689	-4.663096	-0.360432
125	1	0	0.969488	-4.966882	1.488951
126	1	0	3.349088	-4.350378	1.181492
127	1	0	-4.672693	2.061574	-0.801475
128	1	0	-3.988196	-1.668030	-4.083797
129	1	0	2.939154	2.412470	-0.980219
130	1	0	4.875397	-3.018492	-0.123293
131	1	0	2.042837	-0.894896	-1.421974
132	1	0	2.786097	0.106794	-2.677699
133	1	0	-8.068523	1.416690	-0.283058
134	1	0	-6.997907	0.778111	-1.572627
135	1	0	-2.856195	-1.521114	-0.517222
136	1	0	-1.758257	-0.440015	-1.417390

Compound 13, UV and CD data, TD-DFT B3LYP/6-31G(d)
(Rotatory strengths in 10^{-40} erg·esu·cm/Gauss)

state	Energy (eV)	nm	osc. strength	Rotatory Strengths (velocity)	Rotatory Strengths (length)
1	3.6656	338.23	f=0.0151	10.8981	11.7727
2	3.7766	328.3	f=0.0018	11.2126	7.8714
3	3.7805	327.96	f=0.0013	-2.4384	-2.6654
4	3.7917	326.99	f=0.0008	0.7119	0.3942
5	3.843	322.62	f=0.0227	11.5927	7.0076
6	3.8655	320.74	f=0.0014	1.9279	2.6406
7	3.9024	317.71	f=0.0008	1.3678	2.2923
8	3.9389	314.77	f=0.0085	23.3476	21.109
9	3.9525	313.68	f=0.0009	-0.6705	-0.0555
10	3.9617	312.96	f=0.0081	1.7052	-1.471
11	3.9878	310.91	f=0.0345	31.2018	19.8411
12	4.0272	307.87	f=0.1048	58.9465	38.1079
13	4.0734	304.38	f=0.0001	0.0376	0.0251
14	4.1034	302.15	f=0.0052	-10.9341	-10.0577
15	4.1166	301.18	f=0.0308	18.6631	23.7674
16	4.1536	298.5	f=0.0370	41.281	45.3047
17	4.1767	296.84	f=0.0003	1.5341	1.5111
18	4.2653	290.68	f=0.0000	0.0128	0.0242
19	4.2771	289.88	f=0.0454	19.8025	21.0873
20	4.3316	286.23	f=0.0233	39.6927	39.2941
21	4.3779	283.21	f=0.0001	-0.1434	-0.1523
22	4.3793	283.12	f=0.0000	0.0838	0.0812
23	4.4395	279.27	f=0.0002	0.1433	0.2614
24	4.4434	279.03	f=0.0041	1.6712	4.07
25	4.4519	278.5	f=0.0069	-1.2605	0.3201
26	4.4537	278.38	f=0.0229	62.8283	66.1636
27	4.4732	277.17	f=0.0019	2.3864	2.3179
28	4.5027	275.36	f=0.0003	0.0364	0.113
29	4.5418	272.98	f=0.4190	71.9255	68.0603
30	4.5603	271.88	f=0.0006	0.0224	0.0346
31	4.5755	270.98	f=0.2317	-516.5407	-534.2578
32	4.6182	268.47	f=0.0788	85.1202	87.2559
33	4.6336	267.58	f=0.0450	-60.8962	-61.9053
34	4.6548	266.36	f=0.4096	480.0403	493.4035
35	4.6604	266.03	f=0.0893	24.7622	26.0056
36	4.6759	265.16	f=0.0087	20.0328	18.8419
37	4.6955	264.05	f=0.0005	0.553	0.5521
38	4.7288	262.19	f=0.0048	-5.9474	-5.9669
39	4.7394	261.6	f=0.0075	-3.2818	-3.7355
40	4.7523	260.89	f=0.0165	-24.7479	-23.4584
41	4.7594	260.51	f=0.0063	-6.6277	-6.6198
42	4.7686	260	f=0.0020	-2.3722	-1.881

43	4.7729	259.77	f=0.0028	-23.5716	-17.3554
44	4.773	259.76	f=0.0025	-4.4764	-3.6823
45	4.7871	259	f=0.0087	-0.9446	1.1371
46	4.7989	258.36	f=0.0014	3.4396	3.4178
47	4.8077	257.89	f=0.0167	-3.0441	-3.1862
48	4.8311	256.64	f=0.0004	0.0979	0.65
49	4.8491	255.68	f=0.0038	3.6185	2.8897
50	4.8566	255.29	f=0.0023	-3.735	-4.5801
51	4.8601	255.11	f=0.0381	22.5023	22.803
52	4.8713	254.52	f=0.0001	-0.6441	-0.4785
53	4.8957	253.25	f=0.0080	0.8693	0.0026
54	4.8972	253.17	f=0.0012	-0.9429	-1.0023
55	4.9057	252.74	f=0.0014	1.5596	2.5933
56	4.9104	252.49	f=0.0132	2.9584	3.8421
57	4.9389	251.04	f=0.0023	0.8226	0.9236
58	4.9548	250.23	f=0.0053	2.7185	2.3662
59	4.9629	249.82	f=0.0001	0.0653	-0.4249
60	4.9642	249.76	f=0.0097	-11.0669	-11.9769
61	4.9693	249.5	f=0.0006	-1.0023	-1.0957
62	4.9956	248.19	f=0.0015	-6.3185	-6.8454
63	5.0043	247.75	f=0.0010	-1.7136	-2.1616
64	5.0105	247.45	f=0.0112	-3.1601	-1.319
65	5.0236	246.8	f=0.0001	-1.7581	-1.3501
66	5.0282	246.58	f=0.0009	-0.6249	-0.6446
67	5.0441	245.8	f=0.0149	-15.6628	-12.1223
68	5.0544	245.3	f=0.0046	0.0206	0.1698
69	5.077	244.21	f=0.0007	1.7302	1.6744
70	5.0808	244.02	f=0.0252	9.6131	11.0661
71	5.0876	243.7	f=0.0142	-1.1992	0.582
72	5.0958	243.31	f=0.0002	-0.4904	-0.5791
73	5.0967	243.26	f=0.0006	-1.5141	-1.4765
74	5.1041	242.91	f=0.0035	4.3965	3.4964
75	5.1166	242.32	f=0.0093	0.9775	1.0928
76	5.1289	241.74	f=0.0047	-17.178	-17.6827
77	5.1308	241.65	f=0.0096	-8.438	-8.122
78	5.1499	240.75	f=0.0004	-0.5582	-0.5482
79	5.1783	239.43	f=0.0001	-0.3079	-0.2645
80	5.1945	238.68	f=0.0003	-0.1835	-0.2396
81	5.2006	238.41	f=0.0025	-2.8152	-2.9251
82	5.2104	237.96	f=0.0001	0.0357	0.0589
83	5.2147	237.76	f=0.0035	-1.029	-0.6277
84	5.2193	237.55	f=0.0025	-0.3491	0.001
85	5.2245	237.32	f=0.0003	0.0402	0.0313
86	5.229	237.11	f=0.0015	1.9409	2.9607
87	5.24	236.61	f=0.0002	1.3962	1.4991
88	5.253	236.03	f=0.0032	11.4384	12.0473
89	5.2679	235.36	f=0.0008	1.2006	1.1043
90	5.2712	235.21	f=0.0026	-4.5753	-3.9934
91	5.2849	234.6	f=0.0056	-6.8022	-6.682
92	5.2876	234.48	f=0.0015	5.0828	5.5765

