Flexible BODIPY Platform that Offers an Unexpected Regioselective Heterocyclization Reaction Toward Preparation of 2-Pyridone[a]-Fused BODIPYs

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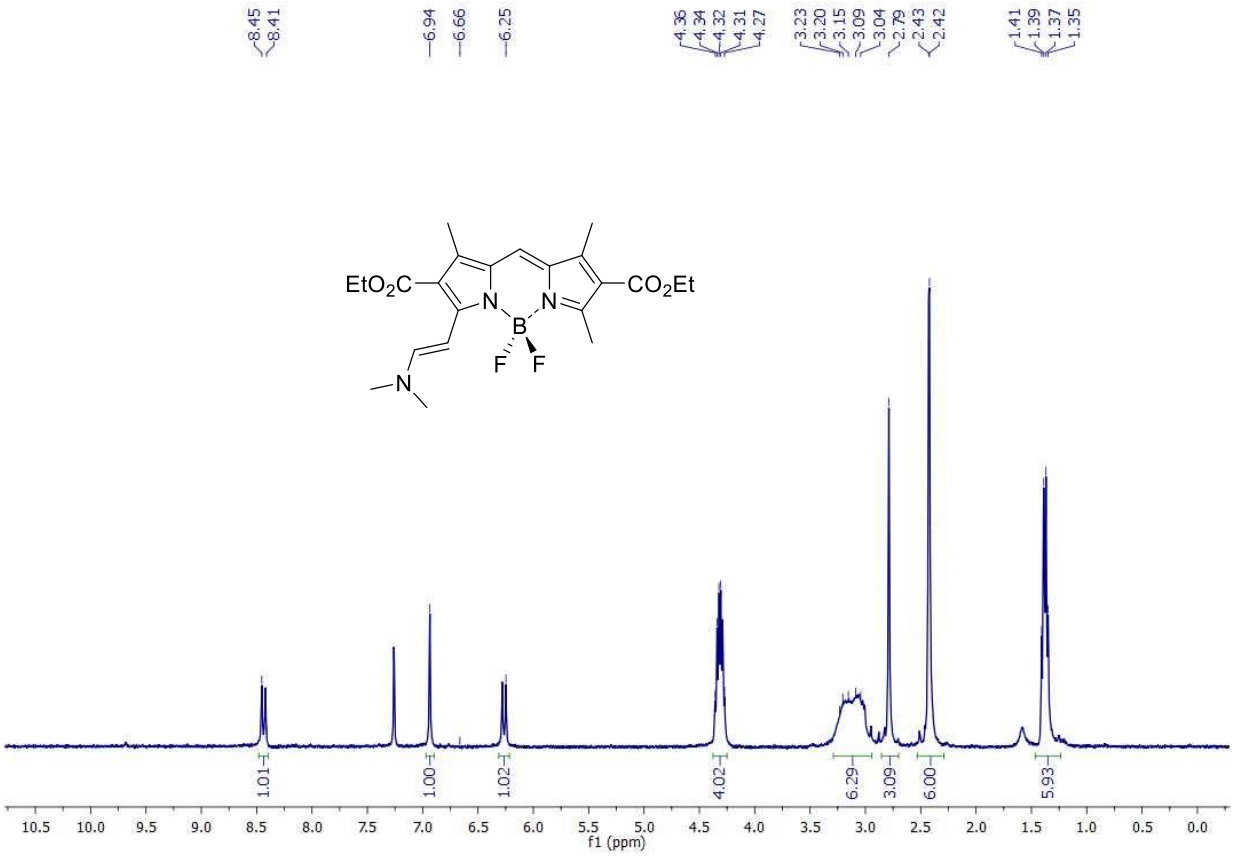

Figure S1. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

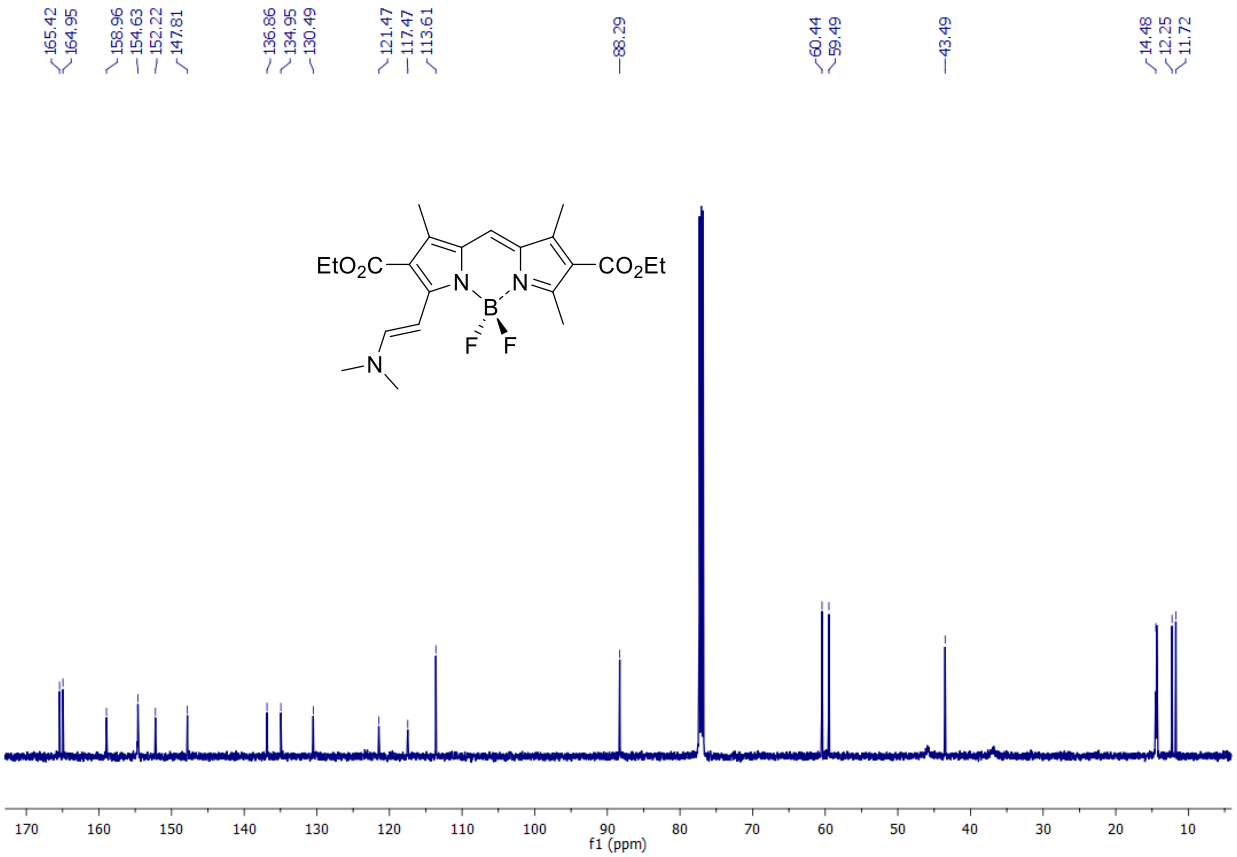

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2** in $CDCl_3$

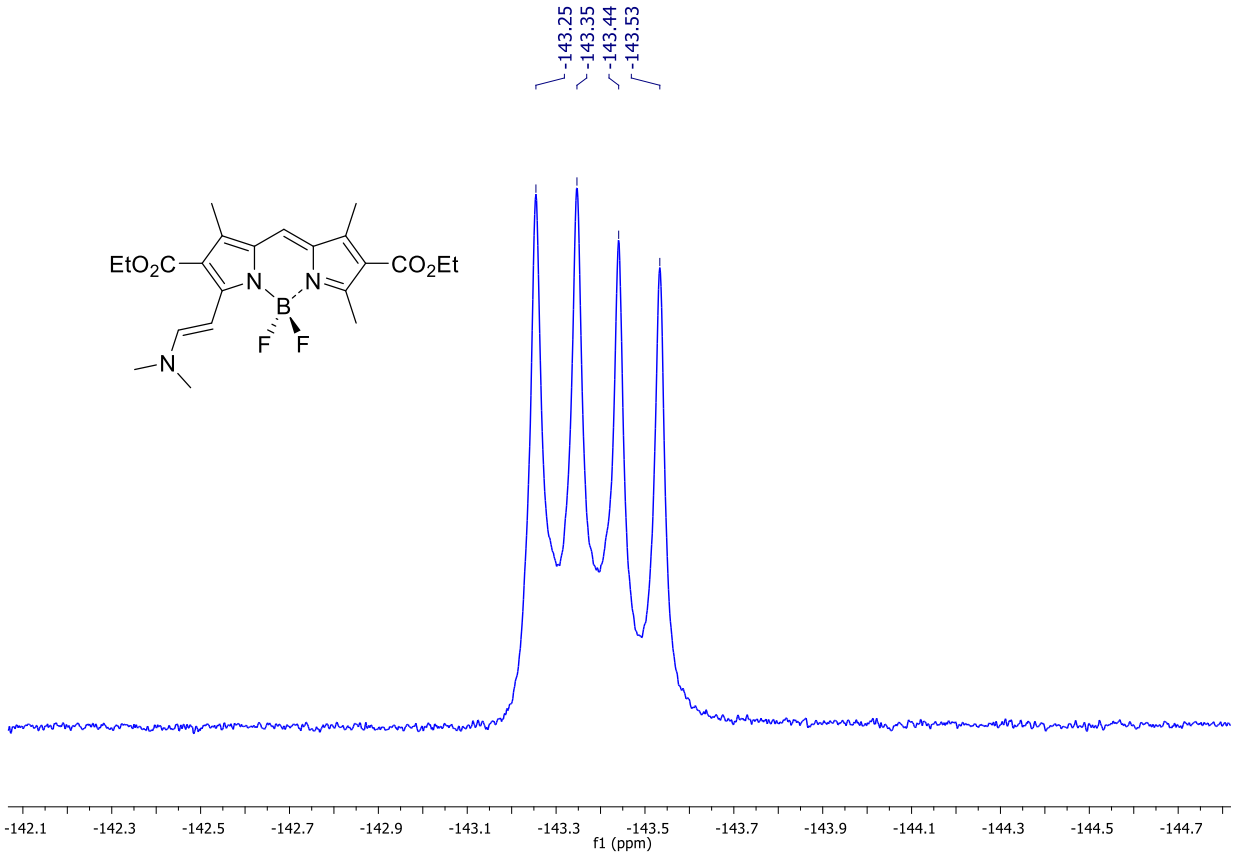

Figure S3. ^{19}F NMR spectrum of compound **2** in $CDCl_3$

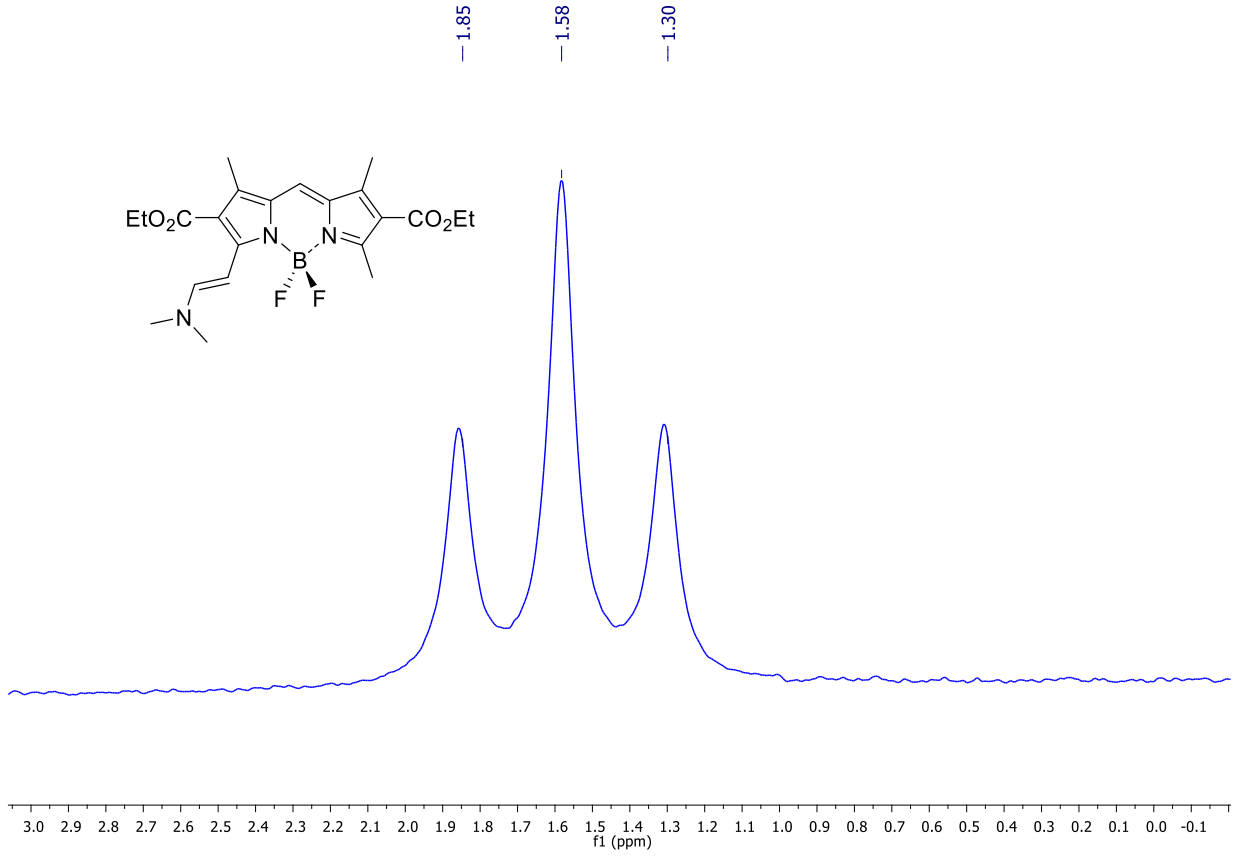

Figure S4. ^{11}B NMR spectrum of compound **2** in $CDCl_3$

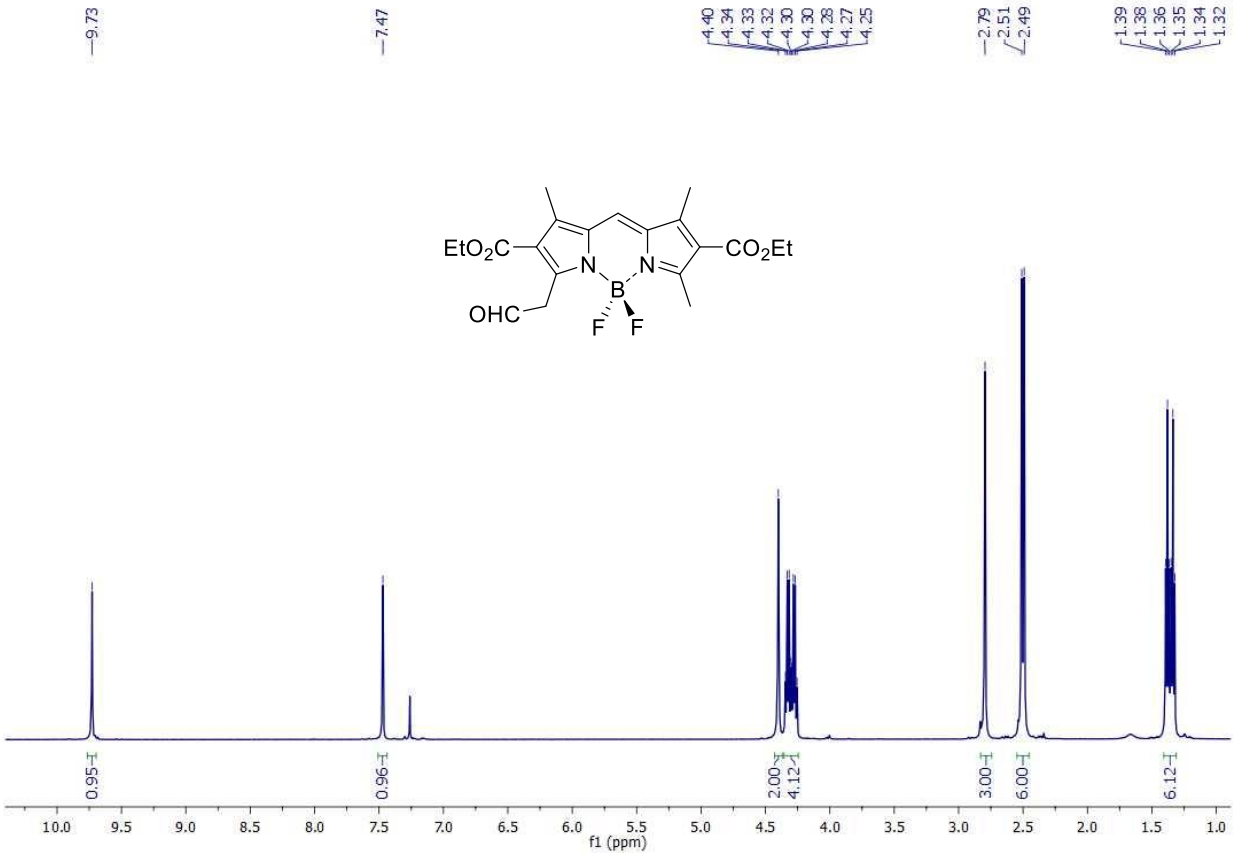

Figure S5. ^{1}H NMR spectrum of compound **3** in $CDCl_3$

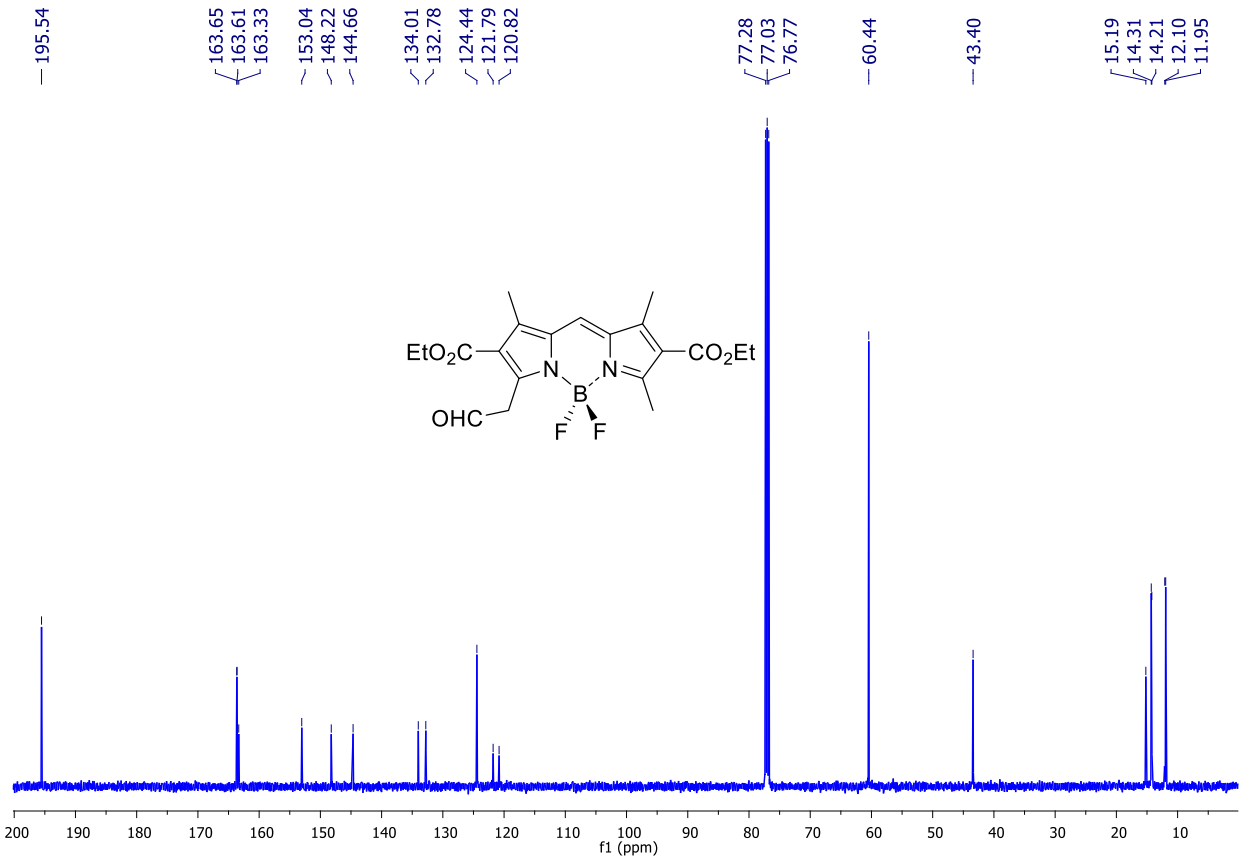

Figure S6. ^{13}C{^{1}H} NMR spectrum of compound **3** in $CDCl_3$

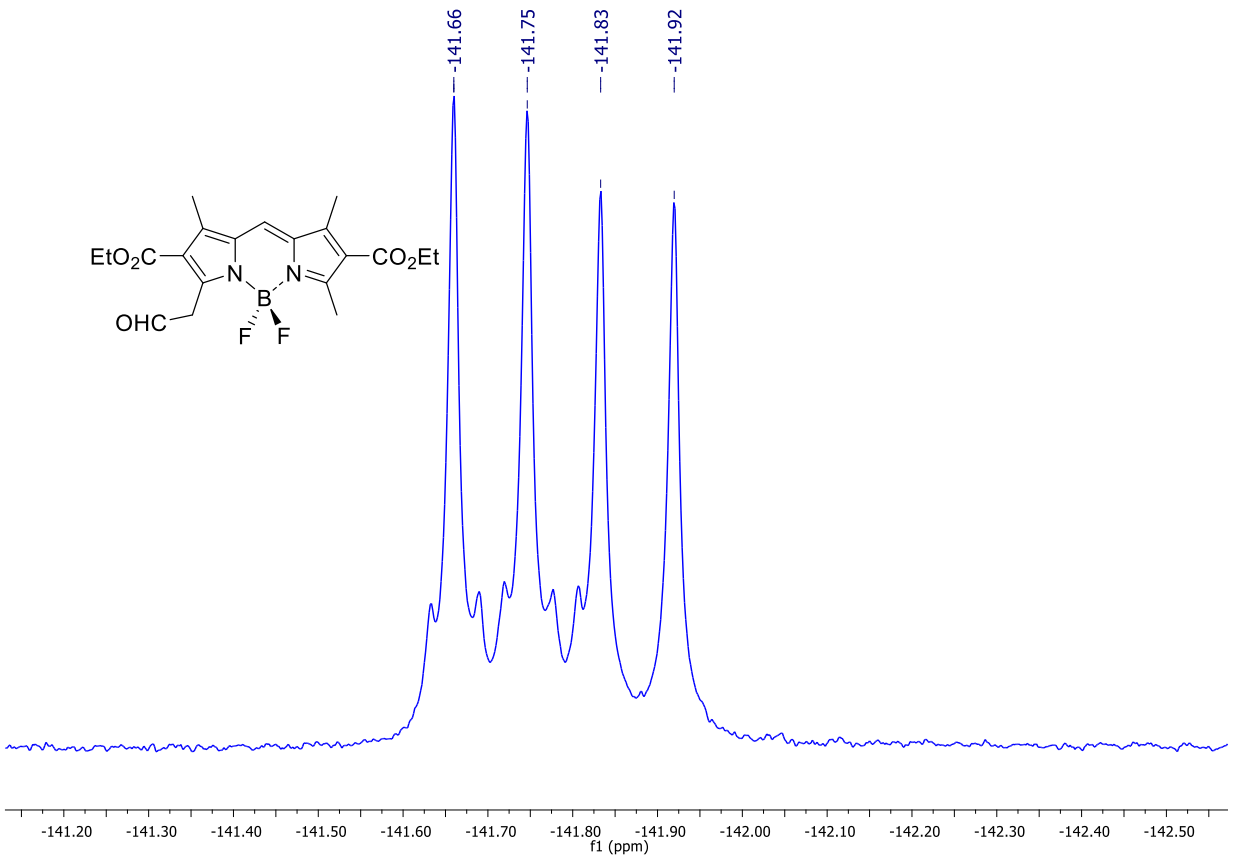

Figure S7. ^{19}F NMR spectrum of compound **3** in $CDCl_3$

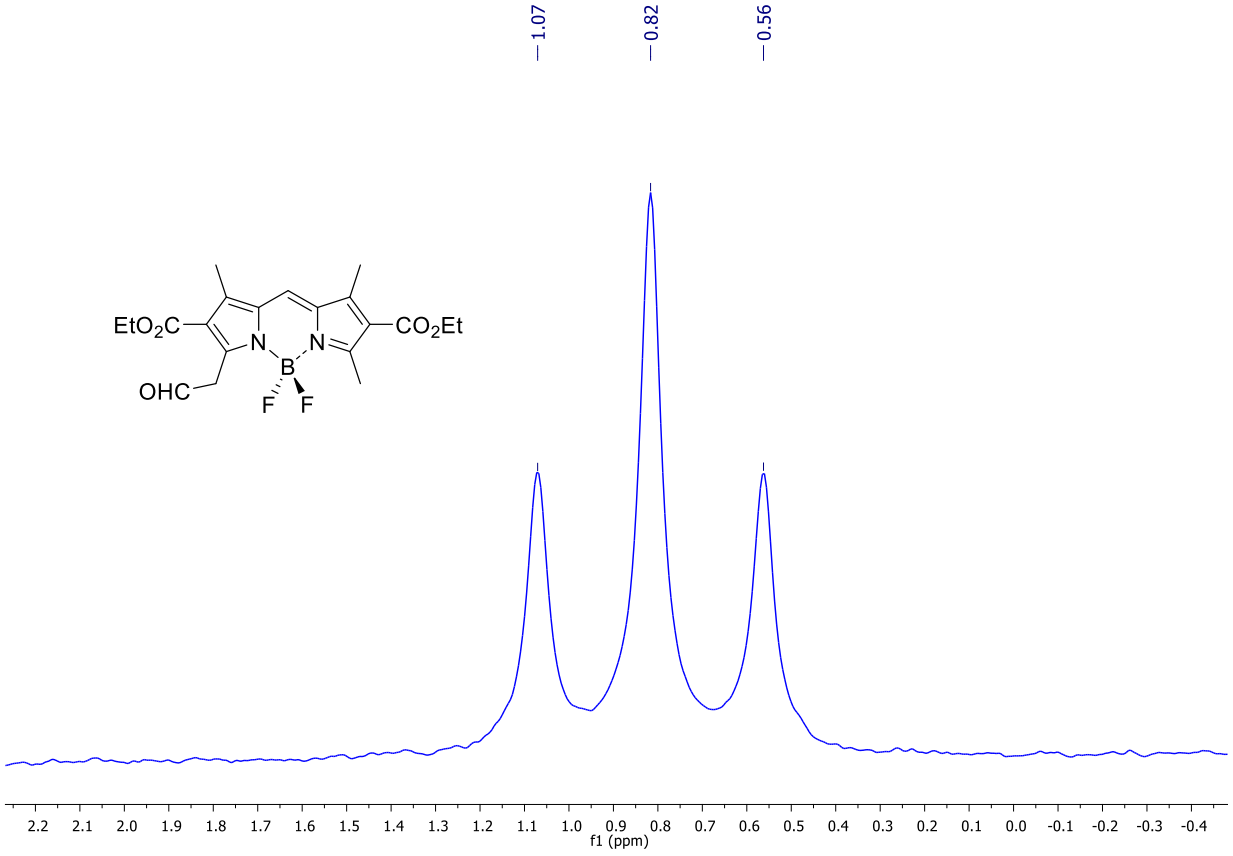

Figure S8. ^{11}B NMR spectrum of compound **3** in $CDCl_3$

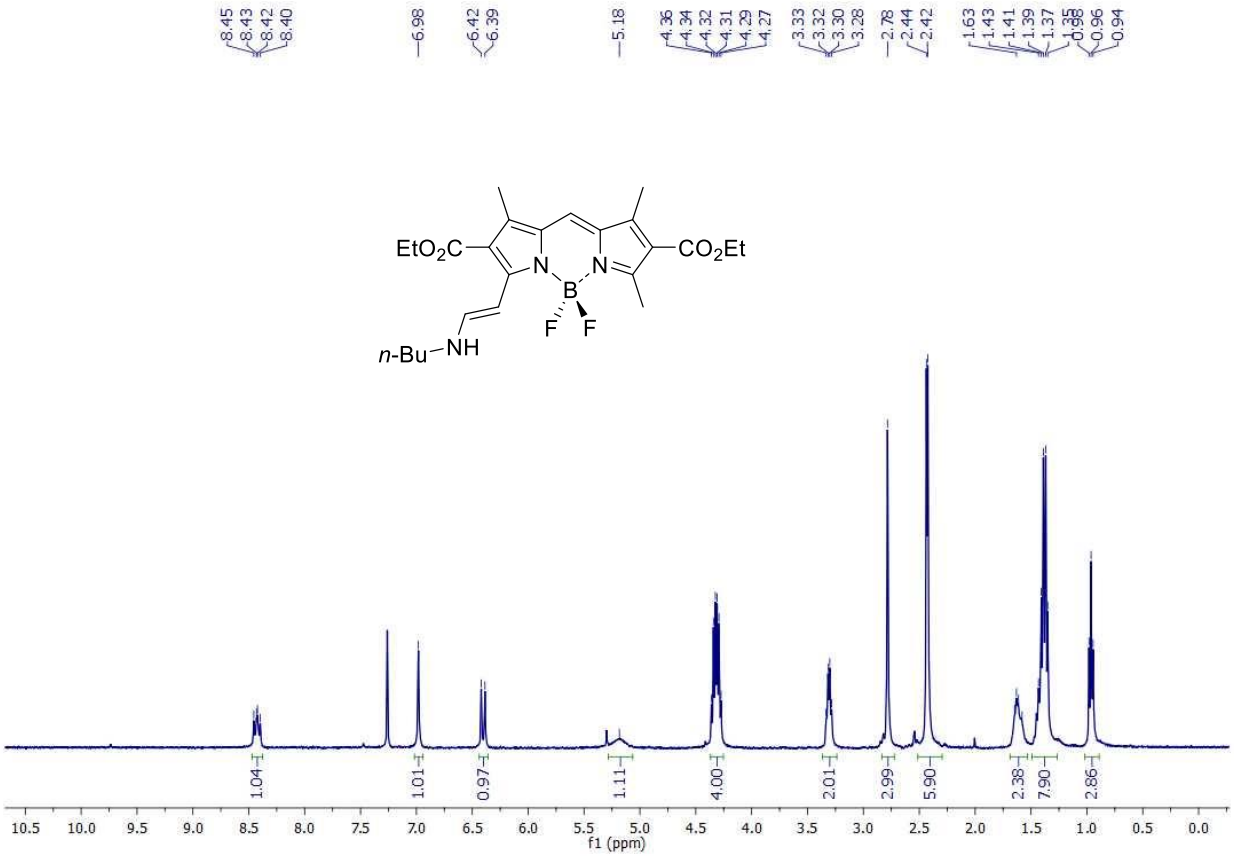

Figure S9. H^1 NMR spectrum of compound **4** in $CDCl_3$

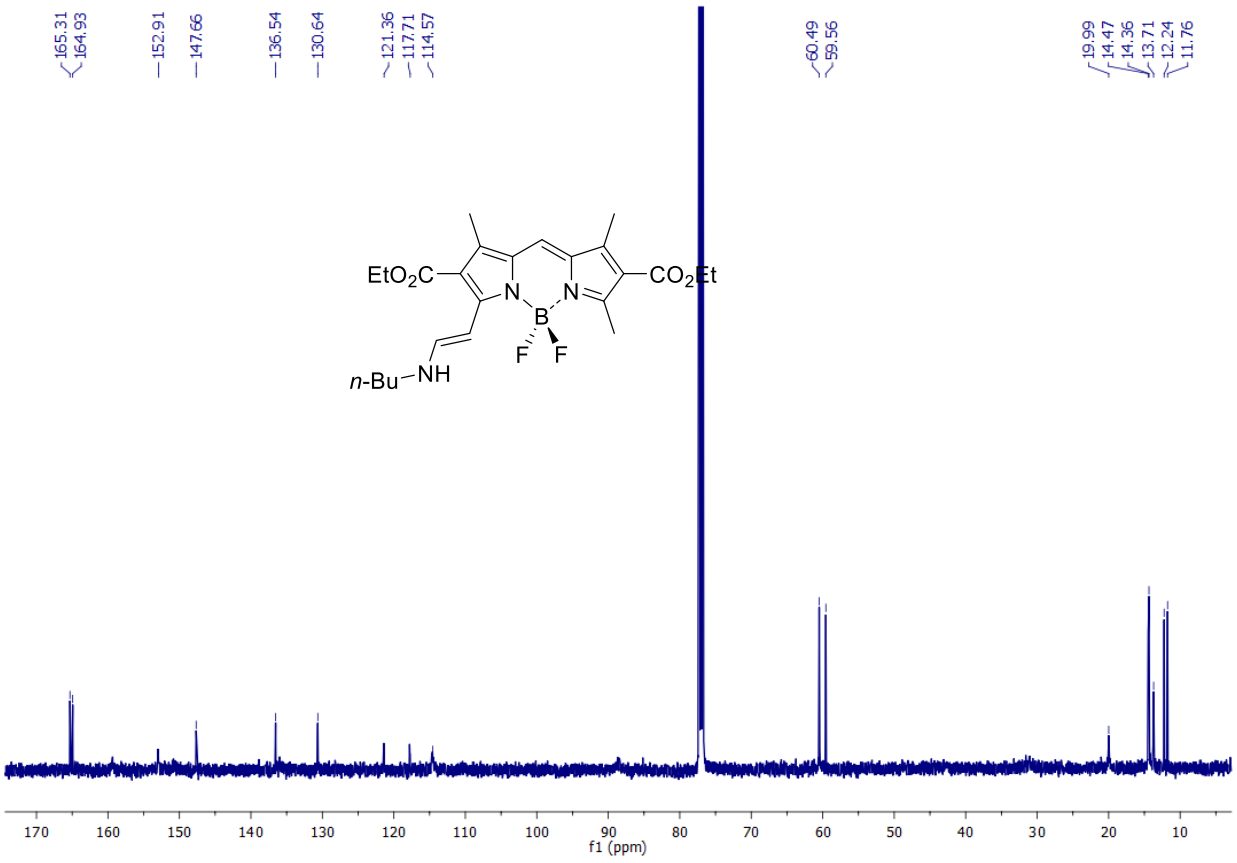

Figure S10. $^{13}C\{^1H\}$ NMR spectrum of compound **4** in $CDCl_3$

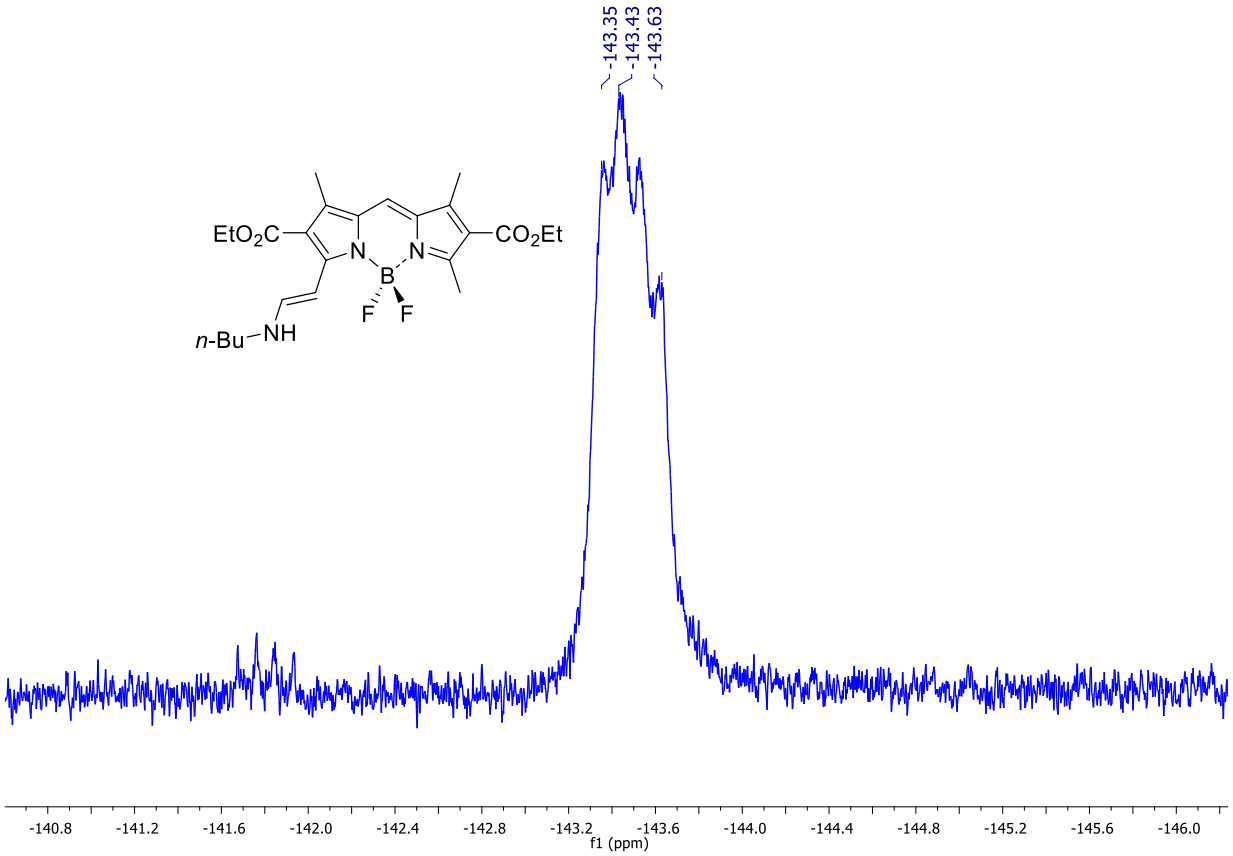

Figure S11. ^{19}F NMR spectrum of compound **4** in $CDCl_3$

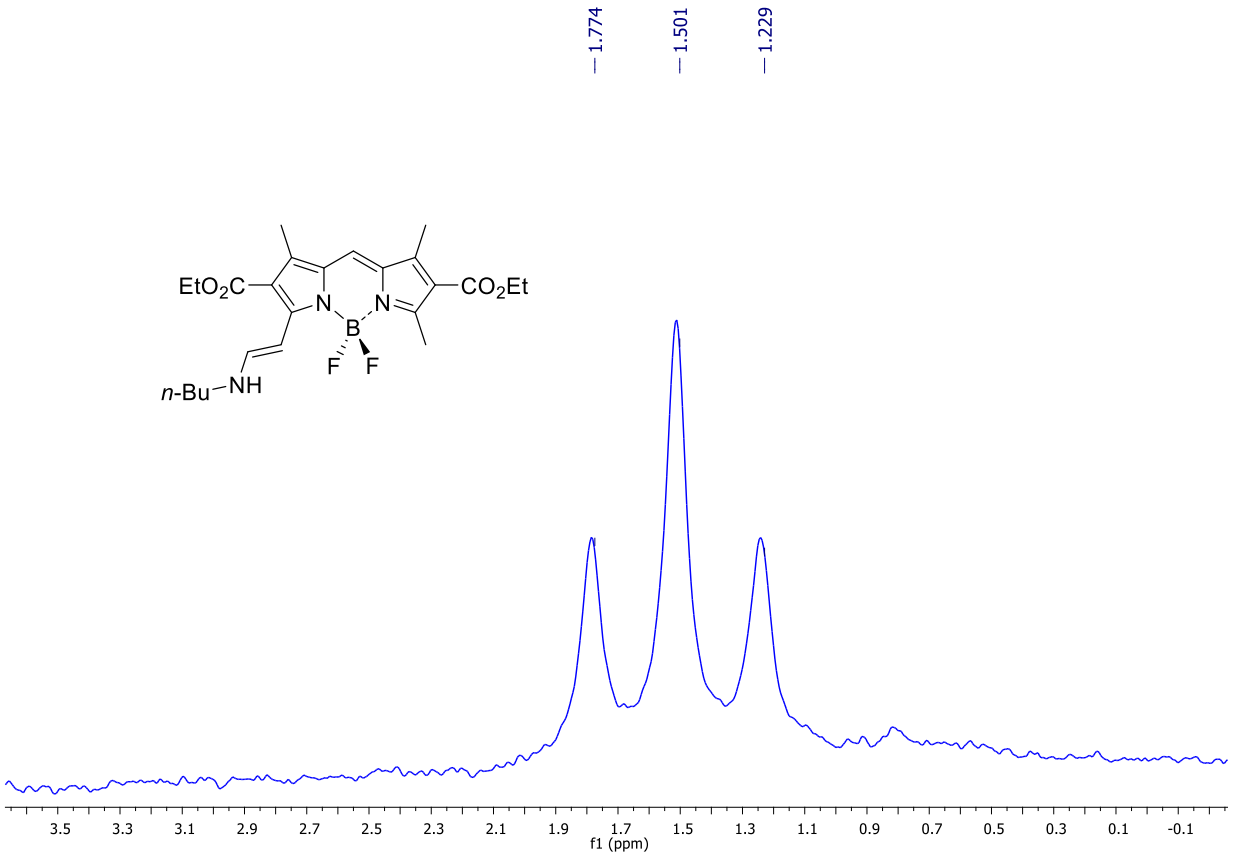

Figure S12. ^{11}B NMR spectrum of compound **4** in $CDCl_3$

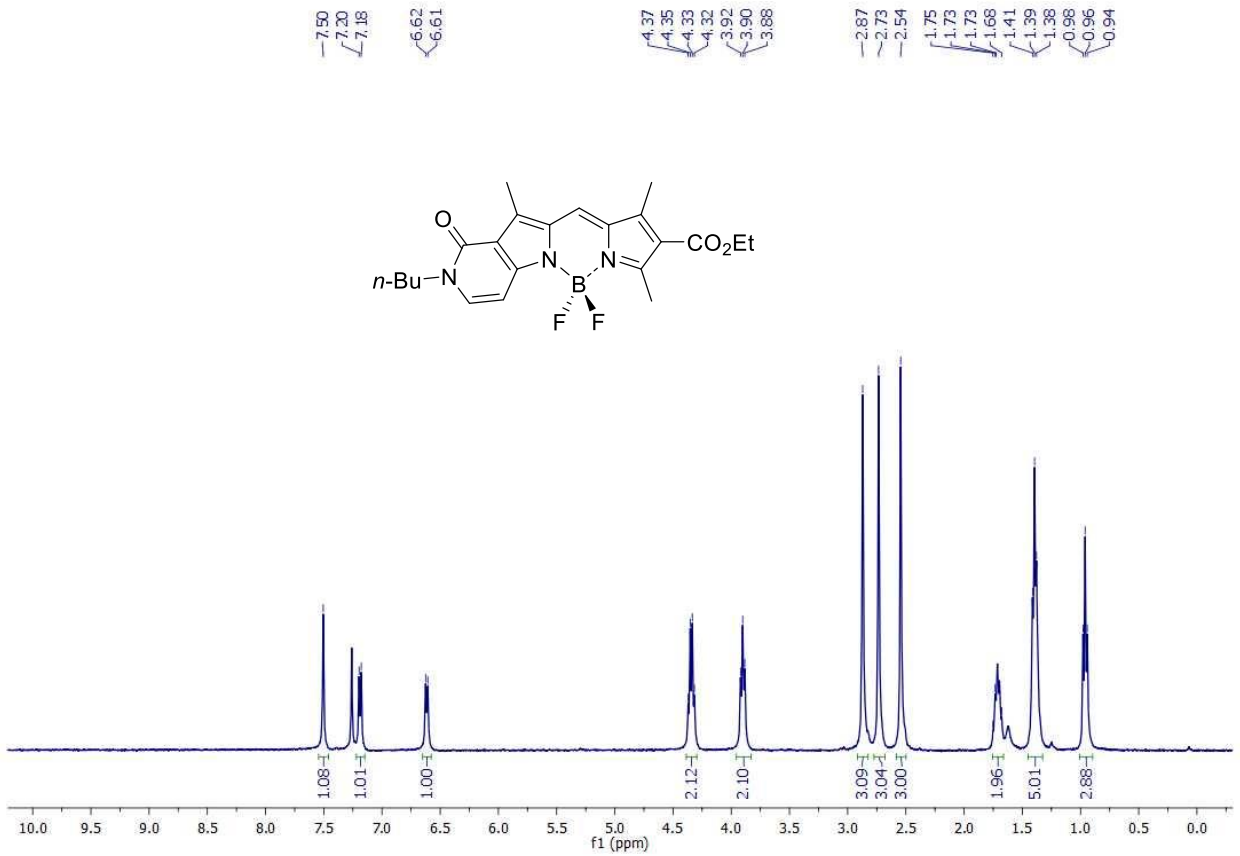

Figure S13. H^1 NMR spectrum of compound **5** in $CDCl_3$ (prepared by method **A)**

