Electronic Supplementary Information

Donor-acceptor type A_2B_2 porphyrins: Synthesis, energy transfer, computational and electrochemical studies

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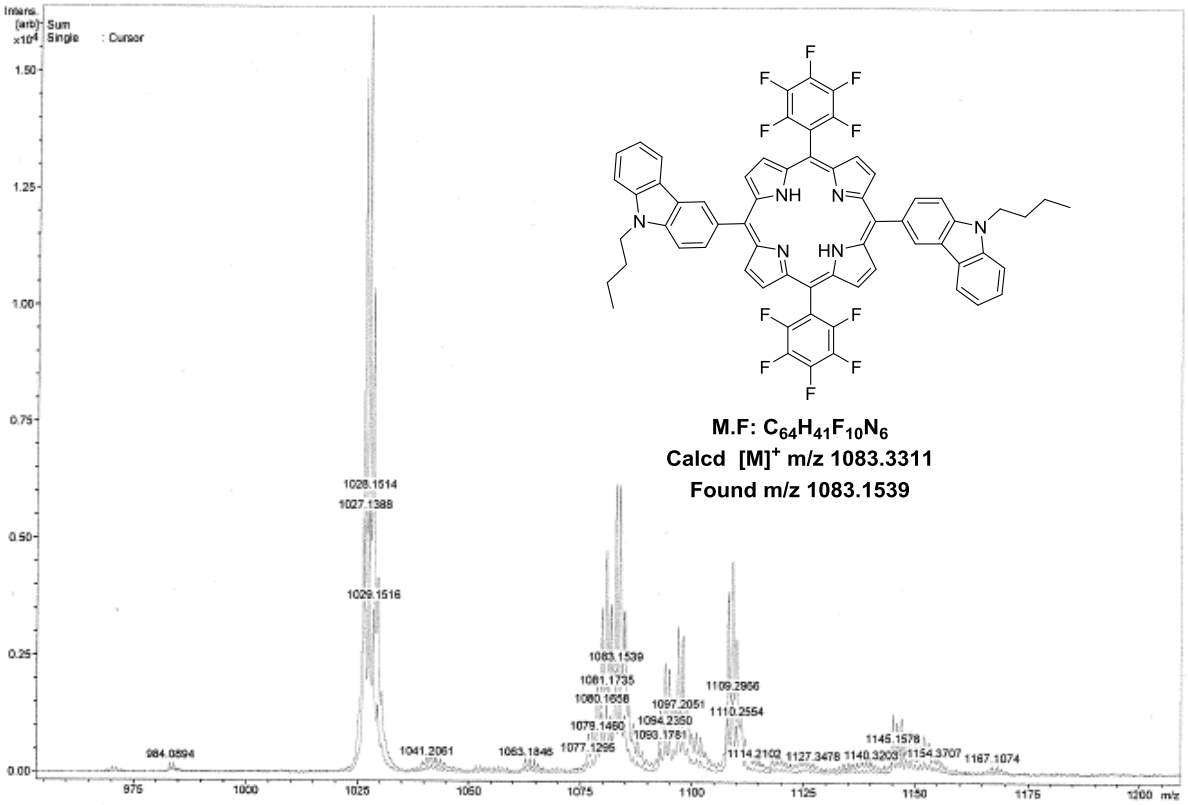