93	5.2906	234.35	f=0.0033	18.543	19.118
94	5.3034	233.78	f=0.0076	14.7661	16.8111
95	5.3163	233.22	f=0.0120	-5.2433	-3.9001
96	5.3263	232.78	f=0.0085	-0.6861	-0.3125
97	5.3268	232.76	f=0.0340	-84.998	-84.0922
98	5.3285	232.68	f=0.0023	-5.5366	-5.3844
99	5.3308	232.58	f=0.0064	13.8321	14.5114
100	5.3575	231.42	f=0.0024	2.6127	2.7164
101	5.3781	230.54	f=0.0008	-2.64	-2.3547
102	5.3932	229.89	f=0.0011	0.4528	0.4917
103	5.3962	229.76	f=0.0016	-0.9232	-1.1131
104	5.4322	228.24	f=0.0089	-15.7514	-16.5047
105	5.4487	227.55	f=0.0304	-31.4561	-32.6497
106	5.4664	226.81	f=0.0024	2.5341	2.6393
107	5.4761	226.41	f=0.2304	-332.2161	-331.4452
108	5.4986	225.48	f=0.0407	33.1303	34.476
109	5.5004	225.41	f=0.0483	60.8354	62.1656
110	5.5044	225.25	f=0.0452	-28.8019	-28.9183
111	5.5056	225.2	f=0.0116	-23.7365	-23.9195
112	5.5062	225.17	f=0.0144	4.8706	5.9705
113	5.5269	224.33	f=0.0129	7.1783	6.9869
114	5.5285	224.26	f=0.0063	8.0579	8.4794
115	5.5353	223.99	f=0.1432	-268.49	-266.5588
116	5.5492	223.43	f=0.1710	230.4432	238.6079
117	5.5568	223.12	f=0.0006	-2.532	-2.4294
118	5.5691	222.63	f=0.0006	-0.5335	-0.4246
119	5.5735	222.45	f=0.0178	-5.8704	-5.7603
120	5.5953	221.59	f=0.0196	-5.4187	-5.6064
121	5.6059	221.17	f=0.0083	-6.2888	-6.4486
122	5.6184	220.67	f=0.0030	5.0861	6.0708
123	5.6249	220.42	f=0.0530	0.3698	0.1331
124	5.6294	220.24	f=0.0144	10.3629	13.353
125	5.63	220.22	f=0.0002	-0.6254	-0.6724
126	5.6321	220.14	f=0.0010	0.8447	0.6822
127	5.6405	219.81	f=0.1204	-80.0992	-77.5101
128	5.6504	219.42	f=0.0297	40.4421	42.909
129	5.6533	219.31	f=0.0286	47.9366	48.342
130	5.6617	218.99	f=0.1834	-31.7775	-27.2251
131	5.6638	218.9	f=0.0040	-0.1122	-4.6422
132	5.676	218.43	f=0.0489	5.4288	7.6523
133	5.6804	218.27	f=0.1001	26.7452	26.8398
134	5.6878	217.98	f=0.0210	72.2826	65.672
135	5.698	217.59	f=0.0529	-376.3649	-368.7343
136	5.7041	217.36	f=0.1971	-252.3	-254.4529
137	5.7111	217.09	f=0.1967	217.0609	218.0482
138	5.7204	216.74	f=0.0501	-19.2778	-18.9373
139	5.7377	216.09	f=0.0934	-155.4225	-156.1607
140	5.7412	215.95	f=0.3276	-202.0871	-204.1056
141	5.7433	215.88	f=0.0959	164.4158	165.2136
142	5.7556	215.42	f=0.0241	21.0875	21.7333

143	5.7591	215.28	f=0.0080	-14.7233	-14.6949
144	5.7636	215.12	f=0.1595	152.9412	155.7575
145	5.7699	214.88	f=0.0369	-16.5768	-13.1801
146	5.7758	214.66	f=0.0226	-17.778	-17.7612
147	5.7769	214.62	f=0.0862	60.7593	62.1331
148	5.7834	214.38	f=0.0903	-1.7016	-1.0392
149	5.7849	214.33	f=0.1166	-3.9752	-4.1548
150	5.7934	214.01	f=0.0011	4.4566	4.6001
151	5.7973	213.87	f=0.0321	-113.3365	-108.1053
152	5.8016	213.71	f=0.0134	31.0526	30.8928
153	5.8136	213.27	f=0.1248	49.623	49.1938
154	5.8206	213.01	f=0.0270	-6.1537	-2.7899
155	5.825	212.85	f=0.0169	7.875	7.1702
156	5.83	212.67	f=0.0071	21.1727	18.7869
157	5.8355	212.47	f=0.1271	57.2215	64.7755
158	5.8449	212.12	f=0.4866	162.182	163.9661
159	5.8589	211.62	f=0.0229	53.1309	51.841
160	5.8624	211.49	f=0.0332	14.2146	14.3193
161	5.8738	211.08	f=0.0046	-8.7778	-8.7244
162	5.8816	210.8	f=0.0046	-5.6254	-5.4889
163	5.888	210.57	f=0.0470	-52.5258	-55.5827
164	5.8907	210.47	f=0.0852	-34.6716	-36.283
165	5.8978	210.22	f=0.0158	18.5954	14.6844
166	5.9029	210.04	f=0.0021	-11.3921	-12.2572
167	5.9111	209.75	f=0.2162	-170.2649	-174.6889
168	5.9147	209.62	f=0.0055	-12.1345	-12.1146
169	5.9187	209.48	f=0.0424	-76.5914	-78.4835
170	5.9235	209.31	f=0.0179	94.9447	94.6721
171	5.9249	209.26	f=0.0135	-24.3283	-24.9321
172	5.9346	208.92	f=0.0189	-59.0223	-61.3482
173	5.9397	208.74	f=0.0255	-2.0232	1.0662
174	5.9412	208.69	f=0.0082	1.3533	1.1367
175	5.9494	208.4	f=0.0120	41.8061	41.0661
176	5.9552	208.2	f=0.0337	33.1802	32.5713
177	5.9617	207.97	f=0.0812	20.65	24.4634
178	5.9692	207.71	f=0.0921	145.0542	142.2161
179	5.9756	207.48	f=0.0452	-70.4306	-70.7417
180	5.9777	207.41	f=0.0265	-50.7799	-53.6319
181	5.9838	207.2	f=0.0188	-17.8121	-17.948
182	5.9883	207.04	f=0.0010	2.1828	2.2158
183	5.9897	207	f=0.0698	84.3732	85.896
184	5.9926	206.9	f=0.0232	-5.1766	-4.9034
185	6.0032	206.53	f=0.0102	-12.5881	-11.1847
186	6.0081	206.36	f=0.0415	57.7745	58.9187
187	6.0134	206.18	f=0.0638	19.405	21.1158
188	6.0231	205.85	f=0.0050	4.2259	4.4744
189	6.0306	205.59	f=0.0020	1.9995	0.675
190	6.0317	205.55	f=0.0036	-7.0744	-7.4594
191	6.0383	205.33	f=0.0187	19.0869	20.4744
192	6.0426	205.18	f=0.0170	17.1249	17.383