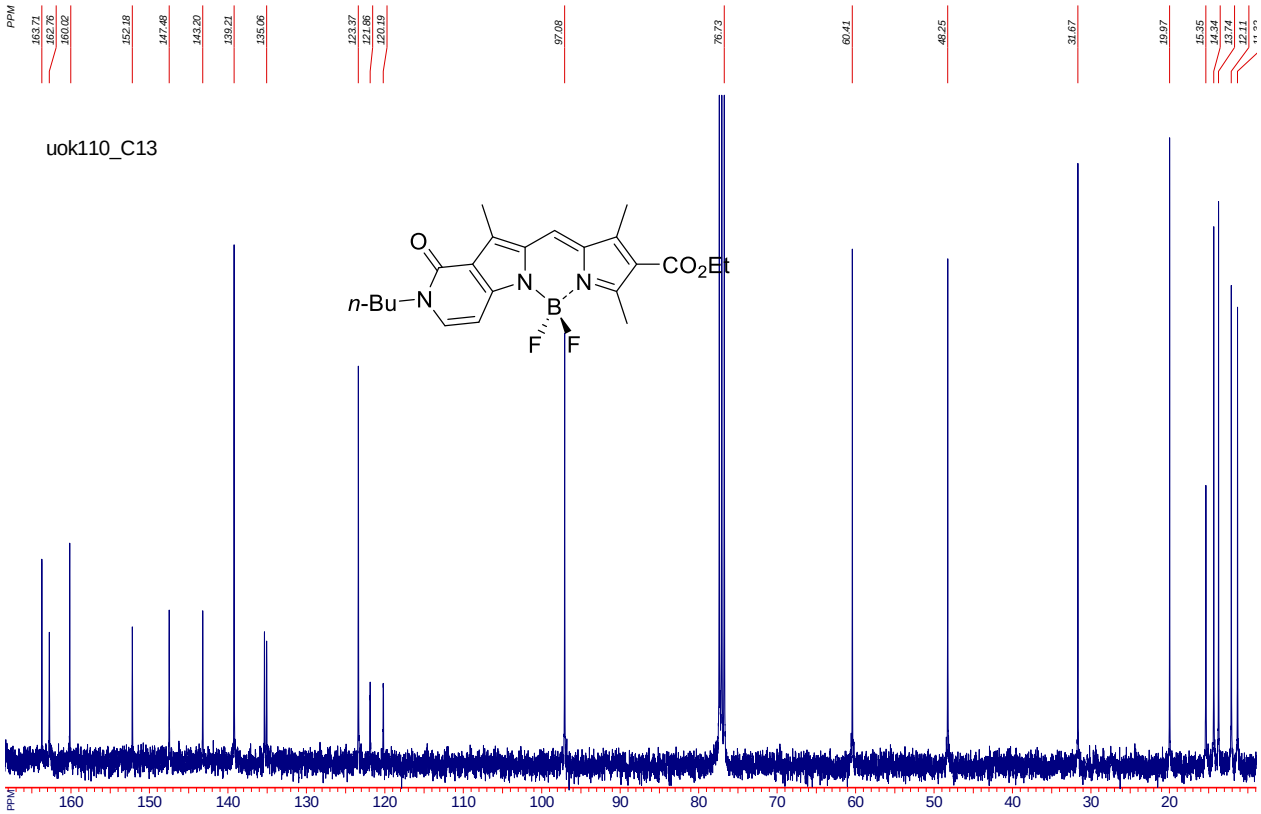

Figure S14. $^{13}C\{^1H\}$ NMR spectrum of compound **5** in $CDCl_3$ (prepared by method **A)**

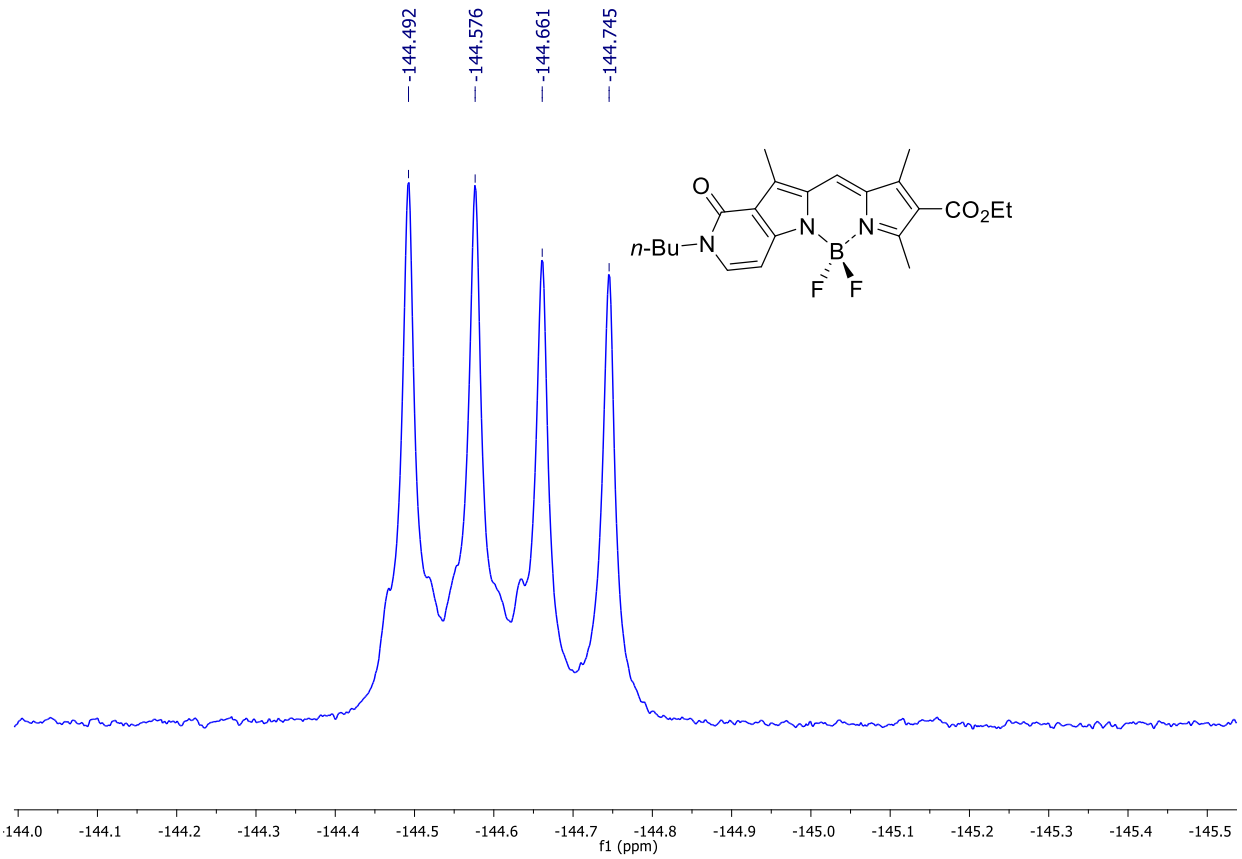

Figure S15. ^{19}F NMR spectrum of compound **5** in $CDCl_3$ (prepared by method **A)**

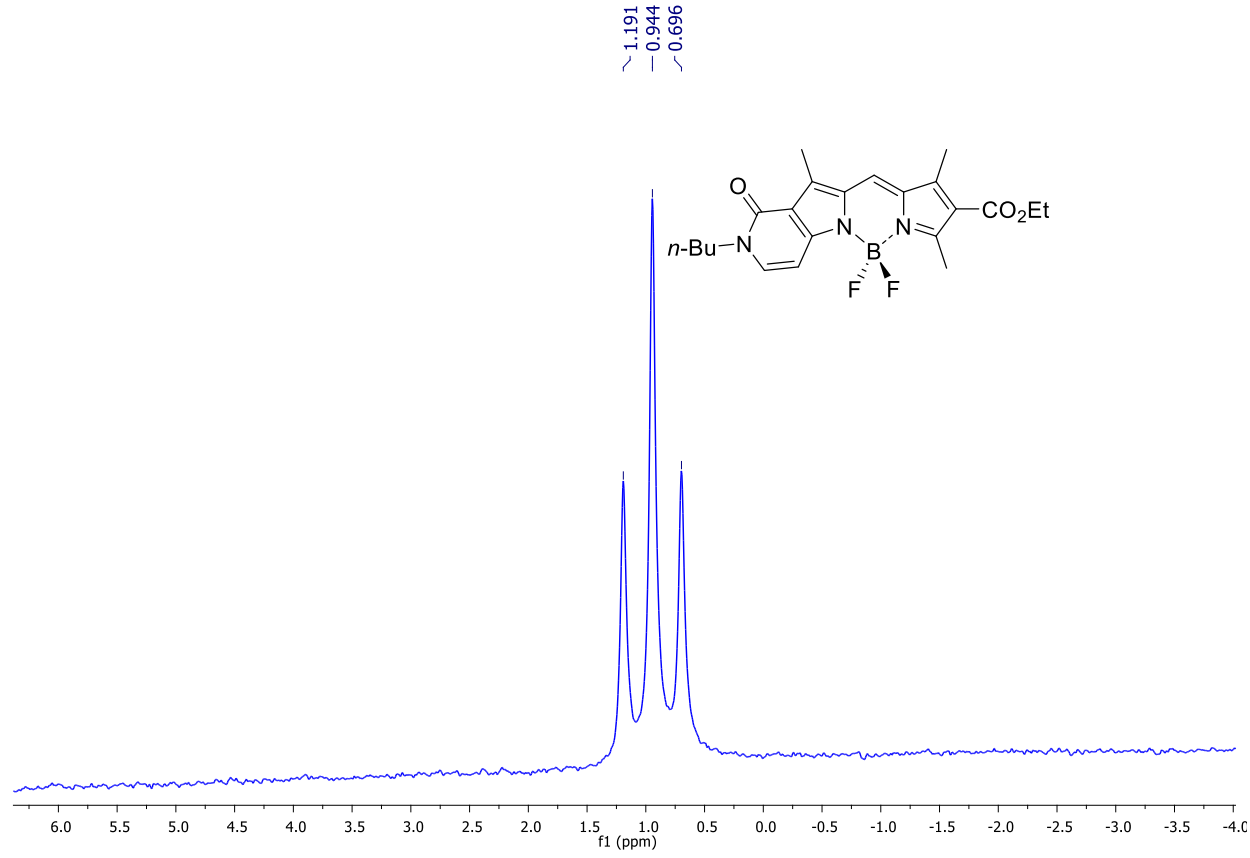

Figure S16. ^{11}B NMR spectrum of compound **5** in $CDCl_3$ (prepared by method **A)**