Figure 1. MALDI-MS of compound **5**

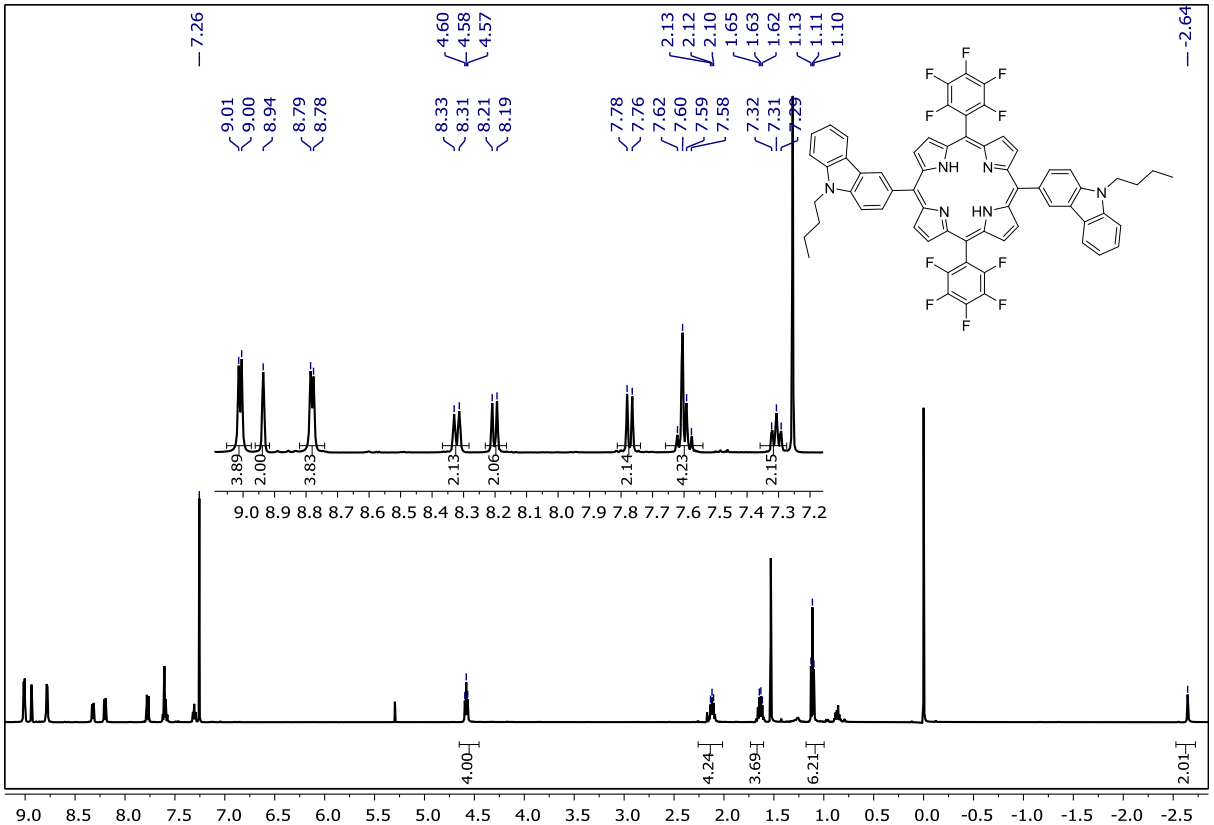


Figure 2. ^{1}H-NMR of compound **5** in $CDCl_3$

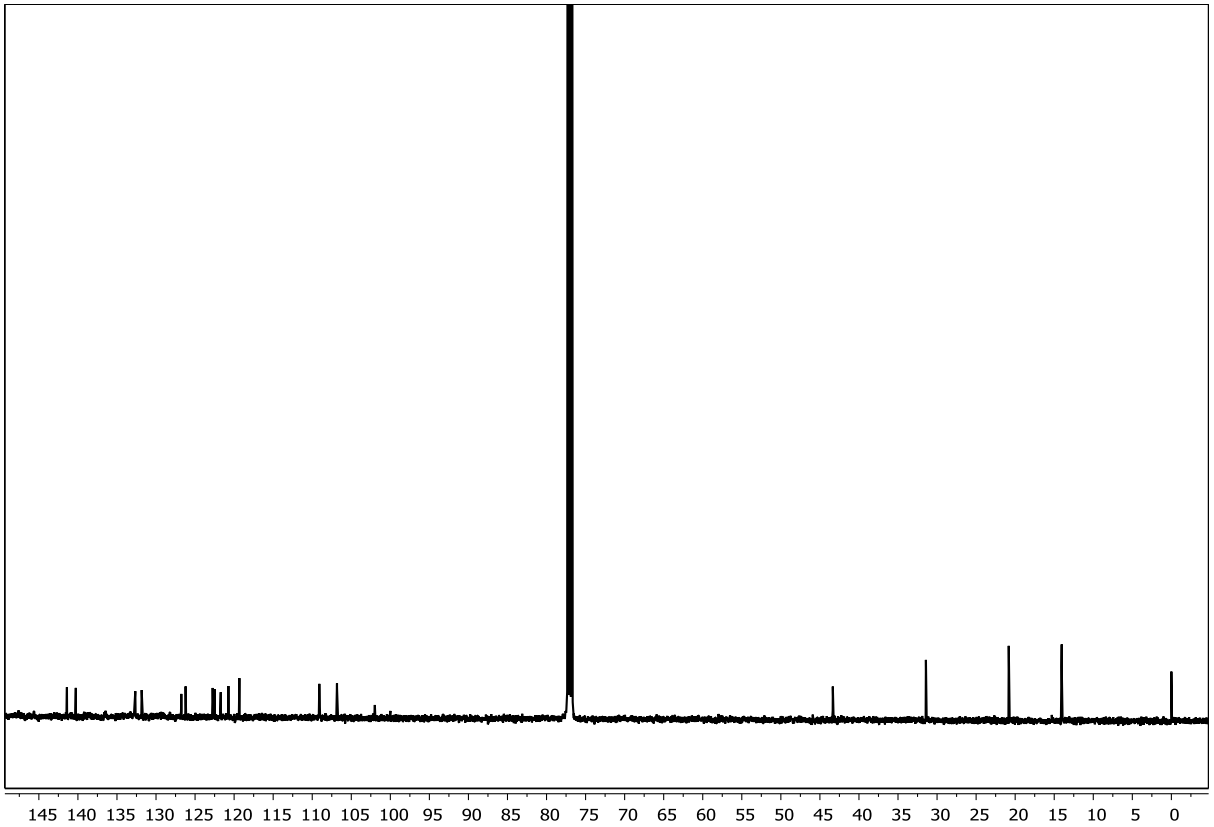


Figure 3. ^{13}C-NMR of compound **5** in $CDCl_3$

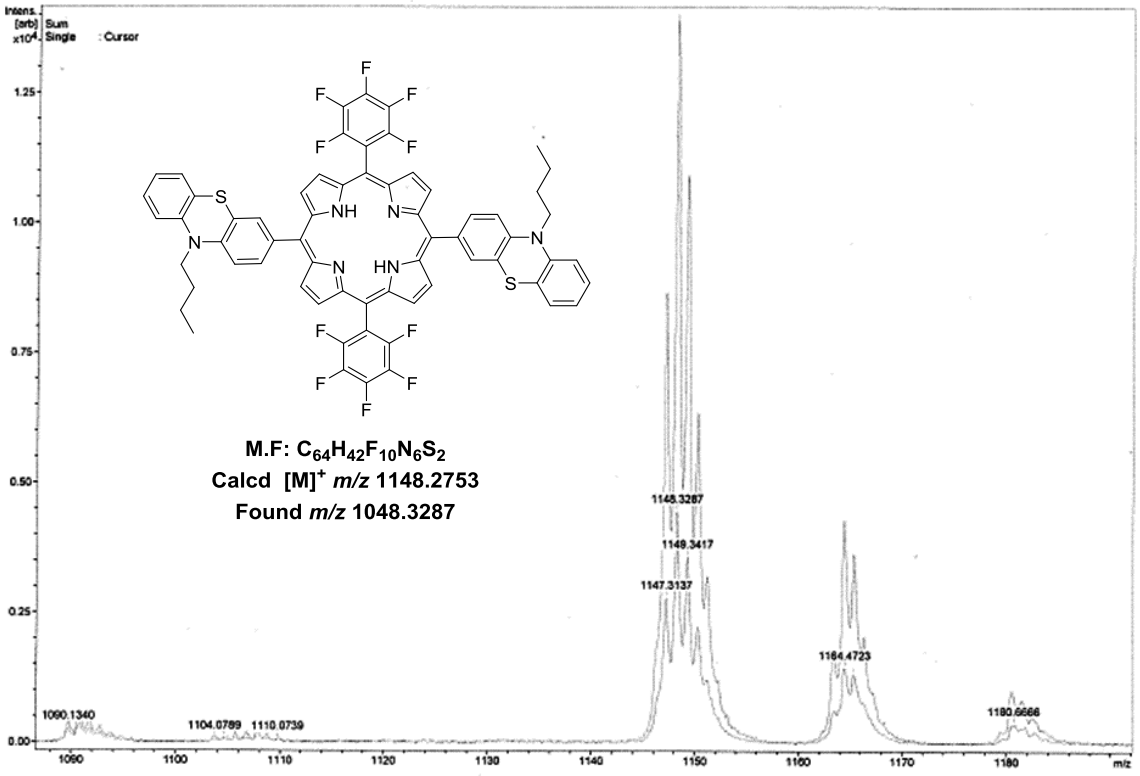


Figure 4. MALDI-MS of compound **6**

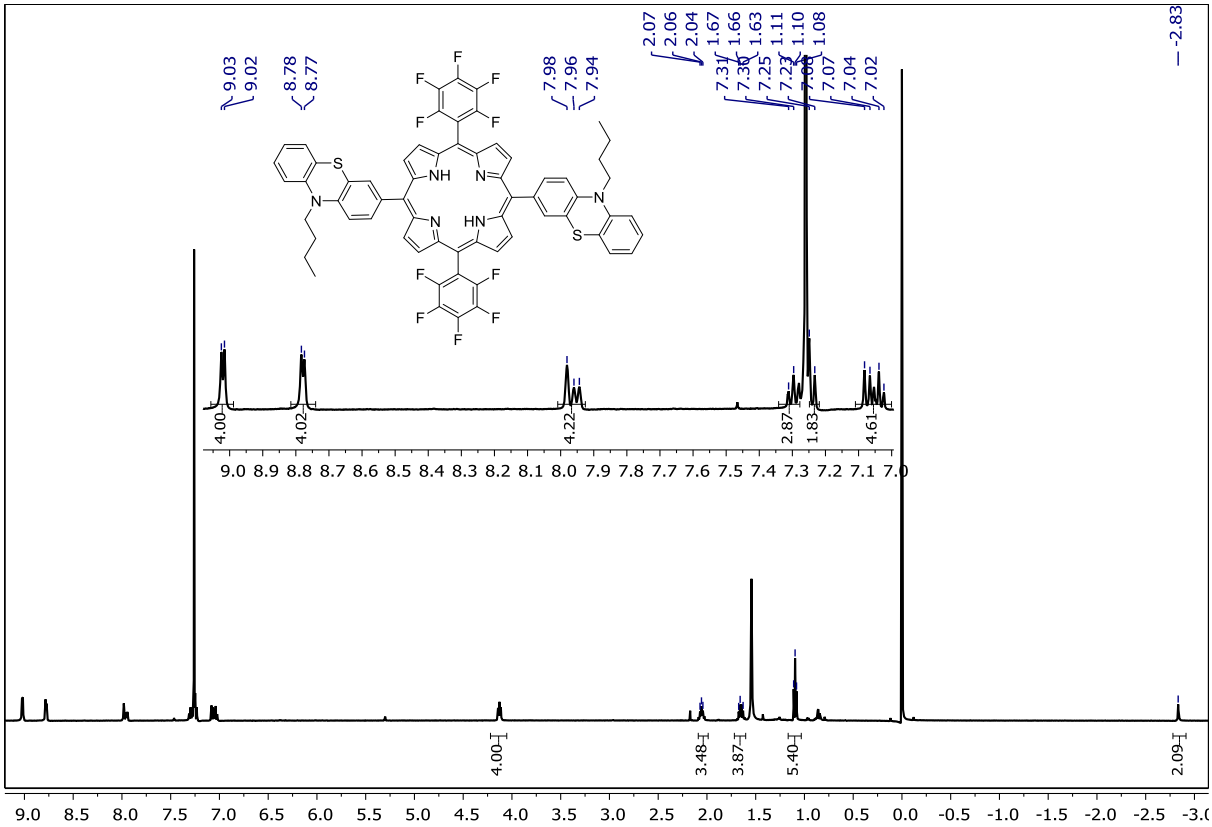


Figure 5. ^{1}H-NMR of compound **6** in $CDCl_3$

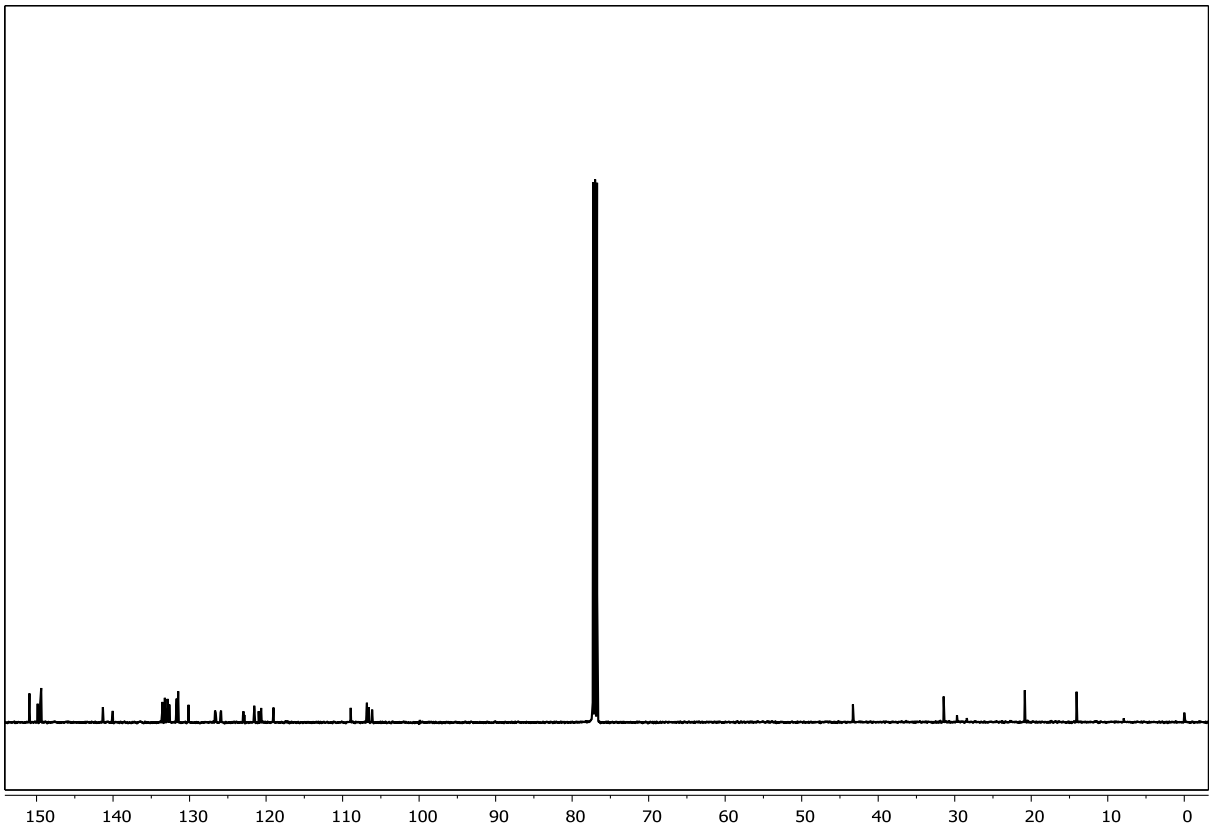


Figure 6. ^{13}C-NMR of compound **6** in $CDCl_3$

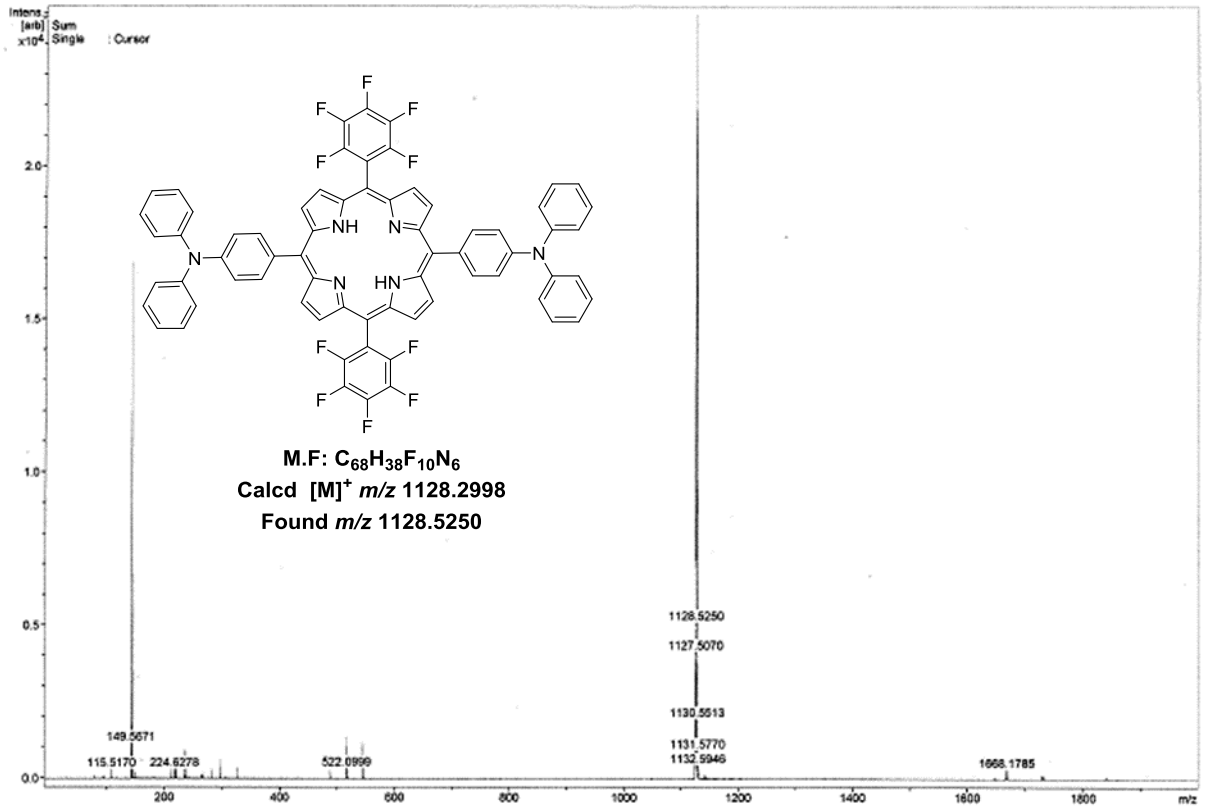


Figure 7. MALDI-MS of compound **7**

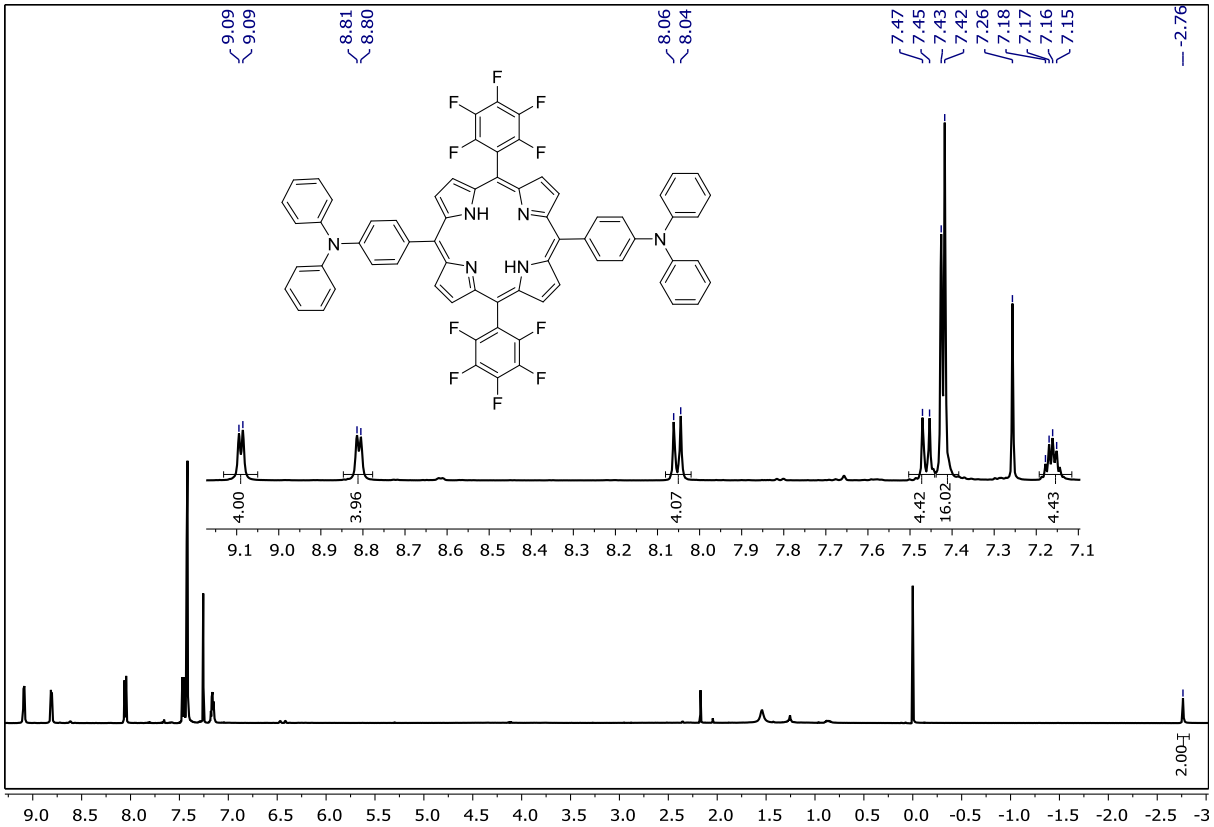


Figure 8. ^{1}H-NMR of compound **7** in $CDCl_3$

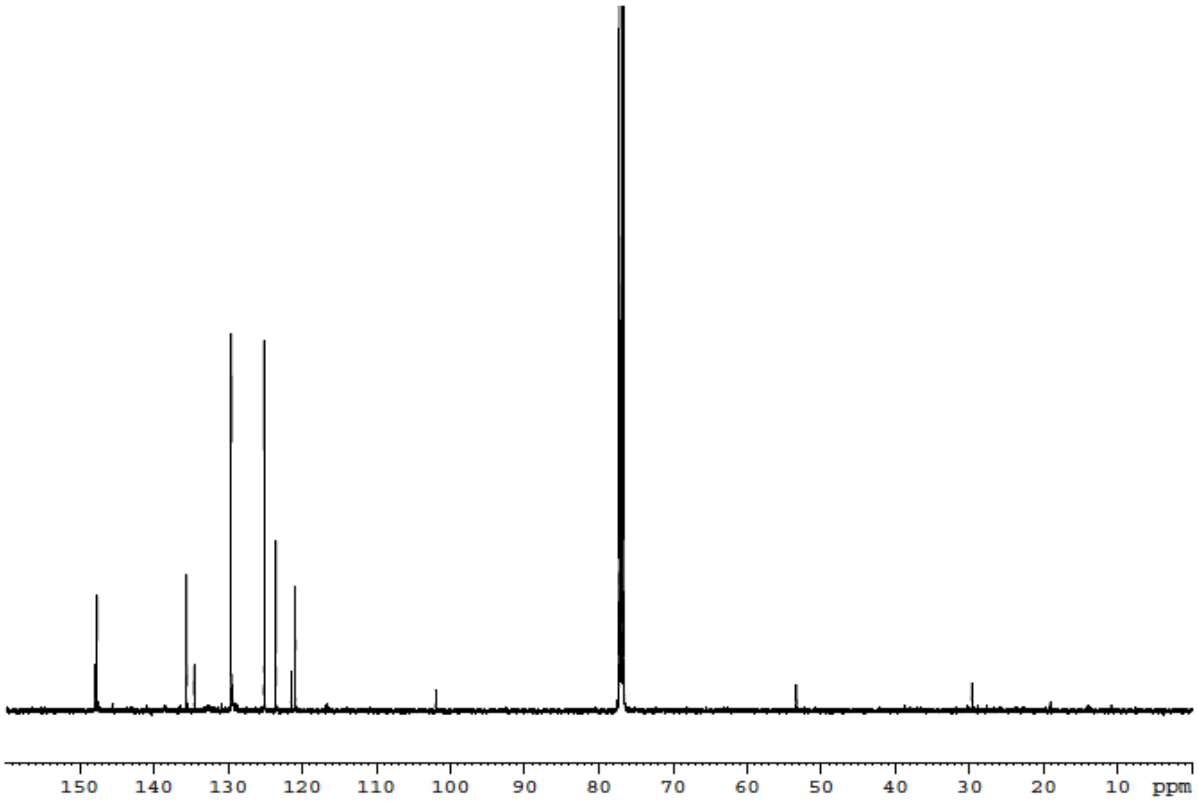


Figure 9. ^{13}C-NMR of compound **7** in $CDCl_3$

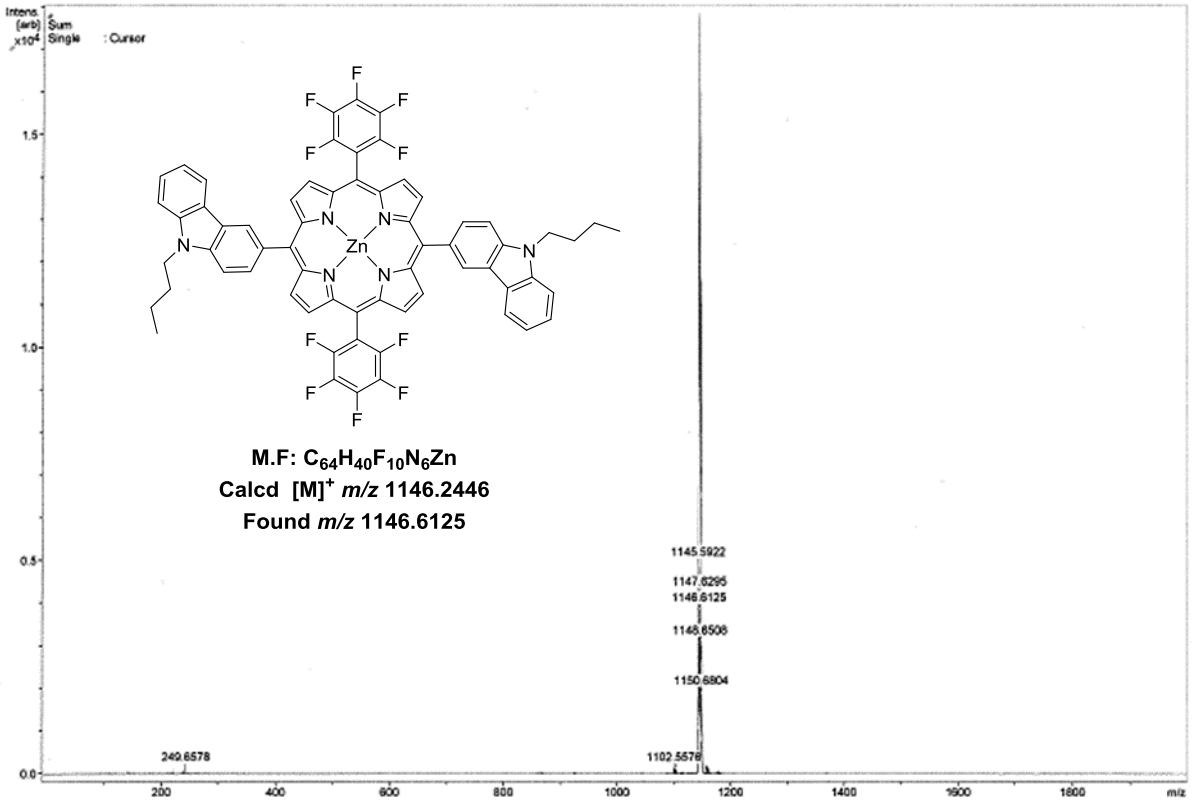


Figure 10. MALDI-MS of compound **8**

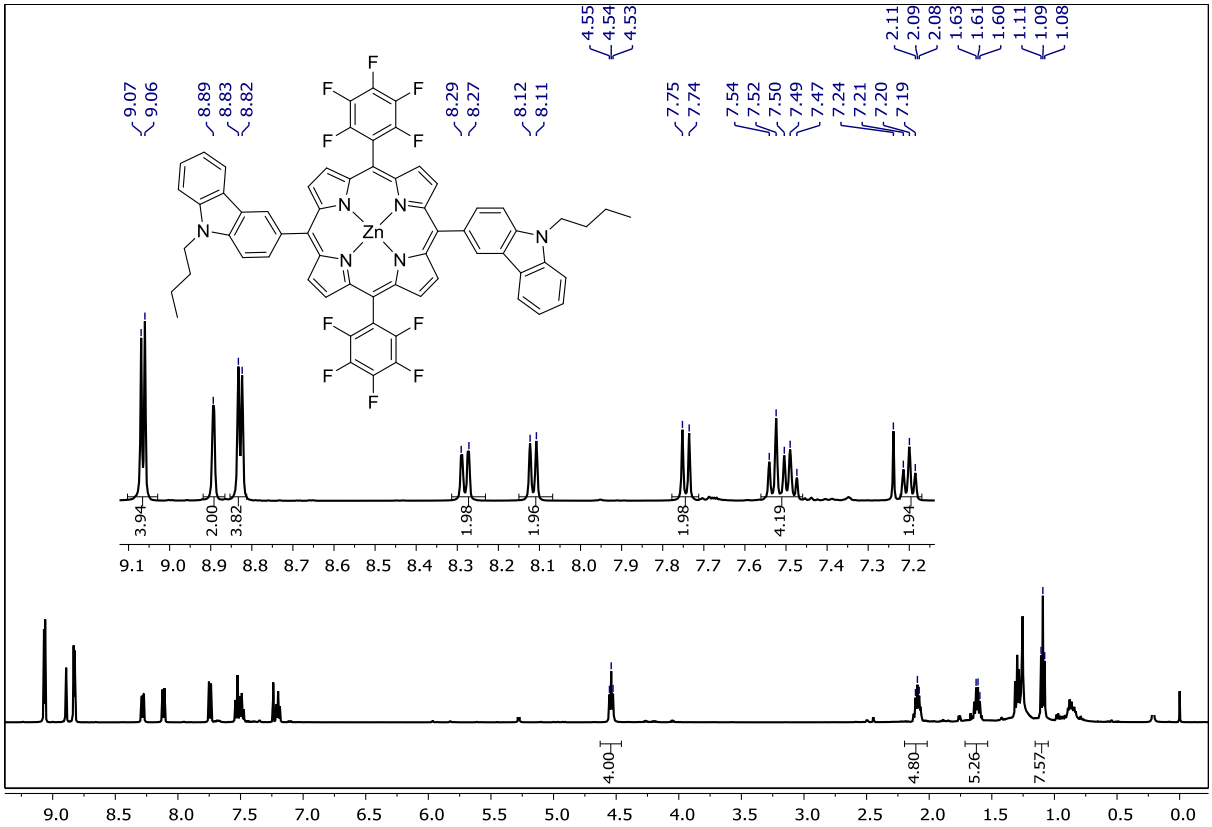


