

Electronic Supplemental Information

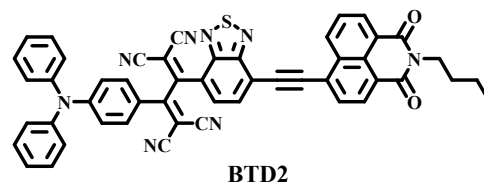
Design and Synthesis of 1,8-Naphthalimide Functionalized Benzothiadiazoles

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RM-YR-122A.001.001.1r.esp

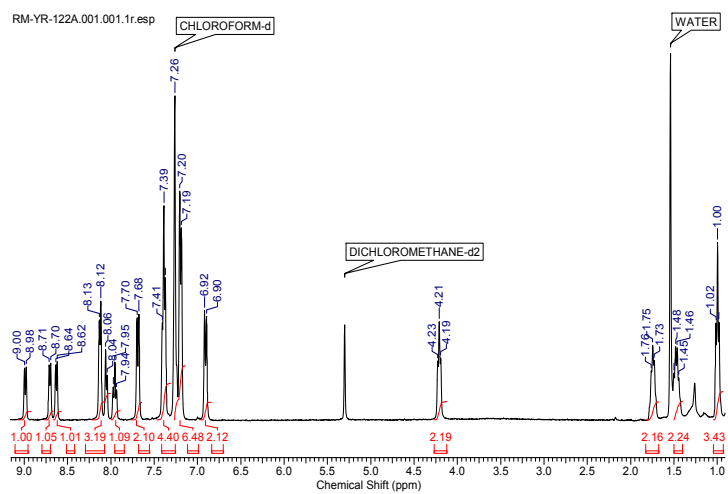
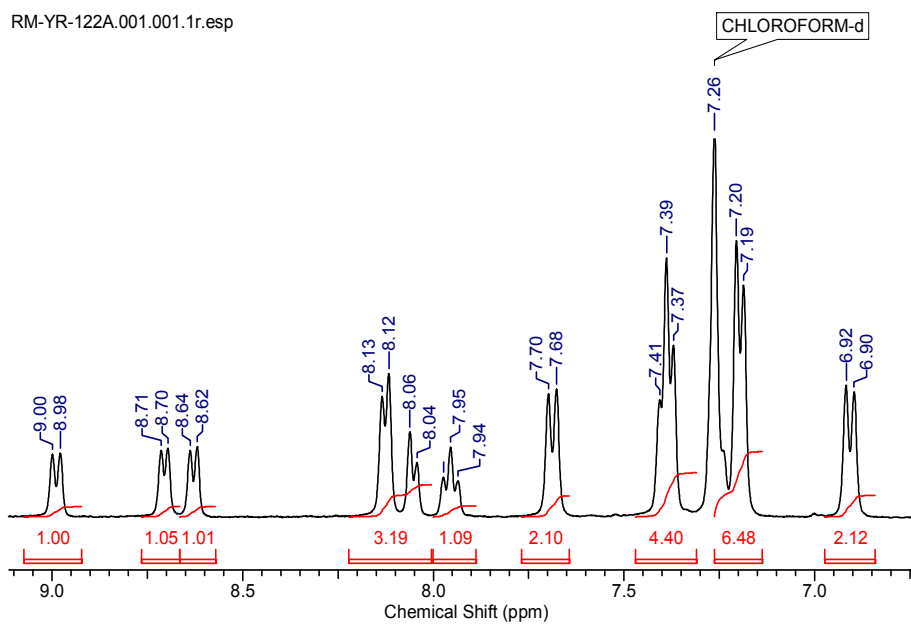
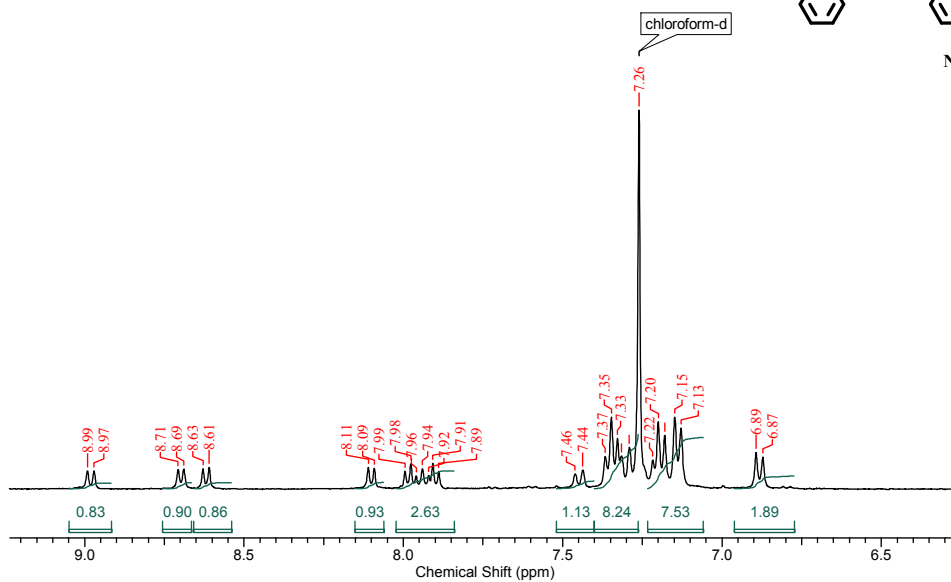
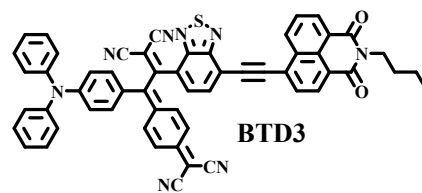


Figure S1. ^1H NMR spectra of **BTD2** in CDCl_3 (400 MHz, 25 °C).