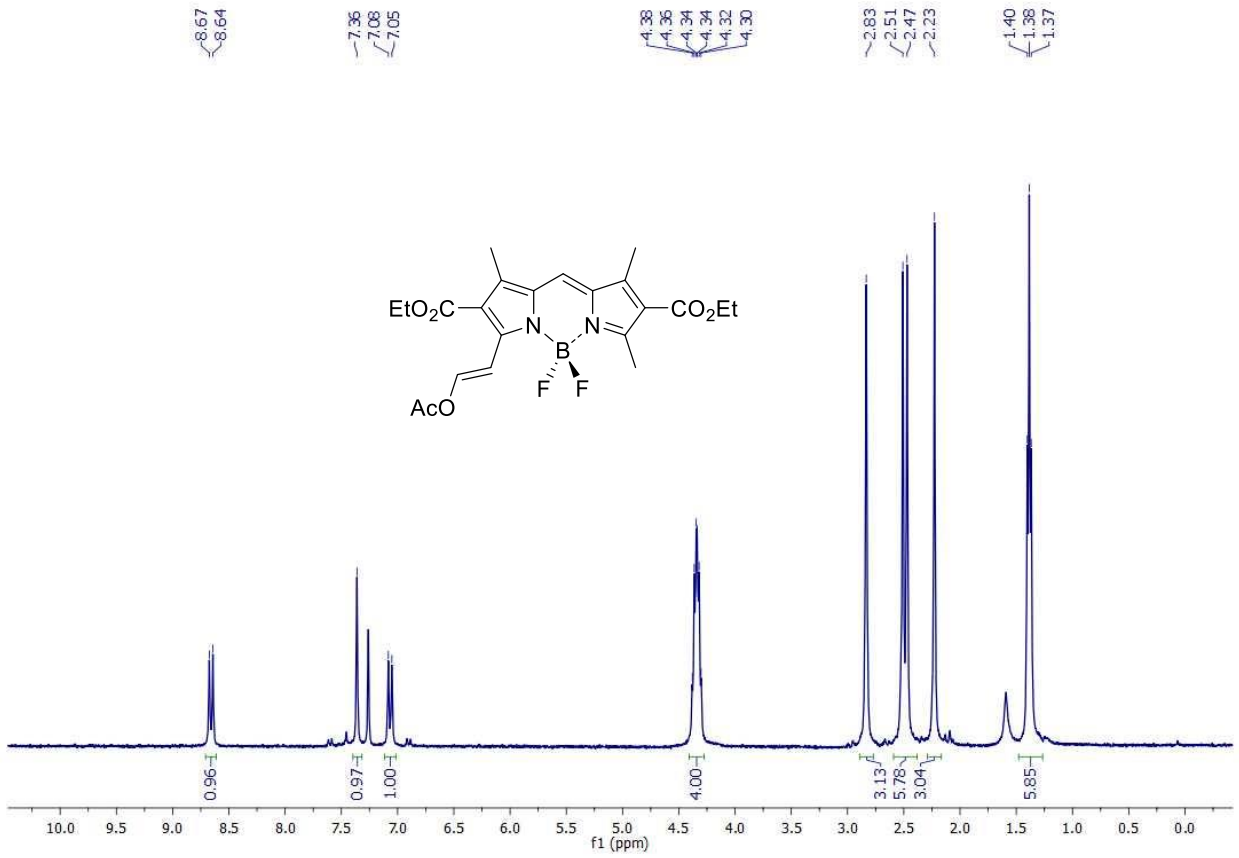

Figure S17. H^1 NMR spectrum of compound **6** in $CDCl_3$

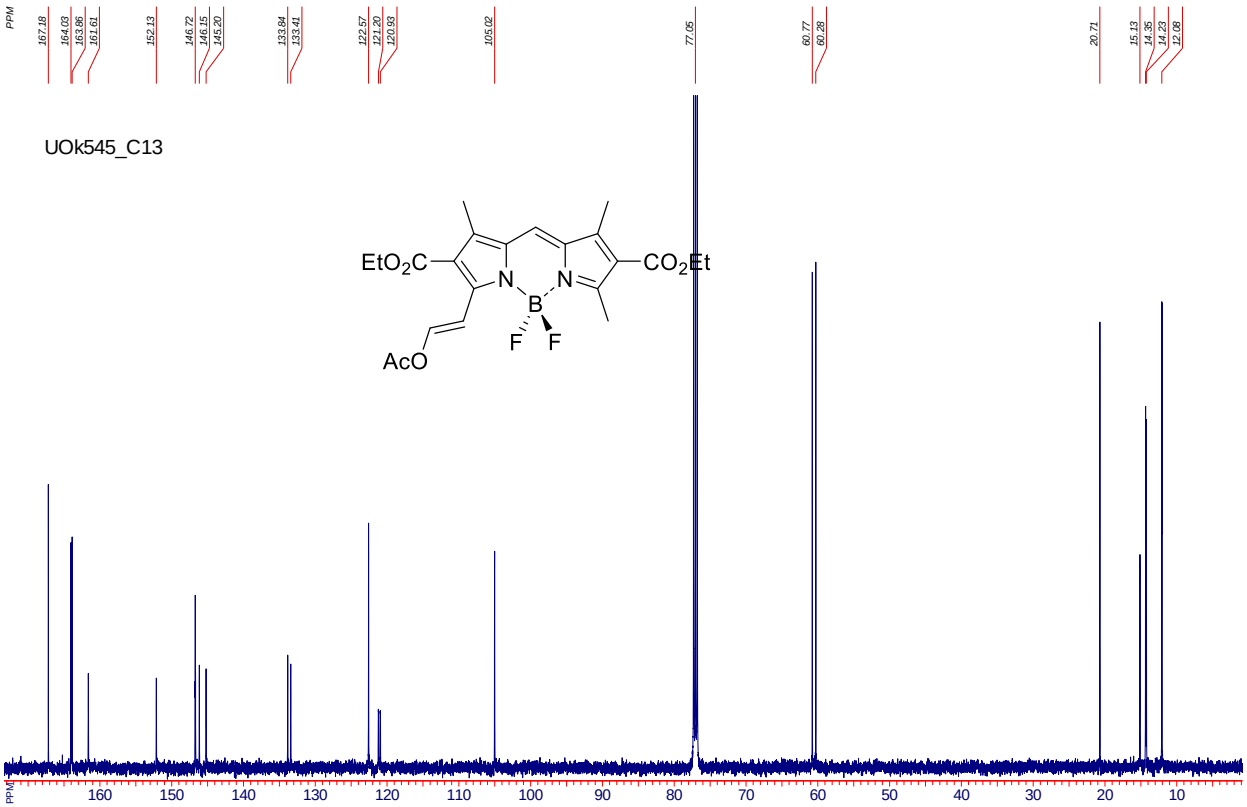

Figure S18. $^{13}C\{^1H\}$ NMR spectrum of compound **6** in $CDCl_3$

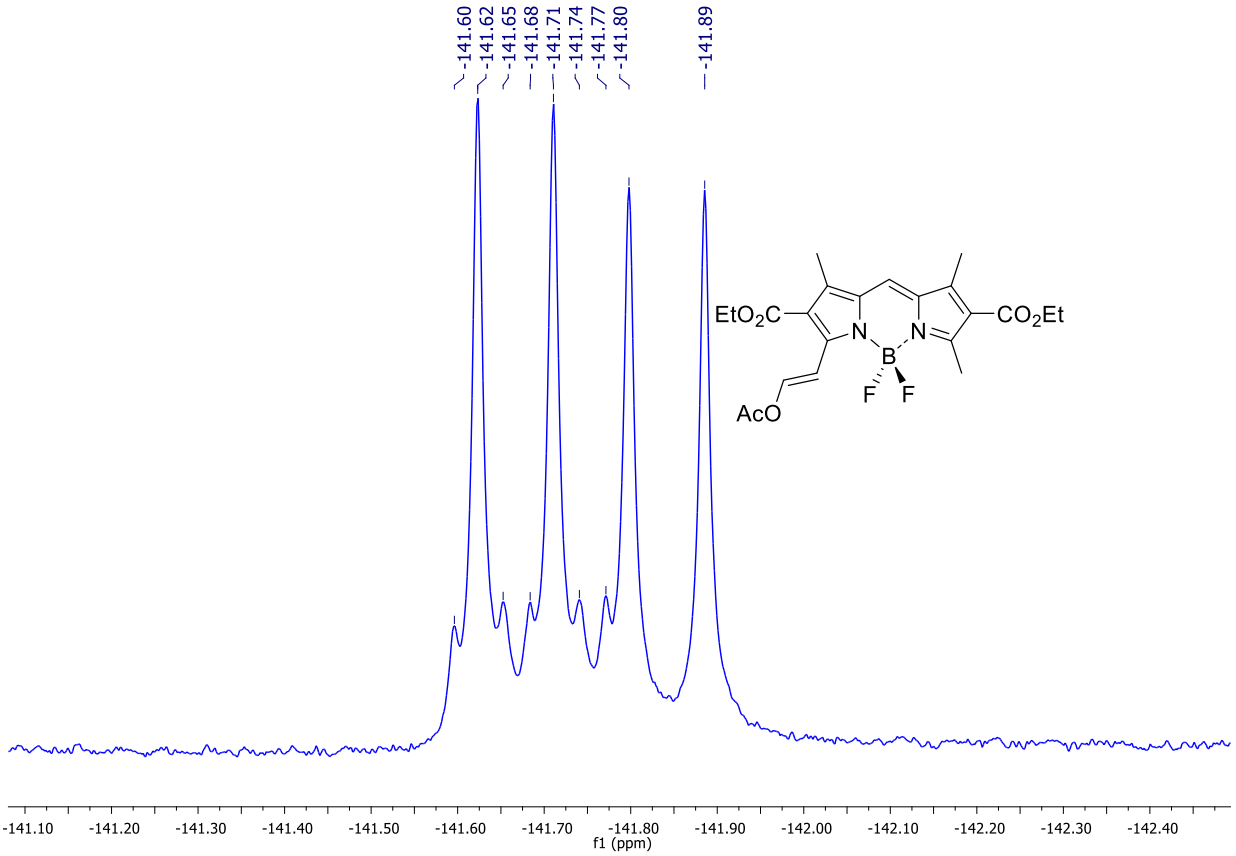

Figure S19. ^{19}F NMR spectrum of compound **6** in $CDCl_3$

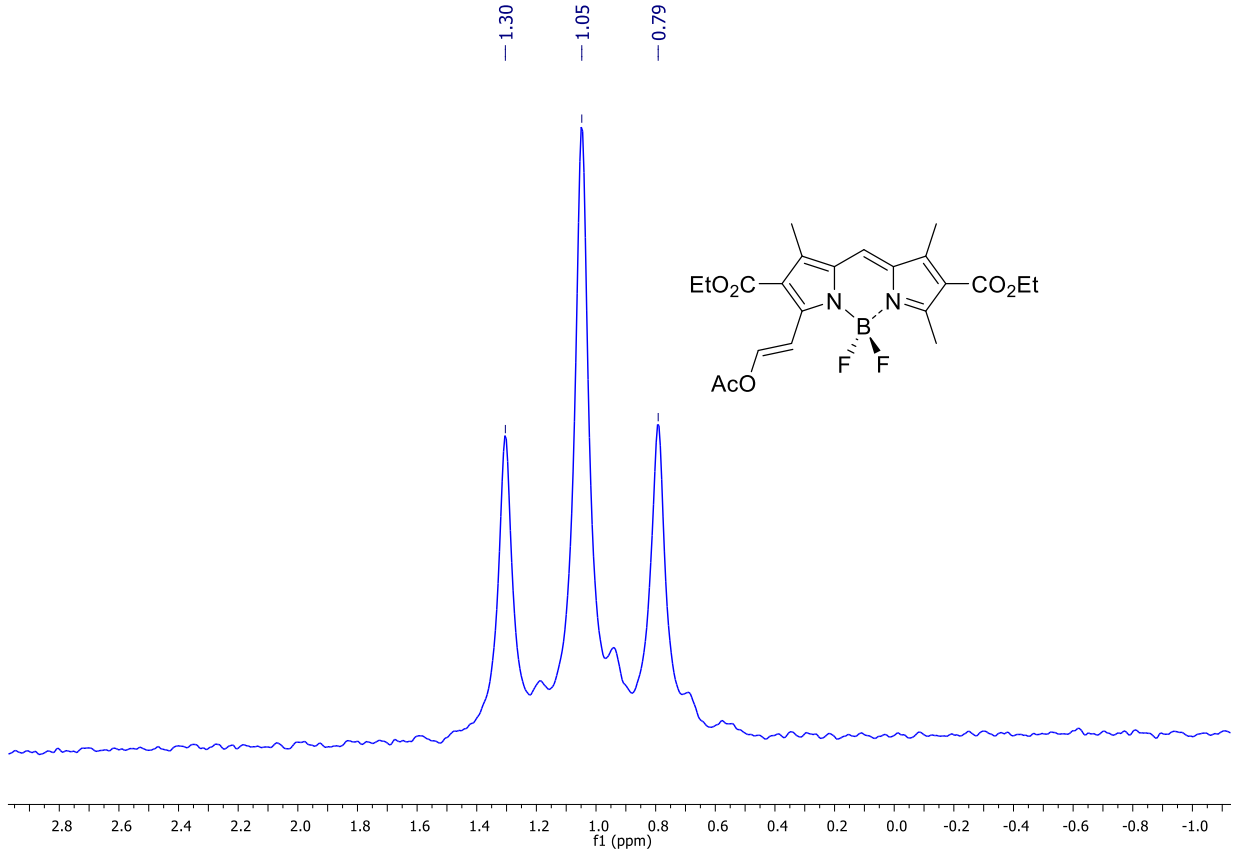

Figure S20. ^{11}B NMR spectrum of compound **6** in $CDCl_3$

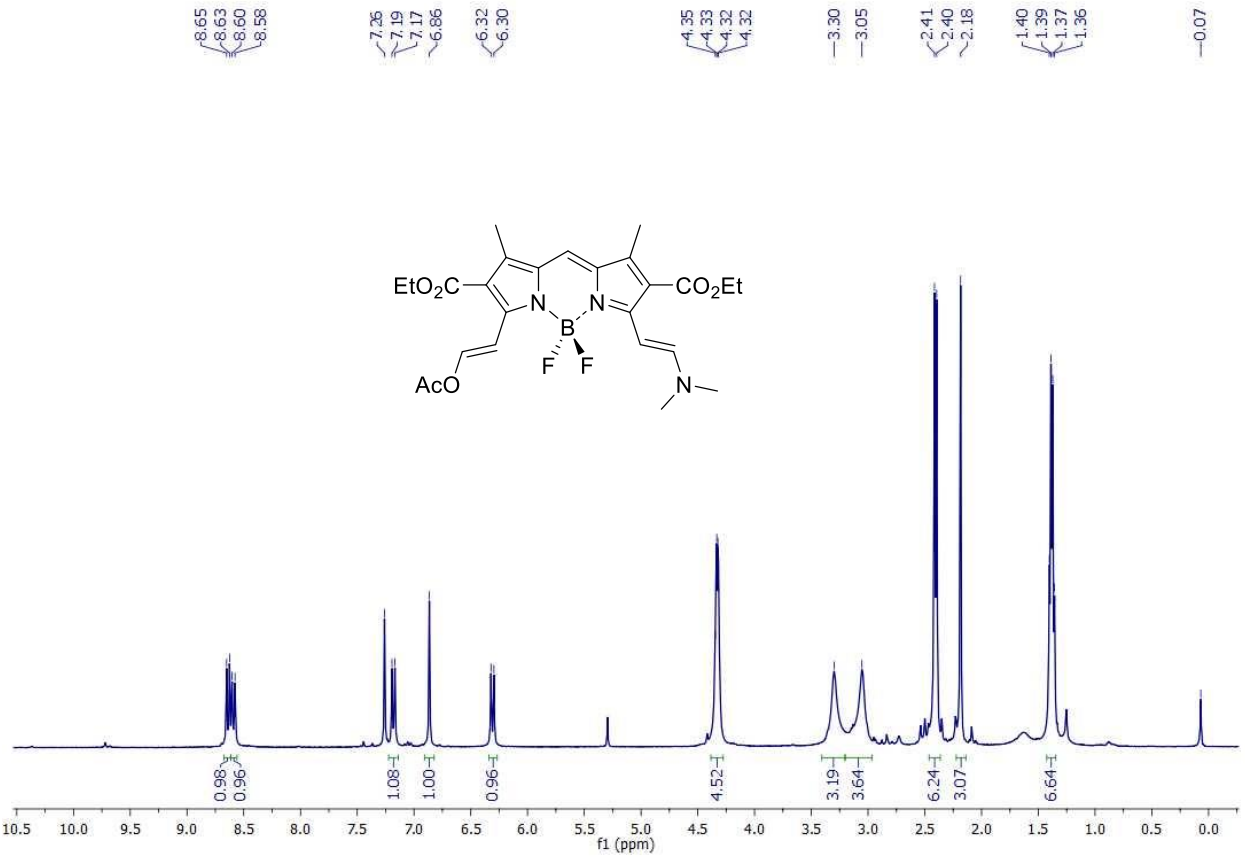

Figure S21. H^1 NMR spectrum of compound **7** in $CDCl_3$

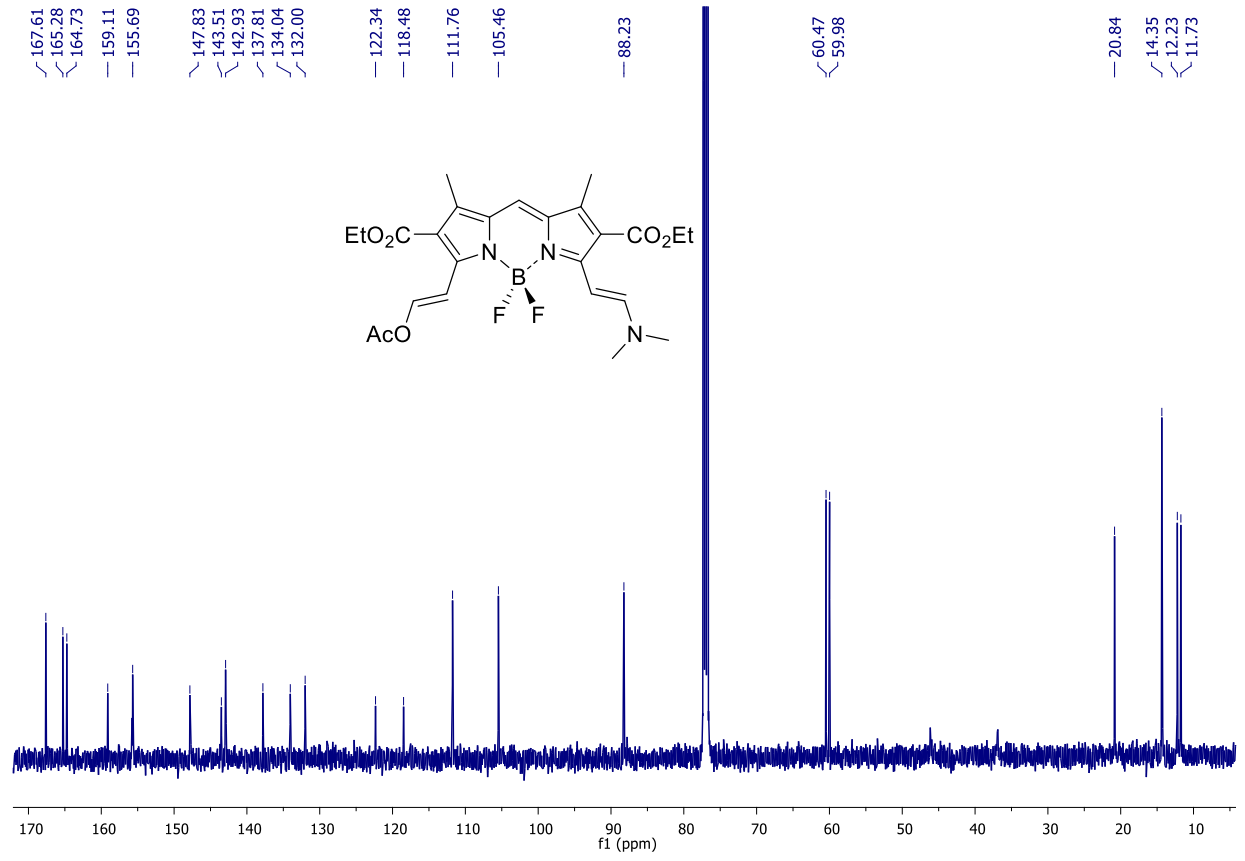

Figure S22. $^{13}C\{^1H\}$ NMR spectrum of compound **7** in $CDCl_3$

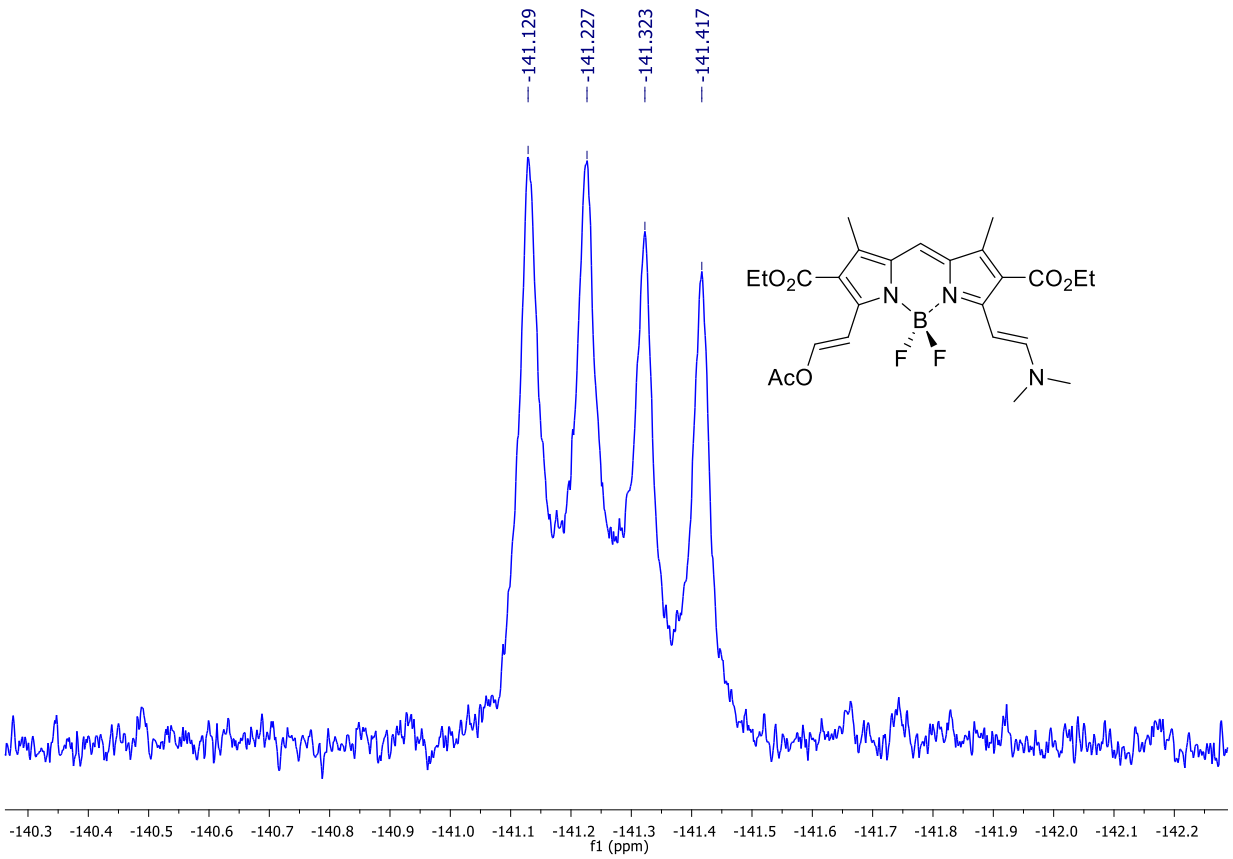

Figure S23. ^{19}F NMR spectrum of compound **7** in $CDCl_3$

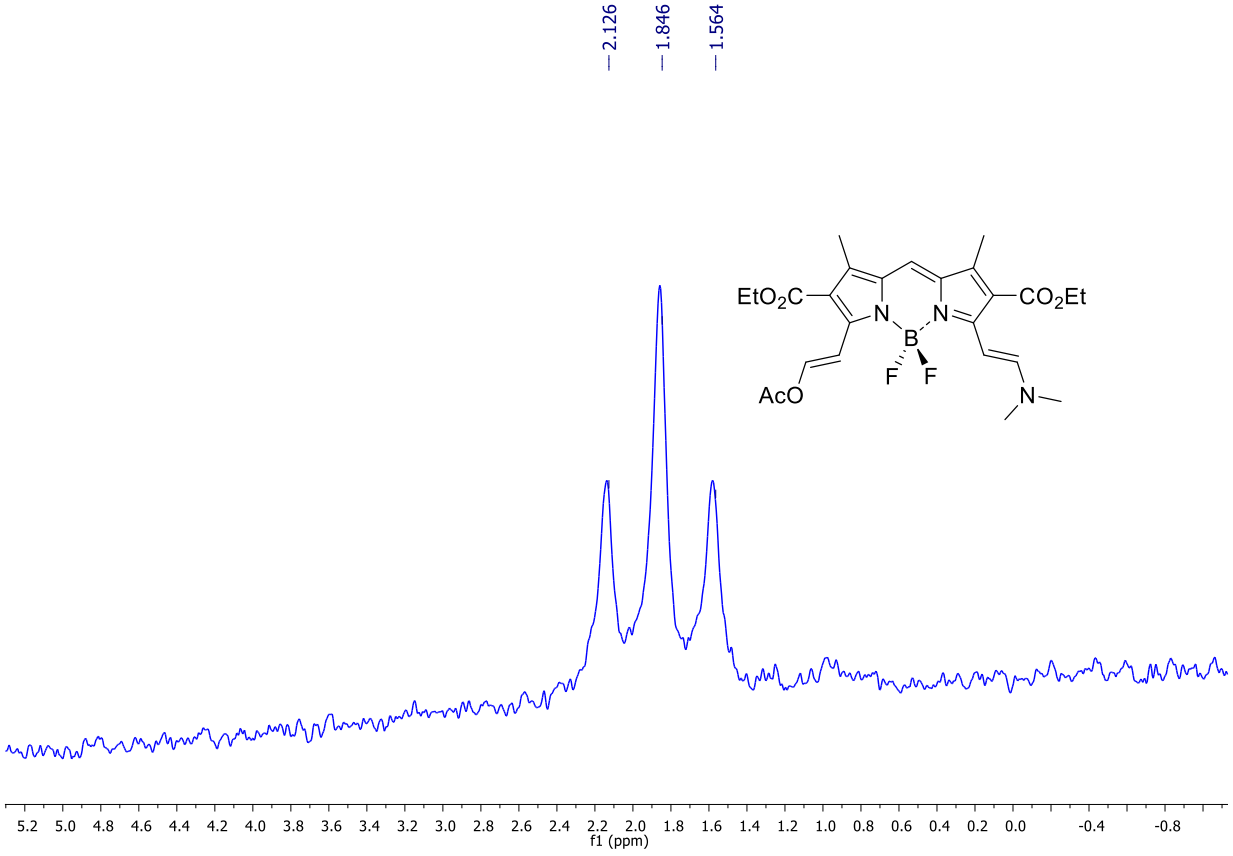

Figure S24. ^{11}B NMR spectrum of compound **7** in $CDCl_3$

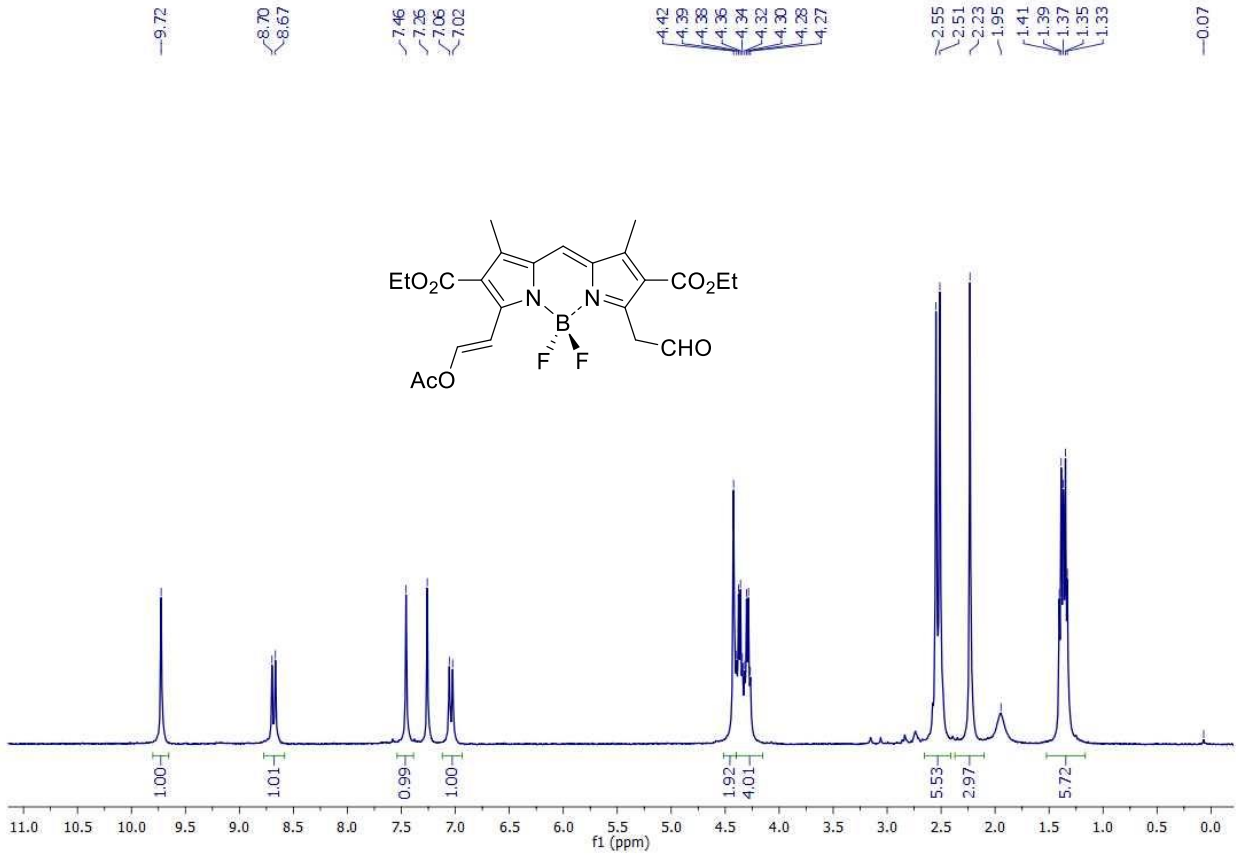

Figure S25. ^{1}H NMR spectrum of compound **8** in $CDCl_3$

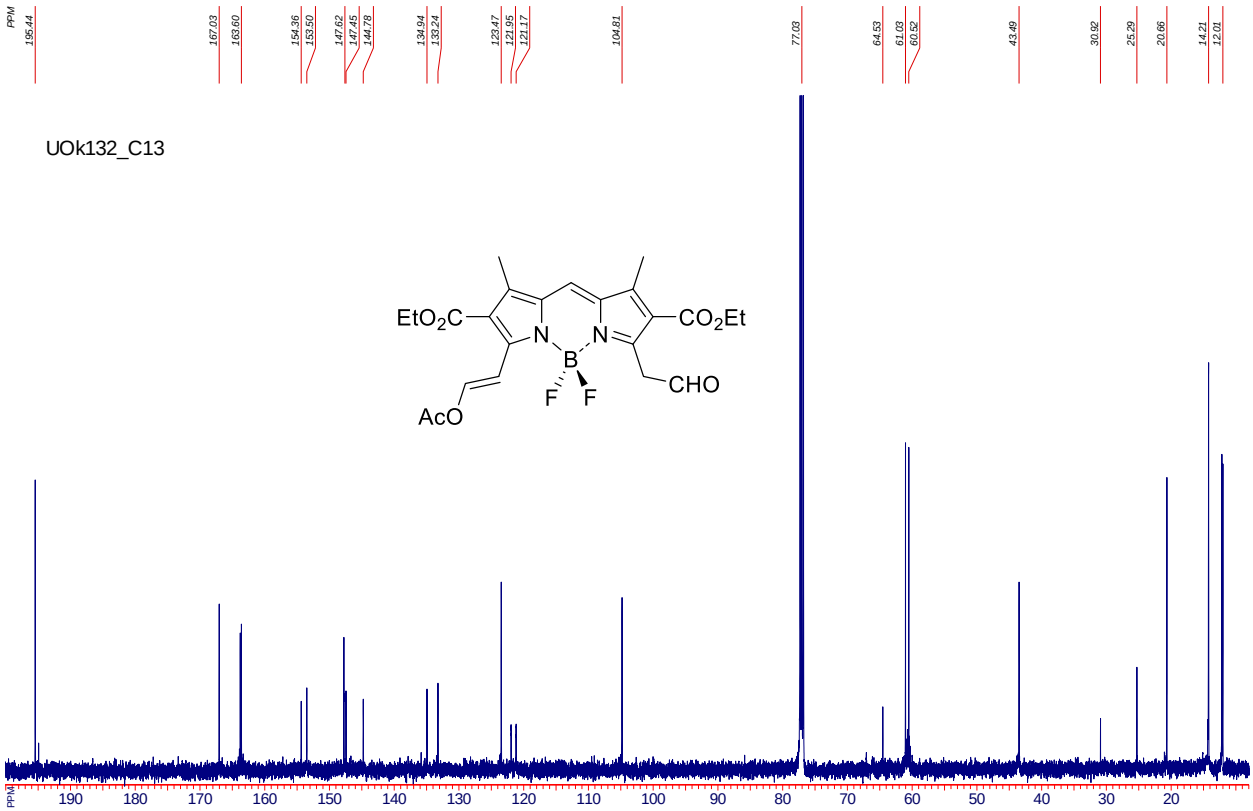

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8** in $CDCl_3$

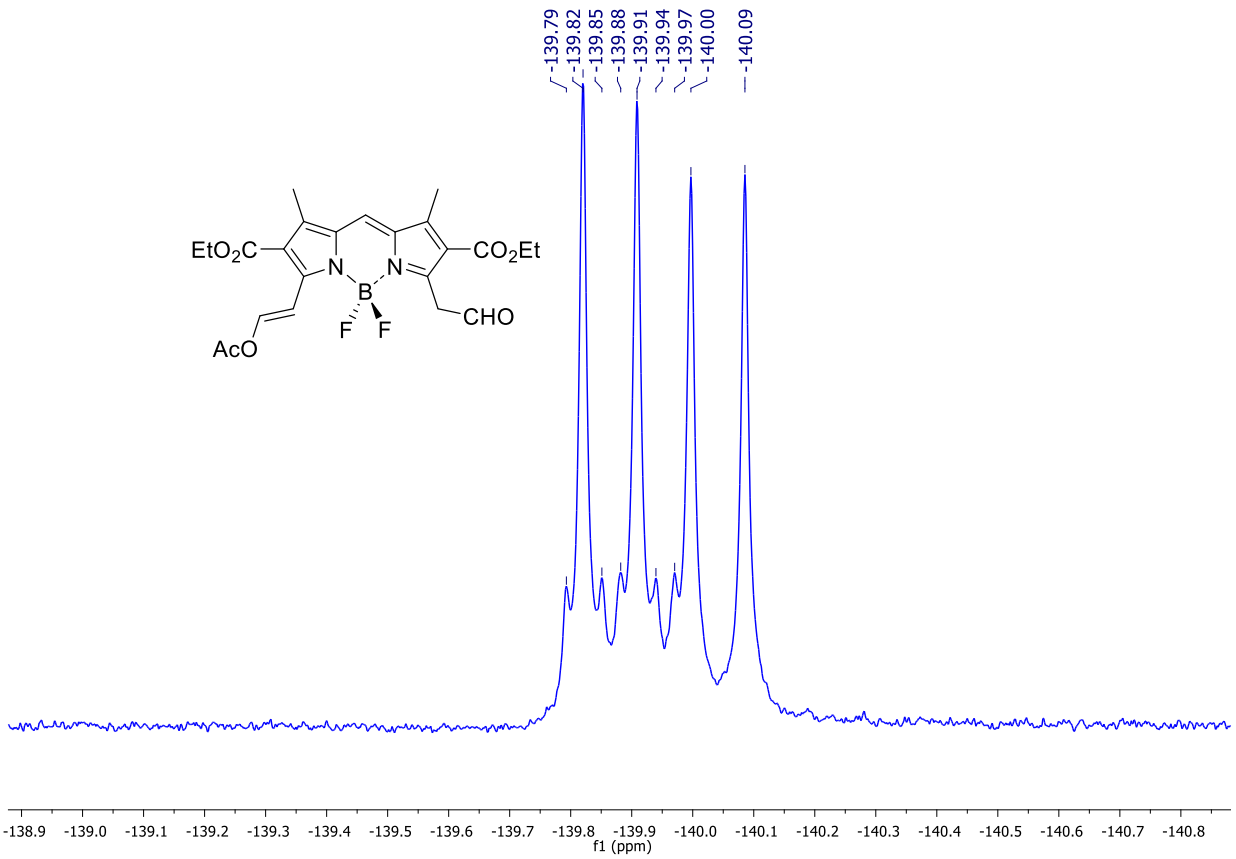

Figure S27. ^{19}F NMR spectrum of compound **8** in $CDCl_3$

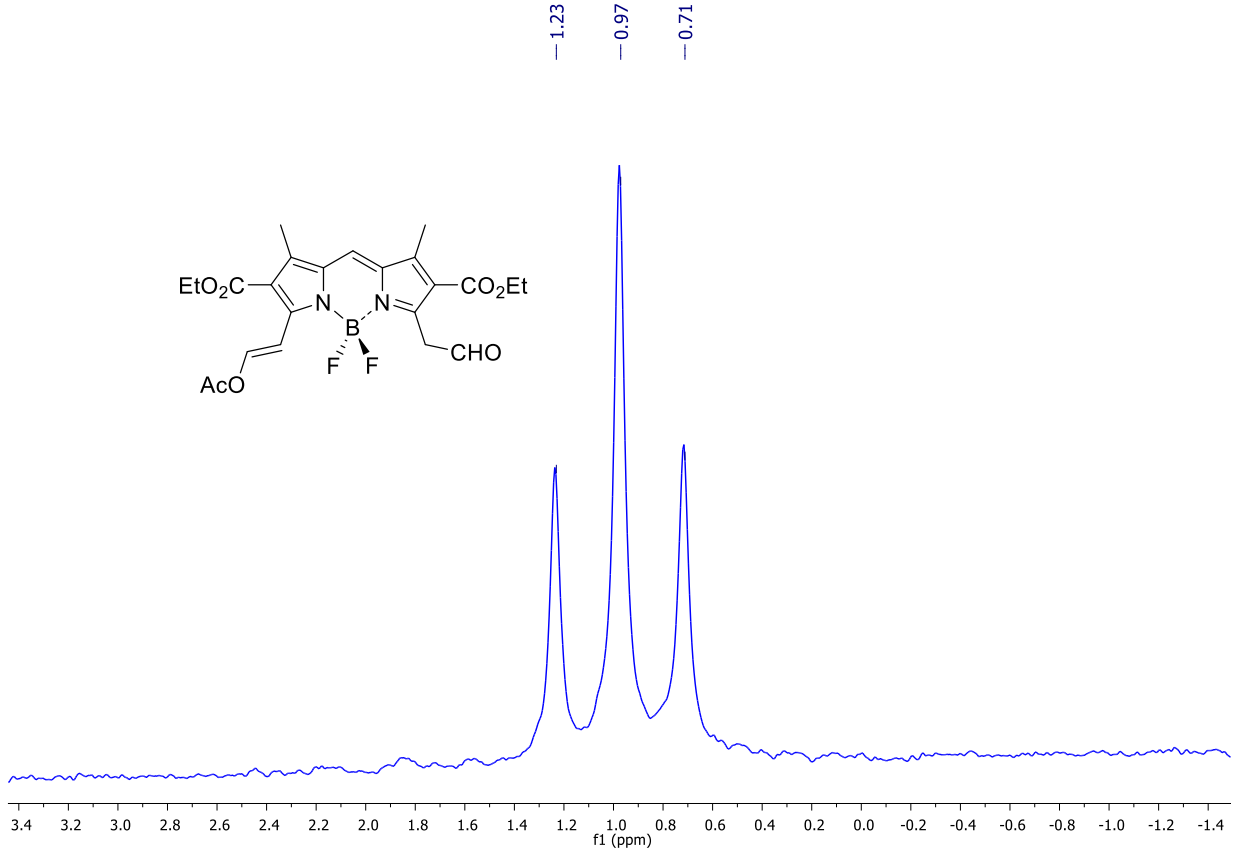

Figure S28. ^{11}B NMR spectrum of compound **8** in $CDCl_3$

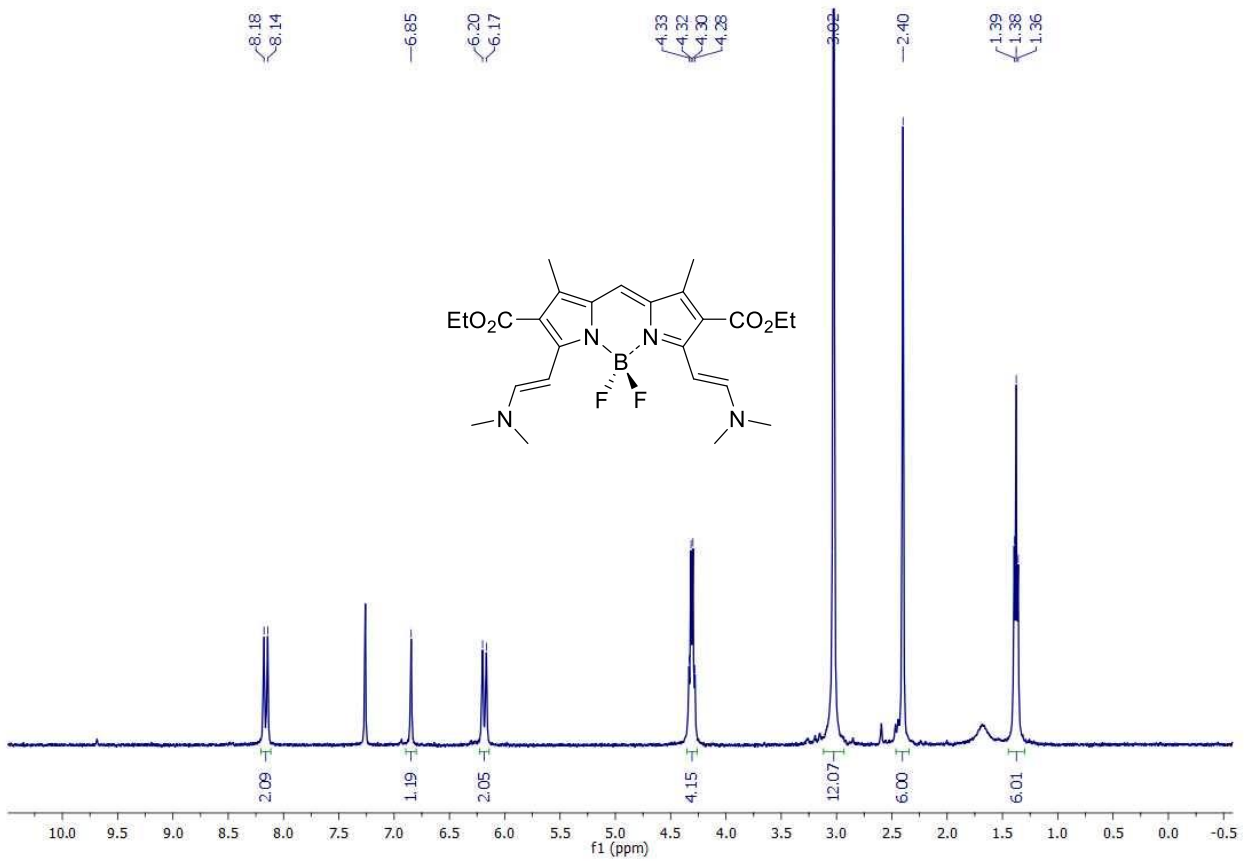

Figure S29. ^{1}H NMR spectrum of compound **9** in $CDCl_3$

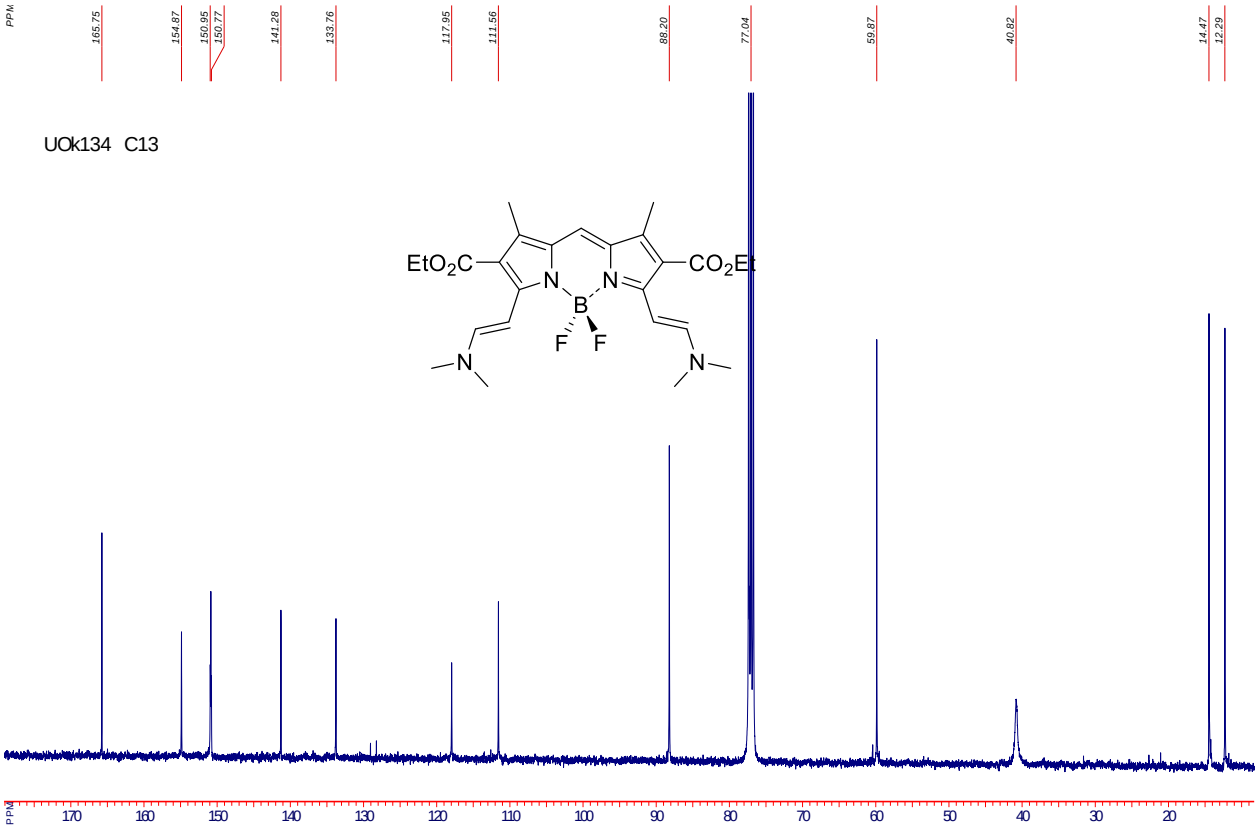

Figure S30. ^{13}C{^{1}H} NMR spectrum of compound **9** in $CDCl_3$

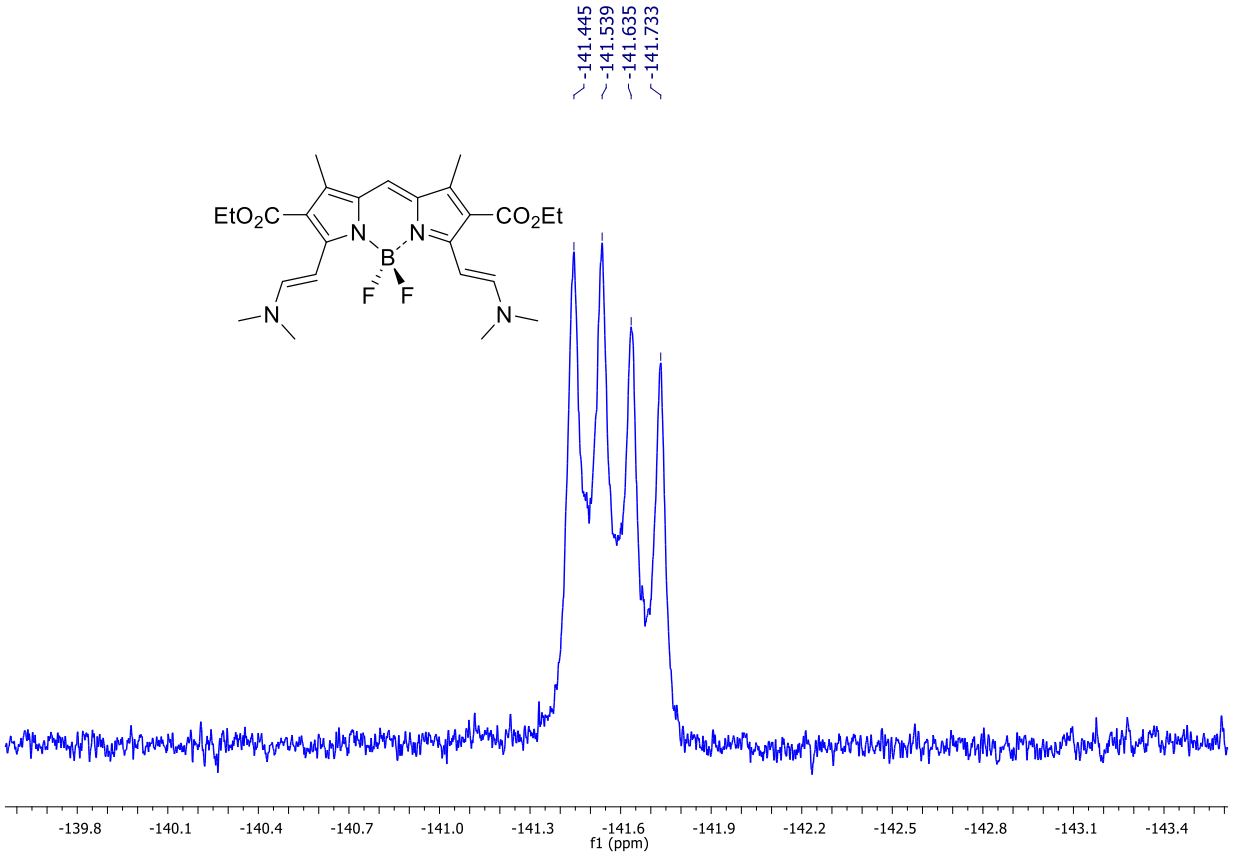

Figure S31. ^{19}F NMR spectrum of compound **9** in $CDCl_3$

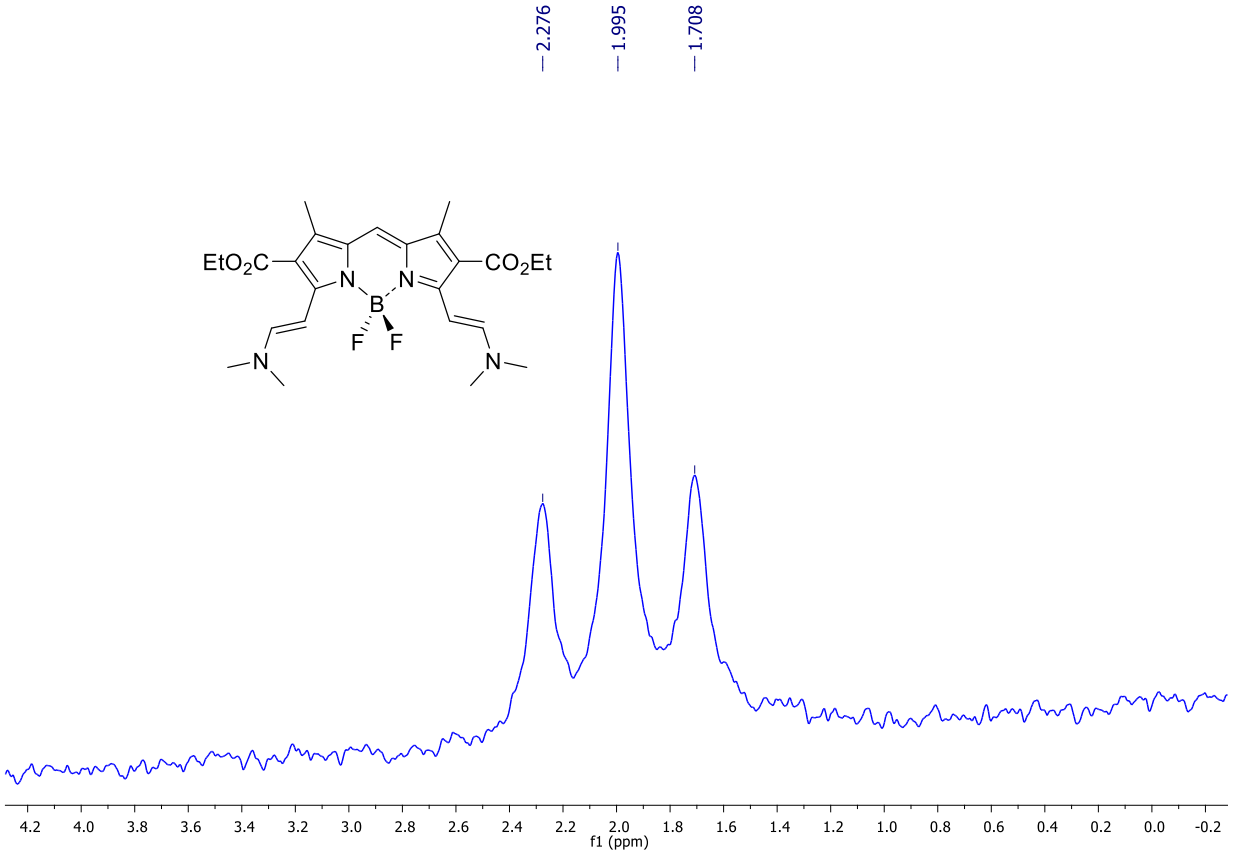

Figure S32. ^{11}B NMR spectrum of compound **9** in $CDCl_3$

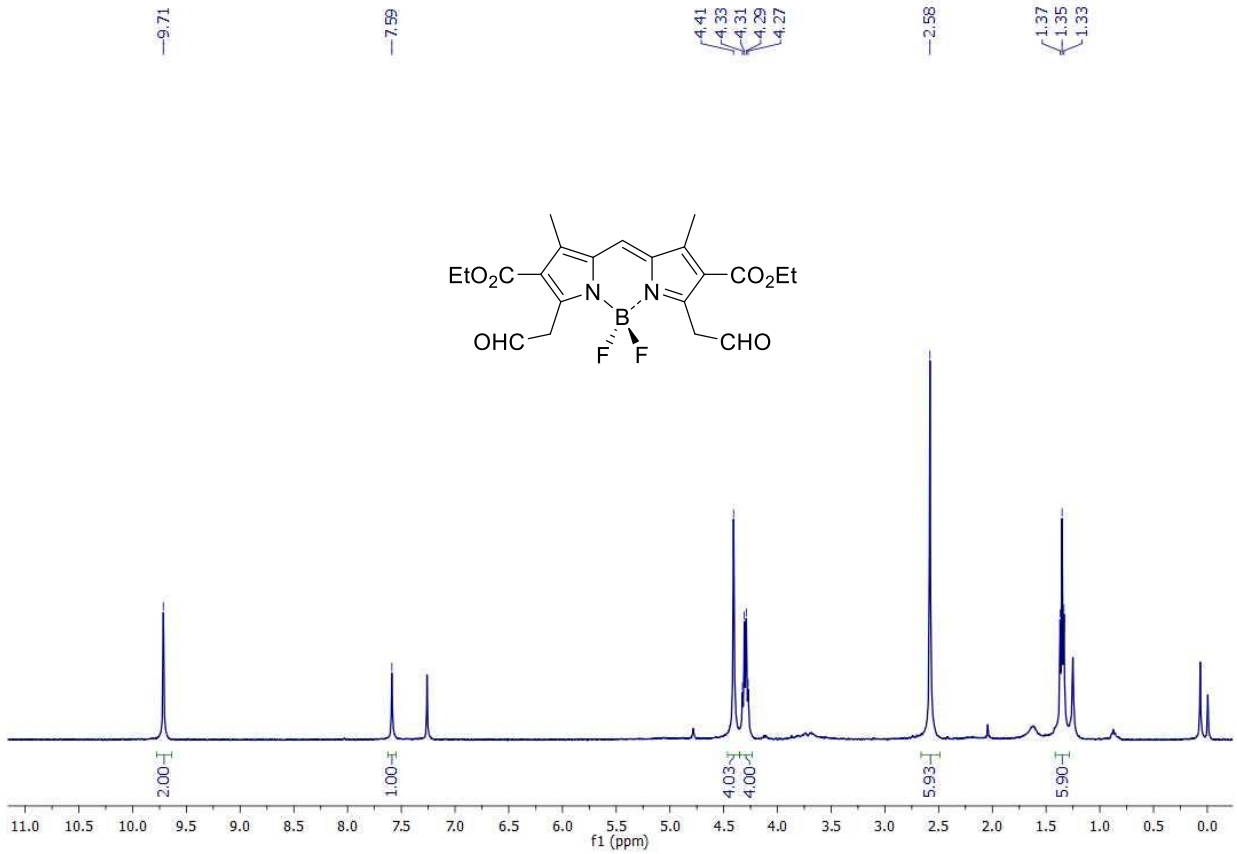

Figure S33. ^{1}H NMR spectrum of compound **10** in $CDCl_3$

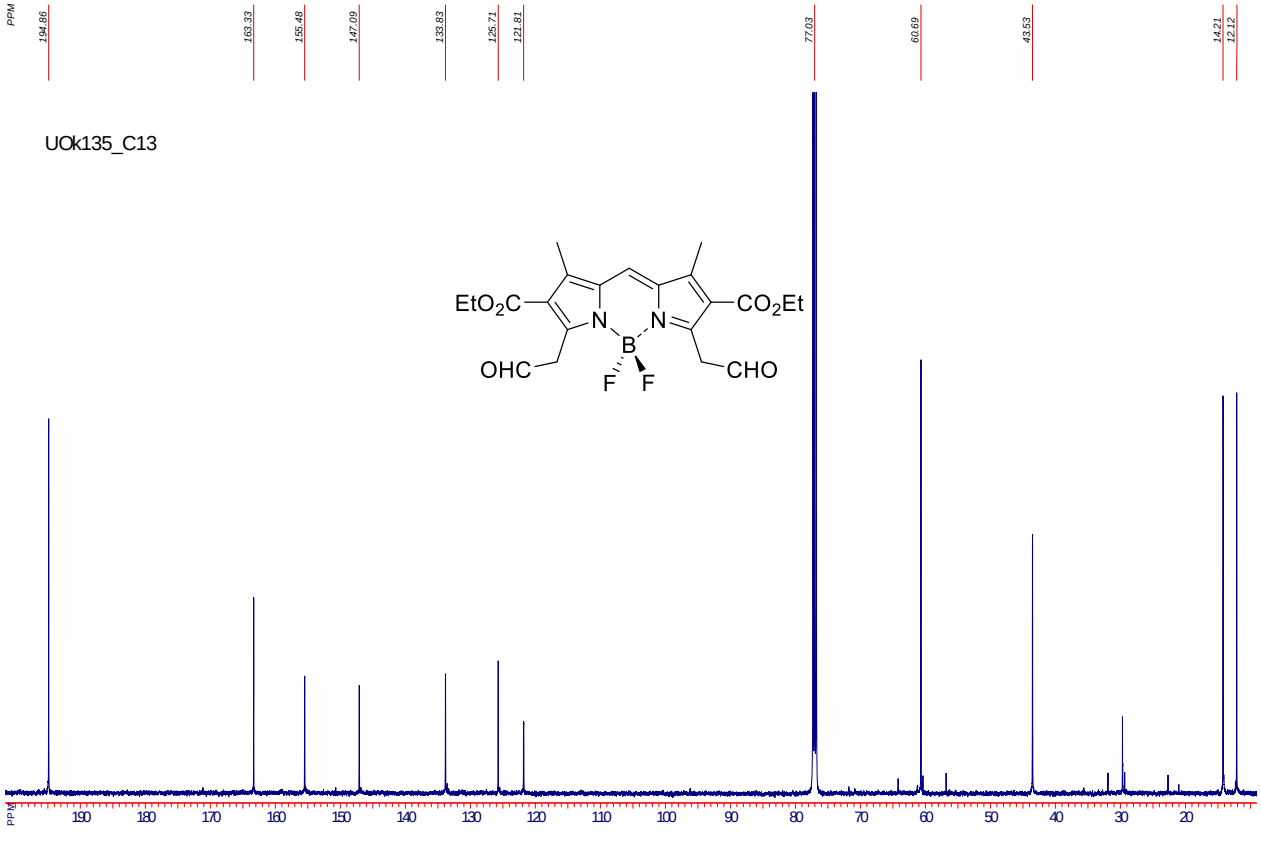

Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of compound **10** in $CDCl_3$

