Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supporting Information

Quinone-Bodipy H-bonding interaction over π-stacking in toluene

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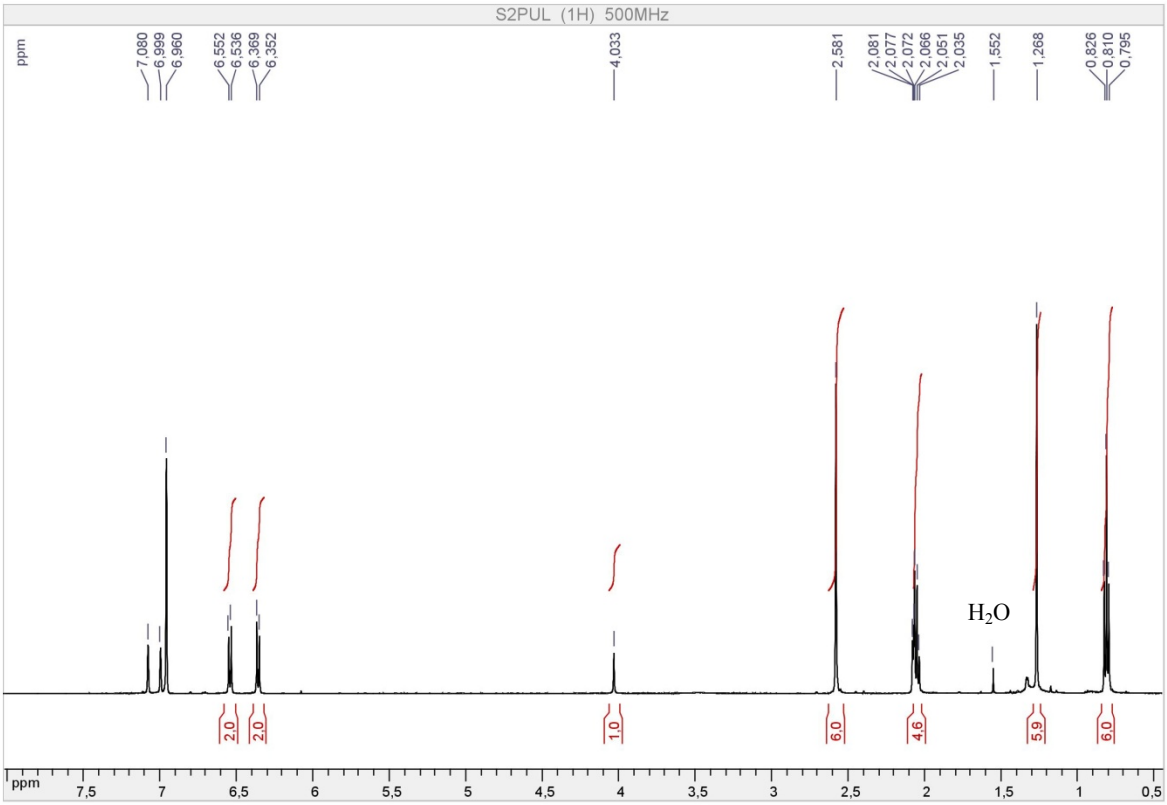
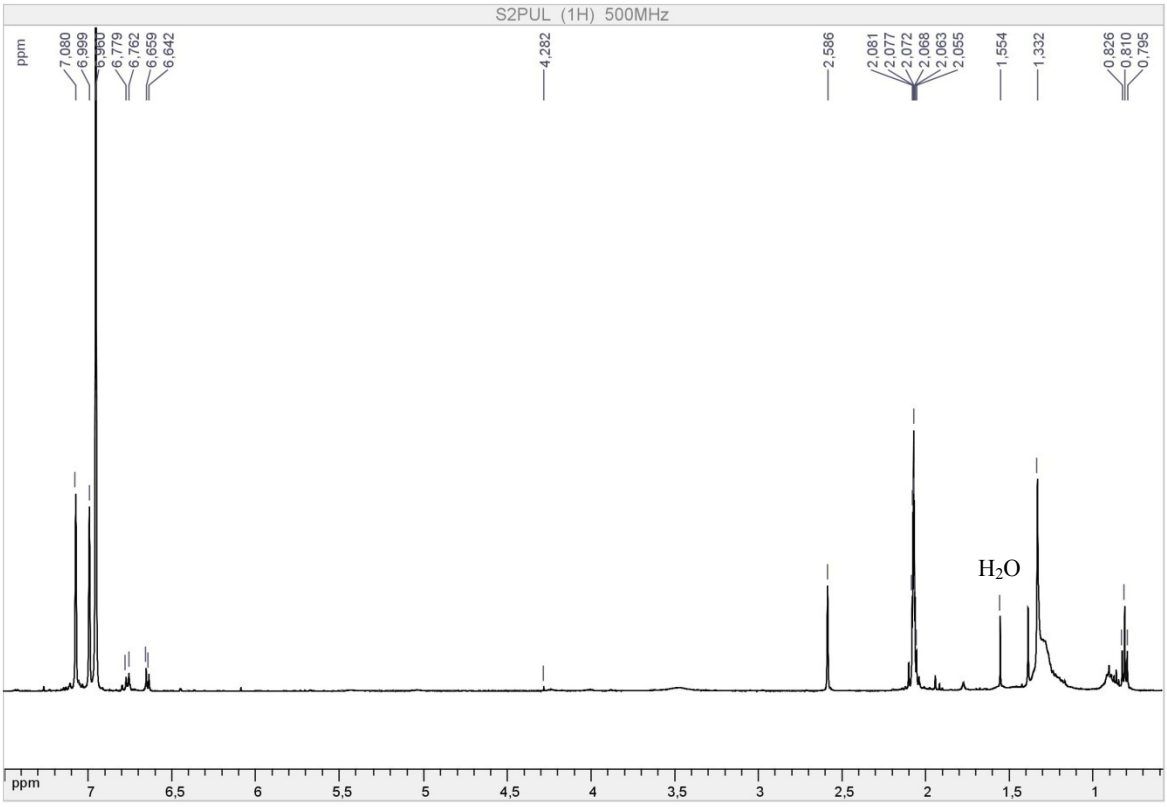
Figure S1. ^{1}H NMR spectra of [a] Dye **1**, [b] **A1**/**1** (1:1), [c] **A3**/**1** (1:1) and [d] **A5**/**1** (1:1) adduct in d_8-toluene at 298K.

[a]



[b]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6.762
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4.282
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2.081
2.077
2.072
2.068
2.063
2.055
1.554
1.332
0.826
0.810
0.795
H2O
ppm
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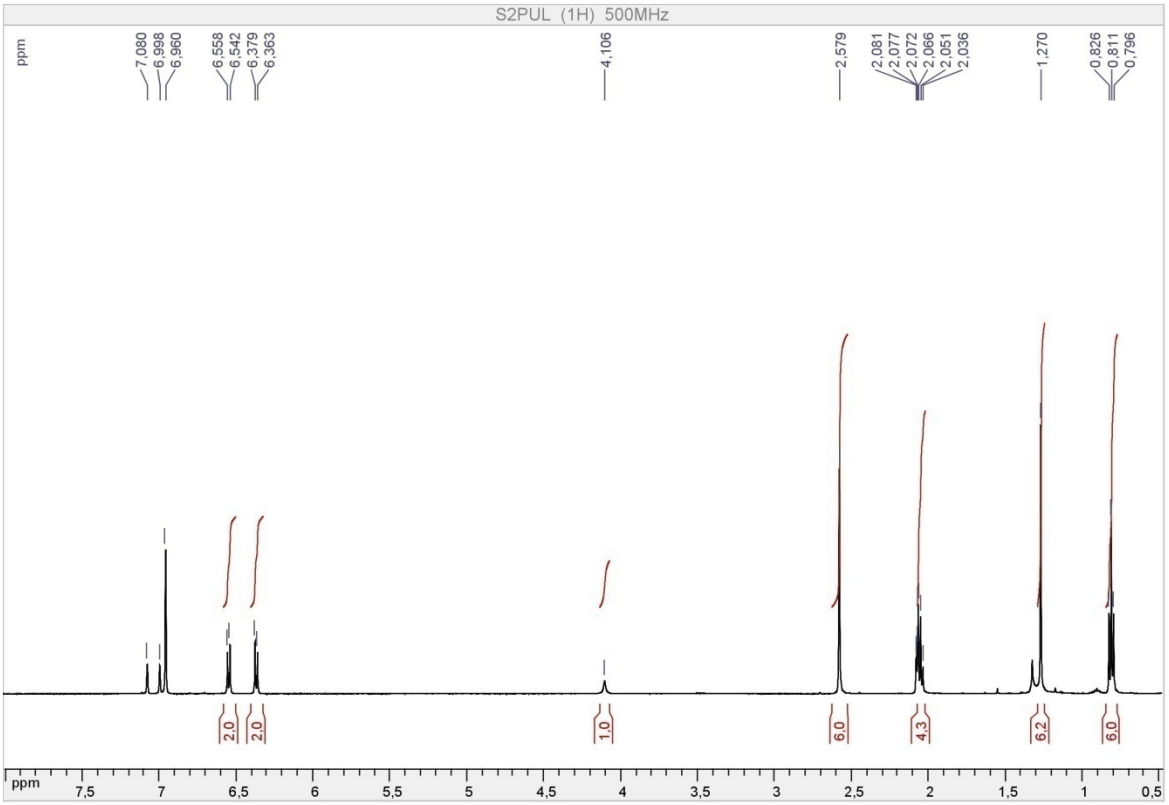
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1