RM-YR-153-127.001.001.1r.esp



RM-YR-153-127.001.001.1r.esp

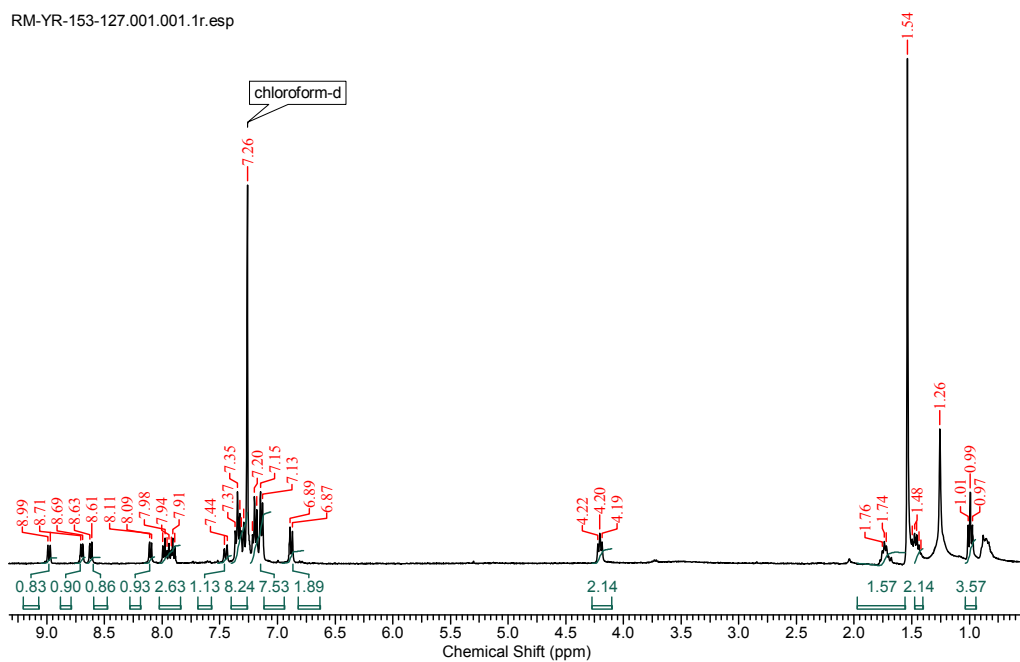
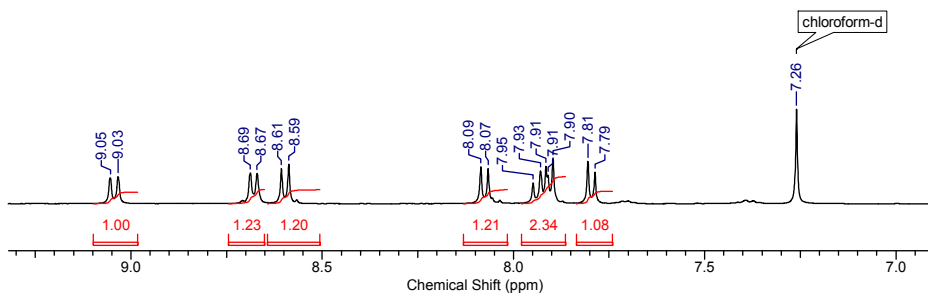
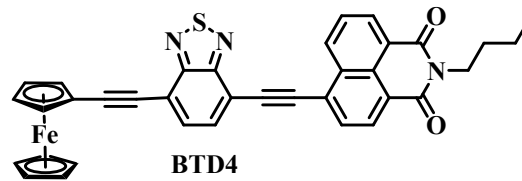


Figure S2. ¹H NMR spectra of BTD3 in CDCl₃ (400 MHz, 25 °C).

RM-YR-550.001.001.1r.esp



RM-YR-550.001.001.1r.esp

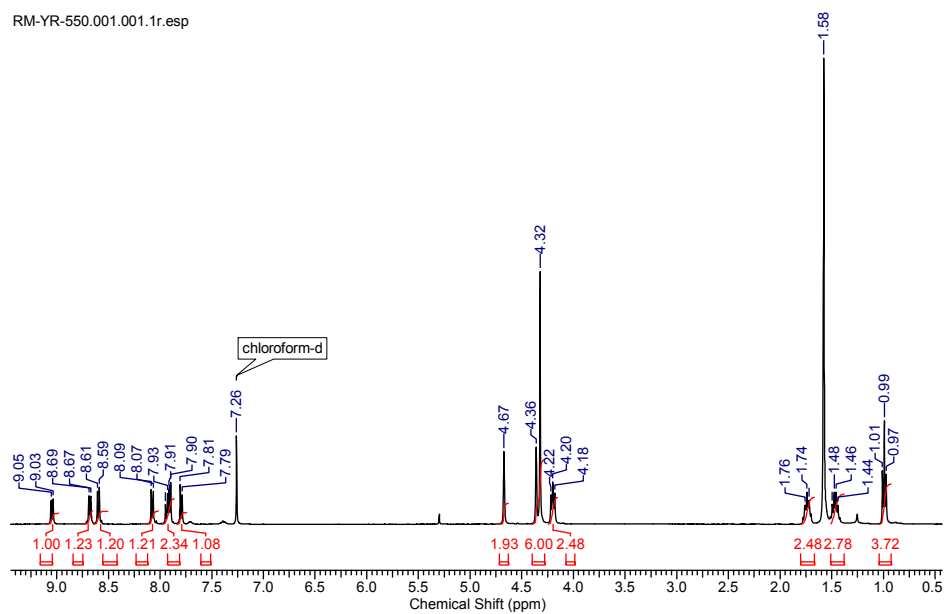
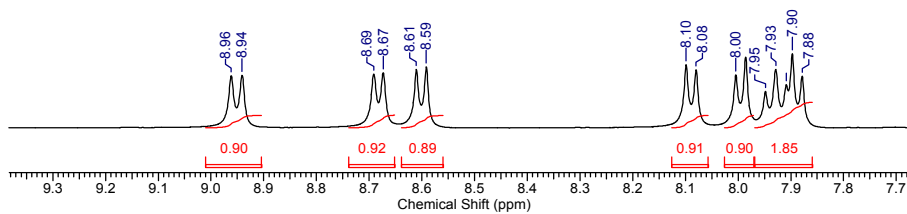
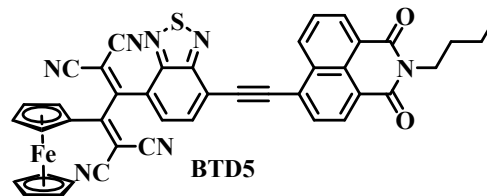


Figure S3. ¹H NMR spectra of **BTD4** in CDCl₃ (400 MHz, 25 °C).

