Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Meso-aryloxy and *meso*-arylaza linked BODIPY dimers: synthesis, structure and properties.

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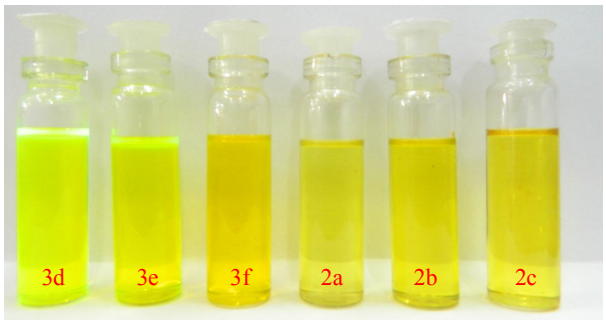


Figure S1. The aryloxy and arylaza BODIPYs in day light.

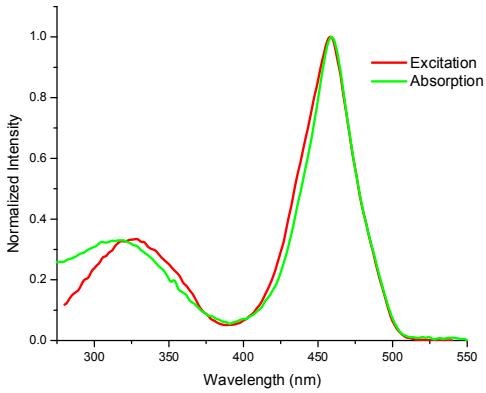


Figure S2. Normalized absorption and excitation spectra of **3d**

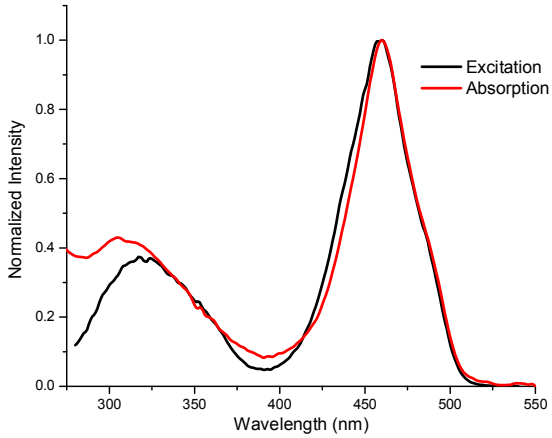


Figure S3. Normalized absorption and excitation spectra of **3e**

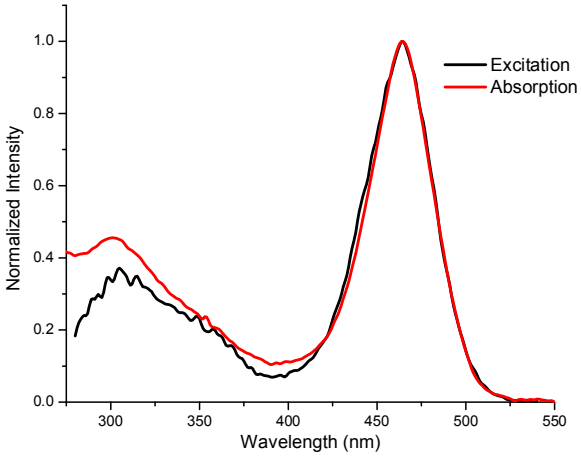


Figure S4. Normalized absorption and excitation spectra of **3f**

Electrochemical Characterizations

Electrochemical characterization of all compounds was done by cyclic voltametry (CV) and Differential pulse voltametry (DPV). Voltamograms were recorded on a CHI620D electrochemical analyzer using glassy carbon as working electrode, Pt wire as the counter electrode, and saturated calomel electrode as the reference electrode (SCE). The scan speed was 100 mVS^{-1}. A solution of tetrabutylammonium- hexafluorophosphate ($TBAPF_6$) in anhydrous $CH_{2c}l_2$ (0.1 M) was employed as the supporting electrolyte. The half-wave oxidation potentials were corrected to ferrocene as per IUPAC guidelines.[1]