193	6.0473	205.02	f=0.0072	4.1284	4.3108
194	6.0524	204.85	f=0.0242	23.2515	24.3256
195	6.0552	204.76	f=0.0043	-13.4112	-14.248
196	6.066	204.39	f=0.0504	43.0579	40.9653
197	6.0754	204.08	f=0.0018	-1.0627	-1.0798
198	6.0785	203.97	f=0.0033	-4.2899	-3.9054
199	6.0797	203.93	f=0.0002	1.6463	1.9681
200	6.0836	203.8	f=0.0165	11.9495	11.2719
201	6.0919	203.52	f=0.0011	-0.091	-0.1277
202	6.0936	203.47	f=0.0163	-7.3984	-7.0946
203	6.1003	203.24	f=0.0083	14.5376	14.2834
204	6.1079	202.99	f=0.0653	-23.3336	-24.4232
205	6.1142	202.78	f=0.0007	-0.4903	-0.5551
206	6.1184	202.64	f=0.0356	-5.8777	-6.5543
207	6.1262	202.38	f=0.0195	-1.9206	-1.9123
208	6.1336	202.14	f=0.0064	-25.6185	-25.593
209	6.1383	201.99	f=0.0167	-0.209	-0.404
210	6.1477	201.68	f=0.0379	-174.3572	-182.7278
211	6.1592	201.3	f=0.0585	140.8613	144.1108
212	6.1635	201.16	f=0.0675	-31.8131	-38.218
213	6.1703	200.94	f=0.0044	10.7695	10.7464
214	6.1839	200.49	f=0.0061	4.8643	5.4061
215	6.1986	200.02	f=0.0091	11.435	12.6695
216	6.2031	199.87	f=0.0690	-39.5113	-41.7649
217	6.2091	199.68	f=0.0242	110.4378	109.5539
218	6.2147	199.5	f=0.0550	325.0619	327.4078
219	6.2193	199.35	f=0.0644	-55.0891	-52.1537
220	6.2279	199.08	f=0.0007	0.6687	0.6626
221	6.2301	199.01	f=0.0051	-9.0225	-8.8774
222	6.2419	198.63	f=0.0011	-0.5603	-0.5244
223	6.2461	198.5	f=0.0189	12.2113	13.3305
224	6.2518	198.32	f=0.0092	11.484	11.9036
225	6.2563	198.17	f=0.0259	15.6721	15.454
226	6.2681	197.8	f=0.0213	-21.7558	-21.4593
227	6.2691	197.77	f=0.0034	1.601	1.212
228	6.2708	197.72	f=0.0329	-6.1998	-8.2979
229	6.2788	197.46	f=0.0305	47.3933	47.6312
230	6.286	197.24	f=0.0057	-2.6474	-3.175
231	6.2881	197.17	f=0.0001	-0.0922	-0.1004
232	6.2964	196.91	f=0.0079	26.1289	25.212
233	6.3102	196.48	f=0.0012	0.8893	0.9077
234	6.3105	196.47	f=0.0185	-20.31	-21.1393
235	6.312	196.43	f=0.0090	0.6752	0.4203
236	6.3171	196.27	f=0.0086	-5.2874	-6.0515
237	6.325	196.02	f=0.0353	15.9998	17.4709
238	6.3306	195.85	f=0.0276	-24.0741	-25.7673
239	6.3364	195.67	f=0.0042	1.6708	1.5969
240	6.3614	194.9	f=0.0001	0.1098	0.101
241	6.3661	194.76	f=0.0002	-0.1188	-0.1098
242	6.3682	194.69	f=0.0092	-8.452	-7.5837

243	6.3701	194.64	f=0.0000	0.0506	0.0604
244	6.3794	194.35	f=0.0032	10.0705	13.6605
245	6.3833	194.23	f=0.0092	-7.1041	-6.2975
246	6.3887	194.07	f=0.0057	-11.3726	-10.4316
247	6.3974	193.8	f=0.0171	11.0603	13.352
248	6.4018	193.67	f=0.0045	10.0867	8.7533
249	6.4093	193.45	f=0.0038	8.303	7.7036
250	6.4106	193.4	f=0.0037	11.7511	11.2682
251	6.4227	193.04	f=0.0161	-6.4716	-7.0982
252	6.4289	192.86	f=0.0002	-1.4357	-1.3294
253	6.4366	192.62	f=0.0098	35.2513	37.7767
254	6.4424	192.45	f=0.0044	-21.4734	-20.6184
255	6.4477	192.29	f=0.0035	14.4312	13.3151
256	6.4609	191.9	f=0.0049	-5.8164	-9.8492
257	6.4618	191.87	f=0.0074	19.8682	16.8736
258	6.4652	191.77	f=0.0099	7.2626	7.1617
259	6.4697	191.64	f=0.0312	-3.8877	-4.3528
260	6.4723	191.56	f=0.0049	-7.4553	-6.4239
261	6.4756	191.46	f=0.0099	4.6033	4.824
262	6.4784	191.38	f=0.0066	-4.9809	-6.4522
263	6.483	191.24	f=0.0038	15.1277	17.003
264	6.4842	191.21	f=0.0000	-0.0189	0.0248
265	6.5088	190.49	f=0.0054	4.2792	4.6695
266	6.512	190.39	f=0.0131	-6.1542	-5.6385
267	6.5148	190.31	f=0.0047	-2.9651	-3.6498
268	6.5197	190.17	f=0.0060	-13.365	-13.8102
269	6.5336	189.76	f=0.0007	2.5908	2.5444
270	6.5362	189.69	f=0.0126	-22.3946	-15.9273
271	6.5492	189.31	f=0.0105	-3.9562	-5.3983
272	6.5542	189.17	f=0.0140	14.4842	13.7548
273	6.5619	188.95	f=0.0090	21.7351	22.6961
274	6.5711	188.68	f=0.0281	-3.3338	-4.4648
275	6.5715	188.67	f=0.0283	-6.7978	-10.6404
276	6.6038	187.75	f=0.0015	-1.5838	-1.417
277	6.6061	187.68	f=0.0140	3.9028	4.1265
278	6.6152	187.42	f=0.0055	-4.6759	-6.7893
279	6.6193	187.31	f=0.0043	3.5322	4.0473
280	6.6211	187.26	f=0.0022	-7.0119	-7.116
281	6.6251	187.14	f=0.0136	-4.9518	-5.1145
282	6.6254	187.14	f=0.0059	6.2471	4.8865
283	6.6269	187.09	f=0.0013	-6.671	-5.6102
284	6.6343	186.88	f=0.0070	10.4627	10.3273
285	6.6372	186.8	f=0.0127	7.2161	6.7317
286	6.6391	186.75	f=0.0056	-4.5685	-4.2078
287	6.6516	186.4	f=0.0082	-5.8616	-7.0513
288	6.6551	186.3	f=0.0055	5.0467	4.8826
289	6.6609	186.14	f=0.0197	-12.5653	-13.481
290	6.6635	186.06	f=0.0027	7.1946	5.606
291	6.6654	186.01	f=0.0131	5.1895	4.0082
292	6.6695	185.9	f=0.0085	-26.3649	-23.6706