RM-MP-450_002001R (3).ESP



RM-MP-450_002001R (3).ESP

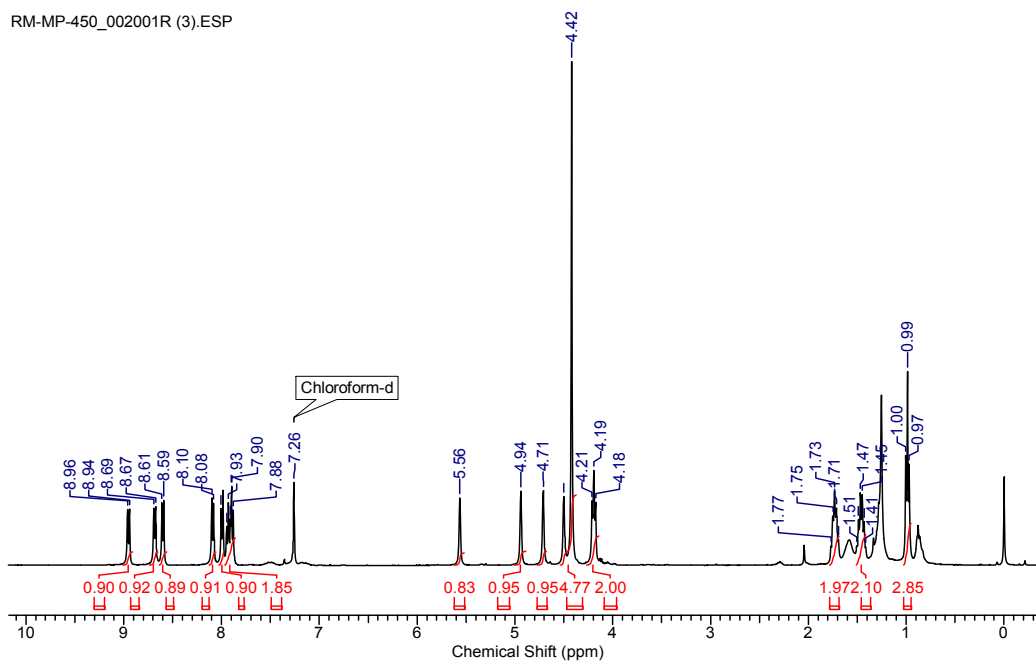
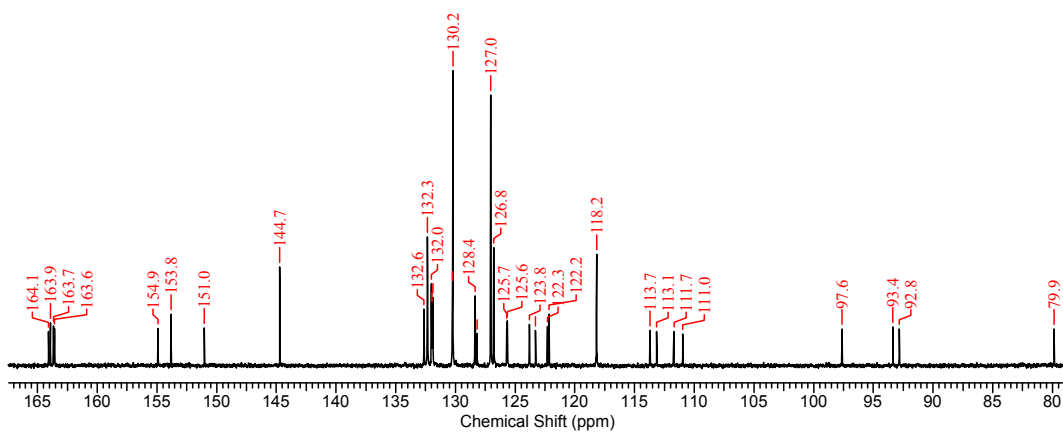
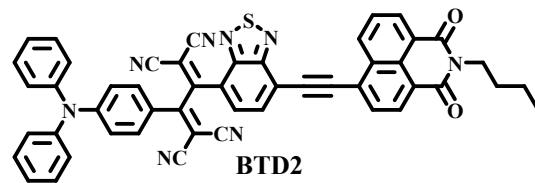


Figure S4. ¹H NMR spectra of BTD5 in CDCl₃ (400 MHz, 25 °C).

RM-YR-122B.003.001.1r.esp



RM-YR-122B.003.001.1r.esp

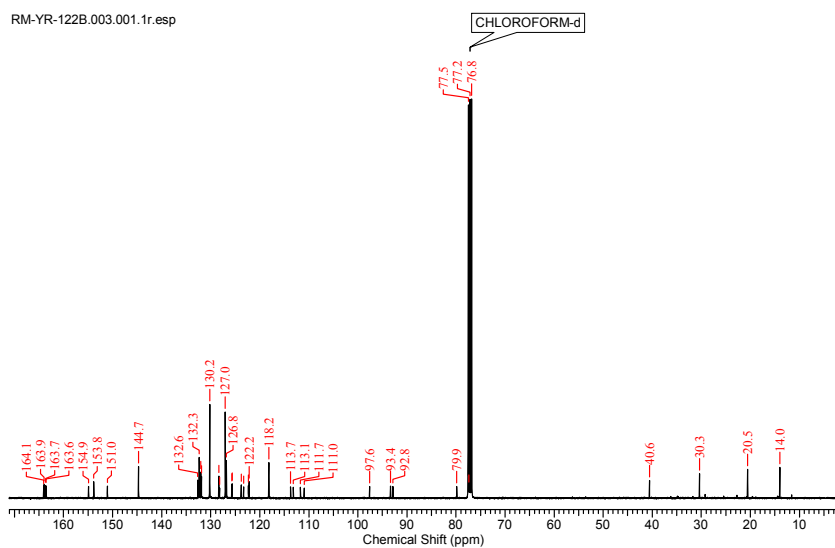


Figure S5. ¹³C NMR spectra of **BTD2** in CDCl₃ (100 MHz, 25 °C).

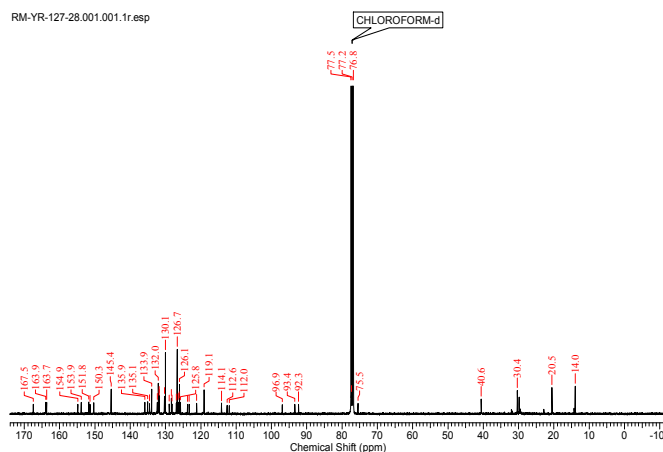
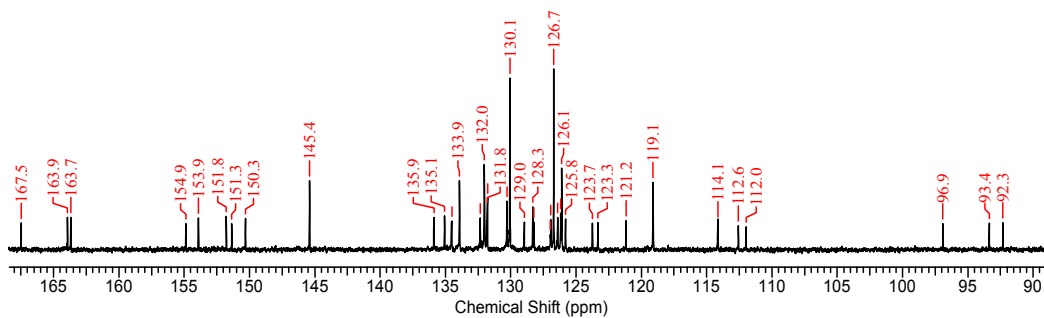
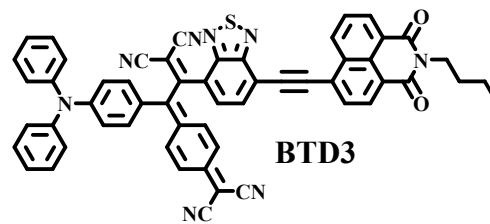
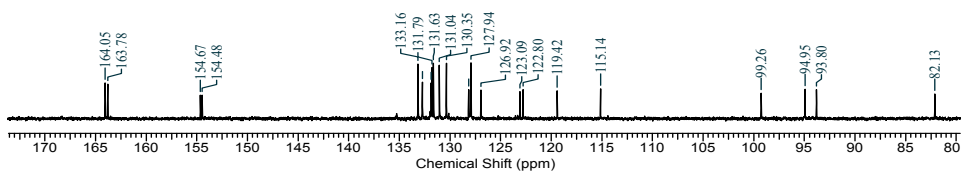
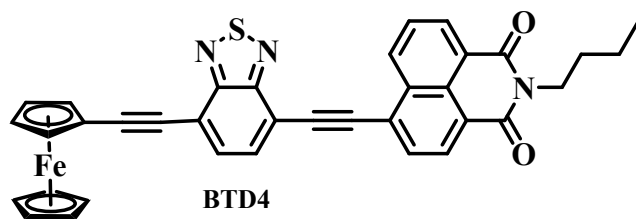


Figure S6. ¹³C NMR spectra of BTD3 in CDCl₃ (100 MHz, 25 °C).