[c]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1,0
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4,3
6,2
6,0
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5,5
5
4,5
4
3,5
3
2,5
2
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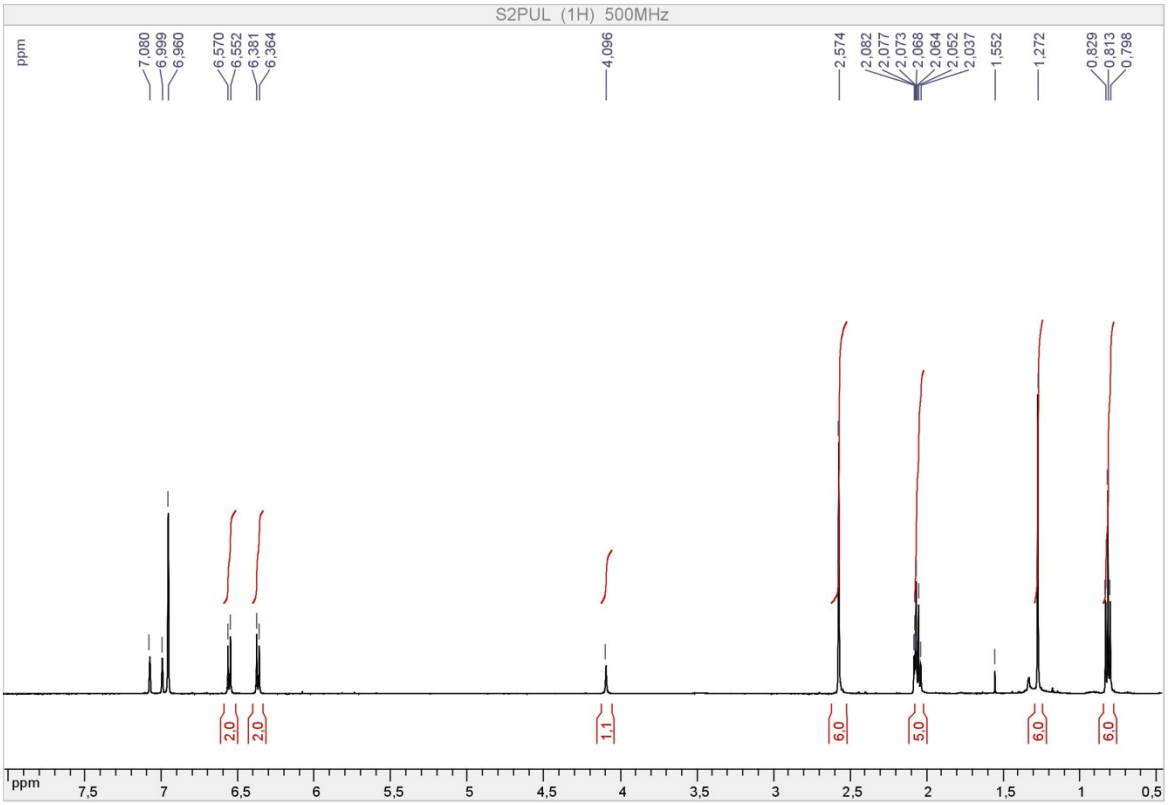
1
0,5

[d]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6,0
ppm
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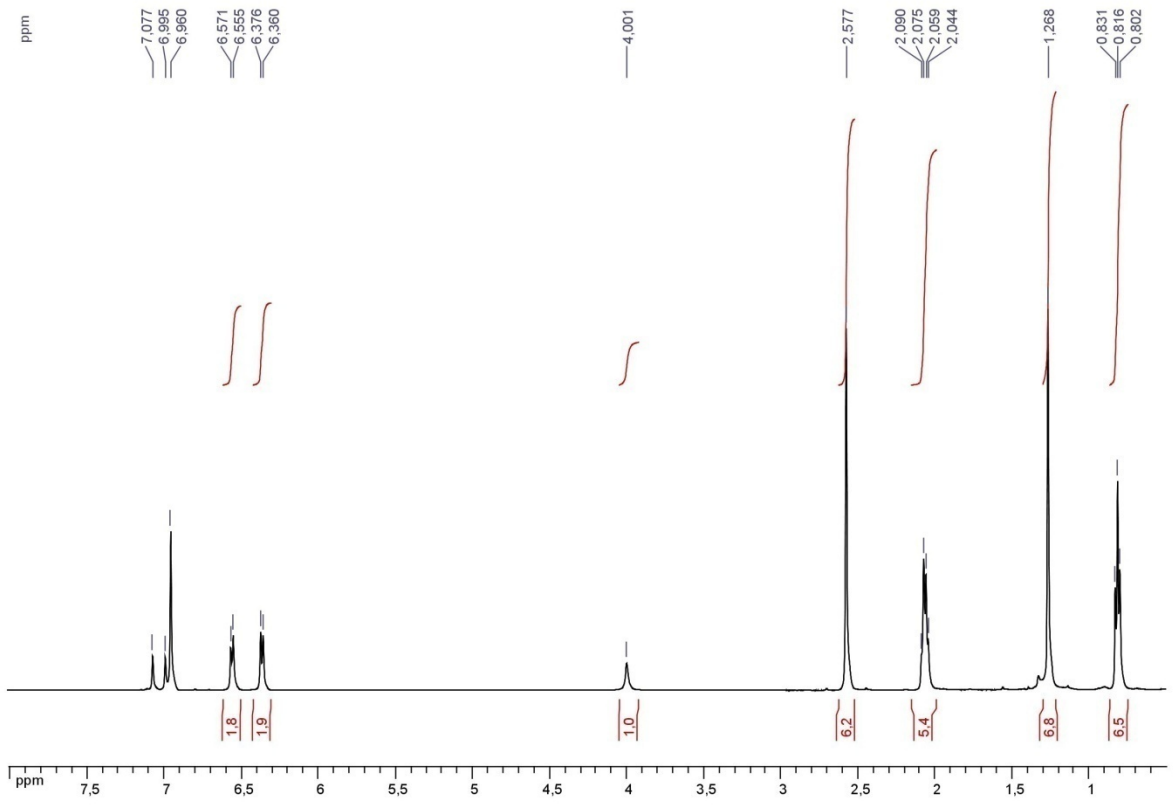
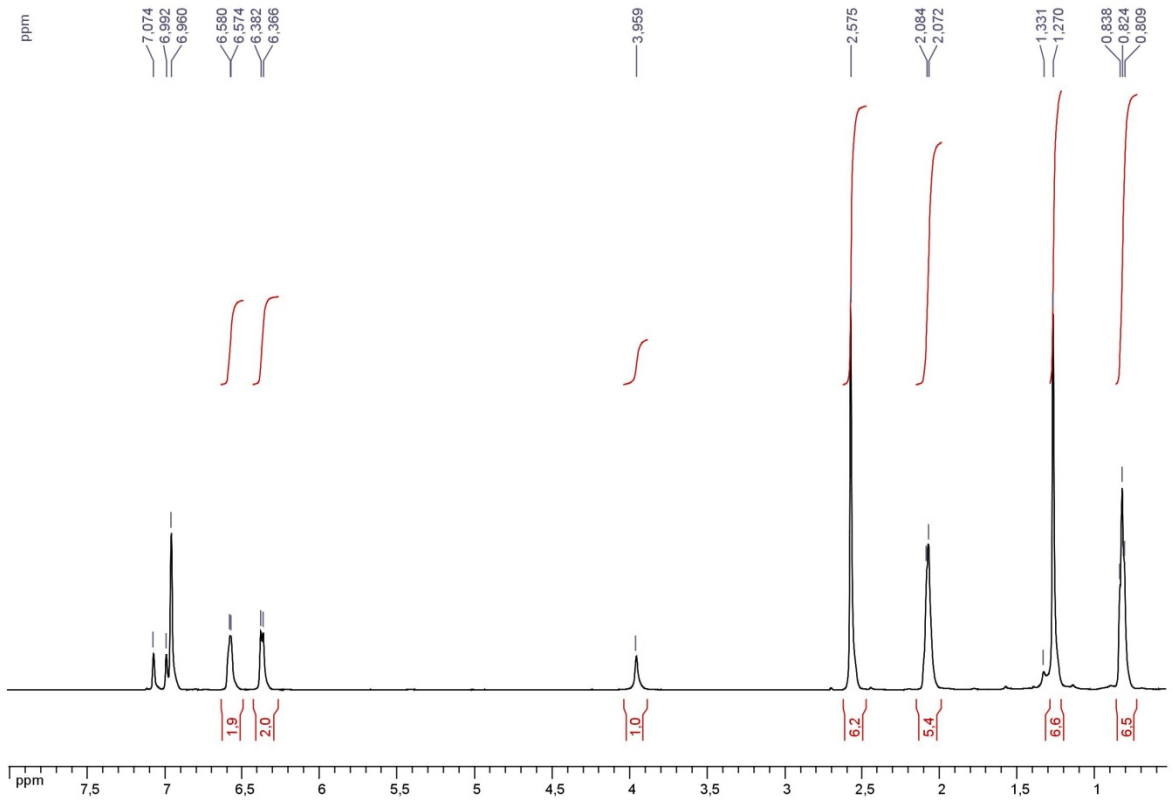
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1
0,5

Figure S2. ^{1}H NMR spectra of **A3/1** (1:1) adduct in d_8-toluene at [a] 313K and [b] 323K.

