

## Supporting Information for

### Design, synthesis and application of fluorescent 2,1,3-benzothiadiazole-triazole-linked biologically active lapachone derivatives

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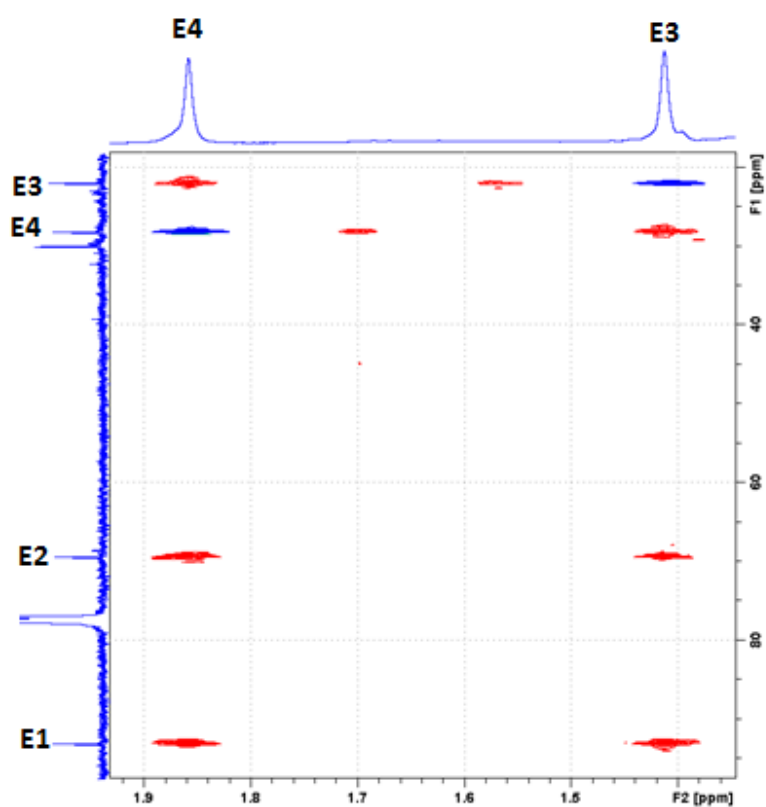
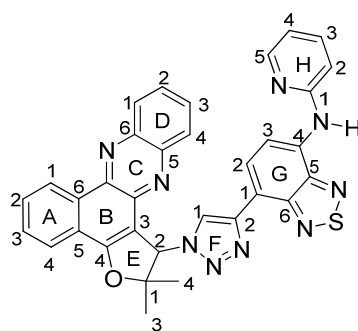
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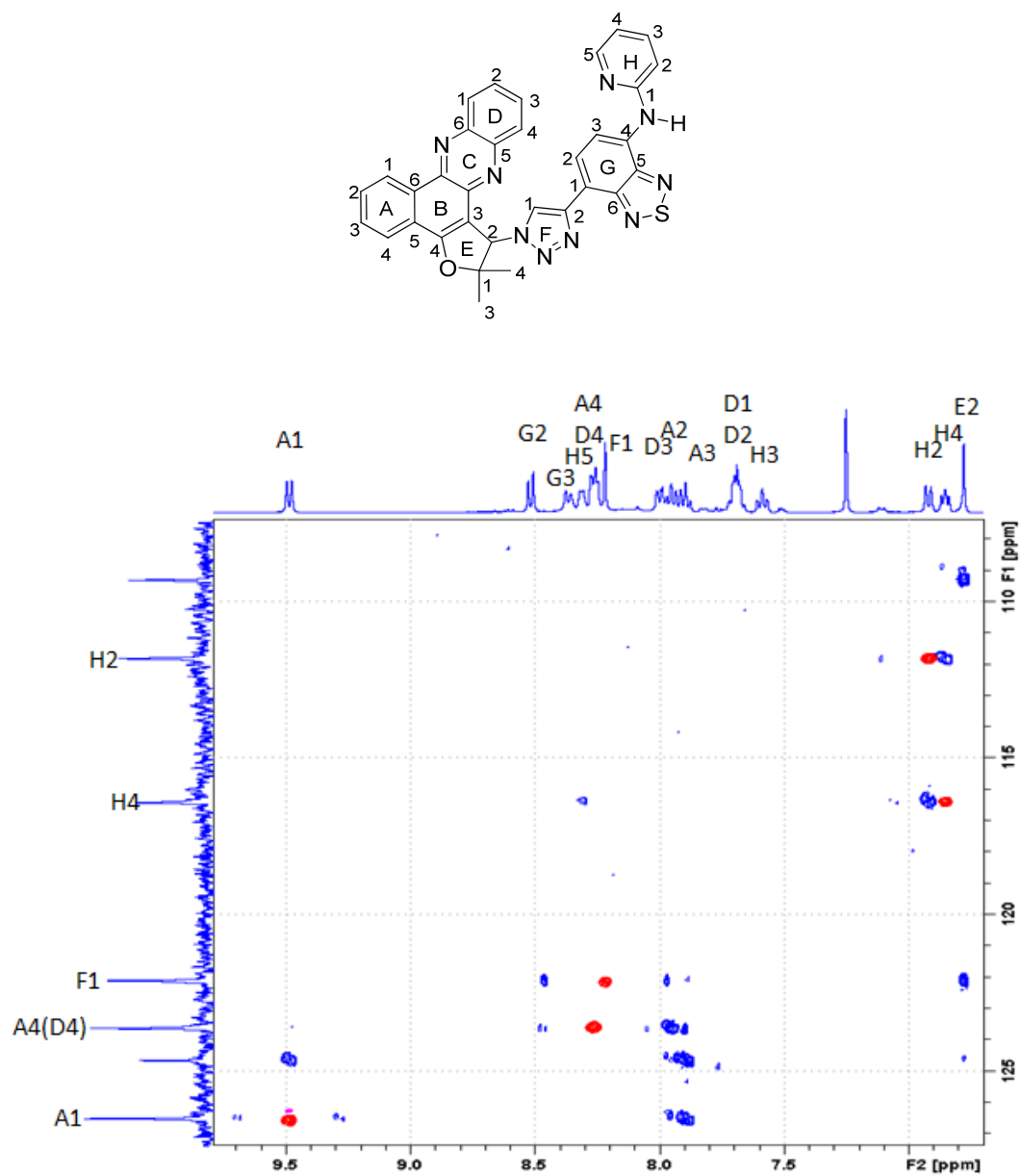
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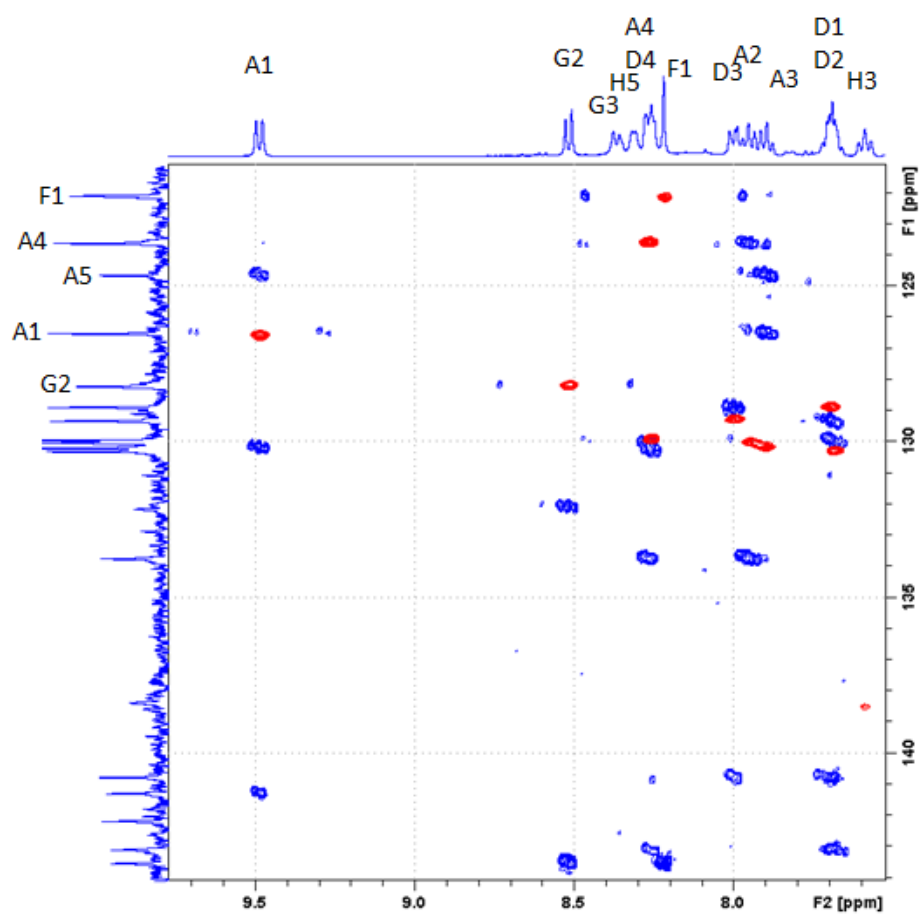
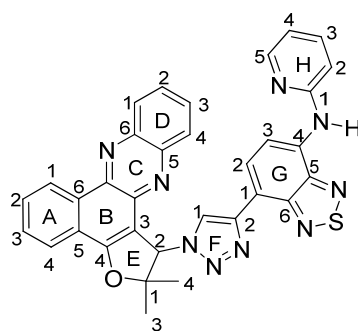
Cartesian coordinates for all the calculated structures \_\_\_\_\_ Pages S12-S20