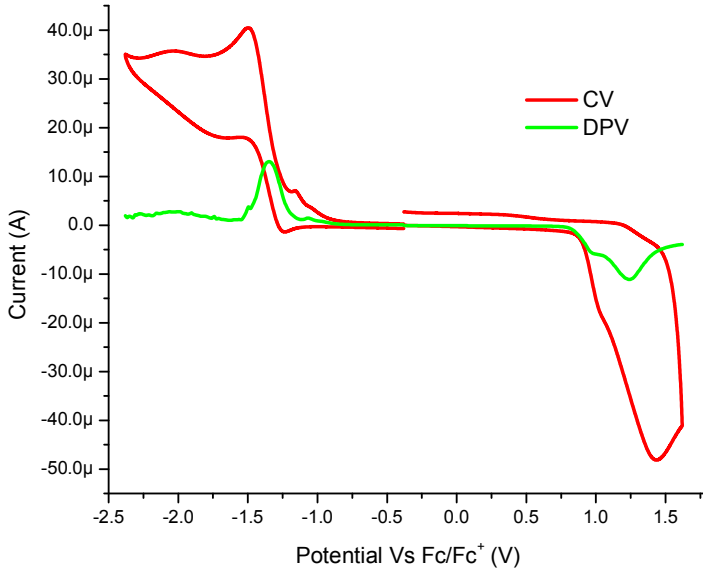


Figure S5. CV and DPV plots of BODIPY dimer **2a.**

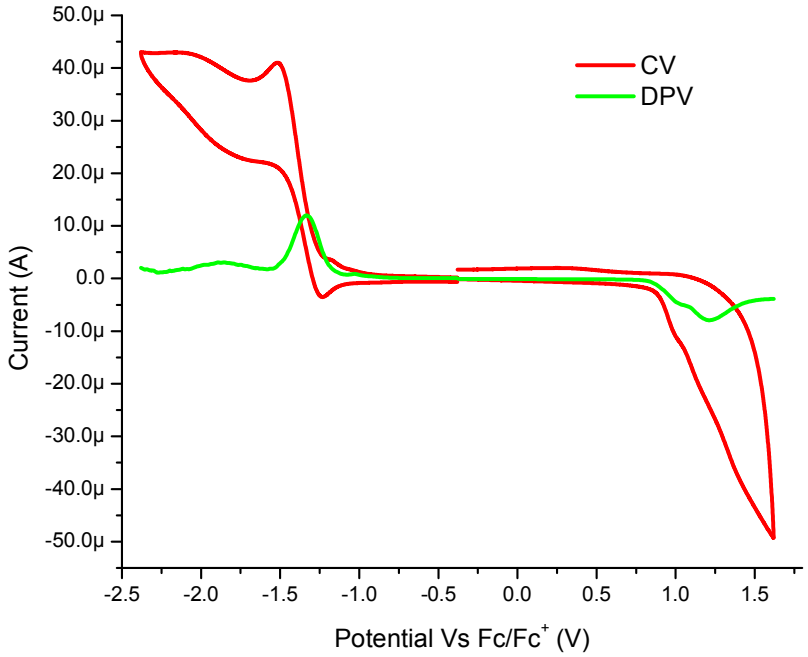


Figure S6. CV and DPV plots of BODIPY dimer **2b.**

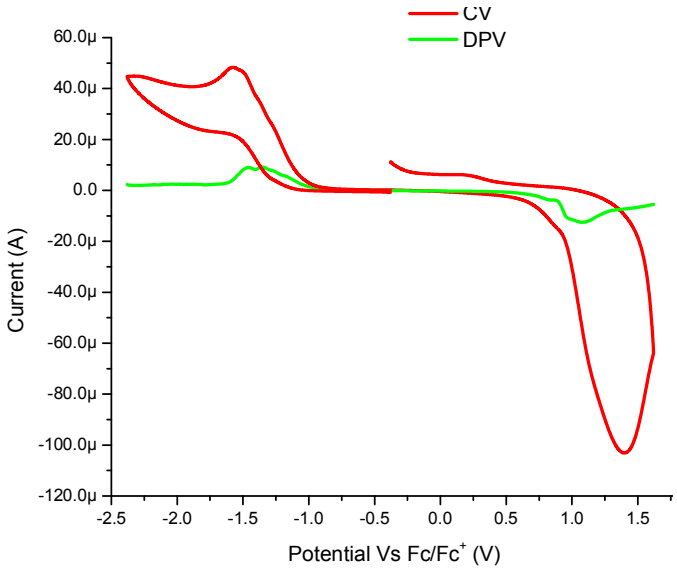


Figure S7. CV and DPV plots of BODIPY dimer **2c.**

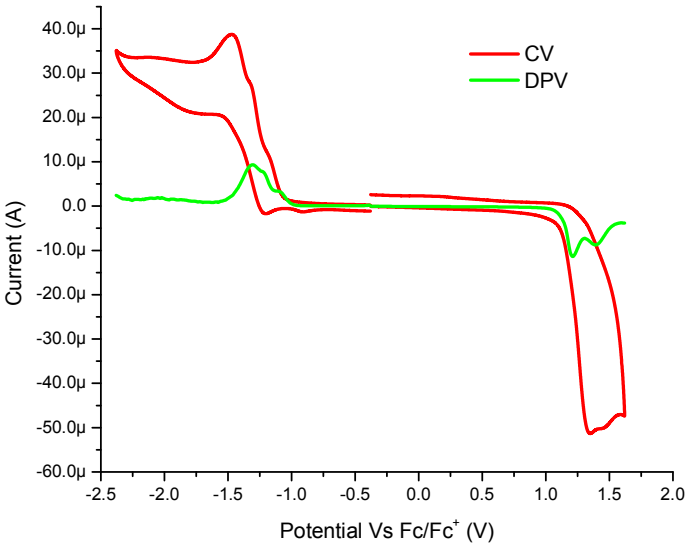


Figure S8. CV and DPV plots of BODIPY dimer **3d.**

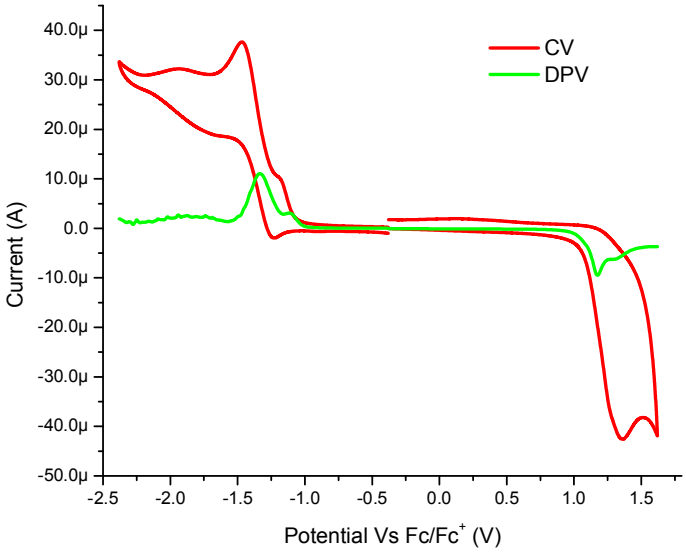


Figure S9. CV and DPV plots of BODIPY dimer **3e.**

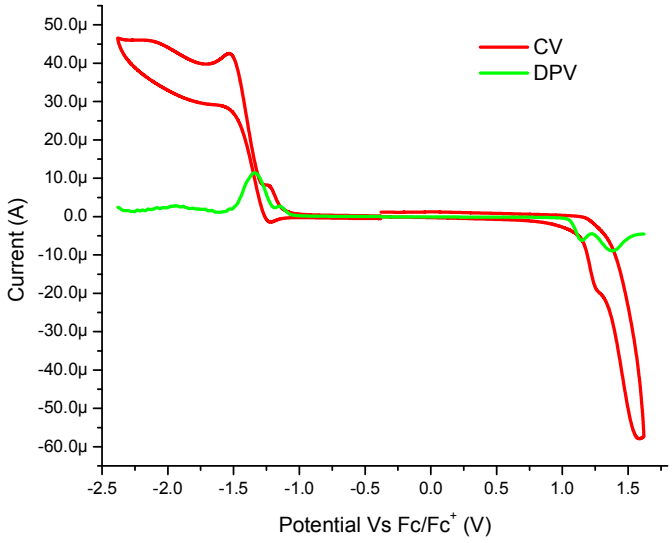


Figure S10. CV and DPV plots of BODIPY dimer **3f.**

Single Crystal X-ray Diffraction Studies.

Single crystal X-ray structural studies of **1**, **2b, 2c** and **3e** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 293(2) K using graphite-monochromated Mo Kα radiation (λ_α = 0.71073 Å) for **1** and at 150(2) K using

graphite-monochromated Cu K\α radiation (λ_α = 1.5418 Å) for **2b, 2c** and **3e**. The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on $F^{2.1}$. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2U_{eq} of their parent atoms. The crystal and refinement data are summarized in Table S2 (ESI). The CCDC 964025, 964026, 966965 and 964027 contain the supplementary crystallographic data for **1, 2b, 2c** and **3e** respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