RM-YR-550A.001.001.1r.esp



RM-YR-550A.001.001.1r.esp

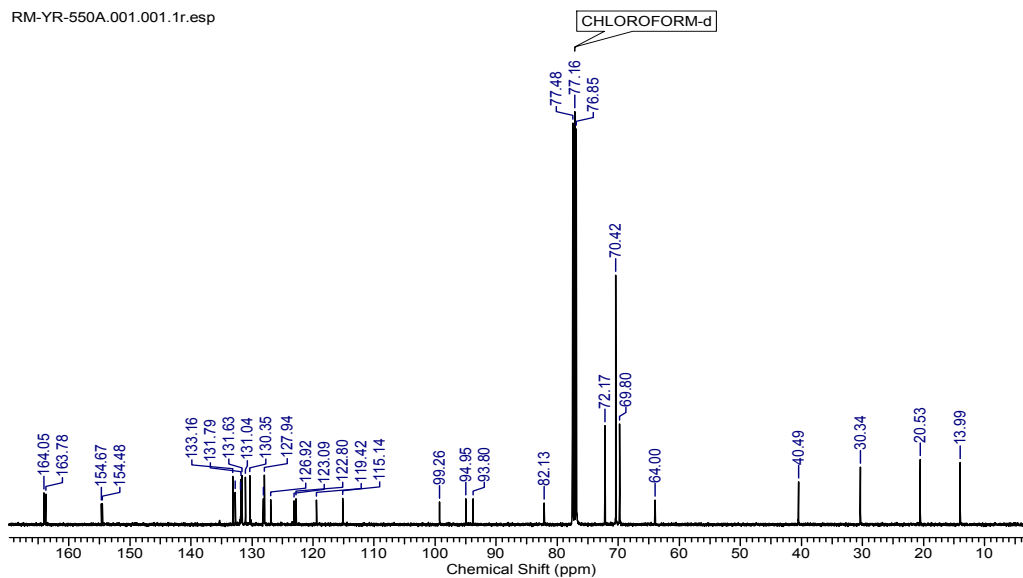
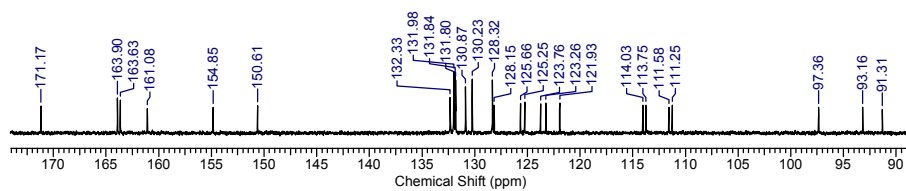
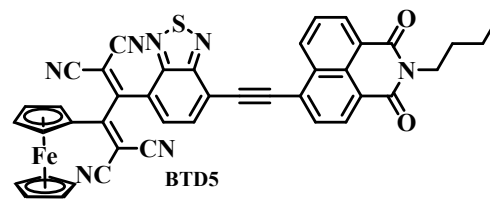


Figure S7. ¹³C NMR spectra of BTD4 in CDCl₃ (100 MHz, 25 °C).

RM-YR-553.001.001.1r.esp



RM-YR-553.001.001.1r.esp

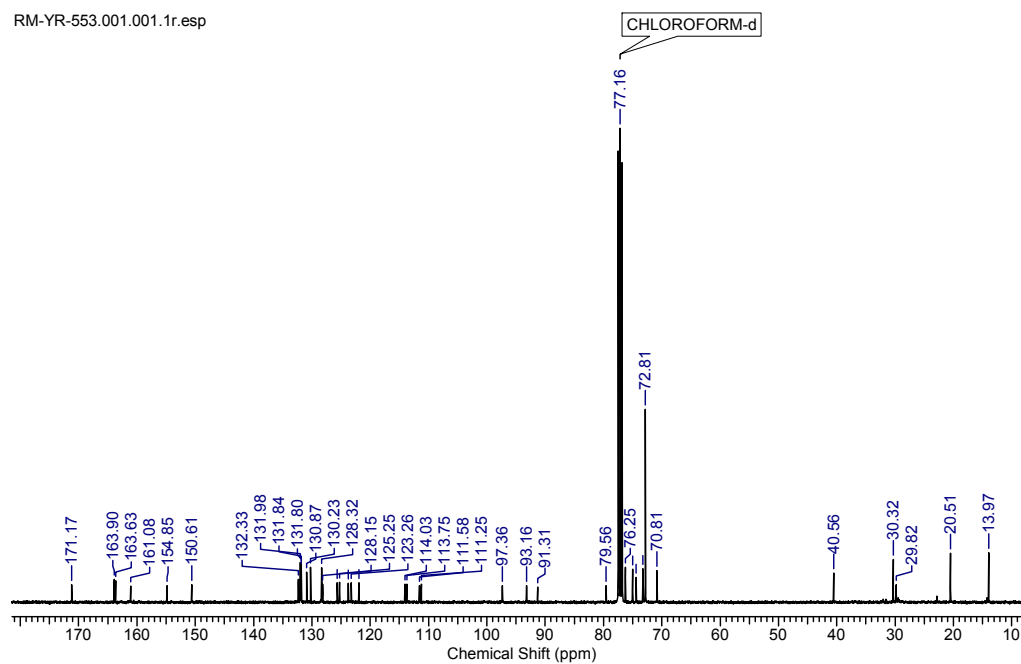


Figure S8. ¹³C NMR spectra of **BTD5** in CDCl₃ (100 MHz, 25 °C).

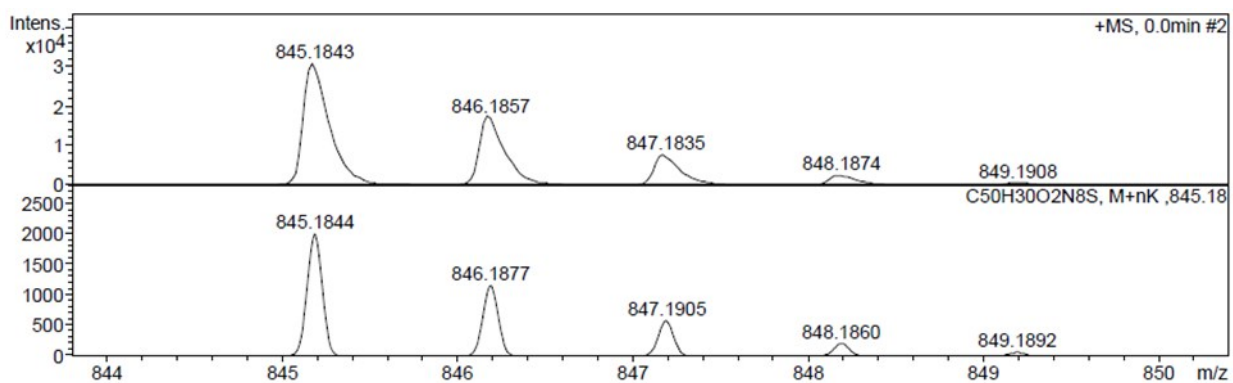
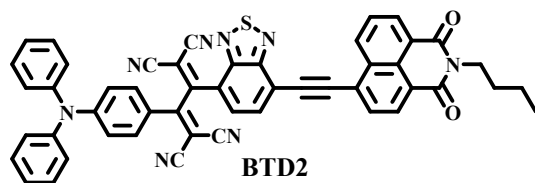


Figure S9. HRMS spectra of **BTD2**.