Figure 11. ^{1}H-NMR of compound **8** in $CDCl_3$

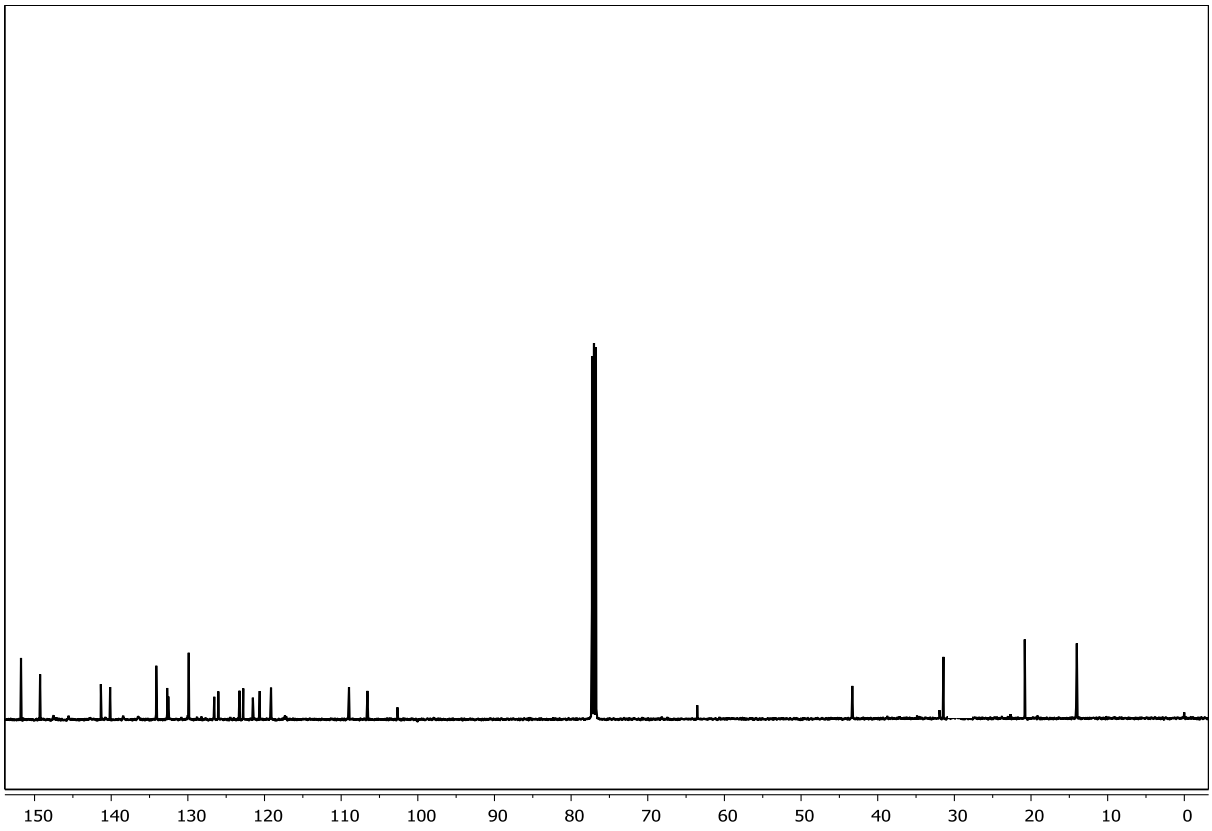


Figure 12. ^{13}C-NMR of compound **8** in $CDCl_3$

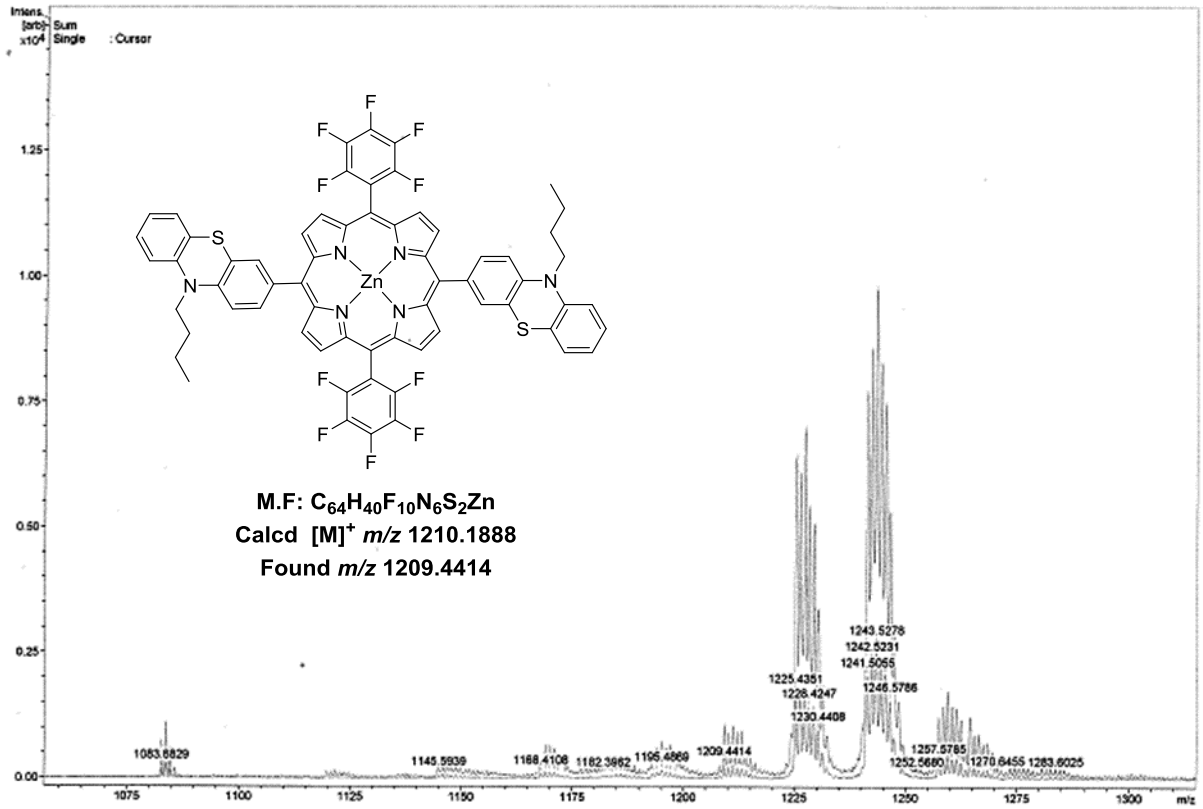


Figure 13. MALDI-MS of compound **9**

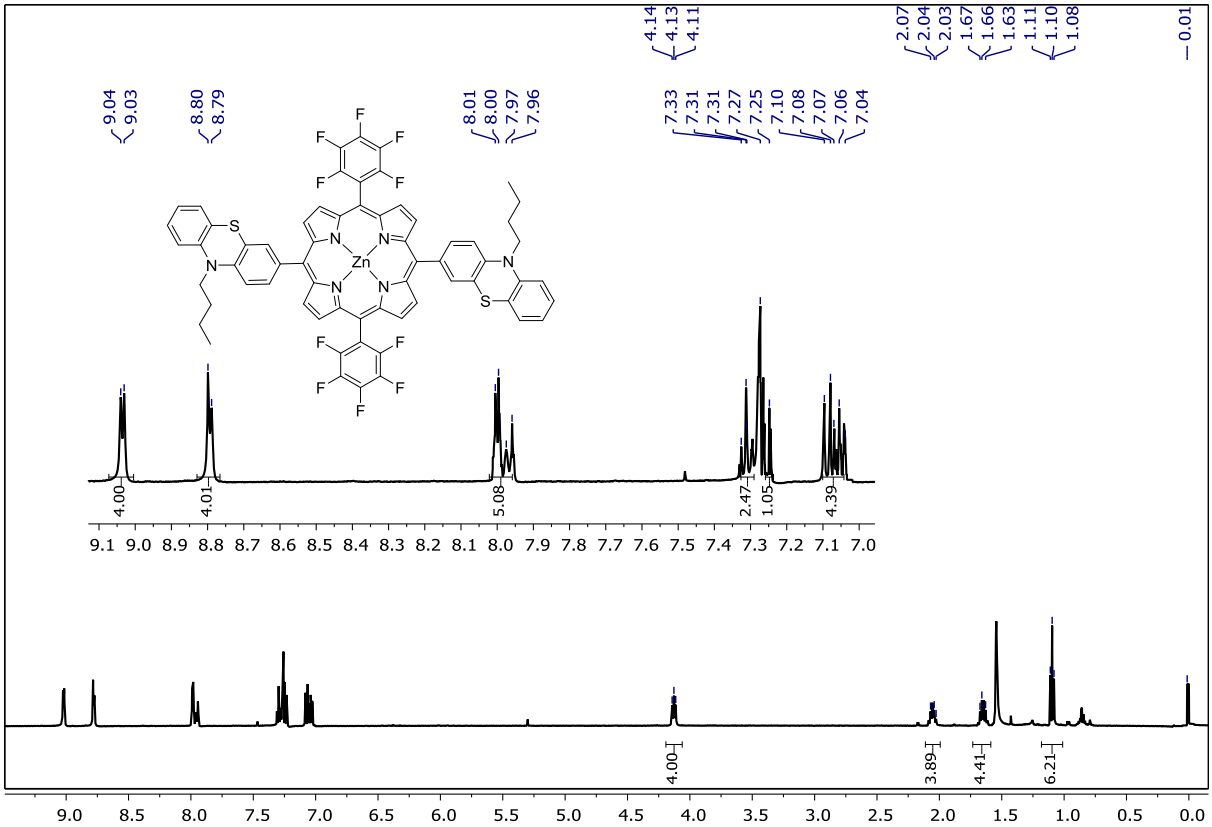


Figure 14. ^{1}H-NMR of compound **9** in $CDCl_3$

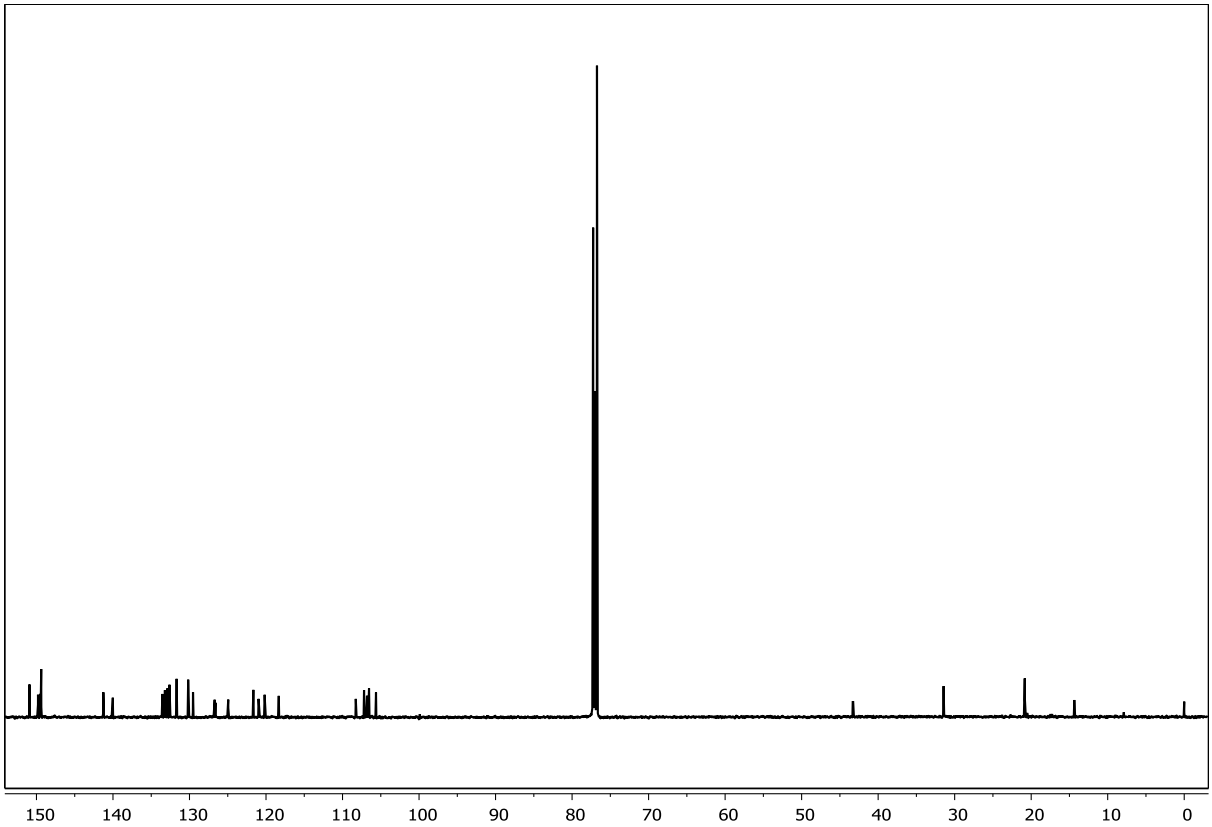


Figure 15. ^{13}C-NMR of compound **9** in $CDCl_3$

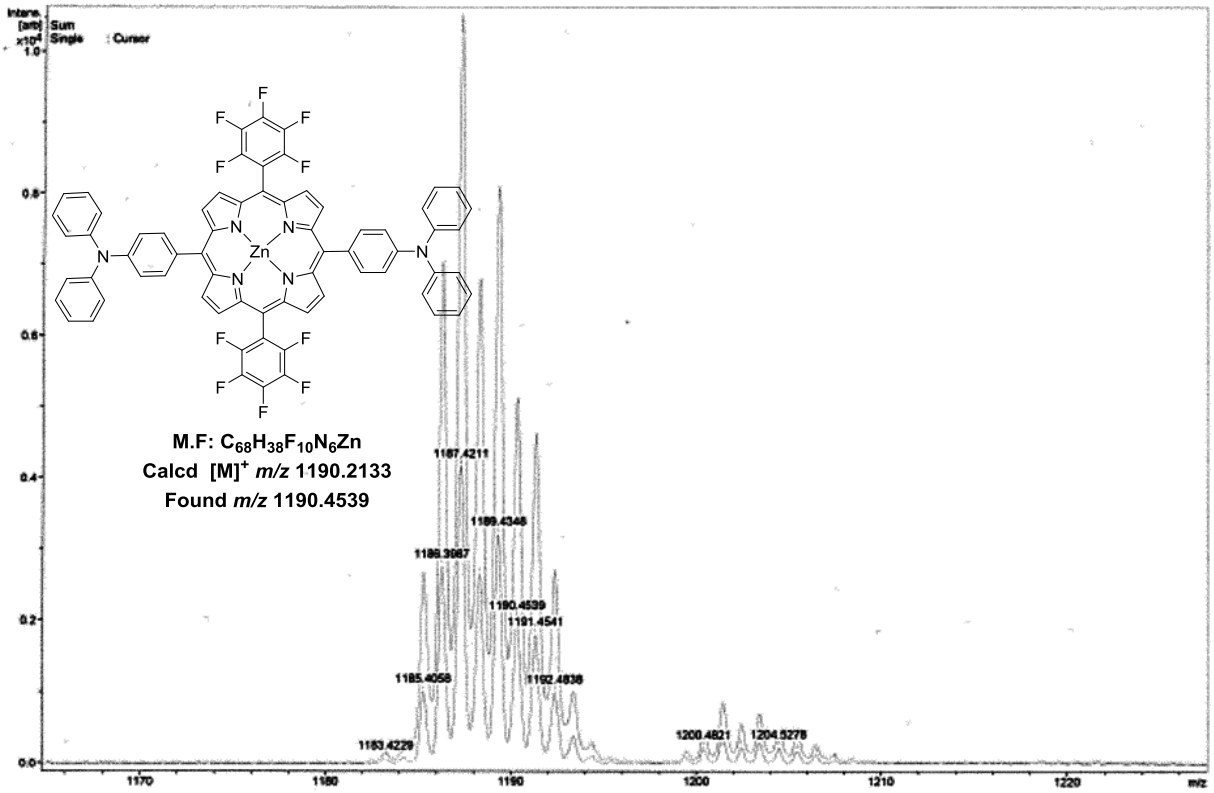


Figure 16. MALDI-MS of compound **10**

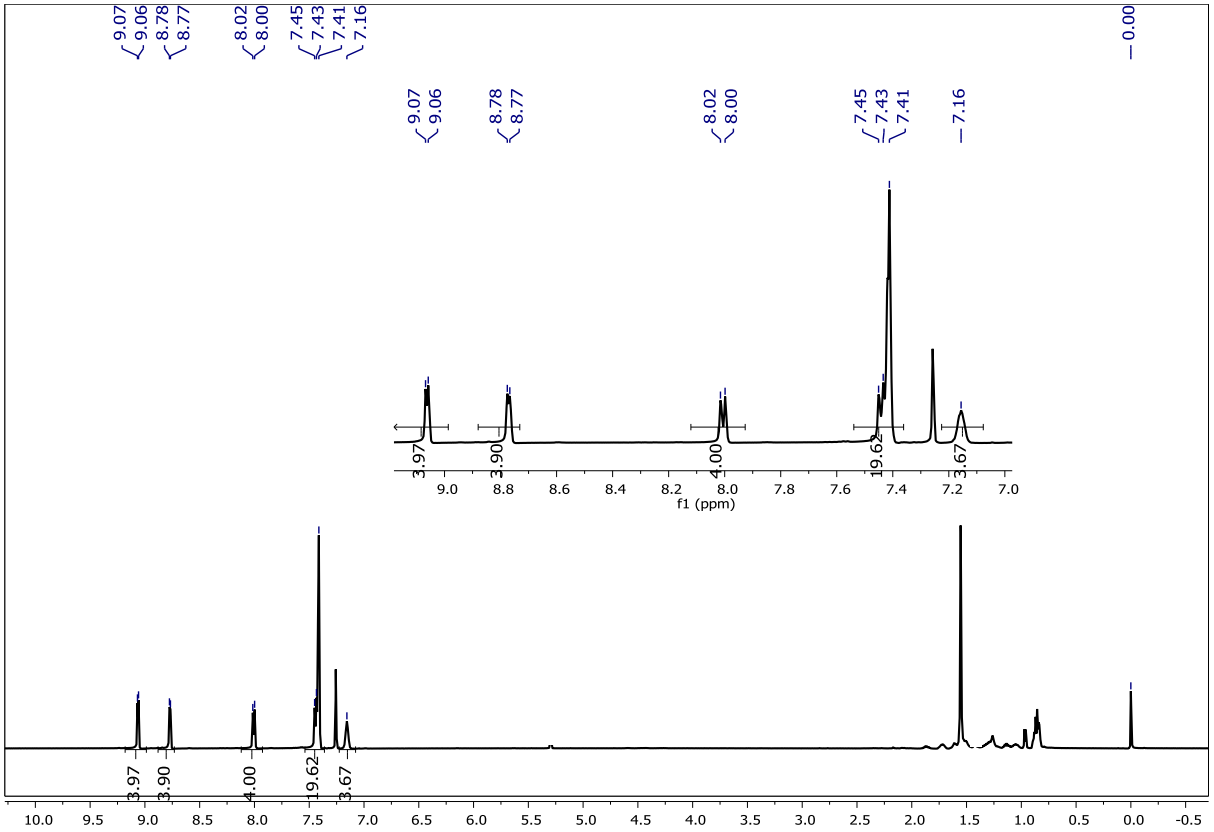


Figure 17. ^{1}H-NMR of compound **10** in $CDCl_3$

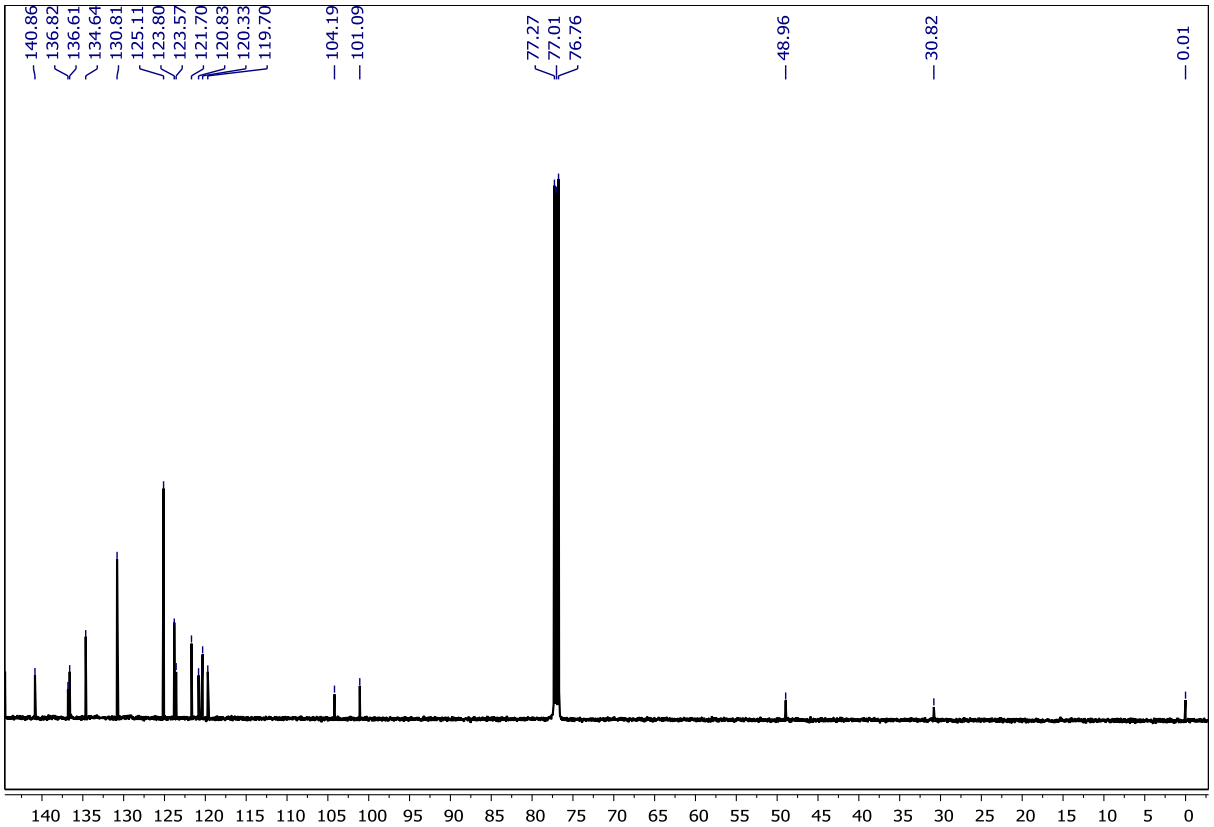


Figure 18. ^{13}C-NMR of compound **10** in $CDCl_3$

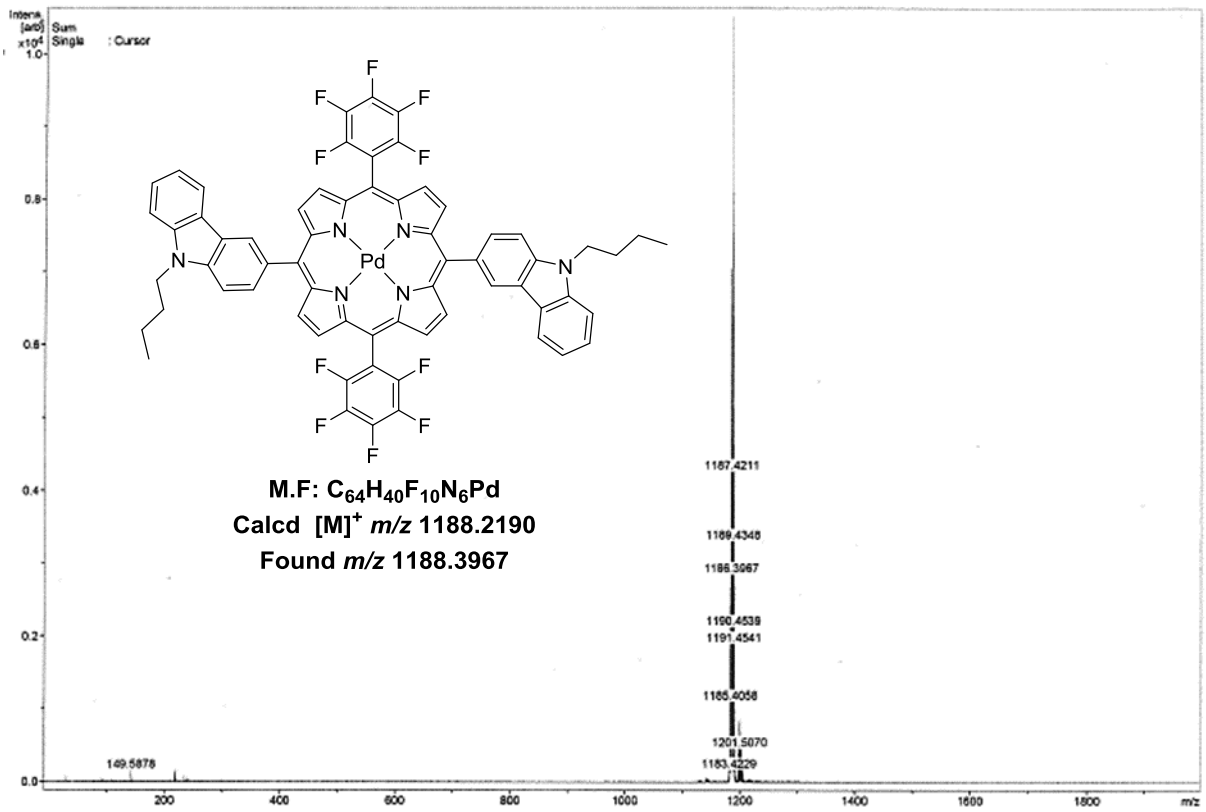


Figure 19. MALDI-MS of compound **11**

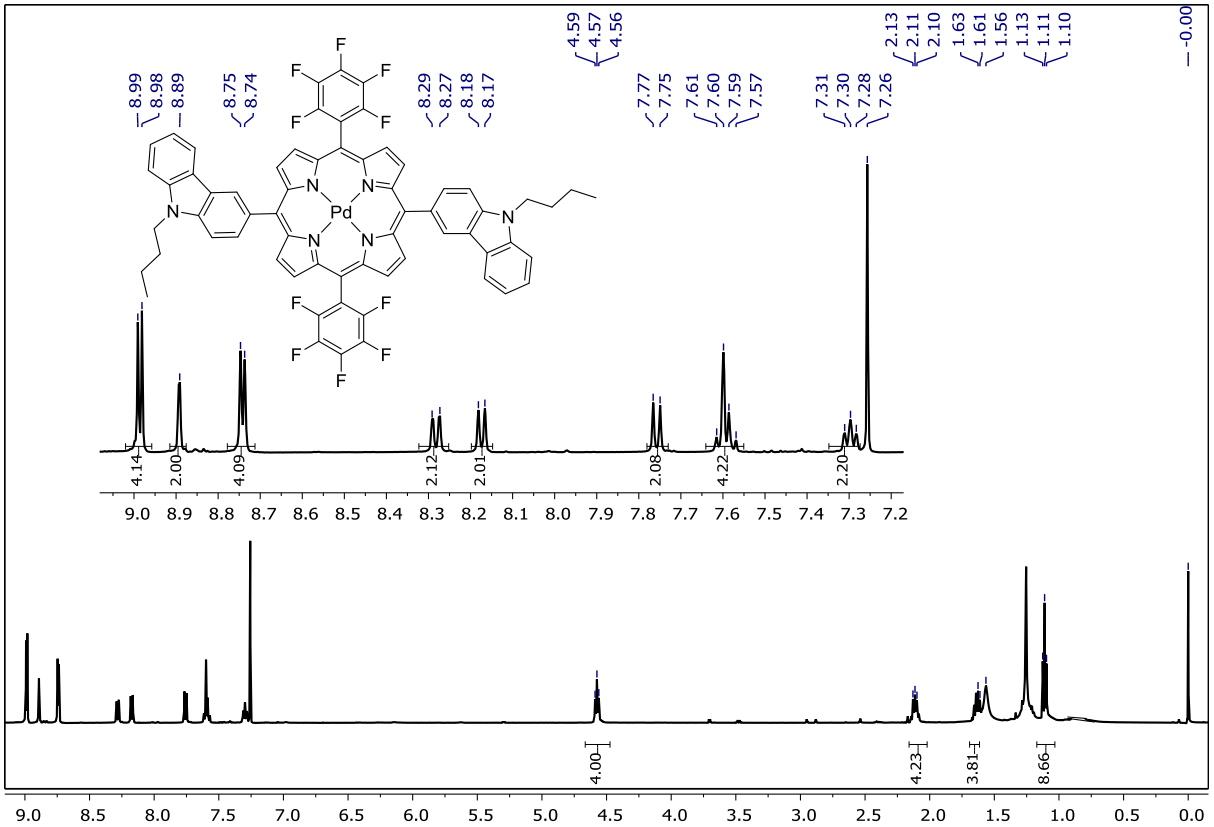


Figure 20. ^{1}H-NMR of compound **11** in $CDCl_3$