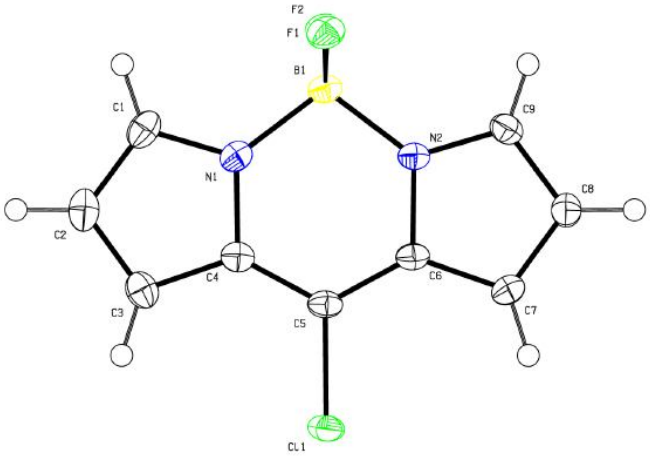


Figure S11. Crystal structure of **1**

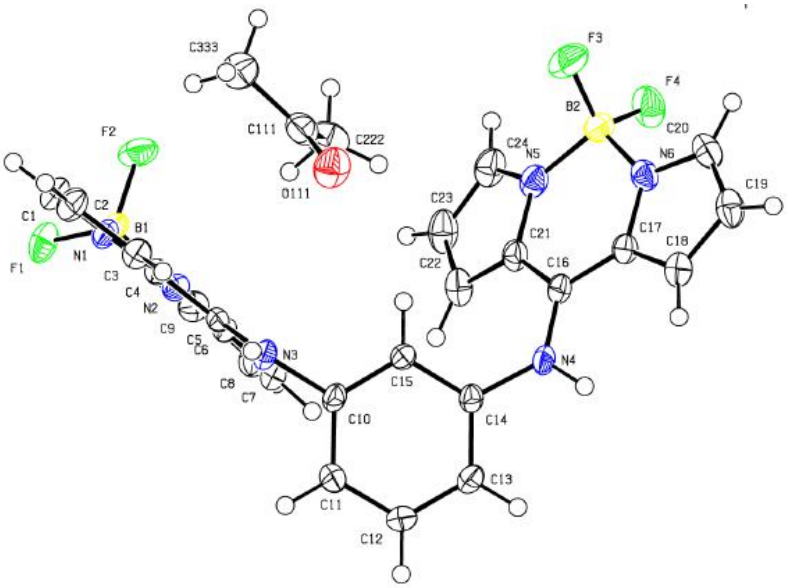


Figure S12. Crystal structure of **2b**

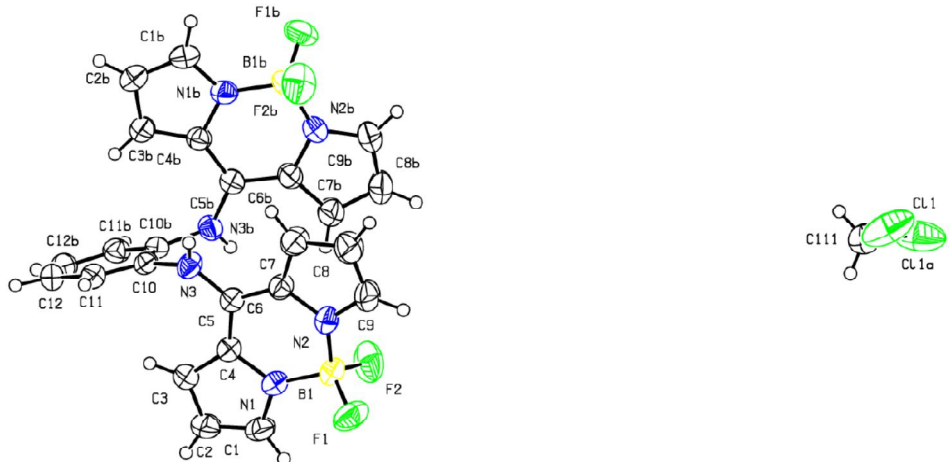


Figure S13. Crystal structure of 2c

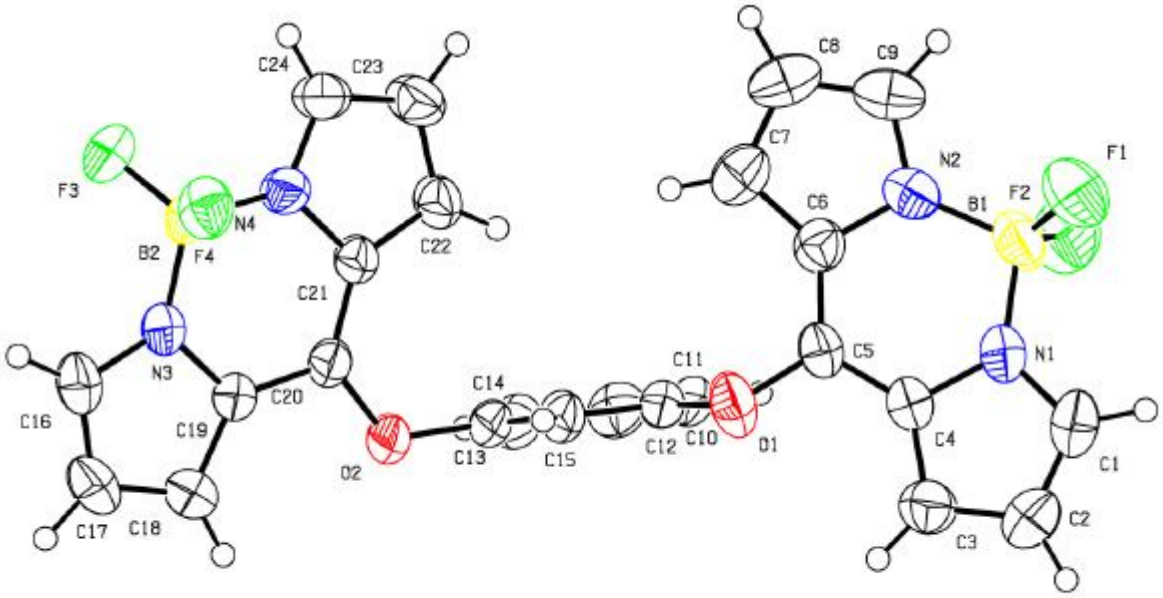


Figure S14. Crystal structure of **3e**

Table S1. Distance and angle of intermolecular interactions in the crystal structures.

	Distance (Å)	Angle (°)
1		
C(1)-H(1)---F(1)	2.720	98.37
C(9)-H(9)---F(1)	2.514	163.63
C(7)-H(7)---F(1)	2.517	161.44
C(3)-H(3)---F(2)	2.651	119.59
C(8)-H(8)---F(2)	2.420	129.12
C(1)-H(1)---Cl(1)	2.865	167.25
C(1)-H(1)---Cl(1)	2.894	134.44
2b		
C(13)-H(13)---F(2)	2.532	152.68