[a]



[b]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0,838
0,824
0,809
1,9
2,0
1,0
6,2
5,4
6,6
6,5
ppm
7,5
7
6,5
6
5,5
5
4,5
4
3,5
3
2,5
2
1,5
1

Figure S3. Ground state titration of the electron acceptors by dye **1** in toluene. Concentration of **1** dye: 0.00, 3.843×10^{-6} , 7.336×10^{-6}, 1.053×10^{-5}, 1.345×10^{-5}, 1.614×10^{-5}, 1.862×10^{-5}, 2.092×10^{-5} and 2.306×10^{-5} mol dm^{-3} [A] At a fixed concentration (1.027×10^{-4} mol dm^{-3}) of the C_{70} solution in toluene [B] at a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the C_{60} solution in toluene [C] At a fixed concentration (1.04×10^{-4} mol dm^{-3}) of the *o*-chloranil solution in toluene. [D] At a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the *p*-chloranil solution in toluene. [E] At a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the DDQ solution in toluene.

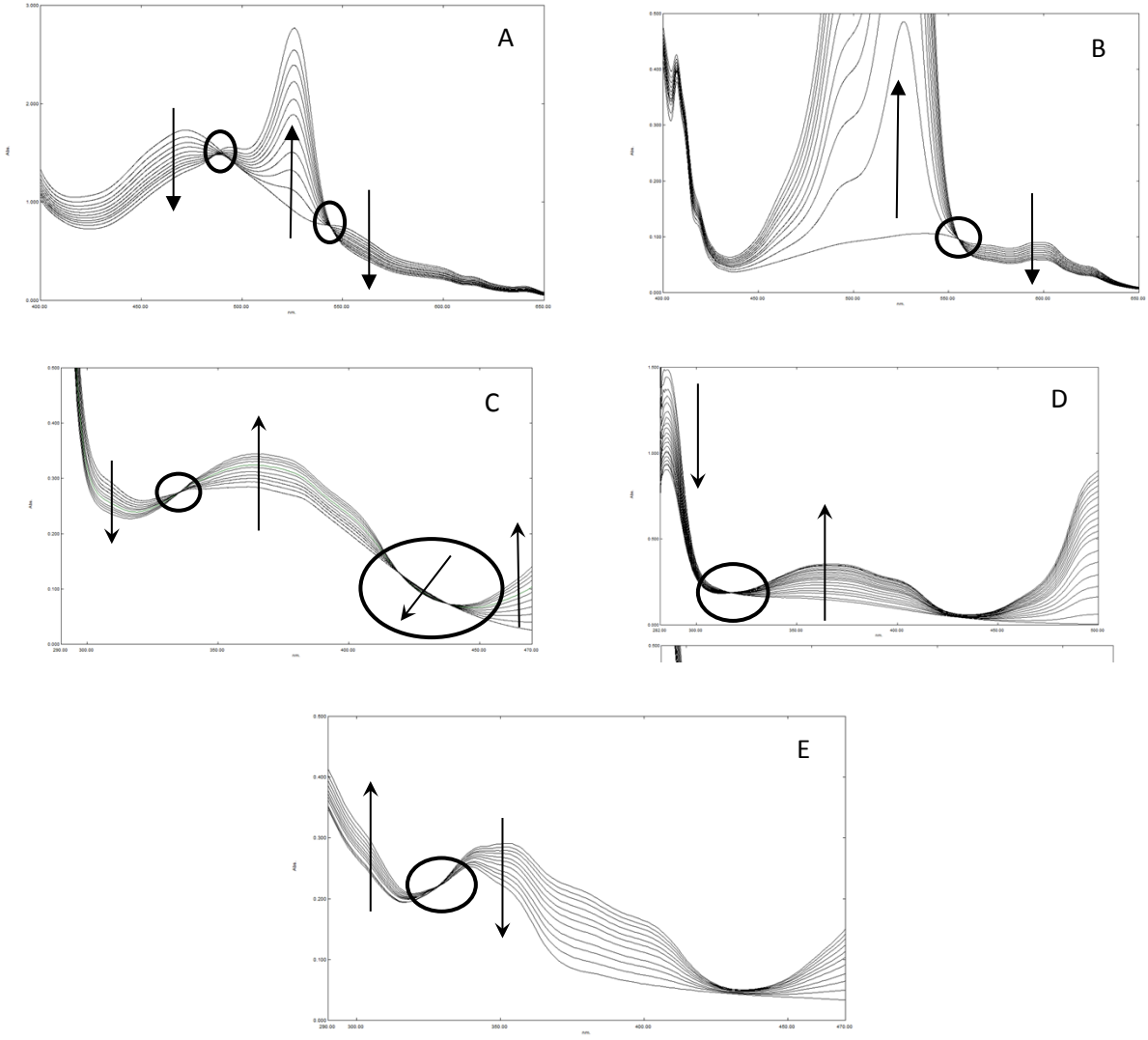
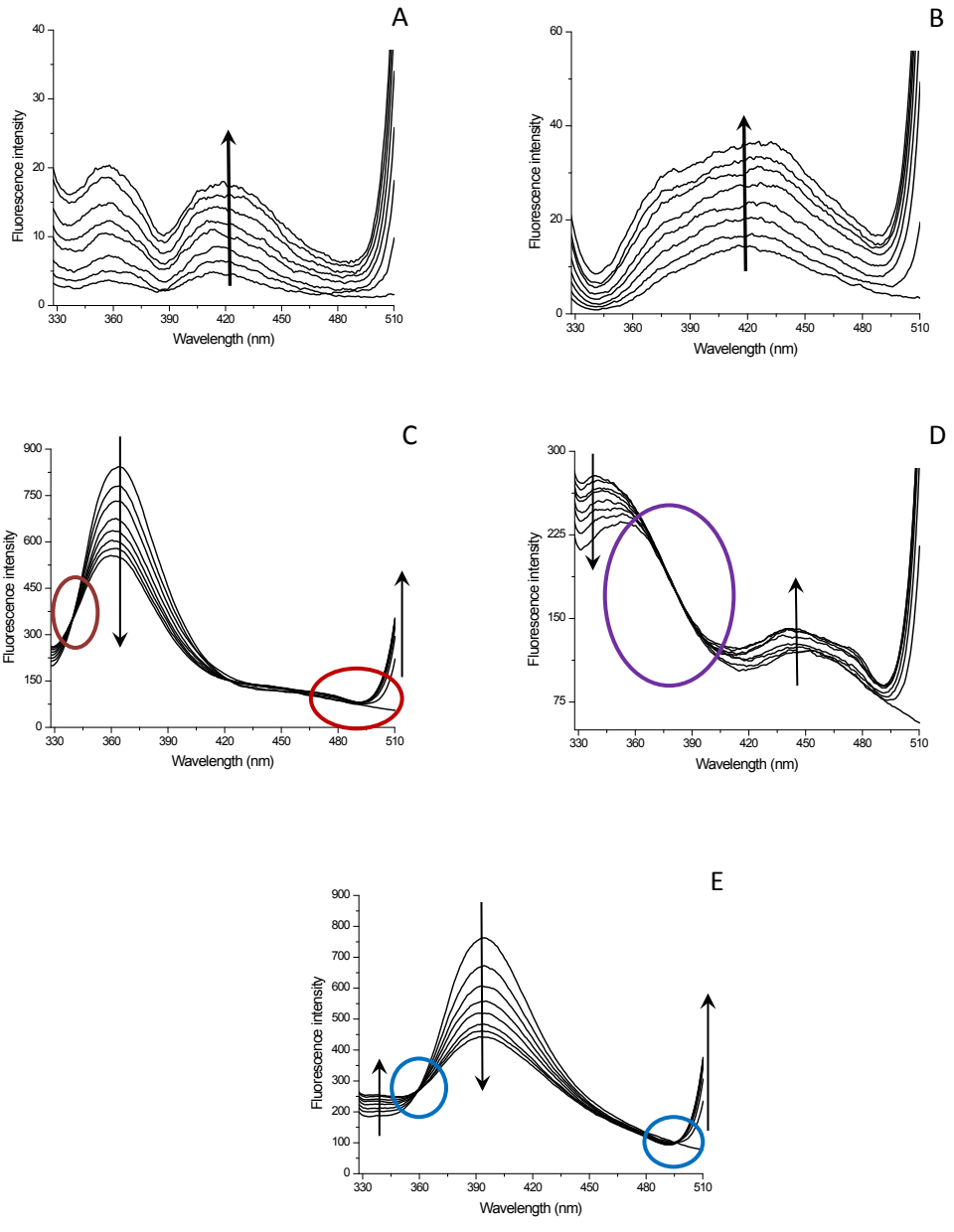