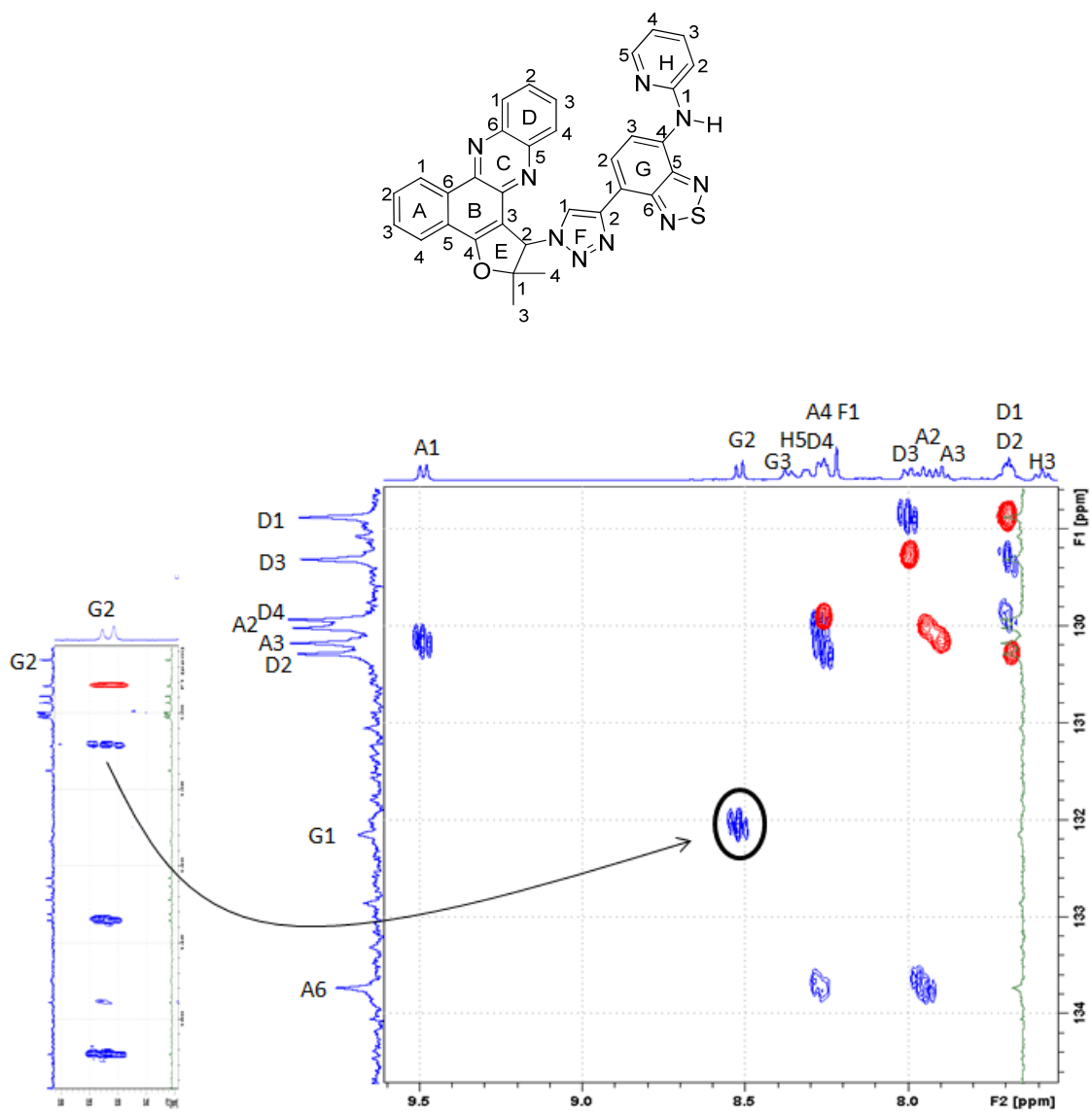
**Figure S1.** Expanded HSQC (blue), HMBC(red) spectra in CDCl<sub>3</sub> for structure **10**.