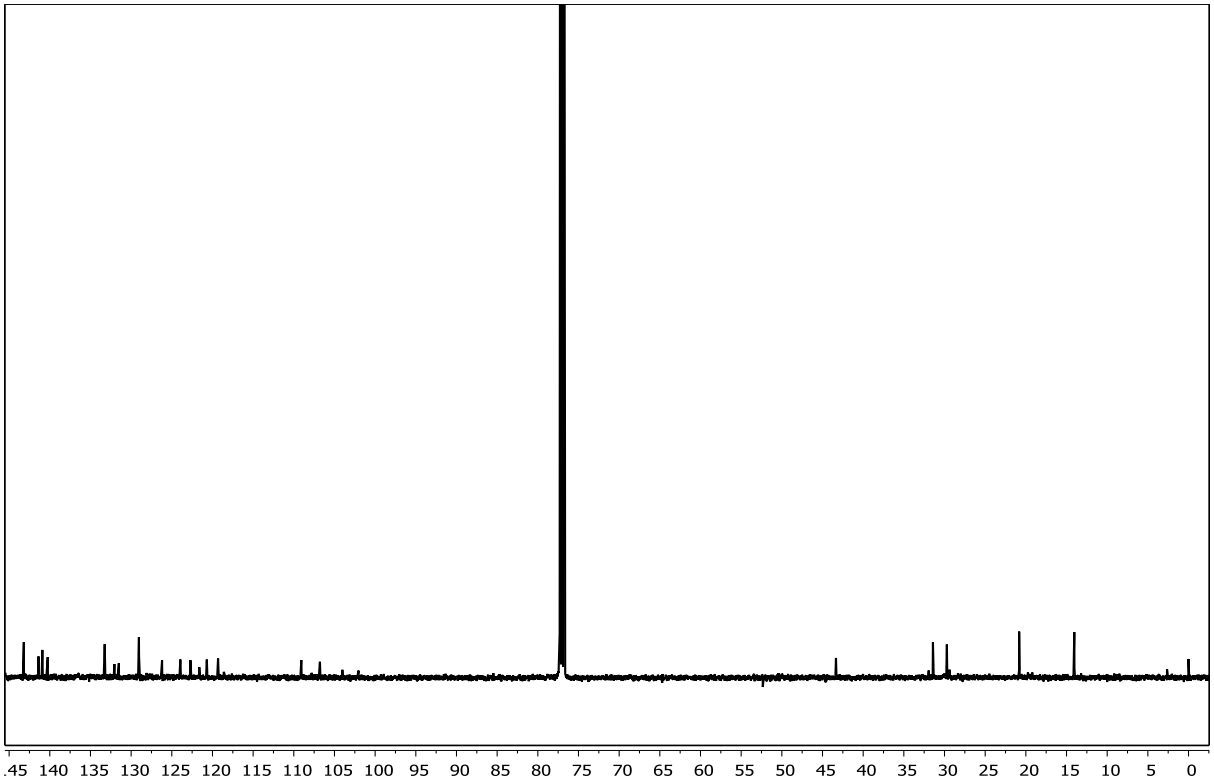


Figure 21. ^{13}C-NMR of compound **11** in $CDCl_3$

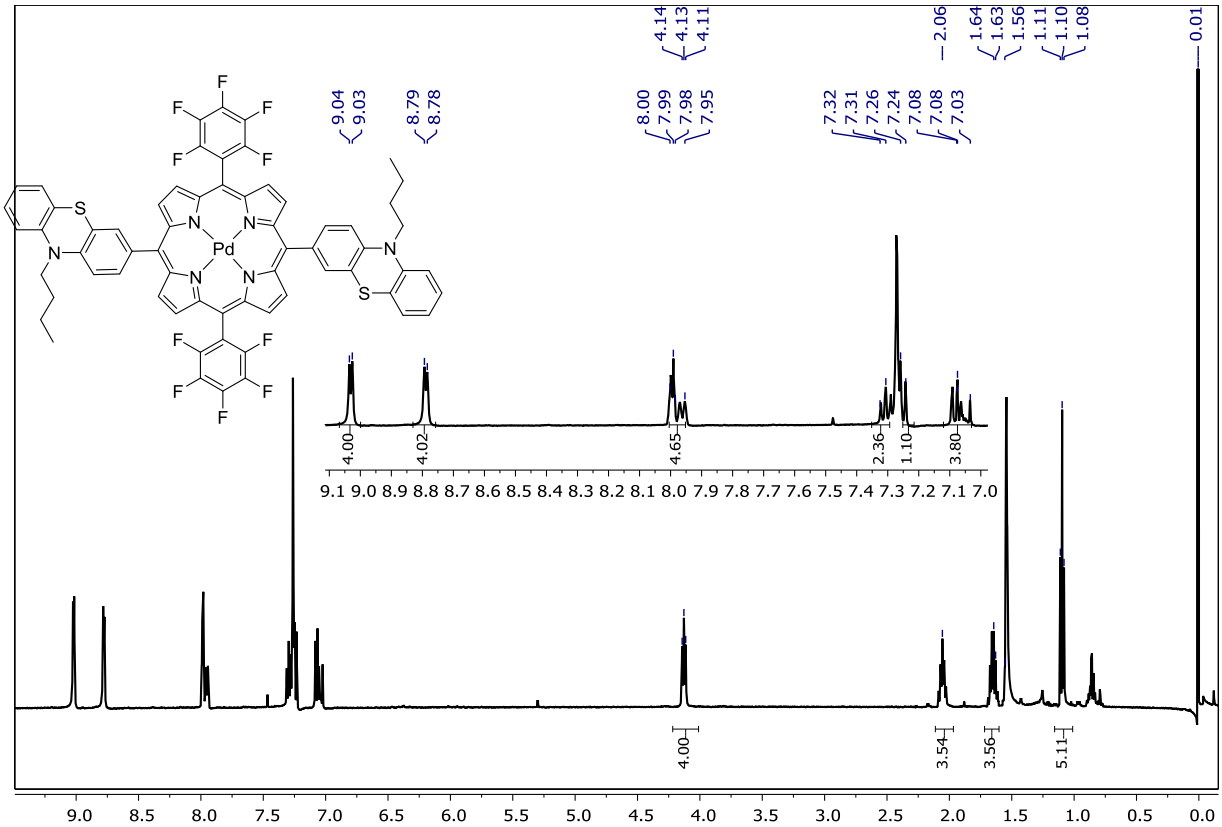


Figure 22. ^{1}H-NMR of compound **12** in $CDCl_3$

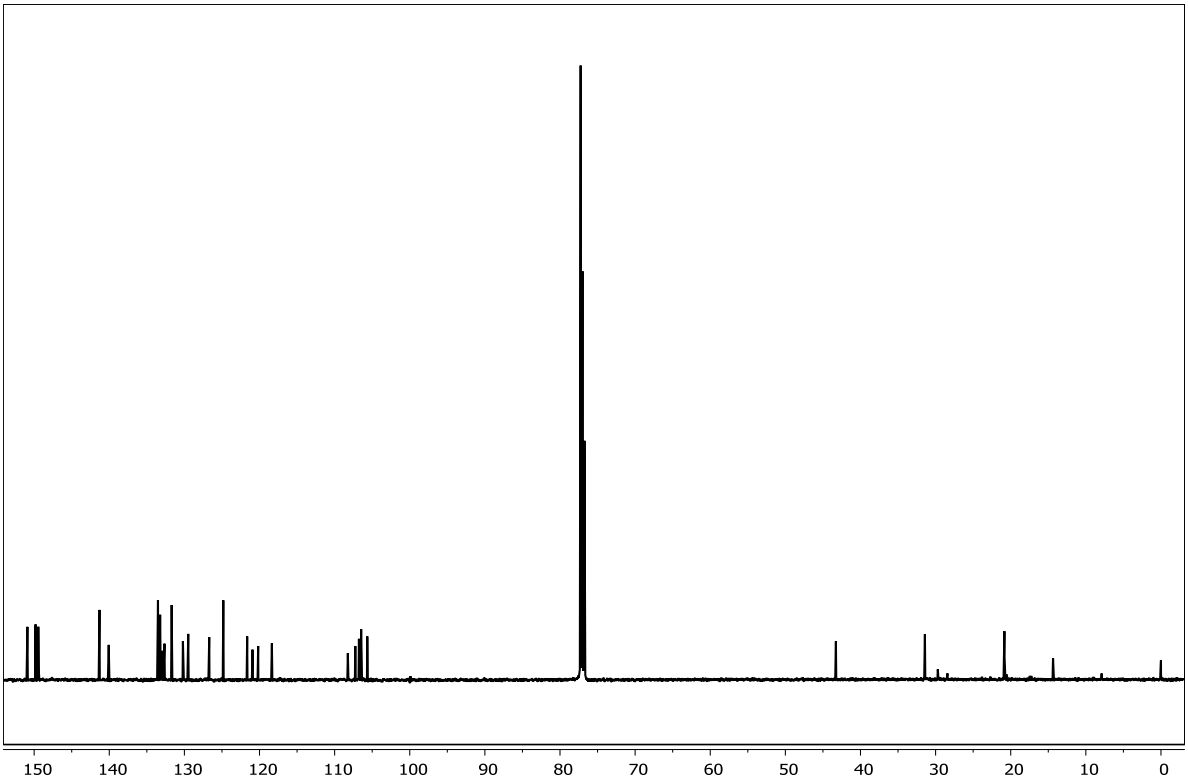


Figure 23. ^{13}C-NMR of compound **12** in $CDCl_3$

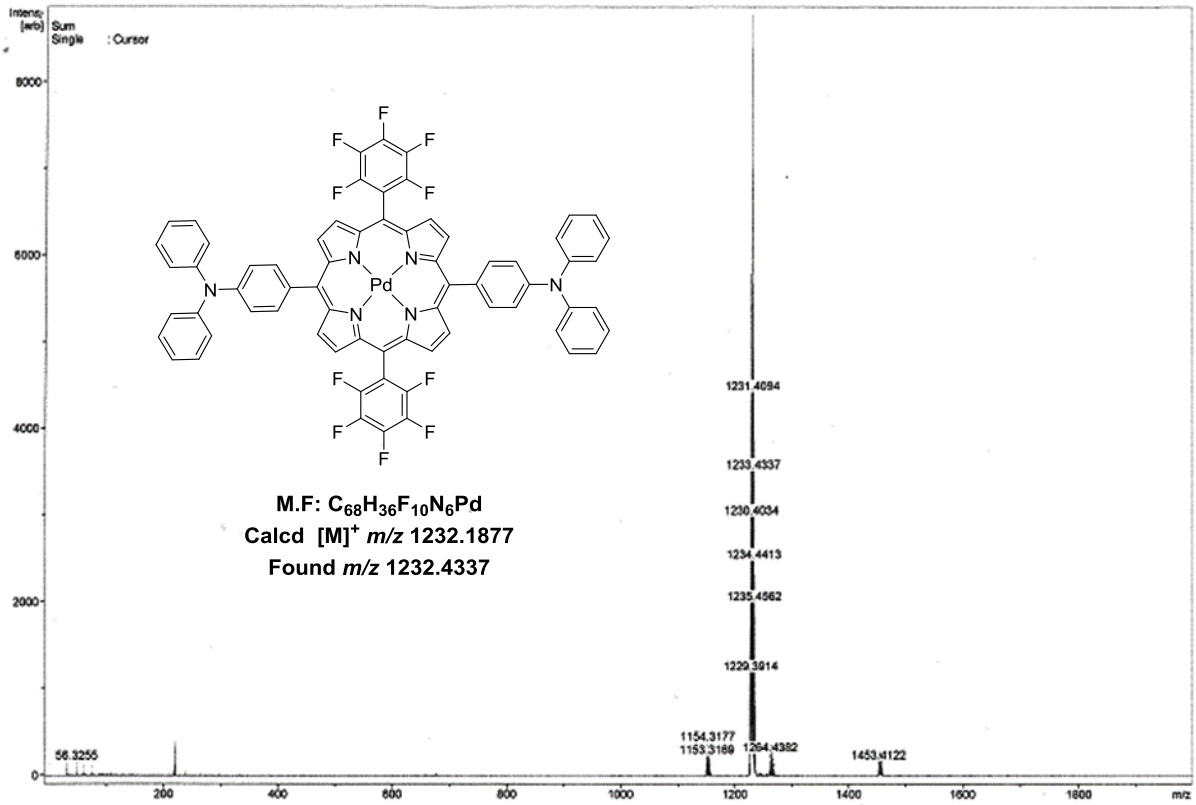


Figure 24. MALDI-MS of compound **13**

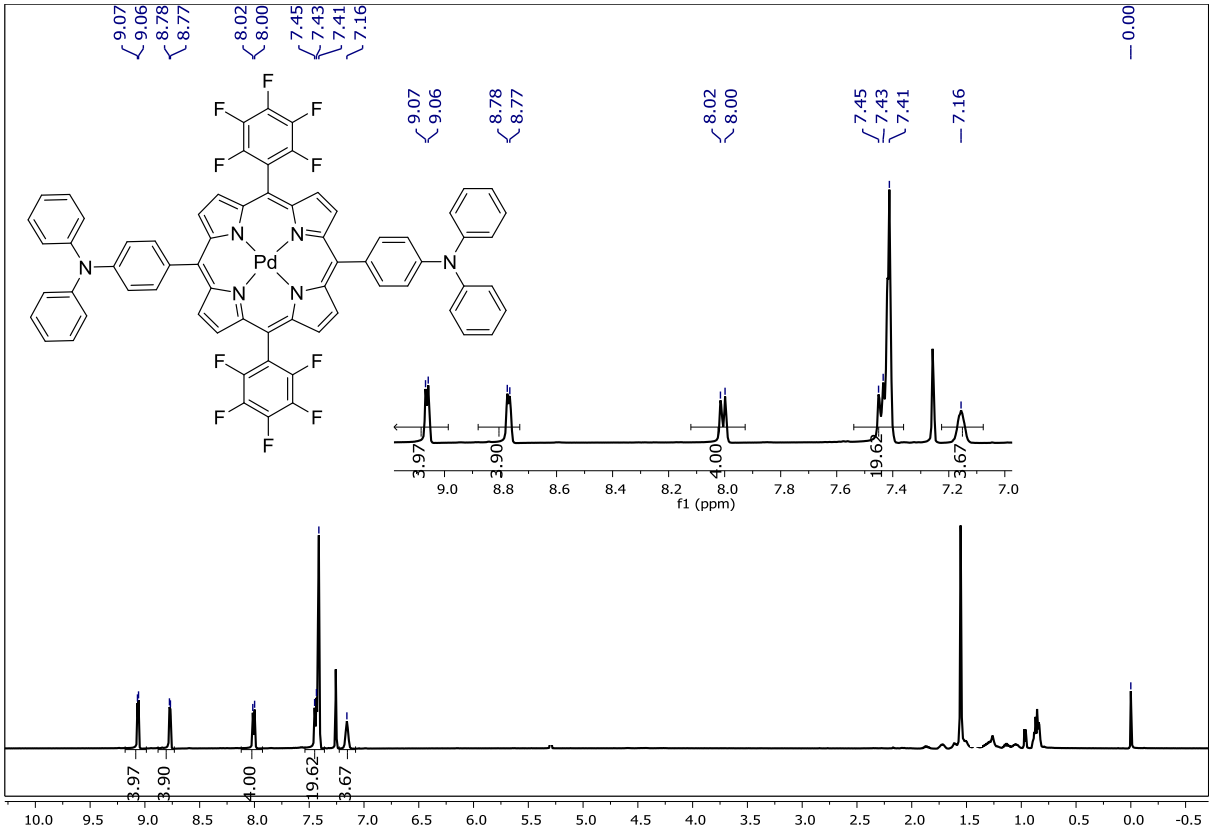


Figure 25. ^{1}H-NMR of compound **13** in $CDCl_3$

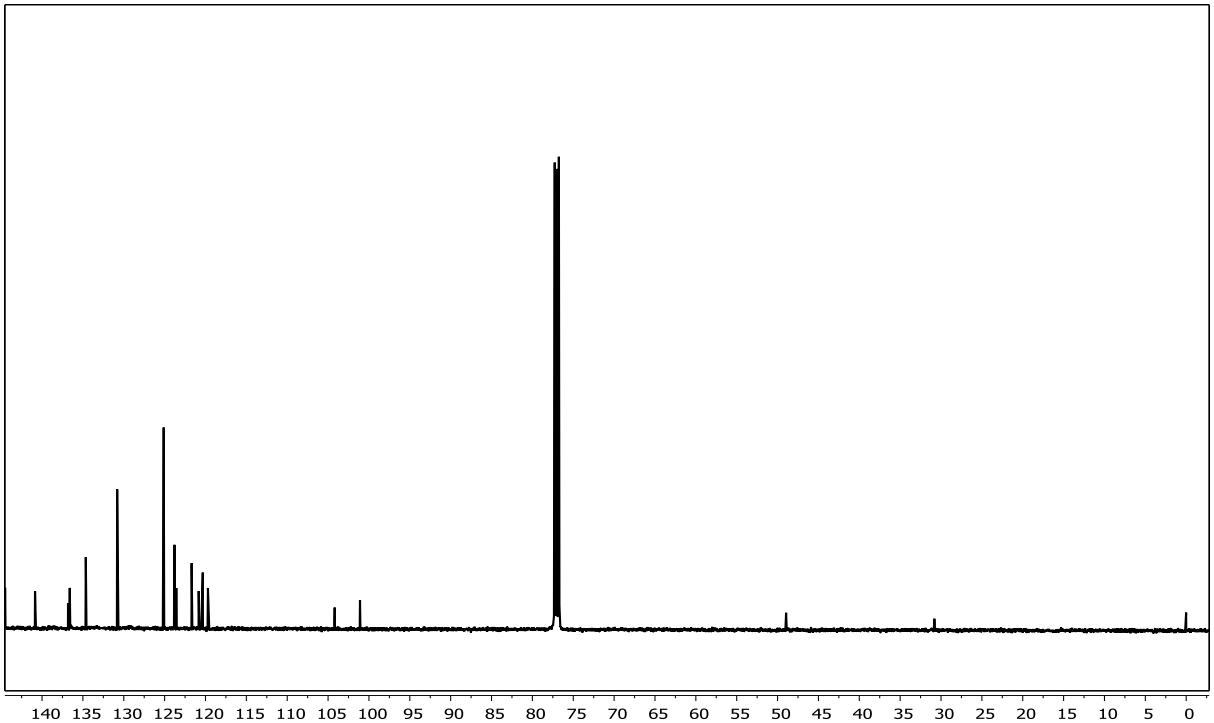


Figure 26. ^{13}C-NMR of compound **13** in $CDCl_3$

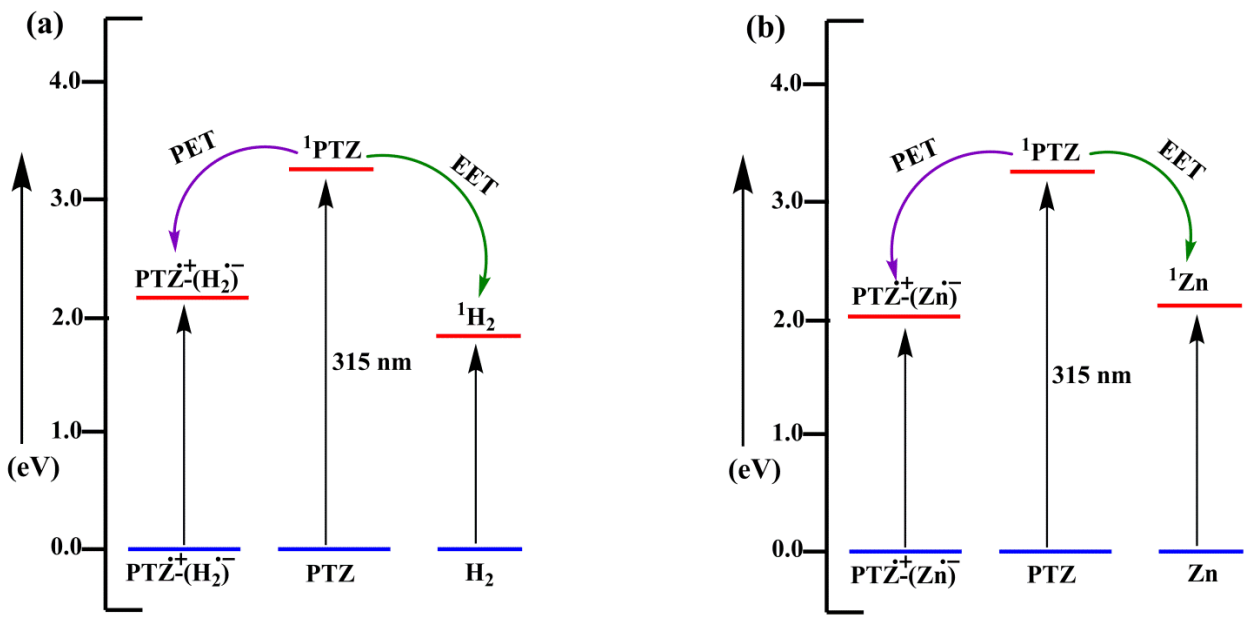


Figure 27. Generalized energy level diagram of porphyrins: (a) **5** and (b) **8**; various energy levels were obtained by absorption, emission and redox data. (EET = excitation energy transfer, PET = photoinduced electron transfer); PTA = N-butylphenothiazine, Zn= ZnTPP, H_2 = H_2TPP.

