Electronic Supplementary Information

Design and synthesis of highly twisted phenanthroimidazole substituted blue-emitting truxene based fluorescent chromophores

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Table of Contents

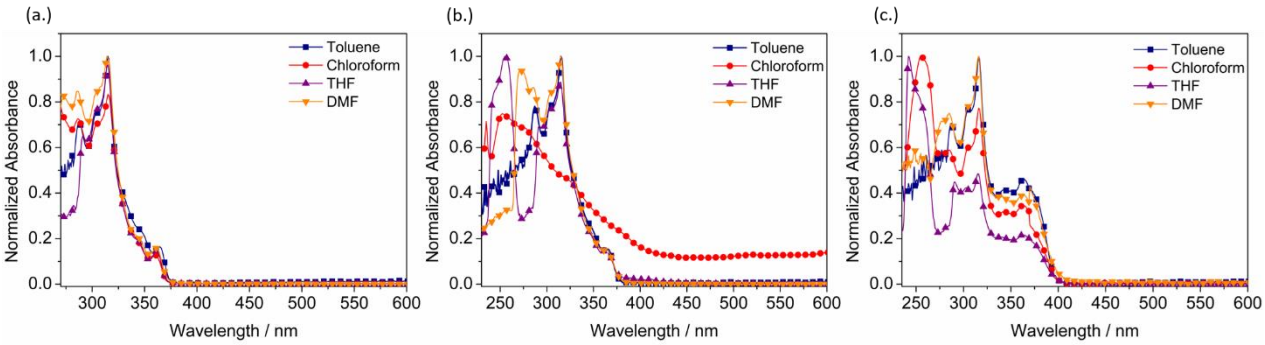


Figure S1. The absorption spectra of the compounds in different solvents (a.) PT_1 (b.) PT_2 and (c.) PT_3

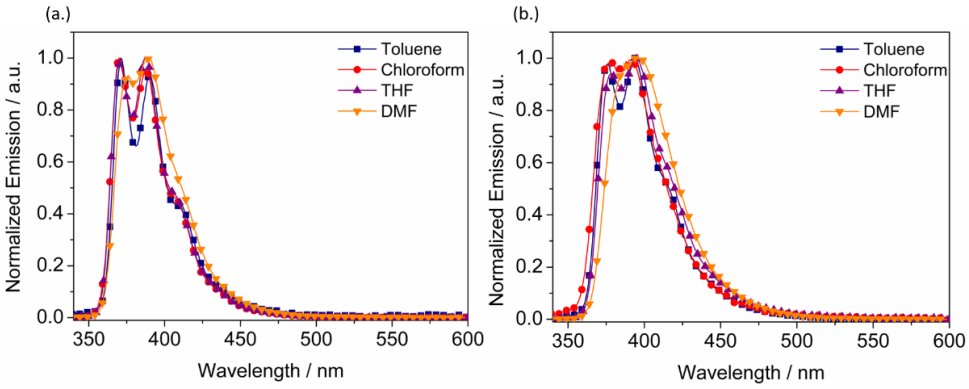


Figure S2. The emission spectra of the compounds in different solvents (a.) PT_1 and (b.) PT_2

Table S1. The absorption properties of the compounds in solvents of different polarities

Compound	Toluene	Chloroform	THF	DMF
PT_1	289, 314, 364	262, 316, 360	256, 315, 364	286, 314, 360
PT_2	286, 312, 364	252, 319,362	258, 315, 368	274, 315, 365
PT_3	288, 315, 364	258, 316, 367	243, 316, 371	255, 316, 367

Table S2. The emission properties of the compounds in solvents of different polarities

Compound	Toluene	Chloroform	THF	DMF
PT_1	386	388	386	389
PT_2	394	396	396	398
PT_3	415	418	421	434

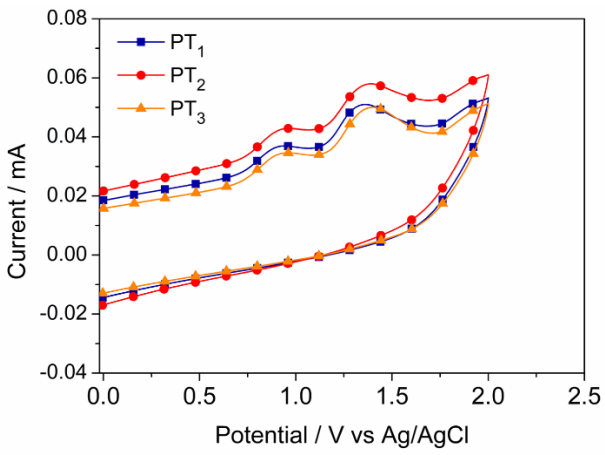
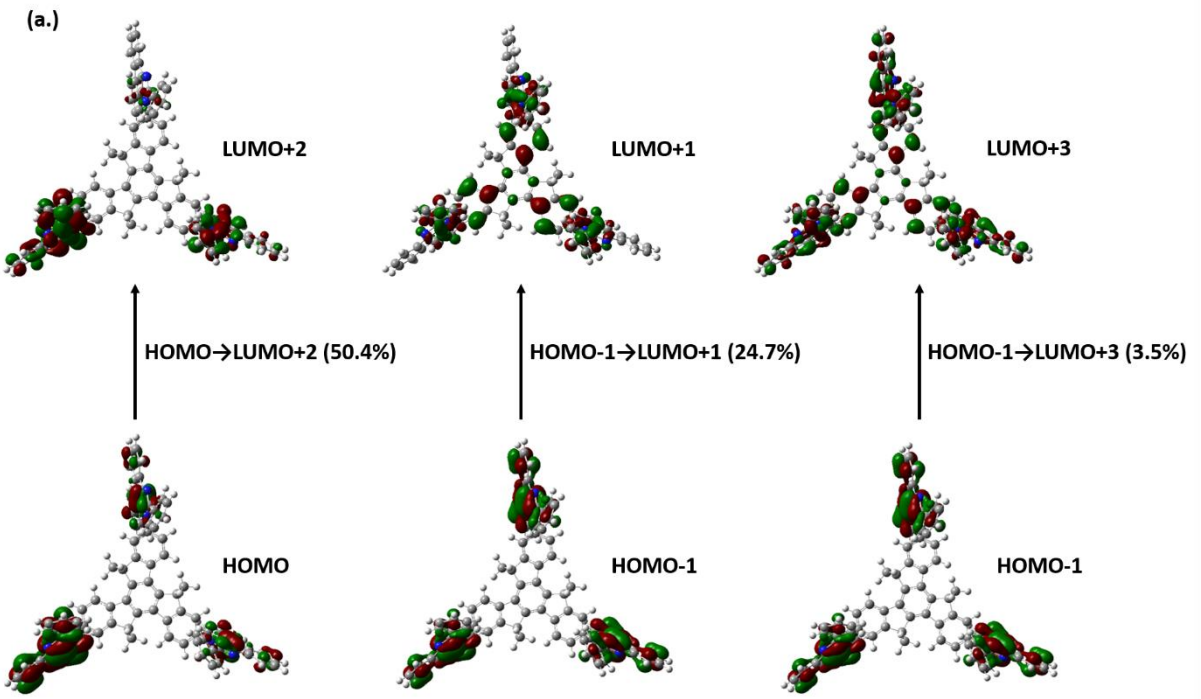


Figure S3. Cyclic voltammogram of the synthesized target molecules at 100 mV/s scan rate in 0.1 M tetrabutylammonium perchlorate solution in DCM.