293	6.6823	185.54	f=0.0224	5.8795	3.3383
294	6.6879	185.39	f=0.0288	22.1043	25.2495
295	6.6938	185.22	f=0.0012	-4.2902	-4.1536
296	6.6983	185.1	f=0.0061	6.0427	6.3917
297	6.7035	184.95	f=0.0670	2.8823	5.7313
298	6.7162	184.61	f=0.0054	-0.0692	0.3379
299	6.7213	184.47	f=0.0067	-14.1591	-14.2534
300	6.7236	184.4	f=0.0028	7.6636	7.8503

Compound 15, UV and CD data, TD-DFT B3LYP/6-31G(d)
(Rotatory strengths in 10^{-40} erg·esu·cm/Gauss)

state	Energy (eV)	nm	osc. strength	Rotatory Strengths (velocity)	Rotatory Strengths (length)
1	3.7647	329.33	f=0.0643	67.1878	55.7632
2	3.7814	327.88	f=0.0002	-0.4863	-0.6101
3	3.7997	326.3	f=0.0001	-0.1189	-0.1624
4	3.8169	324.83	f=0.0001	0.1705	0.1311
5	3.8463	322.35	f=0.0003	-1.1991	0.0661
6	3.861	321.12	f=0.0000	-0.0083	-0.0198
7	3.885	319.14	f=0.0067	2.6662	-0.0086
8	3.8977	318.09	f=0.0154	7.6591	2.8434
9	3.986	311.05	f=0.0015	-3.4138	-2.3119
10	4.0554	305.73	f=0.0282	-25.3233	-23.287
11	4.0593	305.43	f=0.0249	-28.7619	-26.2121
12	4.0603	305.36	f=0.0727	13.4536	7.3168
13	4.0889	303.22	f=0.0017	13.1296	15.2883
14	4.1333	299.97	f=0.0001	0.1654	0.1871
15	4.1427	299.28	f=0.0009	-1.0072	-1.014
16	4.1519	298.62	f=0.0047	-1.3426	-2.2515
17	4.1617	297.92	f=0.0260	65.9983	62.546
18	4.1761	296.89	f=0.0050	-1.1776	-1.9657
19	4.2214	293.7	f=0.0001	0.3726	0.3994
20	4.2549	291.39	f=0.0028	-1.5982	-1.0677
21	4.2566	291.27	f=0.0316	14.6987	14.2454
22	4.2842	289.4	f=0.0472	4.5079	10.9443
23	4.3466	285.25	f=0.0009	4.9847	5.0995
24	4.3549	284.7	f=0.0106	-8.1468	-7.3252
25	4.4018	281.67	f=0.0051	0.3179	-1.0017
26	4.4176	280.66	f=0.0002	-0.1768	-0.4464
27	4.421	280.44	f=0.0007	-0.4916	-0.7916
28	4.4264	280.1	f=0.0029	8.6801	10.1423
29	4.4276	280.03	f=0.0043	-9.1869	-9.774
30	4.4393	279.29	f=0.0229	-1.7277	1.3003
31	4.4482	278.73	f=0.0073	1.4025	0.759
32	4.4627	277.82	f=0.0213	-11.1108	-11.1256
33	4.4644	277.72	f=0.0060	11.2669	11.3967
34	4.4696	277.39	f=0.0046	8.7476	8.4957
35	4.4856	276.41	f=0.0147	-4.2664	-4.8343
36	4.4869	276.32	f=0.0047	-10.2574	-12.0837
37	4.5181	274.42	f=0.0016	2.8015	2.2193
38	4.528	273.82	f=0.0116	11.4851	8.0933
39	4.5364	273.31	f=0.0003	0.9652	1.0199
40	4.5424	272.95	f=0.0067	7.8342	7.9607
41	4.5658	271.55	f=0.0068	12.8541	11.1737
42	4.5798	270.72	f=0.0309	-5.7972	-9.4077
43	4.6007	269.49	f=0.0000	-0.0147	-0.0757

44	4.608	269.06	f=0.0003	0.3597	0.3406
45	4.6137	268.73	f=0.0013	-1.6089	-2.0256
46	4.6186	268.45	f=0.0031	-3.3979	-3.9497
47	4.6287	267.86	f=0.0015	-4.6146	-4.5535
48	4.6349	267.5	f=0.0005	0.3271	0.3624
49	4.6377	267.34	f=0.0010	-2.1168	-2.4715
50	4.6558	266.3	f=0.0001	-0.2201	-0.2597
51	4.6656	265.74	f=0.0010	-2.7982	-2.7618
52	4.6686	265.57	f=0.0050	12.9611	11.6665
53	4.6827	264.77	f=0.0055	-7.7092	-8.1143
54	4.6858	264.6	f=0.0000	-0.1383	-0.1479
55	4.689	264.42	f=0.0007	0.1005	0.1124
56	4.6957	264.04	f=0.0021	0.8708	0.2279
57	4.6985	263.88	f=0.0002	-0.2267	-1.3425
58	4.7057	263.48	f=0.0019	-3.7643	-4.0715
59	4.7138	263.03	f=0.0010	-4.2249	-4.1796
60	4.7164	262.88	f=0.0059	-8.245	-7.5852
61	4.719	262.73	f=0.0004	-1.5348	-1.4592
62	4.7257	262.36	f=0.0010	-6.0277	-5.9693
63	4.7427	261.42	f=0.0023	-3.5813	-2.925
64	4.746	261.24	f=0.0046	19.374	20.1193
65	4.7571	260.63	f=0.0069	-6.1861	-8.0547
66	4.7683	260.02	f=0.0105	-27.398	-27.9996
67	4.7776	259.51	f=0.0000	0.0401	0.0281
68	4.7821	259.27	f=0.0048	-2.2445	-2.5842
69	4.7925	258.7	f=0.0037	-12.2919	-12.7864
70	4.7954	258.55	f=0.1498	41.163	51.1651
71	4.8018	258.2	f=0.0585	-91.0383	-93.8624
72	4.8265	256.88	f=0.0017	6.2736	5.8177
73	4.8349	256.44	f=0.0011	-3.6943	-3.7479
74	4.8381	256.26	f=0.0051	10.1382	10.7986
75	4.855	255.37	f=0.0022	-1.6033	-1.8856
76	4.862	255.01	f=0.0006	-3.2094	-3.0166
77	4.8649	254.85	f=0.0005	1.7691	1.7446
78	4.8734	254.41	f=0.0012	-1.5739	-1.04
79	4.8796	254.09	f=0.0112	-7.6457	-6.8811
80	4.8966	253.21	f=0.0154	-13.1182	-13.1199
81	4.9007	252.99	f=0.0024	-13.616	-14.3625
82	4.9046	252.79	f=0.0135	-12.6857	-13.2377
83	4.9085	252.59	f=0.0014	0.4229	0.4175
84	4.9179	252.11	f=0.0141	-44.432	-46.1516
85	4.9194	252.03	f=0.0120	10.2684	10.7972
86	4.9209	251.95	f=0.0058	-0.7451	-0.7771
87	4.9429	250.83	f=0.0374	-88.3715	-91.5052
88	4.9526	250.34	f=0.0023	2.6156	2.4096
89	4.9552	250.21	f=0.0009	-1.2859	-1.3213
90	4.9643	249.75	f=0.0020	-14.9366	-14.9402
91	4.9827	248.83	f=0.0050	-0.2774	-0.1502
92	4.9838	248.78	f=0.0200	-15.3628	-12.7083
93	4.9886	248.54	f=0.0655	84.5115	85.9669