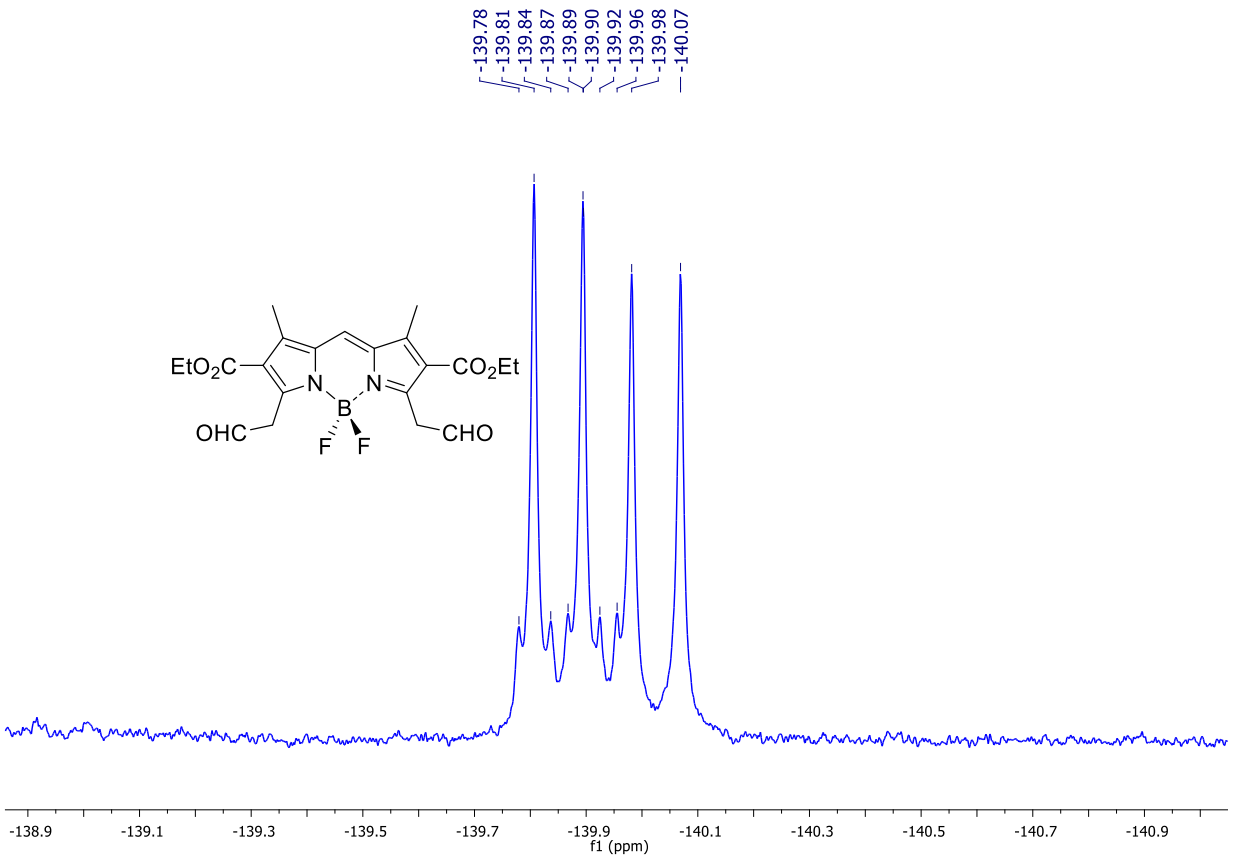

Figure S35. ^{19}F NMR spectrum of compound **10** in $CDCl_3$

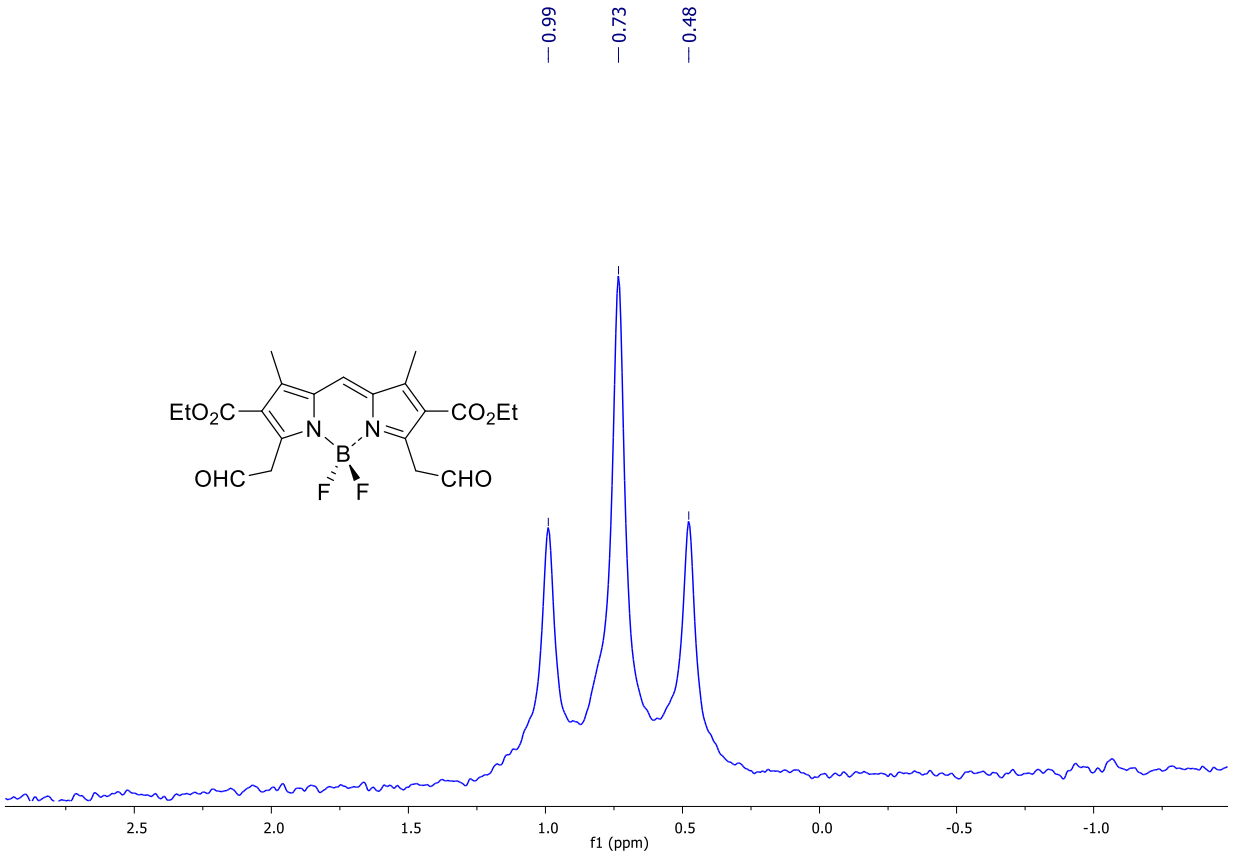

Figure S36. ^{11}B NMR spectrum of compound **10** in $CDCl_3$

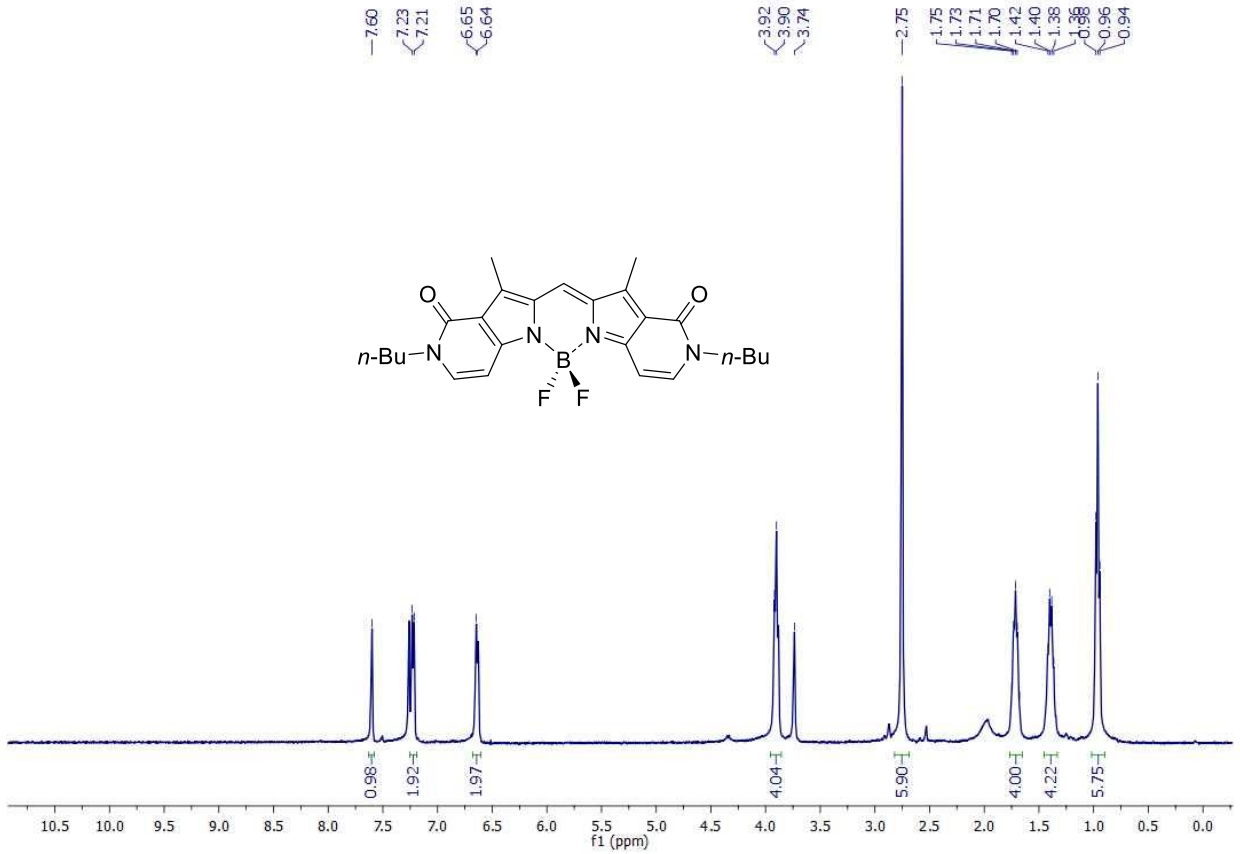

Figure S37. ^{1}H NMR spectrum of compound **11** in $CDCl_3$

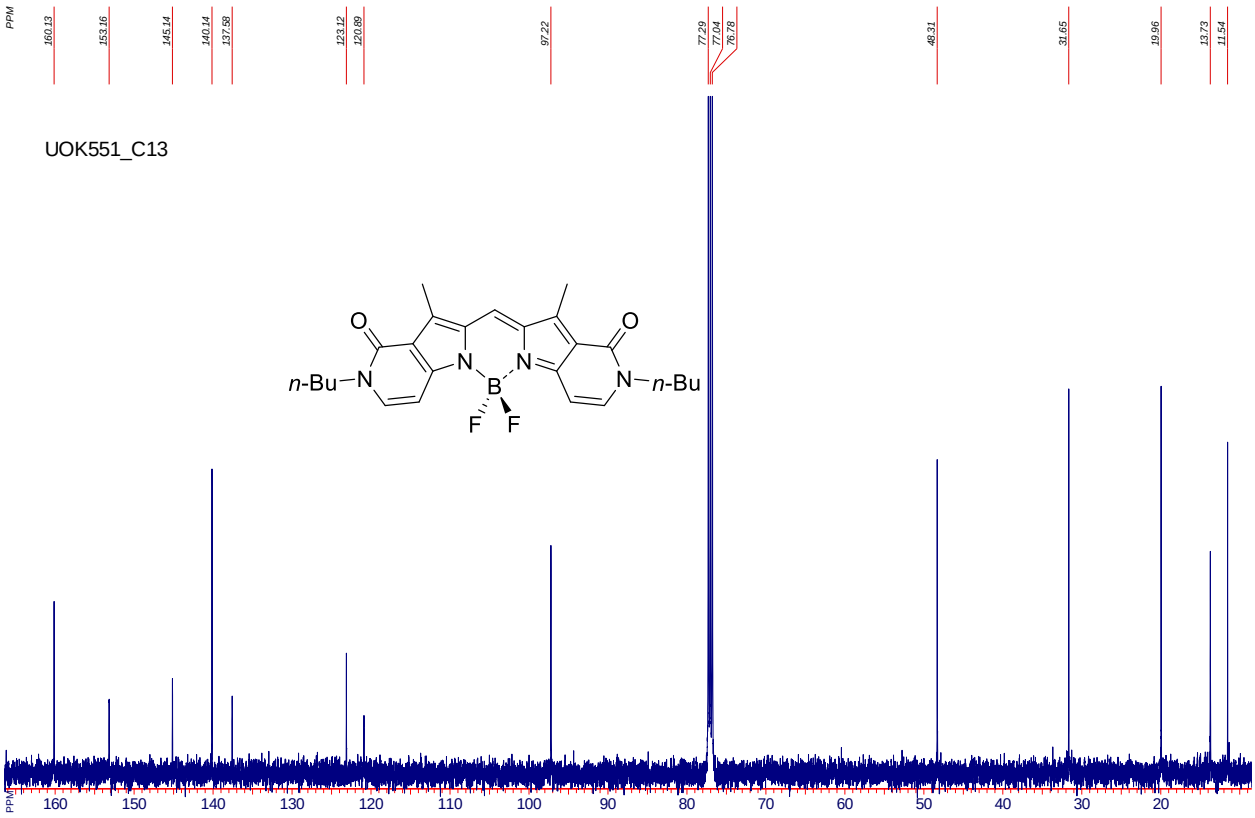

Figure S38. ^{13}C{^{1}H} NMR spectrum of compound **11** in $CDCl_3$

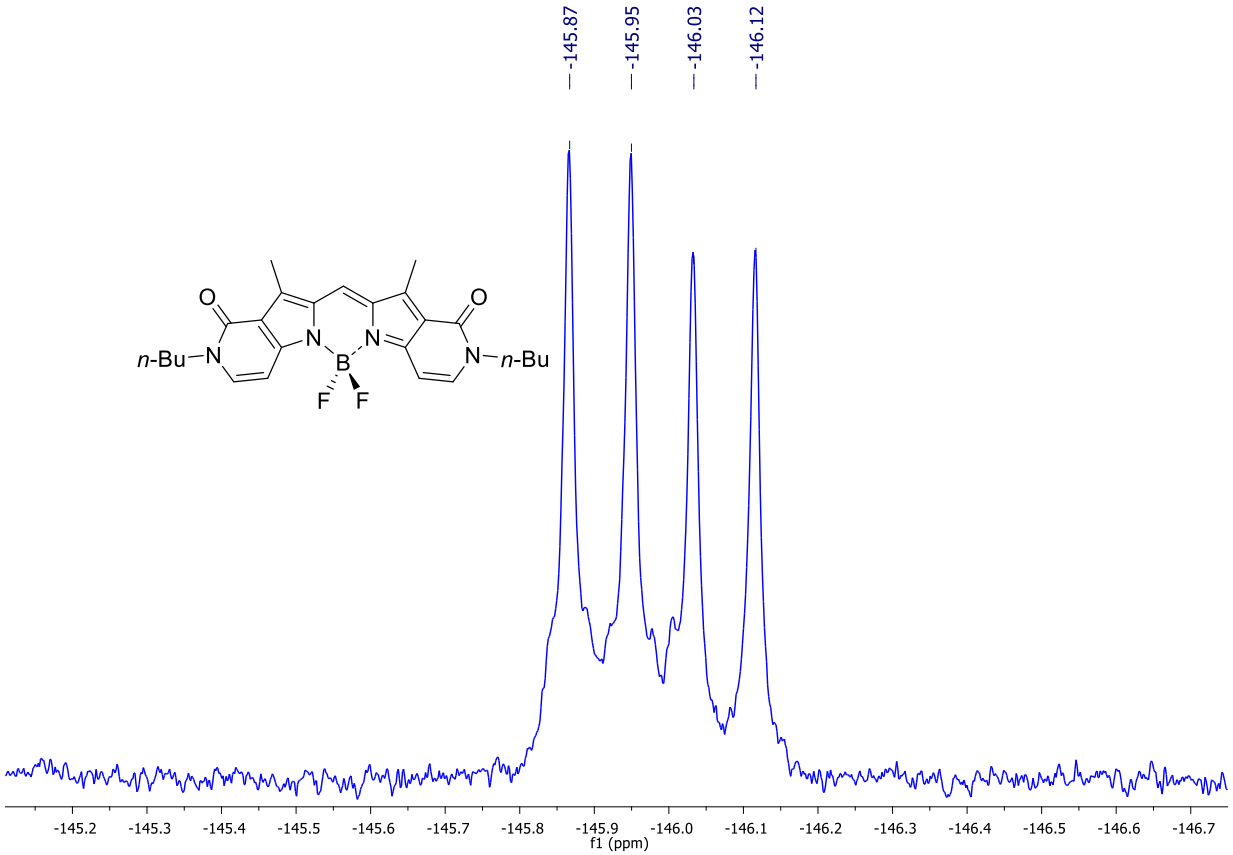

Figure S39. ^{19}F NMR spectrum of compound **11** in $CDCl_3$

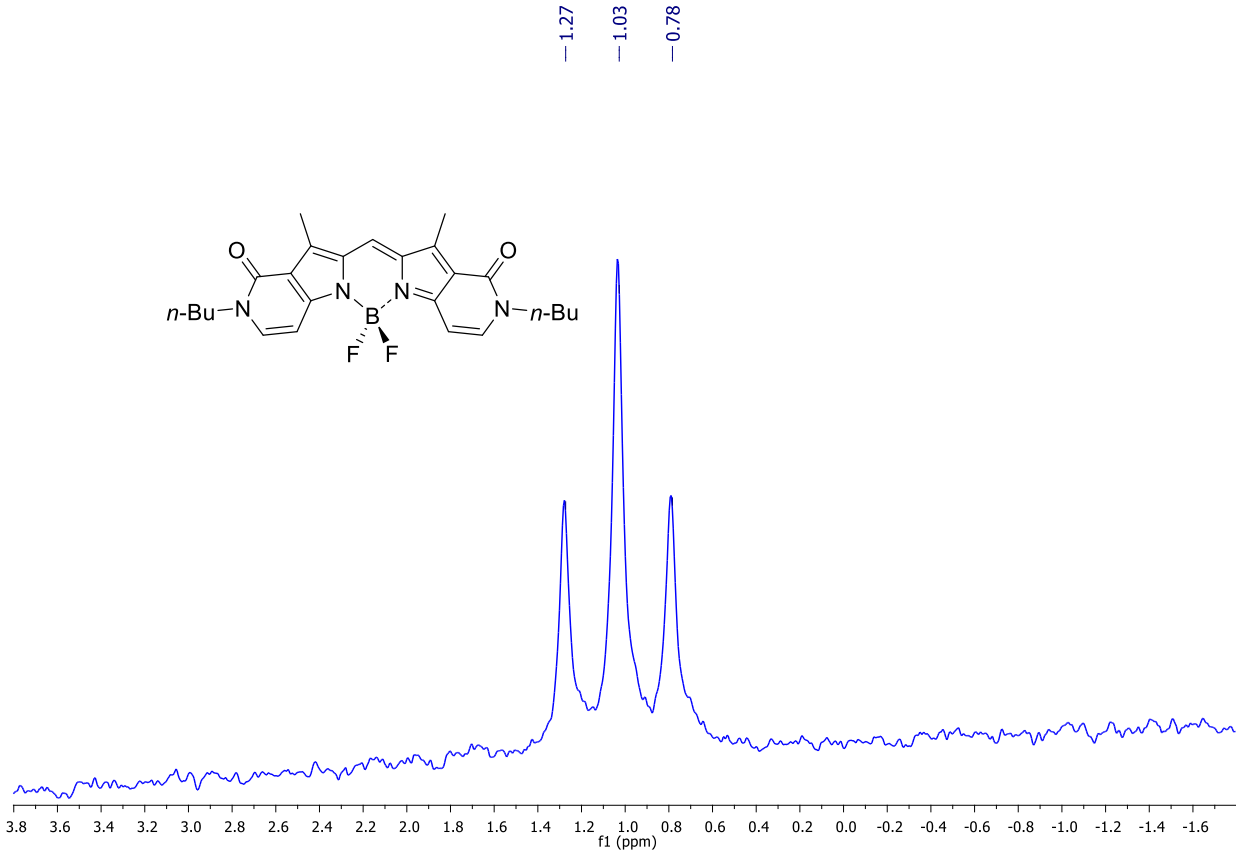

Figure S40. ^{11}B NMR spectrum of compound **11** in $CDCl_3$

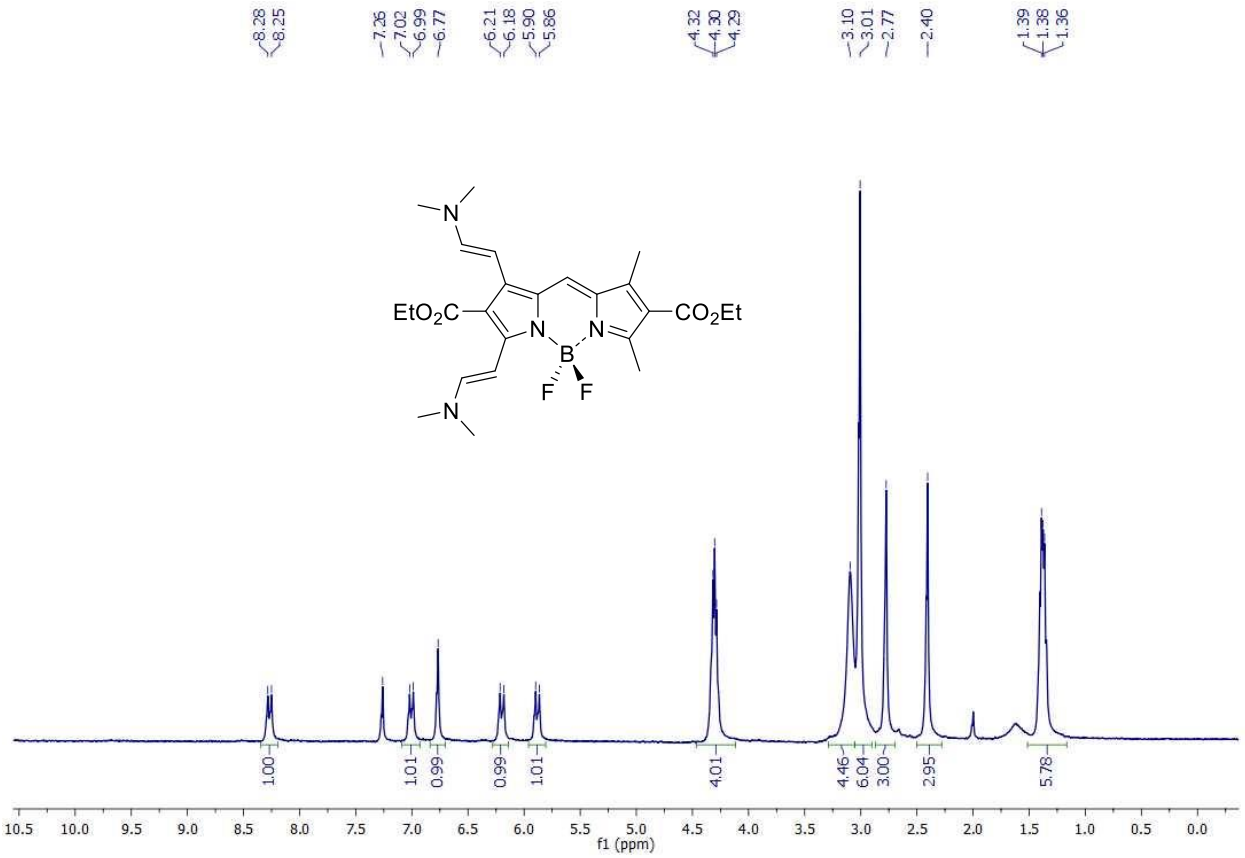

Figure S41. ^{1}H NMR spectrum of compound **12** in $CDCl_3$

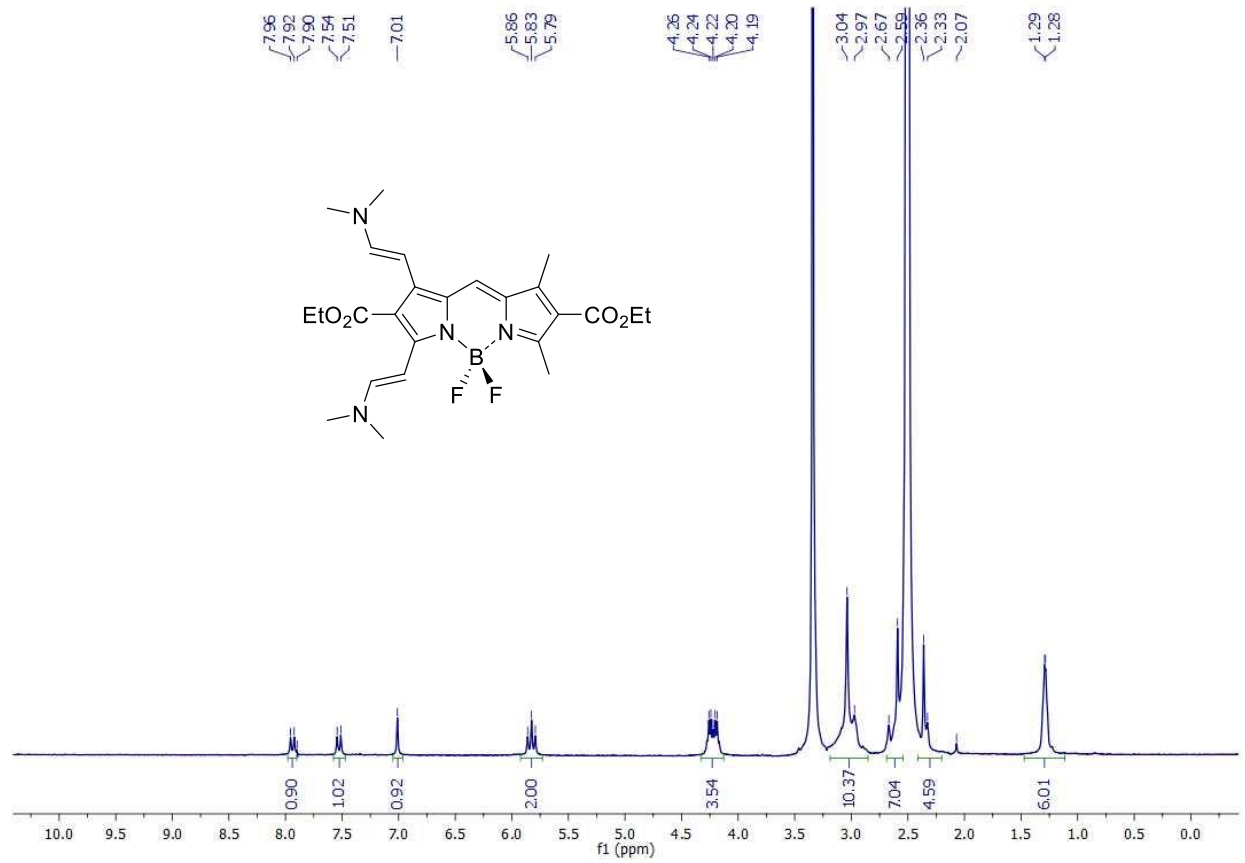

Figure S41a. ^{1}H NMR spectrum of compound **12** in DMSO-d_6

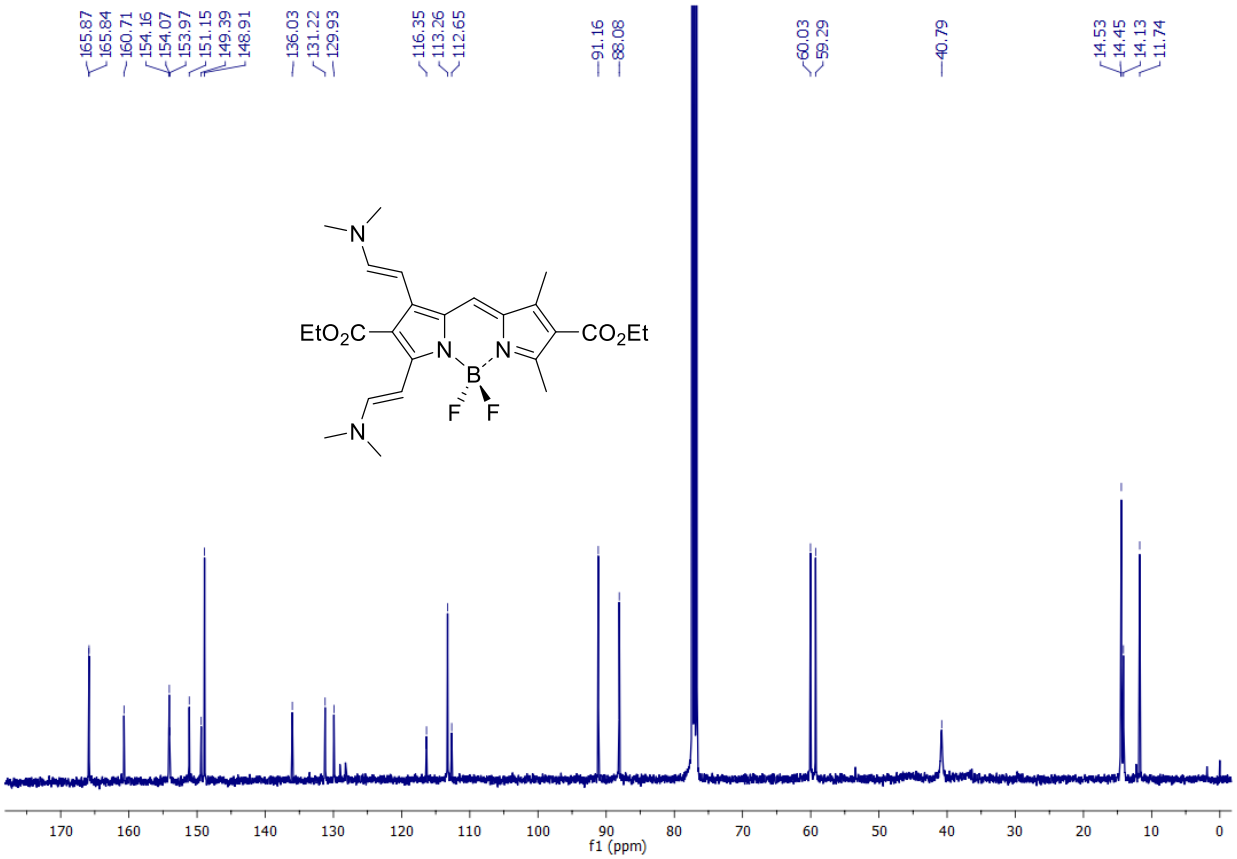

Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of compound **12** in $CDCl_3$

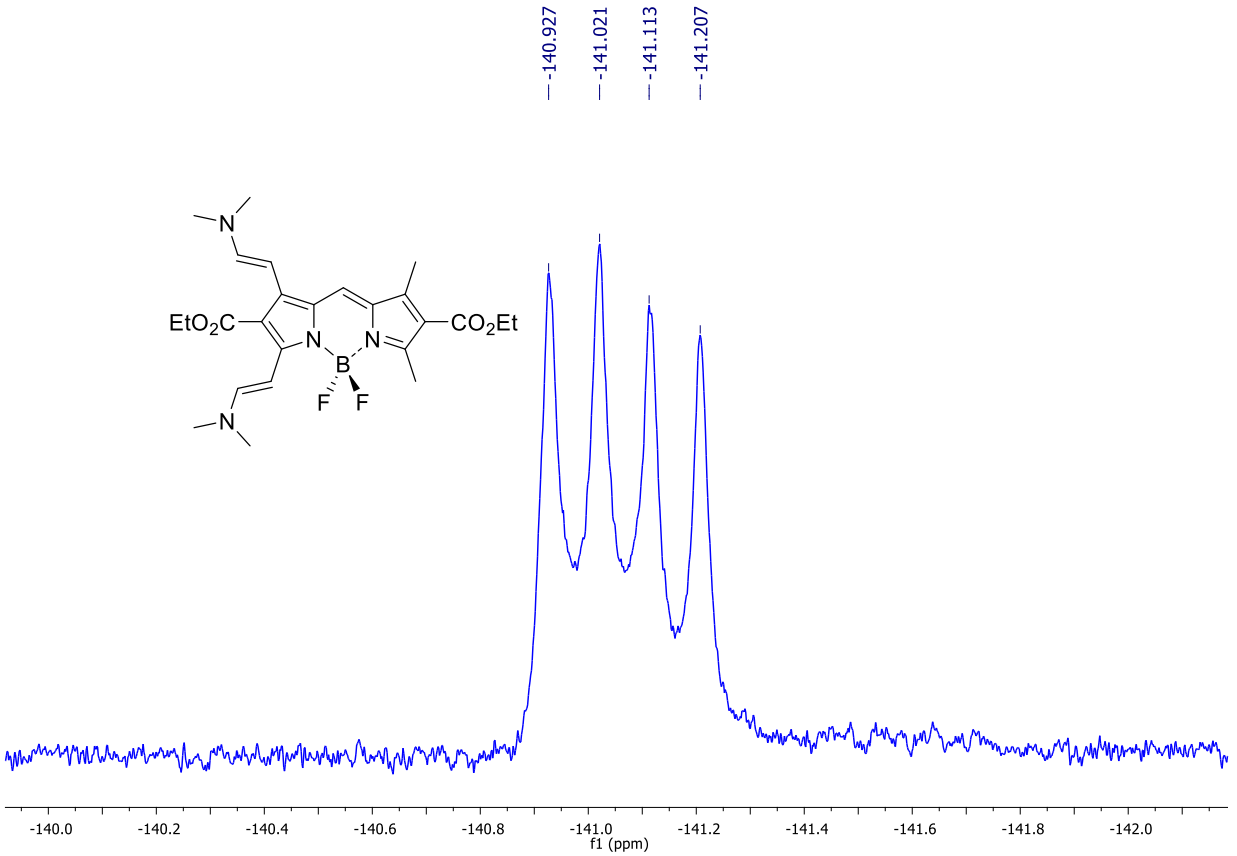

Figure S43. ^{19}F NMR spectrum of compound **12** in $CDCl_3$

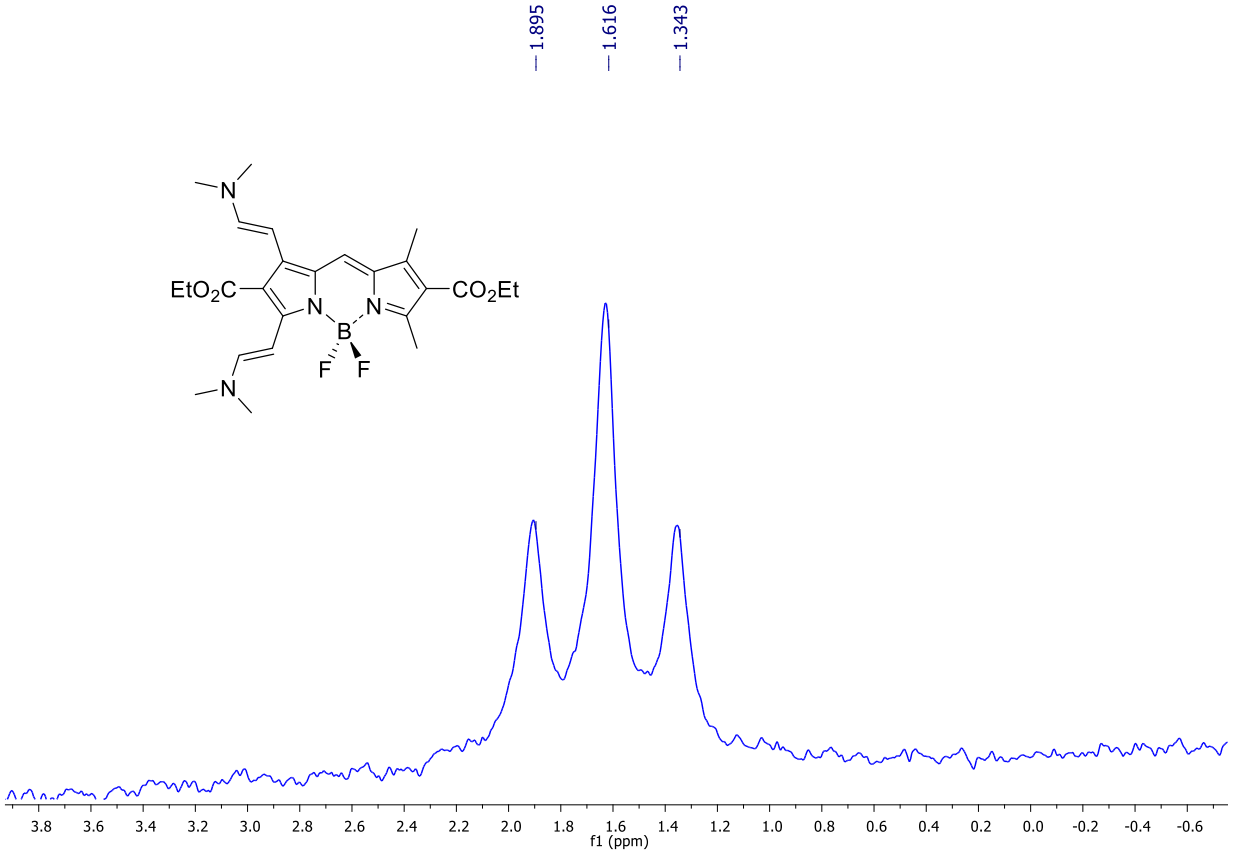

Figure S44. ^{11}B NMR spectrum of compound **12** in $CDCl_3$

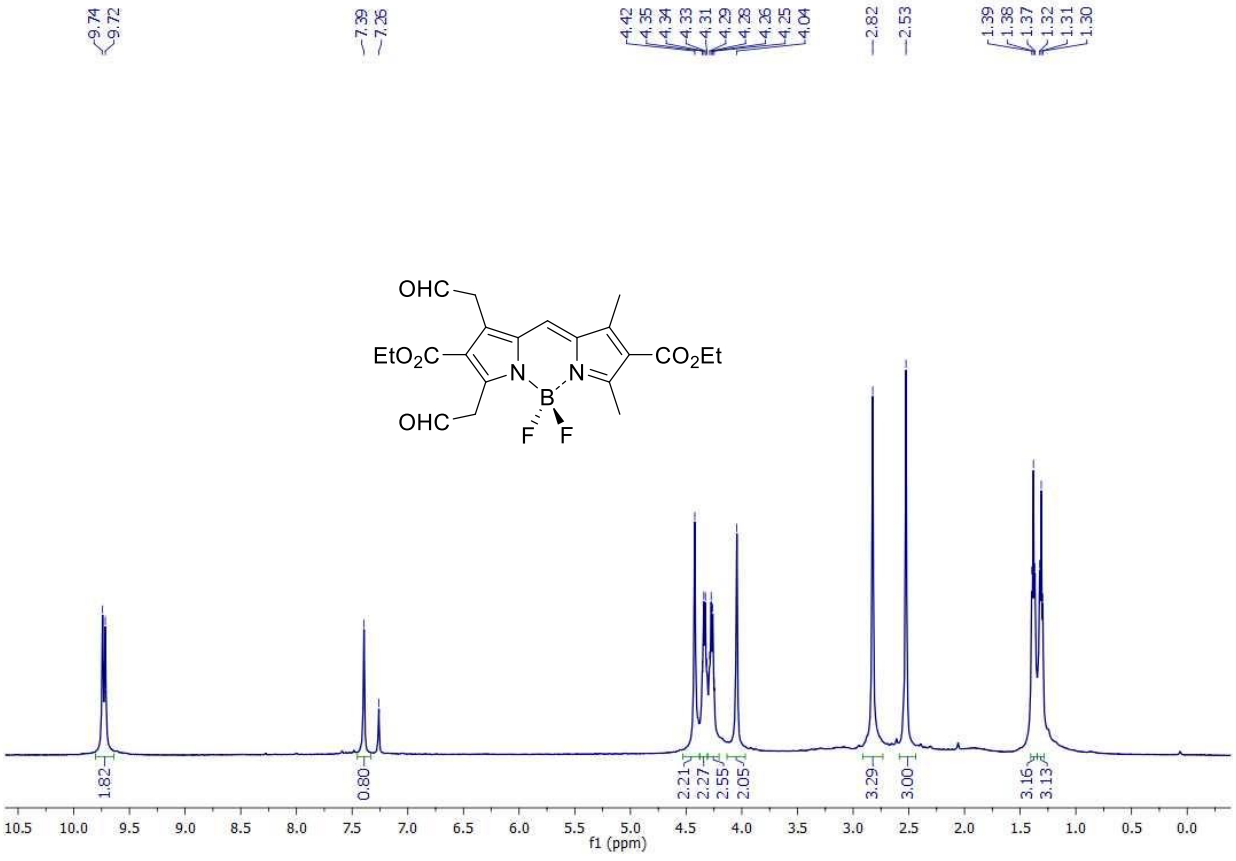

Figure S45. ^{1}H NMR spectrum of compound **13** in $CDCl_3$

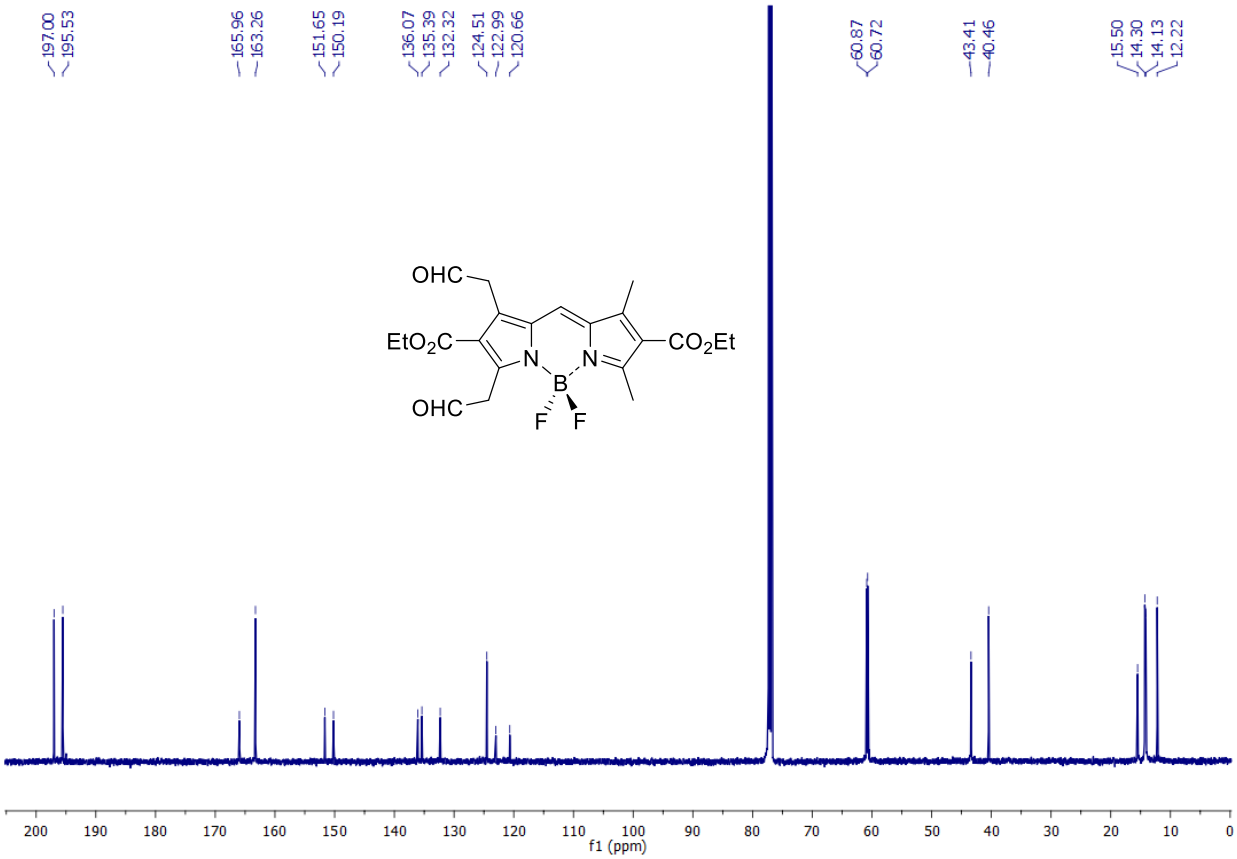

Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum of compound **13** in $CDCl_3$

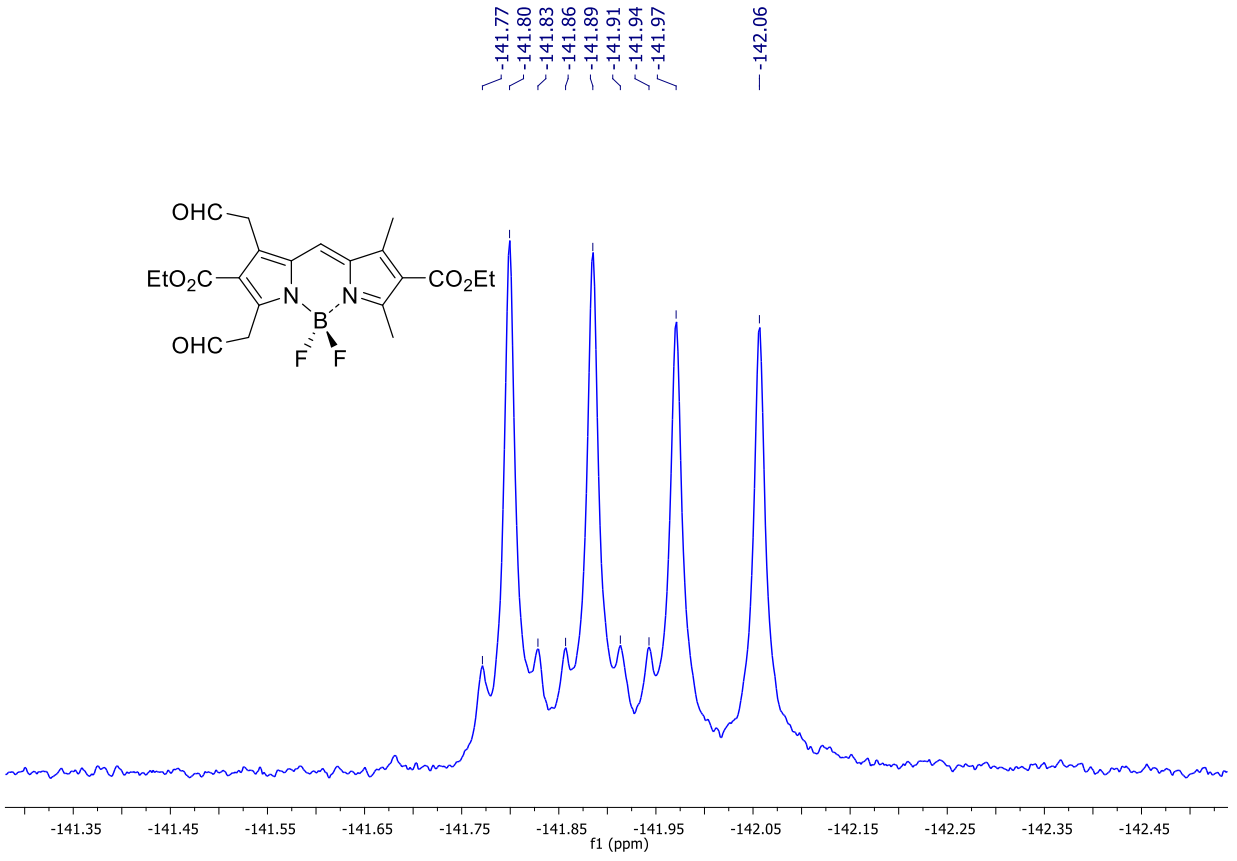

Figure S47. ^{19}F NMR spectrum of compound **13** in $CDCl_3$

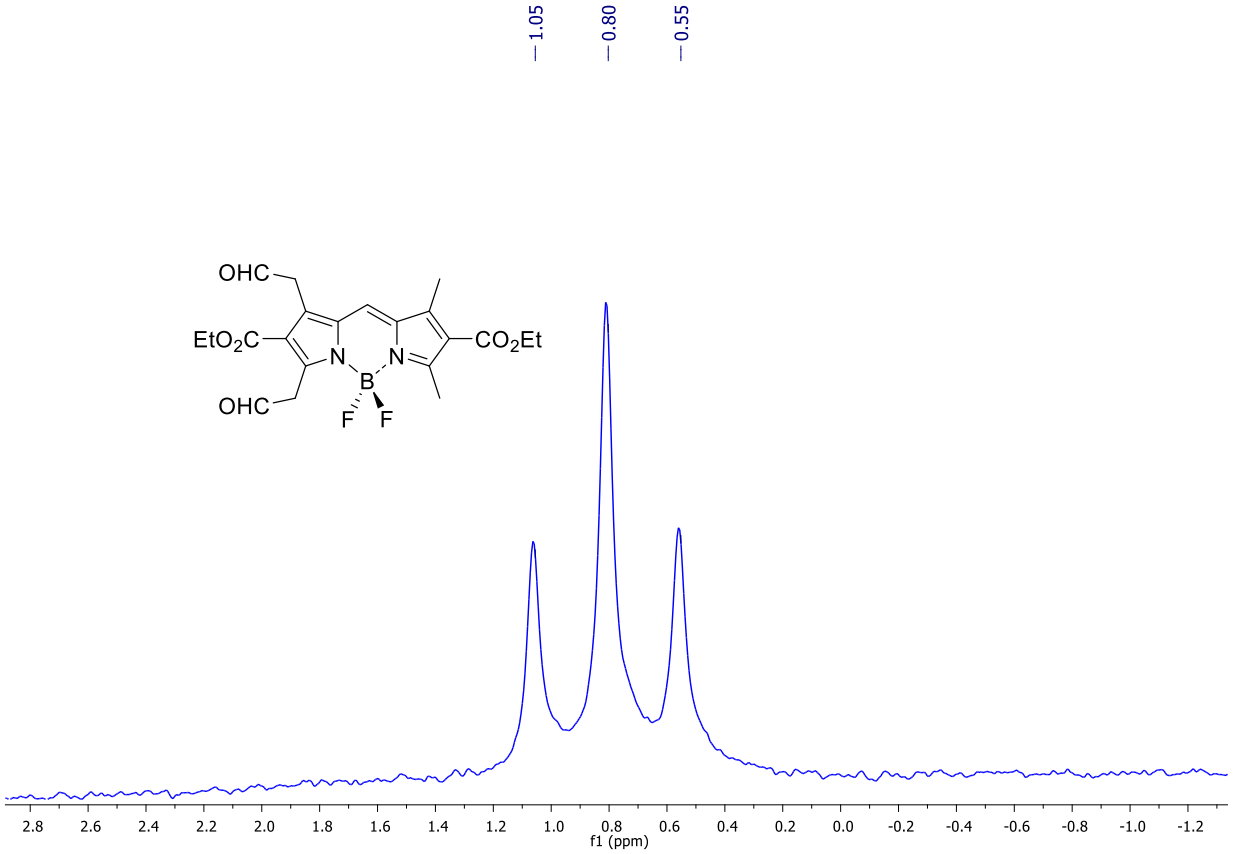

Figure S48. ^{11}B NMR spectrum of compound **13** in $CDCl_3$

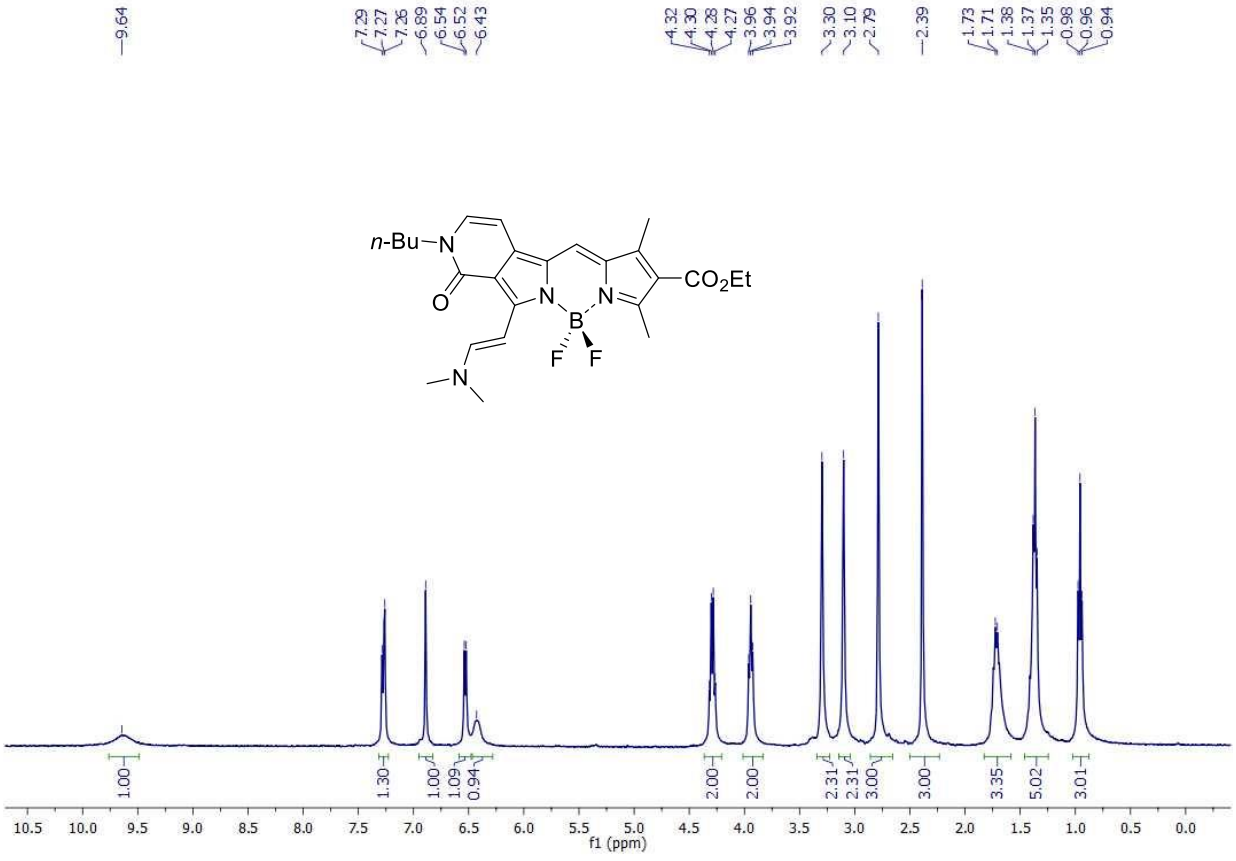

Figure S49. ^{1}H NMR spectrum of compound **14** in $CDCl_3$

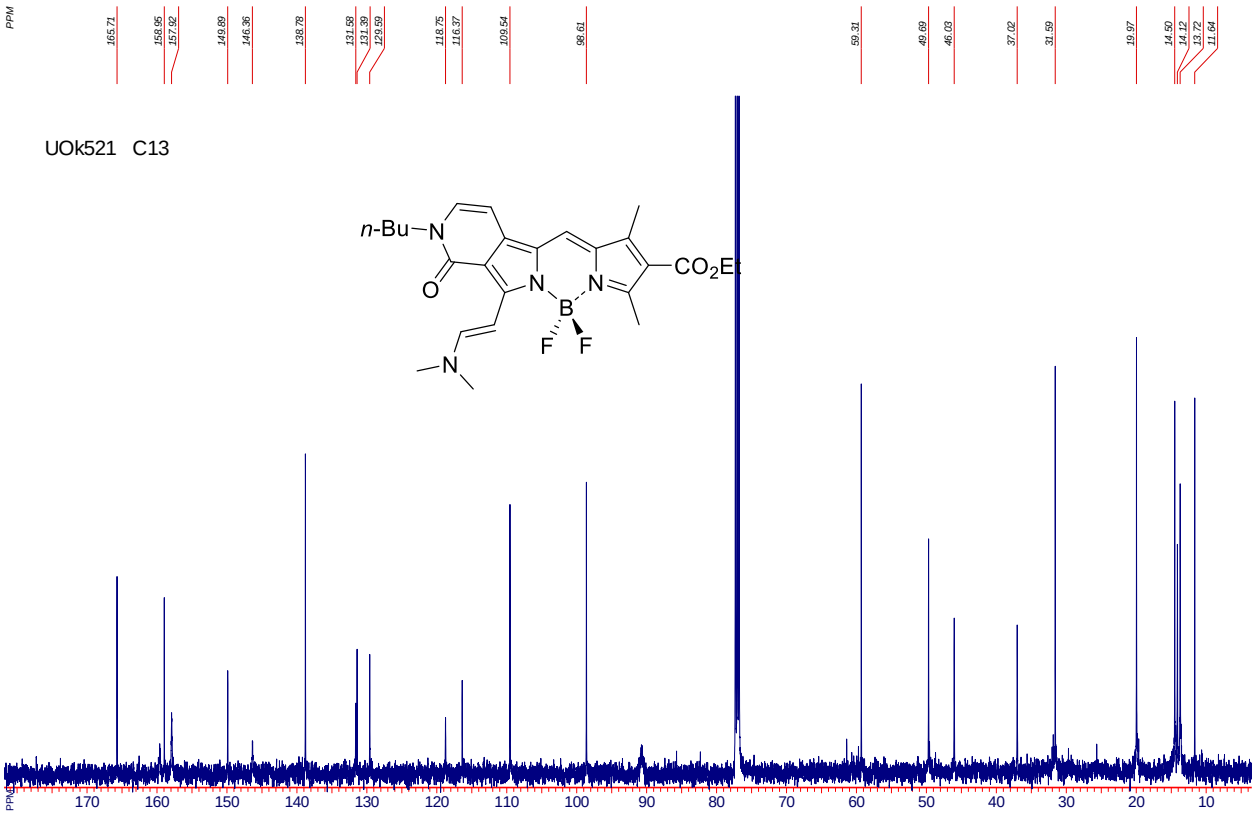

Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of compound **14** in $CDCl_3$