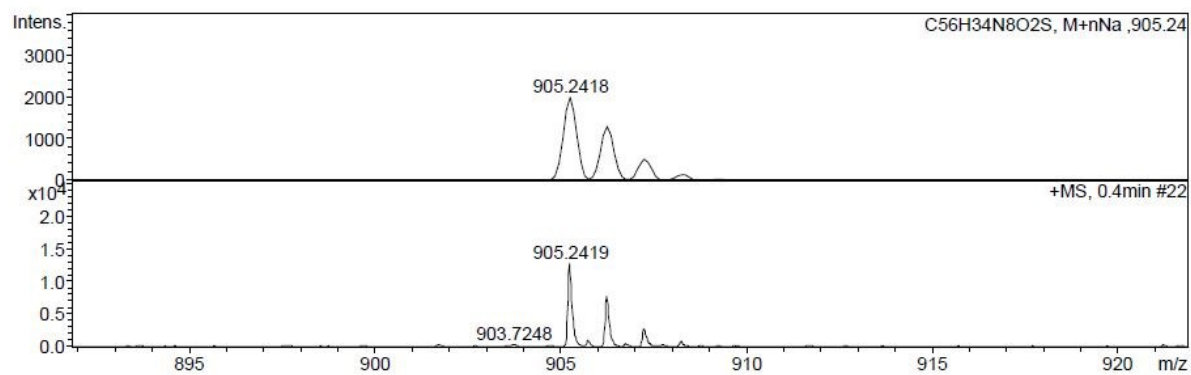
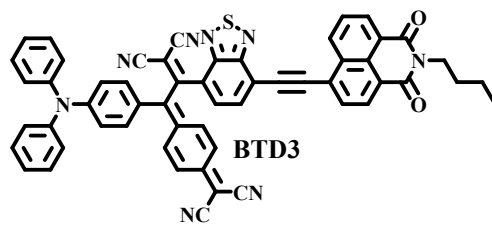
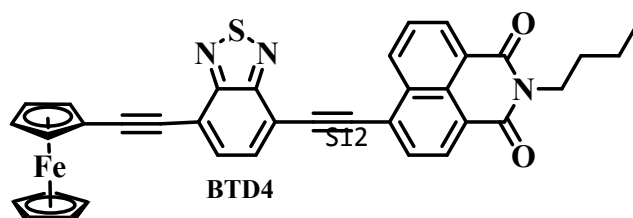


Figure S10. HRMS spectra of BTD3.



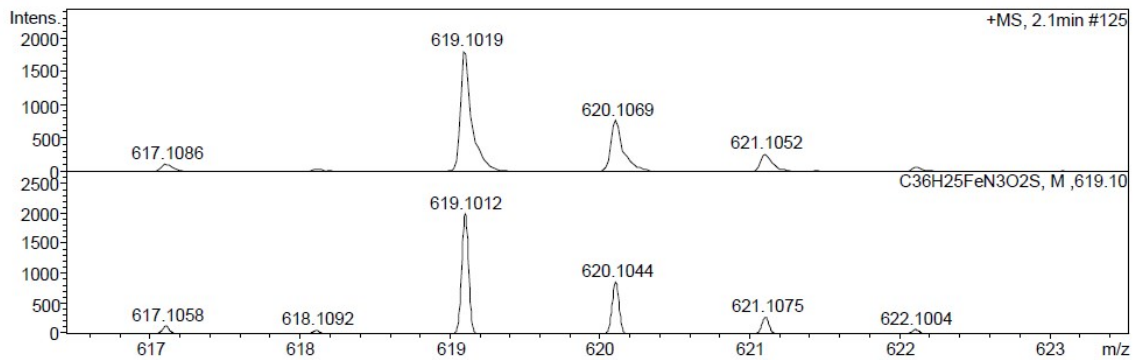
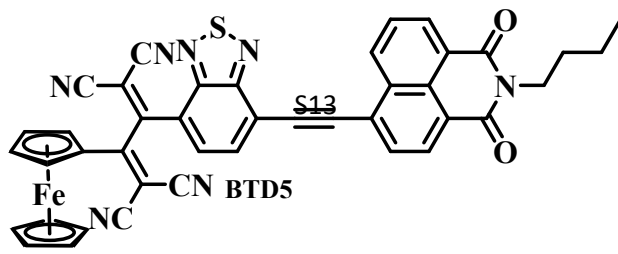


Figure S11. HRMS spectra of **BTD4**.



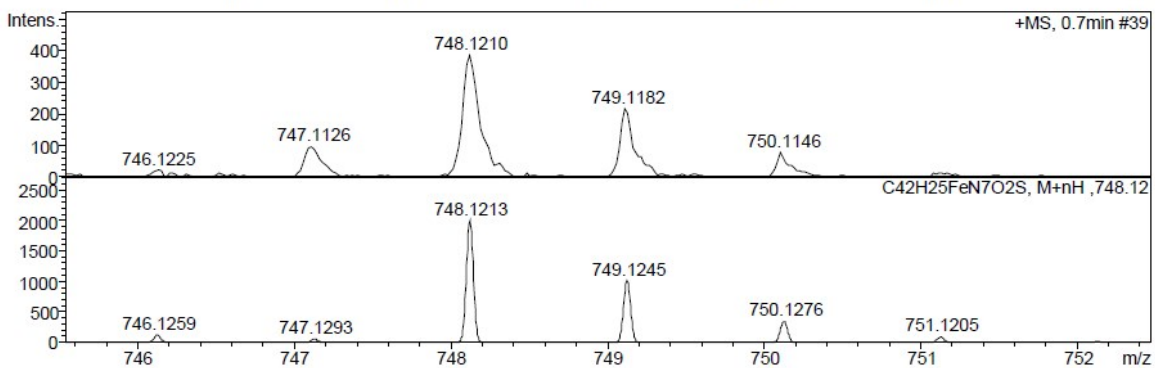


Figure S12. HRMS spectra of **BTD5**.