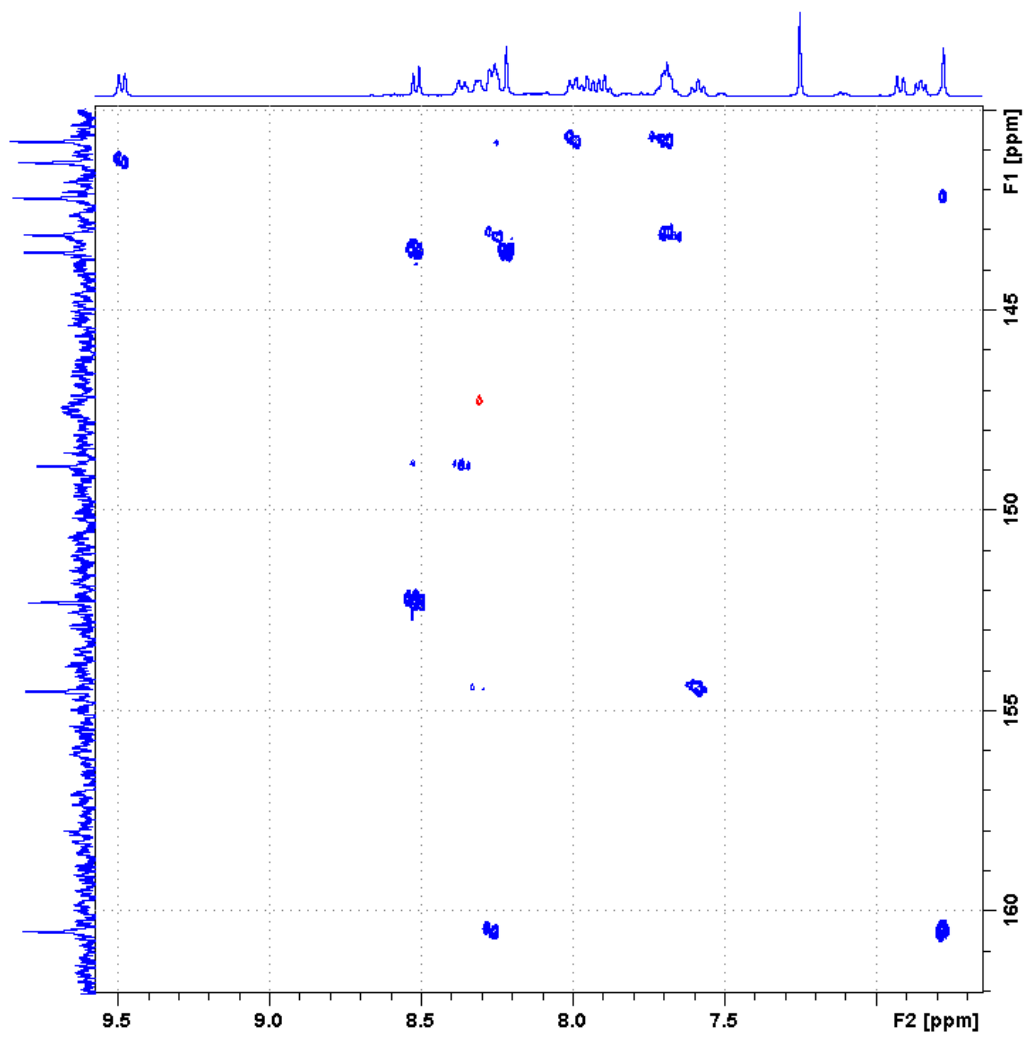
**Figure S2.** Expanded HSQC (red), HMBC(blue) spectra in CDCl<sub>3</sub> for structure 10.



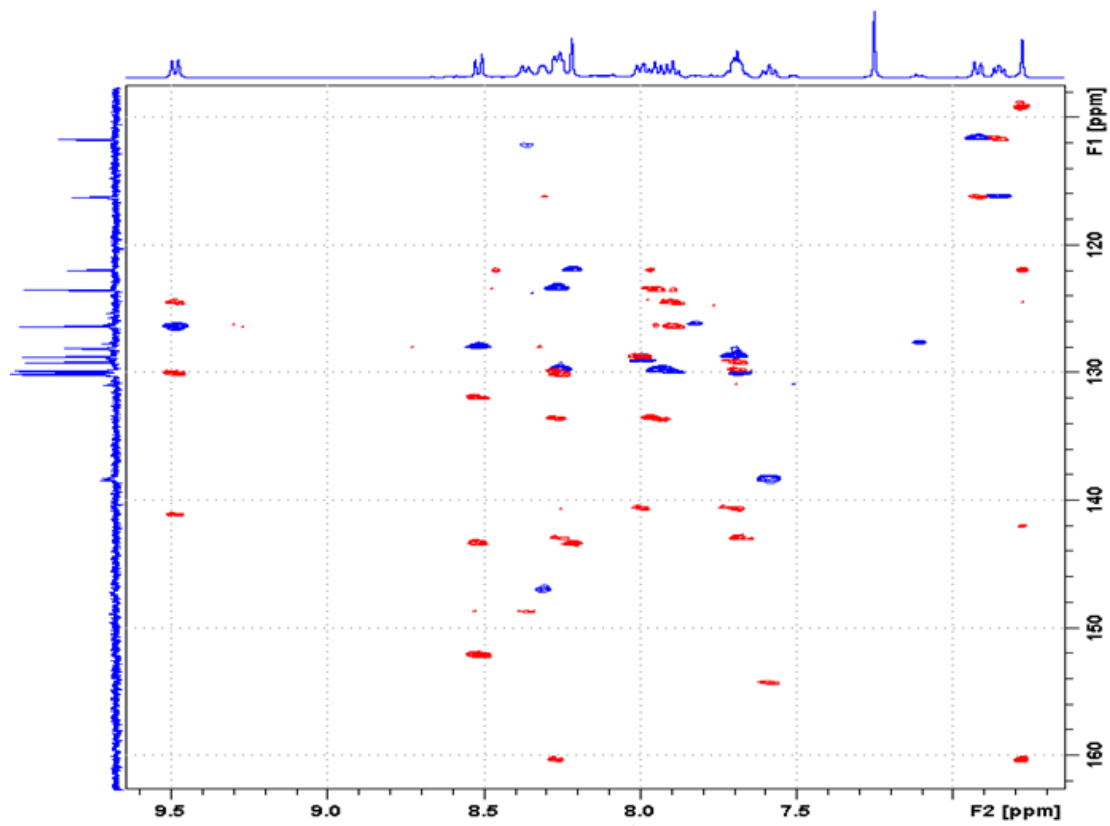
**Figure S3.** Expanded HSQC (red), HMBC(blue) spectra in CDCl<sub>3</sub> for structure **10**.



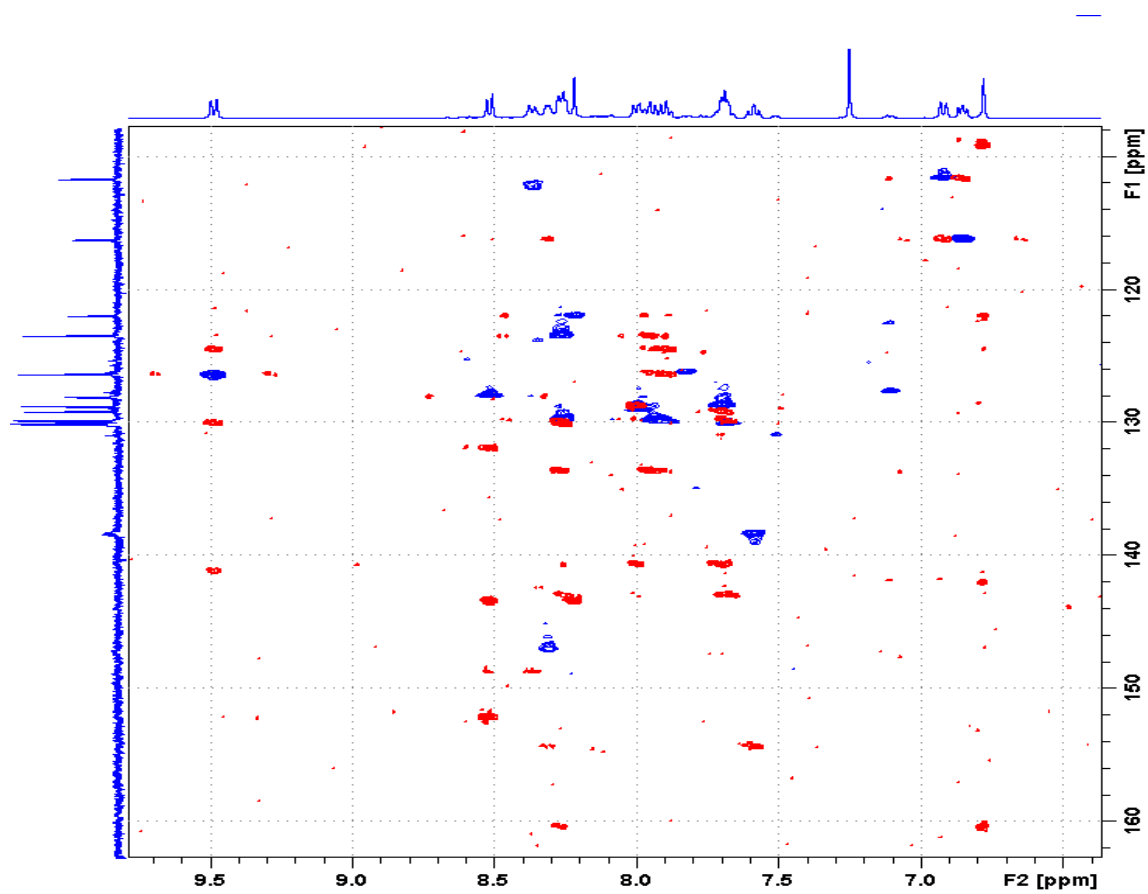
**Figure S4.** Expanded HSQC (red), HMBC(blue) spectra in CDCl<sub>3</sub> for structure 10.