N(3)-H(3)---O(111)	2.059	163.26
N(4)-H(4)---F(1)	2.167	147.33
C(3)-H(3A)---O(111)	2.446	151.51
F(1)---N(4)	2.947	
C(18)-H(18)---F(1)	2.460	152.55
C(12)-H(12)---π (pyrrolic)	2.989	
C(2)-H(2)---F(1)	2.663	148.96
C(19)-H(19)---F(2)	2.377	174.75
C(8)-H(8)---F(3)	2.577	118.36
C(13)-H(13)---π (pyrrolic)	3.289	
C(9)-H(9)---F(4)	2.438	140.98
N(4)-H(4)---F(4)	2.556	120.97
C(20)-H(20)---π (BODIPY)	2.660	
2c		
C(11)-H(11)---F(2)	2.571	125.00
C(12)-H(12)---F(2)	2.658	121.31
C(101)-H(101)---F(1)	2.466	137.05
C(1)-H(1)---Cl(1)	2.850	164.97
N(3)-H(3)---Cl(1)	2.698	121.31
3e		
C(1)-H(1)---F(4)	2.532	132.10
C(18)-H(18)---π (Ph)	3.105	
C(11)-H(11)---F(4)	2.447	146.92
C(13)-H(13)---F(3)	2.669	127.23
C(23)-H(23)---F(2)	2.529	135.12