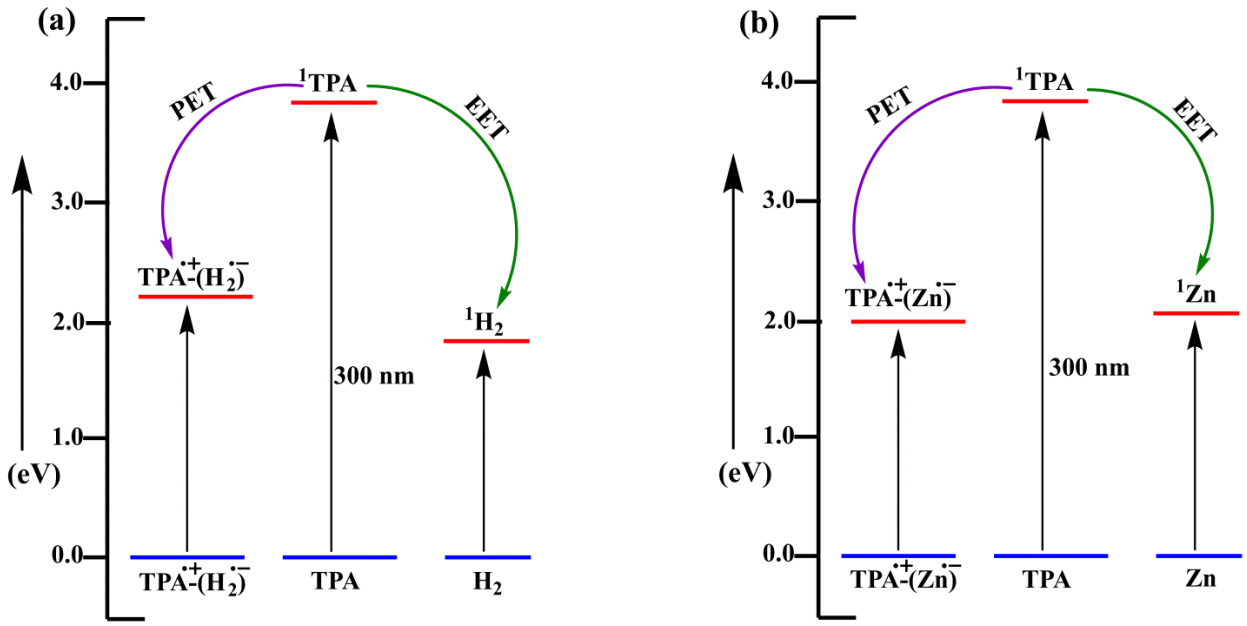


Figure 28. Generalized energy level diagram of porphyrins: (a) **7** and (b) **10**; various energy levels were obtained by absorption, emission and redox data. (EET = excitation energy transfer, PET = photoinduced electron transfer); TPA = triphenylamine, Zn = ZnTPP, H_2 = H_2TPP.

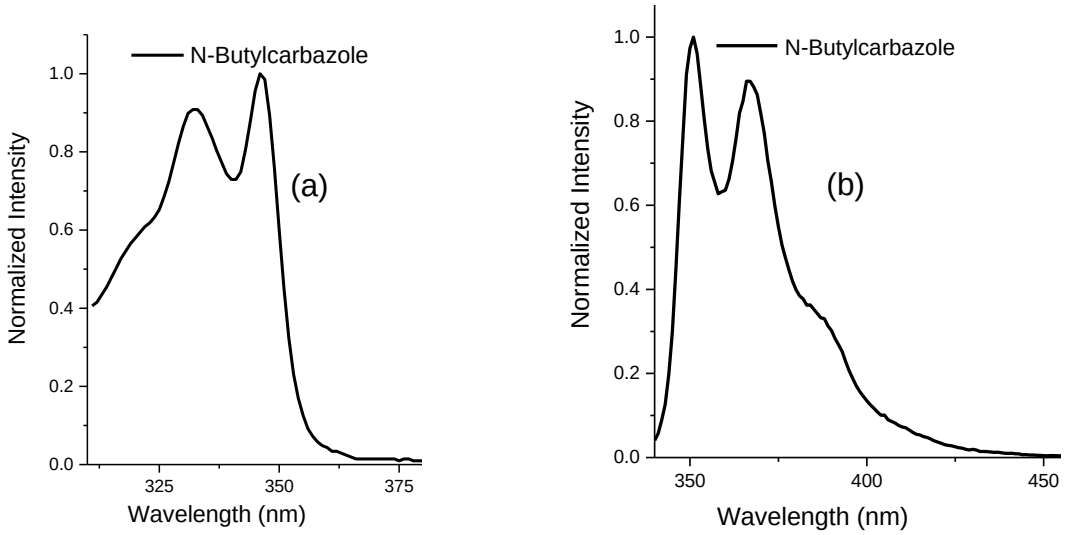


Figure 29. Absorption (a) and Emission spectra of donor (b) *N*-Butylcarbazole (λ_{ex} = 330 nm) in toluene.

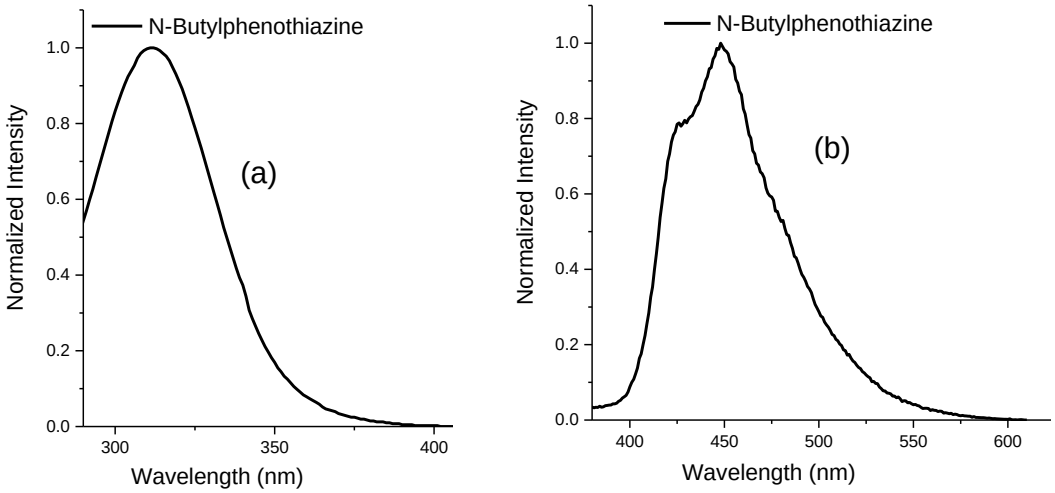


Figure 30. Absorption (a) and Emission spectra of donor (b) *N*-Butylphenothiazine (λ_{ex} = 330 nm) in toluene.

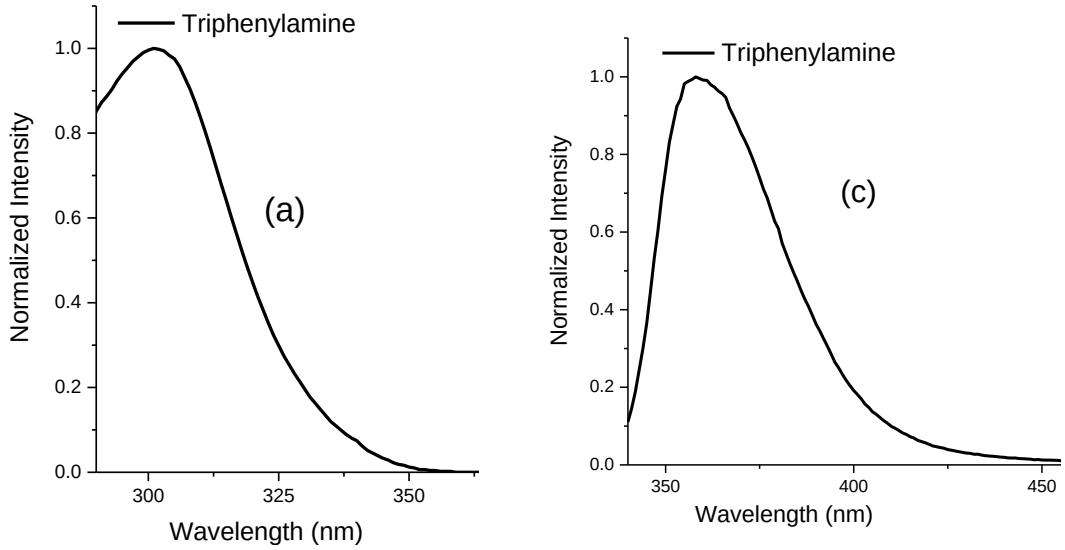


Figure 31. Absorption (a) and Emission spectra of donor (b) triphenylamine (λ_{ex} = 330 nm) in toluene.

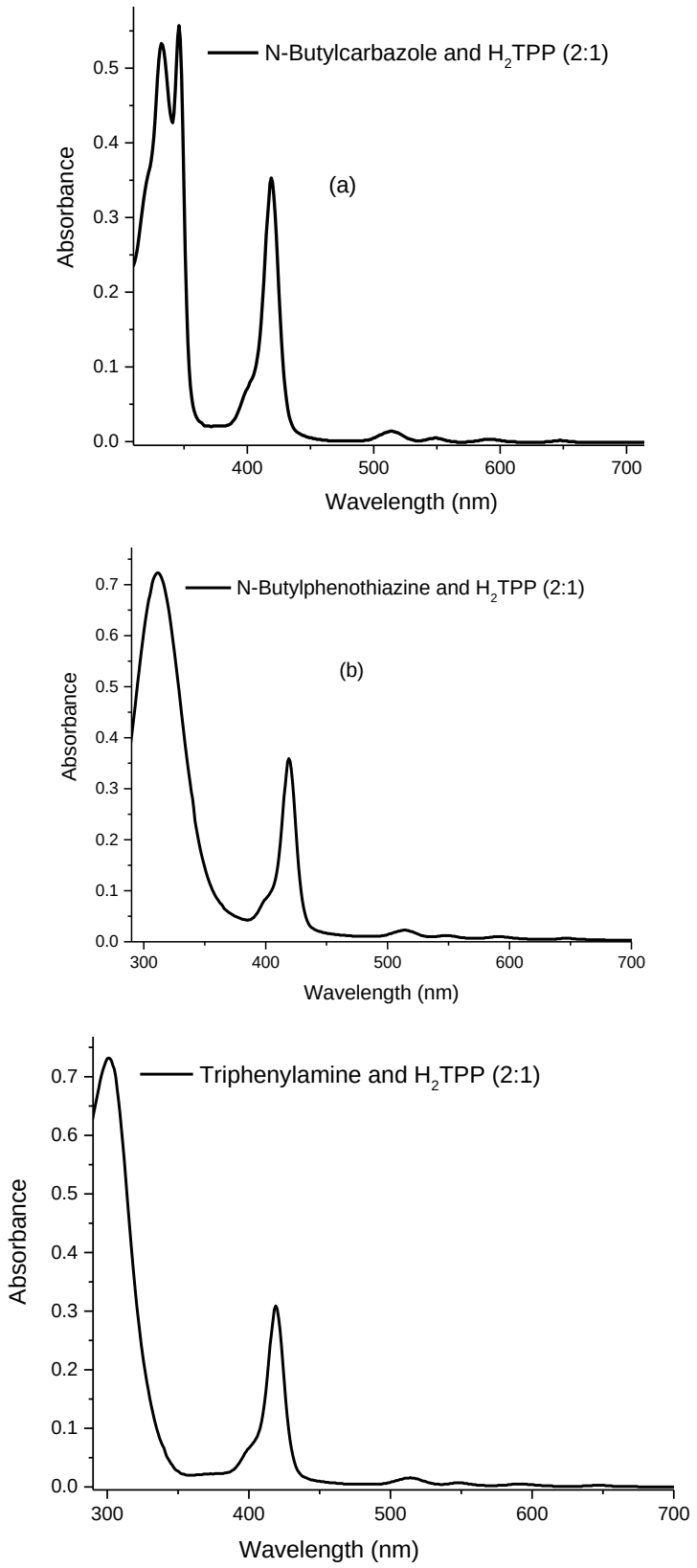
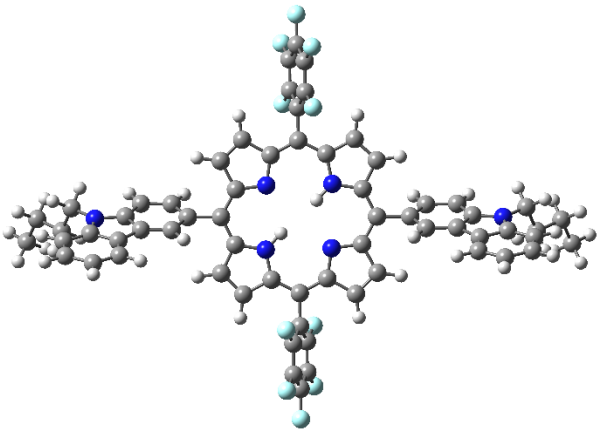
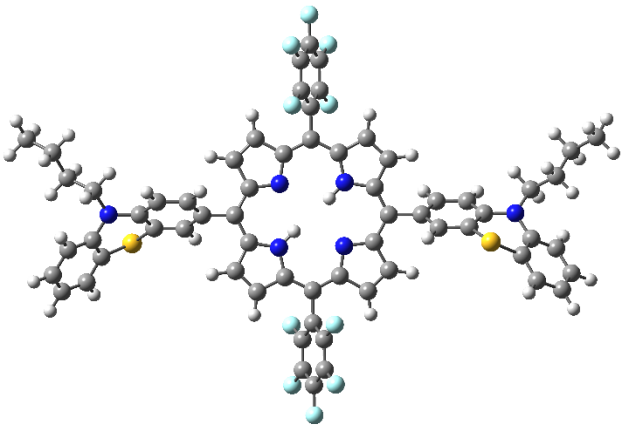


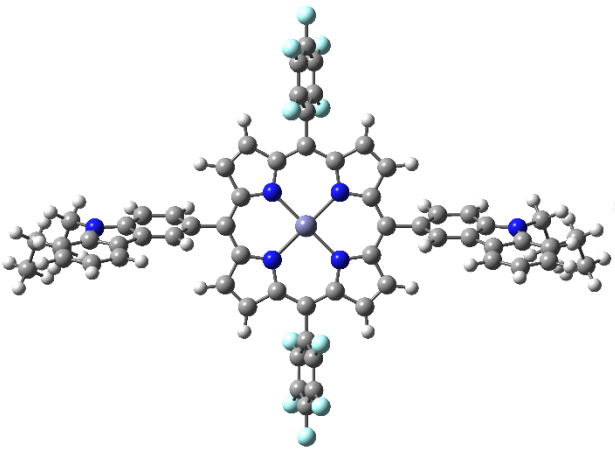
Figure 32. Absorption spectra of (a) *N*-butylcarbazole and H_2TPP (b) *N*-butylphenothiazine and H_2TPP (c) triphenylamine and H_2TPP



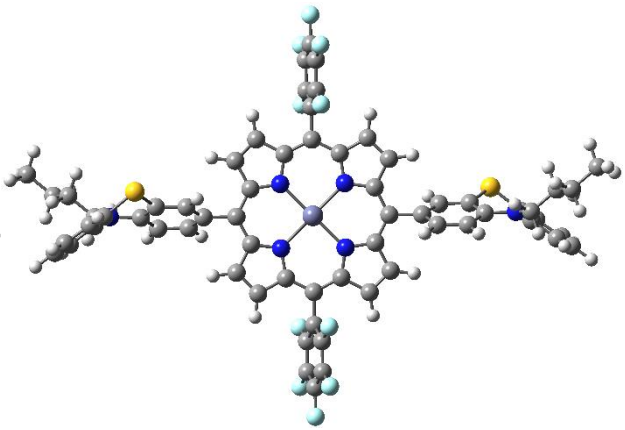
Optimized structure of **5**



Optimized structure of **6**

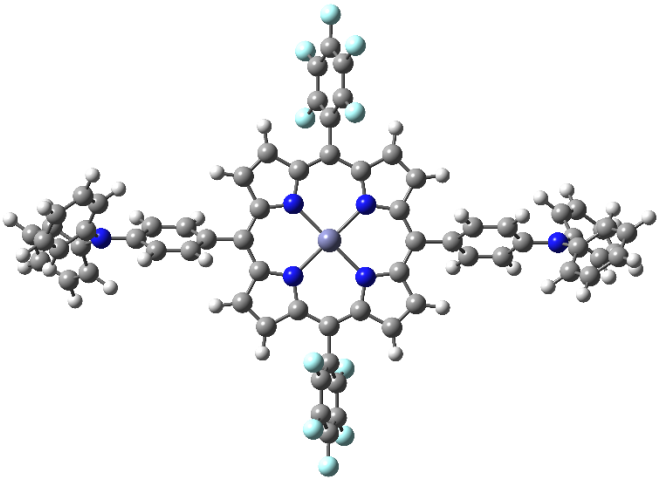


Optimized structure of **8**

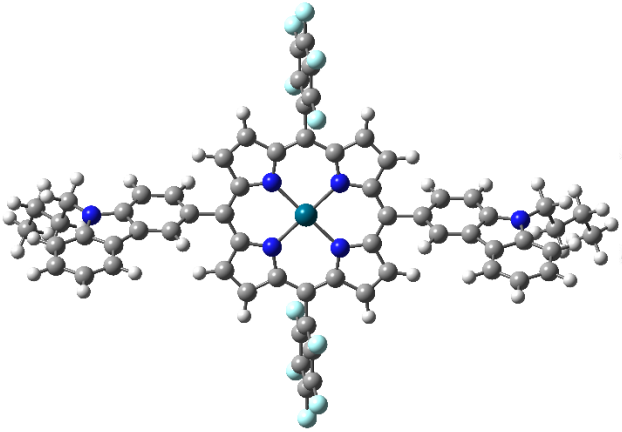


Optimized structure of **9**

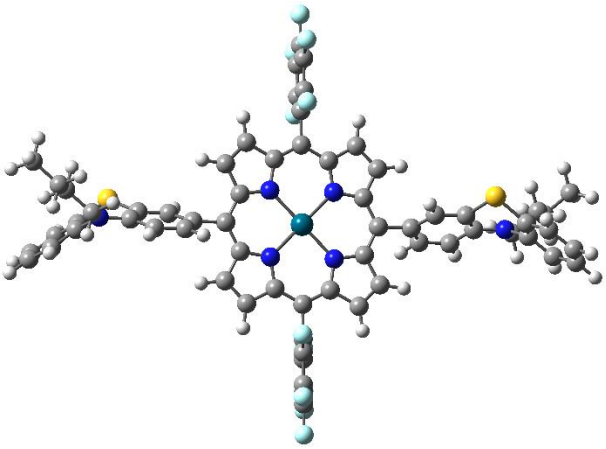
Figure 33. Optimized structures of **5, 6, 8** and **9** excluding **7**