**Figure S5.** Expanded HSQC (red), HMBC(blue) spectra in CDCl<sub>3</sub> for structure **10**.

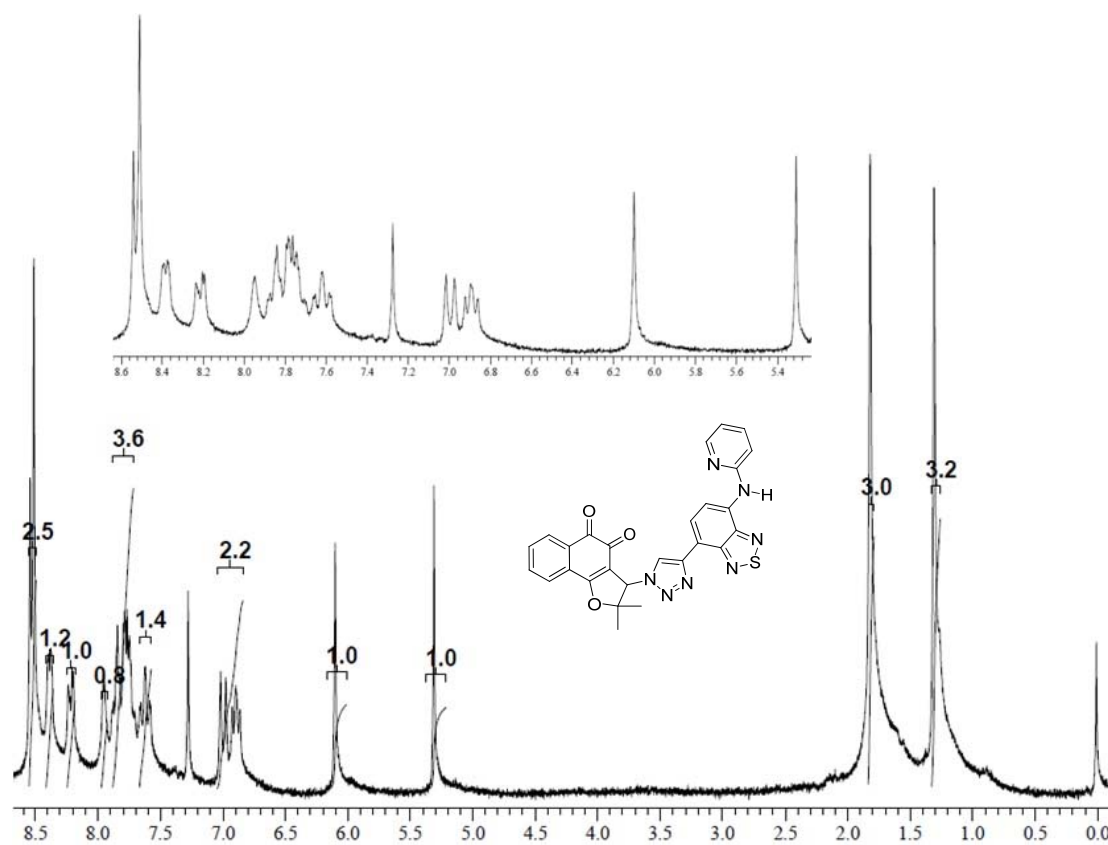


**Figure S6.** Expanded HSQC (red), HMBC(blue) spectra in CDCl<sub>3</sub> for structure **10**.

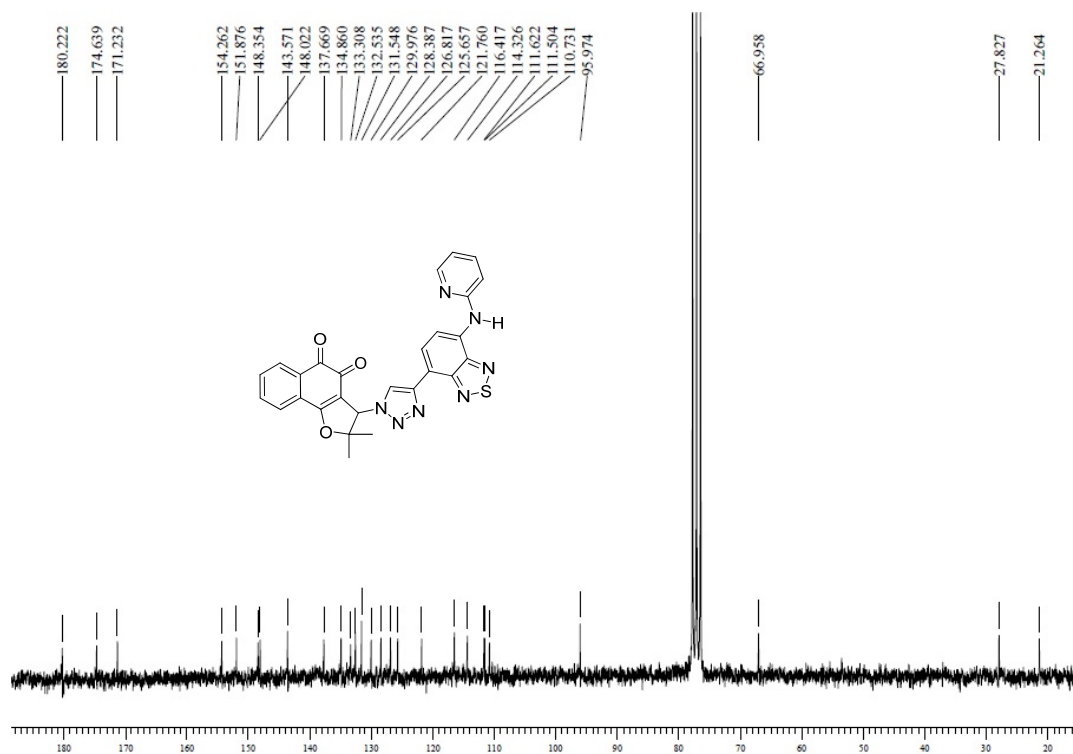


**Figure S7.** Expanded HSQC (red), HMBC(blue) spectra in  $\text{CDCl}_3$  for structure **10**.

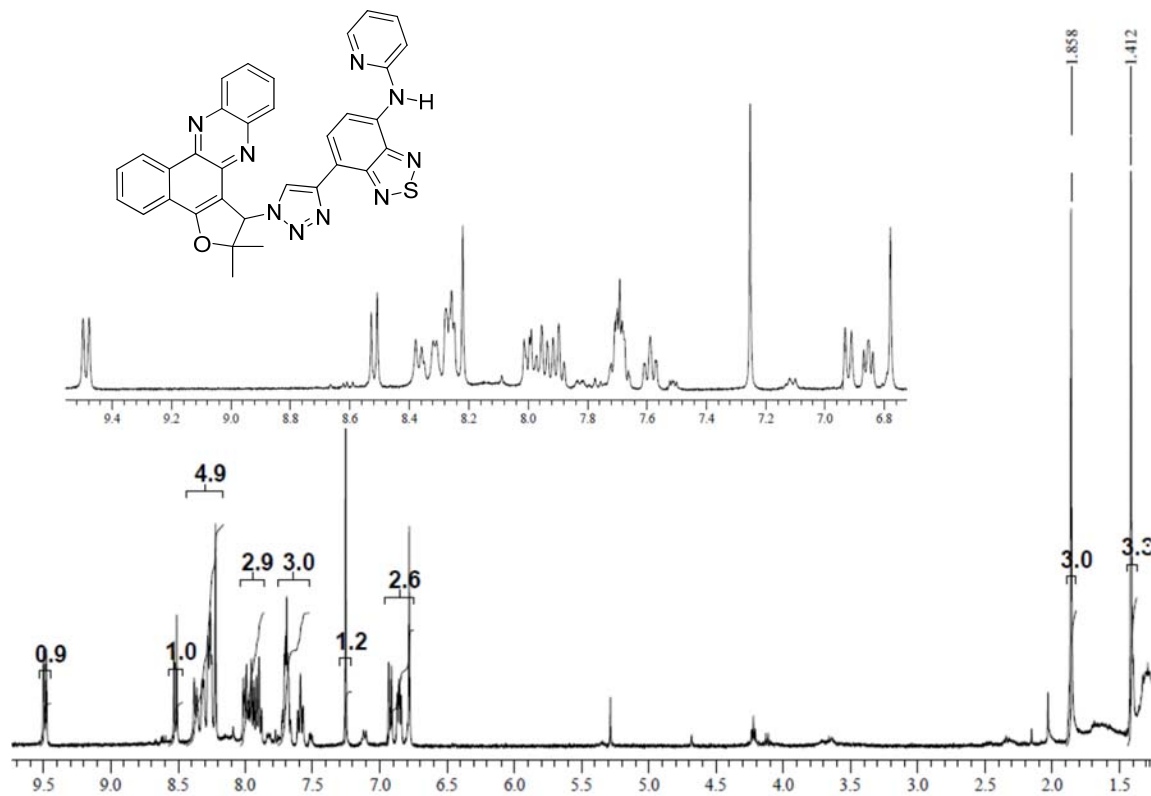




**Figure S8.** <sup>1</sup>H-NMR spectrum showing the expanded aromatic region for structure **9** (200 MHz, CDCl<sub>3</sub>).



**Figure S9.**  $^{13}\text{C}$ -NMR spectrum for structure **9** (50 MHz,  $\text{CDCl}_3$ ).



**Figure S10.** <sup>1</sup>H-NMR spectrum showing the expanded aromatic region for structure **10** (400 MHz, CDCl<sub>3</sub>).

## Cartesian coordinates for all the calculated structures

9 before ESIPT ( $S_0$ )

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.488858	-3.323889	-0.683633
2	6	0	-6.418135	-2.504368	-1.812714
3	6	0	-5.740763	-1.285361	-1.757387
4	6	0	-5.127318	-0.888442	-0.565985
5	6	0	-5.196752	-1.713349	0.579233
6	6	0	-5.881172	-2.927479	0.508525
7	6	0	-4.400371	0.369908	-0.443905
8	6	0	-3.767927	0.804071	0.682631
9	6	0	-3.791543	0.060810	1.923937
10	6	0	-4.555384	-1.300609	1.870180
11	8	0	-4.327600	1.202853	-1.488600
12	6	0	-3.699279	2.472833	-1.023572
13	6	0	-3.100151	2.118671	0.390462
14	8	0	-4.614514	-1.994345	2.866531
15	8	0	-3.273354	0.424839	2.968182
16	6	0	-4.837016	3.480335	-0.876637
17	6	0	-2.688184	2.880975	-2.081663