Figure S4. Excited state titration of the electron acceptors by dye **1** in toluene. Concentration of **1** dye: 0.00, 7.336× 10^{-6} , 1.345×10^{-5}, 1.862 ×10^{-5}, 2.306×10^{-5}, 2.69 ×10^{-5}, 3.026×10^{-5}, 3.323×10^{-5} and 3.587×10^{-5} mol dm^{-3} [A] at a fixed concentration (1.027×10^{-4} mol dm^{-3}) of the C_{70} solution in toluene. [B] At a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the C_{60} solution in toluene. [C] At a fixed concentration (1.04×10^{-4} mol dm^{-3}) of the *o*-chloranil solution in toluene. [D] At a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the *p*-chloranil solution in toluene. [E] At a fixed concentration (1.00×10^{-4} mol dm^{-3}) of the DDQ solution in Toluene.



1. Coordinates of Monte Carlo global minimum conformer of **Dye 1 dimer**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.170000	-1.116000	-2.433000
2	6	0	1.794000	-0.997000	-2.464000
3	6	0	1.069000	0.221000	-2.601000
4	6	0	1.880000	1.381000	-2.692000
5	7	0	3.257000	1.411000	-2.608000
6	6	0	1.324000	-2.304000	-2.278000
7	6	0	2.475000	-3.186000	-2.190000
8	6	0	1.505000	2.718000	-2.868000
9	6	0	3.607000	-2.394000	-2.283000
10	6	0	2.712000	3.527000	-2.847000
11	6	0	3.781000	2.664000	-2.673000
12	5	0	4.121000	0.121000	-2.392000
13	9	0	5.104000	0.015000	-3.423000
14	9	0	4.800000	0.185000	-1.092000
15	6	0	-0.396000	0.273000	-2.558000
16	6	0	-1.048000	0.623000	-1.365000
17	6	0	-1.188000	-0.071000	-3.666000
18	6	0	-2.434000	0.552000	-1.249000
19	1	0	-0.466000	0.931000	-0.501000
20	6	0	-2.585000	-0.129000	-3.557000
21	1	0	-0.708000	-0.335000	-4.604000
22	6	0	-3.192000	0.154000	-2.339000
23	1	0	-2.901000	0.780000	-0.295000
24	1	0	-3.188000	-0.431000	-4.406000
25	6	0	0.130000	3.277000	-3.039000
26	1	0	-0.420000	2.745000	-3.820000
27	1	0	-0.424000	3.235000	-2.098000
28	1	0	0.152000	4.327000	-3.344000
29	6	0	-0.088000	-2.780000	-2.148000
30	1	0	-0.634000	-2.211000	-1.392000
31	1	0	-0.604000	-2.721000	-3.109000
32	1	0	-0.137000	-3.824000	-1.826000
33	6	0	2.457000	-4.670000	-1.990000
34	1	0	1.598000	-5.109000	-2.510000
35	1	0	3.343000	-5.120000	-2.452000
36	6	0	5.052000	-2.710000	-2.219000
37	1	0	5.545000	-2.465000	-3.165000
38	1	0	5.542000	-2.153000	-1.414000
39	1	0	5.221000	-3.773000	-2.025000
40	6	0	5.240000	2.890000	-2.557000
41	1	0	5.765000	2.481000	-3.426000
42	1	0	5.476000	3.957000	-2.501000
43	1	0	5.643000	2.425000	-1.653000
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45	1	0	2.079000	5.374000	-3.716000
46	1	0	3.784000	5.306000	-3.353000
47	6	0	2.553000	5.721000	-1.645000
48	1	0	2.629000	6.805000	-1.772000
49	1	0	1.556000	5.494000	-1.252000
50	1	0	3.288000	5.414000	-0.893000
51	6	0	2.413000	-5.052000	-0.517000
52	1	0	3.287000	-4.665000	0.018000
53	1	0	1.518000	-4.653000	-0.028000
54	1	0	2.402000	-6.141000	-0.408000

55	8	0	-4.545000	0.014000	-2.217000
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59	6	0	-1.069000	-0.221000	2.601000
60	6	0	-1.794000	0.997000	2.464000
61	7	0	-3.170000	1.116000	2.433000
62	6	0	-1.505000	-2.718000	2.868000
63	6	0	-2.712000	-3.527000	2.847000
64	6	0	-1.324000	2.304000	2.278000
65	6	0	-3.781000	-2.664000	2.673000
66	6	0	-2.475000	3.186000	2.190000
67	6	0	-3.607000	2.394000	2.283000
68	5	0	-4.121000	-0.121000	2.392000
69	9	0	-5.104000	-0.015000	3.423000
70	9	0	-4.800000	-0.185000	1.092000
71	6	0	0.396000	-0.273000	2.558000
72	6	0	1.048000	-0.623000	1.365000
73	6	0	1.188000	0.071000	3.666000
74	6	0	2.434000	-0.552000	1.249000
75	1	0	0.466000	-0.931000	0.501000
76	6	0	2.585000	0.129000	3.557000
77	1	0	0.708000	0.335000	4.604000
78	6	0	3.192000	-0.154000	2.339000
79	1	0	2.901000	-0.780000	0.295000
80	1	0	3.188000	0.431000	4.406000
81	6	0	0.088000	2.780000	2.148000
82	1	0	0.604000	2.721000	3.109000
83	1	0	0.634000	2.211000	1.392000
84	1	0	0.137000	3.824000	1.826000
85	6	0	-0.130000	-3.277000	3.039000
86	1	0	0.424000	-3.235000	2.098000
87	1	0	0.420000	-2.745000	3.820000
88	1	0	-0.152000	-4.327000	3.344000
89	6	0	-2.798000	-5.017000	2.972000
90	1	0	-2.079000	-5.374000	3.716000
91	1	0	-3.784000	-5.306000	3.353000
92	6	0	-5.240000	-2.890000	2.557000
93	1	0	-5.765000	-2.481000	3.426000
94	1	0	-5.643000	-2.425000	1.653000
95	1	0	-5.476000	-3.957000	2.501000
96	6	0	-5.052000	2.710000	2.219000
97	1	0	-5.545000	2.465000	3.165000
98	1	0	-5.221000	3.773000	2.025000
99	1	0	-5.542000	2.153000	1.414000
100	6	0	-2.457000	4.670000	1.990000
101	1	0	-1.598000	5.109000	2.510000
102	1	0	-3.343000	5.120000	2.452000
103	6	0	-2.413000	5.052000	0.517000
104	1	0	-2.402000	6.141000	0.408000
105	1	0	-1.518000	4.653000	0.028000
106	1	0	-3.287000	4.665000	-0.018000
107	6	0	-2.553000	-5.721000	1.645000
108	1	0	-3.288000	-5.414000	0.893000
109	1	0	-1.556000	-5.494000	1.252000
110	1	0	-2.629000	-6.805000	1.772000
111	8	0	4.545000	-0.014000	2.217000
112	1	0	4.734000	-0.025000	1.253000