94	4.9955	248.19	f=0.0170	-8.3412	-12.3117
95	5.0053	247.7	f=0.0053	0.9274	0.9822
96	5.0143	247.26	f=0.0090	-0.4774	-2.2447
97	5.0281	246.58	f=0.0121	2.399	7.0615
98	5.033	246.34	f=0.0103	-1.0915	-1.4775
99	5.0627	244.9	f=0.1714	-194.5527	-216.7006
100	5.0681	244.64	f=0.0293	-21.0043	-20.9243
101	5.0724	244.43	f=0.1161	-40.6705	-40.3578
102	5.0747	244.32	f=0.0170	-3.6832	-4.084
103	5.0765	244.23	f=0.0728	158.2326	162.3933
104	5.1028	242.97	f=0.0125	-0.9173	-4.0303
105	5.1116	242.55	f=0.0317	38.0311	35.8504
106	5.1142	242.43	f=0.0035	51.8828	55.218
107	5.1183	242.24	f=0.0374	6.8306	12.6031
108	5.1228	242.02	f=0.0088	73.1673	77.7353
109	5.1242	241.96	f=0.0047	7.5555	8.1271
110	5.141	241.17	f=0.2157	78.2798	71.2828
111	5.151	240.7	f=0.0110	7.4243	8.5706
112	5.1555	240.49	f=0.0060	66.6148	64.9198
113	5.1671	239.95	f=0.0282	18.1792	17.078
114	5.1692	239.85	f=0.0006	-0.0571	-0.0731
115	5.1874	239.01	f=0.3531	-473.9215	-492.9941
116	5.1984	238.5	f=0.1228	-147.5917	-153.2475
117	5.2007	238.4	f=0.0011	-1.4647	-1.7005
118	5.2164	237.68	f=0.0073	-1.8946	-1.9585
119	5.2432	236.47	f=0.0710	-55.9161	-56.3488
120	5.2554	235.92	f=0.0952	-92.9062	-94.4472
121	5.2563	235.88	f=0.0022	4.6568	4.7811
122	5.2627	235.59	f=0.0702	-143.1039	-143.7681
123	5.2726	235.15	f=0.0015	-7.8093	-8.3213
124	5.2771	234.95	f=0.0991	41.6697	37.221
125	5.2815	234.75	f=0.0002	0.3351	0.342
126	5.2821	234.73	f=0.0653	14.6755	14.8054
127	5.2918	234.3	f=0.0070	2.2808	2.5129
128	5.3018	233.85	f=0.0074	5.8207	5.4931
129	5.3105	233.47	f=0.0206	-1.0558	-1.3775
130	5.3136	233.33	f=0.0115	-16.6525	-18.4627
131	5.3173	233.17	f=0.0031	-2.7719	-3.1958
132	5.32	233.05	f=0.0055	11.1183	12.0365
133	5.3352	232.39	f=0.0136	-75.6426	-81.6467
134	5.3368	232.32	f=0.0226	-46.0373	-47.1616
135	5.3404	232.16	f=0.0015	-2.2314	-2.0031
136	5.3436	232.02	f=0.0058	-9.0381	-10.7275
137	5.3479	231.84	f=0.0211	-18.0133	-19.5219
138	5.3548	231.54	f=0.0000	2.6337	1.6942
139	5.3578	231.41	f=0.0025	-2.7455	-3.4309
140	5.3634	231.17	f=0.0018	-2.2481	-2.136
141	5.377	230.58	f=0.0148	-4.5731	-4.6401
142	5.3801	230.45	f=0.0626	-18.0479	-19.2944
143	5.3899	230.03	f=0.0652	-29.4548	-30.7967

144	5.3944	229.84	f=0.0815	-96.8088	-100.2865
145	5.409	229.22	f=0.0020	2.9798	2.8871
146	5.4143	228.99	f=0.0267	-0.1178	-0.3068
147	5.4155	228.94	f=0.0012	-4.4732	-3.562
148	5.4169	228.88	f=0.0211	-13.2309	-14.1906
149	5.4207	228.72	f=0.0049	13.6136	14.1513
150	5.4217	228.68	f=0.0265	-2.617	-3.0735
151	5.4253	228.53	f=0.0076	0.0493	-0.7448
152	5.438	228	f=0.0096	12.4292	12.6298
153	5.4453	227.69	f=0.0790	-66.9625	-70.4417
154	5.4599	227.08	f=0.0018	-1.8781	-1.6546
155	5.4699	226.67	f=0.0052	-22.1547	-24.39
156	5.4938	225.68	f=0.0335	64.0603	69.8761
157	5.4985	225.49	f=0.0164	-11.5577	-11.9871
158	5.5043	225.25	f=0.0007	1.5363	1.5781
159	5.5045	225.24	f=0.0048	-1.1967	1.596
160	5.5103	225	f=0.0123	-7.8324	-9.1158
161	5.5141	224.85	f=0.0024	-1.2052	0.3635
162	5.5186	224.67	f=0.0058	27.5973	28.7796
163	5.5275	224.31	f=0.0057	-16.2196	-16.1806
164	5.5313	224.15	f=0.0616	-52.0738	-54.5681
165	5.5375	223.9	f=0.0115	0.0896	0.0204
166	5.5439	223.64	f=0.0018	-2.1477	-2.1654
167	5.5493	223.42	f=0.0224	0.7971	-2.1514
168	5.5542	223.23	f=0.0231	35.1163	36.7537
169	5.5555	223.17	f=0.0264	16.7729	17.2314
170	5.5738	222.44	f=0.0028	4.5956	5.4563
171	5.5749	222.4	f=0.0118	-16.2347	-16.6199
172	5.5859	221.96	f=0.0137	-35.0395	-22.8784
173	5.5917	221.73	f=0.0011	-4.2907	-3.5367
174	5.5951	221.59	f=0.0042	-66.0801	-62.4086
175	5.5961	221.56	f=0.0076	-86.2937	-80.8998
176	5.5991	221.43	f=0.0026	5.7689	6.1692
177	5.6023	221.31	f=0.0007	-2.4884	-1.9882
178	5.6042	221.23	f=0.0531	118.6259	121.7082
179	5.6061	221.16	f=0.1398	-107.7452	-110.2633
180	5.6065	221.14	f=0.0701	48.7838	49.2067
181	5.6092	221.04	f=0.0091	-14.2334	-10.699
182	5.6176	220.71	f=0.0119	16.6318	18.2347
183	5.6247	220.43	f=0.0288	-8.2794	-8.5002
184	5.6335	220.08	f=0.2004	330.9776	339.026
185	5.6358	219.99	f=0.0119	30.8543	31.3532
186	5.651	219.4	f=0.0425	-80.2069	-81.894
187	5.6545	219.27	f=0.0229	-50.8733	-54.8021
188	5.6555	219.23	f=0.0638	5.6834	6.72
189	5.6653	218.85	f=0.0228	1.0356	0.771
190	5.6673	218.77	f=0.0432	35.751	36.2997
191	5.6731	218.55	f=0.1648	-83.8978	-90.6221
192	5.6779	218.36	f=0.0254	-31.483	-34.2706
193	5.688	217.98	f=0.1186	-13.2083	-14.2758