18	7	0	-1.639462	2.040781	0.427510
19	7	0	-0.934521	3.178430	0.646368
20	7	0	0.328024	2.877178	0.570423
21	6	0	0.464004	1.538239	0.299272
22	6	0	-0.806042	0.994618	0.200948
23	6	0	1.775105	0.910216	0.169974
24	6	0	1.933211	-0.478274	-0.148126
25	6	0	3.258295	-1.055513	-0.263270
26	6	0	4.445524	-0.264795	-0.066655
27	6	0	4.252289	1.070390	0.236776
28	6	0	2.946431	1.622314	0.347912
29	7	0	0.959052	-1.370352	-0.368248
30	16	0	1.686336	-2.813328	-0.688659
31	7	0	3.264399	-2.354750	-0.562695
32	7	0	5.641073	-0.951815	-0.208911
33	6	0	6.953949	-0.523346	-0.095073
34	6	0	7.984480	-1.469093	-0.297337
35	6	0	9.297618	-1.046621	-0.185143
36	6	0	9.565037	0.293175	0.122998
37	6	0	8.479597	1.141734	0.302413
38	7	0	7.198801	0.759068	0.199166
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40	1	0	-6.892491	-2.813616	-2.738974
41	1	0	-5.681921	-0.640741	-2.627397
42	1	0	-5.925262	-3.544220	1.400035
43	1	0	-3.352875	2.901378	1.109633
44	1	0	-4.434738	4.450962	-0.571682
45	1	0	-5.363234	3.602417	-1.826681
46	1	0	-5.555084	3.151925	-0.119135
47	1	0	-3.199392	3.068123	-3.029716
48	1	0	-2.171655	3.792276	-1.771093
49	1	0	-1.940286	2.100231	-2.235687
50	1	0	-1.140515	-0.010801	0.015505
51	1	0	5.114733	1.700901	0.393546
52	1	0	2.860484	2.676042	0.591562
53	1	0	7.744886	-2.501507	-0.534714
54	1	0	10.108787	-1.752923	-0.335621
55	1	0	10.579668	0.662709	0.220028
56	1	0	8.635303	2.191553	0.543331

57	1	0	5.513089	-1.930698	-0.431171
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9 after ESIPT ( $S_0$ )