Table S2. Crystal structure and data refinement parameters

Compound	**1**	**2b**	**2c**	**3e**
Empirical formula	$C_9 H_6 B Cl F_2 N_2$	$C_{27} H_{24} B_2 F_4 N_6 O$	$C_{25} H_{20} B_2 Cl_2 F_4 N_6$	$C_{24} H_{16} B_2 F_4 N_4 O_2$
Formula weight	226.42	546.14	572.99	490.03
Temperature/K	150(2) K	150(2) K	150(2) K	150(2) K
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic,
Space group	$P2_1/c$	$P2_1/c$	$C\ 2/c$	$P\bar{1}$
Unit cell dimensions				
a/Å	7.6805(3)	14.2703(2)	10.7934(2)	9.9907(7)
α/°	90	90	90	81.573(7)
b/ Å	13.5584(4)	8.20790(10)	15.9368(2)	10.7791(9)
β/°	101.345(4)	104.5780(10)	105.658(2)	66.188(8)
c/ Å	9.0977(3)	22.8846(2)	14.8791(2)	11.2843(9)
γ/°	90	90	90	83.531(7)
Volume/ $Å^3$	928.88(5)	2594.16(5)	2464.41(6)	1097.84(15)
Z	4	4	4	2
Calculated density/ Mg/m^3	1.619	1.398	1.544	1.482
Absorption coefficient/mm^{-1}	0.402	0.904	2.898	1.010
$F(000)$	456	1128	1168	500
Crystal size/mm	0.23 x 0.16 x 0.12	0.33 x 0.26 x 0.18	0.23 x 0.18 x 0.13	0.23 x 0.18 x 0.13
θ range from data collection/°	3.52 to 25.00	3.20 to 72.24	5.08 to 72.13	4.15 to 72.07
Reflections collected/unique	6552 / 1632 [R(int) = 0.0162]	17912 / 5056 [R(int) = 0.0190]	7702 / 2408 [R(int) = 0.0154]	7319 / 4205 [R(int) = 0.0128]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Data/restraints/parameters	1632 / 0 / 136	5056 / 0 / 363	2408 / 0 / 182	4205 / 0 / 325
Goodness-of-fit on F^2	1.055	1.026	1.061	1.028
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0253$, $wR_2 = 0.0635$	$R_1 = 0.0378$, $wR_2 = 0.0994$	R1 = 0.0565, $wR_2 = 0.1416$	$R_1 = 0.0393$, $wR_2 = 0.1004$
R indices (all data)	$R_1 = 0.0263$, $wR_2 = 0.0646$	$R_1 = 0.0417$, $wR_2 = 0.1033$	R1 = 0.0602, $wR_2 = 0.1452$	$R_1 = 0.0491$, $wR_2 = 0.1100$
Largest diff. peak and hole/e $Å^{-3}$	0.216 and -0.272	0.374 and -0.250	0.619 and -1.124	0.198 and -0.213
CCDC number	964025	964026	966965	964027

DFT Calculations.

Calculation method: B3LYP/6-31G** with Gaussian 09[2]