194	5.6938	217.75	f=0.0179	32.5458	33.0278
195	5.6988	217.56	f=0.0233	4.6878	3.7055
196	5.701	217.48	f=0.0512	-114.2457	-109.9177
197	5.7061	217.28	f=0.0116	-2.4891	0.0735
198	5.7084	217.2	f=0.0162	-48.4086	-48.0032
199	5.7096	217.15	f=0.0064	2.6858	2.5095
200	5.7114	217.08	f=0.0175	26.1089	27.4731
201	5.7196	216.77	f=0.0745	-7.9351	-6.246
202	5.722	216.68	f=0.0084	-8.4696	-7.7781
203	5.7252	216.56	f=0.0192	-60.8082	-61.2234
204	5.7305	216.36	f=0.0178	44.2695	45.4716
205	5.7366	216.13	f=0.0346	49.9232	49.9701
206	5.7385	216.06	f=0.0120	40.2089	41.9808
207	5.7391	216.04	f=0.0413	-4.3922	-4.4664
208	5.7401	216	f=0.1513	7.5681	7.6356
209	5.7424	215.91	f=0.0032	4.5206	4.5813
210	5.7541	215.47	f=0.0143	16.684	18.0927
211	5.7557	215.41	f=0.0022	7.7262	7.8429
212	5.7572	215.36	f=0.0039	18.188	17.6855
213	5.7604	215.24	f=0.0921	194.0336	199.2174
214	5.7608	215.22	f=0.0083	5.2087	5.1327
215	5.7657	215.04	f=0.0893	-192.0723	-194.6852
216	5.7667	215	f=0.0061	-12.5462	-12.3863
217	5.774	214.73	f=0.0033	-7.1331	-7.0098
218	5.778	214.58	f=0.0191	-6.7483	-7.1591
219	5.7783	214.57	f=0.0395	-57.0589	-61.8102
220	5.7912	214.09	f=0.0611	61.4001	59.1657
221	5.7937	214	f=0.0258	-70.7112	-72.2984
222	5.7971	213.87	f=0.0648	85.7923	84.3042
223	5.7981	213.84	f=0.0216	-117.9767	-123.4915
224	5.8023	213.68	f=0.0078	-51.3843	-53.9543
225	5.8037	213.63	f=0.0361	89.2434	90.3693
226	5.8063	213.53	f=0.0984	158.2796	157.7212
227	5.8117	213.33	f=0.0982	-16.1205	-15.5777
228	5.8147	213.22	f=0.0037	5.631	5.6008
229	5.825	212.85	f=0.0138	2.6956	2.1995
230	5.828	212.74	f=0.0155	7.6775	7.3006
231	5.8297	212.68	f=0.0028	3.7185	2.4378
232	5.8392	212.33	f=0.0852	-99.4058	-100.8814
233	5.8425	212.21	f=0.0010	6.9245	6.5999
234	5.8438	212.16	f=0.0120	-28.6597	-28.564
235	5.8508	211.91	f=0.0262	-41.8139	-41.5876
236	5.8555	211.74	f=0.0058	15.5222	16.1375
237	5.8575	211.67	f=0.0014	-2.253	-2.0457
238	5.8609	211.54	f=0.0128	38.8155	36.6674
239	5.8642	211.43	f=0.0115	36.3442	36.8079
240	5.8687	211.26	f=0.0180	-7.6147	-5.7952
241	5.8748	211.04	f=0.0290	1.8743	1.3051
242	5.8784	210.91	f=0.0144	16.419	15.8543
243	5.88	210.86	f=0.0172	-44.6606	-45.6891

244	5.8818	210.79	f=0.0099	-12.8014	-13.0201
245	5.8876	210.58	f=0.1226	143.7979	145.6316
246	5.9001	210.14	f=0.0447	50.2737	51.0688
247	5.9084	209.84	f=0.0153	12.2774	12.4647
248	5.9162	209.57	f=0.0569	-1.0553	-0.7454
249	5.9215	209.38	f=0.1358	71.9584	78.1876
250	5.927	209.19	f=0.0850	1.0661	4.3645
251	5.929	209.11	f=0.1557	211.2997	212.3158
252	5.9349	208.91	f=0.0139	47.5177	50.5393
253	5.9414	208.68	f=0.0668	-119.3231	-124.1042
254	5.9612	207.99	f=0.3318	238.6274	251.7226
255	5.9738	207.55	f=0.0291	50.7673	50.4585
256	5.9756	207.49	f=0.4561	-119.0444	-114.7468
257	5.9843	207.18	f=0.0040	25.0295	25.4136
258	5.9941	206.84	f=0.0248	-11.3339	-11.5594
259	5.9954	206.8	f=0.0290	12.7839	11.819
260	6.0033	206.53	f=0.0215	-37.3507	-38.6915
261	6.008	206.36	f=0.0251	8.2706	9.2975
262	6.0153	206.11	f=0.0840	27.9772	23.5762
263	6.0206	205.93	f=0.0235	-14.2526	-14.0756
264	6.0308	205.58	f=0.0006	-1.2444	-1.2362
265	6.0488	204.97	f=0.0014	-0.2269	-0.3953
266	6.05	204.93	f=0.0028	-0.4012	-0.3856
267	6.0519	204.87	f=0.0038	2.8722	3.0617
268	6.0553	204.75	f=0.0141	13.6495	14.1685
269	6.0671	204.35	f=0.0064	-4.255	-4.1228
270	6.0733	204.15	f=0.0230	43.6827	44.308
271	6.0785	203.97	f=0.0433	-13.5934	-14.081
272	6.0903	203.58	f=0.0027	0.9912	0.9577
273	6.0918	203.53	f=0.0030	0.4641	0.5593
274	6.0935	203.47	f=0.0128	-22.4318	-23.2871
275	6.1	203.25	f=0.0148	9.6266	10.3278
276	6.1084	202.97	f=0.0052	14.9903	15.1283
277	6.1106	202.9	f=0.0887	-283.6425	-299.3361
278	6.1172	202.68	f=0.0251	-38.3575	-37.9962
279	6.1194	202.61	f=0.0218	34.1664	36.9732
280	6.1228	202.49	f=0.0232	37.4173	36.0849
281	6.127	202.36	f=0.0650	-12.0763	-14.3628
282	6.1329	202.16	f=0.0061	1.8534	0.5956
283	6.1348	202.1	f=0.0446	-76.5903	-76.7939
284	6.138	201.99	f=0.0289	40.9503	39.0491
285	6.1451	201.76	f=0.0055	-7.7796	-7.379
286	6.1601	201.27	f=0.0036	-7.7223	-7.6976
287	6.1633	201.17	f=0.0262	1.0492	0.1399
288	6.1686	200.99	f=0.0145	25.2265	26.3835
289	6.1742	200.81	f=0.0331	75.4566	78.6316
290	6.176	200.75	f=0.0498	96.2623	97.8105
291	6.1837	200.5	f=0.0006	-0.1715	-0.1728
292	6.1889	200.33	f=0.0036	0.6385	0.1322
293	6.1961	200.1	f=0.0018	4.1869	4.1369