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.482690	-3.321758	-0.682687
2	6	0	-6.412169	-2.502219	-1.811768
3	6	0	-5.735097	-1.283046	-1.756441
4	6	0	-5.121749	-0.885976	-0.565039
5	6	0	-5.190980	-1.710900	0.580179
6	6	0	-5.875102	-2.925198	0.509471
7	6	0	-4.395112	0.372553	-0.442959
8	6	0	-3.762774	0.806871	0.683577
9	6	0	-3.786208	0.063604	1.924883
10	6	0	-4.549714	-1.298002	1.871126
11	8	0	-4.322545	1.205516	-1.487654
12	6	0	-3.694537	2.475650	-1.022626
13	6	0	-3.095322	2.121635	0.391408
14	8	0	-4.608673	-1.991753	2.867477
15	8	0	-3.268108	0.427761	2.969128
16	6	0	-4.832521	3.482872	-0.875691
17	6	0	-2.683542	2.884041	-2.080717
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19	7	0	-0.929952	3.181927	0.647314
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21	6	0	0.468976	1.542080	0.300218
22	6	0	-0.800936	0.998146	0.201894
23	6	0	1.780231	0.914379	0.170920
24	6	0	1.938679	-0.474072	-0.147180
25	6	0	3.263905	-1.050985	-0.262324
26	6	0	4.450939	-0.259975	-0.065709
27	6	0	4.257376	1.075162	0.237722
28	6	0	2.951382	1.626765	0.348858
29	7	0	0.964739	-1.366390	-0.367302
30	16	0	1.692378	-2.809187	-0.687713
31	7	0	3.270328	-2.350221	-0.561749
32	7	0	5.646657	-0.946701	-0.207965
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34	6	0	7.990191	-1.463403	-0.296391
35	6	0	9.303225	-1.040608	-0.184197
36	6	0	9.570315	0.299253	0.123944
37	6	0	8.484666	1.147545	0.303359
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42	1	0	-5.919040	-3.541950	1.400981
43	1	0	-3.348238	2.904280	1.110579
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45	1	0	-5.358769	3.604825	-1.825735
46	1	0	-5.550509	3.154286	-0.118189
47	1	0	-3.194796	3.071063	-3.028770
48	1	0	-2.167237	3.795469	-1.770147
49	1	0	-1.935452	2.103480	-2.234741
50	1	0	-1.135162	-0.007355	0.016451
51	1	0	5.119665	1.705885	0.394492
52	1	0	2.865176	2.680472	0.592508
53	1	0	7.750851	-2.495876	-0.533768
54	1	0	10.114568	-1.746711	-0.334675
55	1	0	10.584855	0.669037	0.220974
56	1	0	8.640114	2.197403	0.544277
57	1	0	4.074359	-2.931779	-0.685541

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10 before ESIPT (S<sub>0</sub>)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.962219	-0.252201	3.602413
2	6	0	-5.737506	-1.633361	3.476811
3	6	0	-5.034643	-2.126570	2.388841
4	6	0	-4.543673	-1.242250	1.411225
5	6	0	-4.768630	0.156149	1.530346
6	6	0	-5.486082	0.629504	2.643447
7	6	0	-3.805091	-1.694844	0.260175
8	6	0	-3.315237	-0.859902	-0.700405
9	6	0	-3.527013	0.553210	-0.632859
10	6	0	-4.265677	1.073043	0.502486
11	8	0	-3.555898	-3.004992	0.049920
12	6	0	-2.979989	-3.141244	-1.307931
13	6	0	-2.574665	-1.673630	-1.722632
14	6	0	-4.107464	-3.641562	-2.210570
15	7	0	-1.131649	-1.419534	-1.725795
16	7	0	-0.428523	-1.672376	-2.856540
17	7	0	0.824574	-1.434936	-2.600443
18	6	0	0.954713	-1.025468	-1.296773
19	6	0	-0.308031	-1.017753	-0.726772
20	6	0	2.254419	-0.680874	-0.728655
21	6	0	2.411683	-0.256315	0.631433
22	6	0	3.726121	0.072683	1.148151
23	6	0	4.904016	-0.016111	0.325188
24	6	0	4.712509	-0.429312	-0.980158
25	6	0	3.416984	-0.747486	-1.473503
26	7	0	1.445339	-0.114516	1.547410
27	16	0	2.165728	0.395392	2.937889
28	7	0	3.731736	0.452531	2.426309
29	7	0	6.090508	0.327925	0.955671
30	7	0	-3.058315	1.349449	-1.592278
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32	6	0	-4.025554	3.193816	-0.337927
33	7	0	-4.499315	2.372273	0.627831
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35	6	0	-3.054584	4.923467	-2.328753
36	6	0	-3.776569	5.437470	-1.216308
37	6	0	-4.252412	4.594199	-0.241405
38	6	0	7.394208	0.349009	0.488288
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41	6	0	9.989158	0.398508	-0.405602
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47	1	0	-4.853408	-3.189665	2.273899
48	1	0	-5.655205	1.696880	2.727140
49	1	0	-2.888661	-1.474676	-2.749729
50	1	0	-4.501545	-4.589143	-1.834524
51	1	0	-4.926295	-2.916702	-2.250470
52	1	0	-3.733396	-3.796006	-3.227278
53	1	0	-0.648687	-0.750596	0.258123
54	1	0	5.568454	-0.510663	-1.633445
55	1	0	3.331940	-1.065239	-2.507361
56	1	0	5.962049	0.601262	1.921461
57	1	0	-2.268297	3.160807	-3.291096
58	1	0	-2.687008	5.609577	-3.086012
59	1	0	-3.949577	6.506845	-1.142073
60	1	0	-4.805637	4.960022	0.617536
61	1	0	8.177324	1.027829	2.400985
62	1	0	10.525894	1.069486	1.582984
63	1	0	10.997411	0.401964	-0.804196
64	1	0	9.068522	-0.271132	-2.235490

65	1	0	-1.082440	-3.796453	-0.491037
66	1	0	-2.211627	-5.105911	-0.889382
67	1	0	-1.347194	-4.245212	-2.183918

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**10 after ESIPT ( $S_0$ )**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.956319	-0.244862	3.601612
2	6	0	-5.731565	-1.626287	3.479034
3	6	0	-5.029045	-2.121895	2.391933
4	6	0	-4.538463	-1.239742	1.412167
5	6	0	-4.763464	0.158908	1.528226
6	6	0	-5.480563	0.634717	2.640507
7	6	0	-3.800247	-1.694874	0.261883
8	6	0	-3.310773	-0.862061	-0.700737
9	6	0	-3.522611	0.551186	-0.636290
10	6	0	-4.260918	1.073522	0.498138
11	8	0	-3.551047	-3.005476	0.054483
12	6	0	-2.975594	-3.144741	-1.303255
13	6	0	-2.570501	-1.678037	-1.721388
14	6	0	-4.103348	-3.647151	-2.204383
15	7	0	-1.127502	-1.423863	-1.725615
16	7	0	-0.424747	-1.679200	-2.856030
17	7	0	0.828423	-1.441111	-2.600896
18	6	0	0.958983	-1.028710	-1.298193
19	6	0	-0.303566	-1.019791	-0.727778
20	6	0	2.258863	-0.682764	-0.731295
21	6	0	2.416566	-0.255144	0.627783
22	6	0	3.731161	0.075091	1.143311
23	6	0	4.908780	-0.015479	0.320147
24	6	0	4.716851	-0.431621	-0.984203
25	6	0	3.421177	-0.750978	-1.476389
26	7	0	1.450527	-0.111347	1.543770
27	16	0	2.171361	0.401723	2.932855
28	7	0	3.737190	0.457807	2.420612
29	7	0	6.095467	0.330042	0.949450
30	7	0	-3.054289	1.345298	-1.597654
31	6	0	-3.292684	2.670052	-1.470249
32	6	0	-4.021211	3.192418	-0.347115
33	7	0	-4.494592	2.373016	0.620647
34	6	0	-2.814672	3.569458	-2.463253
35	6	0	-3.051027	4.917654	-2.342150
36	6	0	-3.772662	5.434110	-1.230615
37	6	0	-4.248120	4.593000	-0.253659
38	6	0	7.399005	0.350155	0.481574
39	6	0	8.421779	0.750105	1.371550
40	6	0	9.726282	0.770309	0.910136
41	6	0	9.993646	0.397802	-0.413313
42	6	0	8.916515	0.021601	-1.206177
43	7	0	7.643995	-0.007071	-0.784971
44	6	0	-1.827124	-4.135718	-1.204430
45	1	0	-6.508159	0.137831	4.455012
46	1	0	-6.109605	-2.306896	4.235840
47	1	0	-4.847785	-3.185234	2.279315
48	1	0	-5.649722	1.702268	2.721862
49	1	0	-2.884860	-1.481408	-2.748821
50	1	0	-4.497243	-4.593909	-1.826076
51	1	0	-4.922236	-2.922431	-2.245630
52	1	0	-3.729618	-3.803854	-3.220870
53	1	0	-0.643901	-0.750445	0.256631
54	1	0	5.572578	-0.514387	-1.637599
55	1	0	3.335798	-1.071056	-2.509502
56	1	0	-2.264962	3.152886	-3.300804
57	1	0	-2.683751	5.602085	-3.101073
58	1	0	-3.945709	6.503638	-1.158721
59	1	0	-4.801074	4.960717	0.604649