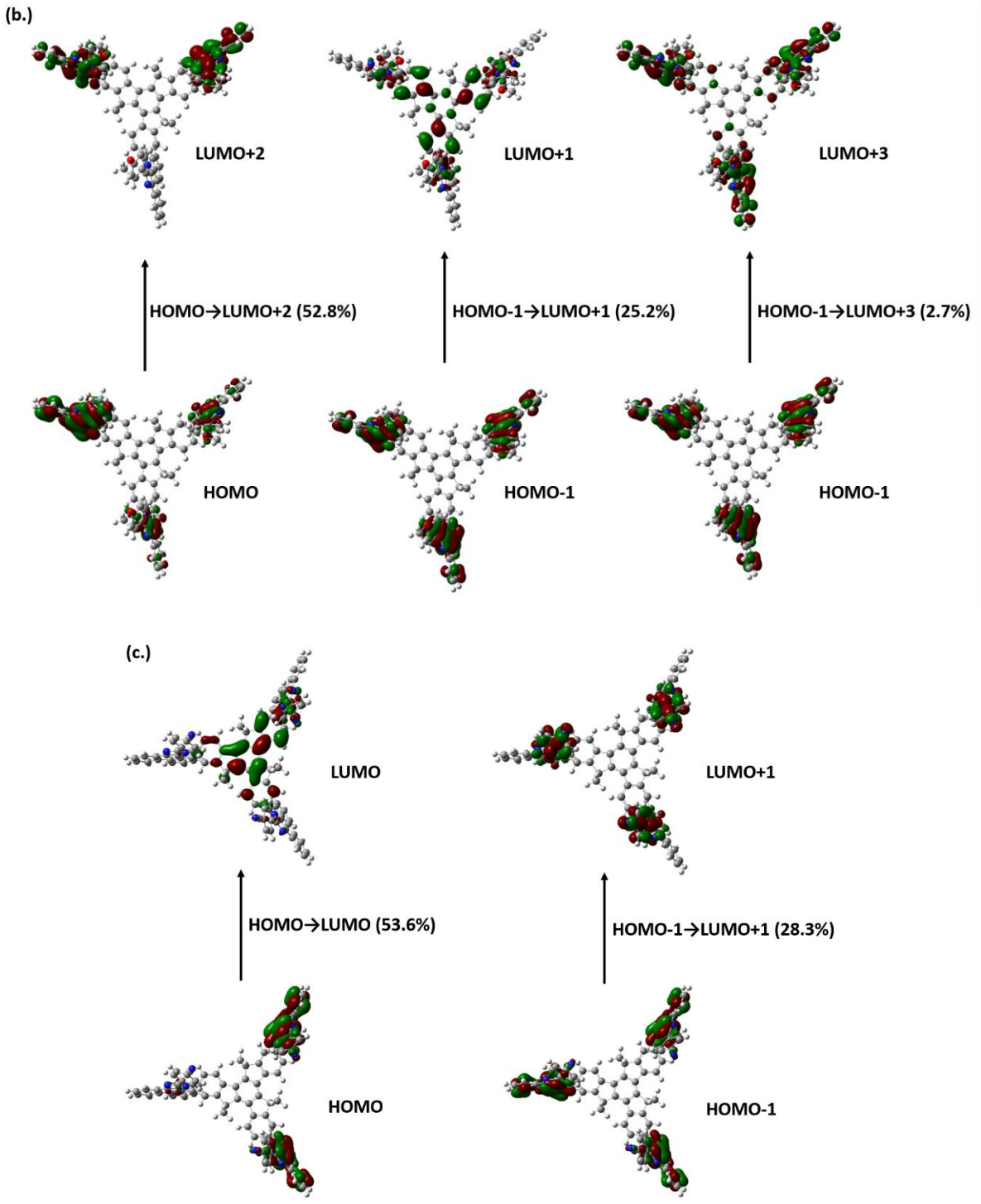
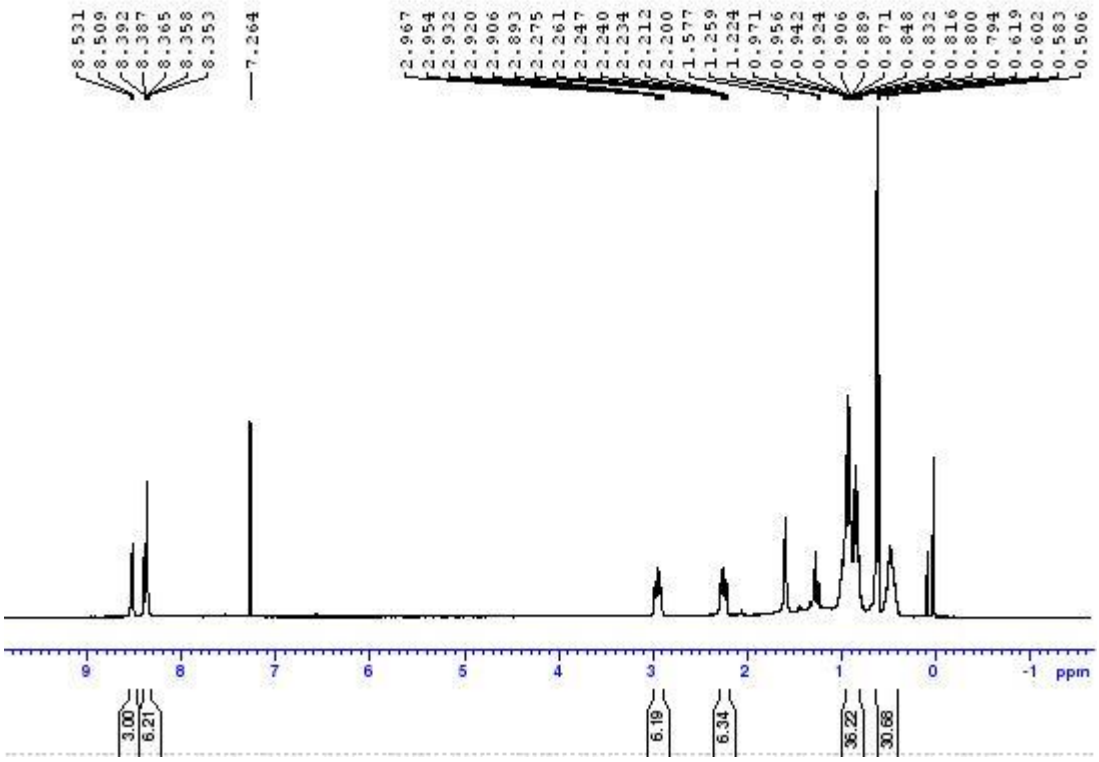
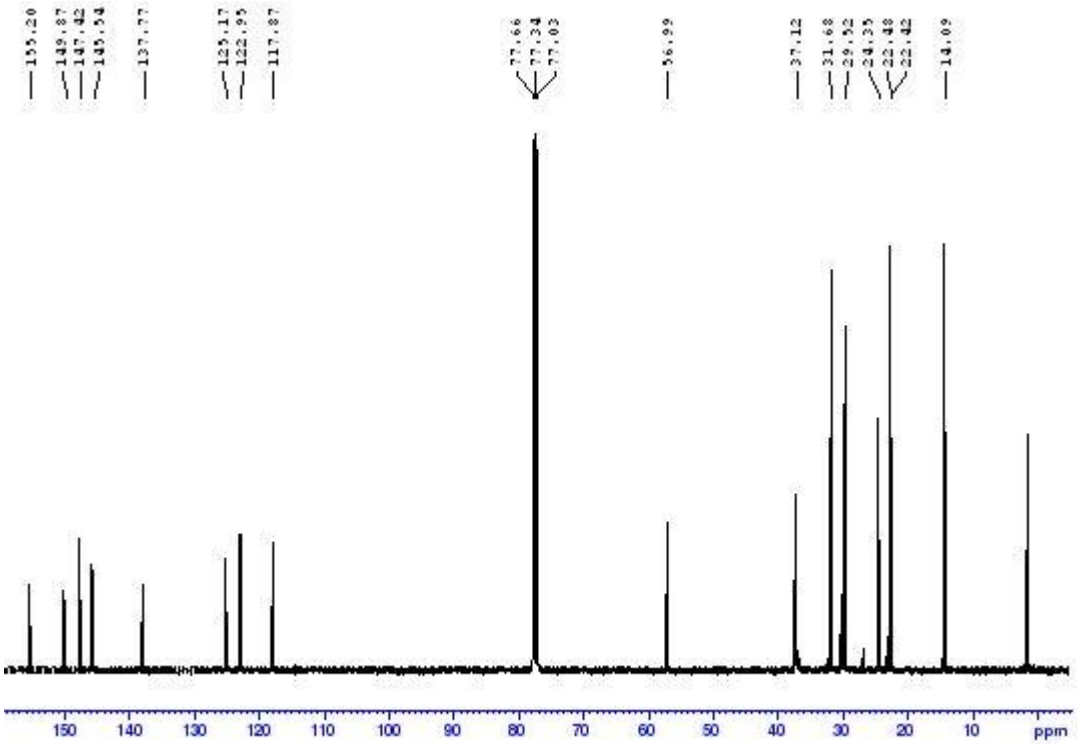


Figure S4. The major transitions in (a.) PT_1 (b.) PT_2 and (c.) PT_3

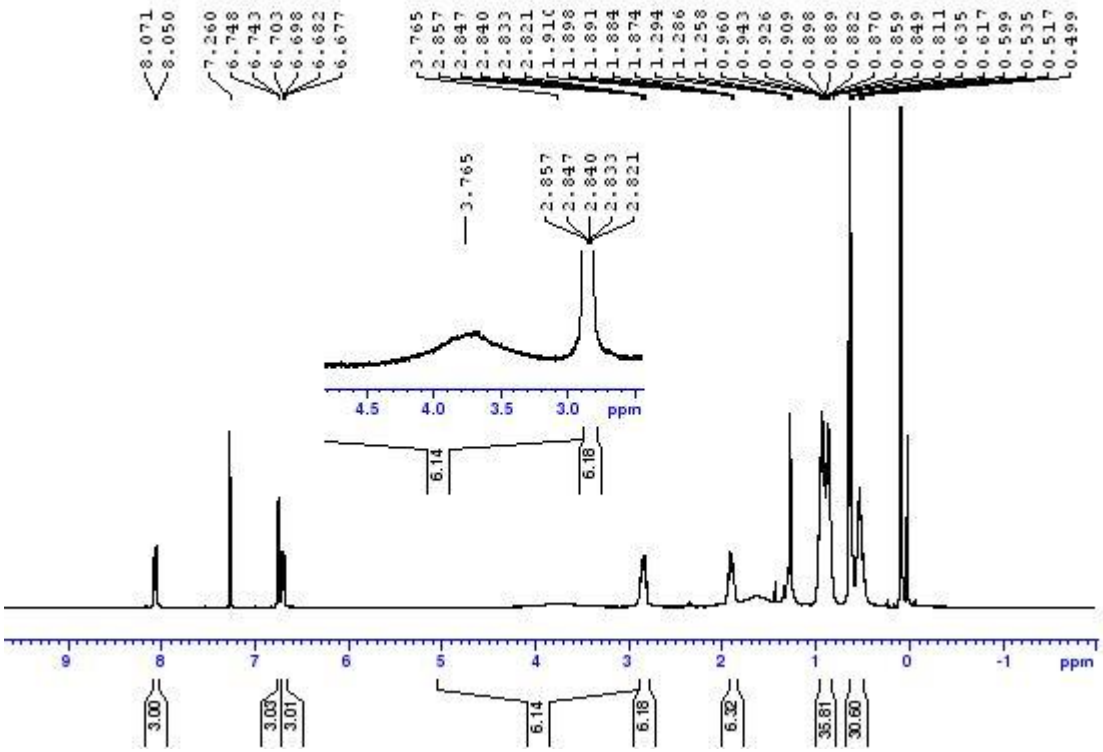
Copies of ^{1}H NMR, ^{13}C NMR and HRMS of the compounds