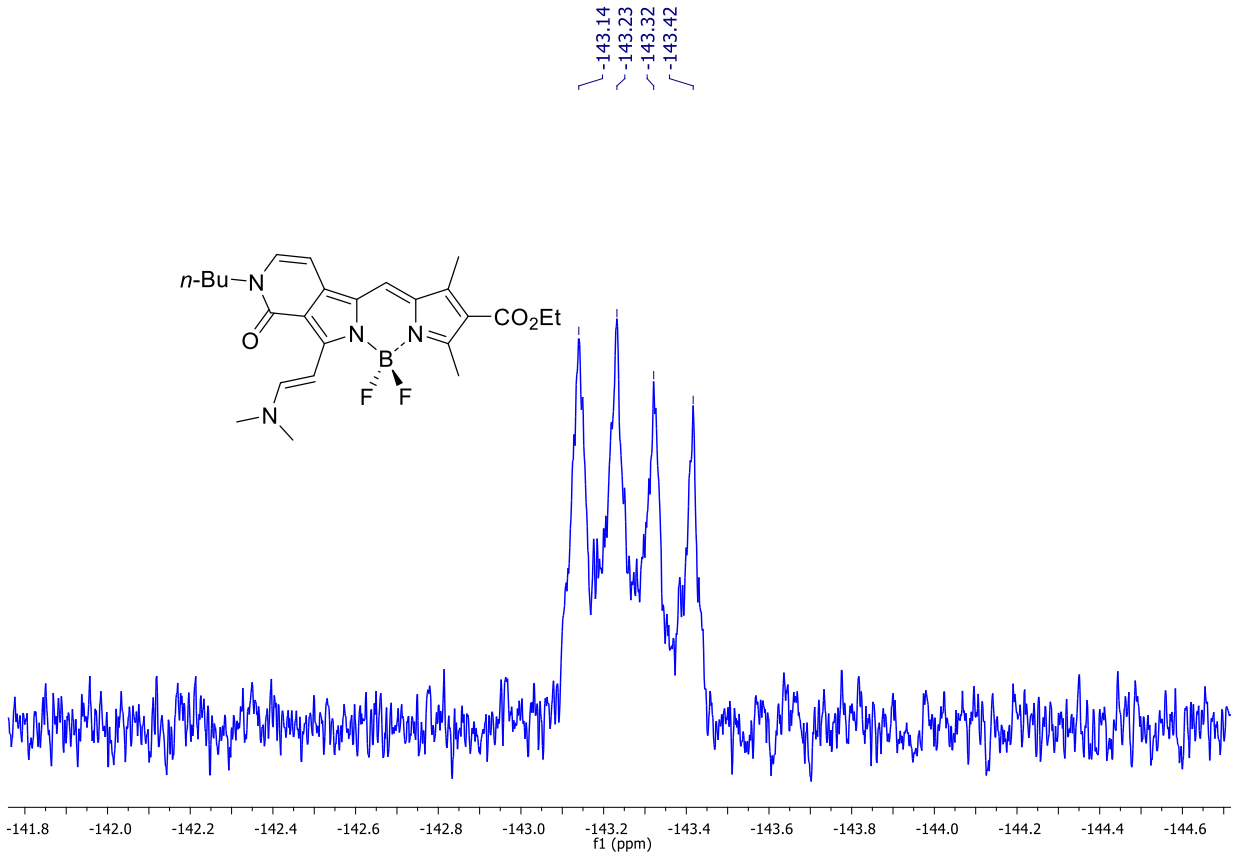

Figure S51. ^{19}F NMR spectrum of compound **14** in $CDCl_3$

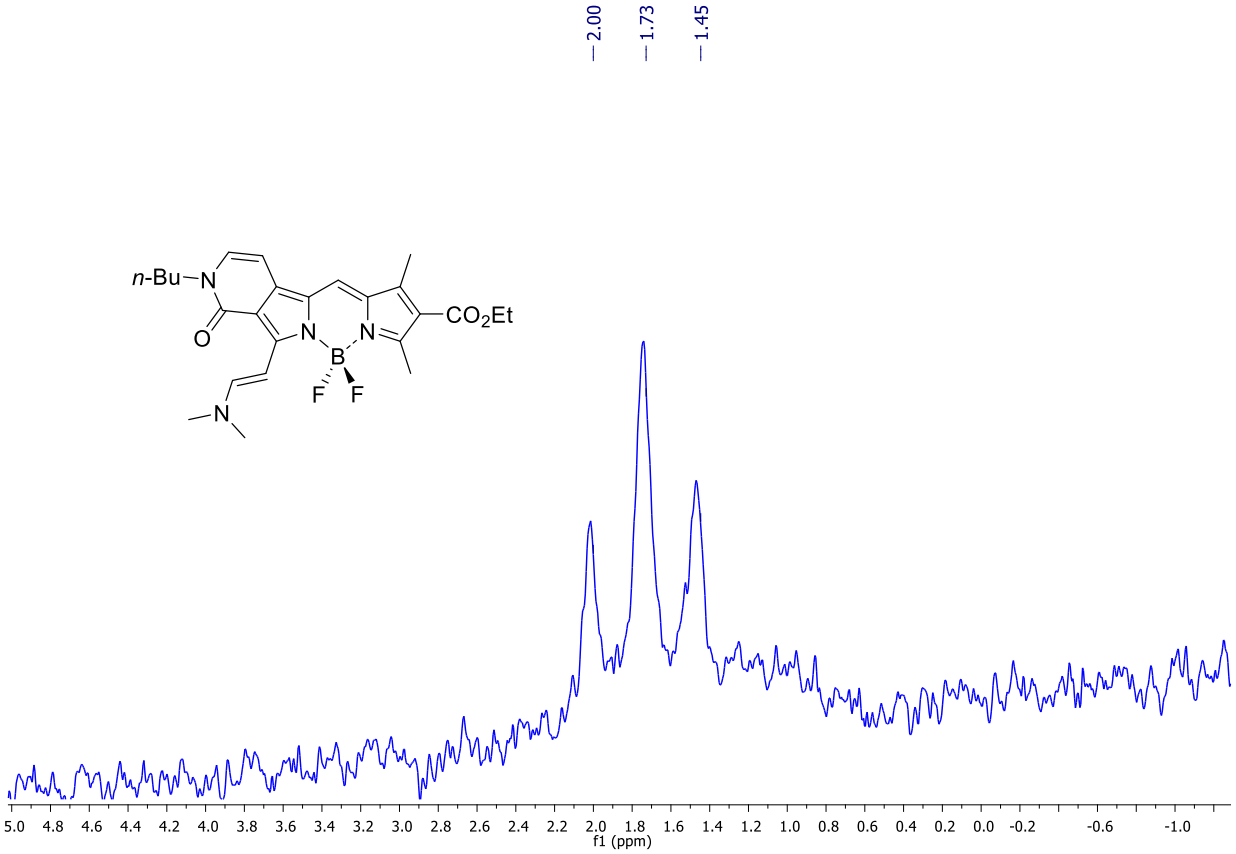

Figure S52. ^{11}B NMR spectrum of compound **14** in $CDCl_3$

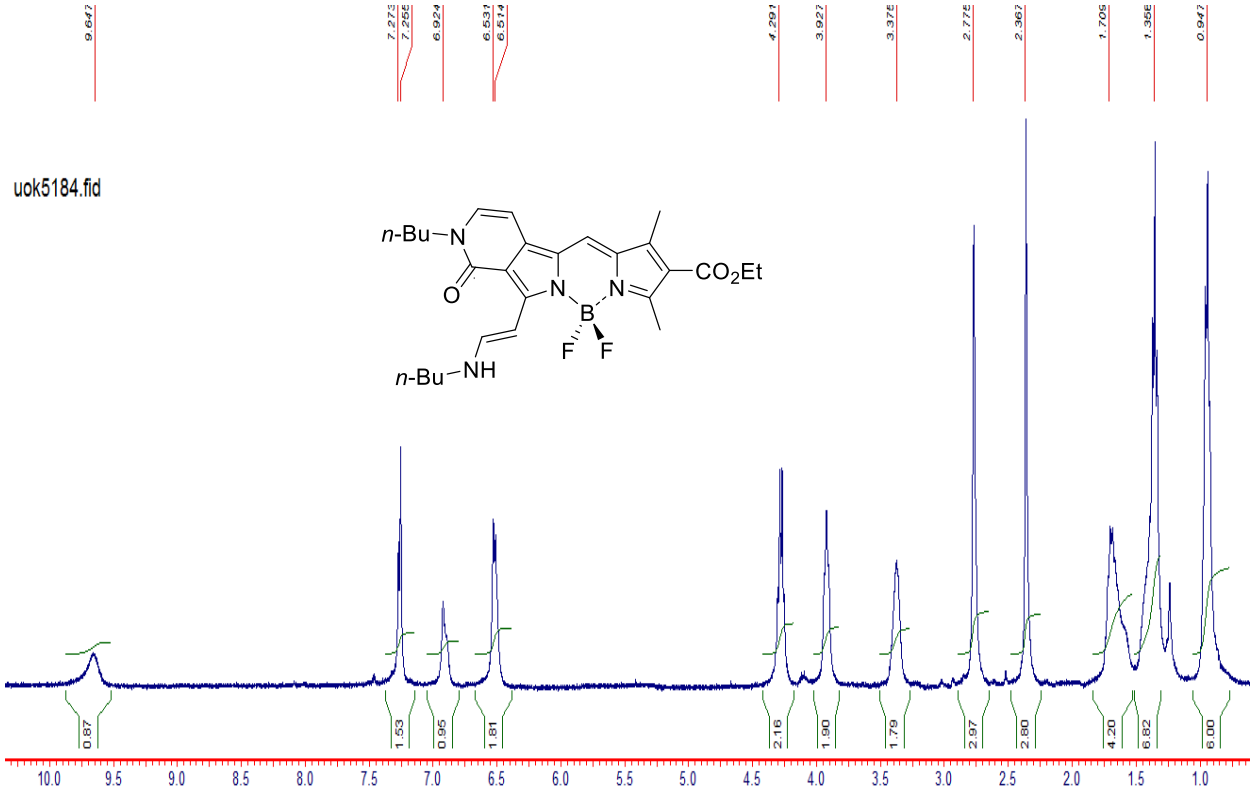

Figure S53. ^{1}H NMR spectrum of compound **15** in $CDCl_3$

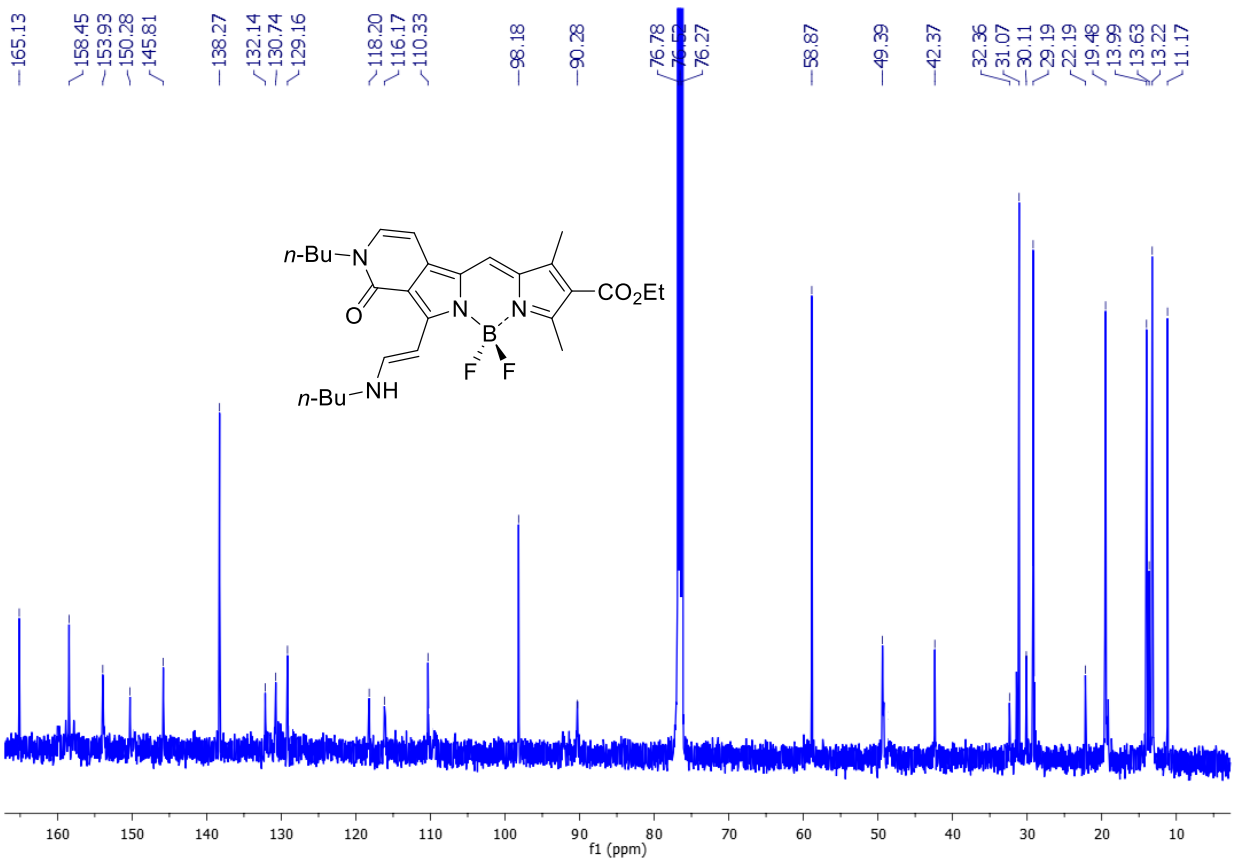

Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of compound **15** in $CDCl_3$