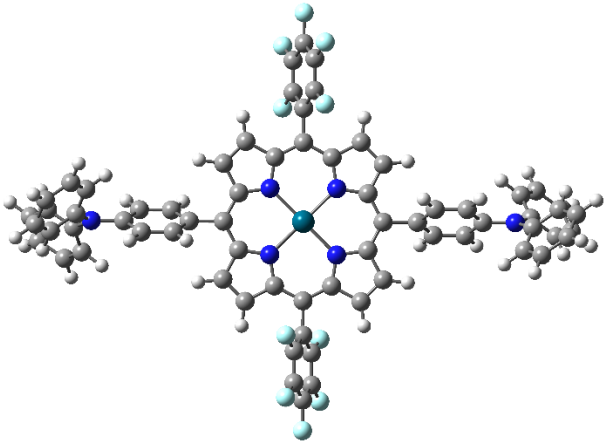
Optimized structure of **10**



Optimized structure of **11**



Optimized structure of **12**



Optimized structure of **13**

Figure 34. Optimized structures of **10-13** excluding **7**

Optimized coordinates of molecules **5-13** are given below:

Porphyrin 5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.230523	-2.601767	-0.181064
2	6	0	-2.502910	-3.267718	-0.265012
3	6	0	-3.491167	-2.313763	-0.243667
4	6	0	-2.867629	-1.021812	-0.135028
5	7	0	-1.499728	-1.247952	-0.103262
6	1	0	-4.553930	-2.475326	-0.310097
7	6	0	-3.509902	0.228464	-0.092678
8	6	0	-2.838600	1.468868	-0.056137
9	6	0	-3.523646	2.757016	0.072562
10	7	0	-1.468932	1.655855	-0.109384
11	6	0	-2.559267	3.714281	0.079340
12	1	0	-4.589127	2.892976	0.163187
13	6	0	-1.275530	3.020275	-0.034964
14	6	0	1.233467	3.078234	-0.077107
15	6	0	2.507543	3.745465	-0.040454
16	7	0	1.501095	1.722681	-0.132325
17	6	0	3.494810	2.790614	-0.056777
18	6	0	2.869053	1.496731	-0.120838
19	1	0	4.558895	2.952758	-0.018314
20	6	0	3.512004	0.246310	-0.141192
21	6	0	2.842577	-0.994946	-0.157477
22	6	0	3.530143	-2.286420	-0.230363
23	7	0	1.471677	-1.180574	-0.136428
24	6	0	2.565653	-3.243306	-0.239719
25	1	0	4.597945	-2.425322	-0.278868
26	6	0	1.279172	-2.546288	-0.188542
27	1	0	2.705945	-4.312153	-0.283256
28	6	0	-0.049941	5.176496	0.022811
29	6	0	0.275563	5.872766	1.192362
30	6	0	-0.401001	5.950673	-1.089015
31	6	0	0.256611	7.263619	1.258652
32	6	0	-0.432056	7.342090	-1.045448
33	6	0	-0.100557	8.001403	0.134238
34	6	0	-0.032824	3.680606	-0.036945
35	6	0	0.047762	-4.700881	-0.271328
36	6	0	0.359777	-5.384666	-1.451855
37	6	0	-0.252998	-5.487301	0.846556
38	6	0	0.379322	-6.775268	-1.521373
39	6	0	-0.244700	-6.879030	0.800167
40	6	0	0.074417	-7.525654	-0.389853
41	6	0	0.036031	-3.205125	-0.205730
42	9	0	0.628761	5.175168	2.327092
43	9	0	0.582435	7.911254	2.427216
44	9	0	-0.729427	5.332733	-2.275826
45	9	0	-0.781218	8.067500	-2.160569
46	9	0	-0.124444	9.373455	0.188330
47	9	0	-0.569979	-4.881078	2.042927
48	9	0	-0.544253	-7.616455	1.921734
49	9	0	0.087685	-8.897636	-0.448000
50	9	0	0.690590	-7.410998	-2.700425
51	9	0	0.660110	-4.674853	-2.593779
52	1	0	2.643808	4.813764	0.002588
53	1	0	-2.696821	4.780160	0.174817
54	1	0	-2.636756	-4.333751	-0.351057
55	6	0	5.010605	0.254579	-0.137458
56	6	0	5.723550	0.795038	-1.236552
57	6	0	5.724162	-0.269745	0.952936
58	6	0	7.118491	0.825438	-1.270053
59	1	0	5.164464	1.181031	-2.082486
60	6	0	7.122531	-0.249414	0.944315
61	1	0	5.183767	-0.676956	1.801401
62	6	0	7.814636	0.305792	-0.172557
63	1	0	7.635116	1.232983	-2.132056
64	6	0	8.134729	-0.689381	1.888253

65	6	0	9.399012	-0.384304	1.305059
66	6	0	8.083796	-1.298911	3.148946
67	6	0	10.598870	-0.684004	1.960209
68	6	0	9.278547	-1.596034	3.807915
69	1	0	7.129367	-1.537167	3.608142
70	6	0	10.520558	-1.290393	3.216828
71	1	0	11.561971	-0.460557	1.514364
72	1	0	9.253114	-2.067968	4.784430
73	1	0	11.436711	-1.532624	3.746018
74	7	0	9.189874	0.226896	0.060545
75	6	0	-5.007490	0.225500	-0.090898
76	6	0	-5.720906	0.812171	-1.166254
77	6	0	-5.721396	-0.357500	0.969507
78	6	0	-7.115500	0.830874	-1.204964
79	1	0	-5.161179	1.246847	-1.987552
80	6	0	-7.119911	-0.349033	0.955440
81	1	0	-5.181726	-0.797242	1.802176
82	6	0	-7.811863	0.252055	-0.137356
83	1	0	-7.632129	1.276036	-2.048128
84	6	0	-8.132376	-0.842167	1.872469
85	6	0	-9.396752	-0.522269	1.297313
86	6	0	-8.081754	-1.508713	3.104018
87	6	0	-10.596795	-0.864120	1.931142
88	6	0	-9.276764	-1.847661	3.742010
89	1	0	-7.127395	-1.758279	3.557370
90	6	0	-10.518774	-1.527263	3.158813
91	1	0	-11.559909	-0.629591	1.491020
92	1	0	-9.251452	-2.363869	4.695860
93	1	0	-11.435132	-1.802642	3.671149
94	7	0	-9.187248	0.148822	0.084074
95	1	0	0.802540	0.987457	-0.160423
96	1	0	-0.801712	-0.512969	-0.060946
97	6	0	10.238171	0.674995	-0.853125
98	6	0	10.707171	-0.408119	-1.843367
99	1	0	11.084258	1.025949	-0.250418
100	1	0	9.861774	1.547663	-1.399928
101	6	0	11.816770	0.100793	-2.781184
102	1	0	9.847166	-0.751572	-2.434545
103	1	0	11.066519	-1.279463	-1.278995
104	6	0	12.296084	-0.970033	-3.774135
105	1	0	12.669043	0.451028	-2.179975
106	1	0	11.451355	0.977827	-3.335960
107	1	0	13.086926	-0.582787	-4.426256
108	1	0	12.694480	-1.845575	-3.246892
109	1	0	11.472424	-1.312324	-4.412612
110	6	0	-10.234644	0.629976	-0.813750
111	6	0	-10.682361	-0.407507	-1.860981
112	1	0	-9.865281	1.533701	-1.312764
113	1	0	-11.089244	0.939812	-0.200718
114	6	0	-11.787736	0.135583	-2.784588
115	1	0	-11.037827	-1.309424	-1.344203
116	1	0	-9.812797	-0.712338	-2.459415
117	6	0	-12.244426	-0.889276	-3.834949
118	1	0	-11.426185	1.043019	-3.290815
119	1	0	-12.650278	0.446323	-2.176332
120	1	0	-13.031564	-0.477643	-4.476499
121	1	0	-11.410010	-1.191374	-4.479762
122	1	0	-12.639967	-1.793833	-3.356835

Porphyrin 6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224714	-2.727039	0.075102
2	6	0	-2.488896	-3.392986	0.240531
3	6	0	-3.476080	-2.439113	0.288825
4	6	0	-2.860291	-1.146754	0.144628

5	7	0	-1.497175	-1.372217	0.031098
6	1	0	-4.532239	-2.603671	0.420812
7	6	0	-3.503137	0.103923	0.124977
8	6	0	-2.836605	1.344502	0.039134
9	6	0	-3.527968	2.630787	-0.076431
10	7	0	-1.466618	1.534051	0.043257
11	6	0	-2.566312	3.589865	-0.114070
12	1	0	-4.595644	2.765406	-0.138302
13	6	0	-1.278488	2.899335	-0.030490
14	6	0	1.229587	2.958398	-0.020714
15	6	0	2.503516	3.623181	0.042685
16	7	0	1.496435	1.603300	-0.087213
17	6	0	3.490353	2.668409	0.007053
18	6	0	2.863998	1.376673	-0.088158
19	1	0	4.554061	2.830510	0.053389
20	6	0	3.504563	0.127015	-0.166213
21	6	0	2.835280	-1.114526	-0.189821
22	6	0	3.514881	-2.401758	-0.355325
23	7	0	1.469908	-1.302651	-0.074201
24	6	0	2.552708	-3.359933	-0.311897
25	1	0	4.574340	-2.538749	-0.499224
26	6	0	1.275607	-2.667946	-0.129535
27	1	0	2.686895	-4.425451	-0.414517
28	6	0	-0.053925	5.058699	-0.022803
29	6	0	-0.481296	5.788910	1.093029
30	6	0	0.352208	5.803069	-1.137136
31	6	0	-0.510139	7.180903	1.103860
32	6	0	0.337915	7.195271	-1.147320
33	6	0	-0.097185	7.887609	-0.021472
34	6	0	-0.037015	3.562997	-0.025092
35	6	0	0.054991	-4.826909	-0.026092
36	6	0	-0.426155	-5.570987	-1.110171
37	6	0	0.556804	-5.556246	1.058727
38	6	0	-0.412573	-6.963209	-1.120864
39	6	0	0.585385	-6.948267	1.068391
40	6	0	0.097235	-7.655001	-0.026441
41	6	0	0.038078	-3.330884	-0.027733
42	9	0	-0.888158	5.125786	2.229946
43	9	0	-0.935888	7.860627	2.220790
44	9	0	0.781621	5.153259	-2.274380
45	9	0	0.743904	7.888510	-2.263418
46	9	0	-0.117989	9.260532	-0.020609
47	9	0	1.040611	-4.891962	2.164251
48	9	0	1.084778	-7.627940	2.154248
49	9	0	0.117566	-9.027900	-0.026449
50	9	0	-0.892851	-7.657040	-2.206511
51	9	0	-0.932075	-4.920688	-2.215066
52	1	0	2.640308	4.689229	0.122780
53	1	0	-2.709138	4.654757	-0.212098
54	1	0	-2.618193	-4.459360	0.327765
55	6	0	4.998901	0.137802	-0.234034
56	6	0	5.776062	-0.470769	0.770432
57	6	0	5.672953	0.748437	-1.306632
58	6	0	7.167586	-0.433057	0.718823
59	1	0	5.287894	-0.951776	1.610891
60	6	0	7.066869	0.752354	-1.376960
61	1	0	5.099358	1.194934	-2.111936
62	6	0	7.847194	0.180600	-0.352776
63	1	0	7.548025	1.182775	-2.246931
64	6	0	9.575469	-1.720793	1.112857
65	6	0	10.251175	-2.881177	1.491658
66	6	0	9.990709	-0.963583	0.001508
67	6	0	11.388625	-3.291883	0.786972
68	1	0	9.894099	-3.450991	2.342753
69	6	0	11.120851	-1.402785	-0.714323
70	6	0	11.819518	-2.545744	-0.314126
71	1	0	11.924687	-4.183201	1.094135
72	1	0	11.453741	-0.854274	-1.587301
73	1	0	12.694480	-2.857488	-0.875219
74	7	0	9.264203	0.196196	-0.391229
75	16	0	8.153016	-1.116269	2.115435
76	6	0	-4.996087	0.105060	0.215513
77	6	0	-5.787396	-0.514568	-0.770932
78	6	0	-5.654792	0.717427	1.296685
79	6	0	-7.178090	-0.487234	-0.693833
80	1	0	-5.312466	-0.993092	-1.620512
81	6	0	-7.046959	0.711281	1.392613

82	1	0	-5.069188	1.176270	2.086036
83	6	0	-7.842244	0.126860	0.386959
84	1	0	-7.514946	1.145036	2.268064
85	6	0	-9.582394	-1.795212	-1.037861
86	6	0	-10.256442	-2.962100	-1.399230
87	6	0	-9.982967	-1.035751	0.077353
88	6	0	-11.378054	-3.377742	-0.672402
89	1	0	-9.910854	-3.533039	-2.254328
90	6	0	-11.097323	-1.479502	0.814888
91	6	0	-11.794701	-2.629344	0.432640
92	1	0	-11.913149	-4.274220	-0.965940
93	1	0	-11.419230	-0.928448	1.690372
94	1	0	-12.657489	-2.944371	1.010497
95	7	0	-9.258301	0.130866	0.452375
96	16	0	-8.183258	-1.184682	-2.069247
97	1	0	0.797243	0.868353	-0.097031
98	1	0	-0.801572	-0.636726	-0.033890
99	6	0	-9.953039	1.213845	1.177117
100	6	0	-11.130003	1.812204	0.385636
101	1	0	-9.219562	2.005591	1.345195
102	1	0	-10.291511	0.880829	2.171151
103	6	0	-11.810623	2.962092	1.151598
104	1	0	-11.870429	1.035743	0.158615
105	1	0	-10.750226	2.175623	-0.578218
106	6	0	-12.983551	3.580489	0.374124
107	1	0	-11.068127	3.742417	1.375361
108	1	0	-12.170480	2.591974	2.123319
109	1	0	-13.450230	4.395082	0.939357
110	1	0	-12.647320	3.988381	-0.586932
111	1	0	-13.756641	2.830785	0.165181
112	6	0	9.963145	1.281639	-1.107937
113	6	0	11.121377	1.892642	-0.298507
114	1	0	9.226380	2.066796	-1.292145
115	1	0	10.321778	0.947730	-2.094612
116	6	0	11.804665	3.046220	-1.056475
117	1	0	11.864559	1.123191	-0.057112
118	1	0	10.722437	2.255364	0.657837
119	6	0	12.961138	3.675060	-0.262831
120	1	0	11.059705	3.820422	-1.292988
121	1	0	12.181930	2.676964	-2.021896
122	1	0	13.430025	4.492136	-0.822645
123	1	0	12.607640	4.082142	0.692363
124	1	0	13.736650	2.931610	-0.041015

Porphyrin 7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.845305	1.223754	0.023589
2	6	0	3.512822	2.493431	0.129698
3	6	0	2.559629	3.482546	0.135942
4	6	0	1.266356	2.862438	0.024817
5	7	0	1.490552	1.495274	-0.027889
6	1	0	2.723828	4.543749	0.218748
7	6	0	0.017315	3.507623	-0.017553
8	6	0	-1.224854	2.840372	-0.065808
9	6	0	-2.510844	3.529138	-0.196949
10	7	0	-1.416241	1.471577	-0.010378
11	6	0	-3.471470	2.568283	-0.194863
12	1	0	-2.644234	4.594526	-0.292312
13	6	0	-2.782107	1.282885	-0.071270
14	6	0	-2.845305	-1.223754	0.023589
15	6	0	-3.512822	-2.493431	0.129698
16	7	0	-1.490552	-1.495274	-0.027889
17	6	0	-2.559629	-3.482546	0.135942
18	6	0	-1.266356	-2.862438	0.024817
19	1	0	-2.723828	-4.543749	0.218748
20	6	0	-0.017315	-3.507623	-0.017553

21	6	0	1.224854	-2.840372	-0.065808
22	6	0	2.510844	-3.529138	-0.196949
23	7	0	1.416241	-1.471577	-0.010378
24	6	0	3.471470	-2.568283	-0.194863
25	1	0	2.644234	-4.594526	-0.292312
26	6	0	2.782107	-1.282885	-0.071270
27	1	0	4.536915	-2.709328	-0.289436
28	6	0	-4.943243	0.062464	-0.022923
29	6	0	-5.687524	-0.372402	-1.126328
30	6	0	-5.673135	0.520495	1.080797
31	6	0	-7.079718	-0.356320	-1.137576
32	6	0	-7.065112	0.551355	1.090337
33	6	0	-7.771845	0.109542	-0.023971
34	6	0	-3.447412	0.043228	-0.024137
35	6	0	4.943243	-0.062464	-0.022923
36	6	0	5.673135	-0.520495	1.080797
37	6	0	5.687524	0.372402	-1.126328
38	6	0	7.065112	-0.551355	1.090337
39	6	0	7.079718	0.356320	-1.137576
40	6	0	7.771845	-0.109542	-0.023971
41	6	0	3.447412	-0.043228	-0.024137
42	9	0	-5.037599	-0.833288	-2.251081
43	9	0	-7.773205	-0.790875	-2.242709
44	9	0	-5.009645	0.957031	2.206425
45	9	0	-7.744826	1.007462	2.195224
46	9	0	-9.144790	0.132217	-0.024289
47	9	0	5.037599	0.833288	-2.251081
48	9	0	7.773205	0.790875	-2.242709
49	9	0	9.144790	-0.132217	-0.024289
50	9	0	7.744826	-1.007462	2.195224
51	9	0	5.009645	-0.957031	2.206425
52	1	0	-4.579627	-2.625365	0.207965
53	1	0	-4.536915	2.709328	-0.289436
54	1	0	4.579627	2.625365	0.207965
55	6	0	-0.024867	-5.003563	-0.006774
56	6	0	0.568390	-5.725744	1.047065
57	6	0	-0.624805	-5.737963	-1.048225
58	6	0	0.568793	-7.119945	1.060399
59	1	0	1.035885	-5.185695	1.863946
60	6	0	-0.638629	-7.132332	-1.038113
61	1	0	-1.083523	-5.208250	-1.876973
62	6	0	-0.038505	-7.847533	0.017369
63	1	0	1.037647	-7.650772	1.880455
64	6	0	0.024867	5.003563	-0.006774
65	6	0	-0.568390	5.725744	1.047065
66	6	0	0.624805	5.737963	-1.048225
67	6	0	-0.568793	7.119945	1.060399
68	1	0	-1.035885	5.185695	1.863946
69	6	0	0.638629	7.132332	-1.038113
70	1	0	1.083523	5.208250	-1.876973
71	6	0	0.038505	7.847533	0.017369
72	1	0	-1.037647	7.650772	1.880455
73	7	0	0.045054	9.269539	0.029556
74	1	0	-1.110820	-7.672584	-1.850084
75	7	0	-0.045054	-9.269539	0.029556
76	6	0	0.078893	-10.004324	-1.193597
77	6	0	1.026037	-9.624734	-2.162343
78	6	0	-0.741366	-11.121088	-1.436135
79	6	0	1.138422	-10.343904	-3.354975
80	1	0	1.668039	-8.771219	-1.975682
81	6	0	-0.610464	-11.844587	-2.624334
82	1	0	-1.474954	-11.414647	-0.693805
83	6	0	0.325029	-11.458822	-3.592213
84	1	0	1.873230	-10.039616	-4.093744
85	1	0	-1.250339	-12.703976	-2.798375
86	1	0	0.419600	-12.018869	-4.516570
87	6	0	-0.174819	-9.981585	1.265514
88	6	0	0.638629	-11.098475	1.529371
89	6	0	-1.121037	-9.579134	2.225864
90	6	0	0.501850	-11.799660	2.730214
91	1	0	1.371663	-11.409395	0.793598
92	6	0	-1.239340	-10.275984	3.431107
93	1	0	-1.757840	-8.725382	2.022993
94	6	0	-0.432804	-11.391148	3.689548
95	1	0	1.136599	-12.659340	2.920761
96	1	0	-1.973280	-9.954139	4.163280
97	1	0	-0.531841	-11.933859	4.623723