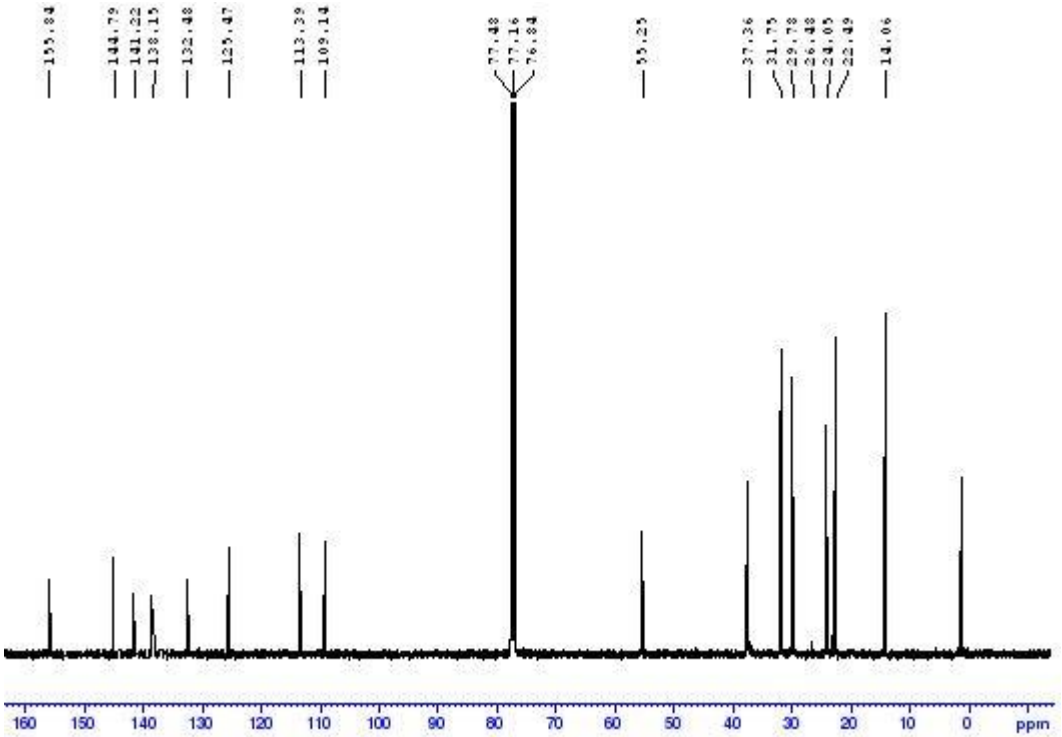
a.) ^{1}H NMR and ^{13}C NMR of 3



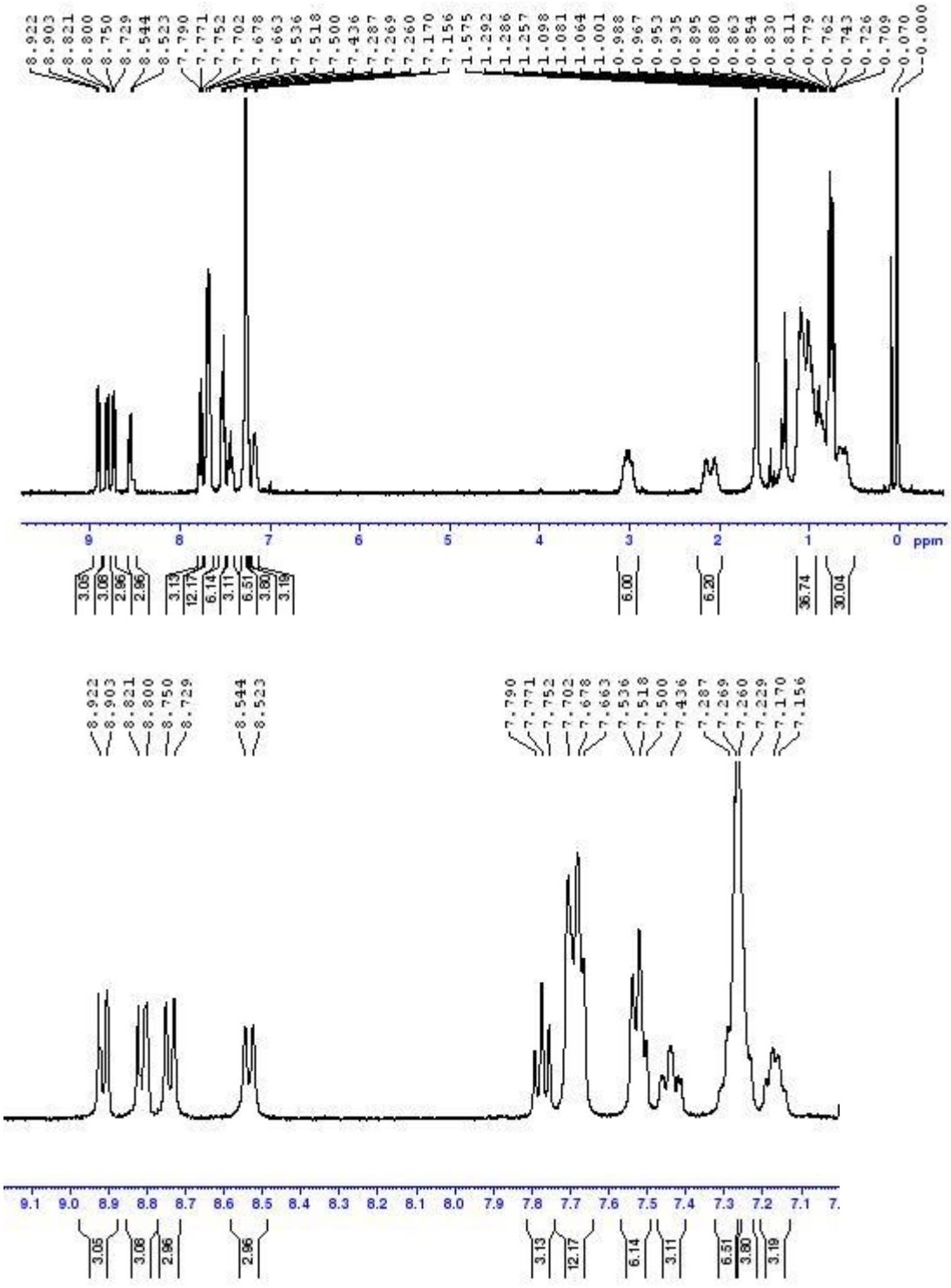


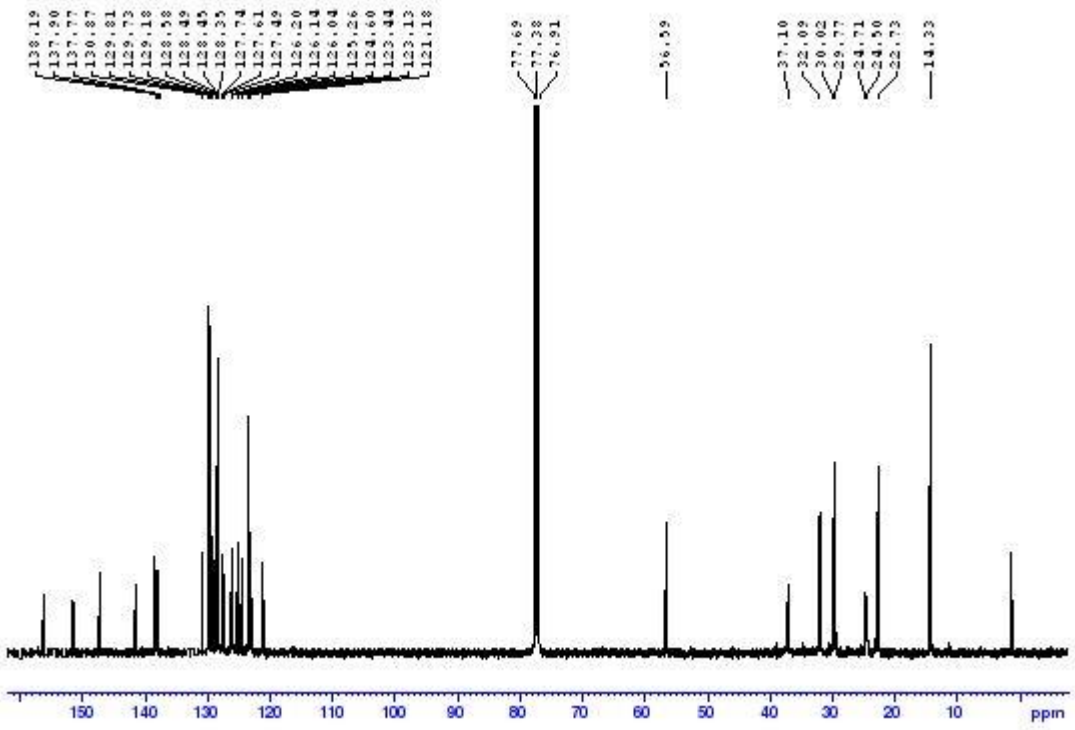
b.) ^{1}H NMR and ^{13}C NMR of 4





c.) ^{1}H NMR, ^{13}C NMR and HRMS of PT$_1$

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129.81
129.73
129.18
128.58
128.49
128.45
128.35
127.74
127.61
127.49
126.20
126.14
126.04
125.26
124.60
123.44
123.13
121.18
77.69
77.38
76.91
56.59
37.10
32.09
30.02
29.77
24.71
24.50