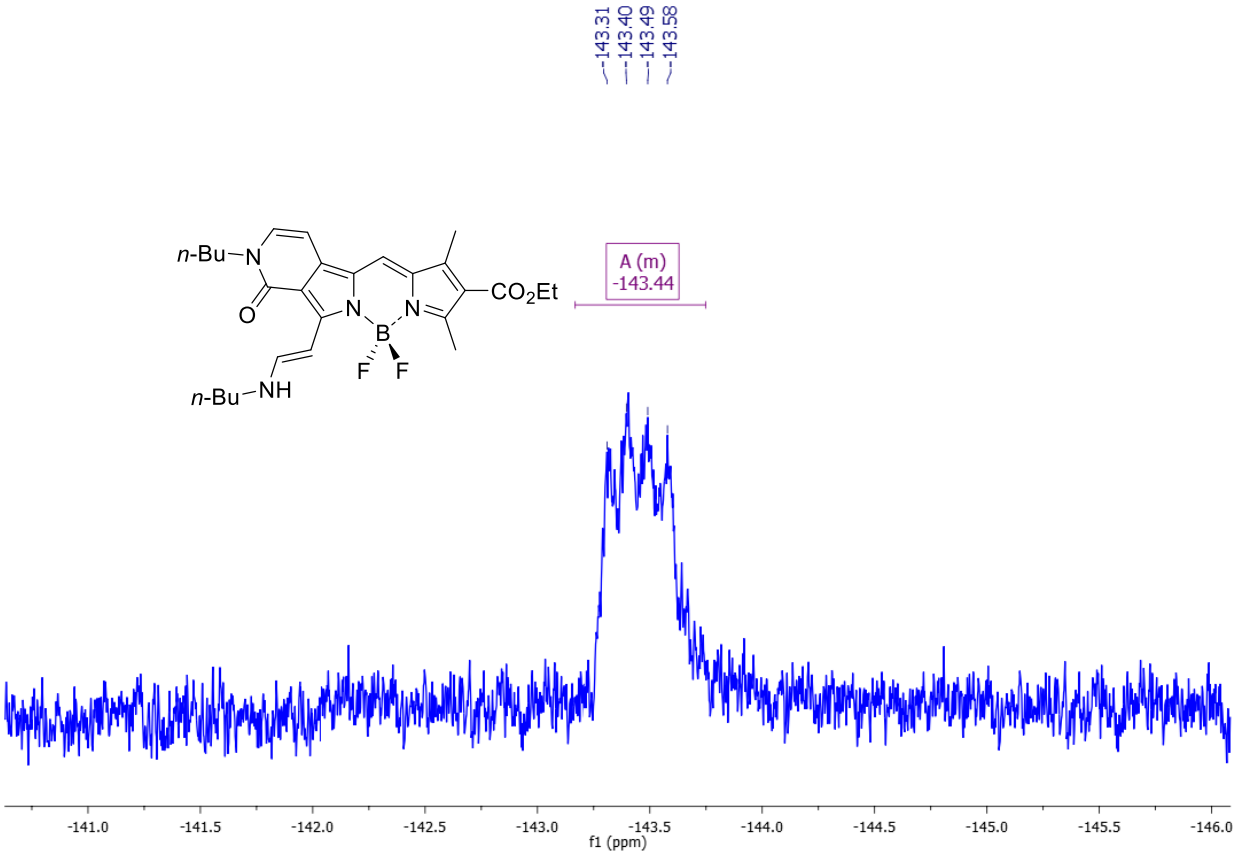

Figure S55. ^{19}F NMR spectrum of compound **15** in $CDCl_3$

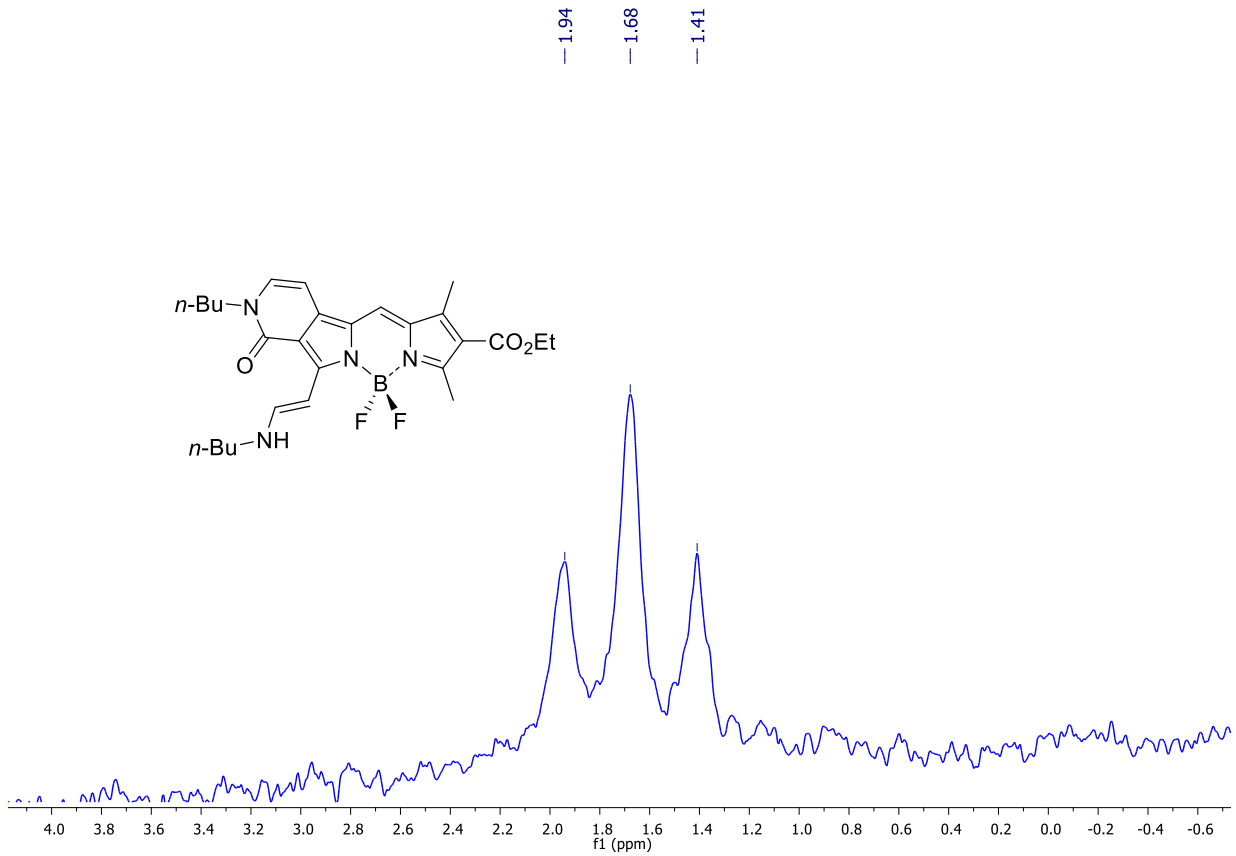

Figure S56. ^{11}B NMR spectrum of compound **15** in $CDCl_3$

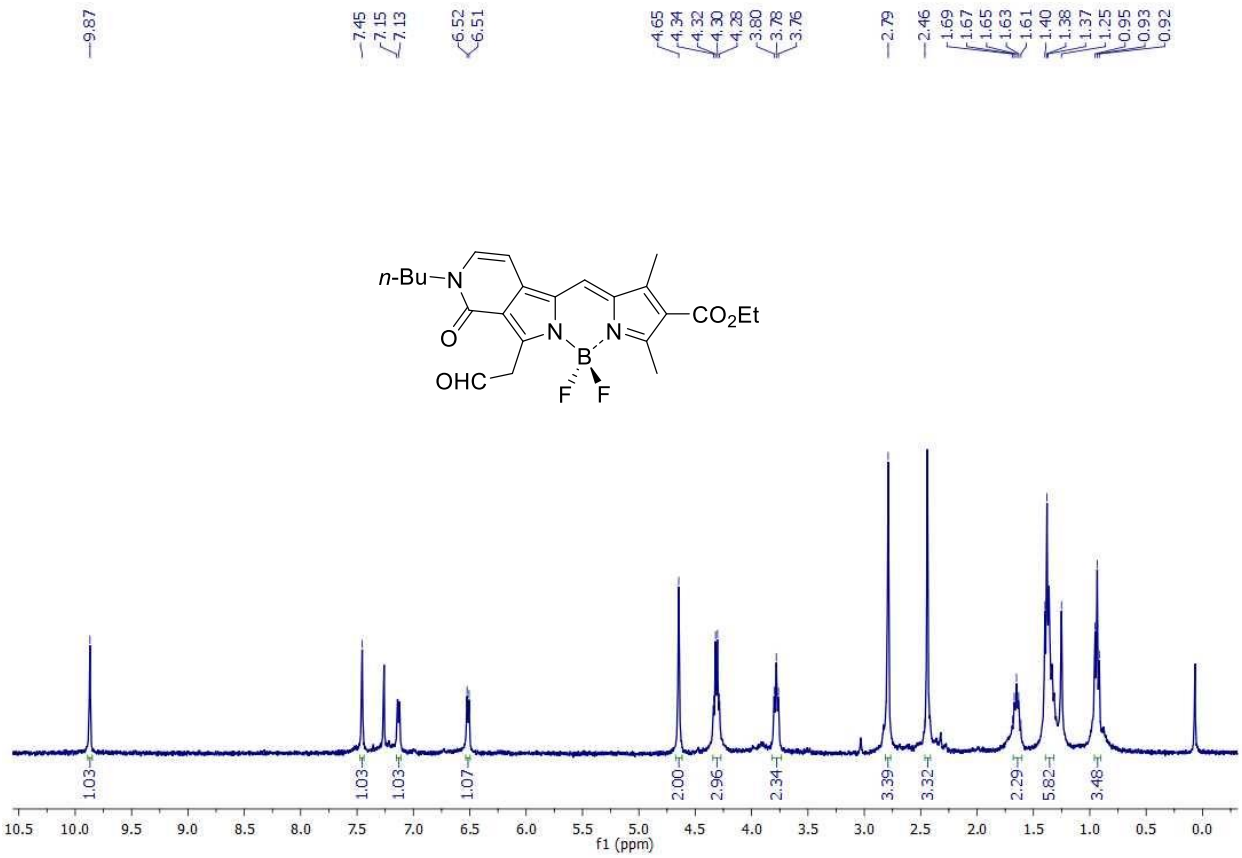

Figure S57. ^{1}H NMR spectrum of compound **16** in $CDCl_3$

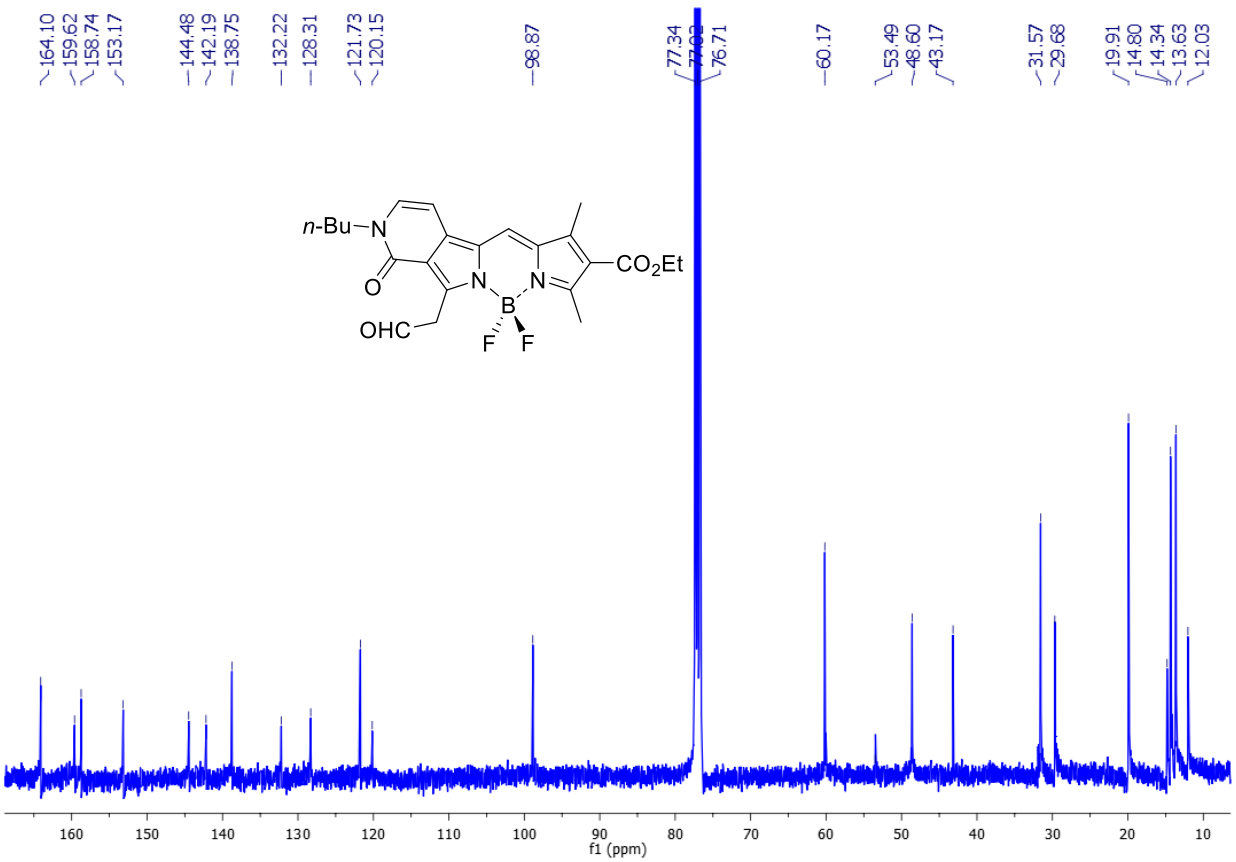

Figure S58. $^{13}C\{^{1}H\}$ NMR spectrum of compound **16** in $CDCl_3$

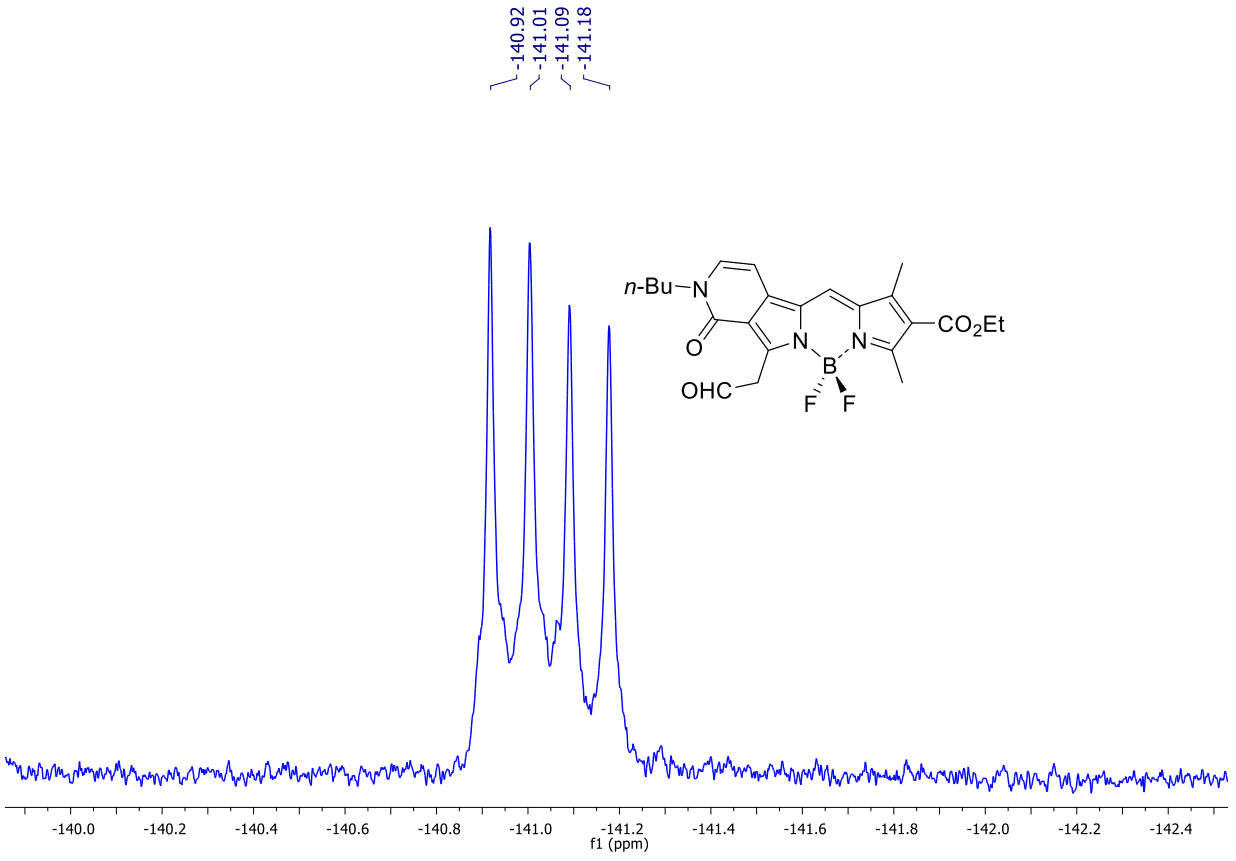

Figure S59. ^{19}F NMR spectrum of compound **16** in $CDCl_3$

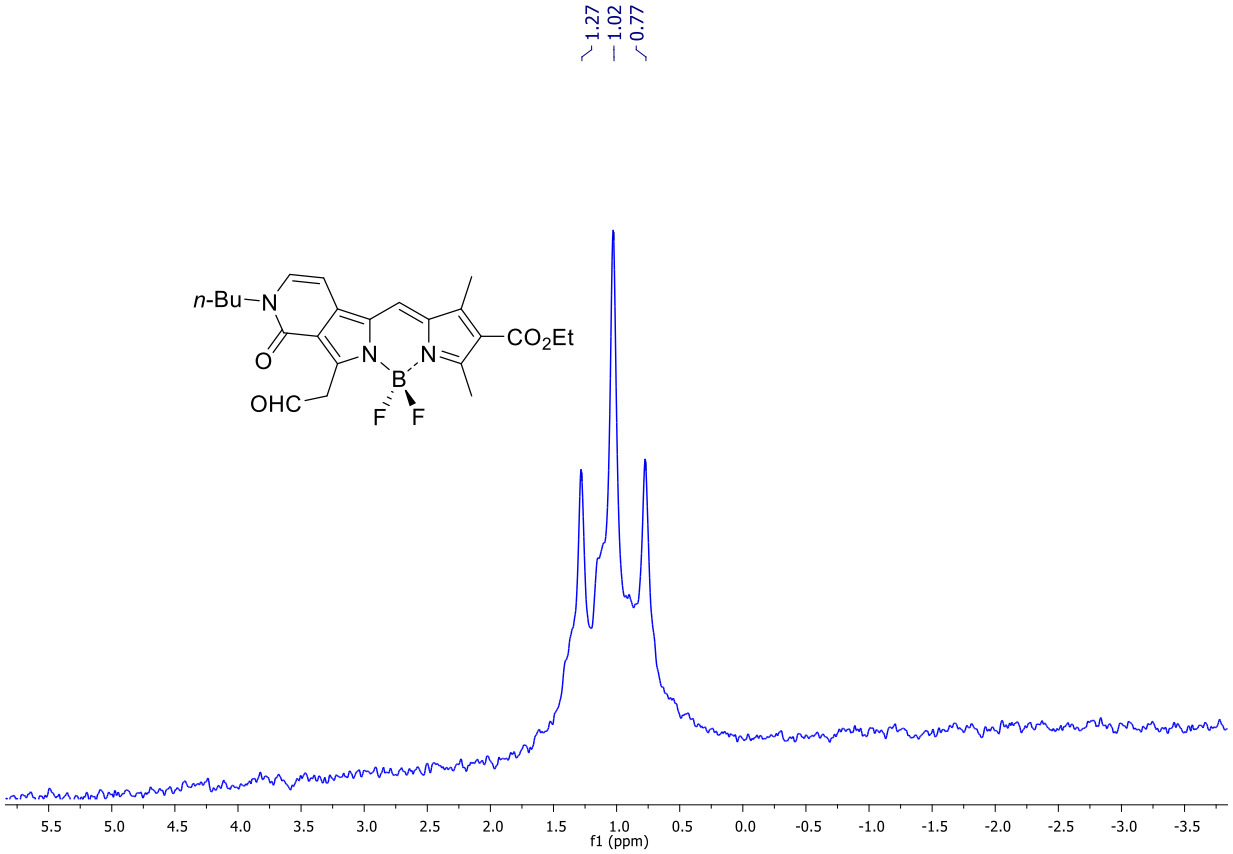

Figure S60. ^{11}B NMR spectrum of compound **16** in $CDCl_3$

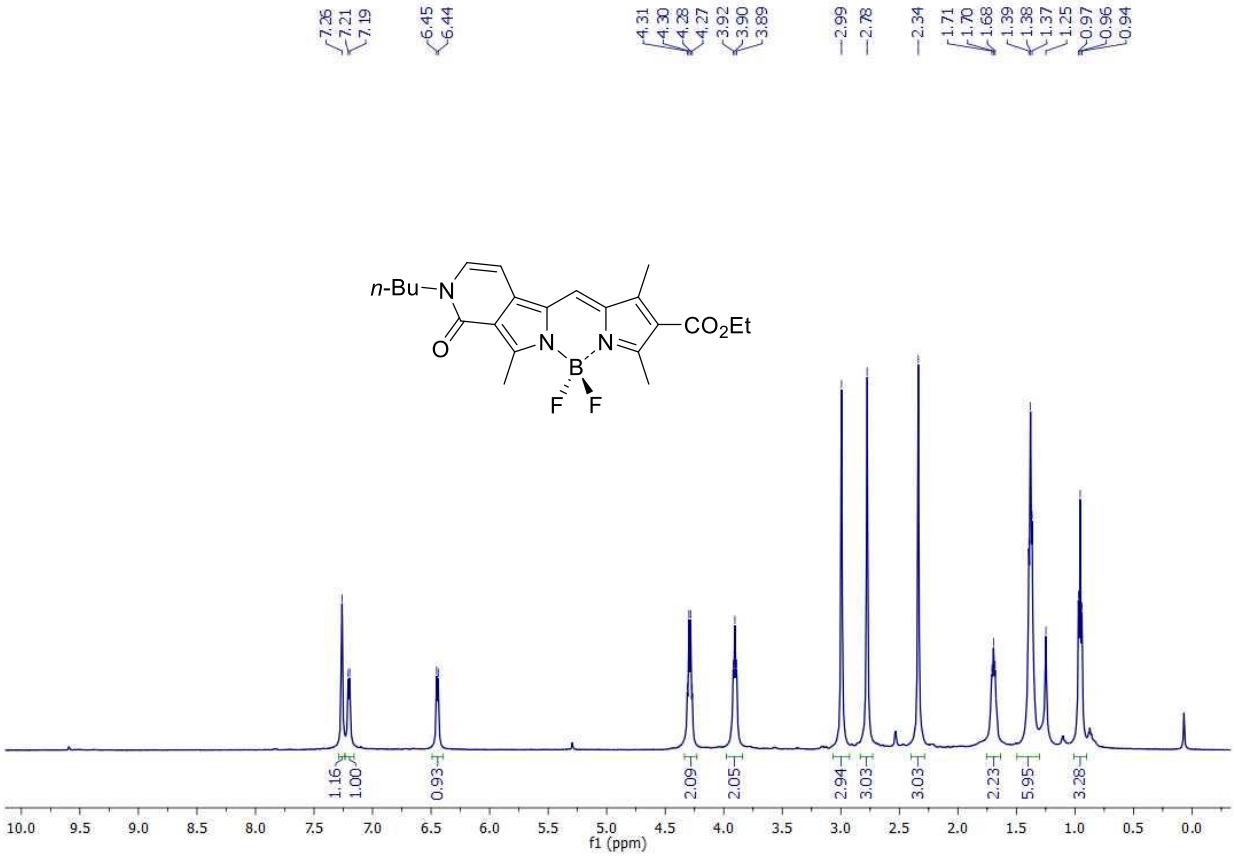

Figure S61. ^{1}H NMR spectrum of compound **17** in $CDCl_3$

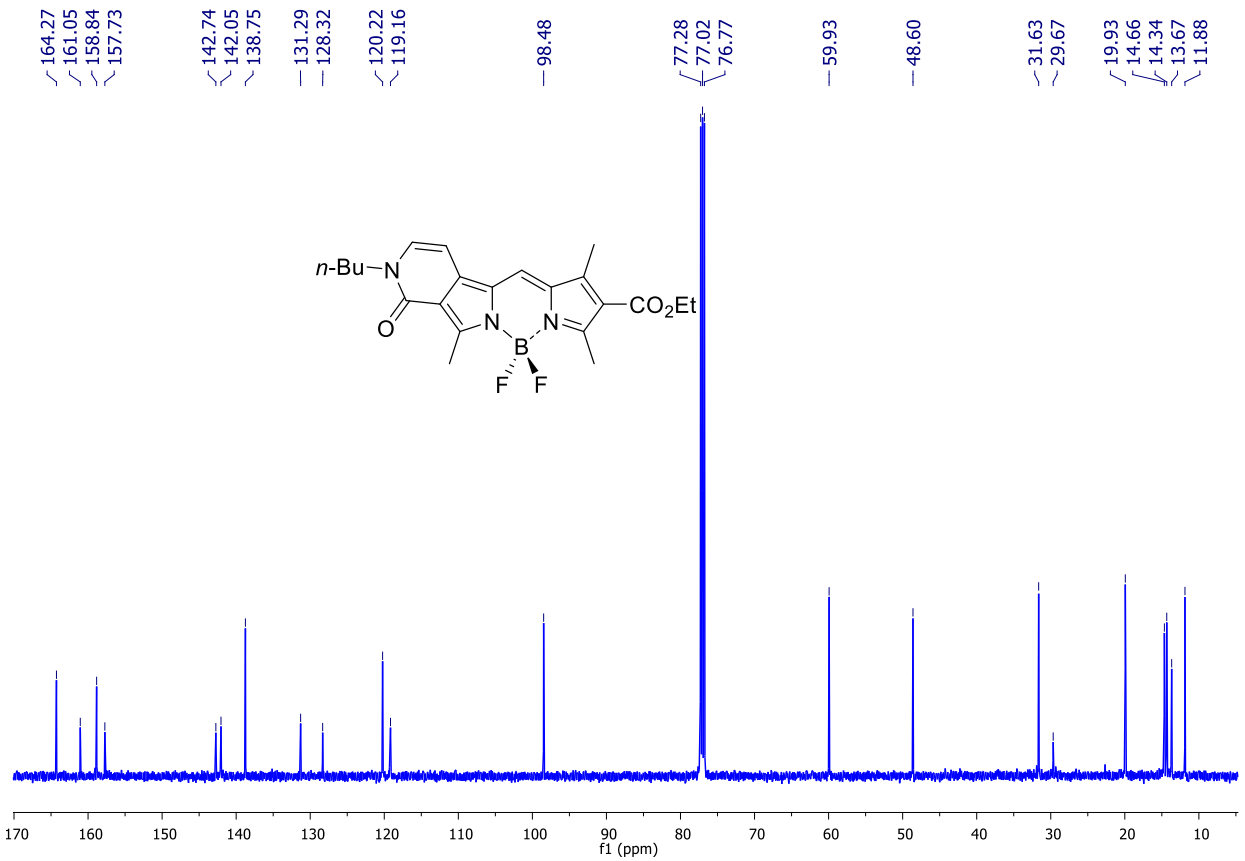

Figure S62. $^{13}C\{^{1}H\}$ NMR spectrum of compound **17** in $CDCl_3$

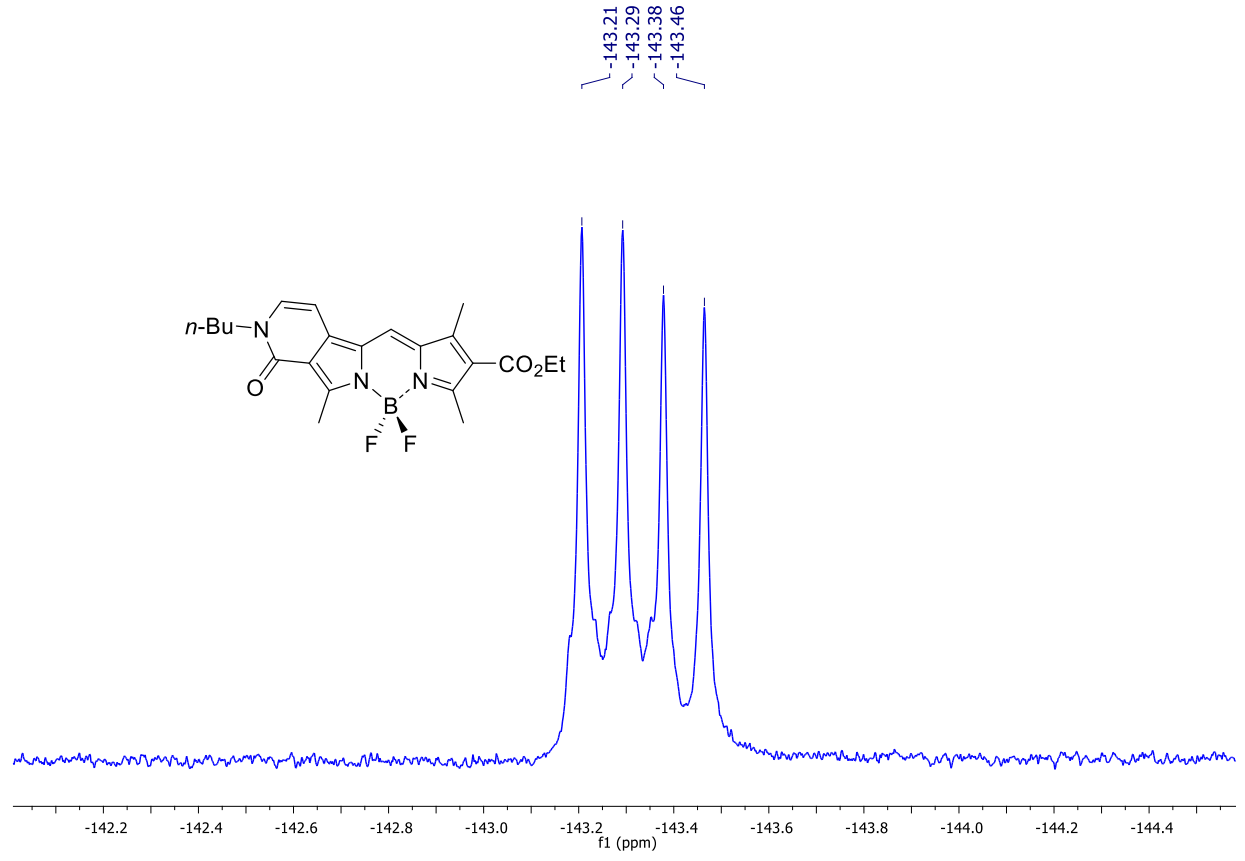

Figure S63. ^{19}F NMR spectrum of compound **17** in $CDCl_3$

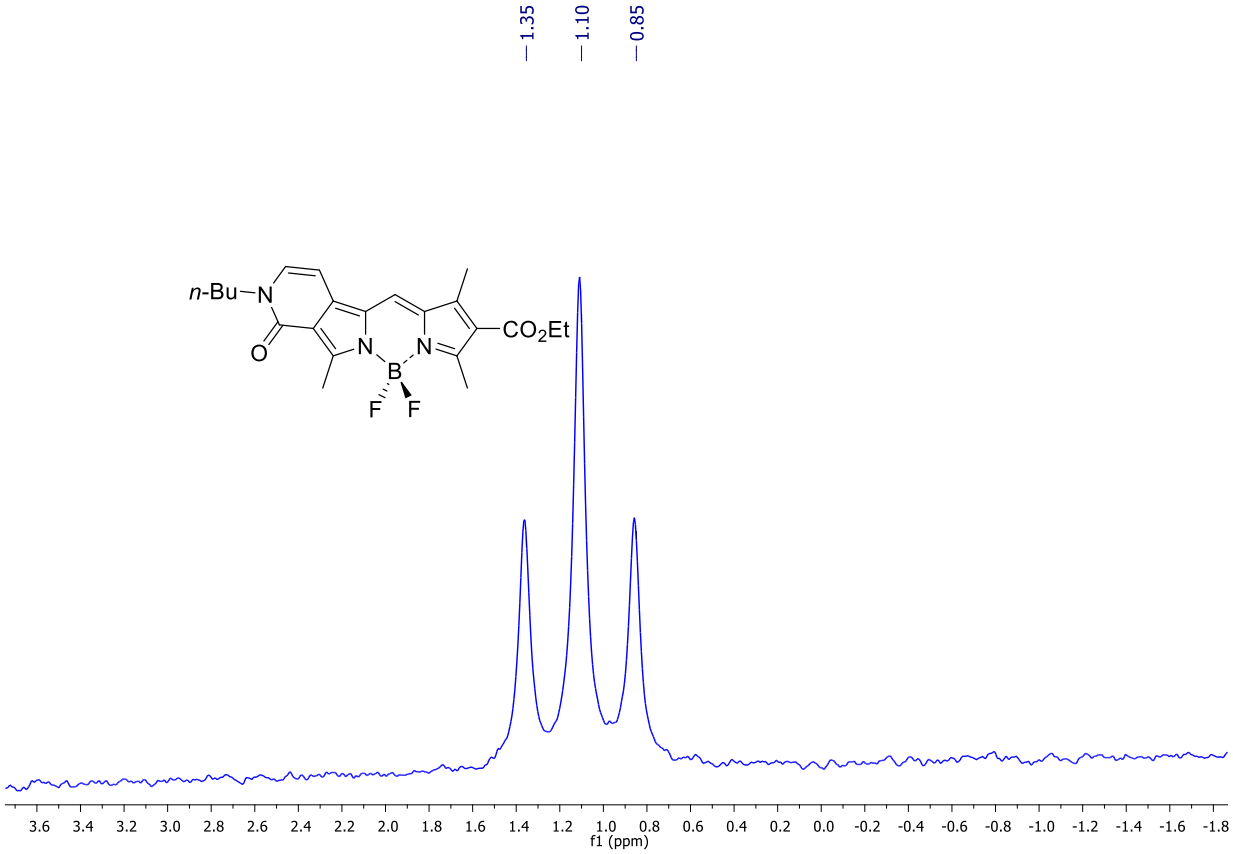

Figure S64. ^{11}B NMR spectrum of compound **17** in $CDCl_3$

High-Resolution Mass Specs

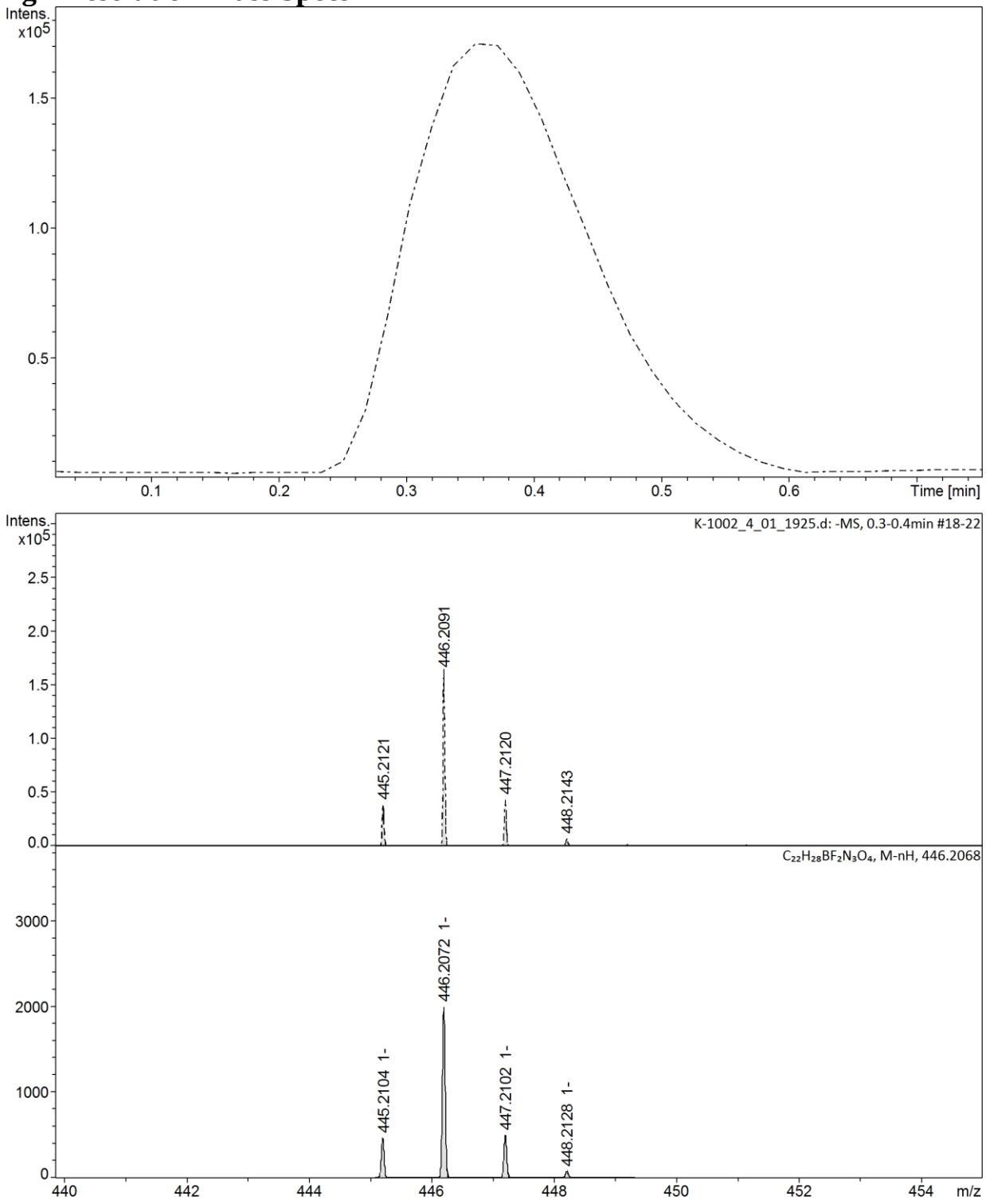

Figure S65. High-resolution mass spectrum of compound **2.**

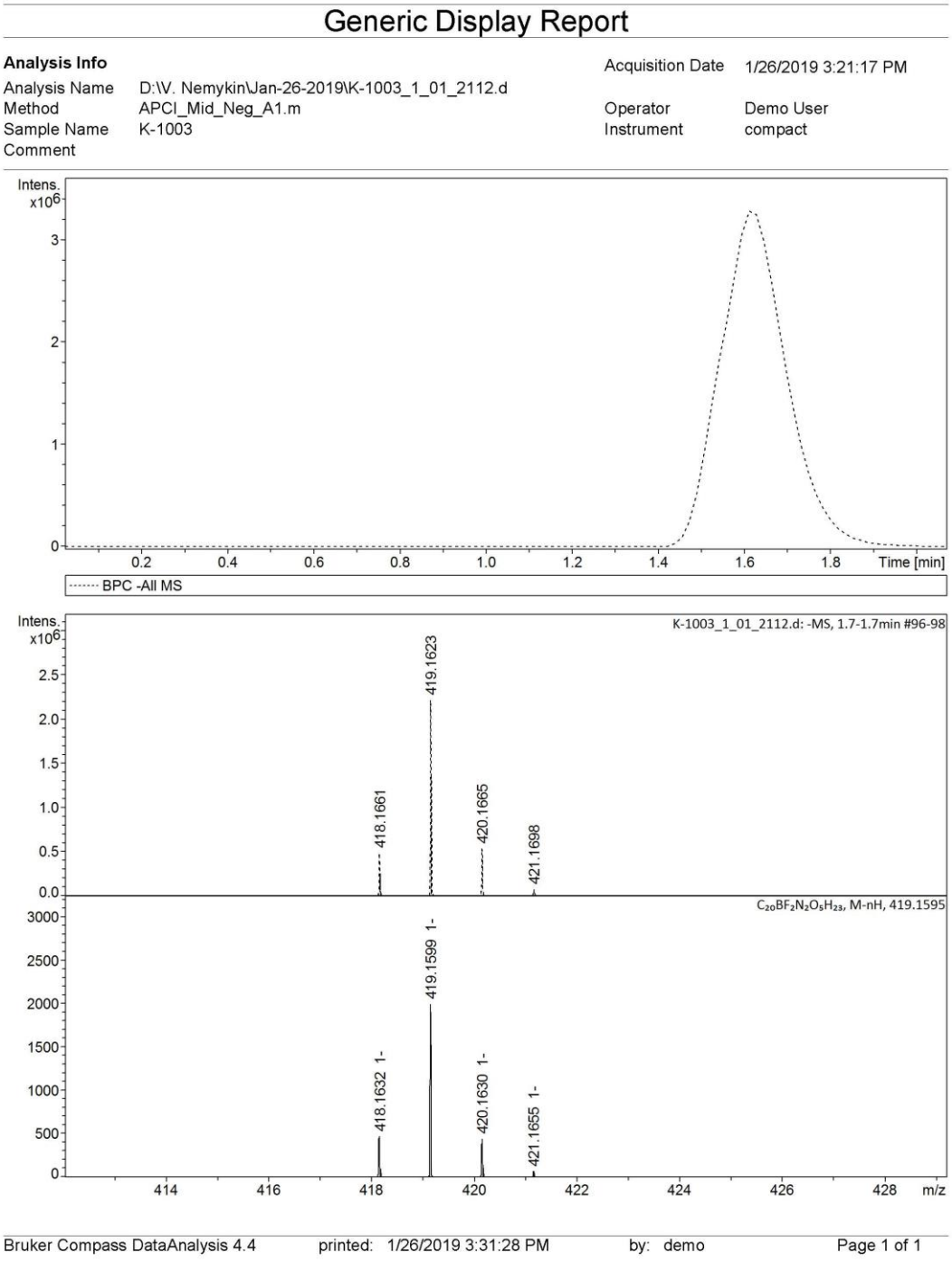

Figure S66. High-resolution mass spectrum of compound **3.**

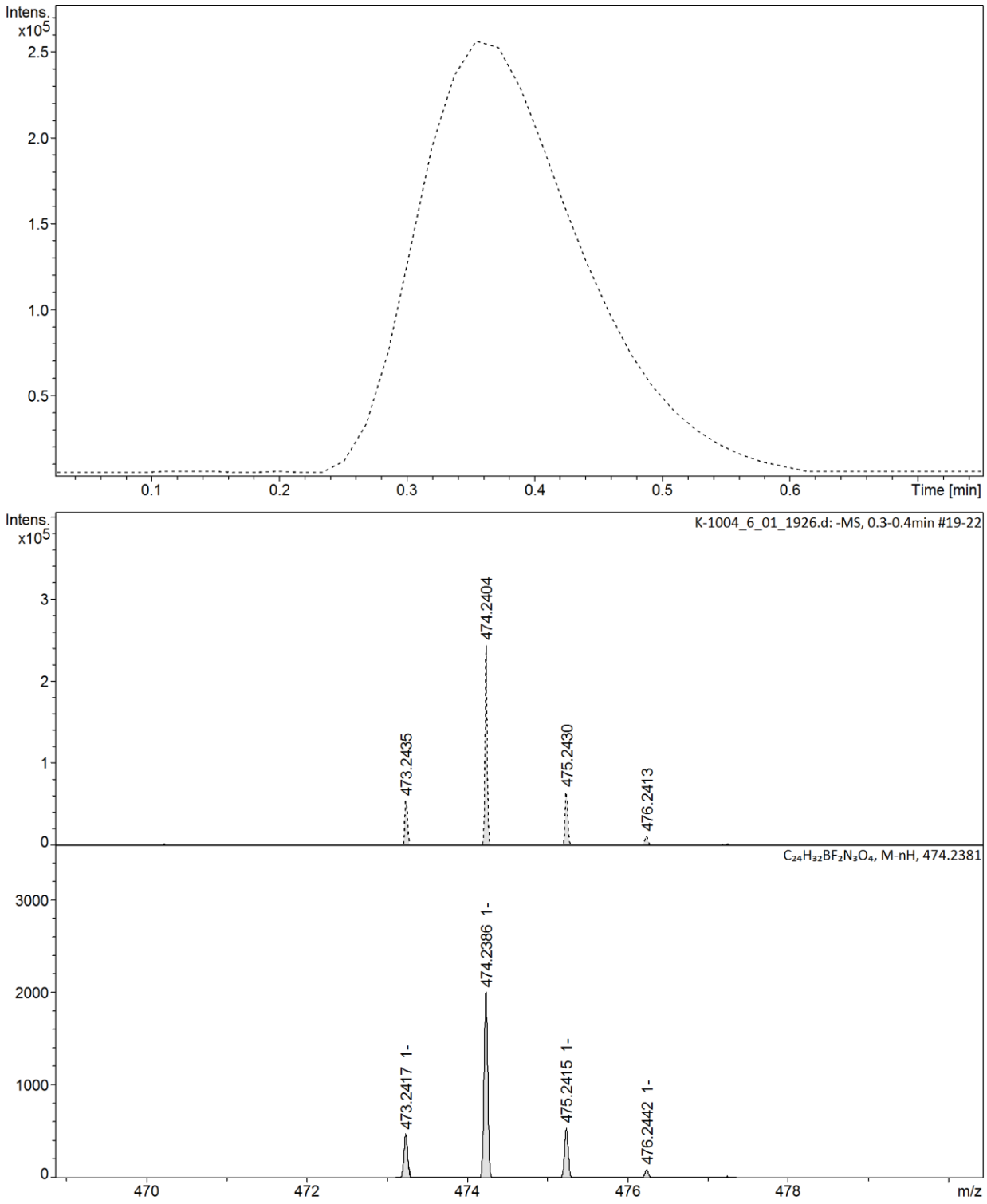

Figure S67. High-resolution mass spectrum of compound **4.**

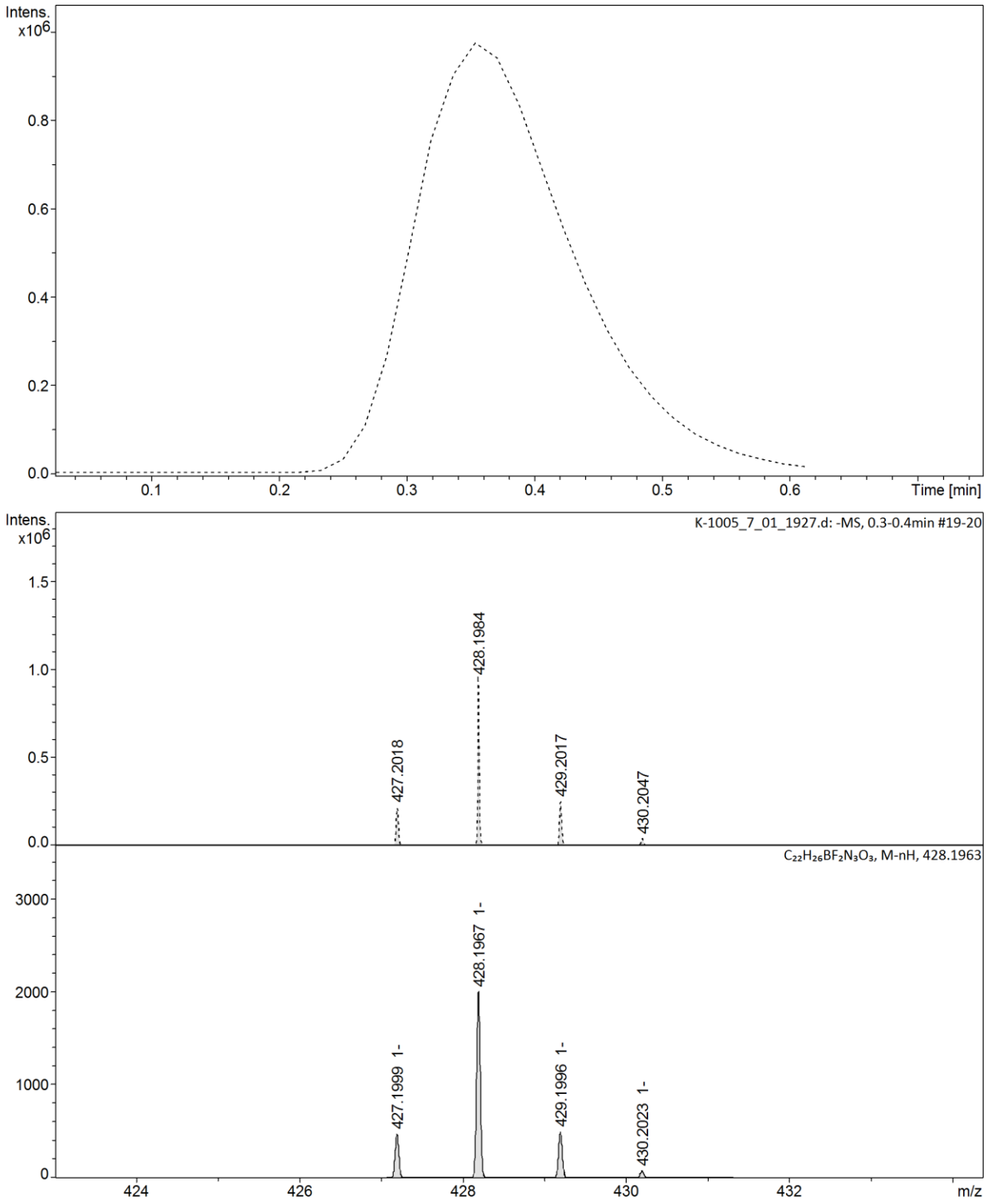

Figure S68. High-resolution mass spectrum of compound **5.**

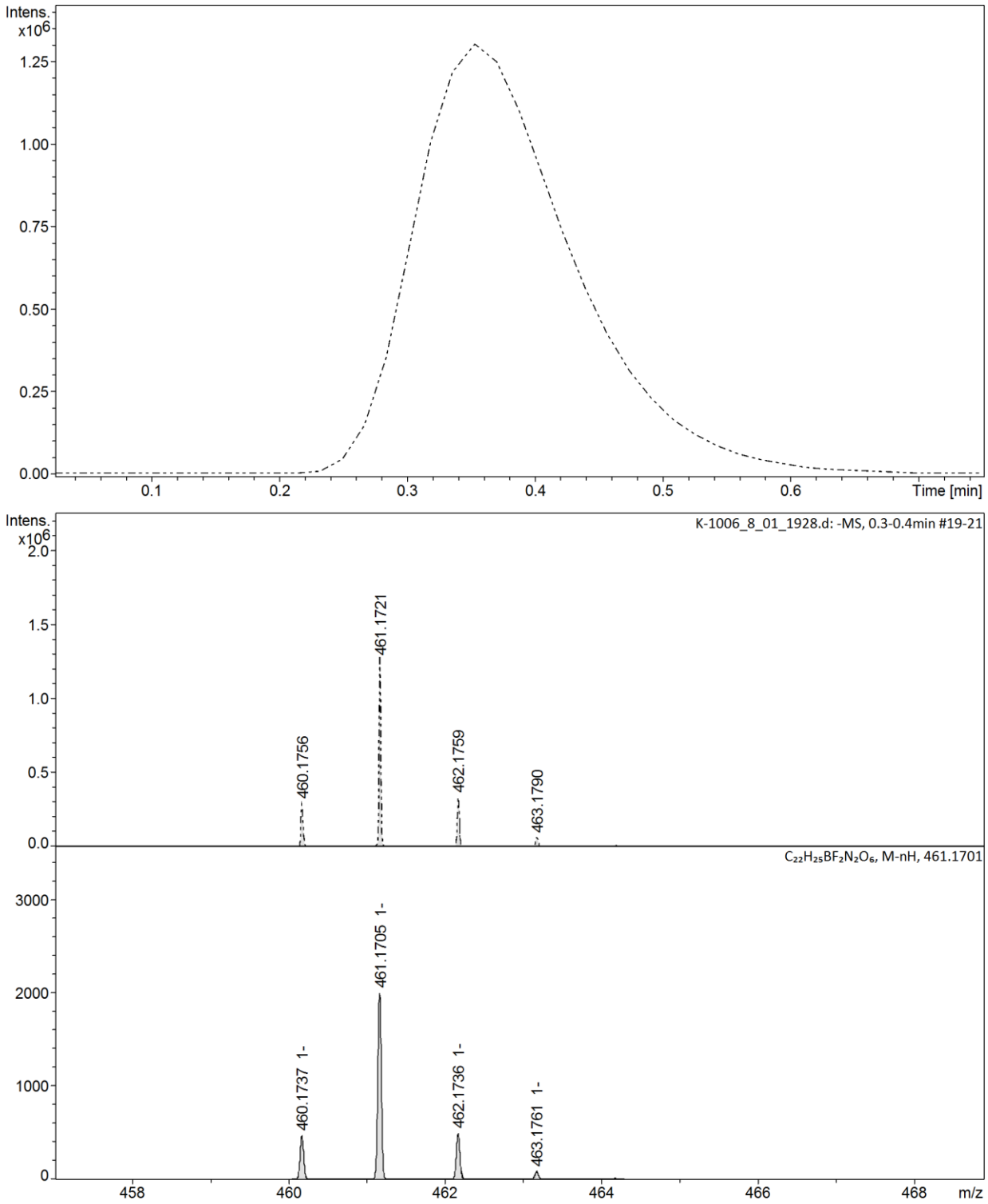

Figure S69. High-resolution mass spectrum of compound **6.**

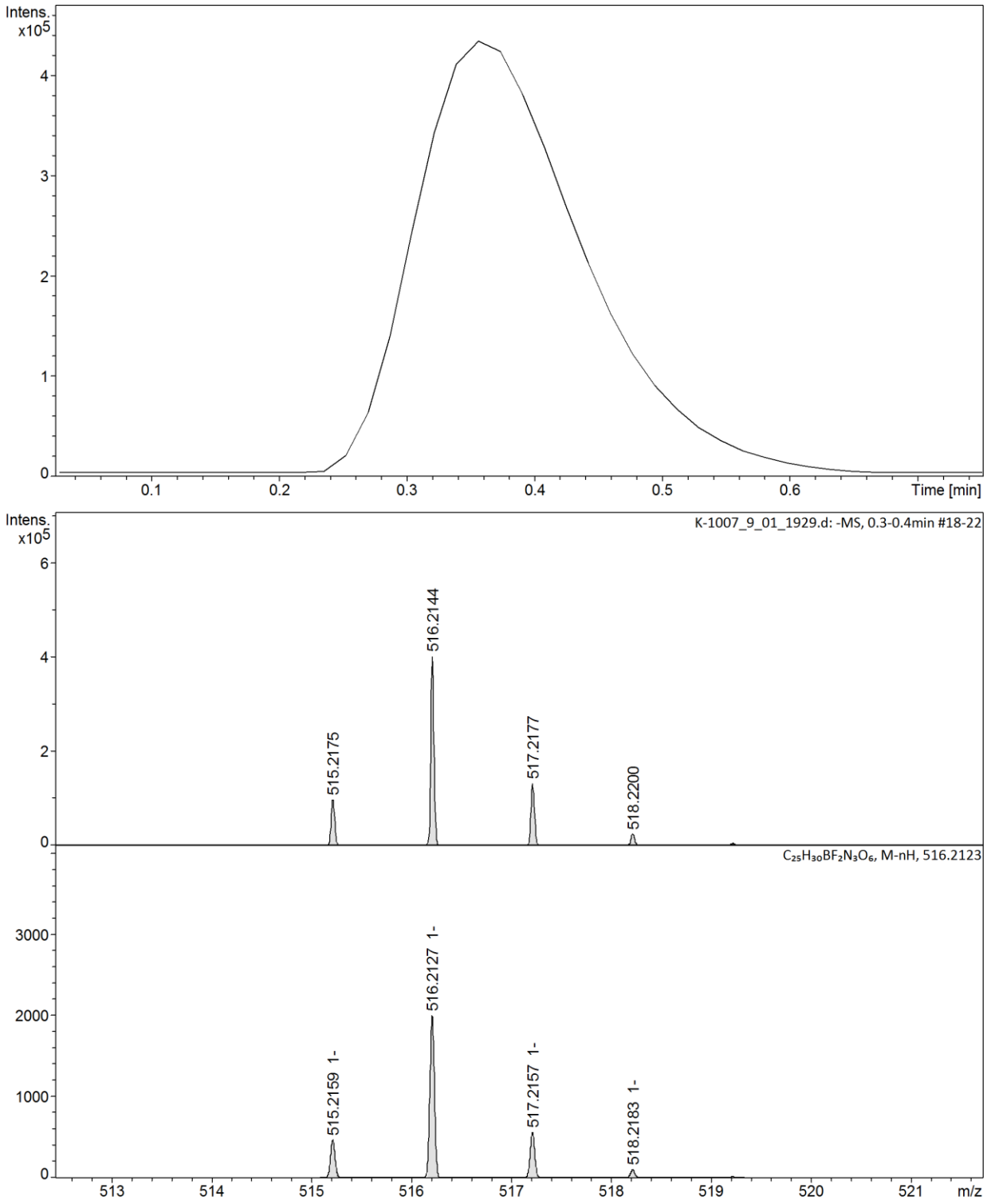

Figure S70. High-resolution mass spectrum of compound **7.**

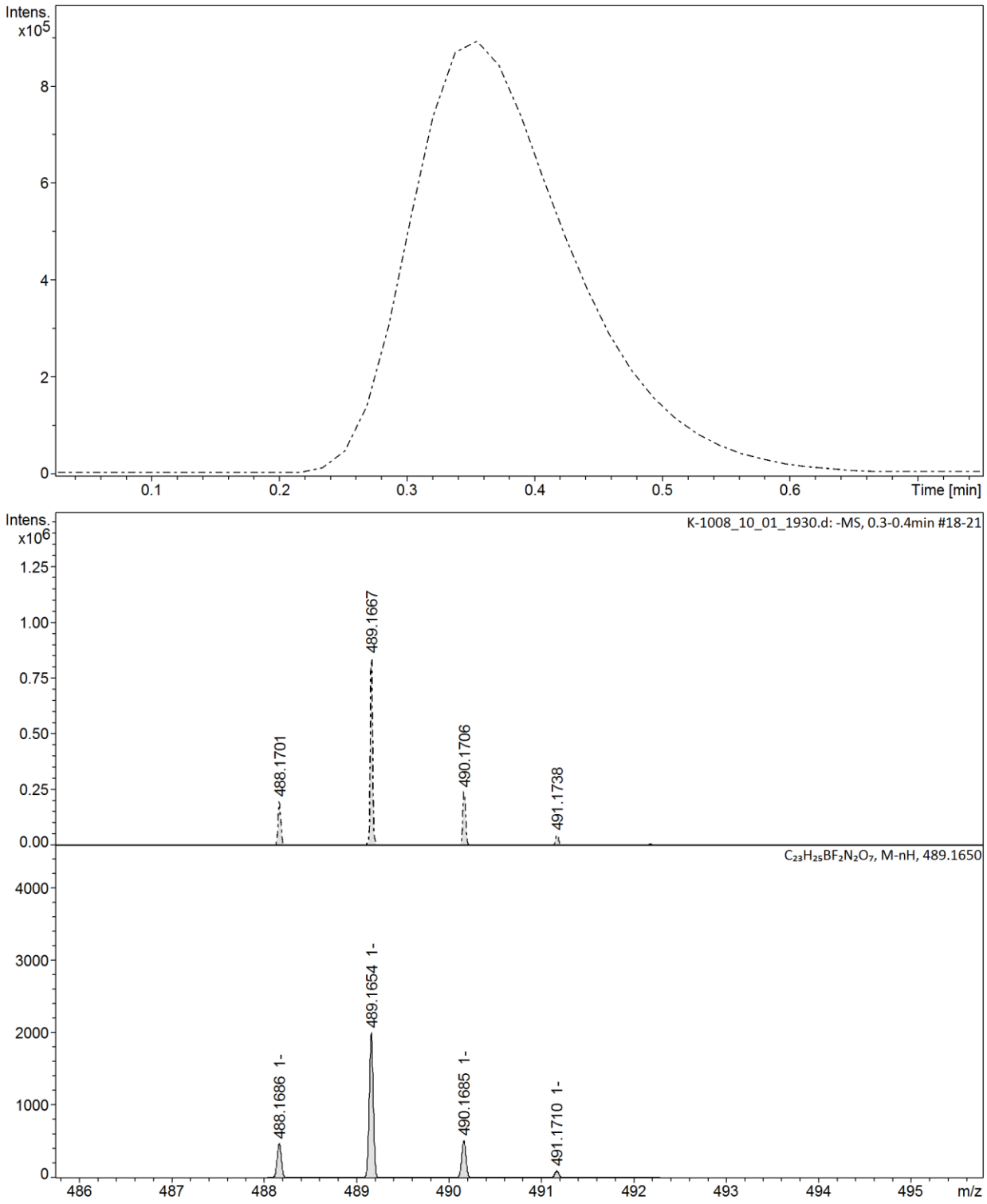

Figure S71. High-resolution mass spectrum of compound **8.**

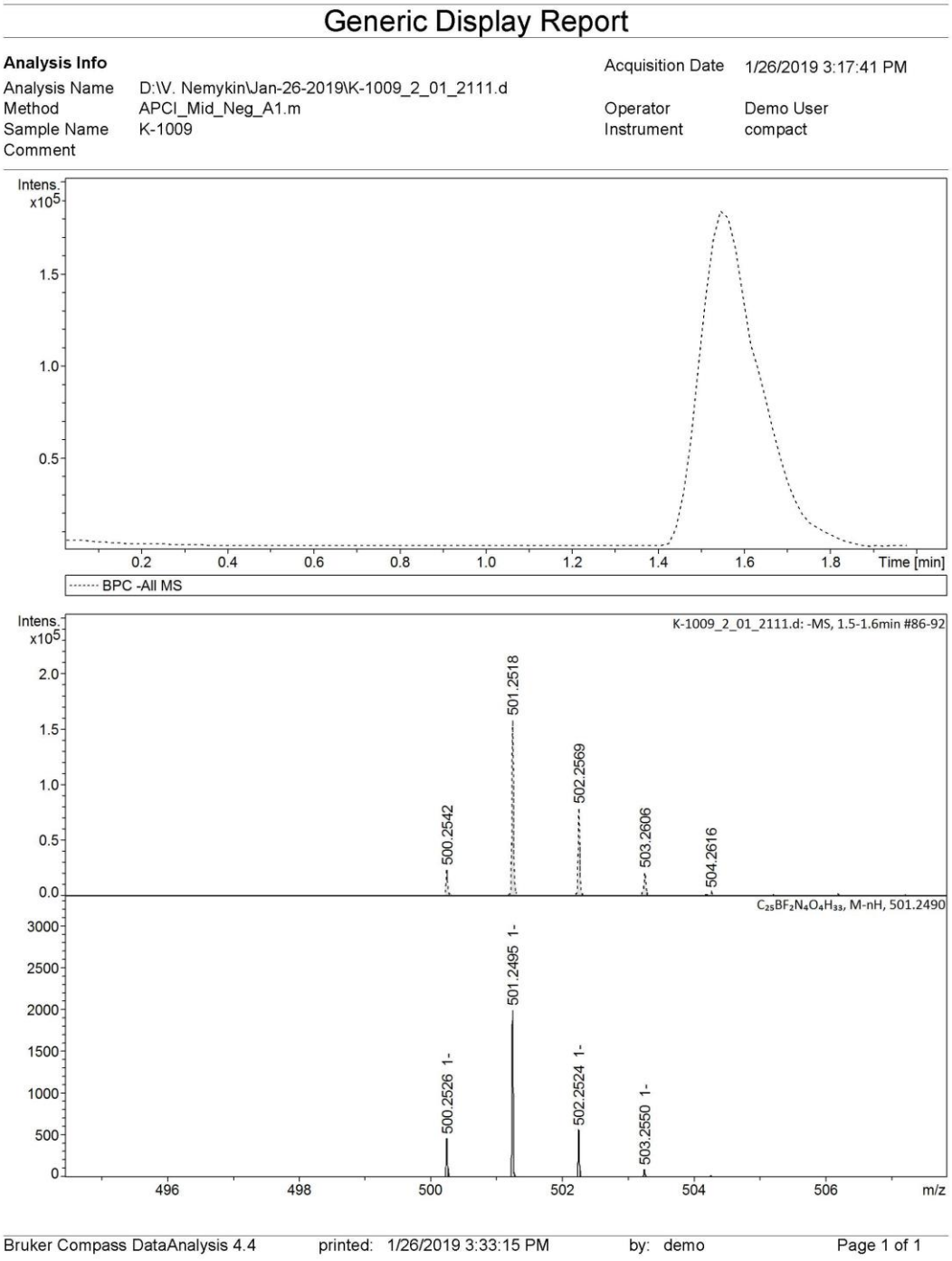

Figure S72. High-resolution mass spectrum of compound **9.**

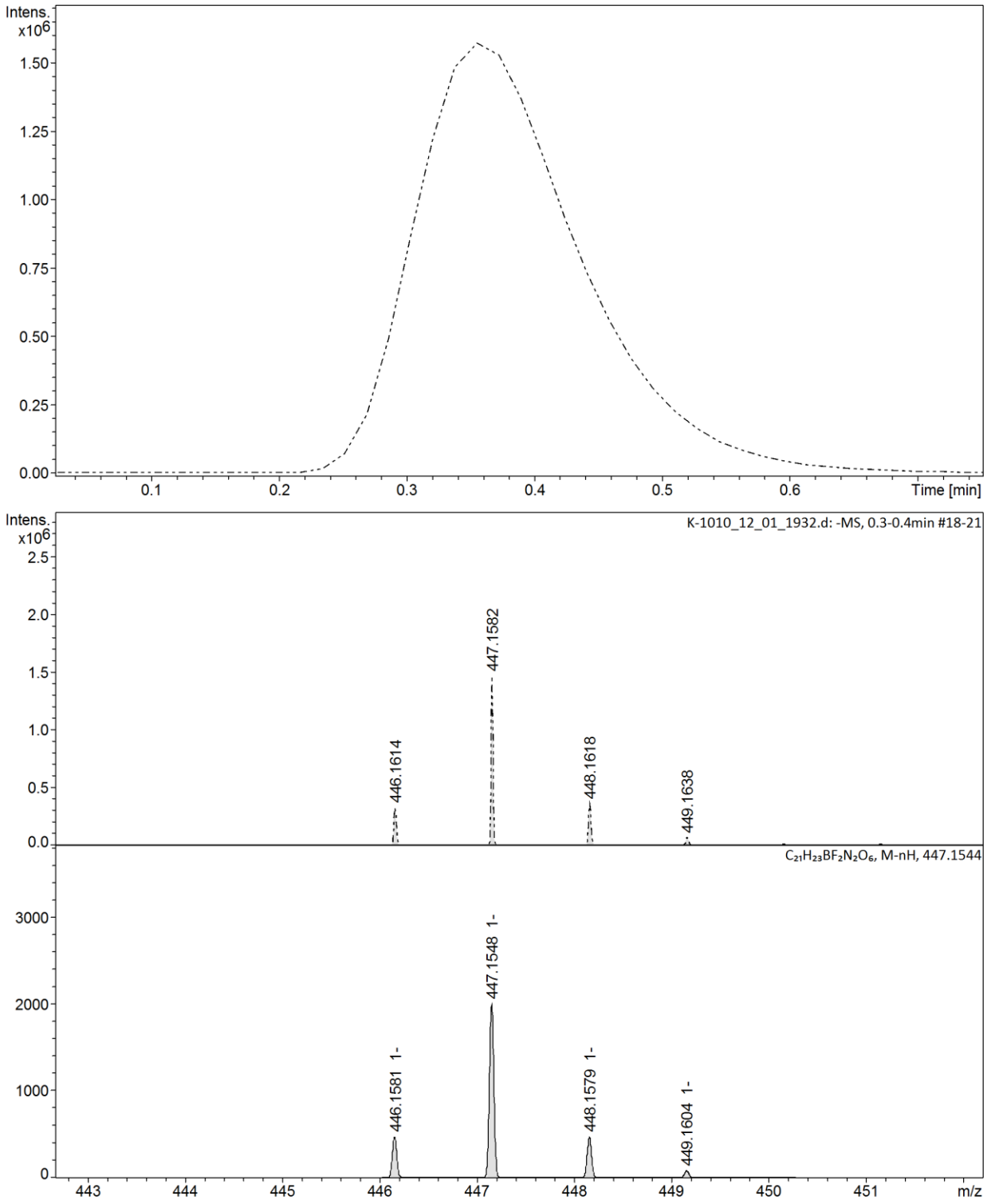

Figure S73. High-resolution mass spectrum of compound **10.**

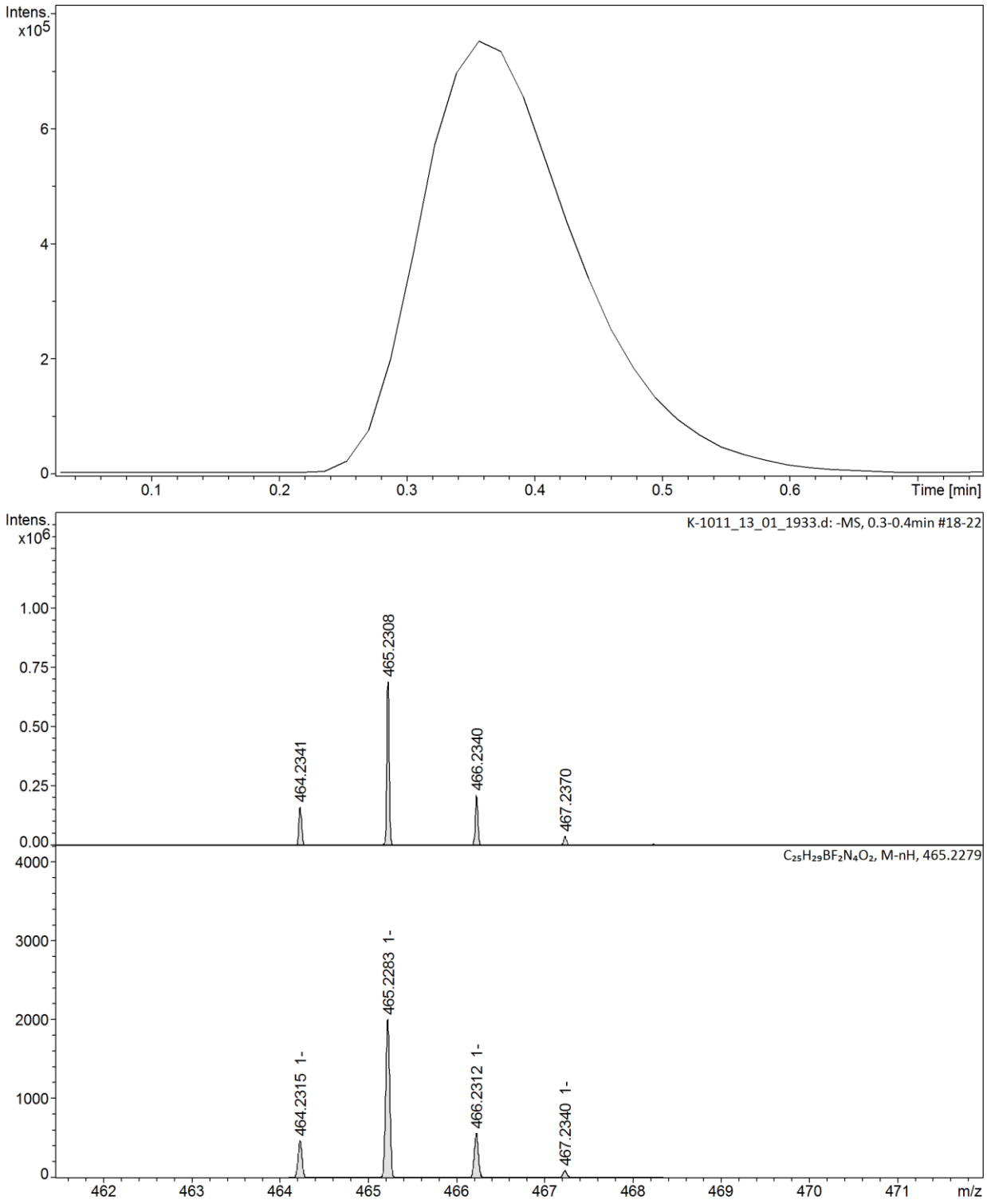

Figure S74. High-resolution mass spectrum of compound **11.**

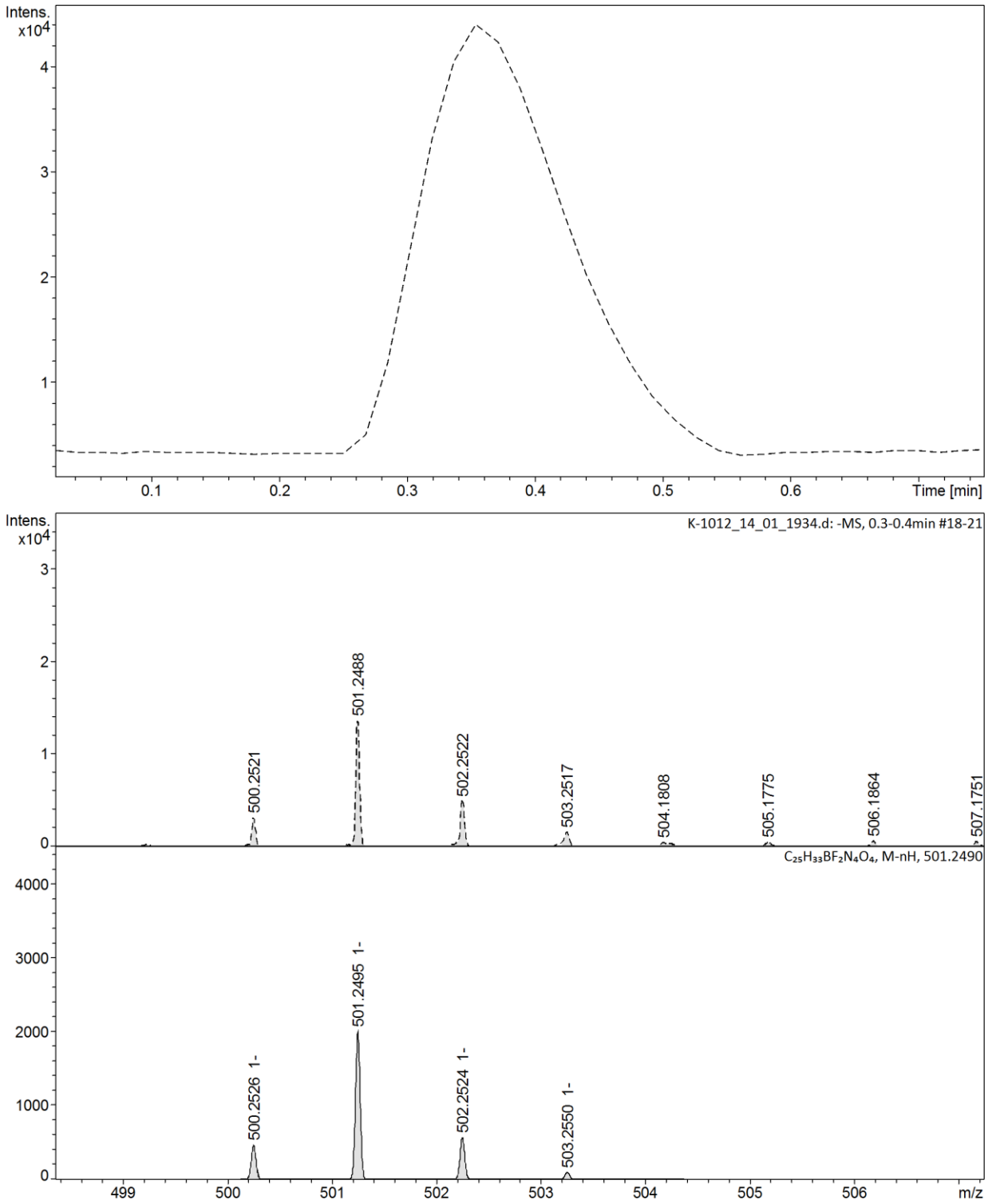

Figure S75. High-resolution mass spectrum of compound **12.**

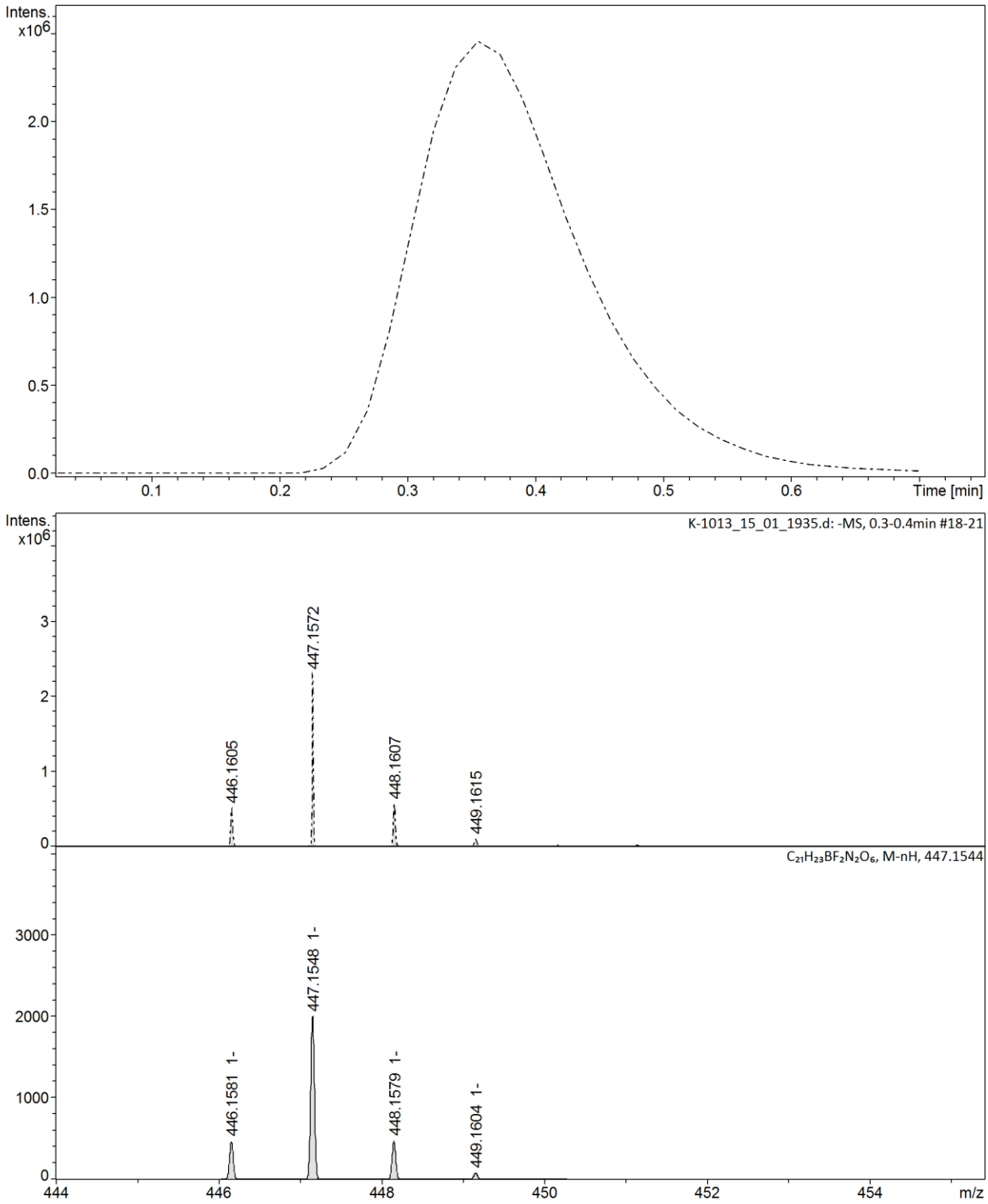

Figure S76. High-resolution mass spectrum of compound **13.**

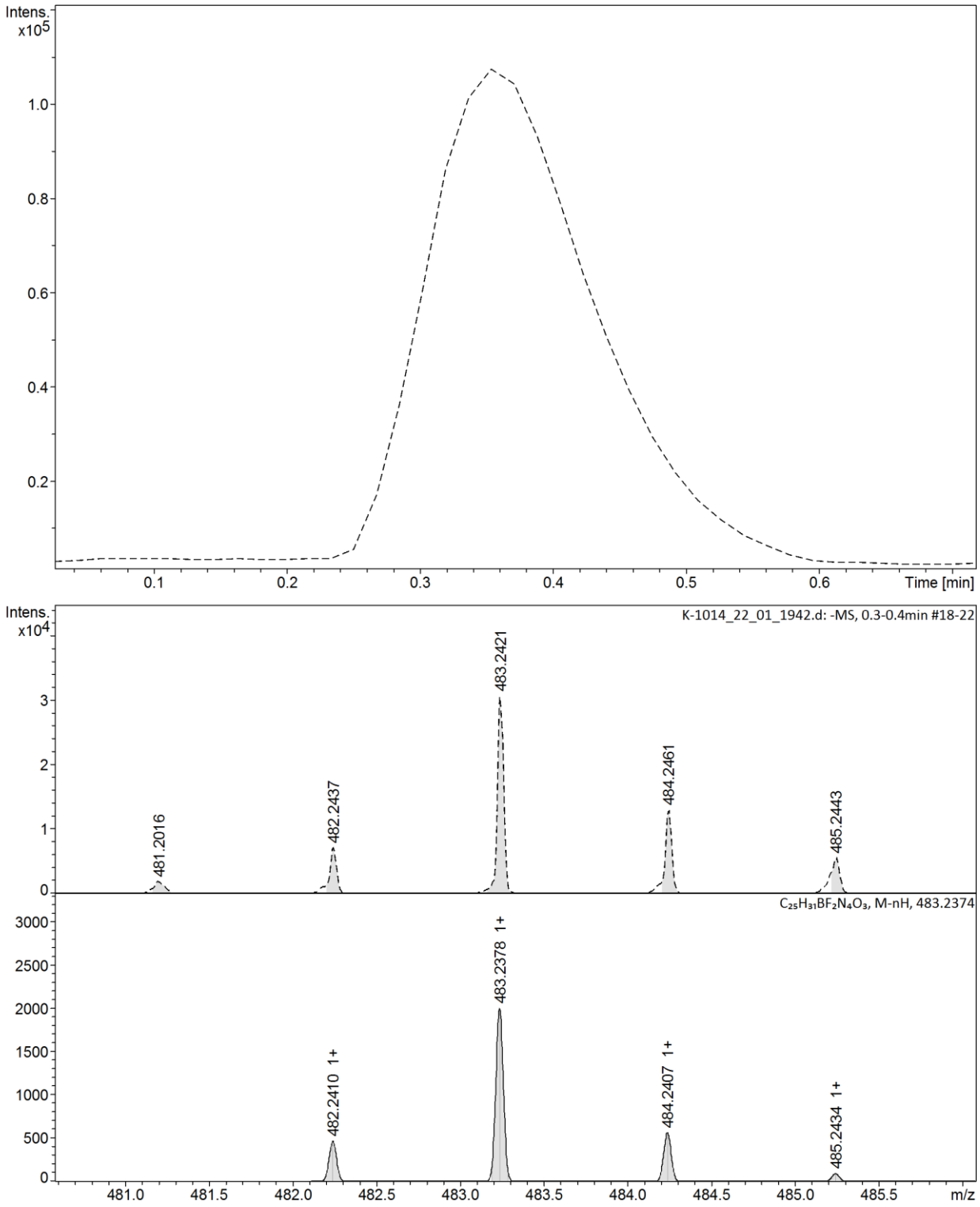

Figure S77 High-resolution mass spectrum of compound **14.**

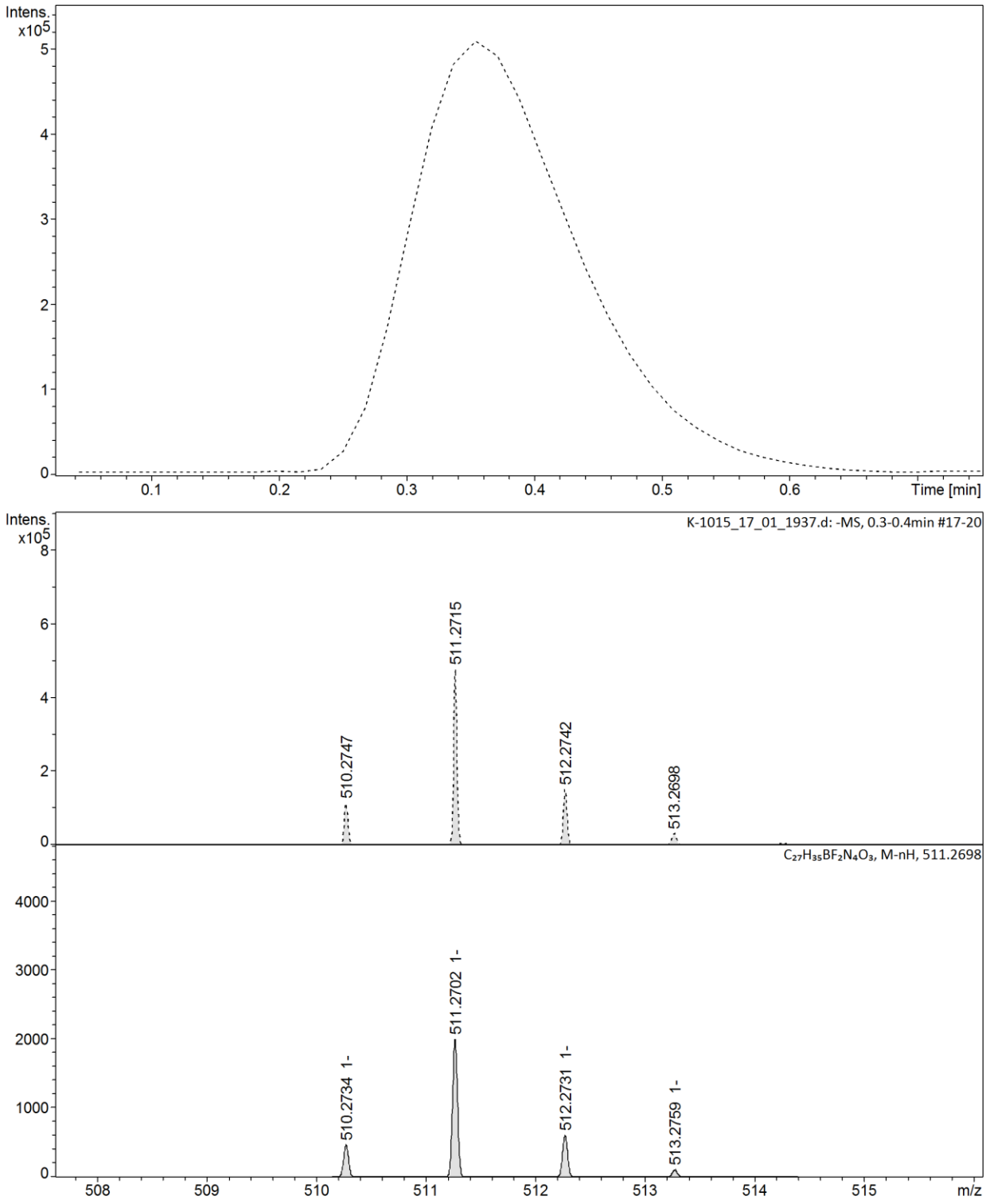

Figure S78. High-resolution mass spectrum of compound **15.**

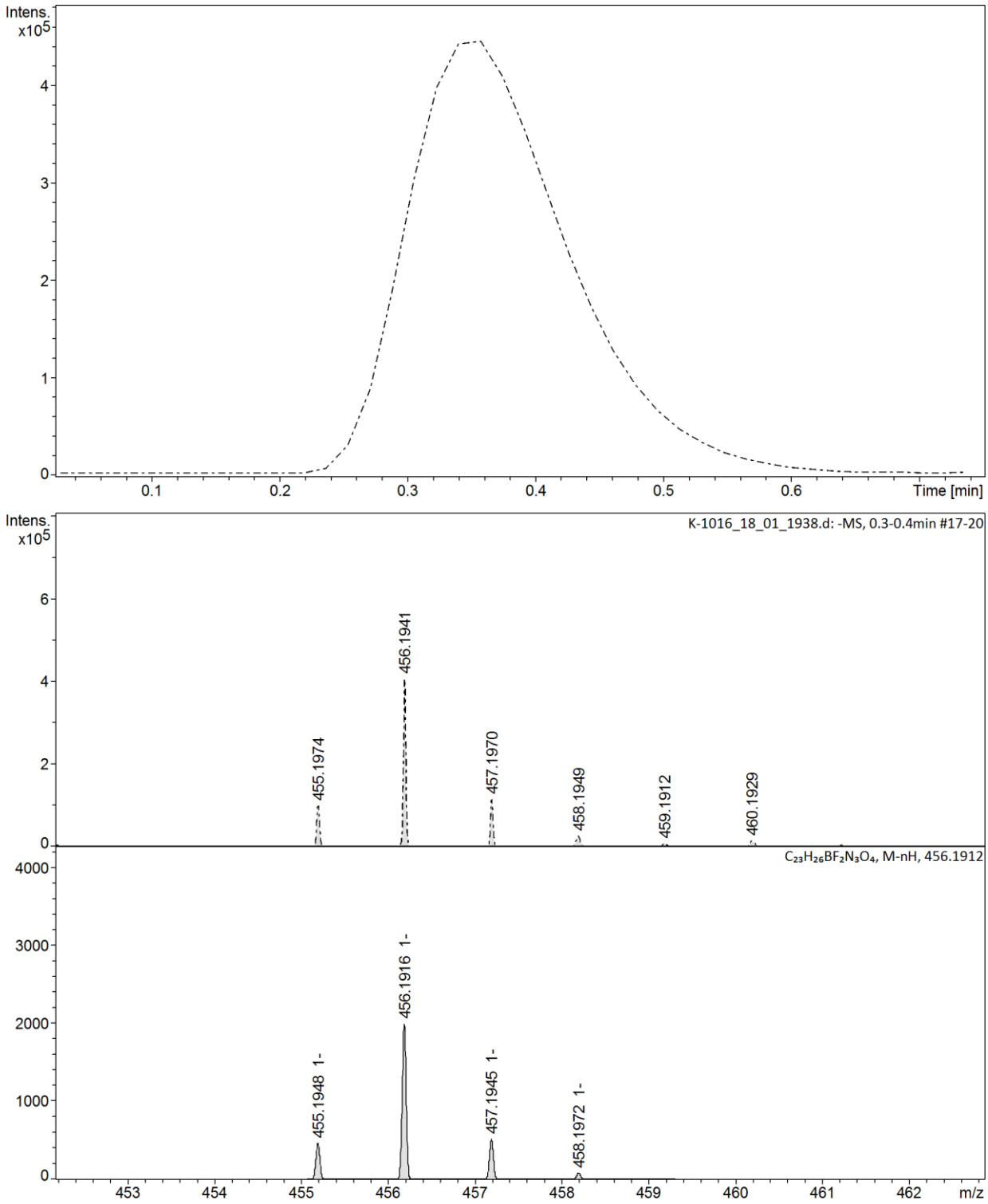

Figure S79. High-resolution mass spectrum of compound **16.**

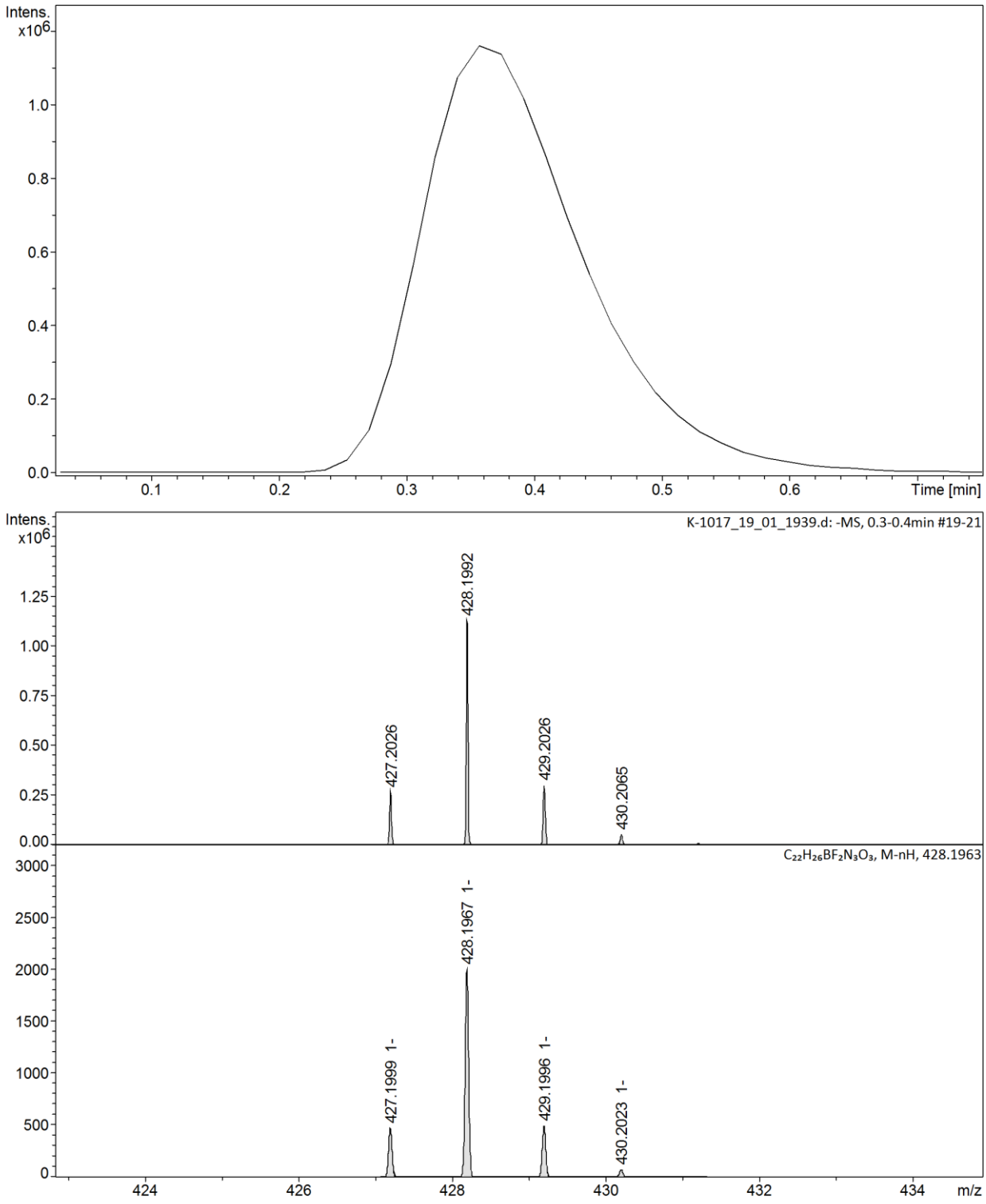

Figure S80. High-resolution mass spectrum of compound **17.**

Table S1. DFT optimized geometry of compound **1.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.496246	-1.178182	-0.158913
2	6	0	-1.188567	-0.634226	-0.100749
3	6	0	-3.367991	-0.075238	-0.153731
4	7	0	-1.276069	0.762168	-0.054954

5	6	0	-2.573979	1.108911	-0.085264
6	5	0	-0.049161	1.731821	-0.015499
7	6	0	-4.834305	-0.063148	-0.213343
8	6	0	0.048472	-1.266880	-0.085857
9	6	0	1.241487	-0.556235	-0.038338
10	6	0	2.582073	-1.015821	-0.005429
11	7	0	1.237898	0.843145	-0.015508
12	6	0	3.380508	0.140161	0.044554
13	1	0	0.083973	-2.348995	-0.111756
14	6	0	3.000785	-2.450430	-0.018931
15	6	0	2.510580	1.271919	0.032989
16	6	0	4.843309	0.245287	0.103993
17	6	0	2.862984	2.719504	0.082810
18	1	0	2.067166	3.325141	-0.347396
19	1	0	3.800369	2.898564	-0.440454
20	1	0	3.009727	3.031824	1.122499
21	1	0	2.138878	-3.119141	-0.030991
22	1	0	3.608752	-2.685189	0.857712
23	1	0	3.617869	-2.665244	-0.894613
24	9	0	-0.068541	2.558167	-1.147331
25	9	0	-0.081652	2.510577	1.149216
26	8	0	-5.522071	0.942323	-0.284831
27	8	0	-5.351029	-1.312231	-0.187943
28	6	0	-6.802587	-1.417057	-0.253396
29	1	0	-7.173354	-0.644235	-0.926630
30	6	0	-7.421652	-1.303920	1.128657
31	1	0	-6.972045	-2.399127	-0.693519
32	1	0	-7.250821	-0.312299	1.551745
33	1	0	-7.004349	-2.054826	1.804048
34	1	0	-8.501181	-1.466571	1.060067
35	8	0	5.446337	-0.960808	0.024879
36	8	0	5.466959	1.288396	0.213682
37	6	0	6.900449	-0.940530	0.083312
38	1	0	7.199673	-0.479477	1.026705
39	1	0	7.267736	-0.317112	-0.734199
40	6	0	7.375598	-2.373417	-0.030968
41	1	0	6.988374	-2.981767	0.789745
42	1	0	8.467743	-2.399034	0.008873
43	1	0	7.056754	-2.817372	-0.976932
44	6	0	-2.821153	-2.635844	-0.217483
45	1	0	-3.421845	-2.863726	-1.100867
46	1	0	-1.917610	-3.246689	-0.246786
47	1	0	-3.413721	-2.935893	0.650144
48	6	0	-3.020725	2.530841	-0.065638
49	1	0	-2.265026	3.166550	0.392507
50	1	0	-3.192628	2.881535	-1.089049
51	1	0	-3.965511	2.622482	0.466952

E_h = -1373.350740 Hartree

Table S2. DFT optimized geometry of compound **2.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.491699	-2.196845	-0.398394
2	6	0	0.323889	-1.396268	-0.256256
3	6	0	2.584473	-1.336290	-0.288545
4	7	0	0.709260	-0.067952	-0.078426
5	6	0	2.073804	0.014455	-0.108097
6	5	0	-0.290824	1.119985	0.036663
7	6	0	3.955149	-1.865005	-0.232787
8	6	0	2.691330	1.288442	-0.003752
9	6	0	-1.005867	-1.769124	-0.279097
10	6	0	-2.035062	-0.831244	-0.124357
11	6	0	-3.433542	-0.997497	-0.111446
12	7	0	-1.732069	0.523225	0.046169
13	6	0	-3.973027	0.298650	0.065094
14	1	0	-1.260262	-2.810603	-0.429513
15	6	0	-4.148889	-2.302891	-0.262254
16	6	0	-2.888015	1.210912	0.158407
17	6	0	-5.377543	0.704066	0.140437
18	6	0	-2.922309	2.694270	0.322400
19	6	0	3.976141	1.603644	-0.389528
20	1	0	-2.003463	3.051008	0.784855
21	1	0	-3.783521	2.988478	0.919452
22	1	0	-3.024922	3.180836	-0.654071
23	1	0	-3.446993	-3.124787	-0.415352
24	1	0	-4.838025	-2.277002	-1.109922
25	1	0	-4.750407	-2.525893	0.622684
26	9	0	-0.057664	1.828451	1.235163
27	9	0	-0.148683	1.997555	-1.051879
28	7	0	4.526750	2.824206	-0.301665
29	6	0	3.781691	3.953615	0.247030
30	6	0	5.834881	3.103539	-0.885657
31	1	0	2.037574	2.088023	0.319164
32	1	0	4.626801	0.851185	-0.811086
33	1	0	6.287917	2.171954	-1.221523
34	1	0	6.485358	3.568225	-0.140607
35	1	0	5.738384	3.779566	-1.740815
36	1	0	3.371530	3.695168	1.225683
37	1	0	2.960998	4.242795	-0.417317
38	1	0	4.459443	4.797739	0.360994
39	8	0	4.271455	-2.969079	-0.645466
40	8	0	4.833696	-1.034010	0.373773
41	6	0	6.200223	-1.519673	0.513278
42	1	0	6.454172	-2.097164	-0.375388
43	6	0	6.358950	-2.337456	1.782800
44	1	0	6.798535	-0.609084	0.543946
45	1	0	5.765567	-3.252408	1.733807
46	1	0	6.048811	-1.759982	2.656951
47	1	0	7.409209	-2.615691	1.909716
48	8	0	-6.222711	-0.354156	0.100575
49	8	0	-5.779337	1.854695	0.228391

50	6	0	-7.636818	-0.026314	0.166736
51	1	0	-7.878719	0.631917	-0.670432
52	1	0	-7.821252	0.520424	1.093932
53	6	0	-8.406193	-1.329364	0.110528
54	1	0	-8.204738	-1.864758	-0.820430
55	1	0	-9.478499	-1.122245	0.161418
56	1	0	-8.142293	-1.976665	0.950289
57	6	0	1.493496	-3.679834	-0.585653
58	1	0	1.886358	-3.943861	-1.570630
59	1	0	2.142152	-4.166185	0.146167
60	1	0	0.488331	-4.093643	-0.490890

E_h = -1545.484892 Hartree

Table S3. DFT optimized geometry of compound **3.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.132939	-1.556675	-0.148847
2	6	0	-0.863762	-0.928624	-0.134377
3	6	0	-3.069912	-0.511810	-0.242386
4	7	0	-1.034938	0.456567	-0.222106
5	6	0	-2.351855	0.714909	-0.291218
6	5	0	0.126104	1.505816	-0.233130
7	6	0	-4.533147	-0.565827	-0.279126
8	6	0	0.413551	-1.477118	-0.046864
9	6	0	1.554917	-0.689846	-0.042703
10	6	0	2.922893	-1.059226	0.047523
11	7	0	1.464450	0.705226	-0.132643
12	6	0	3.645043	0.143757	0.016945
13	1	0	0.517449	-2.553079	0.020947
14	6	0	3.429803	-2.460648	0.154556
15	6	0	2.706504	1.215091	-0.098093
16	6	0	5.097788	0.346535	0.090266
17	6	0	2.970943	2.680447	-0.153237