98	1	0	1.110820	7.672584	-1.850084
99	6	0	-0.078893	10.004324	-1.193597
100	6	0	-1.026037	9.624734	-2.162343
101	6	0	0.741366	11.121088	-1.436135
102	6	0	-1.138422	10.343904	-3.354975
103	1	0	-1.668039	8.771219	-1.975682
104	6	0	0.610464	11.844587	-2.624334
105	1	0	1.474954	11.414647	-0.693805
106	6	0	-0.325029	11.458822	-3.592213
107	1	0	-1.873230	10.039616	-4.093744
108	1	0	1.250339	12.703976	-2.798375
109	1	0	-0.419600	12.018869	-4.516570
110	6	0	0.174819	9.981585	1.265514
111	6	0	1.121037	9.579134	2.225864
112	6	0	-0.638629	11.098475	1.529371
113	6	0	1.239340	10.275984	3.431107
114	1	0	1.757840	8.725382	2.022993
115	6	0	-0.501850	11.799660	2.730214
116	1	0	-1.371663	11.409395	0.793598
117	6	0	0.432804	11.391148	3.689548
118	1	0	1.973280	9.954139	4.163280
119	1	0	-1.136599	12.659340	2.920761
120	1	0	0.531841	11.933859	4.623723
121	1	0	0.754483	0.798002	-0.060907
122	1	0	-0.754483	-0.798002	-0.060907

Porphyrin 8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.237252	3.045491	-0.089950
2	6	0	2.511655	3.724858	-0.075070
3	6	0	3.476260	2.767864	-0.080788
4	6	0	2.807666	1.486870	-0.114229
5	7	0	1.447601	1.689263	-0.114572
6	1	0	4.547169	2.904305	-0.060635
7	6	0	3.468002	0.249152	-0.132087
8	6	0	2.812673	-0.991316	-0.136893
9	6	0	3.484621	-2.269769	-0.198989
10	7	0	1.453443	-1.198801	-0.108468
11	6	0	2.523297	-3.229911	-0.195261
12	1	0	4.554969	-2.402579	-0.247332
13	6	0	1.247456	-2.555428	-0.140075
14	6	0	-1.239447	-2.560555	-0.128390
15	6	0	-2.513547	-3.240396	-0.145583
16	7	0	-1.450171	-1.204340	-0.109967
17	6	0	-3.478440	-2.283883	-0.148973
18	6	0	-2.810489	-1.002219	-0.116799
19	1	0	-4.549012	-2.421387	-0.172556
20	6	0	-3.470208	0.235837	-0.104987
21	6	0	-2.814268	1.475959	-0.094474
22	6	0	-3.487092	2.753622	-0.031698
23	7	0	-1.455221	1.683796	-0.116065
24	6	0	-2.526082	3.714248	-0.026209
25	1	0	-4.557894	2.885210	0.012801
26	6	0	-1.249721	3.040428	-0.078550
27	1	0	-2.663644	4.784713	0.025725
28	6	0	0.009310	-4.697282	-0.167082
29	6	0	0.312138	-5.445559	0.974938
30	6	0	-0.287177	-5.409130	-1.333802
31	6	0	0.322932	-6.838747	0.963378
32	6	0	-0.287392	-6.801900	-1.368866
33	6	0	0.020492	-7.518210	-0.214457
34	6	0	0.005277	-3.201788	-0.141577
35	6	0	-0.011262	5.182059	-0.038908
36	6	0	-0.315266	5.936874	-1.176269
37	6	0	0.286974	5.887202	1.131498
38	6	0	-0.325737	7.329929	-1.156840

39	6	0	0.287574	7.279812	1.174375
40	6	0	-0.021633	8.002671	0.024409
41	6	0	-0.007494	3.686740	-0.072401
42	9	0	0.604411	-4.823968	2.124746
43	9	0	0.615683	-7.525735	2.073540
44	9	0	-0.583726	-4.751534	-2.462355
45	9	0	-0.574972	-7.453728	-2.501415
46	9	0	0.025462	-8.853661	-0.237061
47	9	0	0.584763	5.223223	2.255715
48	9	0	0.576847	7.925241	2.309983
49	9	0	-0.026190	9.337993	0.054441
50	9	0	-0.619689	8.023255	-2.262927
51	9	0	-0.609094	5.321901	-2.329433
52	1	0	-2.647714	-4.312466	-0.157476
53	1	0	2.660318	-4.300647	-0.242736
54	1	0	2.646076	4.796847	-0.058464
55	6	0	-4.968438	0.234186	-0.102515
56	6	0	-5.679810	0.667395	-1.244059
57	6	0	-5.678765	-0.200819	1.022208
58	6	0	-7.071548	0.672777	-1.288966
59	1	0	-5.119778	0.994195	-2.115516
60	6	0	-7.076531	-0.203114	1.005117
61	1	0	-5.138130	-0.530428	1.905365
62	6	0	-7.767372	0.238033	-0.156144
63	1	0	-7.588528	0.998713	-2.186428
64	6	0	-8.088402	-0.579581	1.970143
65	6	0	-9.344881	-0.352091	1.347393
66	6	0	-8.044738	-1.079590	3.276755
67	6	0	-10.547037	-0.624292	2.008515
68	6	0	-9.239292	-1.348003	3.939905
69	1	0	-7.090698	-1.256670	3.766491
70	6	0	-10.474981	-1.121610	3.308473
71	1	0	-11.508842	-0.460015	1.532018
72	1	0	-9.218849	-1.736975	4.953808
73	1	0	-11.395629	-1.340596	3.842613
74	7	0	-9.135597	0.156401	0.067722
75	6	0	4.966092	0.251482	-0.150856
76	6	0	5.660820	0.687076	-1.301750
77	6	0	5.692732	-0.184810	0.962898
78	6	0	7.051794	0.694554	-1.366216
79	1	0	5.088217	1.013838	-2.165035
80	6	0	7.090116	-0.185191	0.926054
81	1	0	5.164953	-0.517161	1.852759
82	6	0	7.764013	0.259140	-0.243913
83	1	0	7.555800	1.022200	-2.270411
84	6	0	8.115966	-0.562631	1.875818
85	6	0	9.363270	-0.332171	1.235996
86	6	0	8.091273	-1.066172	3.181548
87	6	0	10.574953	-0.604720	1.879344
88	6	0	9.295369	-1.335036	3.827018
89	1	0	7.144461	-1.245815	3.684169
90	6	0	10.521790	-1.105566	3.178863
91	1	0	11.529749	-0.438106	1.389731
92	1	0	9.289603	-1.726801	4.840028
93	1	0	11.450121	-1.324949	3.699364
94	7	0	9.135333	0.178954	-0.039504
95	46	0	-0.001090	0.242434	-0.112232
96	6	0	-10.174066	0.440759	-0.909985
97	6	0	-10.564161	-0.774131	-1.765964
98	1	0	-9.821862	1.259329	-1.548057
99	1	0	-11.048740	0.823854	-0.371786
100	6	0	-11.665370	-0.450430	-2.783517
101	1	0	-10.894278	-1.584798	-1.102761
102	1	0	-9.670934	-1.144067	-2.286805
103	6	0	-12.058566	-1.657527	-3.641702
104	1	0	-11.330088	0.368470	-3.436187
105	1	0	-12.552188	-0.073676	-2.253937
106	1	0	-12.843657	-1.395511	-4.359644
107	1	0	-11.199866	-2.036571	-4.208841
108	1	0	-12.434398	-2.479649	-3.020720
109	6	0	10.159553	0.465958	-1.031325
110	6	0	10.539335	-0.747541	-1.893937
111	1	0	11.041171	0.849673	-0.505035
112	1	0	9.797281	1.284719	-1.663523
113	6	0	11.627582	-0.422259	-2.924829
114	1	0	9.639769	-1.117217	-2.403971
115	1	0	10.878061	-1.558921	-1.235961

116	6	0	12.010534	-1.628383	-3.788997
117	1	0	12.520792	-0.045698	-2.405980
118	1	0	11.283943	0.397154	-3.572506
119	1	0	12.786434	-1.365393	-4.516511
120	1	0	12.394477	-2.450877	-3.173488
121	1	0	11.144939	-2.007337	-4.345635

Porphyrin 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.240856	2.733894	0.076841
2	6	0	-2.512786	3.410947	0.174277
3	6	0	-3.474416	2.452405	0.224177
4	6	0	-2.806997	1.172748	0.142586
5	7	0	-1.449904	1.377225	0.063224
6	1	0	-4.542072	2.589141	0.309440
7	6	0	-3.463614	-0.067075	0.145027
8	6	0	-2.808640	-1.306346	0.089096
9	6	0	-3.481374	-2.584493	0.031231
10	7	0	-1.449395	-1.511882	0.067079
11	6	0	-2.519521	-3.543243	-0.008574
12	1	0	-4.552580	-2.718692	0.012420
13	6	0	-1.243110	-2.868049	0.018262
14	6	0	1.243099	-2.868049	-0.018258
15	6	0	2.519509	-3.543245	0.008586
16	7	0	1.449387	-1.511883	-0.067063
17	6	0	3.481363	-2.584496	-0.031195
18	6	0	2.808632	-1.306349	-0.089070
19	1	0	4.552568	-2.718697	-0.012365
20	6	0	3.463607	-0.067079	-0.145001
21	6	0	2.806991	1.172743	-0.142576
22	6	0	3.474411	2.452399	-0.224189
23	7	0	1.449899	1.377223	-0.063223
24	6	0	2.512780	3.410942	-0.174316
25	1	0	4.542066	2.589134	-0.309451
26	6	0	1.240851	2.733891	-0.076866
27	1	0	2.647783	4.482541	-0.202098
28	6	0	-0.000005	-5.008033	-0.000018
29	6	0	-0.338263	-5.738897	1.143826
30	6	0	0.338254	-5.738869	-1.143881
31	6	0	-0.344214	-7.131979	1.155237
32	6	0	0.344206	-7.131950	-1.155325
33	6	0	-0.000004	-7.830131	-0.000053
34	6	0	-0.000006	-3.513040	-0.000003
35	6	0	-0.000001	4.873959	-0.000043
36	6	0	-0.198315	5.603671	1.176245
37	6	0	0.198316	5.603632	-1.176354
38	6	0	-0.203067	6.996874	1.188364
39	6	0	0.203072	6.996834	-1.188519
40	6	0	0.000003	7.694722	-0.000089
41	6	0	-0.000002	3.377886	-0.000020
42	9	0	-0.669221	-5.099991	2.273502
43	9	0	-0.671358	-7.801129	2.266521
44	9	0	0.669212	-5.099936	-2.273541
45	9	0	0.671351	-7.801074	-2.266625
46	9	0	-0.000003	-9.165533	-0.000069
47	9	0	0.394699	4.963177	-2.336191
48	9	0	0.396173	7.666243	-2.330490
49	9	0	0.000006	9.030107	-0.000111
50	9	0	-0.396165	7.666319	2.330315
51	9	0	-0.394699	4.963254	2.336102
52	1	0	2.657388	-4.613264	0.067472
53	1	0	-2.657403	-4.613261	-0.067466
54	1	0	-2.647789	4.482548	0.202034
55	6	0	4.958871	-0.069702	-0.212273
56	6	0	5.729850	0.381782	0.869775

57	6	0	5.631640	-0.536296	-1.348864
58	6	0	7.121949	0.405441	0.800970
59	1	0	5.238028	0.725668	1.775057
60	6	0	7.024940	-0.548390	-1.409609
61	1	0	5.059309	-0.905488	-2.194940
62	6	0	7.798723	-0.055170	-0.347088
63	1	0	7.507968	-0.951155	-2.293148
64	6	0	9.471065	-0.016697	2.042275
65	6	0	10.133393	-0.425225	3.200564
66	6	0	9.918291	-0.429118	0.772136
67	6	0	11.277271	-1.220504	3.114486
68	1	0	9.754811	-0.106023	4.167432
69	6	0	11.047917	-1.258922	0.702964
70	6	0	11.729043	-1.634441	1.862093
71	1	0	11.801965	-1.517545	4.017639
72	1	0	11.401199	-1.613956	-0.258953
73	1	0	12.609479	-2.265643	1.779144
74	7	0	9.211120	-0.013221	-0.384685
75	16	0	8.074815	1.087785	2.143448
76	6	0	-4.958878	-0.069700	0.212310
77	6	0	-5.729865	0.381758	-0.869744
78	6	0	-5.631640	-0.536270	1.348915
79	6	0	-7.121964	0.405416	-0.800931
80	1	0	-5.238048	0.725630	-1.775035
81	6	0	-7.024940	-0.548366	1.409669
82	1	0	-5.059303	-0.905440	2.194997
83	6	0	-7.798730	-0.055173	0.347140
84	1	0	-7.507962	-0.951108	2.293221
85	6	0	-9.471081	-0.016753	-2.042217
86	6	0	-10.133407	-0.425312	-3.200496
87	6	0	-9.918296	-0.429157	-0.772067
88	6	0	-11.277269	-1.220611	-3.114398
89	1	0	-9.754836	-0.106119	-4.167371
90	6	0	-11.047898	-1.258992	-0.702878
91	6	0	-11.729022	-1.634545	-1.861997
92	1	0	-11.801964	-1.517674	-4.017544
93	1	0	-11.401157	-1.614028	0.259047
94	1	0	-12.609441	-2.265768	-1.779033
95	7	0	-9.211128	-0.013223	0.384742
96	16	0	-8.074841	1.087739	-2.143413
97	46	0	-0.000003	-0.067209	0.000015
98	6	0	-9.898529	0.008811	1.679508
99	6	0	-11.087656	0.980038	1.709118
100	1	0	-9.168937	0.345952	2.418926
101	1	0	-10.215856	-0.999510	1.991522
102	6	0	-11.772056	1.012770	3.082544
103	1	0	-11.821585	0.708383	0.941790
104	1	0	-10.720991	1.980968	1.447645
105	6	0	-12.951475	1.989741	3.134529
106	1	0	-11.036854	1.286728	3.852686
107	1	0	-12.122619	0.003259	3.341359
108	1	0	-13.420782	1.994262	4.124690
109	1	0	-12.627046	3.013754	2.913685
110	1	0	-13.721209	1.721028	2.400916
111	6	0	9.898525	0.008771	-1.679448
112	6	0	11.087699	0.979940	-1.709054
113	1	0	9.168951	0.345929	-2.418878
114	1	0	10.215815	-0.999568	-1.991443
115	6	0	11.772104	1.012644	-3.082477
116	1	0	11.821612	0.708242	-0.941724
117	1	0	10.721085	1.980886	-1.447574
118	6	0	12.951568	1.989557	-3.134457
119	1	0	11.036917	1.286638	-3.852620
120	1	0	12.122619	0.003116	-3.341294
121	1	0	13.420875	1.994059	-4.124618
122	1	0	12.627189	3.013586	-2.913609
123	1	0	13.721290	1.720805	-2.400845

Porphyrin 10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.242427	-2.800355	-0.048026
2	6	0	-2.515202	-3.474808	-0.149699
3	6	0	-3.478010	-2.516055	-0.152241
4	6	0	-2.810154	-1.238730	-0.044740
5	7	0	-1.451470	-1.444522	0.001360
6	1	0	-4.546675	-2.650275	-0.227692
7	6	0	-3.468214	0.000029	0.000021
8	6	0	-2.810134	1.238778	0.044762
9	6	0	-3.477965	2.516113	0.152298
10	7	0	-1.451444	1.444554	-0.001387
11	6	0	-2.515149	3.474858	0.149662
12	1	0	-4.546625	2.650347	0.227801
13	6	0	-1.242381	2.800390	0.047975
14	6	0	1.242421	2.800376	-0.048004
15	6	0	2.515191	3.474827	-0.149734
16	7	0	1.451466	1.444541	0.001405
17	6	0	3.478002	2.516075	-0.152279
18	6	0	2.810156	1.238753	-0.044733
19	1	0	4.546665	2.650299	-0.227773
20	6	0	3.468219	-0.000007	0.000020
21	6	0	2.810130	-1.238758	0.044753
22	6	0	3.477961	-2.516091	0.152295
23	7	0	1.451440	-1.444533	-0.001426
24	6	0	2.515139	-3.474834	0.149699
25	1	0	4.546620	-2.650330	0.227816
26	6	0	1.242377	-2.800370	0.047944
27	1	0	2.649594	-4.544186	0.226042
28	6	0	0.000035	4.940339	-0.000076
29	6	0	0.419789	5.671585	1.116427
30	6	0	-0.419726	5.671516	-1.116623
31	6	0	0.426758	7.064637	1.127229
32	6	0	-0.426685	7.064567	-1.127514
33	6	0	0.000039	7.762834	-0.000165
34	6	0	0.000024	3.445552	-0.000027
35	6	0	-0.000046	-4.940318	-0.000087
36	6	0	0.419661	-5.671508	-1.116646
37	6	0	-0.419758	-5.671548	1.116440
38	6	0	0.426621	-7.064559	-1.127518
39	6	0	-0.426725	-7.064600	1.127261
40	6	0	-0.000051	-7.762811	-0.000141
41	6	0	-0.000032	-3.445530	-0.000061
42	9	0	0.830843	5.033212	2.219777
43	9	0	0.833438	7.733805	2.211911
44	9	0	-0.830795	5.033078	-2.219929
45	9	0	-0.833367	7.733668	-2.212236
46	9	0	0.000042	9.098249	-0.000207
47	9	0	-0.830774	-5.033161	2.219796
48	9	0	-0.833363	-7.733753	2.211968
49	9	0	-0.000058	-9.098227	-0.000168
50	9	0	0.833252	-7.733675	-2.212251
51	9	0	0.830675	-5.033082	-2.219979
52	1	0	2.649657	4.544176	-0.226098
53	1	0	-2.649604	4.544214	0.225962
54	1	0	-2.649670	-4.544161	-0.226028
55	6	0	4.963949	-0.000023	0.000046
56	6	0	5.690014	-0.518443	-1.084264
57	6	0	5.689991	0.518392	1.084372
58	6	0	7.081873	-0.526420	-1.086534
59	1	0	5.154536	-0.926217	-1.937214
60	6	0	7.081852	0.526342	1.086681
61	1	0	5.154500	0.926181	1.937305
62	6	0	7.802221	-0.000045	0.000085
63	1	0	7.618288	-0.939131	-1.934583
64	6	0	-4.963950	0.000038	0.000047
65	6	0	-5.690009	0.518455	-1.084265
66	6	0	-5.689981	-0.518380	1.084375
67	6	0	-7.081870	0.526433	-1.086530
68	1	0	-5.154530	0.926235	-1.937209
69	6	0	-7.081844	-0.526352	1.086678
70	1	0	-5.154483	-0.926168	1.937304
71	6	0	-7.802206	0.000040	0.000085
72	1	0	-7.618295	0.939148	-1.934569

73	7	0	-9.218312	0.000032	0.000098
74	1	0	7.618250	0.939046	1.934744
75	7	0	9.218315	-0.000050	0.000099
76	6	0	9.935587	-0.251568	1.204239
77	6	0	9.539092	-1.284612	2.068753
78	6	0	11.055351	0.526190	1.539918
79	6	0	10.243041	-1.523476	3.247968
80	1	0	8.680208	-1.896306	1.811014
81	6	0	11.764235	0.267851	2.712101
82	1	0	11.364652	1.328705	0.877804
83	6	0	11.361327	-0.753348	3.575693
84	1	0	9.922203	-2.326789	3.905987
85	1	0	12.628780	0.879364	2.956770
86	1	0	11.911864	-0.946797	4.491840
87	6	0	9.935581	0.251473	-1.204055
88	6	0	11.055181	-0.526452	-1.539876
89	6	0	9.539230	1.284696	-2.068419
90	6	0	11.764054	-0.268107	-2.712066
91	1	0	11.364368	-1.329094	-0.877863
92	6	0	10.243161	1.523570	-3.247643
93	1	0	8.680472	1.896513	-1.810554
94	6	0	11.361286	0.753269	-3.575514
95	1	0	12.628475	-0.879748	-2.956855
96	1	0	9.922442	2.327020	-3.905553
97	1	0	11.911813	0.946726	-4.491666
98	1	0	-7.618246	-0.939070	1.934731
99	6	0	-9.935572	0.251547	1.204240
100	6	0	-9.539072	1.284583	2.068765
101	6	0	-11.055334	-0.526212	1.539924
102	6	0	-10.243016	1.523434	3.247986
103	1	0	-8.680191	1.896282	1.811030
104	6	0	-11.764212	-0.267887	2.712114
105	1	0	-11.364643	-1.328726	0.877813
106	6	0	-11.361299	0.753304	3.575713
107	1	0	-9.922173	2.326741	3.906010
108	1	0	-12.628753	-0.879405	2.956782
109	1	0	-11.911826	0.946748	4.491868
110	6	0	-9.935565	-0.251520	-1.204051
111	6	0	-9.539181	-1.284721	-2.068428
112	6	0	-11.055202	0.526358	-1.539867
113	6	0	-10.243111	-1.523616	-3.247648
114	1	0	-8.680398	-1.896510	-1.810577
115	6	0	-11.764073	0.267993	-2.712054
116	1	0	-11.364422	1.328988	-0.877854
117	6	0	-11.361270	-0.753362	-3.575510
118	1	0	-9.922361	-2.327049	-3.905564
119	1	0	-12.628519	0.879602	-2.956830
120	1	0	-11.911791	-0.946838	-4.491661
121	46	0	0.000002	0.000014	-0.000019