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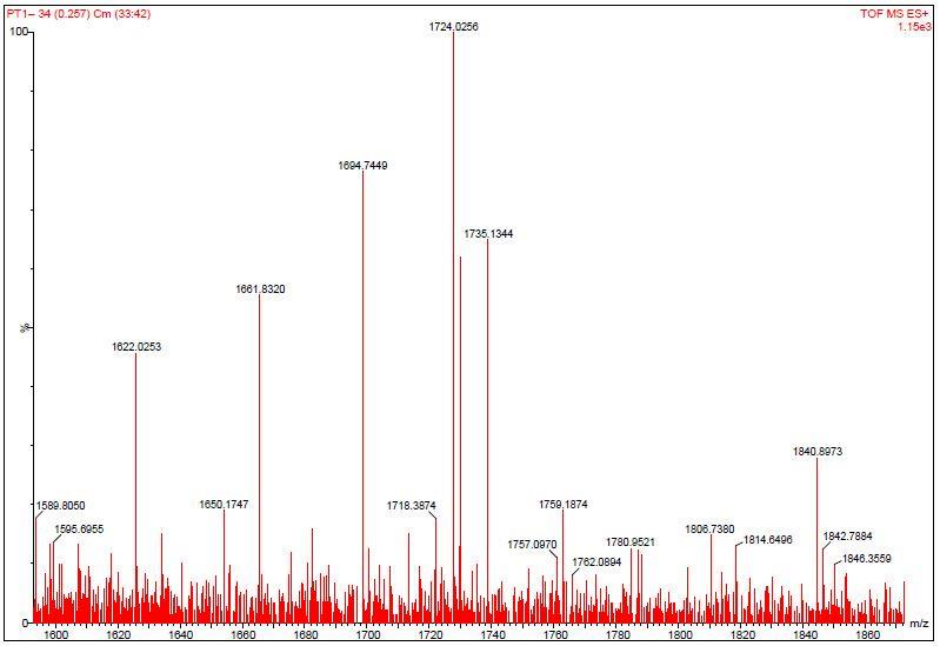
90
80
70
60
50
40
30
20
10
ppm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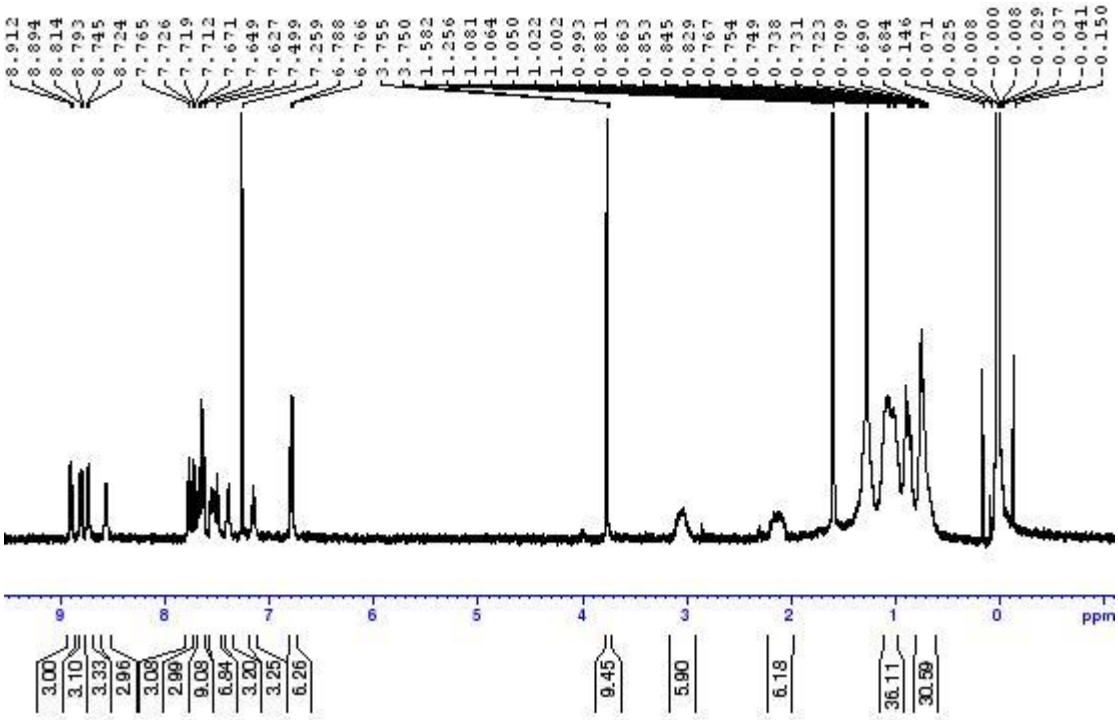
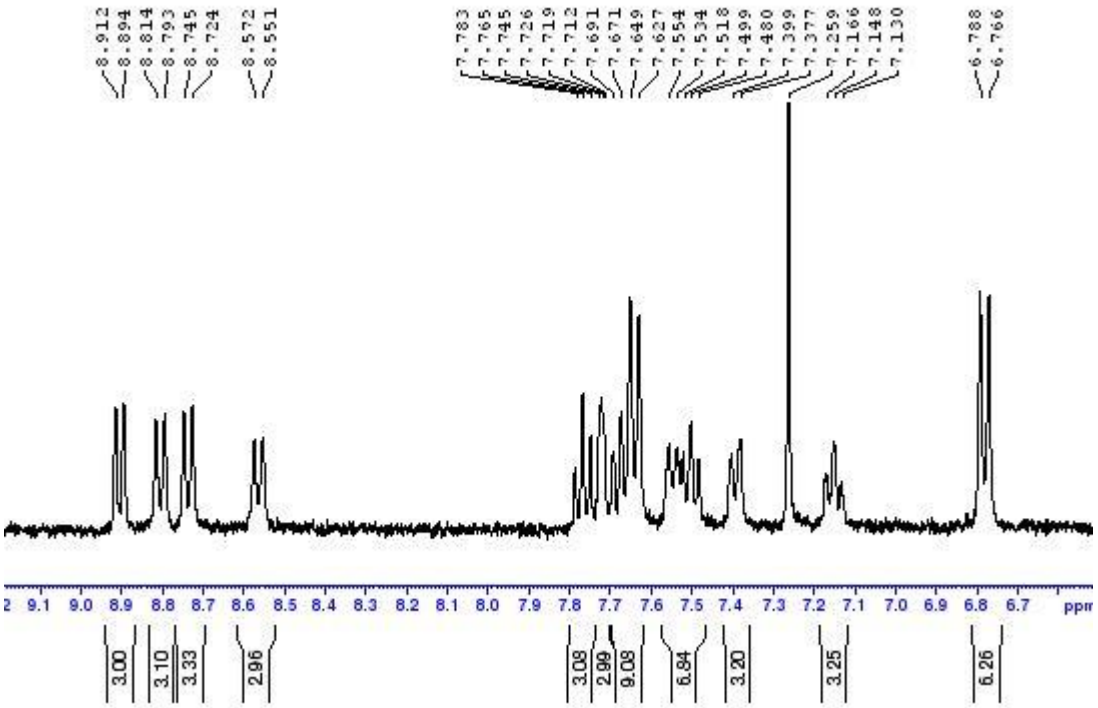
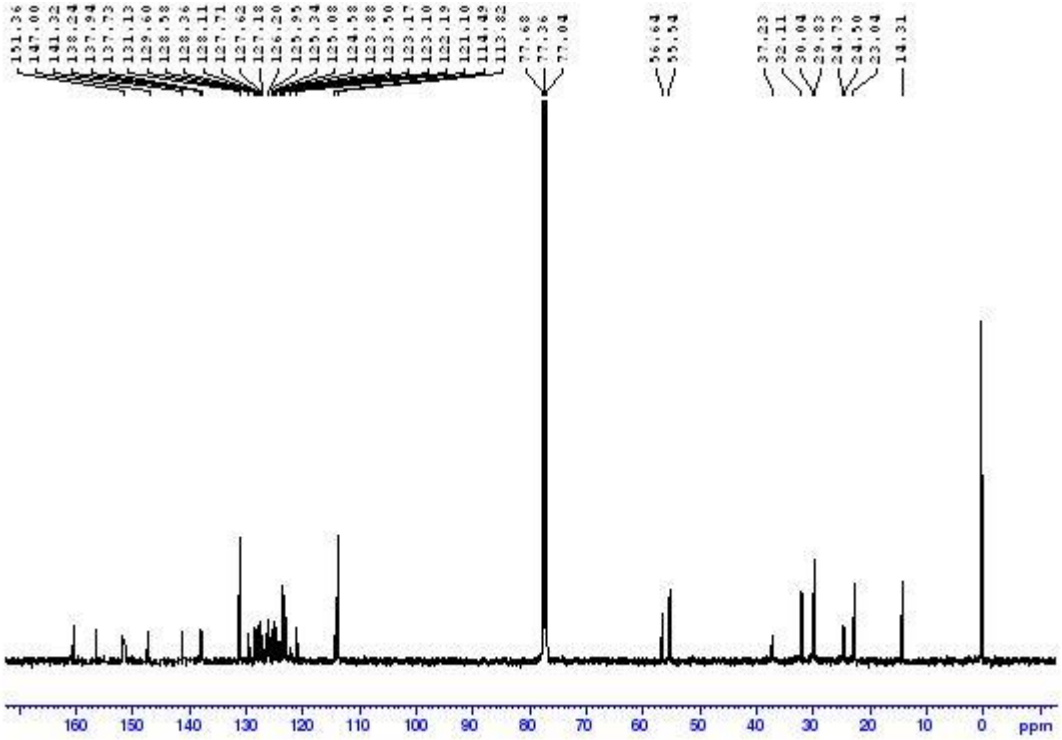
100
%
0
1724.0256
1694.7449
1735.1344
1661.8320
1622.0253
1840.8973
1589.8050
1650.1747
1718.3874
1759.1874
1596.6955
1757.0970
1780.9521
1806.7380
1814.6496
1842.7884
1762.0894
1846.3559
1600
1620
1640
1660
1680
1700
1720
1740
1760
1780
1800
1820
1840
1860
m/z