DFT calculation

BTD2

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-7.001003	-1.358137	0.288294
2	6	0	-8.142798	-1.301075	-0.505102
3	6	0	-7.127969	-1.392740	1.674586
4	6	0	-9.397521	-1.279340	0.084232
5	6	0	-8.384888	-1.353920	2.257572
6	1	0	-6.239298	-1.446535	2.291274
7	6	0	-9.523984	-1.300283	1.465967
8	1	0	-10.280691	-1.235958	-0.541580
9	1	0	-8.473384	-1.378120	3.336931
10	1	0	-10.504966	-1.276778	1.924012
11	6	0	-5.490067	-2.379425	-1.337992
12	6	0	-5.842457	-3.707925	-1.118279
13	6	0	-4.944359	-2.008286	-2.564525
14	6	0	-5.649647	-4.652051	-2.114968
15	6	0	-4.739456	-2.960265	-3.550830
16	1	0	-4.683474	-0.971847	-2.739573
17	6	0	-5.093211	-4.284661	-3.332005
18	1	0	-5.929203	-5.683013	-1.934690
19	1	0	-4.314677	-2.661416	-4.501583
20	1	0	-4.939760	-5.025029	-4.107270
21	6	0	-4.698251	-0.537398	0.076118
22	6	0	-3.347914	-0.890240	-0.066474
23	6	0	-4.994332	0.706417	0.650016
24	6	0	-2.347394	-0.035191	0.340528
25	1	0	-3.089128	-1.852143	-0.486885
26	6	0	-3.985926	1.560115	1.044085
27	1	0	-6.025011	0.997173	0.798086
28	6	0	-2.635523	1.223731	0.882882
29	1	0	-1.319681	-0.353478	0.223629
30	1	0	-4.248789	2.494698	1.522559
31	7	0	-5.712525	-1.405629	-0.321748
32	6	0	-0.466695	1.463384	2.105764
33	6	0	6.369469	-1.144736	-2.033136
34	6	0	6.831731	-2.466191	-1.739061
35	6	0	7.055940	-0.358299	-2.936751
36	6	0	6.181446	-3.324739	-0.822800
37	6	0	7.993952	-2.930686	-2.397367
38	6	0	8.206728	-0.835010	-3.575967

39	1	0	6.696198	0.639935	-3.148838
40	6	0	6.671232	-4.580370	-0.579264
41	1	0	5.290808	-2.975660	-0.313930
42	6	0	8.478120	-4.229265	-2.128601
43	6	0	8.670733	-2.098870	-3.314510
44	1	0	8.747672	-0.219474	-4.282847
45	6	0	7.826988	-5.038618	-1.234157
46	1	0	6.165997	-5.228578	0.125655
47	1	0	8.223802	-6.028420	-1.048381
48	6	0	9.892274	-2.578379	-4.007719
49	6	0	9.695370	-4.733187	-2.809632
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51	8	0	10.503970	-1.881746	-4.786368
52	7	0	10.308598	-3.877389	-3.726078
53	6	0	11.512086	-4.367490	-4.411248
54	1	0	11.534381	-3.893588	-5.390685
55	1	0	11.393314	-5.442738	-4.529489
56	6	0	12.788959	-4.055375	-3.640826
57	1	0	12.727084	-4.513374	-2.649143
58	1	0	12.863650	-2.973027	-3.499360
59	6	0	14.031177	-4.564939	-4.364969
60	1	0	14.078680	-4.114579	-5.362188
61	1	0	13.942178	-5.645619	-4.519208
62	6	0	15.319652	-4.263013	-3.607653
63	1	0	15.312088	-4.728193	-2.618614
64	1	0	16.194492	-4.636027	-4.143951
65	1	0	15.449513	-3.186951	-3.466477
66	1	0	-8.040814	-1.278850	-1.582952
67	1	0	-6.272414	-3.993303	-0.166324
68	6	0	-1.574393	2.126659	1.346874
69	6	0	-0.582527	1.318280	3.444381
70	6	0	0.463500	0.820848	4.284714
71	6	0	-1.768318	1.748748	4.123563
72	7	0	1.303339	0.477456	4.987323
73	7	0	-2.718580	2.087672	4.671131
74	6	0	-1.561274	3.481183	1.160036
75	6	0	-0.601568	4.341575	1.828677
76	6	0	-2.479079	4.146275	0.253020
77	6	0	-0.591231	5.673951	1.657720
78	1	0	0.109768	3.897268	2.512883
79	6	0	-2.462946	5.476786	0.067474
80	1	0	-3.164626	3.540098	-0.321740
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84	6	0	-1.518084	7.686921	0.591241
85	6	0	-2.440454	8.327620	-0.284061
86	7	0	-3.192075	8.825167	-0.997908
87	6	0	-0.579075	8.519315	1.264126
88	7	0	0.189482	9.174307	1.813966
89	6	0	5.203902	-0.646634	-1.389923
90	6	0	4.215531	-0.258273	-0.825800

91	6	0	3.052950	0.154904	-0.133259
92	6	0	2.430545	-0.725996	0.811084
93	6	0	2.457078	1.374929	-0.326288
94	6	0	1.262067	-0.315059	1.538283
95	6	0	1.296899	1.772514	0.384122
96	1	0	2.888255	2.063252	-1.040982
97	6	0	0.702148	0.990089	1.340043
98	1	0	0.888190	2.751413	0.171253
99	7	0	2.813029	-1.963933	1.092411
100	7	0	0.781764	-1.268066	2.325952
101	16	0	1.759110	-2.549411	2.176949

HF=-3140.1639741 Hartree

BTD3

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.195232	-1.038653	-1.812023
2	6	0	6.631525	-2.368256	-1.515097
3	6	0	6.896690	-0.268401	-2.718178
4	6	0	5.965055	-3.210731	-0.595471
5	6	0	7.783288	-2.857837	-2.173693
6	6	0	8.036495	-0.769830	-3.357802
7	1	0	6.556358	0.736135	-2.932496
8	6	0	6.429595	-4.475425	-0.349178
9	1	0	5.082381	-2.842301	-0.086256
10	6	0	8.241427	-4.165202	-1.901851
11	6	0	8.475261	-2.042317	-3.094172
12	1	0	8.588533	-0.167367	-4.067371
13	6	0	7.574934	-4.958664	-1.004283
14	1	0	5.911750	-5.111363	0.357708
15	1	0	7.951479	-5.955987	-0.816521
16	6	0	9.684381	-2.548603	-3.789097
17	6	0	9.446644	-4.695499	-2.583459
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20	7	0	10.074326	-3.855217	-3.505024
21	6	0	11.263421	-4.372905	-4.194400
22	1	0	11.289557	-3.904524	-5.176443
23	1	0	11.122195	-5.446123	-4.306220
24	6	0	12.551352	-4.083183	-3.433710