60	1	0	8.182735	1.033313	2.392475
61	1	0	10.531022	1.073274	1.573579
62	1	0	11.001763	0.400424	-0.812258
63	1	0	9.072425	-0.275998	-2.241378
64	1	0	-1.077726	-3.798001	-0.485542
65	1	0	-2.206970	-5.108418	-0.880561
66	1	0	-1.343032	-4.250575	-2.177321
67	1	0	4.534528	0.726014	2.961276

9 before ESIPT ( $S_1$ )

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.488858	-3.323889	-0.683633
2	6	0	-6.418135	-2.504368	-1.812714
3	6	0	-5.740763	-1.285361	-1.757387
4	6	0	-5.127318	-0.888442	-0.565985
5	6	0	-5.196752	-1.713349	0.579233
6	6	0	-5.881172	-2.927479	0.508525
7	6	0	-4.400371	0.369908	-0.443905
8	6	0	-3.767927	0.804071	0.682631
9	6	0	-3.791543	0.060810	1.923937
10	6	0	-4.555384	-1.300609	1.870180
11	8	0	-4.327600	1.202853	-1.488600
12	6	0	-3.699279	2.472833	-1.023572
13	6	0	-3.100151	2.118671	0.390462
14	8	0	-4.614514	-1.994345	2.866531
15	8	0	-3.273354	0.424839	2.968182
16	6	0	-4.837016	3.480335	-0.876637
17	6	0	-2.688184	2.880975	-2.081663
18	7	0	-1.639462	2.040781	0.427510
19	7	0	-0.934521	3.178430	0.646368
20	7	0	0.328024	2.877178	0.570423
21	6	0	0.464004	1.538239	0.299272
22	6	0	-0.806042	0.994618	0.200948
23	6	0	1.775105	0.910216	0.169974
24	6	0	1.933211	-0.478274	-0.148126
25	6	0	3.258295	-1.055513	-0.263270
26	6	0	4.445524	-0.264795	-0.066655
27	6	0	4.252289	1.070390	0.236776
28	6	0	2.946431	1.622314	0.347912
29	7	0	0.959052	-1.370352	-0.368248
30	16	0	1.686336	-2.813328	-0.688659
31	7	0	3.264399	-2.354750	-0.562695
32	7	0	5.641073	-0.951815	-0.208911
33	6	0	6.953949	-0.523346	-0.095073
34	6	0	7.984480	-1.469093	-0.297337
35	6	0	9.297618	-1.046621	-0.185143
36	6	0	9.565037	0.293175	0.122998
37	6	0	8.479597	1.141734	0.302413
38	7	0	7.198801	0.759068	0.199166
39	1	0	-7.018568	-4.270232	-0.732382
40	1	0	-6.892491	-2.813616	-2.738974
41	1	0	-5.681921	-0.640741	-2.627397
42	1	0	-5.925262	-3.544220	1.400035
43	1	0	-3.352875	2.901378	1.109633
44	1	0	-4.434738	4.450962	-0.571682
45	1	0	-5.363234	3.602417	-1.826681
46	1	0	-5.555084	3.151925	-0.119135
47	1	0	-3.199392	3.068123	-3.029716
48	1	0	-2.171655	3.792276	-1.771093
49	1	0	-1.940286	2.100231	-2.235687
50	1	0	-1.140515	-0.010801	0.015505
51	1	0	5.114733	1.700901	0.393546
52	1	0	2.860484	2.676042	0.591562



53	1	0	7.744886	-2.501507	-0.534714
54	1	0	10.108787	-1.752923	-0.335621
55	1	0	10.579668	0.662709	0.220028
56	1	0	8.635303	2.191553	0.543331
57	1	0	5.513089	-1.930698	-0.431171

9 after ESIPT ( $S_1$ )

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.515560	-3.278621	-0.822806
2	6	0	-6.471976	-2.398884	-1.907101
3	6	0	-5.788764	-1.186203	-1.804013
4	6	0	-5.142624	-0.855622	-0.609587
5	6	0	-5.184986	-1.741332	0.490410
6	6	0	-5.874725	-2.948845	0.372247
7	6	0	-4.409463	0.393791	-0.438694
8	6	0	-3.752853	0.769780	0.695040
9	6	0	-3.750050	-0.038488	1.895313
10	6	0	-4.508197	-1.399814	1.783848
11	8	0	-4.357414	1.277203	-1.441494
12	6	0	-3.711282	2.520854	-0.929996
13	6	0	-3.093791	2.100350	0.458545
14	8	0	-4.533044	-2.151945	2.738580
15	8	0	-3.211401	0.269394	2.947288
16	6	0	-4.838375	3.529626	-0.723582
17	6	0	-2.711842	2.965598	-1.984243
18	7	0	-1.633228	2.030752	0.476430
19	7	0	-0.934821	3.167356	0.702598
20	7	0	0.330824	2.875341	0.611686
21	6	0	0.474299	1.540126	0.324967
22	6	0	-0.794357	0.990162	0.229845
23	6	0	1.785583	0.921782	0.183236
24	6	0	1.954856	-0.451596	-0.091015
25	6	0	3.304335	-0.972076	-0.199891
26	6	0	4.529262	-0.212944	-0.059791
27	6	0	4.280863	1.156902	0.211788
28	6	0	2.976877	1.657950	0.321877
29	7	0	1.011057	-1.404099	-0.275059
30	16	0	1.699809	-2.863739	-0.557351
31	7	0	3.291324	-2.272206	-0.452574
32	7	0	5.616051	-0.980182	-0.217744
33	6	0	6.902707	-0.516949	-0.136474
34	6	0	7.935274	-1.473226	-0.324328
35	6	0	9.258151	-1.073958	-0.256090
36	6	0	9.549108	0.272045	-0.002058
37	6	0	8.476162	1.145391	0.170197
38	7	0	7.191588	0.784925	0.109178
39	1	0	-7.050457	-4.219418	-0.908511
40	1	0	-6.972636	-2.655915	-2.835504
41	1	0	-5.751267	-0.495168	-2.638847
42	1	0	-5.897422	-3.612793	1.230045
43	1	0	-3.345482	2.845539	1.217055
44	1	0	-4.423309	4.481299	-0.378699
45	1	0	-5.374545	3.700319	-1.660525
46	1	0	-5.550817	3.172907	0.026524
47	1	0	-3.234242	3.190076	-2.918027
48	1	0	-2.187609	3.861984	-1.645138
49	1	0	-1.968832	2.188444	-2.175781
50	1	0	-1.131483	-0.013605	0.040890
51	1	0	5.127164	1.814729	0.336864
52	1	0	2.860044	2.715809	0.537165
53	1	0	7.657528	-2.503554	-0.518156
54	1	0	10.057516	-1.796202	-0.397670
55	1	0	10.570328	0.632467	0.060730
56	1	0	8.661275	2.200451	0.369841
57	1	0	4.190802	-2.752774	-0.547094