d.) ^{1}H NMR, ^{13}C NMR and HRMS of PT_2



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141.32
138.24
137.94
137.73
131.13
129.60
128.58
128.36
128.11
127.71
127.62
127.18
126.20
125.95
125.24
125.08
124.58
123.88
123.50
123.17
123.10
122.19
121.10
114.49
113.82
77.68
77.36
77.04
56.64
55.54
37.23
32.11
30.04
29.83
24.73
24.50
23.04
14.31
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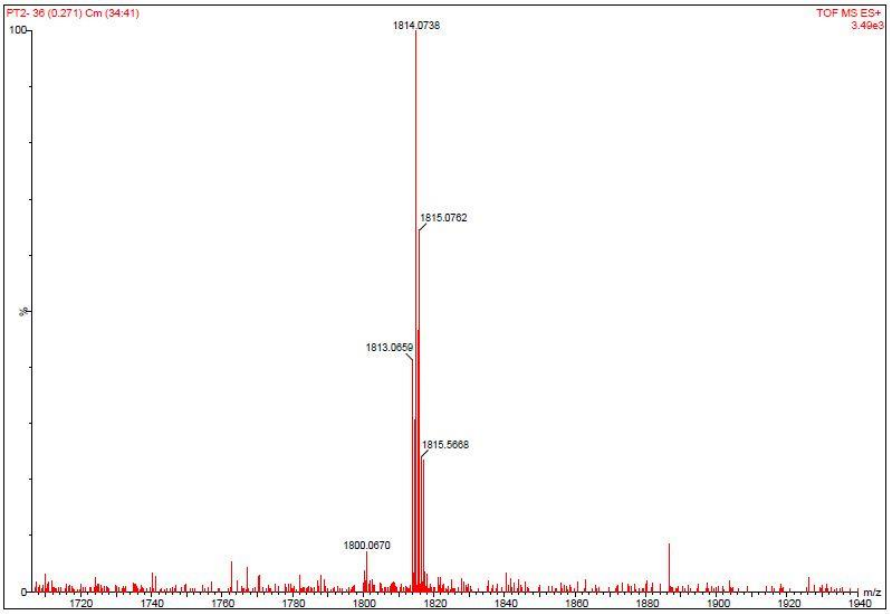
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


PT2- 36 (0.271) Cm (34:41)
TOF MS ES+
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100
%
0
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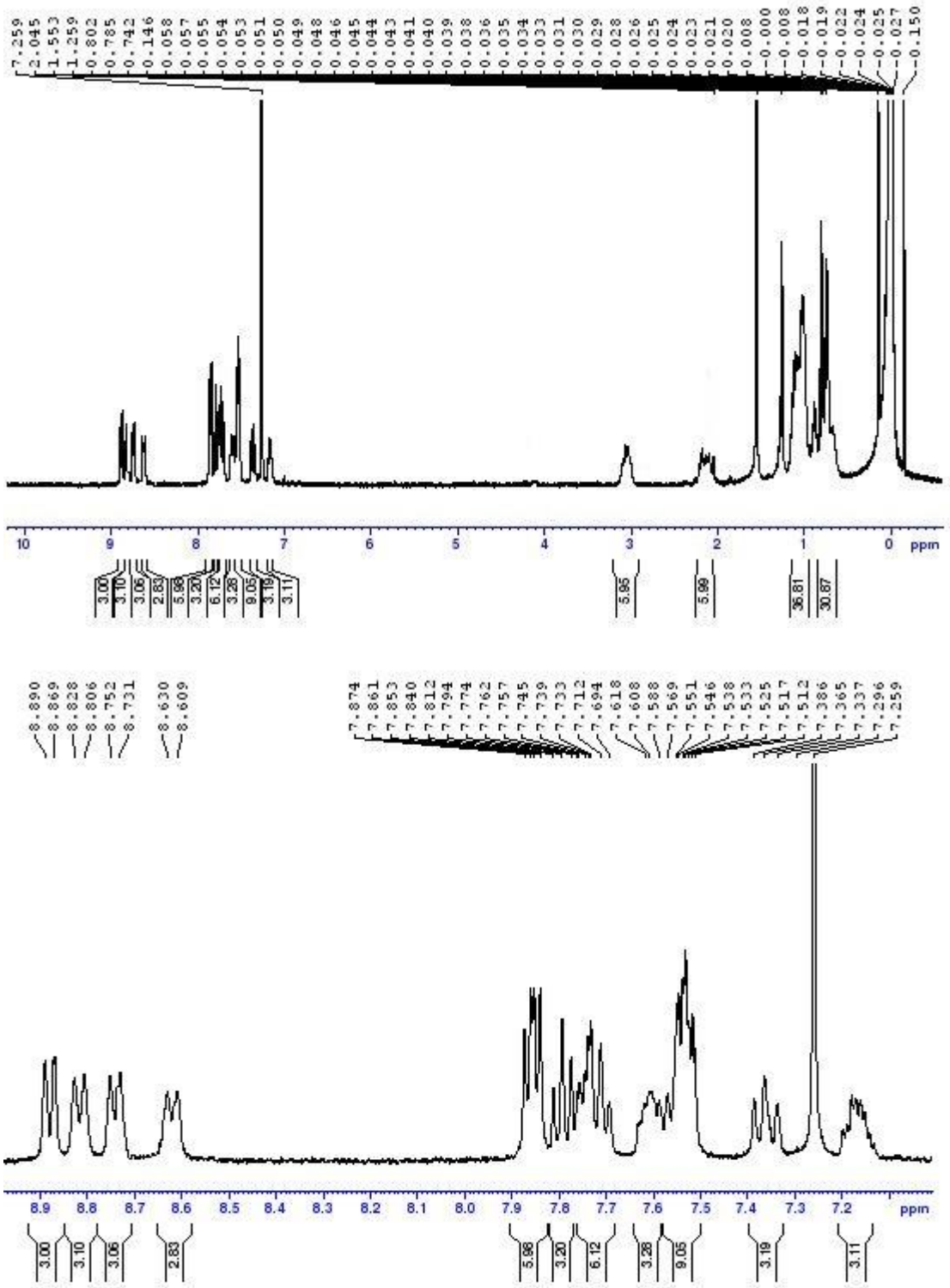
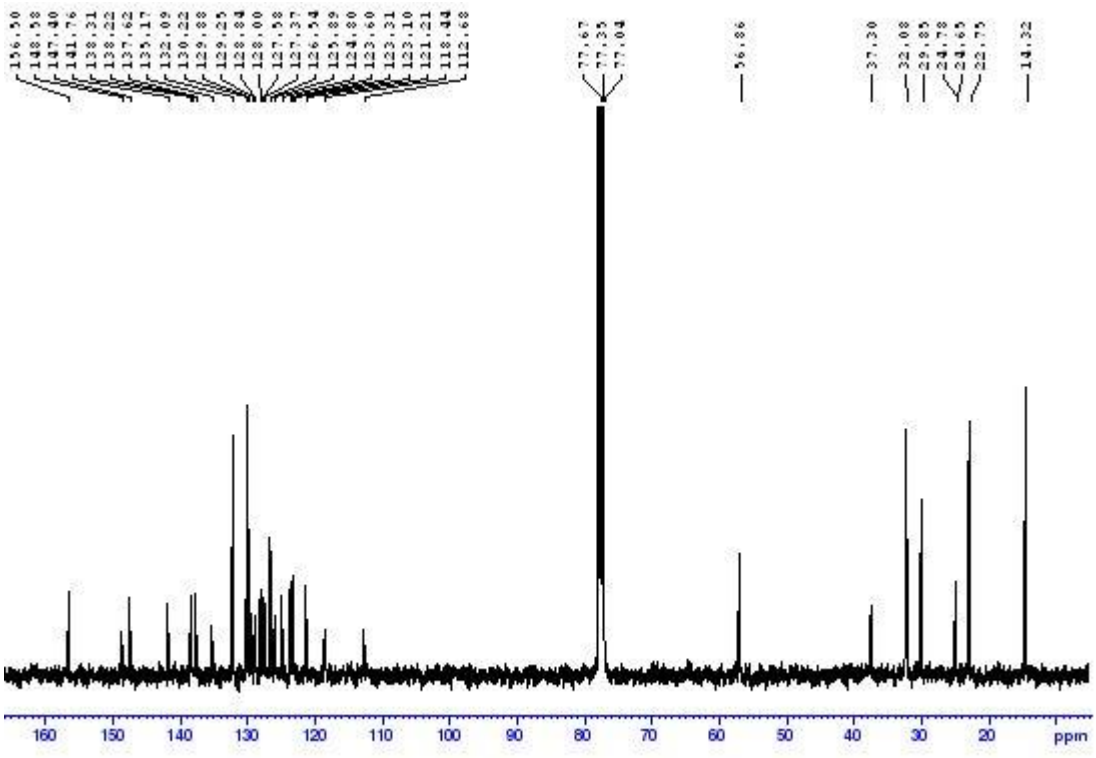
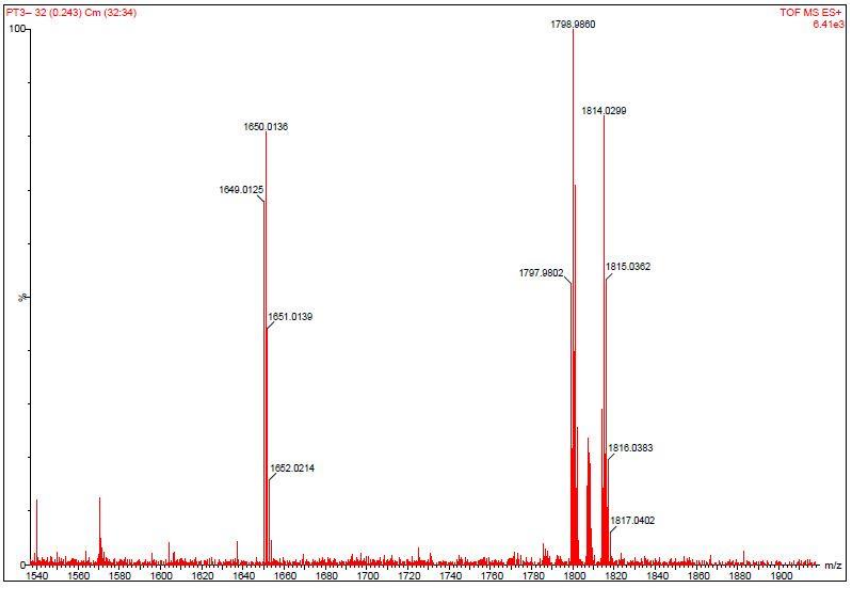
1815.0762
1813.0659
1815.5668
1800.0670
1720
1740
1760
1780
1800
1820
1840
1860
1880
1900
1920
1940
m/z