---

2. Coordinates of Monte Carlo global minimum conformer of **A1/1 adduct**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.214789	-1.457941	1.919947
2	6	0	-4.714748	-0.313271	1.332619
3	6	0	-4.982422	-0.142692	-0.051316
4	6	0	-4.598440	-1.242929	-0.863272
5	7	0	-4.094317	-2.444130	-0.404224
6	6	0	-4.855953	0.595513	2.389220
7	6	0	-4.404594	-0.059116	3.605139
8	6	0	-4.610028	-1.370697	-2.257657
9	6	0	-4.020014	-1.344591	3.260123
10	6	0	-4.108908	-2.693246	-2.588890
11	6	0	-3.795167	-3.323734	-1.396472
12	5	0	-3.903425	-2.745324	1.107985
13	9	0	-4.782422	-3.748868	1.487792
14	9	0	-2.650713	-3.165396	1.355273
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16	6	0	-7.041872	1.071525	-0.734515
17	6	0	-4.918141	2.184927	-0.982187
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21	1	0	-3.838170	2.201302	-0.874446
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23	1	0	-8.772489	2.196999	-1.354601
24	1	0	-4.967067	4.170049	-1.784586
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27	1	0	-4.434548	0.553508	-3.178732
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30	1	0	-4.653499	2.621956	1.736936
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33	6	0	-4.346800	0.531862	4.979628
34	1	0	-5.197210	1.205831	5.136987
35	1	0	-4.453681	-0.255906	5.733510
36	6	0	-3.484498	-2.474654	4.055366
37	1	0	-4.064790	-3.386654	3.885798
38	1	0	-2.439462	-2.670305	3.793234
39	1	0	-3.518218	-2.262704	5.127413
40	6	0	-3.251654	-4.668178	-1.089998
41	1	0	-3.898445	-5.204892	-0.389545
42	1	0	-3.166941	-5.281298	-1.991934
43	1	0	-2.251362	-4.591204	-0.653420
44	6	0	-3.953562	-3.282898	-3.957082
45	1	0	-4.750008	-2.920213	-4.616083
46	1	0	-4.081715	-4.370815	-3.913798
47	6	0	-2.598516	-2.964346	-4.572295
48	1	0	-2.524877	-3.399354	-5.573421
49	1	0	-2.444038	-1.884303	-4.657568
50	1	0	-1.784616	-3.373750	-3.964302
51	6	0	-3.046845	1.283264	5.224982
52	1	0	-2.180658	0.621061	5.116630
53	1	0	-2.926431	2.110706	4.518087
54	1	0	-3.033103	1.697862	6.238157

55	8	0	-7.616205	4.385296	-2.128348
56	1	0	-6.958627	5.072658	-2.322616
57	6	0	5.224021	-2.733459	-0.661125
58	6	0	5.544053	-2.323167	0.761325
59	6	0	4.480126	-2.904603	1.666743
60	6	0	3.503504	-3.673503	0.804418
61	6	0	3.961508	-3.568708	-0.633172
62	6	0	5.544918	-1.926280	-1.749025
63	6	0	6.176315	-1.117967	1.052802
64	6	0	3.059710	-3.574467	-1.694441
65	6	0	4.079891	-2.266481	2.836971
66	6	0	2.158967	-3.782963	1.139282
67	6	0	4.522655	-0.829887	2.916052
68	6	0	5.467813	-0.312251	2.111632
69	6	0	5.890238	-0.512057	-1.362767
70	6	0	6.175801	-0.147895	-0.099794
71	6	0	4.385499	-1.697585	-2.686799
72	6	0	3.265259	-2.439578	-2.662131
73	6	0	2.582682	-2.117051	2.960795
74	6	0	1.714171	-2.802640	2.195785
75	6	0	1.629160	-3.339178	-1.270206
76	6	0	1.223285	-3.431097	0.009100
77	6	0	5.805707	1.217600	0.363430
78	6	0	5.375055	1.117301	1.708962
79	6	0	4.297053	-0.261473	-3.068965
80	6	0	5.213008	0.459540	-2.264253
81	6	0	1.965012	-1.808491	-3.020441
82	6	0	0.970788	-2.353551	-2.174051
83	6	0	0.424512	-2.162895	1.817601
84	6	0	0.131855	-2.541150	0.486591
85	6	0	2.228311	-0.742274	3.412035
86	6	0	3.407192	0.040051	3.383394
87	6	0	5.279163	2.197539	-0.497115
88	6	0	4.406482	1.994364	2.228431
89	6	0	1.865683	-0.489096	-3.502125
90	6	0	3.358270	1.421141	3.120941
91	6	0	4.962486	1.792949	-1.896977
92	6	0	0.967622	-0.161925	3.177134
93	6	0	-0.145291	-1.590807	-1.787047
94	6	0	0.007121	-0.918780	2.326684
95	6	0	3.108321	0.334110	-3.527848
96	6	0	-0.583709	-1.686877	-0.369488
97	6	0	0.906450	1.244564	3.138662
98	6	0	2.978183	1.722248	-3.344166
99	6	0	2.087330	2.024835	3.109135
100	6	0	3.893147	2.442256	-2.539362
101	6	0	-1.178017	-0.555294	0.212083
102	6	0	4.485855	3.201387	0.089244
103	6	0	-0.893358	-0.177098	1.543233
104	6	0	4.056185	3.101022	1.433762
105	6	0	-0.351124	-0.366934	-2.450416
106	6	0	0.643100	0.178126	-3.296806
107	6	0	-1.016918	1.304143	1.628679
108	6	0	-1.492773	0.673876	-0.557126
109	6	0	2.739759	3.788497	1.543917
110	6	0	-1.098937	0.766557	-1.838288
111	6	0	-0.150364	1.988866	2.395792
112	6	0	0.536170	1.663083	-3.230972
113	6	0	3.447747	3.952853	-0.667509
114	6	0	1.657436	2.404161	-3.254587
115	6	0	1.794601	3.270861	2.348337
116	6	0	3.163183	3.588698	-1.930500

117	6	0	2.420774	4.530349	0.271172
118	6	0	1.788369	3.720958	-2.531561
119	6	0	-0.698883	2.077742	-2.477309
120	6	0	-1.591618	1.868309	0.356346
121	6	0	0.323332	3.383822	2.055212
122	6	0	0.790270	3.933323	-1.584503
123	6	0	1.110302	4.343614	-0.162053
124	6	0	-0.471235	3.097083	-1.556495
125	6	0	-0.926213	2.991387	-0.117887
126	6	0	0.047384	3.761189	0.743420

3. Coordinates of Monte Carlo global minimum conformer of **A2/1 adduct**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.080596	1.259377	-1.833617
2	6	0	4.413326	1.193332	-0.494803
3	6	0	4.647718	-0.000320	0.237155
4	6	0	4.413700	-1.193006	-0.495010
5	7	0	4.079741	-1.259778	-1.833789
6	6	0	4.431513	2.524780	-0.063750
7	6	0	4.094068	3.366022	-1.200383
8	6	0	4.431260	-2.525313	-0.063823
9	6	0	3.888831	2.527691	-2.283438
10	6	0	4.094120	-3.365893	-1.199467
11	6	0	3.888435	-2.527596	-2.283444
12	5	0	3.996975	-0.000631	-2.733046
13	9	0	5.077588	-0.000047	-3.640486
14	9	0	2.785183	-0.000518	-3.472903
15	6	0	5.136685	0.000339	1.617136
16	6	0	4.260851	0.000408	2.713619
17	6	0	6.519512	0.000211	1.868457
18	6	0	4.749872	0.000528	4.021950
19	1	0	3.188926	0.000314	2.540766
20	6	0	7.014503	-0.000237	3.175359
21	1	0	7.210804	0.000409	1.026890
22	6	0	6.121051	-0.000073	4.241583
23	1	0	4.059420	0.000252	4.859358
24	1	0	8.086779	0.000007	3.330723
25	6	0	4.701941	-3.049601	1.306971
26	1	0	5.708164	-2.782463	1.638157
27	1	0	3.962575	-2.670862	2.017599
28	1	0	4.638345	-4.139949	1.350527
29	6	0	4.701766	3.049446	1.306388
30	1	0	3.962869	2.670540	2.017603
31	1	0	5.708714	2.783041	1.637691
32	1	0	4.637613	4.139998	1.349810
33	6	0	3.972488	4.858272	-1.214931
34	1	0	4.712512	5.302728	-0.540606
35	1	0	4.214383	5.245438	-2.211446
36	6	0	3.517519	2.790269	-3.693556
37	1	0	4.187662	2.269468	-4.385011
38	1	0	2.491161	2.464015	-3.888709
39	1	0	3.573085	3.857158	-3.931429
40	6	0	3.517430	-2.791239	-3.693905
41	1	0	4.187649	-2.270205	-4.384580
42	1	0	3.573060	-3.857661	-3.930215
43	1	0	2.490670	-2.464382	-3.888427
44	6	0	3.972402	-4.858180	-1.213884