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**10 before ESIPT (S<sub>1</sub>)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.962219	-0.252201	3.602413
2	6	0	-5.737506	-1.633361	3.476811
3	6	0	-5.034643	-2.126570	2.388841
4	6	0	-4.543673	-1.242250	1.411225
5	6	0	-4.768630	0.156149	1.530346
6	6	0	-5.486082	0.629504	2.643447
7	6	0	-3.805091	-1.694844	0.260175
8	6	0	-3.315237	-0.859902	-0.700405
9	6	0	-3.527013	0.553210	-0.632859
10	6	0	-4.265677	1.073043	0.502486
11	8	0	-3.555898	-3.004992	0.049920
12	6	0	-2.979989	-3.141244	-1.307931
13	6	0	-2.574665	-1.673630	-1.722632
14	6	0	-4.107464	-3.641562	-2.210570
15	7	0	-1.131649	-1.419534	-1.725795
16	7	0	-0.428523	-1.672376	-2.856540
17	7	0	0.824574	-1.434936	-2.600443
18	6	0	0.954713	-1.025468	-1.296773
19	6	0	-0.308031	-1.017753	-0.726772
20	6	0	2.254419	-0.680874	-0.728655
21	6	0	2.411683	-0.256315	0.631433
22	6	0	3.726121	0.072683	1.148151
23	6	0	4.904016	-0.016111	0.325188
24	6	0	4.712509	-0.429312	-0.980158
25	6	0	3.416984	-0.747486	-1.473503
26	7	0	1.445339	-0.114516	1.547410
27	16	0	2.165728	0.395392	2.937889
28	7	0	3.731736	0.452531	2.426309
29	7	0	6.090508	0.327925	0.955671
30	7	0	-3.058315	1.349449	-1.592278
31	6	0	-3.296674	2.673928	-1.461981
32	6	0	-4.025554	3.193816	-0.337927
33	7	0	-4.499315	2.372273	0.627831
34	6	0	-2.818269	3.575532	-2.452801
35	6	0	-3.054584	4.923467	-2.328753
36	6	0	-3.776569	5.437470	-1.216308
37	6	0	-4.252412	4.594199	-0.241405
38	6	0	7.394208	0.349009	0.488288
39	6	0	8.416701	0.746899	1.379509
40	6	0	9.721363	0.768060	0.918588
41	6	0	9.989158	0.398508	-0.405602
42	6	0	8.912276	0.024153	-1.199677
43	7	0	7.639610	-0.005388	-0.778972
44	6	0	-1.831612	-4.132510	-1.210937
45	1	0	-6.514328	0.128609	4.456481
46	1	0	-6.115845	-2.315644	4.231958
47	1	0	-4.853408	-3.189665	2.273899
48	1	0	-5.655205	1.696880	2.727140
49	1	0	-2.888661	-1.474676	-2.749729
50	1	0	-4.501545	-4.589143	-1.834524
51	1	0	-4.926295	-2.916702	-2.250470
52	1	0	-3.733396	-3.796006	-3.227278
53	1	0	-0.648687	-0.750596	0.258123
54	1	0	5.568454	-0.510663	-1.633445
55	1	0	3.331940	-1.065239	-2.507361
56	1	0	5.962049	0.601262	1.921461
57	1	0	-2.268297	3.160807	-3.291096
58	1	0	-2.687008	5.609577	-3.086012
59	1	0	-3.949577	6.506845	-1.142073
60	1	0	-4.805637	4.960022	0.617536
61	1	0	8.177324	1.027829	2.400985

62	1	0	10.525894	1.069486	1.582984
63	1	0	10.997411	0.401964	-0.804196
64	1	0	9.068522	-0.271132	-2.235490
65	1	0	-1.082440	-3.796453	-0.491037
66	1	0	-2.211627	-5.105911	-0.889382
67	1	0	-1.347194	-4.245212	-2.183918

10 after ESIPT ( $S_1$ )

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.917396	-0.235063	3.629196
2	6	0	-5.691911	-1.616680	3.509502
3	6	0	-4.998197	-2.115226	2.418064
4	6	0	-4.517122	-1.236055	1.430837
5	6	0	-4.742776	0.162721	1.544088
6	6	0	-5.450977	0.641590	2.660865
7	6	0	-3.788485	-1.694704	0.275662
8	6	0	-3.308867	-0.864998	-0.694616
9	6	0	-3.522387	0.548096	-0.633271
10	6	0	-4.250386	1.074057	0.506266
11	8	0	-3.538613	-3.005608	0.072072
12	6	0	-2.976133	-3.149192	-1.291535
13	6	0	-2.573192	-1.684061	-1.716907
14	6	0	-4.113307	-3.652830	-2.179950
15	7	0	-1.131482	-1.429126	-1.728559
16	7	0	-0.434571	-1.684770	-2.858777
17	7	0	0.821970	-1.448882	-2.608150
18	6	0	0.959238	-1.037184	-1.305668
19	6	0	-0.302041	-1.027298	-0.730720
20	6	0	2.258700	-0.692129	-0.743727
21	6	0	2.424430	-0.262565	0.589979
22	6	0	3.762136	0.057087	1.051660
23	6	0	4.979198	-0.021909	0.272296
24	6	0	4.735566	-0.459599	-1.054198
25	6	0	3.442271	-0.766355	-1.500345
26	7	0	1.486425	-0.094447	1.550901
27	16	0	2.165420	0.425907	2.947707
28	7	0	3.745886	0.443436	2.318644
29	7	0	6.056233	0.336666	0.985031
30	7	0	-3.064488	1.339654	-1.601858
31	6	0	-3.303222	2.664424	-1.477012
32	6	0	-4.020762	3.190366	-0.348401
33	7	0	-4.483437	2.373960	0.627038
34	6	0	-2.836154	3.560568	-2.478268
35	6	0	-3.072696	4.908956	-2.359876
36	6	0	-3.783618	5.428910	-1.242998
37	6	0	-4.248146	4.591105	-0.257962
38	6	0	7.333828	0.350308	0.492165
39	6	0	8.356791	0.758158	1.388765
40	6	0	9.670684	0.794107	0.957405
41	6	0	9.963177	0.425395	-0.361598
42	6	0	8.900329	0.037961	-1.176221
43	7	0	7.624255	-0.005234	-0.783981
44	6	0	-1.827504	-4.140583	-1.201685
45	1	0	-6.463090	0.149898	4.485548
46	1	0	-6.063208	-2.295188	4.271544
47	1	0	-4.817213	-3.178801	2.307123
48	1	0	-5.621478	1.709170	2.739389
49	1	0	-2.893670	-1.491217	-2.743152
50	1	0	-4.503982	-4.598672	-1.795993
51	1	0	-4.932148	-2.927696	-2.214640
52	1	0	-3.749828	-3.811741	-3.199794
53	1	0	-0.645970	-0.757782	0.252349
54	1	0	5.576703	-0.553609	-1.723790
55	1	0	3.328836	-1.094606	-2.529164
56	1	0	-2.294614	3.141256	-3.319752

57	1	0	-2.714060	5.590831	-3.125187
58	1	0	-3.957479	6.498488	-1.173722
59	1	0	-4.793248	4.961591	0.604198
60	1	0	8.078672	1.033914	2.400172
61	1	0	10.462221	1.104233	1.634188
62	1	0	10.977726	0.437543	-0.745391
63	1	0	9.086707	-0.256080	-2.208790
64	1	0	-1.070308	-3.800510	-0.492188
65	1	0	-2.204163	-5.112512	-0.871707
66	1	0	-1.353400	-4.257349	-2.179218
67	1	0	4.637220	0.696115	2.755307

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