e.) ^{1}H NMR, ^{13}C NMR and HRMS of PT_3







Coordinates of optimized geometries from DFT calculations

PT_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.917610	1.073743	0.361538
2	6	0	0.482213	1.328812	0.361262
3	6	0	1.388694	0.257802	0.361538
4	6	0	0.909678	-1.082015	0.361262
5	6	0	-0.471084	-1.331546	0.361538
6	6	0	-1.391891	-0.246797	0.361262
7	6	0	-1.215043	-2.671952	0.363578
8	6	0	-2.663229	-2.216422	0.366394
9	6	0	-2.766402	-0.811750	0.362707
10	6	0	2.921499	0.283718	0.363578
11	6	0	3.251092	-1.198213	0.366394
12	6	0	2.086197	-1.989899	0.362707
13	6	0	-1.706457	2.388234	0.363578
14	6	0	-0.587863	3.414635	0.366394
15	6	0	0.680205	2.801649	0.362707
16	6	0	-3.787391	-3.031608	0.373684
17	6	0	-5.056676	-2.442665	0.370261
18	6	0	-5.181003	-1.052661	0.362241
19	6	0	-4.047253	-0.239951	0.360844
20	6	0	4.519145	-1.764172	0.373684
21	6	0	4.643748	-3.157877	0.370261
22	6	0	3.502133	-3.960550	0.362241
23	6	0	2.231431	-3.385049	0.360844
24	6	0	-0.731755	4.795781	0.373684
25	6	0	0.412928	5.600542	0.370261
26	6	0	1.678870	5.013211	0.362241
27	6	0	1.815823	3.625000	0.360844
28	1	0	-3.703374	-4.113897	0.377444
29	1	0	-6.170554	-0.608480	0.357879
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33	1	0	1.379956	-4.047511	0.355509
34	1	0	-1.711052	5.264164	0.377444

35	1	0	2.558318	5.648097	0.357879
36	1	0	2.815270	3.218833	0.355509
37	6	0	-2.543155	2.570343	1.655781
38	1	0	-1.887022	2.566060	2.530891
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40	1	0	-3.282519	1.782485	1.797455
41	6	0	-0.962562	-3.487325	-0.930575
42	1	0	0.088785	-3.732966	-1.078583
43	1	0	-1.528865	-4.423774	-0.907080
44	1	0	-1.293134	-2.917411	-1.803506
45	6	0	-0.954405	-3.487609	1.655781
46	1	0	-1.278762	-2.917239	2.530891
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66	6	0	7.918105	-4.571520	-0.183371
67	6	0	-7.071541	-3.495448	1.471618
68	6	0	-6.782775	-3.958281	-0.699843

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71	7	0	5.943167	-3.759757	0.382189
72	7	0	-6.227629	-3.267055	0.382189
73	7	0	0.341255	9.139019	1.142799
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75	7	0	-8.085250	-4.273974	1.142799
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77	6	0	0.546605	6.239878	3.426922
78	6	0	1.670709	8.374827	3.577787
79	6	0	0.949480	5.944477	4.729000
80	1	0	-0.066754	5.527117	2.890596
81	6	0	2.068932	8.074759	4.876323
82	1	0	1.934320	9.321650	3.120541
83	6	0	1.714782	6.854762	5.457491
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86	1	0	2.027430	6.619339	6.470540
87	6	0	6.003499	-4.517118	2.828168
88	6	0	5.130591	-3.593313	3.426922
89	6	0	6.417458	-5.634290	3.577787
90	6	0	4.673328	-3.794512	4.729000
91	1	0	4.820001	-2.705748	2.890596
92	6	0	5.958481	-5.829127	4.876323
93	1	0	7.105626	-6.335995	3.120541
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98	6	0	-6.913689	-2.940623	2.828168
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112	6	0	-0.551587	6.109754	-4.016310
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125	6	0	6.681194	-2.849272	-4.822195
126	1	0	4.682984	-2.111771	-4.442296
127	1	0	8.635740	-3.671518	-4.921237
128	1	0	6.671538	-2.591163	-5.876861
129	6	0	-6.408497	-4.062152	-2.085814
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133	1	0	-4.700626	-2.734549	-2.067810
134	6	0	-6.893507	-5.020312	-4.272378
135	6	0	-5.808139	-4.361448	-4.822195
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137	1	0	-7.497498	-5.643011	-4.921237
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148	1	0	-1.173232	13.344948	-3.211515
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154	6	0	10.187440	-4.792722	-3.130242
155	6	0	11.281868	-5.442807	-2.586039
156	1	0	12.144675	-6.335144	-0.812143
157	1	0	10.225544	-4.512538	-4.176394
158	1	0	12.143680	-5.656425	-3.211515
159	6	0	-8.761817	-5.409174	-0.986511
160	6	0	-9.895458	-6.046418	-0.443647
161	6	0	-8.412732	-5.585212	-2.354686
162	6	0	-10.686618	-6.858789	-1.233571
163	1	0	-10.121448	-5.883169	0.604730
164	6	0	-9.244339	-6.426221	-3.130242
165	6	0	-10.354544	-7.048981	-2.586039
166	1	0	-11.558733	-7.350026	-0.812143
167	1	0	-9.020745	-6.599312	-4.176394
168	1	0	-10.970448	-7.688523	-3.211515

PT_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.960030	-1.036030	-0.138758
2	6	0	-0.428510	-1.347118	-0.139353
3	6	0	-1.377243	-0.313395	-0.138758
4	6	0	-0.952384	1.044660	-0.139353
5	6	0	0.417213	1.349425	-0.138758
6	6	0	1.380894	0.302458	-0.139353
7	6	0	1.106853	2.718521	-0.133552
8	6	0	2.572170	2.321175	-0.128931
9	6	0	2.731787	0.921892	-0.136338
10	6	0	-2.907735	-0.400698	-0.133552
11	6	0	-3.296282	1.066977	-0.128931
12	6	0	-2.164275	1.904851	-0.136338
13	6	0	1.800882	-2.317823	-0.133552
14	6	0	0.724111	-3.388153	-0.128931
15	6	0	-0.567512	-2.826743	-0.136338
16	6	0	3.662035	3.181506	-0.116259
17	6	0	4.954461	2.645142	-0.119601
18	6	0	5.134573	1.261230	-0.133809
19	6	0	4.034958	0.402792	-0.139476
20	6	0	-4.586283	1.580662	-0.116259
21	6	0	-4.767991	2.968118	-0.119601
22	6	0	-3.659544	3.816055	-0.133809
23	6	0	-2.366307	3.292980	-0.139476
24	6	0	0.924248	-4.762168	-0.116259
25	6	0	-0.186470	-5.613261	-0.119601
26	6	0	-1.475029	-5.077285	-0.133809
27	6	0	-1.668651	-3.695772	-0.139476
28	1	0	3.533450	4.259359	-0.107744
29	1	0	6.141389	0.857769	-0.137891

30	1	0	4.226091	-0.658988	-0.148319
31	1	0	-5.455438	0.930378	-0.107744
32	1	0	-3.813544	4.889715	-0.137891
33	1	0	-1.542345	3.989396	-0.148319
34	1	0	1.921988	-5.189737	-0.107744
35	1	0	-2.327845	-5.747483	-0.137891
36	1	0	-2.683746	-3.330408	-0.148319
37	6	0	2.643797	-2.463520	1.159002
38	1	0	1.988231	-2.479749	2.034350
39	1	0	3.206854	-3.402145	1.141392
40	1	0	3.353768	-1.648488	1.297190
41	6	0	0.824604	3.524800	-1.427145
42	1	0	-0.235648	3.726814	-1.577516
43	1	0	1.351821	4.483717	-1.400684
44	1	0	1.180695	2.970341	-2.299993
45	6	0	0.811572	3.521356	1.159002
46	1	0	1.153410	2.961733	2.034350
47	1	0	1.342917	4.478289	1.141392
48	1	0	-0.249251	3.728692	1.297190
49	6	0	-3.464868	-1.048272	-1.427145
50	1	0	-3.109691	-2.067484	-1.577516
51	1	0	-4.558924	-1.071147	-1.400684
52	1	0	-3.162738	-0.462658	-2.299993
53	6	0	-3.455369	-1.057836	1.159002
54	1	0	-3.141641	-0.481984	2.034350
55	1	0	-4.549771	-1.076145	1.141392
56	1	0	-3.104516	-2.080204	1.297190
57	6	0	2.640265	-2.476528	-1.427145
58	1	0	3.345339	-1.659330	-1.577516
59	1	0	3.207102	-3.412570	-1.400684
60	1	0	1.982043	-2.507683	-2.299993
61	6	0	-0.196214	-7.876249	0.999550
62	6	0	0.367740	-7.854104	-1.168635
63	6	0	0.380717	-9.139171	-0.640301