45	1	0	4.711873	-5.303232	-0.539155
46	1	0	4.214048	-5.245398	-2.210371
47	6	0	2.578862	-5.325459	-0.823820
48	1	0	2.527762	-6.418602	-0.836131
49	1	0	2.311689	-4.984969	0.182559
50	1	0	1.824519	-4.942646	-1.519168
51	6	0	2.578509	5.325980	-0.824386
52	1	0	1.824762	4.942668	-1.519446
53	1	0	2.311585	4.985262	0.182089
54	1	0	2.527969	6.418710	-0.836937
55	8	0	6.562205	0.000177	5.532543
56	1	0	7.532938	-0.000175	5.514434
57	6	0	-5.771953	1.213378	-0.858677
58	6	0	-6.136284	-0.000255	-0.055904
59	6	0	-5.963821	-0.000019	1.288262
60	6	0	-5.409093	1.213079	1.972787
61	6	0	-5.079386	2.309289	1.247674
62	6	0	-5.269783	2.309822	-0.239624
63	6	0	-5.183231	0.749777	-2.156641
64	6	0	-5.182923	-0.749915	-2.156603
65	6	0	-5.772308	-1.212602	-0.858781
66	6	0	-5.270280	-2.309353	-0.239028
67	6	0	-5.408473	-1.213121	1.972643
68	6	0	-4.510493	0.749967	3.080211
69	6	0	-3.369878	1.427239	3.356442
70	6	0	-3.005547	2.640871	2.553669
71	6	0	-3.817636	3.059074	1.552581
72	6	0	-3.228130	3.522513	0.253567
73	6	0	-4.126418	3.059118	-0.854038
74	6	0	-3.594362	2.640270	-2.027190
75	6	0	-4.149090	1.427172	-2.711715
76	6	0	-4.148703	-1.427614	-2.711945
77	6	0	-3.005338	-0.678318	-3.326359
78	6	0	-3.005211	0.677729	-3.326308
79	6	0	-1.743341	1.428266	-3.022593
80	6	0	-2.107231	2.640817	-2.218740
81	6	0	-1.294836	3.060919	-1.217645
82	6	0	-1.883679	3.523767	0.081511
83	6	0	-0.986054	3.060875	1.188974
84	6	0	-1.518331	2.641620	2.363094
85	6	0	-4.511161	-0.749505	3.080288
86	6	0	0.069267	-0.750138	2.493658
87	6	0	-0.963899	-1.427752	3.048693
88	6	0	-1.518712	-2.641054	2.363192
89	6	0	-0.985888	-3.061075	1.190218
90	6	0	0.157683	-2.310826	0.575587
91	6	0	1.011100	0.000201	0.392813
92	6	0	0.655456	1.213450	1.193750
93	6	0	0.069166	0.750508	2.493404
94	6	0	-0.964079	1.427987	3.048707
95	6	0	-2.107615	0.678286	3.661170
96	6	0	-2.107657	-0.677558	3.662094
97	6	0	-3.005722	-2.640849	2.553551
98	6	0	-3.817619	-3.058839	1.552998
99	6	0	-3.228008	-3.522862	0.254019
100	6	0	-1.884055	-3.523719	0.081421
101	6	0	-1.295729	-3.061015	-1.217337
102	6	0	-0.033895	-2.311027	-0.911455
103	6	0	0.289281	-1.212121	-1.635533
104	6	0	0.835677	0.000076	-0.949067
105	6	0	0.157910	2.311635	0.575357
106	6	0	-0.033874	2.310480	-0.911469

107	6	0	0.289138	1.211748	-1.635971
108	6	0	-0.603827	0.749710	-2.746374
109	6	0	-0.603519	-0.749982	-2.746336
110	6	0	-1.743366	-1.428428	-3.022390
111	6	0	-2.107406	-2.640903	-2.218858
112	6	0	-3.594330	-2.640495	-2.027524
113	6	0	-4.126400	-3.058796	-0.853621
114	6	0	-3.369491	-1.427547	3.356212
115	6	0	-5.079762	-2.309136	1.247078
116	6	0	0.654894	-1.213484	1.193862

4. Coordinates of Monte Carlo global minimum conformer of **A3/1 adduct**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.505566	-0.434918	2.409293
2	6	0	-3.313656	0.240212	2.242796
3	6	0	-3.161958	1.525534	1.659796
4	6	0	-4.369601	2.122513	1.207026
5	7	0	-5.634764	1.588098	1.334136
6	6	0	-2.347085	-0.618846	2.781559
7	6	0	-3.024321	-1.816098	3.249404
8	6	0	-4.568404	3.342586	0.549683
9	6	0	-4.376294	-1.647603	3.004460
10	6	0	-5.998749	3.542981	0.401643
11	6	0	-6.624213	2.411974	0.898561
12	5	0	-5.886343	0.154606	1.908453
13	9	0	-6.762429	0.228496	2.969876
14	9	0	-6.362166	-0.533958	1.096032
15	6	0	-1.877561	2.230854	1.623546
16	6	0	-1.566796	3.179209	2.614947
17	6	0	-0.923948	1.982167	0.622131
18	6	0	-0.347364	3.859899	2.602569
19	1	0	-2.289817	3.384797	3.401796
20	6	0	0.304307	2.648376	0.617063
21	1	0	-1.127401	1.243224	-0.147565
22	6	0	0.580806	3.584574	1.606723
23	1	0	-0.120316	4.589525	3.371566
24	1	0	1.034158	2.413050	-0.152264
25	6	0	-3.541738	4.311869	0.062785
26	1	0	-3.092707	4.856175	0.898095
27	1	0	-2.763092	3.805322	-0.513968
28	1	0	-3.976049	5.056794	-0.610968
29	6	0	-0.869249	-0.413125	2.878734
30	1	0	-0.417360	-0.378153	1.884627
31	1	0	-0.634162	0.501518	3.429607
32	1	0	-0.375275	-1.229691	3.413803
33	6	0	-2.396569	-3.019420	3.884861
34	1	0	-1.589267	-2.711248	4.558825
35	1	0	-3.129954	-3.531433	4.519538
36	6	0	-5.546118	-2.508866	3.299080
37	1	0	-6.013492	-2.199560	4.239877
38	1	0	-6.303338	-2.466073	2.512626
39	1	0	-5.248377	-3.557231	3.398283
40	6	0	-8.053830	2.044063	1.023369
41	1	0	-8.233940	1.006558	0.727430
42	1	0	-8.389937	2.171140	2.057441
43	1	0	-8.681322	2.673638	0.385175
44	6	0	-6.686752	4.742464	-0.173357

45	1	0	-6.101415	5.645153	0.035505
46	1	0	-7.651269	4.891942	0.328169
47	6	0	-6.919124	4.622552	-1.671227
48	1	0	-7.412906	5.523277	-2.051034
49	1	0	-5.974799	4.500658	-2.212065
50	1	0	-7.555496	3.763406	-1.905689
51	6	0	-1.859829	-4.002268	2.855855
52	1	0	-2.653071	-4.343747	2.181977
53	1	0	-1.073728	-3.546306	2.244185
54	1	0	-1.434546	-4.878762	3.353199
55	8	0	1.768703	4.256027	1.637359
56	1	0	2.368740	3.838611	0.976561
57	7	0	5.756666	-1.603261	-1.408799
58	6	0	4.474304	-2.110686	-1.401024
59	6	0	3.310038	-1.434422	-1.855648
60	6	0	3.537936	-0.126336	-2.358715
61	7	0	4.759696	0.508684	-2.427713
62	6	0	4.605290	-3.391066	-0.849964
63	6	0	6.014206	-3.619009	-0.577157
64	6	0	2.629444	0.801499	-2.883858
65	6	0	6.691489	-2.462715	-0.926480
66	6	0	3.374122	1.988046	-3.267174
67	6	0	4.704022	1.758434	-2.955384
68	5	0	6.069870	-0.130432	-1.834847
69	9	0	7.057271	-0.130516	-2.800694
70	9	0	6.461766	0.496816	-0.909092
71	6	0	1.985190	-2.057665	-1.849700
72	6	0	1.578839	-2.872705	-2.920583
73	6	0	1.091650	-1.856955	-0.784649
74	6	0	0.319278	-3.475825	-2.921966
75	1	0	2.256530	-3.037084	-3.755482
76	6	0	-0.175481	-2.448927	-0.789560
77	1	0	1.382178	-1.221121	0.049826
78	6	0	-0.547206	-3.256884	-1.859063
79	1	0	0.015777	-4.106072	-3.750919
80	1	0	-0.854287	-2.263182	0.037579
81	6	0	1.149095	0.664374	-3.038957
82	1	0	0.899796	-0.173490	-3.694028
83	1	0	0.666772	0.533870	-2.067685
84	1	0	0.699353	1.555683	-3.486328
85	6	0	3.533608	-4.388645	-0.555747
86	1	0	2.755530	-3.954939	0.078478
87	1	0	3.092139	-4.769932	-1.480647
88	1	0	3.919699	-5.253903	-0.008817
89	6	0	6.633355	-4.860226	-0.013219
90	1	0	6.099621	-5.744359	-0.378781
91	1	0	7.661188	-4.963563	-0.380071
92	6	0	8.125411	-2.093651	-0.866664
93	1	0	8.559554	-2.080127	-1.870622
94	1	0	8.269047	-1.108576	-0.413207
95	1	0	8.694930	-2.808710	-0.264779
96	6	0	5.918944	2.589626	-3.117782
97	1	0	6.503728	2.244258	-3.975155
98	1	0	5.661601	3.639912	-3.286830
99	1	0	6.555791	2.555492	-2.229362
100	6	0	2.825127	3.241673	-3.877517
101	1	0	2.015546	2.997032	-4.574032
102	1	0	3.597742	3.729454	-4.484430
103	6	0	2.321156	4.224494	-2.832165
104	1	0	1.941122	5.130574	-3.315253
105	1	0	1.509246	3.791277	-2.238949
106	1	0	3.121761	4.516815	-2.144313