18	1	0	2.134415	3.209704	-0.605601
19	1	0	3.887638	2.877989	-0.706216
20	1	0	3.119114	3.068524	0.860343
21	1	0	2.612397	-3.182649	0.177058
22	1	0	4.029341	-2.587394	1.058828
23	1	0	4.081258	-2.700384	-0.689046
24	9	0	0.086242	2.238282	-1.427802
25	9	0	-0.003862	2.368333	0.861330
26	8	0	-5.251750	0.423550	-0.251645
27	8	0	-5.003906	-1.825028	-0.350786
28	6	0	-6.454794	-1.980170	-0.380200
29	1	0	-6.873839	-1.167529	-0.973042
30	6	0	-7.028999	-2.009696	1.024907
31	1	0	-6.601299	-2.926647	-0.898750
32	1	0	-6.880904	-1.052528	1.528550
33	1	0	-6.563264	-2.799788	1.618876

34	1	0	-8.103579	-2.207234	0.974442
35	8	0	5.775674	-0.820577	0.120410
36	8	0	5.650576	1.433465	0.123091
37	6	0	7.224573	-0.702688	0.202587
38	1	0	7.471320	-0.141327	1.105882
39	1	0	7.570908	-0.131769	-0.661064
40	6	0	7.790718	-2.106366	0.226411
41	1	0	7.423162	-2.663242	1.091495
42	1	0	8.880983	-2.057051	0.288529
43	1	0	7.523891	-2.652614	-0.681397
44	6	0	-2.905289	2.095992	-0.394845
45	1	0	-2.100694	2.824284	-0.512834
46	1	0	-3.551172	2.179610	-1.272892
47	6	0	-3.747956	2.517965	0.810458
48	1	0	-3.728297	1.846735	1.689719
49	8	0	-4.372353	3.552505	0.829261
50	6	0	-2.377187	-3.028888	-0.072819
51	1	0	-3.020093	-3.271816	0.776551
52	1	0	-2.893936	-3.381330	-0.968833
53	1	0	-1.444623	-3.585640	0.029313

E_h = -1486.699545 Hartree

Table S4. DFT optimized geometry of compound **4.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.616488	2.507593	-0.310536
2	6	0	-0.428639	1.550609	-0.188345
3	6	0	1.815880	1.823880	-0.091377
4	7	0	0.126611	0.309225	0.112631
5	5	0	-0.707029	-0.996730	0.277333
6	6	0	3.149434	2.435654	-0.129344
7	6	0	-1.792789	1.724957	-0.325690
8	6	0	-2.689430	0.661881	-0.162963
9	6	0	-4.095842	0.627842	-0.229856
10	7	0	-2.212439	-0.619107	0.127455
11	6	0	-4.460905	-0.712929	0.038245
12	1	0	-2.180897	2.708075	-0.558996
13	6	0	-4.973114	1.804182	-0.521128
14	6	0	-3.266374	-1.453093	0.249484
15	6	0	-5.801837	-1.297645	0.105451
16	6	0	-3.099774	-2.900712	0.573111
17	1	0	-2.161737	-3.277955	0.166927
18	1	0	-3.938138	-3.473500	0.182641
19	1	0	-3.078683	-3.046237	1.658834
20	1	0	-4.383460	2.710762	-0.669684
21	1	0	-5.676463	1.982362	0.296206
22	1	0	-5.572987	1.633698	-1.418498
23	9	0	-0.345228	-1.930702	-0.713137
24	9	0	-0.493536	-1.567777	1.547448

25	8	0	4.221789	1.850180	-0.177326
26	8	0	3.076896	3.786136	-0.121192
27	6	0	4.337578	4.509081	-0.204874
28	1	0	5.004285	3.965887	-0.874485
29	6	0	4.952161	4.697949	1.171190
30	1	0	4.060200	5.461074	-0.656534
31	1	0	5.233647	3.737938	1.607799
32	1	0	4.252232	5.201093	1.842782
33	1	0	5.851574	5.315063	1.088438
34	8	0	-6.768567	-0.403268	-0.212981
35	8	0	-6.059552	-2.452327	0.410971
36	6	0	-8.129769	-0.908467	-0.160028
37	1	0	-8.323887	-1.273220	0.850807
38	1	0	-8.212352	-1.752162	-0.848423
39	6	0	-9.049321	0.232418	-0.542224
40	1	0	-8.945170	1.069257	0.152497
41	1	0	-10.087260	-0.109848	-0.513830
42	1	0	-8.833388	0.587960	-1.552570
43	6	0	0.383821	3.952068	-0.624205
44	1	0	0.657258	4.583494	0.224407
45	1	0	0.997903	4.275160	-1.466587
46	1	0	-0.663049	4.137191	-0.868031
47	6	0	1.490602	0.424873	0.174954
48	6	0	2.247078	-0.728866	0.495953
49	6	0	3.617135	-0.884878	0.516638
50	1	0	1.652689	-1.600675	0.745976
51	7	0	4.222788	-2.028886	0.860568
52	1	0	4.274327	-0.067611	0.250131
53	6	0	5.665208	-2.251975	0.791110
54	1	0	6.144992	-1.271685	0.747045
55	1	0	5.981390	-2.730645	1.723292
56	6	0	6.076770	-3.108239	-0.412503
57	1	0	5.548452	-4.068642	-0.369119
58	1	0	5.749693	-2.608050	-1.331384
59	6	0	7.589455	-3.353116	-0.457460
60	1	0	7.906656	-3.840976	0.472435
61	1	0	8.112080	-2.389377	-0.494345
62	6	0	8.010891	-4.209993	-1.654054
63	1	0	9.092973	-4.369321	-1.664856
64	1	0	7.528738	-5.192394	-1.624715
65	1	0	7.734169	-3.731470	-2.598944
66	1	0	3.646733	-2.828104	1.095655

E_h = -1624.143278 Hartree

Table S5. DFT optimized geometry of compound **5.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.788773	1.179729	-0.004732
2	6	0	-1.415859	0.823483	-0.021233

3	7	0	-1.308106	-0.573943	-0.028873
4	6	0	-2.545361	-1.097027	-0.014341
5	6	0	-3.497788	-0.033558	0.005188
6	6	0	-0.280400	1.625050	-0.021132
7	6	0	1.000327	1.079185	-0.017207
8	7	0	1.177775	-0.307816	-0.012537
9	6	0	2.510835	-0.546818	0.000152
10	6	0	3.211698	0.694958	0.003293
11	6	0	2.264025	1.727463	-0.007399
12	6	0	2.520236	3.197737	-0.009681
13	6	0	-3.316398	2.578131	0.004160
14	5	0	0.042935	-1.365042	-0.042524
15	9	0	0.139857	-2.140237	-1.209811
16	9	0	0.123176	-2.200366	1.080688
17	6	0	-4.948878	-0.244688	0.034961
18	8	0	-5.504300	-1.328591	0.102054
19	8	0	-5.633817	0.919988	-0.018628
20	6	0	-7.071360	0.788032	0.014202
21	1	0	-0.392812	2.702198	-0.019862
22	1	0	-7.415012	0.211204	-0.844503
23	1	0	-7.382784	0.296311	0.935804
24	6	0	3.212133	-1.772127	0.010563
25	6	0	4.577857	-1.692989	0.023541
26	6	0	4.656962	0.754057	0.018045
27	7	0	5.277264	-0.514166	0.027047
28	8	0	5.346457	1.774973	0.022860
29	1	0	-7.449101	1.806188	-0.027881
30	6	0	6.745700	-0.518389	0.041935
31	1	0	2.719961	-2.733944	0.010316
32	1	0	5.190130	-2.585559	0.032322
33	6	0	-2.787836	-2.567715	-0.000370
34	1	0	-1.954491	-3.099849	-0.456428
35	1	0	-2.893128	-2.918193	1.032319
36	1	0	-3.716694	-2.802837	-0.516195
37	1	0	7.107182	-0.004780	0.932829
38	1	0	7.091110	-1.549720	0.043089
39	1	0	7.124802	-0.000839	-0.839229
40	1	0	1.594295	3.774100	0.016819
41	1	0	3.132405	3.481522	0.850131
42	1	0	3.082514	3.486683	-0.902054
43	1	0	-3.951106	2.747791	0.877054
44	1	0	-2.508814	3.311465	0.015909
45	1	0	-3.938387	2.762322	-0.875144

E_h = -1311.757156 Hartree

Table S6. DFT optimized geometry of compound **6.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276701	-2.223761	-0.124344

2	6	0	-0.133264	-1.388100	-0.099279
3	6	0	-2.390158	-1.367835	-0.127833
4	7	0	-0.538408	-0.057768	-0.099617
5	5	0	0.447405	1.159663	-0.045356
6	6	0	-3.797163	-1.791452	-0.150586
7	6	0	1.214187	-1.732926	-0.071713
8	6	0	2.219370	-0.775559	-0.044940
9	6	0	3.628865	-0.921307	-0.007902
10	7	0	1.899990	0.586013	-0.045240
11	6	0	4.145682	0.385710	0.021758
12	1	0	1.487281	-2.780462	-0.068348
13	6	0	4.358523	-2.225521	-0.001422
14	6	0	3.043545	1.292418	-0.005566
15	6	0	5.547055	0.817953	0.080615
16	6	0	3.062456	2.782540	0.028023
17	1	0	2.151255	3.190075	-0.405958
18	1	0	3.935739	3.161211	-0.499718
19	1	0	3.136592	3.130377	1.064245
20	1	0	3.667786	-3.070019	-0.013672
21	1	0	4.994036	-2.310698	0.883041
22	1	0	5.017360	-2.305167	-0.869340
23	9	0	0.260177	1.977333	-1.172608
24	9	0	0.232864	1.900721	1.122498
25	8	0	-4.768650	-1.071011	0.012729
26	8	0	-3.913498	-3.116697	-0.380758
27	6	0	-5.267134	-3.656802	-0.403386
28	1	0	-5.917357	-2.932708	-0.893899
29	6	0	-5.750113	-3.990238	0.997189
30	1	0	-5.176985	-4.547773	-1.023512
31	1	0	-5.834566	-3.088404	1.606245
32	1	0	-5.068313	-4.688702	1.488523
33	1	0	-6.737029	-4.458424	0.939869
34	8	0	6.406080	-0.223843	0.038735
35	8	0	5.920701	1.976829	0.161666
36	6	0	7.817611	0.124662	0.104816
37	1	0	7.989745	0.685533	1.025585
38	1	0	8.049840	0.775309	-0.740654
39	6	0	8.603585	-1.168626	0.065903
40	1	0	8.349768	-1.807349	0.915161
41	1	0	9.672818	-0.945816	0.112198
42	1	0	8.408167	-1.719103	-0.857399
43	6	0	-1.225066	-3.718729	-0.135835
44	1	0	-1.811556	-4.136558	0.684618
45	1	0	-1.650708	-4.115012	-1.060274
46	1	0	-0.199331	-4.078907	-0.045891
47	6	0	-1.898269	-0.010870	-0.110704
48	6	0	-2.517066	1.292024	-0.138435
49	6	0	-3.816607	1.618102	-0.009589
50	1	0	-1.828900	2.118083	-0.271277
51	1	0	-4.641896	0.940229	0.139117
52	8	0	-4.126771	2.952992	-0.073451
53	6	0	-5.587158	4.806524	-0.026232

54	1	0	-5.214501	5.143919	-0.996195
55	1	0	-6.630303	5.090975	0.091514
56	1	0	-4.979067	5.287886	0.743233
57	6	0	-5.456127	3.316945	0.079922
58	8	0	-6.334324	2.515741	0.268801