64	6	0	-6.722925	4.108051	0.999550
65	6	0	-6.985724	3.608580	-1.168635
66	6	0	-8.105113	4.239875	-0.640301
67	6	0	6.919139	3.768198	0.999550
68	6	0	6.617984	4.245524	-1.168635
69	6	0	7.724396	4.899296	-0.640301
70	7	0	0.000000	-7.032554	-0.096746
71	7	0	-6.090371	3.516277	-0.096746
72	7	0	6.090371	3.516277	-0.096746
73	7	0	0.029607	-9.138220	0.683762
74	7	0	-7.928734	4.543470	0.683762
75	7	0	7.899127	4.594750	0.683762
76	6	0	-0.628749	-7.466003	2.345245
77	6	0	-0.336081	-6.224203	2.941126
78	6	0	-1.341993	-8.405647	3.106789
79	6	0	-0.757538	-5.934276	4.230922
80	1	0	0.241528	-5.481019	2.406482
81	6	0	-1.768743	-8.125488	4.402135
82	1	0	-1.554859	-9.372395	2.664724
83	1	0	-0.526779	-4.980222	4.692996
84	1	0	-2.321357	-8.878048	4.951663
85	6	0	-6.151374	4.277515	2.345245
86	6	0	-5.222277	3.403156	2.941126
87	6	0	-6.608507	5.365023	3.106789
88	6	0	-4.760465	3.623186	4.230922
89	1	0	-4.867466	2.531340	2.406482
90	6	0	-6.152507	5.594520	4.402135
91	1	0	-7.339302	6.032745	2.664724
92	1	0	-4.049610	2.946315	4.692996
93	1	0	-6.527936	6.449378	4.951663
94	6	0	6.780123	3.188489	2.345245
95	6	0	5.558358	2.821047	2.941126
96	6	0	7.950500	3.040624	3.106789
97	6	0	5.518003	2.311091	4.230922

98	1	0	4.625938	2.949679	2.406482
99	6	0	7.921250	2.530968	4.402135
100	1	0	8.894162	3.339650	2.664724
101	1	0	4.576389	2.033907	4.692996
102	1	0	8.849294	2.428670	4.951663
103	6	0	0.649199	-7.582445	-2.553295
104	6	0	0.565119	-6.304116	-3.153459
105	6	0	1.015252	-8.711943	-3.362554
106	6	0	0.848445	-6.118666	-4.494121
107	1	0	0.264123	-5.453851	-2.557721
108	6	0	1.299674	-8.474229	-4.725412
109	6	0	1.225396	-7.211829	-5.286751
110	1	0	0.772967	-5.126401	-4.929245
111	1	0	1.579387	-9.303485	-5.363996
112	1	0	1.450816	-7.074009	-6.339968
113	6	0	-6.891189	3.229000	-2.553295
114	6	0	-5.742084	2.662651	-3.153459
115	6	0	-8.052390	3.476738	-3.362554
116	6	0	-5.723143	2.324559	-4.494121
117	1	0	-4.855236	2.498188	-2.557721
118	6	0	-7.988734	3.111564	-4.725412
119	6	0	-6.858325	2.544690	-5.286751
120	1	0	-4.826077	1.893791	-4.929245
121	1	0	-8.846748	3.283953	-5.363996
122	1	0	-6.851680	2.280561	-6.339968
123	6	0	6.241990	4.353445	-2.553295
124	6	0	5.176965	3.641465	-3.153459
125	6	0	7.037138	5.235206	-3.362554
126	6	0	4.874698	3.794108	-4.494121
127	1	0	4.591112	2.955663	-2.557721
128	6	0	6.689061	5.362665	-4.725412
129	6	0	5.632929	4.667138	-5.286751
130	1	0	4.053110	3.232609	-4.929245
131	1	0	7.267361	6.019532	-5.363996

132	1	0	5.400863	4.793448	-6.339968
133	6	0	0.741452	-10.281278	-1.429829
134	6	0	0.776394	-11.576433	-0.875017
135	6	0	1.074273	-10.065747	-2.796610
136	6	0	1.139364	-12.660740	-1.650990
137	1	0	0.516043	-11.691357	0.171813
138	6	0	1.443684	-11.199286	-3.557791
139	6	0	1.476290	-12.466648	-3.001839
140	1	0	1.167236	-13.657292	-1.220037
141	1	0	1.712082	-11.090536	-4.602124
142	1	0	1.765191	-13.314149	-3.616592
143	6	0	-9.274574	4.498523	-1.429829
144	6	0	-10.413682	5.115840	-0.875017
145	6	0	-9.254329	4.102526	-2.796610
146	6	0	-11.534205	5.343651	-1.650990
147	1	0	-10.383034	5.398772	0.171813
148	6	0	-10.420708	4.349376	-3.557791
149	6	0	-11.534579	4.954819	-3.001839
150	1	0	-12.411180	5.817790	-1.220037
151	1	0	-10.460727	4.062562	-4.602124
152	1	0	-12.412987	5.128374	-3.616592
153	6	0	8.533122	5.782755	-1.429829
154	6	0	9.637288	6.460593	-0.875017
155	6	0	8.180057	5.963221	-2.796610
156	6	0	10.394840	7.317088	-1.650990
157	1	0	9.866991	6.292585	0.171813
158	6	0	8.977024	6.849910	-3.557791
159	6	0	10.058288	7.511829	-3.001839
160	1	0	11.243943	7.839502	-1.220037
161	1	0	8.748645	7.027974	-4.602124
162	1	0	10.647795	8.185775	-3.616592
163	6	0	-5.216064	4.722432	4.972104
164	6	0	-1.481714	-6.878460	4.972104
165	6	0	6.697778	2.156028	4.972104

166	8	0	-4.696027	4.850163	6.225787
167	8	0	-1.852351	-6.491960	6.225787
168	8	0	6.548378	1.641797	6.225787
169	6	0	-5.136259	5.934819	7.029610
170	1	0	-4.605177	5.840984	7.977758
171	1	0	-4.891555	6.902367	6.573453
172	1	0	-6.216755	5.888621	7.214645
173	6	0	-2.571575	-7.415541	7.029610
174	1	0	-2.755852	-6.908692	7.977758
175	1	0	-3.531848	-7.687394	6.573453
176	1	0	-1.991317	-8.328178	7.214645
177	6	0	7.707834	1.480721	7.029610
178	1	0	7.361029	1.067708	7.977758
179	1	0	8.423403	0.785027	6.573453
180	1	0	8.208073	2.439558	7.214645

PT_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109843	-0.874164	0.008199
2	6	0	-1.308459	0.534719	0.007812
3	6	0	-0.202127	1.398234	0.008199
4	6	0	1.117310	0.865799	0.007812
5	6	0	1.311970	-0.524070	0.008199
6	6	0	0.191149	-1.400518	0.007812
7	6	0	2.621780	-1.320779	0.008535
8	6	0	2.108364	-2.749487	0.009029
9	6	0	0.700555	-2.796637	0.006789
10	6	0	-0.167062	2.930917	0.008535
11	6	0	1.326943	3.200641	0.009029

12	6	0	2.071681	2.005017	0.006789
13	6	0	-2.454718	-1.610139	0.008535
14	6	0	-3.435308	-0.451154	0.009029
15	6	0	-2.772237	0.791620	0.006789
16	6	0	2.877990	-3.905576	0.010857
17	6	0	2.237445	-5.149523	0.002112
18	6	0	0.843583	-5.218970	-0.004146
19	6	0	0.077263	-4.053327	0.001278
20	6	0	1.943334	4.445200	0.010857
21	6	0	3.340895	4.512446	0.002112
22	6	0	4.097969	3.340049	-0.004146
23	6	0	3.471652	2.093575	0.001278
24	6	0	-4.821323	-0.539624	0.010857
25	6	0	-5.578340	0.637077	0.002112
26	6	0	-4.941552	1.878921	-0.004146
27	6	0	-3.548915	1.959751	0.001278
28	1	0	3.962785	-3.865648	0.013822
29	1	0	0.360068	-6.189982	-0.013251
30	1	0	-0.996397	-4.157808	-0.001398
31	1	0	1.366357	5.364697	0.013822
32	1	0	5.180648	3.406819	-0.013251
33	1	0	4.098966	1.215998	-0.001398
34	1	0	-5.329142	-1.499048	0.013822
35	1	0	-5.540715	2.783163	-0.013251
36	1	0	-3.102568	2.941809	-0.001398
37	6	0	-2.673239	-2.438632	1.300386
38	1	0	-2.642159	-1.784171	2.176184
39	1	0	-3.652749	-2.926966	1.277651
40	1	0	-1.917360	-3.210428	1.443201
41	6	0	3.444857	-1.099992	-1.286611
42	1	0	3.735603	-0.059914	-1.432061
43	1	0	4.356194	-1.705953	-1.266354
44	1	0	2.859767	-1.402677	-2.159677
45	6	0	3.448537	-1.095776	1.300386