107	6	0	6.645715	-4.865190	1.508279
108	1	0	7.227063	-4.024330	1.900549
109	1	0	5.632310	-4.792077	1.915347
110	1	0	7.095133	-5.791149	1.880018
111	8	0	-1.771618	-3.856416	-1.903557
112	1	0	-2.313477	-3.497827	-1.164268
113	6	0	-5.938891	-2.806813	-0.519534
114	6	0	-7.120819	-2.190982	-0.967908
115	6	0	-7.063679	-0.945663	-1.620128
116	6	0	-5.819005	-0.316456	-1.825549
117	6	0	-4.637914	-0.933360	-1.376786
118	6	0	-4.694790	-2.173966	-0.721292
119	17	0	-3.082623	-0.238391	-1.754039
120	17	0	-5.735233	1.171175	-2.731914
121	17	0	-8.646200	-3.025315	-0.779433
122	8	0	-3.722621	-2.729775	-0.491247
123	6	0	4.588358	2.105712	0.785979
124	6	0	5.932932	2.428204	1.031807
125	6	0	6.782708	1.484949	1.637621
126	6	0	6.285403	0.215986	1.998772
127	6	0	4.936893	-0.101927	1.762247
128	6	0	4.090265	0.838957	1.154095
129	17	0	6.507636	4.036724	0.662504
130	8	0	2.970349	0.625032	1.098958
131	17	0	7.318980	-0.924898	2.819668
132	8	0	-5.994561	-3.997369	-0.073032
133	17	0	-8.524679	-0.220949	-2.241951
134	17	0	8.436446	1.909601	1.998997
135	17	0	4.262823	-1.606915	2.344803
136	8	0	3.793458	3.024051	0.396429

5. Coordinates of Monte Carlo global minimum conformer of **A4/1 adduct**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.572821	0.793212	-2.146198
2	6	0	-4.266537	0.370172	-2.273897
3	6	0	-3.785633	-0.936611	-1.996163
4	6	0	-4.775835	-1.860241	-1.569013
5	7	0	-6.112536	-1.579383	-1.381113
6	6	0	-3.576697	1.499322	-2.732259
7	6	0	-4.547246	2.560264	-2.945682
8	6	0	-4.652494	-3.219249	-1.254740
9	6	0	-5.777039	2.079562	-2.530761
10	6	0	-5.970900	-3.718048	-0.901254
11	6	0	-6.847313	-2.647488	-0.974036
12	5	0	-6.693438	-0.129605	-1.537707
13	9	0	-7.772207	-0.161581	-2.389268
14	9	0	-7.059050	0.288832	-0.502939
15	6	0	-2.385965	-1.315801	-2.194790
16	6	0	-1.457120	-1.230857	-1.144996
17	6	0	-1.939175	-1.769399	-3.448261
18	6	0	-0.115420	-1.572620	-1.343553
19	1	0	-1.784068	-0.887336	-0.165966
20	6	0	-0.600740	-2.114238	-3.648789
21	1	0	-2.645312	-1.844348	-4.272610
22	6	0	0.301084	-2.003654	-2.598304
23	1	0	0.584112	-1.496494	-0.517204
24	1	0	-0.263884	-2.454904	-4.621285

25	6	0	-3.420931	-4.064068	-1.262044
26	1	0	-3.000159	-4.134133	-2.267149
27	1	0	-2.672418	-3.668017	-0.570654
28	1	0	-3.624448	-5.088127	-0.936134
29	6	0	-2.113885	1.652497	-2.993587
30	1	0	-1.528220	1.381291	-2.111389
31	1	0	-1.804709	1.045236	-3.848161
32	1	0	-1.846619	2.687501	-3.223965
33	6	0	-4.281662	3.921939	-3.513718
34	1	0	-3.481151	3.863636	-4.258914
35	1	0	-5.166154	4.273890	-4.058248
36	6	0	-7.121426	2.699331	-2.483602
37	1	0	-7.754287	2.302950	-3.282883
38	1	0	-7.614674	2.513377	-1.525170
39	1	0	-7.062491	3.784973	-2.609213
40	6	0	-8.303608	-2.537175	-0.723712
41	1	0	-8.544822	-1.654748	-0.125053
42	1	0	-8.849534	-2.475095	-1.670134
43	1	0	-8.678792	-3.407537	-0.176638
44	6	0	-6.331743	-5.122292	-0.528163
45	1	0	-5.742233	-5.828386	-1.123495
46	1	0	-7.378417	-5.321586	-0.786968
47	6	0	-6.122859	-5.405869	0.951012
48	1	0	-6.365426	-6.449816	1.173711
49	1	0	-5.085924	-5.225853	1.251989
50	1	0	-6.767464	-4.771200	1.567436
51	6	0	-3.912243	4.944381	-2.451248
52	1	0	-4.742718	5.106503	-1.757564
53	1	0	-3.042274	4.621621	-1.870360
54	1	0	-3.672661	5.904620	-2.917986
55	8	0	1.604085	-2.327154	-2.837381
56	1	0	2.136348	-2.028205	-2.064443
57	7	0	6.088857	1.585379	1.243796
58	6	0	4.748242	1.842472	1.439752
59	6	0	3.783718	0.909171	1.901372
60	6	0	4.290103	-0.391759	2.165305
61	7	0	5.603622	-0.786159	2.030648
62	6	0	4.589805	3.184493	1.072098
63	6	0	5.881484	3.682229	0.627515
64	6	0	3.618156	-1.543848	2.591253
65	6	0	6.790800	2.648277	0.773381
66	6	0	4.593594	-2.616049	2.701471
67	6	0	5.826362	-2.084843	2.361138
68	5	0	6.703098	0.157729	1.434448
69	9	0	7.755405	0.232184	2.303133
70	9	0	7.108356	-0.267654	0.401675
71	6	0	2.378496	1.262637	2.110788
72	6	0	1.435859	1.131668	1.077531
73	6	0	1.940243	1.736040	3.359799
74	6	0	0.091539	1.450379	1.287994
75	1	0	1.754326	0.770141	0.102089
76	6	0	0.597527	2.055389	3.571683
77	1	0	2.656010	1.845514	4.171139
78	6	0	-0.316758	1.900815	2.537432
79	1	0	-0.618842	1.341292	0.473215
80	1	0	0.267180	2.411698	4.542471
81	6	0	2.162737	-1.714408	2.883712
82	1	0	1.843447	-1.045415	3.686084
83	1	0	1.563276	-1.537618	1.987014
84	1	0	1.928549	-2.728441	3.221445
85	6	0	3.344308	4.008699	1.091019
86	1	0	2.608586	3.617528	0.382998

87	1	0	2.913940	4.045925	2.094262
88	1	0	3.535992	5.046979	0.805156
89	6	0	6.189497	5.052771	0.110344
90	1	0	7.024290	5.006458	-0.598714
91	1	0	5.338936	5.438015	-0.464223
92	6	0	8.250067	2.561533	0.526004
93	1	0	8.789841	2.396477	1.463699
94	1	0	8.488794	1.743285	-0.160603
95	1	0	8.638081	3.482726	0.082359
96	6	0	7.187382	-2.669369	2.316668
97	1	0	7.836140	-2.189099	3.056100
98	1	0	7.173025	-3.740208	2.542238
99	1	0	7.638603	-2.549842	1.328552
100	6	0	4.332632	-4.034406	3.104668
101	1	0	5.069517	-4.698101	2.638487
102	1	0	3.360481	-4.361822	2.719357
103	6	0	4.374374	-4.222994	4.613043
104	1	0	4.180799	-5.269813	4.869691
105	1	0	5.354633	-3.949507	5.018351
106	1	0	3.620220	-3.605934	5.112629
107	6	0	6.535639	6.027975	1.225234
108	1	0	5.706497	6.132313	1.932813
109	1	0	7.414625	5.691193	1.784650
110	1	0	6.754671	7.016327	0.810587
111	8	0	-1.624068	2.197926	2.788301
112	1	0	-2.158565	1.868157	2.029617
113	6	0	-5.627988	2.036446	1.356209
114	6	0	-6.959623	1.873701	1.762278
115	6	0	-7.401327	0.618758	2.217998
116	6	0	-6.517153	-0.475187	2.263671
117	6	0	-5.183887	-0.310905	1.858588
118	6	0	-4.743126	0.944206	1.403154
119	17	0	-4.031003	-1.605620	2.055630
120	17	0	-7.064584	-1.987621	2.938218
121	17	0	-8.054444	3.233707	1.795484
122	8	0	-3.503142	1.141205	1.213240
123	6	0	5.671734	-2.101598	-1.418049
124	6	0	6.978483	-1.854876	-1.861190
125	6	0	7.326365	-0.574964	-2.333399
126	6	0	6.371292	0.458031	-2.360328
127	6	0	5.061192	0.205900	-1.928566
128	6	0	4.715273	-1.072071	-1.454518
129	17	0	3.817612	1.414857	-2.122632
130	17	0	8.157910	-3.140514	-1.921271
131	8	0	3.495230	-1.349070	-1.235699
132	17	0	5.182661	-3.710432	-0.945530
133	17	0	6.803418	2.006075	-3.044560
134	8	0	8.459440	-0.392976	-2.870899
135	8	0	-8.558051	0.509692	2.725512
136	17	0	-5.019408	3.611426	0.920213