294	6.1966	200.08	f=0.0146	-9.7303	-9.7292
295	6.2075	199.73	f=0.0071	2.428	2.5538
296	6.2095	199.67	f=0.0480	-1.375	-1.3622
297	6.2164	199.45	f=0.0538	40.6174	43.5644
298	6.2219	199.27	f=0.0049	11.7454	11.4623
299	6.2289	199.05	f=0.0082	7.9785	7.8392
300	6.2356	198.83	f=0.0284	-26.2911	-24.8115
301	6.2371	198.79	f=0.0156	23.4094	22.9722
302	6.242	198.63	f=0.0002	-0.0088	0.0215
303	6.2435	198.58	f=0.0023	3.3107	2.9275
304	6.2504	198.36	f=0.0039	5.2745	4.8495
305	6.2541	198.25	f=0.0108	5.3305	5.9872
306	6.2576	198.13	f=0.0445	28.9896	30.321
307	6.2615	198.01	f=0.0148	63.8939	66.0068
308	6.2732	197.64	f=0.0048	-3.5474	-3.7303
309	6.2739	197.62	f=0.0085	9.755	10.1434
310	6.278	197.49	f=0.0076	4.7833	4.1343
311	6.2853	197.26	f=0.0144	7.3373	7.2497
312	6.2892	197.14	f=0.0163	35.2398	35.8589
313	6.293	197.02	f=0.0254	-0.5082	0.4553
314	6.2987	196.84	f=0.0063	-0.3974	-0.5998
315	6.3047	196.65	f=0.0005	-0.4184	-0.434
316	6.3152	196.33	f=0.0040	2.6373	2.5505
317	6.3191	196.2	f=0.0002	1.5233	1.8027
318	6.3322	195.8	f=0.0094	8.7016	8.001
319	6.3339	195.75	f=0.0037	2.8171	2.9369
320	6.341	195.53	f=0.0005	-2.3903	-2.2195
321	6.3437	195.44	f=0.0036	12.5975	13.3894
322	6.3528	195.16	f=0.0085	-0.2155	-1.171
323	6.3684	194.69	f=0.0073	-19.6198	-18.0181
324	6.3734	194.53	f=0.0160	-9.7323	-9.6617
325	6.3749	194.49	f=0.0190	43.7226	52.2627
326	6.3774	194.41	f=0.0020	-9.3074	-9.5825
327	6.3782	194.39	f=0.0004	1.3527	1.5486
328	6.3871	194.12	f=0.0243	-50.3877	-50.6239
329	6.3922	193.96	f=0.0003	0.2713	0.3798
330	6.393	193.94	f=0.0013	-5.1203	-4.4566
331	6.396	193.85	f=0.0085	-2.9172	-2.7133
332	6.399	193.76	f=0.0005	0.2449	0.2432
333	6.4012	193.69	f=0.0032	-11.8971	-12.0322
334	6.4024	193.65	f=0.0083	-15.1067	-15.5844
335	6.4117	193.37	f=0.0239	23.0186	18.8241
336	6.4161	193.24	f=0.0076	-19.2134	-19.3487
337	6.4204	193.11	f=0.0046	10.1028	10.9545
338	6.4229	193.04	f=0.0063	1.4542	1.6841
339	6.4235	193.02	f=0.0039	11.2708	11.0467
340	6.4269	192.91	f=0.0043	-14.2427	-17.2922
341	6.428	192.88	f=0.0051	11.0173	12.0078
342	6.43	192.82	f=0.0162	40.1957	41.166
343	6.434	192.7	f=0.0292	-8.6518	-9.5376

344	6.4441	192.4	f=0.0322	-14.6711	-15.7858
345	6.4463	192.33	f=0.0052	-1.2129	-1.1008
346	6.4494	192.24	f=0.0106	20.6124	21.7177
347	6.4505	192.21	f=0.0027	-5.9313	-5.0819
348	6.4552	192.07	f=0.0044	9.5035	9.6541
349	6.4587	191.96	f=0.0033	7.881	5.7805
350	6.4606	191.91	f=0.0082	0.6112	0.2612
351	6.4633	191.83	f=0.0092	-11.7897	-12.2229
352	6.4649	191.78	f=0.0309	40.589	40.881
353	6.467	191.72	f=0.0162	28.9496	28.6508
354	6.4699	191.63	f=0.0103	5.3953	6.4107
355	6.4842	191.21	f=0.0073	2.4146	1.0248
356	6.4882	191.09	f=0.0112	9.3299	10.1694
357	6.4961	190.86	f=0.0306	9.6449	9.9106
358	6.499	190.77	f=0.0050	16.8097	15.5522
359	6.5055	190.58	f=0.0320	6.1241	10.9139
360	6.5137	190.34	f=0.0362	56.2507	55.025
361	6.5155	190.29	f=0.0079	-11.9312	-13.1873
362	6.5164	190.27	f=0.0099	15.4219	14.6863
363	6.5198	190.16	f=0.0107	-24.4156	-23.8736
364	6.5211	190.13	f=0.0166	-17.4717	-16.1376
365	6.5222	190.1	f=0.0023	1.6158	-0.0993
366	6.5278	189.93	f=0.0044	14.0304	14.0594
367	6.5335	189.77	f=0.0186	-1.8311	-1.4402
368	6.5369	189.67	f=0.0065	-3.7284	-4.6629
369	6.5395	189.59	f=0.0162	3.491	3.6216
370	6.5502	189.28	f=0.0025	2.8417	2.5433
371	6.5527	189.21	f=0.0011	-2.9587	-3.3944
372	6.5539	189.18	f=0.0012	-3.4472	-3.6242
373	6.5564	189.1	f=0.0076	0.3573	0.4513
374	6.5599	189	f=0.0065	2.8367	3.6895
375	6.5627	188.92	f=0.0052	1.3478	1.1793
376	6.5731	188.62	f=0.0069	19.5092	22.4728
377	6.5785	188.47	f=0.0057	1.5816	1.8411
378	6.58	188.43	f=0.0294	2.0045	0.9195
379	6.5816	188.38	f=0.0080	-8.1474	-8.0766
380	6.5902	188.13	f=0.0091	-6.4026	-6.3712
381	6.592	188.08	f=0.0012	-0.1427	-0.1265
382	6.5957	187.98	f=0.0035	2.7139	3.1679
383	6.5992	187.88	f=0.0006	1.0618	1.2327
384	6.6014	187.82	f=0.0003	0.271	0.1622
385	6.6024	187.79	f=0.0019	6.2566	6.012
386	6.6049	187.72	f=0.0047	2.4278	2.2958
387	6.6063	187.68	f=0.0029	1.0908	1.2947
388	6.6102	187.57	f=0.0004	-0.121	-0.0831
389	6.6138	187.46	f=0.0013	-2.0882	-2.0281
390	6.6153	187.42	f=0.0030	8.9637	9.3809
391	6.6212	187.25	f=0.0030	-2.1496	-2.6728
392	6.6276	187.07	f=0.0211	22.6172	22.5646
393	6.6293	187.02	f=0.0014	-1.5223	-1.836