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26	1	0	12.649701	-3.001838	-3.299300
27	6	0	13.777788	-4.623277	-4.162598
28	1	0	13.827740	-4.180753	-5.163231
29	1	0	13.665258	-5.702872	-4.308861
30	6	0	15.077574	-4.343218	-3.416285
31	1	0	15.067192	-4.801345	-2.423986
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34	6	0	5.039426	-0.516721	-1.170380
35	6	0	4.057803	-0.109917	-0.607579
36	6	0	2.898451	0.323118	0.078397
37	6	0	2.238305	-0.557160	0.996380
38	6	0	2.364956	1.578166	-0.071973
39	6	0	1.050832	-0.141399	1.686739
40	6	0	1.208126	1.993492	0.630742
41	1	0	2.844751	2.276786	-0.744309
42	6	0	0.512867	1.168865	1.477719
43	1	0	0.860186	3.007473	0.473670
44	7	0	2.633160	-1.779777	1.325245
45	7	0	0.595794	-1.055584	2.531190
46	16	0	1.583781	-2.330796	2.431261
47	6	0	-0.696926	1.644845	2.167406
48	6	0	-0.670102	3.034563	2.729310
49	6	0	-1.825902	0.907723	2.283944
50	6	0	-1.630059	3.993358	2.191557
51	6	0	0.263378	3.305061	3.684130
52	6	0	-2.021438	-0.344437	1.620213
53	6	0	-2.953324	1.368601	3.037828
54	6	0	-2.082160	3.867104	0.869090
55	6	0	-2.161966	5.042586	2.954777
56	6	0	1.106540	2.278893	4.214178
57	6	0	0.507216	4.608462	4.214740
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59	7	0	-3.865839	1.708946	3.645326
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62	6	0	-3.082730	5.916763	2.427673
63	1	0	-1.875730	5.165405	3.989249
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67	1	0	-3.311454	4.618628	-0.697156
68	1	0	-3.480667	6.705377	3.050261
69	7	0	-4.451100	6.672321	0.568129
70	6	0	-5.368713	7.371765	1.410311
71	6	0	-4.561117	6.872013	-0.840925
72	6	0	-5.509542	8.749714	1.284149
73	6	0	-6.144991	6.679288	2.335555
74	6	0	-5.792413	6.722007	-1.470560
75	6	0	-3.445851	7.243405	-1.586790
76	6	0	-6.419952	9.428792	2.079175

77	1	0	-4.906676	9.282036	0.558998
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79	1	0	-6.039893	5.605025	2.426020
80	6	0	-5.904005	6.939646	-2.835288
81	1	0	-6.658389	6.439446	-0.885105
82	6	0	-3.561308	7.445145	-2.953270
83	1	0	-2.492220	7.373587	-1.090003
84	6	0	-7.185107	8.741936	3.011078
85	1	0	-6.524504	10.501886	1.974857
86	1	0	-7.640622	6.821822	3.857487
87	6	0	-4.790044	7.296436	-3.581964
88	1	0	-6.866485	6.821520	-3.318022
89	1	0	-2.688918	7.734266	-3.526774
90	1	0	-7.891607	9.275182	3.634970
91	1	0	-4.879453	7.461798	-4.648456

HF=-2909.2132976 Hartree

BTD4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.101148	-1.119110	-0.688711
2	6	0	-0.429699	0.071145	-0.431212
3	6	0	-2.502045	-1.188000	-0.865532
4	6	0	-1.238879	1.260912	-0.352138
5	6	0	-3.326226	-0.069340	-0.796268
6	6	0	-2.675855	1.190627	-0.533128
7	1	0	-2.955100	-2.153653	-1.063119
8	1	0	-0.524446	-2.035806	-0.755708
9	6	0	-4.726239	-0.144501	-0.966328
10	6	0	-5.933665	-0.210640	-1.110391
11	6	0	-7.335315	-0.276306	-1.285905
12	6	0	-8.244368	0.843249	-1.317754
13	6	0	-8.124036	-1.471893	-1.456062
14	6	0	-9.558062	0.338819	-1.522027
15	1	0	-7.958632	1.878089	-1.195024
16	6	0	-9.484492	-1.085662	-1.606308
17	1	0	-7.734129	-2.479725	-1.455494
18	1	0	-10.461790	0.930493	-1.568949
19	1	0	-10.322653	-1.757769	-1.727469
20	26	0	-8.746652	-0.440030	0.233957
21	6	0	-7.756352	-0.456442	2.060616
22	6	0	-8.492726	-1.667714	1.891275

23	6	0	-8.678120	0.632106	2.012829
24	1	0	-6.681846	-0.373507	2.149820
25	6	0	-9.871941	-1.327387	1.741075
26	1	0	-8.075726	-2.664513	1.851973
27	6	0	-9.986325	0.093546	1.816086
28	1	0	-8.425547	1.681254	2.080866
29	1	0	-10.682845	-2.021467	1.567466
30	1	0	-10.898837	0.663745	1.708703
31	7	0	-3.286434	2.373847	-0.427964
32	7	0	-0.788791	2.495610	-0.114717
33	16	0	-2.107304	3.476749	-0.124624
34	6	0	0.970160	0.133041	-0.249750
35	6	0	2.175266	0.209707	-0.086538
36	6	0	3.572881	0.340509	0.111337
37	6	0	4.443392	-0.803781	0.033640
38	6	0	4.115090	1.598697	0.386191
39	6	0	3.973086	-2.111286	-0.242157
40	6	0	5.842104	-0.612465	0.243630
41	6	0	5.492277	1.765310	0.588788
42	1	0	3.449975	2.453619	0.441544
43	6	0	4.846697	-3.179109	-0.309538
44	1	0	2.909570	-2.257879	-0.400469
45	6	0	6.720818	-1.723848	0.169135
46	6	0	6.352352	0.680585	0.521937
47	1	0	5.909523	2.743596	0.801758
48	6	0	6.227337	-2.987253	-0.104845
49	1	0	4.469520	-4.174566	-0.522431
50	1	0	6.926134	-3.815279	-0.156406
51	6	0	8.179681	-1.545638	0.381580
52	6	0	7.803662	0.888811	0.742252
53	8	0	8.972288	-2.476348	0.306570
54	8	0	8.281881	1.993330	0.970858
55	6	0	10.069211	-0.058094	0.903531
56	1	0	10.173154	0.763070	1.614146
57	1	0	10.443795	-0.979936	1.350574
58	6	0	10.828424	0.255689	-0.390175
59	1	0	10.674436	-0.565830	-1.100418
60	1	0	10.404564	1.161849	-0.839633
61	6	0	12.329371	0.453493	-0.144378
62	1	0	12.744449	-0.452271	0.317918
63	1	0	12.474580	1.263329	0.583396
64	6	0	13.105018	0.774481	-1.425927
65	1	0	14.172110	0.911862	-1.223019
66	1	0	13.006721	-0.032738	-2.160536
67	1	0	12.733404	1.693636	-1.892671
68	7	0	8.623522	-0.248914	0.681525