6. Coordinates of Monte Carlo global minimum conformer of **A5/1 adduct**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-6.159106	-1.295655	1.469809
2	6	0	-4.824831	-1.511164	1.741374
3	6	0	-3.861965	-0.505736	2.020448
4	6	0	-4.367270	0.820737	2.029785

5	7	0	-5.681905	1.184445	1.824585
6	6	0	-4.672492	-2.901229	1.671786
7	6	0	-5.968789	-3.478062	1.357272
8	6	0	-3.694607	2.033005	2.227008
9	6	0	-6.862324	-2.429485	1.217235
10	6	0	-4.672671	3.105600	2.148355
11	6	0	-5.906215	2.521122	1.918066
12	5	0	-6.766389	0.155663	1.356579
13	9	0	-7.850553	0.247918	2.160714
14	9	0	-7.107640	0.376847	0.274217
15	6	0	-2.463171	-0.815951	2.321913
16	6	0	-1.506770	-0.927071	1.299196
17	6	0	-2.045175	-1.008742	3.649978
18	6	0	-0.170880	-1.212539	1.591739
19	1	0	-1.809881	-0.786557	0.263970
20	6	0	-0.709545	-1.291243	3.945857
21	1	0	-2.770514	-0.930501	4.456745
22	6	0	0.216991	-1.383466	2.916000
23	1	0	0.547721	-1.297707	0.782216
24	1	0	-0.395052	-1.431224	4.975501
25	6	0	-2.237146	2.255921	2.467160
26	1	0	-1.917584	1.783124	3.398716
27	1	0	-1.642068	1.877602	1.632364
28	1	0	-1.994852	3.318723	2.564769
29	6	0	-3.431266	-3.709005	1.868733
30	1	0	-2.672945	-3.443598	1.127605
31	1	0	-3.031040	-3.572437	2.876722
32	1	0	-3.614828	-4.780187	1.748380
33	6	0	-6.294459	-4.933173	1.208799
34	1	0	-5.720361	-5.519865	1.935337
35	1	0	-7.348604	-5.107047	1.457615
36	6	0	-8.309212	-2.391194	0.897276
37	1	0	-8.892230	-2.152117	1.792099
38	1	0	-8.529998	-1.645202	0.128511
39	1	0	-8.657673	-3.356546	0.517089
40	6	0	-7.269753	3.088596	1.788621
41	1	0	-7.747686	2.767322	0.859118
42	1	0	-7.896560	2.772790	2.629174
43	1	0	-7.251829	4.182145	1.785663
44	6	0	-4.410804	4.575268	2.288507
45	1	0	-5.165326	5.145715	1.734425
46	1	0	-3.451101	4.831958	1.826196
47	6	0	-4.415898	5.026242	3.741291
48	1	0	-4.224682	6.101855	3.804945
49	1	0	-5.383084	4.824230	4.214341
50	1	0	-3.643800	4.509372	4.321631
51	6	0	-6.022091	-5.451385	-0.193953
52	1	0	-6.646635	-4.936602	-0.930608
53	1	0	-4.975179	-5.303974	-0.479747
54	1	0	-6.244758	-6.521497	-0.252958
55	8	0	1.516149	-1.641862	3.243355
56	1	0	2.056458	-1.551656	2.425247
57	7	0	5.668631	-1.221301	-1.771234
58	6	0	4.356199	-0.856410	-1.979714
59	6	0	3.851695	0.471819	-1.967679
60	6	0	4.812196	1.472752	-1.666807
61	7	0	6.148065	1.253962	-1.403590
62	6	0	3.681480	-2.066515	-2.176622
63	6	0	4.655798	-3.142100	-2.086010
64	6	0	4.655283	2.859103	-1.557102
65	6	0	5.890469	-2.559091	-1.857323
66	6	0	5.937245	3.426284	-1.174571

67	6	0	6.844639	2.382377	-1.109548
68	5	0	6.757920	-0.191705	-1.315568
69	9	0	7.821313	-0.275147	-2.141148
70	9	0	7.124695	-0.420664	-0.238693
71	6	0	2.452772	0.783518	-2.267476
72	6	0	1.497364	0.893686	-1.244435
73	6	0	2.034779	0.977275	-3.595800
74	6	0	0.161542	1.178895	-1.537942
75	1	0	1.797542	0.750940	-0.209850
76	6	0	0.699212	1.258551	-3.892384
77	1	0	2.760118	0.899034	-4.402567
78	6	0	-0.227394	1.350067	-2.861304
79	1	0	-0.557063	1.263098	-0.728159
80	1	0	0.384652	1.398791	-4.921064
81	6	0	3.418538	3.671884	-1.762349
82	1	0	2.991694	3.496459	-2.753439
83	1	0	2.675694	3.449662	-0.991277
84	1	0	3.620331	4.745307	-1.706714
85	6	0	2.224426	-2.289053	-2.423074
86	1	0	1.627349	-1.911727	-1.588149
87	1	0	1.908739	-1.810853	-3.353738
88	1	0	1.981411	-3.350007	-2.525380
89	6	0	4.391192	-4.611846	-2.214914
90	1	0	5.138862	-5.179013	-1.648697
91	1	0	3.426661	-4.861398	-1.756930
92	6	0	7.251462	-3.129352	-1.719004
93	1	0	7.893687	-2.791643	-2.539468
94	1	0	7.712606	-2.831532	-0.772946
95	1	0	7.235497	-4.222680	-1.746065
96	6	0	8.297328	2.340051	-0.816123
97	1	0	8.857541	2.007087	-1.694570
98	1	0	8.679285	3.326326	-0.538865
99	1	0	8.514211	1.660103	0.013500
100	6	0	6.241135	4.868468	-0.904790
101	1	0	7.049874	4.947957	-0.169736
102	1	0	5.375240	5.353870	-0.442299
103	6	0	6.636697	5.622160	-2.165370
104	1	0	6.850200	6.669073	-1.930576
105	1	0	7.531614	5.185747	-2.622409
106	1	0	5.834932	5.597632	-2.911591
107	6	0	4.406147	-5.076909	-3.662194
108	1	0	3.640834	-4.563061	-4.253707
109	1	0	5.378027	-4.881518	-4.128991
110	1	0	4.212392	-6.153376	-3.717493
111	8	0	-1.527630	1.604844	-3.186724
112	1	0	-2.064836	1.507402	-2.368533
113	6	0	-5.059988	-0.494654	-1.900899
114	6	0	-6.367695	-0.785958	-2.316764
115	6	0	-7.306169	0.255261	-2.442366
116	6	0	-6.948838	1.573610	-2.135628
117	6	0	-5.640340	1.863773	-1.716288
118	6	0	-4.699884	0.833432	-1.608000
119	17	0	-6.817024	-2.402032	-2.792728
120	8	0	-3.481395	1.131376	-1.423204
121	6	0	5.003604	0.513801	1.942453
122	6	0	6.302662	0.860479	2.340771
123	6	0	7.276563	-0.143104	2.483619
124	6	0	6.964503	-1.480919	2.209108
125	6	0	5.667263	-1.824894	1.797737
126	6	0	4.690316	-0.831944	1.673100
127	17	0	6.697449	2.504881	2.771108
128	8	0	3.483116	-1.175008	1.493940

129	17	0	3.734192	1.709391	1.924770
130	8	0	8.399808	0.135150	2.995047
131	8	0	-8.435425	0.027923	-2.964773
132	17	0	-3.838095	-1.738380	-1.881875
133	6	0	5.306135	-3.196101	1.591067
134	6	0	7.967290	-2.484962	2.400776
135	7	0	8.729692	-3.337128	2.603519
136	7	0	5.052628	-4.326665	1.510884
137	6	0	-7.915467	2.616339	-2.306130
138	6	0	-5.230195	3.218504	-1.489351
139	7	0	-4.937494	4.337728	-1.393034
140	7	0	-8.648593	3.497882	-2.487758