E_h = -1639.400848 Hartree

Table S7. DFT optimized geometry of compound **7**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.079831	-2.508360	-0.106398
2	6	0	-0.833247	-1.855555	-0.048652
3	6	0	-3.059781	-1.490158	-0.117462
4	7	0	-1.034416	-0.482135	-0.018228
5	5	0	0.118579	0.573879	0.019419
6	6	0	-4.509476	-1.694871	-0.170803
7	6	0	0.463007	-2.390342	-0.021947
8	6	0	1.578816	-1.578831	0.021855
9	6	0	2.956123	-1.937774	0.052806
10	7	0	1.472084	-0.192135	0.038994
11	6	0	3.680560	-0.744894	0.100688
12	1	0	0.588516	-3.464742	-0.039393
13	6	0	3.443589	-3.352555	0.047218
14	6	0	5.145778	-0.657425	0.165563
15	1	0	2.616850	-4.053001	0.173267
16	1	0	4.166349	-3.523753	0.846650
17	1	0	3.951872	-3.585128	-0.891613
18	9	0	0.037572	1.400101	-1.119151
19	9	0	-0.001689	1.373143	1.173995
20	8	0	-5.361506	-0.825606	-0.279698
21	8	0	-4.833582	-3.007377	-0.093243
22	6	0	-6.250625	-3.331082	-0.157799
23	1	0	-6.728162	-2.654751	-0.866765
24	6	0	-6.894905	-3.251783	1.215455
25	1	0	-6.266790	-4.346644	-0.552551
26	1	0	-6.877973	-2.228600	1.595261
27	1	0	-6.377866	-3.902280	1.925280
28	1	0	-7.937539	-3.576407	1.149867
29	8	0	5.734100	-1.819516	-0.192356
30	8	0	5.807391	0.312921	0.504982
31	6	0	7.186922	-1.838851	-0.117908
32	1	0	7.481580	-1.632164	0.912940
33	1	0	7.572760	-1.037941	-0.751367
34	6	0	7.642911	-3.205889	-0.582478
35	1	0	7.242583	-3.993931	0.059525
36	1	0	8.734359	-3.256020	-0.546790
37	1	0	7.324636	-3.395857	-1.610180
38	6	0	-2.252475	-3.995006	-0.150174
39	1	0	-2.799803	-4.354272	0.724413

40	1	0	-2.828114	-4.299935	-1.026805
41	1	0	-1.285990	-4.501086	-0.181693
42	6	0	-2.375827	-0.228411	-0.060466
43	6	0	-2.792276	1.154659	-0.011177
44	6	0	-4.019970	1.685671	-0.146082
45	1	0	-1.986990	1.860242	0.153171
46	1	0	-4.943145	1.157107	-0.318352
47	8	0	-4.111209	3.059335	-0.050737
48	6	0	-5.243182	5.127380	-0.064671
49	1	0	-4.563260	5.521172	-0.823885
50	1	0	-6.226344	5.578873	-0.177360
51	1	0	-4.825401	5.381268	0.912339
52	6	0	-5.354037	3.636841	-0.202555
53	8	0	-6.355636	2.999832	-0.415025
54	6	0	2.725574	0.360724	0.090040
55	6	0	2.838041	1.772810	0.069668
56	6	0	3.981418	2.539627	0.187113
57	1	0	1.895464	2.291228	-0.043313
58	7	0	4.002993	3.876812	0.102595
59	1	0	4.938486	2.068695	0.365133
60	6	0	2.788582	4.651659	-0.140478
61	6	0	5.234642	4.622807	0.343519
62	1	0	2.110661	4.596437	0.716885
63	1	0	2.270817	4.277276	-1.026379
64	1	0	3.064823	5.691292	-0.306574
65	1	0	6.058293	3.925001	0.484337
66	1	0	5.136140	5.243343	1.239274
67	1	0	5.454269	5.269151	-0.510174

E_h = -1811.532248 Hartree

Table S8. DFT optimized geometry of compound **8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.651108	-2.346222	-0.195521
2	6	0	-0.450699	-1.596289	-0.096333
3	6	0	-2.701687	-1.417337	-0.157502
4	7	0	-0.764550	-0.243753	-0.005892
5	5	0	0.302011	0.895702	0.116741
6	6	0	-4.134381	-1.740374	-0.231001
7	6	0	0.865952	-2.037190	-0.087055
8	6	0	1.938676	-1.155846	0.012316
9	6	0	3.334323	-1.397133	0.023718
10	7	0	1.709270	0.218358	0.115642
11	6	0	3.935467	-0.129576	0.128923
12	1	0	1.064474	-3.098715	-0.161529
13	6	0	3.987574	-2.737812	-0.067595
14	6	0	5.353272	0.238148	0.155432
15	1	0	3.252098	-3.535630	-0.180158
16	1	0	4.582353	-2.939481	0.826700

17	1	0	4.673894	-2.777815	-0.916856
18	9	0	0.210121	1.772198	-0.974140
19	9	0	0.118940	1.605304	1.311604
20	8	0	-5.057511	-0.950920	-0.114771
21	8	0	-4.334755	-3.055959	-0.453541
22	6	0	-5.720570	-3.499541	-0.543588
23	1	0	-6.293087	-2.731791	-1.063514
24	6	0	-6.292145	-3.796919	0.831314
25	1	0	-5.663012	-4.395386	-1.160578
26	1	0	-6.345309	-2.890743	1.437464
27	1	0	-5.683357	-4.538872	1.353778
28	1	0	-7.304261	-4.197925	0.725273
29	8	0	6.171361	-0.827342	0.231664
30	8	0	5.760291	1.390572	0.109951
31	6	0	7.598084	-0.526705	0.247540
32	1	0	7.803258	0.101199	1.116553
33	1	0	7.836496	0.042973	-0.652475
34	6	0	8.336167	-1.846619	0.305528
35	1	0	8.072345	-2.404883	1.206822
36	1	0	9.412933	-1.658952	0.321804
37	1	0	8.109021	-2.462039	-0.568058
38	6	0	-1.699716	-3.836125	-0.312857
39	1	0	-2.295582	-4.271513	0.491627
40	1	0	-2.171835	-4.135979	-1.250686
41	1	0	-0.699031	-4.268132	-0.275191
42	6	0	-2.116947	-0.100378	-0.037363
43	6	0	-2.640486	1.240477	0.031677
44	6	0	-3.921926	1.654332	0.067446
45	1	0	-1.889995	2.020838	0.062898
46	1	0	-4.802741	1.032013	0.051066
47	8	0	-4.129355	3.006618	0.132788
48	6	0	-5.455163	4.956895	0.253244
49	1	0	-4.919313	5.377446	-0.600609
50	1	0	-6.482960	5.312343	0.262207
51	1	0	-4.938694	5.286165	1.158106
52	6	0	-5.441498	3.460233	0.178657
53	8	0	-6.387826	2.717571	0.160866
54	6	0	2.898281	0.841237	0.191186
55	6	0	3.034655	2.321161	0.310895
56	1	0	3.671572	2.573712	1.162643
57	1	0	2.061797	2.785315	0.482484
58	6	0	3.664474	2.985267	-0.915376
59	1	0	3.824880	2.342216	-1.801197
60	8	0	3.942270	4.161119	-0.939432

E_h = -1752.748811 Hartree

Table S9. DFT optimized geometry of compound **9**.

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

1	6	0	-2.461490	-2.187403	-0.178490
2	6	0	-1.160212	-1.638860	-0.135638
3	6	0	-3.357689	-1.101630	-0.148846
4	7	0	-1.249886	-0.251026	-0.081750
5	5	0	-0.013777	0.696056	-0.044707
6	6	0	-4.815869	-1.216041	-0.155339
7	6	0	0.073193	-2.282194	-0.139582
8	6	0	1.266419	-1.568854	-0.097588
9	6	0	2.597813	-2.042357	-0.079426
10	7	0	1.275338	-0.177617	-0.064461
11	6	0	3.428984	-0.907146	-0.038116
12	1	0	0.105125	-3.363040	-0.172830
13	6	0	2.961525	-3.494351	-0.113205
14	6	0	4.891800	-0.937437	-0.026959
15	1	0	2.070756	-4.117180	-0.209667
16	1	0	3.491012	-3.790102	0.795407
17	1	0	3.628322	-3.715598	-0.949175
18	9	0	-0.032095	1.559276	-1.163600
19	9	0	-0.043529	1.484302	1.129126
20	8	0	-5.629030	-0.301022	-0.135941
21	8	0	-5.218116	-2.511674	-0.190138
22	6	0	-6.651784	-2.747393	-0.203835
23	1	0	-7.123440	-1.984946	-0.823914
24	6	0	-7.223571	-2.757699	1.203756
25	1	0	-6.749876	-3.720807	-0.684118
26	1	0	-7.126209	-1.776044	1.671063
27	1	0	-6.712781	-3.497666	1.824987
28	1	0	-8.285872	-3.016770	1.166294
29	8	0	5.374246	-2.198321	0.098905
30	8	0	5.652800	0.017003	-0.120824
31	6	0	6.821127	-2.318002	0.096903
32	1	0	7.219061	-1.722362	0.921163
33	1	0	7.202398	-1.902019	-0.838131
34	6	0	7.152110	-3.788564	0.244734
35	1	0	6.755610	-4.187658	1.181421
36	1	0	8.237610	-3.918835	0.249164
37	1	0	6.740859	-4.369128	-0.584416
38	6	0	-2.738253	-3.657702	-0.241717
39	1	0	-3.330297	-3.909977	-1.124036
40	1	0	-1.808674	-4.228221	-0.276626
41	1	0	-3.313163	-3.990041	0.625663
42	6	0	-2.571259	0.120774	-0.088270
43	6	0	-2.868696	1.512660	-0.029734
44	6	0	-4.092186	2.140429	-0.099300
45	1	0	-1.991804	2.137275	0.072971
46	7	0	-4.259385	3.476852	-0.080566
47	1	0	-5.001214	1.561310	-0.180693
48	6	0	-3.125665	4.386697	0.034654
49	6	0	-5.594687	4.061625	-0.048422
50	1	0	-2.385316	4.172853	-0.740423
51	1	0	-2.644528	4.297233	1.014507
52	1	0	-3.480962	5.408149	-0.091954

53	1	0	-6.335934	3.275356	-0.183778
54	1	0	-5.705159	4.795966	-0.851152
55	1	0	-5.778060	4.559399	0.909654
56	6	0	2.572740	0.269169	-0.032865
57	6	0	2.790863	1.676340	0.005667
58	6	0	3.982493	2.362734	0.073152
59	1	0	1.879575	2.258064	-0.021496
60	7	0	4.081676	3.703431	0.160496
61	1	0	4.922759	1.829124	0.061327
62	6	0	2.899384	4.556772	0.169773
63	6	0	5.381286	4.359936	0.079981
64	1	0	2.200342	4.228340	0.942772
65	1	0	2.387702	4.536378	-0.798704
66	1	0	3.205982	5.579200	0.385200
67	1	0	6.168289	3.609279	0.136639
68	1	0	5.500139	5.062528	0.909174
69	1	0	5.483602	4.909065	-0.862275

E_h = -1717.610586 Hartree

Table S10. DFT optimized geometry of compound **10**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.496214	-1.610554	-0.275518
2	6	0	-1.185030	-1.076697	-0.185347
3	6	0	-3.356245	-0.499929	-0.283177
4	7	0	-1.260420	0.320159	-0.147060
5	5	0	-0.033528	1.279247	-0.011813
6	6	0	-4.820693	-0.448401	-0.330359
7	6	0	0.046532	-1.718923	-0.133316
8	6	0	1.242305	-1.017476	-0.033349
9	6	0	2.579475	-1.487570	0.023904
10	7	0	1.244907	0.380551	0.028088
11	6	0	3.380527	-0.337545	0.115319
12	1	0	0.075628	-2.800831	-0.171084
13	6	0	3.000544	-2.920253	-0.013555
14	6	0	4.839768	-0.213537	0.180002
15	1	0	2.145736	-3.588197	-0.126833
16	1	0	3.531269	-3.189643	0.902782
17	1	0	3.691328	-3.098596	-0.840952
18	9	0	0.029960	2.143774	-1.111322
19	9	0	-0.141942	2.017567	1.172508
20	8	0	-5.467741	0.582347	-0.213767
21	8	0	-5.375905	-1.660055	-0.515187
22	6	0	-6.834505	-1.710319	-0.556619
23	1	0	-7.191908	-0.824531	-1.081070
24	6	0	-7.416582	-1.813402	0.841780
25	1	0	-7.043552	-2.598771	-1.150670
26	1	0	-7.203165	-0.913438	1.421555
27	1	0	-7.011719	-2.680769	1.368707

28	1	0	-8.502203	-1.928663	0.775734
29	8	0	5.461979	-1.399245	0.297627
30	8	0	5.435368	0.853132	0.130094
31	6	0	6.918674	-1.346330	0.353762
32	1	0	7.203298	-0.726738	1.205996
33	1	0	7.276841	-0.864371	-0.557721
34	6	0	7.414625	-2.769902	0.486246
35	1	0	7.032583	-3.234568	1.398138
36	1	0	8.506693	-2.770240	0.532789
37	1	0	7.107802	-3.373806	-0.370857
38	6	0	-2.842733	-3.062056	-0.341780
39	1	0	-3.511083	-3.337361	0.477432
40	1	0	-3.373115	-3.288924	-1.269728
41	1	0	-1.953354	-3.691339	-0.289128
42	6	0	-2.554148	0.674266	-0.211410
43	6	0	2.518566	0.795881	0.122507
44	6	0	2.902912	2.233654	0.212402
45	1	0	3.524393	2.401698	1.096038
46	1	0	2.019315	2.867088	0.311189
47	6	0	3.708968	2.735915	-0.988773
48	1	0	3.795206	2.050075	-1.852131
49	8	0	4.194263	3.841890	-1.018556
50	6	0	-3.010070	2.093545	-0.195288
51	1	0	-3.671000	2.284784	-1.044685
52	1	0	-2.161600	2.774726	-0.282930
53	6	0	-3.797409	2.476064	1.061169
54	1	0	-3.835772	1.724771	1.872234
55	8	0	-4.323359	3.556406	1.185390

E_h = -1600.048538 Hartree

Table S11. DFT optimized geometry of compound **11**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.540824	1.676667	0.025016
2	6	0	-1.214001	1.167525	0.070608
3	7	0	-1.242761	-0.231773	0.056245
4	6	0	-2.541308	-0.611237	0.000600
5	6	0	-3.370662	0.548950	-0.020891
6	6	0	-0.000016	1.849335	0.087562
7	6	0	1.213997	1.167562	0.070396
8	7	0	1.242775	-0.231729	0.056219
9	6	0	2.541333	-0.611179	0.000705
10	6	0	3.370687	0.549010	-0.020856
11	6	0	2.540804	1.676729	0.024703
12	6	0	2.953456	3.111411	0.014607
13	6	0	-2.953605	3.111306	0.014517
14	5	0	0.000021	-1.153684	0.194153
15	9	0	0.000012	-2.131754	-0.813788
16	9	0	0.000065	-1.789436	1.447791

17	6	0	-4.812348	0.452568	-0.081880
18	8	0	-5.606759	1.393888	-0.106749
19	1	0	-0.000052	2.931997	0.095095
20	6	0	3.106768	-1.904245	-0.034371
21	6	0	4.472234	-1.972347	-0.089348
22	6	0	4.812373	0.452585	-0.081924
23	7	0	5.293372	-0.874687	-0.111691
24	8	0	5.606837	1.393851	-0.106853
25	6	0	6.751688	-1.034560	-0.171915
26	1	0	2.512415	-2.806444	-0.027966
27	1	0	4.984620	-2.925333	-0.120967
28	6	0	-3.106777	-1.904288	-0.034567
29	1	0	-2.512448	-2.806504	-0.028255
30	6	0	-4.472250	-1.972355	-0.089452
31	1	0	-4.984655	-2.925329	-0.121135
32	7	0	-5.293382	-0.874681	-0.111598
33	6	0	-6.751700	-1.034524	-0.171855
34	1	0	-6.986030	-2.096600	-0.188427
35	1	0	-7.210305	-0.567172	0.699592
36	1	0	-7.138952	-0.555095	-1.070980
37	1	0	7.210276	-0.567504	0.699704
38	1	0	6.985981	-2.096639	-0.188814
39	1	0	7.139000	-0.554860	-1.070865
40	1	0	-2.099197	3.783851	0.103999
41	1	0	-3.486587	3.350900	-0.910051
42	1	0	-3.645450	3.316680	0.835396
43	1	0	3.500425	3.347390	-0.902540
44	1	0	2.097712	3.784094	0.088871
45	1	0	3.632701	3.320397	0.845216

E_h = -1328.812386 Hartree

Table S12. DFT optimized geometry of compound **12**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457813	1.395995	-0.148044
2	6	0	-0.169454	0.728762	-0.077524
3	6	0	-2.420825	0.352512	-0.095953
4	7	0	-0.371757	-0.648461	-0.020053
5	6	0	-1.712459	-0.903835	-0.050696
6	5	0	0.768979	-1.706473	-0.040286
7	6	0	-3.856043	0.541335	0.126931
8	6	0	-2.170779	-2.250063	-0.093091
9	6	0	-1.522932	2.818855	-0.178485
10	6	0	1.095357	1.262800	-0.087310
11	6	0	2.246551	0.449267	-0.022368
12	6	0	3.606035	0.790466	0.002758
13	7	0	2.120658	-0.941530	0.022414
14	6	0	4.313452	-0.441893	0.054778
15	1	0	1.224322	2.335236	-0.157939

16	6	0	4.150167	2.185125	-0.021699
17	6	0	3.358886	-1.487342	0.063495
18	6	0	5.756975	-0.665145	0.092846
19	6	0	3.578048	-2.964927	0.078215
20	6	0	-3.399880	-2.637503	-0.571386
21	1	0	2.730214	-3.474402	0.534333
22	1	0	4.494113	-3.206069	0.614325
23	1	0	3.691543	-3.344344	-0.943811
24	1	0	3.346769	2.921469	-0.091405
25	1	0	4.823623	2.332866	-0.869917
26	1	0	4.731263	2.399033	0.879307
27	6	0	-2.609766	3.604990	-0.497643
28	9	0	0.642511	-2.562591	1.078766
29	9	0	0.711056	-2.483246	-1.213261
30	7	0	-3.862704	-3.899606	-0.608940
31	6	0	-3.057927	-5.008079	-0.107422
32	6	0	-5.067108	-4.234153	-1.361589
33	1	0	-1.445923	-3.004068	0.183677
34	1	0	-4.085095	-1.906493	-0.982306
35	1	0	-5.605640	-3.320079	-1.608764
36	1	0	-5.714044	-4.875930	-0.759059
37	1	0	-4.815535	-4.758534	-2.289581
38	1	0	-2.669824	-4.768008	0.884284
39	1	0	-2.216943	-5.223109	-0.775745
40	1	0	-3.687709	-5.893559	-0.034491
41	8	0	-4.541060	1.447727	-0.329674
42	8	0	-4.377484	-0.390738	0.962858
43	6	0	-5.804333	-0.303140	1.228864
44	1	0	-6.309627	0.029292	0.321487
45	6	0	-6.084345	0.626387	2.397234
46	1	0	-6.092023	-1.330097	1.454799
47	1	0	-5.803701	1.652409	2.152148
48	1	0	-5.530198	0.309833	3.284187
49	1	0	-7.152163	0.608114	2.634676
50	7	0	-2.624108	4.950527	-0.481240
51	6	0	-1.448420	5.722855	-0.098175
52	6	0	-3.756759	5.686880	-1.032707
53	1	0	-4.077559	6.459831	-0.329950
54	1	0	-4.583648	4.999652	-1.205632
55	1	0	-3.487868	6.163865	-1.981256
56	1	0	-1.050348	5.356949	0.850861
57	1	0	-1.737038	6.765899	0.022693
58	1	0	-0.664014	5.659932	-0.860849
59	1	0	-0.582585	3.323183	0.018075
60	1	0	-3.541657	3.138394	-0.787920
61	8	0	6.458687	0.495347	0.164885
62	8	0	6.312950	-1.754202	0.065421
63	6	0	7.902064	0.349327	0.205217
64	1	0	8.224002	-0.174933	-0.697284
65	1	0	8.164481	-0.267270	1.067655
66	6	0	8.494615	1.740186	0.298127
67	1	0	8.216498	2.343931	-0.569142

68	1	0	9.585288	1.671573	0.332542
69	1	0	8.154792	2.250772	1.202447

E_h = -1717.676099 Hartree

Table S13. DFT optimized geometry of compound **13**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.025664	-1.165766	-0.073530
2	6	0	0.718572	-0.629922	-0.015209
3	6	0	2.894798	-0.075284	0.112236
4	7	0	0.800989	0.747218	0.200264
5	6	0	2.098911	1.088867	0.285045
6	5	0	-0.425438	1.716951	0.293984
7	6	0	4.359633	-0.046318	0.117400
8	6	0	-0.524699	-1.252056	-0.141090
9	6	0	-1.711721	-0.544852	-0.063191
10	6	0	-3.056637	-0.995442	-0.169021
11	7	0	-1.711173	0.840654	0.144701
12	6	0	-3.853331	0.148885	-0.028335
13	1	0	-0.561354	-2.321874	-0.306292
14	6	0	-3.471916	-2.413290	-0.388013
15	6	0	-2.983536	1.267767	0.166179
16	6	0	-5.318082	0.261798	-0.068154
17	6	0	-3.342997	2.702034	0.345171
18	1	0	-2.537712	3.246777	0.834126
19	1	0	-4.264112	2.791869	0.918310
20	1	0	-3.529064	3.160084	-0.632305
21	1	0	-2.609328	-3.072612	-0.492369
22	1	0	-4.087288	-2.502016	-1.286001
23	1	0	-4.081358	-2.768808	0.446153
24	9	0	-0.420481	2.362837	1.537298
25	9	0	-0.358433	2.657451	-0.738317
26	8	0	5.026840	0.975296	0.150529
27	8	0	4.889897	-1.286103	0.083663
28	6	0	6.347624	-1.384107	0.078923
29	1	0	6.741759	-0.604092	0.729721
30	6	0	6.895132	-1.277013	-1.332613
31	1	0	6.539002	-2.362167	0.517507
32	1	0	6.693663	-0.291430	-1.756244
33	1	0	6.455427	-2.040008	-1.979283
34	1	0	7.978325	-1.426799	-1.313371
35	8	0	-5.919633	-0.941092	-0.171034
36	8	0	-5.937391	1.311100	-0.016750
37	6	0	-7.375130	-0.913199	-0.222442
38	1	0	-7.675521	-0.304124	-1.077190
39	1	0	-7.739493	-0.431665	0.687016
40	6	0	-7.848913	-2.345763	-0.342566
41	1	0	-7.466577	-2.810452	-1.254373
42	1	0	-8.941220	-2.365023	-0.380101

43	1	0	-7.525078	-2.938985	0.515808
44	6	0	2.380382	-2.602025	-0.282724
45	1	0	1.485692	-3.200442	-0.484638
46	1	0	3.037840	-2.725786	-1.147050
47	6	0	2.560679	2.488050	0.511786
48	1	0	1.725334	3.130473	0.795674
49	1	0	3.285532	2.515435	1.329472
50	6	0	3.253350	3.116755	-0.700335
51	1	0	3.256141	2.525107	-1.635192
52	8	0	3.752599	4.215796	-0.655985
53	6	0	3.086576	-3.251088	0.909472
54	1	0	3.057049	-2.688908	1.862847
55	8	0	3.620801	-4.333147	0.839369

E_h = -1600.145481 Hartree

Table S14. DFT optimized geometry of compound **14**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.022532	-2.044920	-1.099359
2	9	0	0.030267	-1.995034	1.194830
3	8	0	5.225255	0.988552	-0.019728
4	8	0	-5.652085	-1.842048	-0.119268
5	8	0	-6.037127	0.375863	0.026216
6	7	0	0.891879	-0.054902	0.007241
7	7	0	-1.568126	-0.591249	0.014648
8	7	0	4.285346	3.055084	-0.015365
9	6	0	2.814444	1.162874	-0.001772
10	6	0	1.734426	2.064797	0.004036
11	6	0	0.529353	1.292498	0.010082
12	6	0	-0.780917	1.704741	0.013386
13	1	0	-1.000437	2.765319	0.012978
14	6	0	-1.841628	0.778948	0.011430
15	6	0	-3.231430	0.972864	-0.003379
16	6	0	-3.802838	-0.327475	-0.017726
17	6	0	-2.740819	-1.265698	-0.002969
18	6	0	-2.795578	-2.758185	-0.023501
19	1	0	-2.742329	-3.127832	-1.053674
20	1	0	-3.734070	-3.106723	0.401889
21	1	0	-1.953187	-3.179444	0.524949
22	6	0	-3.917510	2.303234	-0.008091
23	1	0	-4.568238	2.409619	-0.879774
24	1	0	-3.193566	3.120615	-0.019890
25	1	0	-4.553558	2.422368	0.872884
26	6	0	-5.216441	-0.702189	-0.043582
27	6	0	-7.458408	0.079195	0.000392
28	1	0	-7.693190	-0.564148	0.851237
29	1	0	-7.680722	-0.473593	-0.914871
30	6	0	-8.198030	1.399242	0.063071
31	1	0	-9.275643	1.215008	0.047113

32	1	0	-7.946062	2.030903	-0.792164
33	1	0	-7.957092	1.941214	0.980821
34	6	0	1.928675	3.463115	0.000896
35	1	0	1.109627	4.169894	0.005524
36	6	0	3.218472	3.908624	-0.008896
37	1	0	3.466387	4.962099	-0.012200
38	6	0	4.175035	1.644474	-0.012669
39	6	0	5.654451	3.586083	-0.026574
40	1	0	5.604736	4.672704	-0.026076
41	1	0	6.178061	3.236300	-0.916118
42	5	0	-0.145060	-1.220253	0.029339
43	1	0	6.192521	3.236136	0.854204
44	6	0	2.257794	-0.183195	0.000884
45	6	0	2.835151	-1.472945	-0.001623
46	6	0	4.188651	-1.755742	0.003691
47	1	0	2.131171	-2.294185	-0.007337
48	7	0	4.701727	-2.991344	0.007452
49	1	0	4.906960	-0.943097	0.004864
50	6	0	3.844573	-4.175225	0.007052
51	6	0	6.145980	-3.205694	0.006461
52	1	0	3.220952	-4.198832	-0.890827
53	1	0	3.197401	-4.180768	0.888209
54	1	0	4.473095	-5.063256	0.024519
55	1	0	6.653039	-2.242464	0.007795
56	1	0	6.444618	-3.766066	-0.883873
57	1	0	6.445075	-3.769026	0.894709

E_h = -1523.211024 Hartree

Table S15. DFT optimized geometry of compound **15**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.233528	-1.944892	0.659467
2	9	0	0.413073	-1.584943	-1.599274
3	8	0	-4.293552	2.065973	-0.248265
4	8	0	5.927724	-2.602906	0.060347
5	8	0	6.679163	-0.482518	0.221287
6	7	0	-0.204566	0.297977	-0.189937
7	7	0	2.125305	-0.654501	-0.142487
8	7	0	-3.026023	3.926947	0.047953
9	6	0	-1.892619	1.823030	-0.125159
10	6	0	-0.680004	2.518019	0.034785
11	6	0	0.376822	1.553411	-0.006823
12	6	0	1.734049	1.728023	0.110267
13	1	0	2.127391	2.726693	0.255250
14	6	0	2.622069	0.636972	0.052110
15	6	0	4.019112	0.582074	0.170276
16	6	0	4.363671	-0.790805	0.048799
17	6	0	3.164822	-1.520695	-0.147327
18	6	0	2.968021	-2.990882	-0.323219

19	1	0	2.718391	-3.460541	0.634678
20	1	0	3.882236	-3.451852	-0.689472
21	1	0	2.144728	-3.186564	-1.010856
22	6	0	4.913492	1.762811	0.386676
23	1	0	5.495982	1.654996	1.305320
24	1	0	4.336724	2.687470	0.454823
25	1	0	5.633231	1.867790	-0.429177
26	6	0	5.690588	-1.404419	0.106207
27	6	0	8.026414	-1.019387	0.291849
28	1	0	8.219470	-1.590672	-0.618813
29	1	0	8.082562	-1.704349	1.140557
30	6	0	8.973571	0.152824	0.441052
31	1	0	10.002326	-0.213440	0.495076
32	1	0	8.761642	0.714543	1.354022
33	1	0	8.896134	0.831160	-0.412108
34	6	0	-0.639000	3.919159	0.201956
35	1	0	0.284297	4.468815	0.326924
36	6	0	-1.834326	4.577684	0.201000
37	1	0	-1.903400	5.651030	0.321399
38	6	0	-3.151450	2.527788	-0.122557
39	6	0	-4.285021	4.682653	0.055403
40	1	0	-4.055399	5.737851	0.185507
41	1	0	-4.918833	4.335244	0.871208
42	5	0	0.623501	-1.017569	-0.325737
43	1	0	-4.812471	4.528240	-0.885665
44	6	0	-1.569637	0.409915	-0.265976
45	6	0	-2.356672	-0.748367	-0.445955
46	6	0	-3.732353	-0.793000	-0.555893
47	1	0	-1.811900	-1.684090	-0.498793
48	7	0	-4.425123	-1.920822	-0.743035
49	1	0	-4.315224	0.120953	-0.497948
50	6	0	-5.883650	-1.997551	-0.798014
51	1	0	-6.258236	-0.981149	-0.935978
52	1	0	-6.162713	-2.574541	-1.685418
53	1	0	-3.919850	-2.797733	-0.786993
54	6	0	-6.488105	-2.631158	0.460179
55	1	0	-6.053721	-3.627874	0.606007
56	1	0	-6.202301	-2.030673	1.331471
57	6	0	-8.014617	-2.742619	0.374960
58	1	0	-8.286788	-3.334556	-0.507571
59	1	0	-8.443699	-1.744810	0.221909
60	6	0	-8.627850	-3.377596	1.625686
61	1	0	-9.716056	-3.447742	1.540491
62	1	0	-8.239200	-4.388502	1.785365
63	1	0	-8.400030	-2.788247	2.519616

E_h = -1601.865881 Hartree

Table S16. DFT optimized geometry of compound **16**.

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

1	9	0	-0.192279	2.383144	-0.925621
2	9	0	-0.109579	2.256164	1.363552
3	8	0	-5.542093	0.181301	0.199354
4	8	0	5.483341	1.472436	0.168427
5	8	0	5.609289	-0.762864	-0.116557
6	7	0	-1.214509	0.468164	0.145980
7	7	0	1.287330	0.730791	0.086058
8	7	0	-5.031826	-2.053580	0.064349
9	6	0	-3.248606	-0.480305	0.124531
10	6	0	-2.313595	-1.532354	0.022922
11	6	0	-1.025098	-0.917165	0.035441
12	6	0	0.246022	-1.457894	-0.035861
13	1	0	0.351362	-2.533348	-0.112459
14	6	0	1.390649	-0.662034	-0.007386
15	6	0	2.756938	-1.022234	-0.049927
16	6	0	3.474674	0.188018	0.027831
17	6	0	2.530089	1.250620	0.107189
18	6	0	2.777523	2.716730	0.219797
19	1	0	3.683565	2.989078	-0.318011
20	1	0	2.930180	2.991134	1.269361
21	1	0	1.928680	3.283193	-0.160111
22	6	0	3.277019	-2.420161	-0.151748
23	1	0	3.875827	-2.546691	-1.056863
24	1	0	2.465076	-3.148798	-0.170857
25	1	0	3.931269	-2.653755	0.691361
26	6	0	4.927151	0.393935	0.037124
27	6	0	7.059187	-0.641252	-0.111655
28	1	0	7.363549	-0.196030	0.837725
29	1	0	7.349316	0.037369	-0.916197
30	6	0	7.628564	-2.031276	-0.301385
31	1	0	8.720543	-1.979993	-0.304156
32	1	0	7.303472	-2.461473	-1.251604
33	1	0	7.318904	-2.696128	0.508438
34	6	0	-2.763107	-2.869403	-0.057948
35	1	0	-2.096184	-3.717850	-0.134576
36	6	0	-4.117028	-3.070686	-0.030558
37	1	0	-4.543525	-4.063969	-0.084423
38	6	0	-4.671862	-0.691979	0.137530
39	6	0	-6.471767	-2.343123	0.079188
40	1	0	-6.611791	-3.421229	0.054344
41	1	0	-6.948236	-1.884814	-0.787629
42	5	0	-0.051976	1.522596	0.172729
43	1	0	-6.917525	-1.929769	0.983498
44	6	0	-2.531960	0.736994	0.206147
45	6	0	-3.104293	2.106801	0.332197
46	1	0	-3.700463	2.177578	1.247243
47	1	0	-2.315212	2.857654	0.402470
48	6	0	-4.026990	2.497772	-0.825038
49	1	0	-4.031576	1.828491	-1.705773
50	8	0	-4.691617	3.506497	-0.803960

E_h = -1464.428991 Hartree

Table S17. DFT optimized geometry of compound **17**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-0.272256	2.572198	-1.145920
2	9	0	-0.239861	2.560177	1.150441
3	8	0	-5.837836	0.814805	-0.019566
4	8	0	5.287580	1.287134	0.096656
5	8	0	5.243190	-0.965854	-0.029484
6	7	0	-1.467397	0.803944	0.000822
7	7	0	1.048247	0.864150	-0.013523
8	7	0	-5.458841	-1.442143	0.003580
9	6	0	-2.760011	1.181707	-0.010623
10	6	0	-3.572734	0.018185	-0.007634
11	6	0	-2.718866	-1.107219	0.006834
12	6	0	-1.384938	-0.596195	0.009614
13	6	0	-0.163084	-1.239223	0.015080
14	1	0	-0.141557	-2.322409	0.024877
15	6	0	1.043359	-0.534575	0.007132
16	6	0	2.375878	-1.001320	0.019478
17	6	0	3.186948	0.153448	0.013914
18	6	0	2.327827	1.287492	-0.009011
19	6	0	2.686663	2.735369	-0.006372
20	1	0	3.622580	2.894051	-0.538537
21	1	0	2.836440	3.082985	1.021761
22	1	0	1.891966	3.330068	-0.454263
23	6	0	2.786086	-2.439113	0.038954
24	1	0	3.377755	-2.687057	-0.845629
25	1	0	1.919131	-3.101138	0.070128
26	1	0	3.414918	-2.653283	0.906277
27	6	0	4.649847	0.247968	0.032236
28	6	0	6.697394	-0.954422	-0.008687
29	1	0	7.024781	-0.473579	0.915419
30	1	0	7.048912	-0.353330	-0.849635
31	6	0	7.160495	-2.393029	-0.100821
32	1	0	8.253138	-2.425876	-0.087490
33	1	0	6.815045	-2.856858	-1.027769
34	1	0	6.789688	-2.979316	0.743253
35	6	0	-3.254531	-2.413548	0.016510
36	1	0	-2.643167	-3.306020	0.026283
37	6	0	-4.618695	-2.523039	0.014480
38	1	0	-5.111409	-3.486791	0.021932
39	6	0	-5.011259	-0.099129	-0.009237
40	6	0	-6.914856	-1.632193	0.003189
41	1	0	-7.128370	-2.698596	0.018910
42	1	0	-7.344472	-1.178986	-0.890196
43	6	0	-3.190794	2.607248	-0.041962
44	5	0	-0.227403	1.762241	-0.001817
45	1	0	-2.633697	3.193542	0.690918

46	1	0	-2.984768	3.038262	-1.026677
47	1	0	-4.258856	2.672986	0.152785
48	1	0	-7.347884	-1.152028	0.880612

E_h = -1351.083286 Hartree

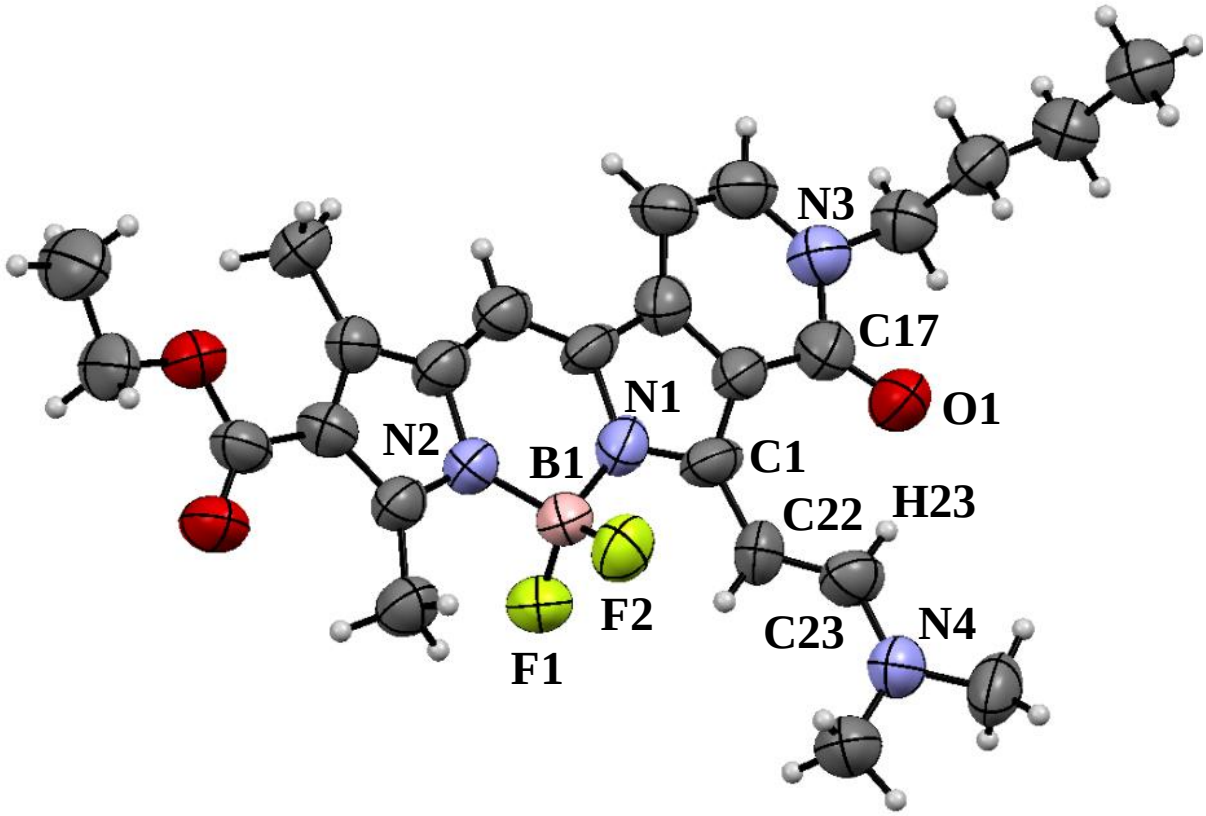

Figure S81. X-ray structure of BODIPY **14**. Thermal ellipsoids are at 50% probability level. Single crystal of BODIPY **14** suitable for X-ray crystallographic analysis were obtained by slow evaporation from their DCM/methanol solutions. X-ray diffraction data for **14** was collected on Rigaku RAPID II Image Plate system using graphite-monochromated Cu-Kα radiation (λ = 1.54187 Å) at 123 K. All diffractometer manipulations, including data collection, integration and scaling were carried out using the Bruker APEX3 software suite.[87] Absorption corrections were applied using SADABS.

Crystal data for **14** $C_{25}H_{31}B_1F_2N_4O_3 \cdot C_7H_8$: MW = 576.48, monoclinic, space group P_{21}/c, a = 15.1030(5), b = 12.2789(3), c = 16.4063(12) Å, β = 95.270(7)°, V = 3029.7(3) $Å^3$, Z = 4, μ = 0.732 mm^{-1}, 17365 reflections, (1392 I > 2σ(I)), θ_{max} = 58.936; final R_1 = 0.0948, R_w(all) = 0.2199. Additional crystallographic information for all compounds may be found in the CIF included as Supporting Information or accessible from the Cambridge Structural Database: CCDC-1882628.

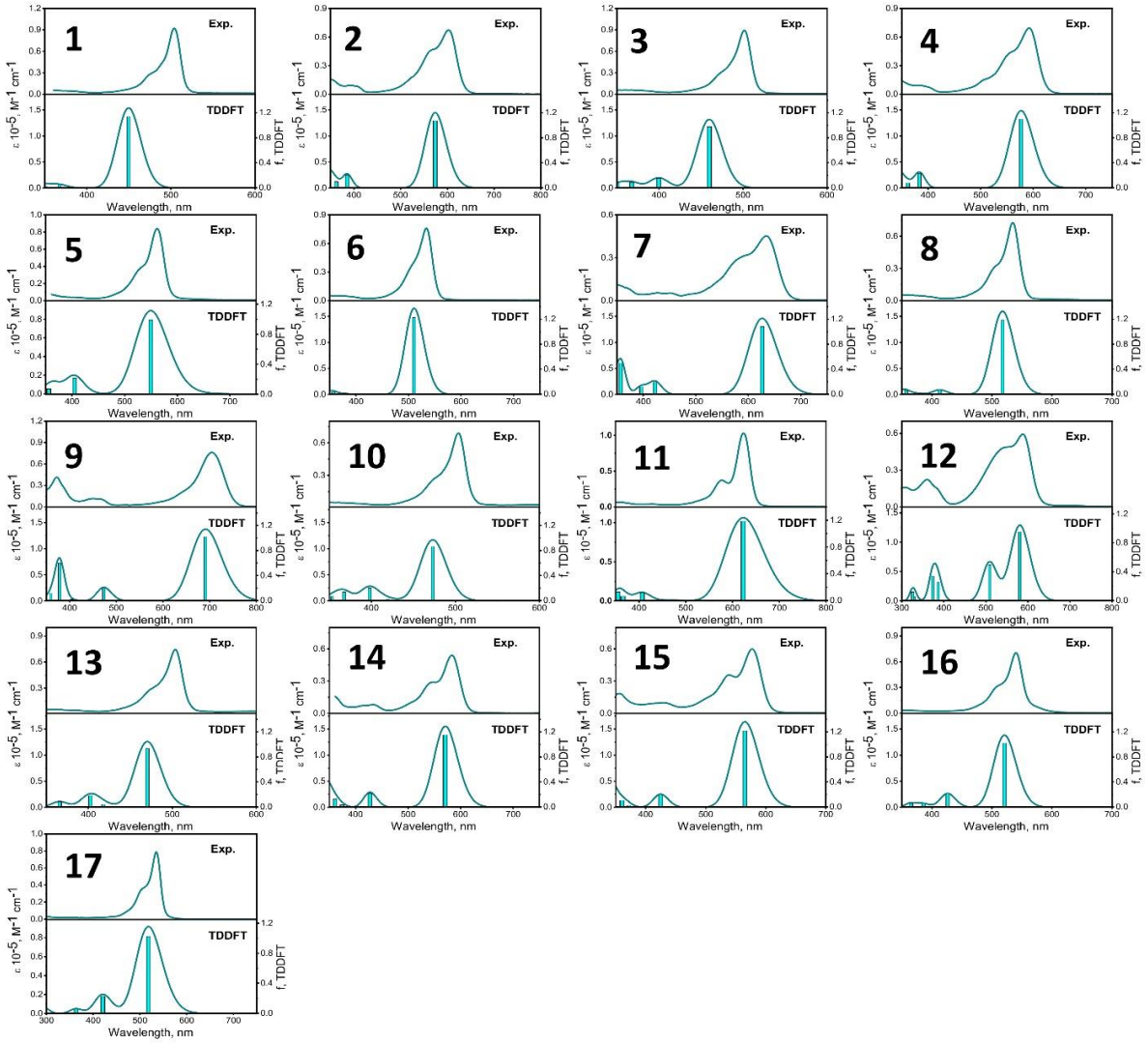

Figure S82. Comparison between experimental and TDDFT-predicted UV-vis spectra of BODIPYs **1** – **17** in DCM.