HF=-2223.1724646 Hartree

BTD5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.998998	-0.981921	-1.213982
2	6	0	4.946437	-0.861995	-0.055075
3	6	0	4.518524	-1.144564	-2.476024
4	6	0	5.692235	-1.960897	0.299648
5	6	0	5.930335	-1.093605	-2.727697
6	6	0	3.724436	-1.366671	-3.649446
7	6	0	5.516187	-3.237189	-0.326309
8	6	0	6.668502	-1.940572	1.344750
9	7	0	7.065801	-1.026152	-2.971689
10	7	0	3.122387	-1.546476	-4.628689
11	7	0	5.388430	-4.289308	-0.806585
12	7	0	7.477823	-1.949132	2.181361
13	6	0	4.941190	0.425076	0.627858
14	6	0	4.485228	1.664966	0.038893
15	6	0	5.325037	0.725769	1.990280
16	6	0	4.564223	2.683339	1.022717
17	1	0	4.159171	1.795872	-0.982729
18	6	0	5.073086	2.102292	2.224159
19	1	0	5.721192	0.025504	2.708735
20	1	0	4.318557	3.725629	0.875015
21	1	0	5.273556	2.627026	3.147927
22	1	0	8.181208	0.291111	-0.952423
23	6	0	8.128641	1.219805	-0.401229
24	6	0	8.465649	1.409239	0.972348
25	6	0	7.655422	2.462134	-0.918544
26	6	0	8.206983	2.774409	1.302469
27	1	0	8.812060	0.641345	1.649916
28	6	0	7.704221	3.425095	0.135129
29	1	0	7.302248	2.634780	-1.925694
30	1	0	8.330307	3.226271	2.277203
31	1	0	7.386301	4.456730	0.070002
32	26	0	6.454635	1.858166	0.674873
33	6	0	2.557028	-0.861051	-0.949718
34	6	0	1.958675	-1.407830	0.241518
35	6	0	1.698379	-0.189920	-1.811515
36	6	0	0.536419	-1.263915	0.487089
37	6	0	0.313551	-0.038865	-1.571259
38	1	0	2.097787	0.270586	-2.707158
39	6	0	-0.307866	-0.557767	-0.442137
40	1	0	-0.280996	0.509221	-2.293634

41	6	0	-1.688078	-0.406999	-0.190361
42	6	0	-2.875721	-0.288013	0.054020
43	6	0	-4.251074	-0.170319	0.378170
44	6	0	-5.150820	0.573364	-0.463426
45	6	0	-4.734418	-0.784548	1.536006
46	6	0	-4.738655	1.225000	-1.651876
47	6	0	-6.522469	0.659725	-0.078868
48	6	0	-6.086766	-0.688176	1.894865
49	1	0	-4.044524	-1.342031	2.160206
50	6	0	-5.643489	1.929198	-2.421661
51	1	0	-3.696616	1.160803	-1.947655
52	6	0	-7.434079	1.388509	-0.884851
53	6	0	-6.974152	0.022984	1.103883
54	1	0	-6.460971	-1.164701	2.794349
55	6	0	-6.997407	2.013342	-2.039268
56	1	0	-5.312254	2.422479	-3.330096
57	1	0	-7.718334	2.562862	-2.634808
58	6	0	-8.867231	1.491157	-0.503295
59	6	0	-8.399776	0.112165	1.512643
60	7	0	-9.260316	0.833608	0.674344
61	6	0	-10.675523	0.935651	1.092919
62	1	0	-11.078496	1.814547	0.589725
63	1	0	-10.672596	1.102158	2.171658
64	6	0	-11.506982	-0.311783	0.765328
65	1	0	-12.506974	-0.146146	1.189184
66	1	0	-11.085179	-1.169619	1.301620
67	6	0	-11.636159	-0.633037	-0.729010
68	1	0	-10.640257	-0.813333	-1.152965
69	1	0	-12.035052	0.240262	-1.259275
70	6	0	-12.524384	-1.853695	-0.990794
71	1	0	-12.595927	-2.072325	-2.061140
72	1	0	-12.128864	-2.747121	-0.494061
73	1	0	-13.541776	-1.692513	-0.616102
74	8	0	-8.817686	-0.415151	2.535711
75	8	0	-9.674513	2.117197	-1.176833
76	16	0	1.451542	-2.507395	2.309875
77	7	0	2.587485	-2.095305	1.199675
78	7	0	0.124505	-1.837107	1.619640

HF=-2670.7436779 Hartree

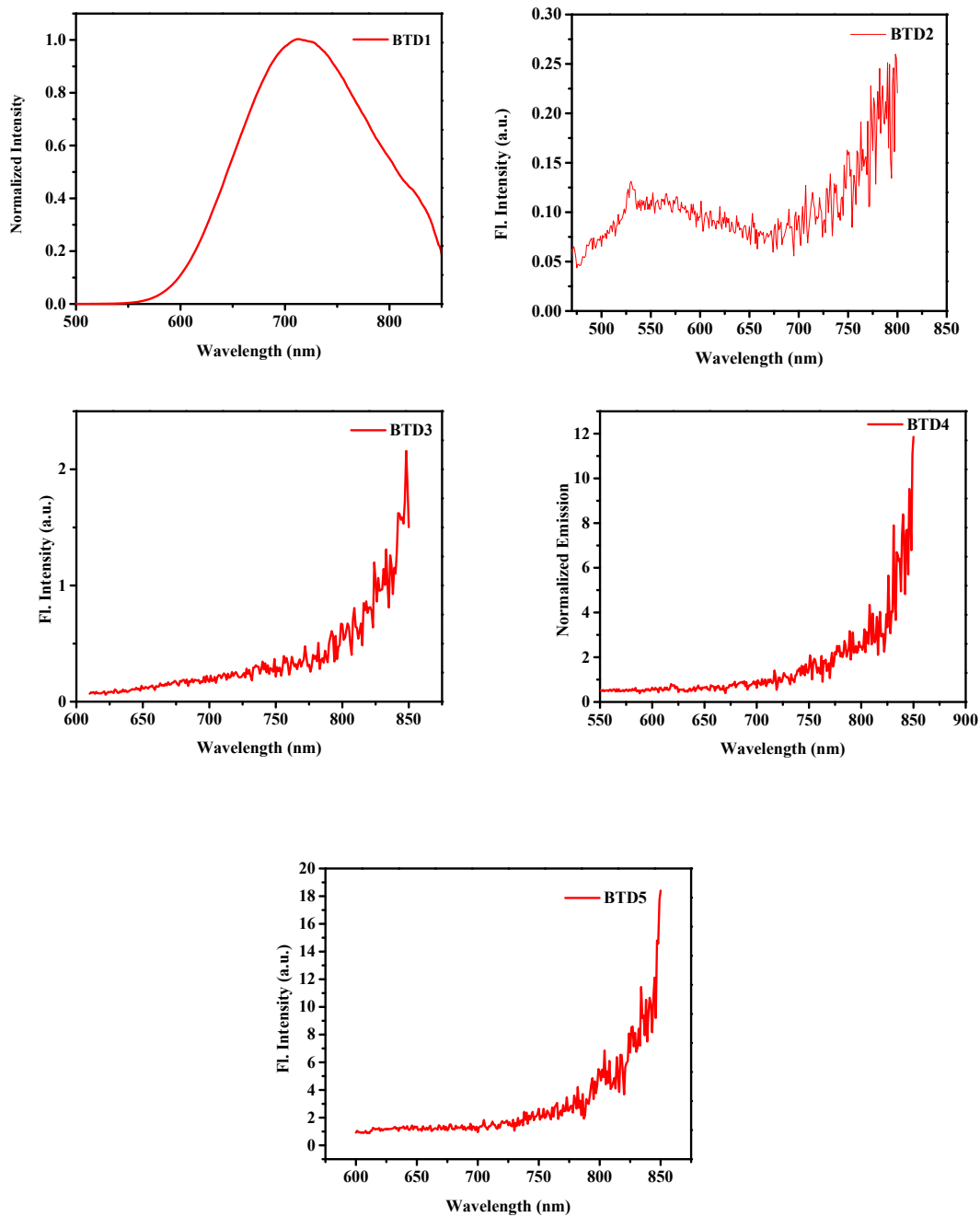


Figure S13: Fluorescence spectra of **BTD1–5** in DCM.