Porphyrin 11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.259616	-2.563115	-0.134297
2	6	0	-2.535871	-3.243422	-0.161074
3	6	0	-3.501369	-2.283174	-0.163727
4	6	0	-2.828798	-1.001560	-0.123286
5	7	0	-1.468562	-1.206386	-0.108529
6	1	0	-4.571448	-2.425537	-0.195337
7	6	0	-3.478854	0.251506	-0.120443
8	6	0	-2.828668	1.504574	-0.113238
9	6	0	-3.502503	2.785290	-0.074898
10	7	0	-1.468741	1.710265	-0.121951
11	6	0	-2.537727	3.746460	-0.071536
12	1	0	-4.573016	2.926179	-0.047248
13	6	0	-1.260839	3.067146	-0.093717
14	6	0	1.253663	3.066918	-0.081119

15	6	0	2.528523	3.745660	-0.004955
16	7	0	1.463173	1.711097	-0.133422
17	6	0	3.494160	2.785160	-0.009409
18	6	0	2.822768	1.505691	-0.096033
19	1	0	4.563183	2.925688	0.054166
20	6	0	3.474018	0.252894	-0.113234
21	6	0	2.823969	-1.000423	-0.128942
22	6	0	3.495322	-2.280298	-0.214436
23	7	0	1.464183	-1.206041	-0.091423
24	6	0	2.529756	-3.240691	-0.216869
25	1	0	4.564183	-2.421428	-0.277362
26	6	0	1.254867	-2.561904	-0.141784
27	1	0	2.670701	-4.310313	-0.282929
28	6	0	-0.002348	5.198744	-0.032688
29	6	0	-0.320392	5.897771	1.136289
30	6	0	0.320751	5.961504	-1.159551
31	6	0	-0.322553	7.290027	1.187754
32	6	0	0.330366	7.354384	-1.131784
33	6	0	0.005854	8.020202	0.047864
34	6	0	-0.003796	3.702815	-0.075555
35	6	0	-0.000153	-4.694292	-0.188213
36	6	0	-0.313844	-5.395773	-1.356833
37	6	0	0.319272	-5.454676	0.941329
38	6	0	-0.315423	-6.788067	-1.405564
39	6	0	0.329360	-6.847656	0.916381
40	6	0	0.009179	-7.515898	-0.263090
41	6	0	-0.002308	-3.198266	-0.148137
42	9	0	-0.635593	5.227544	2.252620
43	9	0	-0.630871	7.928434	2.322637
44	9	0	0.633751	5.354244	-2.312230
45	9	0	0.642585	8.054423	-2.228922
46	9	0	0.009279	9.355557	0.086054
47	9	0	0.628137	-4.844956	2.093641
48	9	0	0.637912	-7.545384	2.015834
49	9	0	0.013135	-8.851301	-0.298754
50	9	0	-0.619570	-7.428792	-2.540429
51	9	0	-0.625436	-4.727808	-2.475792
52	1	0	2.669340	4.815160	0.063474
53	1	0	-2.680965	4.817641	-0.052241
54	1	0	-2.678328	-4.314717	-0.178947
55	6	0	4.971822	0.253607	-0.115682
56	6	0	5.681469	0.747902	-1.233979
57	6	0	5.687423	-0.239596	0.982036
58	6	0	7.072942	0.757732	-1.282373
59	1	0	5.119345	1.118466	-2.086272
60	6	0	7.085010	-0.237468	0.962065
61	1	0	5.150142	-0.615834	1.848340
62	6	0	7.772554	0.265632	-0.175639
63	1	0	7.586832	1.131077	-2.163031
64	6	0	8.099750	-0.660459	1.904763
65	6	0	9.354437	-0.397215	1.292658
66	6	0	8.060358	-1.227321	3.183927
67	6	0	10.558720	-0.699111	1.936669
68	6	0	9.257080	-1.525168	3.830543
69	1	0	7.107888	-1.433197	3.665405
70	6	0	10.490900	-1.262583	3.209658
71	1	0	11.518921	-0.507389	1.467212
72	1	0	9.239647	-1.965875	4.823126
73	1	0	11.413247	-1.505619	3.730288
74	7	0	9.141489	0.176279	0.041409
75	6	0	-4.977657	0.251399	-0.127244
76	6	0	-5.683423	0.696222	-1.268141
77	6	0	-5.696124	-0.194836	0.988119
78	6	0	-7.074879	0.702949	-1.321555
79	1	0	-5.118533	1.030712	-2.133509
80	6	0	-7.093813	-0.196239	0.962898
81	1	0	-5.161376	-0.533532	1.871383
82	6	0	-7.777740	0.257272	-0.197464
83	1	0	-7.586308	1.037888	-2.218930
84	6	0	-8.111508	-0.582074	1.918172
85	6	0	-9.364373	-0.347328	1.290717
86	6	0	-8.075810	-1.095961	3.219597
87	6	0	-10.570437	-0.625809	1.942036
88	6	0	-9.274297	-1.370681	3.873092
89	1	0	-7.124698	-1.278988	3.712853
90	6	0	-10.506225	-1.136891	3.237085
91	1	0	-11.529371	-0.455893	1.461713

92	1	0	-9.259835	-1.770432	4.882913
93	1	0	-11.430060	-1.360983	3.763563
94	7	0	-9.147518	0.174378	0.017738
95	30	0	-0.002538	0.252019	-0.112337
96	6	0	-10.180121	0.467694	-0.963369
97	6	0	-10.565999	-0.739842	-1.831601
98	1	0	-9.823809	1.291387	-1.592528
99	1	0	-11.057749	0.846749	-0.427052
100	6	0	-11.662549	-0.408029	-2.851533
101	1	0	-10.899039	-1.556071	-1.176720
102	1	0	-9.670228	-1.105290	-2.351253
103	6	0	-12.052318	-1.608478	-3.720536
104	1	0	-11.324264	0.415730	-3.496518
105	1	0	-12.551597	-0.035055	-2.323002
106	1	0	-12.834186	-1.340880	-4.439955
107	1	0	-11.191238	-1.983566	-4.286714
108	1	0	-12.431075	-2.435114	-3.107362
109	6	0	10.178613	0.511999	-0.921234
110	6	0	10.579176	-0.660840	-1.829398
111	1	0	11.049856	0.877096	-0.365017
112	1	0	9.821086	1.355570	-1.522604
113	6	0	11.684242	-0.286463	-2.825065
114	1	0	9.690535	-1.011446	-2.371067
115	1	0	10.910131	-1.498853	-1.201512
116	6	0	12.093397	-1.454042	-3.729224
117	1	0	12.564170	0.075229	-2.273870
118	1	0	11.346778	0.556013	-3.445822
119	1	0	12.882531	-1.157153	-4.428973
120	1	0	12.469988	-2.298487	-3.139407
121	1	0	11.242356	-1.815335	-4.319072

Porphyrin 12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.255192	2.740653	0.066690
2	6	0	2.528310	3.421012	0.157299
3	6	0	3.492530	2.460745	0.207934
4	6	0	2.822484	1.179443	0.133670
5	7	0	1.464950	1.383764	0.054871
6	1	0	4.559594	2.604961	0.292319
7	6	0	3.470836	-0.074567	0.150804
8	6	0	2.822748	-1.328062	0.109910
9	6	0	3.497974	-2.607466	0.052304
10	7	0	1.463051	-1.533941	0.091543
11	6	0	2.533828	-3.568226	0.012119
12	1	0	4.568565	-2.748522	0.030434
13	6	0	1.256482	-2.890135	0.037240
14	6	0	-1.256477	-2.890137	-0.037253
15	6	0	-2.533820	-3.568231	-0.012136
16	7	0	-1.463049	-1.533943	-0.091550
17	6	0	-3.497969	-2.607472	-0.052317
18	6	0	-2.822746	-1.328067	-0.109919
19	1	0	-4.568559	-2.748531	-0.030445
20	6	0	-3.470836	-0.074574	-0.150809
21	6	0	-2.822487	1.179437	-0.133672
22	6	0	-3.492536	2.460738	-0.207926
23	7	0	-1.464954	1.383761	-0.054874
24	6	0	-2.528319	3.421006	-0.157291
25	1	0	-4.559600	2.604952	-0.292306
26	6	0	-1.255198	2.740649	-0.066694
27	1	0	-2.669651	4.492231	-0.182035
28	6	0	0.000005	-5.022878	-0.000013
29	6	0	0.342123	-5.754827	1.142171
30	6	0	-0.342110	-5.754819	-1.142203
31	6	0	0.348251	-7.147848	1.153765
32	6	0	-0.348236	-7.147839	-1.153808
33	6	0	0.000009	-7.846330	-0.000024

34	6	0	0.000003	-3.527160	-0.000008
35	6	0	-0.000005	4.873572	-0.000004
36	6	0	-0.220793	5.604187	-1.171749
37	6	0	0.220781	5.604188	1.171740
38	6	0	-0.225905	6.997344	-1.184064
39	6	0	0.225891	6.997346	1.184054
40	6	0	-0.000008	7.695502	-0.000005
41	6	0	-0.000004	3.376514	-0.000004
42	9	0	0.675857	-5.116653	2.271975
43	9	0	0.678776	-7.816927	2.264404
44	9	0	-0.675847	-5.116637	-2.272001
45	9	0	-0.678759	-7.816910	-2.264452
46	9	0	0.000010	-9.181967	-0.000030
47	9	0	0.438876	4.964196	2.328494
48	9	0	0.440557	7.666699	2.322507
49	9	0	-0.000009	9.031124	-0.000006
50	9	0	-0.440573	7.666697	-2.322517
51	9	0	-0.438887	4.964194	-2.328502
52	1	0	-2.678097	-4.637605	0.049831
53	1	0	2.678107	-4.637600	-0.049852
54	1	0	2.669640	4.492237	0.182050
55	6	0	-4.966454	-0.077121	-0.215209
56	6	0	-5.736235	0.390558	0.861240
57	6	0	-5.643415	-0.559354	-1.343201
58	6	0	-7.128365	0.415015	0.794898
59	1	0	-5.242798	0.745988	1.761109
60	6	0	-7.036806	-0.570145	-1.401553
61	1	0	-5.073618	-0.940941	-2.185434
62	6	0	-7.808067	-0.060354	-0.345142
63	1	0	-7.522025	-0.984377	-2.278632
64	6	0	-9.476517	0.013280	2.045958
65	6	0	-10.138238	-0.377978	3.210526
66	6	0	-9.927014	-0.414706	0.782029
67	6	0	-11.284637	-1.170906	3.136839
68	1	0	-9.757268	-0.046989	4.172493
69	6	0	-11.059408	-1.241761	0.725681
70	6	0	-11.739794	-1.599859	1.890740
71	1	0	-11.808742	-1.454379	4.044692
72	1	0	-11.415391	-1.608192	-0.230970
73	1	0	-12.622322	-2.229355	1.817521
74	7	0	-9.220703	-0.016106	-0.381109
75	16	0	-8.077844	1.116118	2.130268
76	6	0	4.966454	-0.077112	0.215207
77	6	0	5.736236	0.390580	-0.861237
78	6	0	5.643415	-0.559350	1.343197
79	6	0	7.128366	0.415039	-0.794893
80	1	0	5.242799	0.746017	-1.761104
81	6	0	7.036806	-0.570143	1.401548
82	1	0	5.073619	-0.940942	2.185429
83	6	0	7.808065	-0.060346	0.345142
84	1	0	7.522027	-0.984378	2.278627
85	6	0	9.476532	0.013332	-2.045949
86	6	0	10.138267	-0.377901	-3.210518
87	6	0	9.927020	-0.414675	-0.782023
88	6	0	11.284672	-1.170821	-3.136835
89	1	0	9.757302	-0.046900	-4.172482
90	6	0	11.059423	-1.241718	-0.725680
91	6	0	11.739824	-1.599789	-1.890739
92	1	0	11.808786	-1.454275	-4.044689
93	1	0	11.415405	-1.608160	0.230968
94	1	0	12.622358	-2.229276	-1.817522
95	7	0	9.220699	-0.016101	0.381117
96	16	0	8.077849	1.116158	-2.130253
97	30	0	0.000000	-0.074825	-0.000004
98	6	0	9.909911	-0.008687	1.674936
99	6	0	11.095607	0.966348	1.715461
100	1	0	10.231274	-1.019827	1.973430
101	1	0	9.180154	0.316135	2.419682
102	6	0	11.780774	0.985555	3.088759
103	1	0	10.725111	1.968915	1.465914
104	1	0	11.830084	0.706431	0.944568
105	6	0	12.956347	1.966495	3.151684
106	1	0	12.135404	-0.025548	3.335556
107	1	0	11.044969	1.247611	3.862471
108	1	0	13.426074	1.961380	4.141653
109	1	0	13.726874	1.709489	2.414707
110	1	0	12.627723	2.991698	2.942886

111	6	0	-9.909933	-0.008652	-1.674920
112	6	0	-11.095628	0.966387	-1.715402
113	1	0	-10.231300	-1.019781	-1.973449
114	1	0	-9.180191	0.316201	-2.419664
115	6	0	-11.780806	0.985642	-3.088695
116	1	0	-10.725130	1.968944	-1.465823
117	1	0	-11.830100	0.706443	-0.944513
118	6	0	-12.956385	1.966578	-3.151577
119	1	0	-12.135432	-0.025454	-3.335528
120	1	0	-11.045008	1.247731	-3.862402
121	1	0	-13.426114	1.961500	-4.141545
122	1	0	-13.726909	1.709538	-2.414609
123	1	0	-12.627766	2.991774	-2.942738

Porphyrin 13

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.256821	-2.815063	0.024411
2	6	0	2.530810	-3.493050	0.116809
3	6	0	3.496056	-2.532476	0.120040
4	6	0	2.825481	-1.253326	0.021565
5	7	0	1.466361	-1.459040	-0.025507
6	1	0	4.564137	-2.674021	0.194843
7	6	0	3.475967	0.000029	0.000011
8	6	0	2.825470	1.253372	-0.021517
9	6	0	3.496038	2.532534	-0.119921
10	7	0	1.466348	1.459073	0.025553
11	6	0	2.530792	3.493099	-0.116606
12	1	0	4.564119	2.674086	-0.194707
13	6	0	1.256804	2.815096	-0.024311
14	6	0	-1.256826	2.815096	0.024423
15	6	0	-2.530822	3.493095	0.116699
16	7	0	-1.466366	1.459072	-0.025446
17	6	0	-3.496066	2.532526	0.119952
18	6	0	-2.825485	1.253368	0.021554
19	1	0	-4.564151	2.674074	0.194690
20	6	0	-3.475973	0.000018	-0.000024
21	6	0	-2.825472	-1.253325	-0.021571
22	6	0	-3.496046	-2.532481	-0.119970
23	7	0	-1.466351	-1.459029	0.025495
24	6	0	-2.530809	-3.493048	-0.116697
25	1	0	-4.564130	-2.674024	-0.194738
26	6	0	-1.256811	-2.815056	-0.024380
27	1	0	-2.671577	-4.562116	-0.190759
28	6	0	-0.000009	4.947766	0.000069
29	6	0	-0.411208	5.679957	-1.119109
30	6	0	0.411210	5.679950	1.119245
31	6	0	-0.418201	7.072958	-1.130217
32	6	0	0.418204	7.072950	1.130360
33	6	0	0.000000	7.771485	0.000074
34	6	0	-0.000013	3.452193	0.000064
35	6	0	0.000016	-4.947734	0.000048
36	6	0	-0.411413	-5.679912	1.119157
37	6	0	0.411431	-5.679940	-1.119044
38	6	0	-0.418401	-7.072912	1.130287
39	6	0	0.418442	-7.072941	-1.130127
40	6	0	0.000026	-7.771457	0.000091
41	6	0	0.000007	-3.452161	0.000019
42	9	0	-0.812964	5.042120	-2.226738
43	9	0	-0.816229	7.742045	-2.218474
44	9	0	0.812971	5.042107	2.226867
45	9	0	0.816236	7.742032	2.218618
46	9	0	0.000004	9.107136	0.000078
47	9	0	0.813394	-5.042125	-2.226602
48	9	0	0.816685	-7.742041	-2.218296
49	9	0	0.000038	-9.107110	0.000112
50	9	0	-0.816632	-7.741984	2.218478
51	9	0	-0.813387	-5.042067	2.226697

52	1	0	-2.671586	4.562166	0.190759
53	1	0	2.671550	4.562172	-0.190645
54	1	0	2.671577	-4.562114	0.190952
55	6	0	-4.971850	0.000005	-0.000044
56	6	0	-5.699294	-0.526593	1.079898
57	6	0	-5.699273	0.526589	-1.080010
58	6	0	-7.091136	-0.534665	1.082275
59	1	0	-5.164214	-0.940068	1.930290
60	6	0	-7.091113	0.534658	-1.082415
61	1	0	-5.164175	0.940069	-1.930388
62	6	0	-7.811455	-0.000004	-0.000077
63	1	0	-7.627645	-0.953393	1.927372
64	6	0	4.971845	0.000028	-0.000001
65	6	0	5.699295	0.526623	1.079941
66	6	0	5.699263	-0.526576	-1.079959
67	6	0	7.091136	0.534684	1.082316
68	1	0	5.164219	0.940106	1.930332
69	6	0	7.091104	-0.534655	-1.082367
70	1	0	5.164163	-0.940055	-1.930336
71	6	0	7.811450	0.000010	-0.000034
72	1	0	7.627651	0.953414	1.927408
73	7	0	9.228020	0.000007	-0.000049
74	1	0	-7.627608	0.953391	-1.927519
75	7	0	-9.228028	0.000009	-0.000091
76	6	0	-9.944606	-0.250459	-1.204579
77	6	0	-9.544789	-1.279842	-2.072034
78	6	0	-11.066640	0.524874	-1.538620
79	6	0	-10.247742	-1.517578	-3.252048
80	1	0	-8.684073	-1.889572	-1.815812
81	6	0	-11.774407	0.267615	-2.711697
82	1	0	-11.378513	1.324771	-0.874559
83	6	0	-11.368285	-0.749987	-3.578033
84	1	0	-9.924279	-2.318134	-3.912161
85	1	0	-12.640666	0.877297	-2.954925
86	1	0	-11.918018	-0.942578	-4.494849
87	6	0	-9.944611	0.250417	1.204411
88	6	0	-11.066574	-0.524999	1.538482
89	6	0	-9.544848	1.279837	2.071848
90	6	0	-11.774332	-0.267786	2.711577
91	1	0	-11.378404	-1.324924	0.874433
92	6	0	-10.247788	1.517527	3.251878
93	1	0	-8.684183	1.889627	1.815596
94	6	0	-11.368265	0.749852	3.577894
95	1	0	-12.640539	-0.877532	2.954830
96	1	0	-9.924370	2.318111	3.911979
97	1	0	-11.917991	0.942409	4.494722
98	1	0	7.627593	-0.953391	-1.927472
99	6	0	9.944589	0.250422	-1.204554
100	6	0	9.544775	1.279797	-2.072019
101	6	0	11.066593	-0.524945	-1.538605
102	6	0	10.247704	1.517494	-3.252054
103	1	0	8.684078	1.889551	-1.815788
104	6	0	11.774339	-0.267726	-2.711705
105	1	0	11.378463	-1.324838	-0.874537
106	6	0	11.368222	0.749870	-3.578050
107	1	0	9.924245	2.318044	-3.912176
108	1	0	12.640577	-0.877433	-2.954940
109	1	0	11.917939	0.942431	-4.494882
110	6	0	9.944610	-0.250454	1.204437
111	6	0	9.544818	-1.279860	2.071874
112	6	0	11.066618	0.524908	1.538491
113	6	0	10.247772	-1.517592	3.251888
114	1	0	8.684118	-1.889609	1.815639
115	6	0	11.774388	0.267654	2.711568
116	1	0	11.378469	1.324822	0.874440
117	6	0	11.368291	-0.749973	3.577887
118	1	0	9.924330	-2.318166	3.911990
119	1	0	12.640628	0.877357	2.954808
120	1	0	11.918027	-0.942561	4.494702
121	30	0	0.000013	0.000010	0.000006