46	1	0	2.866216	-1.396091	2.176184
47	1	0	4.361202	-1.699891	1.277651
48	1	0	3.738992	-0.055268	1.443201
49	6	0	-0.769807	3.533329	-1.286611
50	1	0	-1.815915	3.265084	-1.432061
51	1	0	-0.700698	4.625551	-1.266354
52	1	0	-0.215130	3.177970	-2.159677
53	6	0	-0.775298	3.534409	1.300386
54	1	0	-0.224058	3.180262	2.176184
55	1	0	-0.708452	4.626857	1.277651
56	1	0	-1.821633	3.265696	1.443201
57	6	0	-2.675049	-2.433337	-1.286611
58	1	0	-1.919688	-3.205171	-1.432061
59	1	0	-3.655496	-2.919598	-1.266354
60	1	0	-2.644637	-1.775293	-2.159677
61	6	0	-7.851263	0.814548	1.093545
62	6	0	-7.841755	0.299697	-1.083132
63	6	0	-9.133984	0.386490	-0.574759
64	6	0	4.631051	6.392120	1.093545
65	6	0	4.180423	6.641311	-1.083132
66	6	0	4.901702	7.717017	-0.574759
67	6	0	3.220212	-7.206667	1.093545
68	6	0	3.661332	-6.941008	-1.083132
69	6	0	4.232281	-8.103507	-0.574759
70	7	0	-7.009599	0.567199	0.007256
71	7	0	3.996008	5.786892	0.007256
72	7	0	3.013591	-6.354091	0.007256
73	7	0	-9.123421	0.709853	0.753502
74	7	0	5.176462	7.546188	0.753502
75	7	0	3.946959	-8.256041	0.753502
76	6	0	-7.441431	1.169292	2.461355
77	6	0	-6.213322	0.815278	3.047962
78	6	0	-8.377888	1.877650	3.241809
79	6	0	-5.921863	1.175021	4.358998

80	1	0	-5.483897	0.240267	2.493548
81	6	0	-8.093336	2.238161	4.549512
82	1	0	-9.331856	2.132671	2.795993
83	6	0	-6.854766	1.895236	5.120737
84	1	0	-4.973165	0.891932	4.802233
85	1	0	-8.820536	2.789234	5.136106
86	6	0	4.733353	5.859822	2.461355
87	6	0	3.812713	4.973256	3.047962
88	6	0	5.815037	6.316638	3.241809
89	6	0	3.978530	4.540974	4.358998
90	1	0	2.950025	4.629061	2.493548
91	6	0	5.984972	5.889954	4.549512
92	1	0	6.512876	7.015289	2.795993
93	6	0	5.068706	4.988783	5.120737
94	1	0	3.259018	3.860921	4.802233
95	1	0	6.825815	6.244192	5.136106
96	6	0	2.708079	-7.029115	2.461355
97	6	0	2.400610	-5.788534	3.047962
98	6	0	2.562851	-8.194289	3.241809
99	6	0	1.943334	-5.715995	4.358998
100	1	0	2.533872	-4.869327	2.493548
101	6	0	2.108364	-8.128115	4.549512
102	1	0	2.818980	-9.147960	2.795993
103	6	0	1.786060	-6.884019	5.120737
104	1	0	1.714147	-4.752853	4.802233
105	1	0	1.994721	-9.033425	5.136106
106	6	0	-7.571950	0.027128	-2.471103
107	6	0	-6.281506	0.012661	-3.049508
108	6	0	-8.715994	-0.221307	-3.303271
109	6	0	-6.099519	-0.256188	-4.393826
110	1	0	-5.417902	0.225032	-2.435047
111	6	0	-8.481872	-0.495255	-4.668696
112	6	0	-7.208469	-0.518623	-5.209716
113	1	0	-5.097730	-0.257979	-4.813152

114	1	0	-9.321337	-0.687715	-5.325637
115	1	0	-7.074067	-0.731740	-6.265889
116	6	0	3.809468	6.543937	-2.471103
117	6	0	3.151717	5.433613	-3.049508
118	6	0	4.166340	7.658926	-3.303271
119	6	0	2.827894	5.410432	-4.393826
120	1	0	2.903835	4.579525	-2.435047
121	6	0	3.812032	7.593144	-4.668696
122	6	0	3.155094	6.502028	-5.209716
123	1	0	2.325449	4.543753	-4.813152
124	1	0	4.065090	8.416372	-5.325637
125	1	0	2.903328	6.492192	-6.265889
126	6	0	3.762481	-6.571065	-2.471103
127	6	0	3.129788	-5.446274	-3.049508
128	6	0	4.549654	-7.437619	-3.303271
129	6	0	3.271624	-5.154244	-4.393826
130	1	0	2.514067	-4.804557	-2.435047
131	6	0	4.669840	-7.097889	-4.668696
132	6	0	4.053375	-5.983405	-5.209716
133	1	0	2.772281	-4.285775	-4.813152
134	1	0	5.256247	-7.728657	-5.325637
135	1	0	4.170739	-5.760452	-6.265889
136	6	0	-10.290999	0.144860	-1.389164
137	6	0	-11.592802	0.212267	-0.855023
138	6	0	-10.080418	-0.175238	-2.759025
139	6	0	-12.690891	-0.037038	-1.656570
140	1	0	-11.704449	0.459097	0.195417
141	6	0	-11.227560	-0.427543	-3.546516
142	6	0	-12.502637	-0.360728	-3.011031
143	1	0	-13.693476	0.013845	-1.242440
144	1	0	-11.124688	-0.681887	-4.594780
145	1	0	-13.361078	-0.561018	-3.645379
146	6	0	5.270952	8.839837	-1.389164
147	6	0	5.980230	9.933528	-0.855023

148	6	0	4.888449	8.817517	-2.759025
149	6	0	6.313370	11.009153	-1.656570
150	1	0	6.249815	9.906802	0.195417
151	6	0	5.243517	9.937124	-3.546516
152	6	0	5.938919	11.007965	-3.011031
153	1	0	6.858728	11.851976	-1.242440
154	1	0	4.971812	9.975206	-4.594780
155	1	0	6.194683	11.851542	-3.645379
156	6	0	5.020047	-8.984697	-1.389164
157	6	0	5.612572	-10.145795	-0.855023
158	6	0	5.191969	-8.642280	-2.759025
159	6	0	6.377521	-10.972115	-1.656570
160	1	0	5.454635	-10.365899	0.195417
161	6	0	5.984043	-9.509581	-3.546516
162	6	0	6.563718	-10.647238	-3.011031
163	1	0	6.834748	-11.865820	-1.242440
164	1	0	6.152876	-9.293319	-4.594780
165	1	0	7.166395	-11.290524	-3.645379
166	6	0	-6.548130	2.273965	6.467941
167	7	0	-6.296745	2.584633	7.561007
168	6	0	5.243376	4.533864	6.467941
169	7	0	5.386730	4.160825	7.561007
170	6	0	1.304754	-6.807829	6.467941
171	7	0	0.910015	-6.745458	7.561007

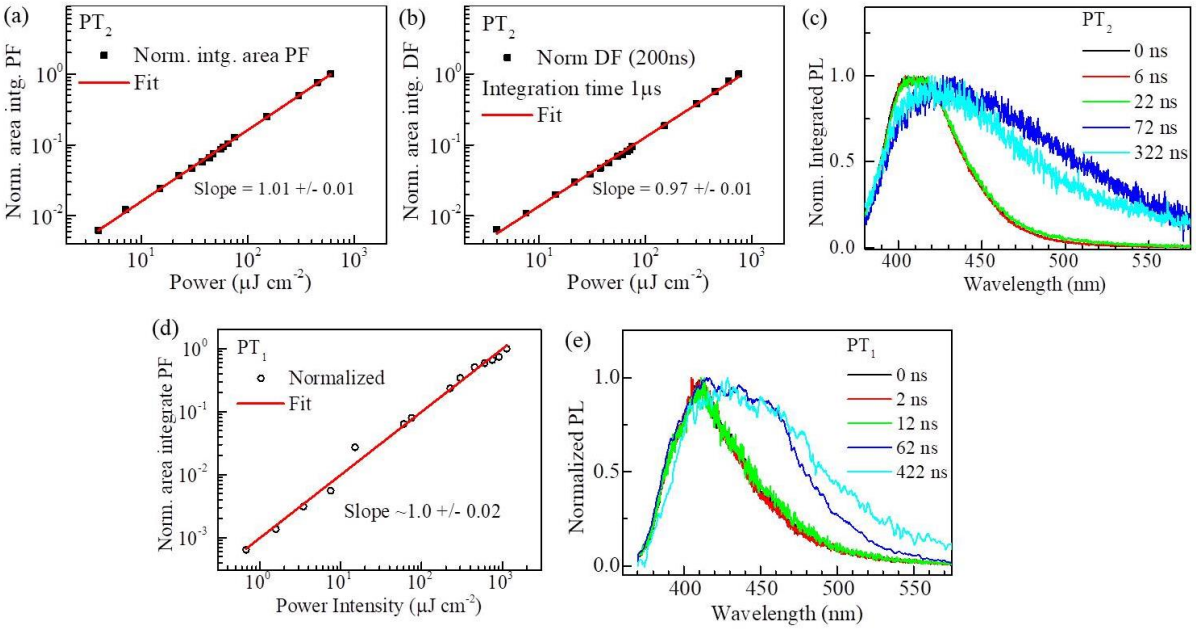

Figure S5. (a)- (c) Fluence and spectral shift in PT_2 (d)- (e) Fluence and spectral shift in PT_1

Spectral relaxation was observed in $PT_{1\text{-}2}$ but not in PT_3. The spectral relaxation in these small molecule system can be attributed to solvent-solute interaction that involve (1) exciplex formation or (2) dipolar interactions between the reorientation of the solvent molecules around the complex that is formed because of the excitation of the solute.[1] The presence/absence of the spectral shift also serves as a comparison of the relaxation lifetime of the solute with fluorescence lifetime. Since relaxation (e.g. torsion) time for star-shaped molecules is in 10's ps while fluorescence lifetime is in nanosecond (prompt), the longer lifetime governs the spectral shift process.[2]

1. W. R. Ware, S. K. Lee, G. J. Brant and P. P. Chow, *J. Chem. Phys.*, 1971, **54**, 4729-4737.
2. M. Fujitsuka, D. W. Cho, H.-H. Huang, J.-S. Yang and T. Majima, *J. Phys. Chem. B*, 2011, **115**, 13502-13507.