394	6.633	186.92	f=0.0017	-1.8901	-1.9229
395	6.6351	186.86	f=0.0010	-2.4589	-3.0062
396	6.6368	186.81	f=0.0015	0.7262	0.6753
397	6.645	186.58	f=0.0001	0.8645	1.1323
398	6.647	186.53	f=0.0037	4.8279	5.1239
399	6.6538	186.34	f=0.0142	29.5831	28.3248
400	6.655	186.3	f=0.0203	-0.06	0.3914
401	6.6589	186.19	f=0.0020	-2.0418	-1.8148
402	6.6618	186.11	f=0.0246	-21.8741	-23.6121
403	6.6638	186.06	f=0.0097	11.3472	11.0172
404	6.6671	185.96	f=0.0036	8.3661	7.8888
405	6.6737	185.78	f=0.0121	21.3374	19.4439
406	6.6762	185.71	f=0.0283	95.3077	96.6279
407	6.6842	185.49	f=0.0030	-13.1295	-14.5891
408	6.6861	185.44	f=0.0034	3.1865	2.0348
409	6.6893	185.35	f=0.0266	11.6858	11.8767
410	6.6914	185.29	f=0.0128	12.2167	12.2628
411	6.6932	185.24	f=0.0084	5.9315	5.5666
412	6.6951	185.19	f=0.0235	22.6965	21.9184
413	6.6967	185.14	f=0.0047	12.3112	12.4954
414	6.6973	185.13	f=0.0050	7.452	7.6421
415	6.7009	185.03	f=0.0144	18.7961	18.6755
416	6.7042	184.93	f=0.0004	0.4537	0.4461
417	6.7112	184.74	f=0.0069	-5.6835	-5.6984
418	6.7179	184.56	f=0.0018	3.2048	3.3613
419	6.7183	184.55	f=0.0009	-1.3723	-0.7652
420	6.7212	184.47	f=0.0006	-0.3265	-0.3564
421	6.723	184.42	f=0.0006	0.0914	0.1556
422	6.7245	184.38	f=0.0061	18.4225	16.9068
423	6.7257	184.34	f=0.0023	-2.3669	-2.3413
424	6.7266	184.32	f=0.0016	-1.5667	-1.7519
425	6.7268	184.31	f=0.0014	-1.6856	-1.7564
426	6.7309	184.2	f=0.0268	32.299	32.4207
427	6.7483	183.73	f=0.0026	6.7476	7.1172
428	6.7489	183.71	f=0.0139	-7.1294	-7.1432
429	6.7513	183.64	f=0.0044	2.8815	3.1742
430	6.7543	183.56	f=0.0299	51.1767	51.257
431	6.757	183.49	f=0.0096	-8.1495	-8.4129
432	6.7595	183.42	f=0.0052	12.419	11.8037
433	6.7657	183.25	f=0.0014	0.9171	0.8417
434	6.7662	183.24	f=0.0003	-0.4162	-0.5509
435	6.7715	183.1	f=0.0093	2.3775	4.3434
436	6.7775	182.94	f=0.0033	-1.5491	-0.735
437	6.7788	182.9	f=0.0040	1.9146	1.8909
438	6.7809	182.84	f=0.0052	2.1662	1.6607
439	6.786	182.7	f=0.0018	1.1711	1.0871
440	6.7966	182.42	f=0.0045	-1.0357	-1.0333
441	6.7974	182.4	f=0.0110	-5.784	-5.8241
442	6.7995	182.34	f=0.0040	6.5587	6.2558
443	6.8032	182.24	f=0.0033	9.9793	8.5931

444	6.8038	182.23	f=0.0006	0.824	0.7923
445	6.8075	182.13	f=0.0015	1.733	1.7858
446	6.8091	182.09	f=0.0005	-0.9836	-1.1416
447	6.8162	181.9	f=0.0042	13.703	15.8652
448	6.817	181.88	f=0.0134	9.8649	10.2327
449	6.8234	181.7	f=0.0079	-16.5691	-16.7589
450	6.8252	181.66	f=0.0008	-1.4486	-1.3726
451	6.8338	181.43	f=0.0197	-22.5995	-25.3577
452	6.8375	181.33	f=0.0043	3.1658	3.0019
453	6.8479	181.05	f=0.0033	12.9197	10.6678
454	6.8527	180.93	f=0.0111	-9.851	-10.5695
455	6.8642	180.62	f=0.0001	0.3637	0.3036
456	6.8666	180.56	f=0.0071	0.3674	-0.1021
457	6.8688	180.5	f=0.0145	-31.8166	-34.9506
458	6.8733	180.39	f=0.0018	1.0137	1.0278
459	6.8756	180.33	f=0.0034	-1.1393	-1.3819
460	6.8794	180.23	f=0.1478	-49.4579	-49.9896
461	6.8906	179.93	f=0.0111	1.8997	2.5508
462	6.8913	179.91	f=0.0119	-12.7035	-13.5066
463	6.8958	179.8	f=0.0196	-4.7915	-5.7722
464	6.9106	179.41	f=0.0081	-5.7942	-6.1577
465	6.913	179.35	f=0.0121	-2.8259	-2.8907
466	6.9138	179.33	f=0.0031	10.6769	10.0044
467	6.9172	179.24	f=0.0031	-7.7514	-7.9185
468	6.9193	179.18	f=0.0019	-4.0749	-4.6176
469	6.9227	179.1	f=0.0077	8.3977	8.6849
470	6.9254	179.03	f=0.0044	2.9829	2.948
471	6.9302	178.91	f=0.0123	-8.2477	-9.4513
472	6.9346	178.79	f=0.0172	13.6771	12.9056
473	6.9405	178.64	f=0.0050	12.9256	12.5981
474	6.9432	178.57	f=0.0116	12.1362	11.1539
475	6.9441	178.55	f=0.1460	-21.5581	-21.2896
476	6.9513	178.36	f=0.0027	-3.6543	-3.5597
477	6.9529	178.32	f=0.0014	3.8648	3.839
478	6.9545	178.28	f=0.0291	-10.3786	-10.5337
479	6.9607	178.12	f=0.0107	-10.74	-10.8418
480	6.9617	178.1	f=0.0056	-12.4639	-11.0459
481	6.9631	178.06	f=0.0361	34.5384	35.2192
482	6.9708	177.86	f=0.0118	-10.1568	-9.6508
483	6.9752	177.75	f=0.0049	24.2034	21.3751
484	6.9876	177.43	f=0.0142	-10.5912	-11.1985
485	6.9897	177.38	f=0.0007	2.7113	2.6388
486	6.9903	177.37	f=0.0019	1.8266	1.2899
487	6.9952	177.24	f=0.0018	-1.6611	-1.5795
488	6.9961	177.22	f=0.0050	0.8681	0.8843
489	7.0021	177.07	f=0.0027	3.232	3.6507
490	7.0052	176.99	f=0.0016	0.5949	0.5799
491	7.0059	176.97	f=0.0030	1.9185	2.4346
492	7.0155	176.73	f=0.0236	1.1008	-0.2586
493	7.0194	176.63	f=0.0019	2.6291	2.4266

494	7.0218	176.57	f=0.0150	10.5497	9.3575
495	7.0303	176.36	f=0.0084	-5.651	-5.7003
496	7.0365	176.2	f=0.0288	-25.1431	-27.3133
497	7.0411	176.09	f=0.0009	0.2821	0.087
498	7.0448	175.99	f=0.0007	-1.5413	-1.6109
499	7.0464	175.95	f=0.0015	3.4799	3.584
500	7.0575	175.68	f=0.0064	-3.0616	-3.5559

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- 1 The use of a relatively small basis set is dictated by the very large molecular size and by the need to limit the computational work into reasonable times (about 15 days on 8 cores servers). For the same reason we had to avoid to include the presence of the solvent in the calculations.
 - 2 P.J. Stephens, D.M. McCann, F.J. Devlin, J. R. Cheeseman and M.J. Frisch, *J. Am. Chem. Soc.*, 2004, **126**, 7514-7521.
 - 3 Gaussview 4.1.2, Semichem Inc., 2006.