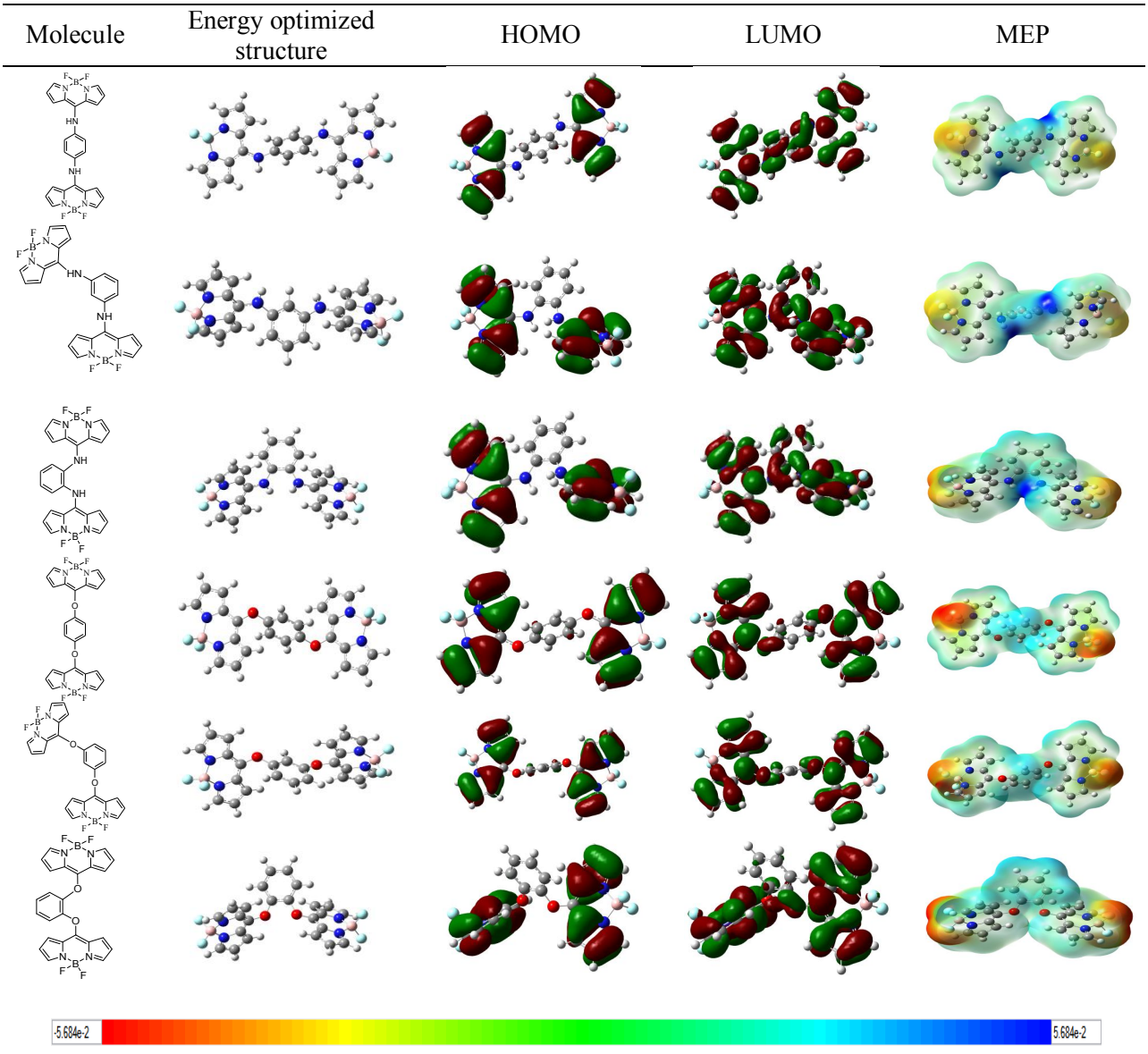


Figure S15. The energy optimized structures, HOMO-LUMO energy levels and MEP of the *meso* arylaza (**2a-2c**) and aryloxy (**3d-3f**) BODIPY dimers.

DFT Data for BODIPY dimer **3d**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.725104	-2.749661	-0.399696
2	1	0	3.873703	-3.371373	-0.638014
3	6	0	6.038747	-3.147132	-0.176353
4	1	0	6.432155	-4.154083	-0.197161
5	6	0	6.781853	-1.976402	0.077586
6	1	0	7.832306	-1.866893	0.311362
7	7	0	5.987998	-0.897252	0.007436
8	5	0	6.354913	0.571561	0.415630
9	6	0	3.880936	3.214010	-0.669072
10	6	0	3.074194	2.086544	-0.773100
11	1	0	2.040282	2.053228	-1.083148
12	6	0	3.876735	0.971568	-0.421788
13	6	0	3.659298	-0.419492	-0.469568
14	6	0	4.703084	-1.339115	-0.285380
15	7	0	5.152250	1.438508	-0.105805
16	9	0	6.434674	0.664340	1.793095
17	6	0	5.151414	2.770545	-0.255041

18	1	0	6.050780	3.340279	-0.064618
19	9	0	7.522877	0.968104	-0.199790
20	1	0	3.601795	4.238328	-0.873750
21	6	0	1.252631	-0.437090	-0.382712
22	6	0	0.225122	-0.392027	-1.323572
23	6	0	1.038372	-0.055559	0.942127
24	6	0	-1.038363	0.055561	-0.942166
25	1	0	0.423169	-0.700304	-2.344725
26	6	0	-0.225113	0.392030	1.323533
27	1	0	1.845219	-0.106790	1.665364
28	6	0	-1.252623	0.437090	0.382674
29	1	0	-1.845210	0.106793	-1.665403
30	1	0	-0.423160	0.700308	2.344686
31	6	0	-3.659292	0.419490	0.469550
32	6	0	-4.703073	1.339115	0.285344
33	6	0	-3.876742	-0.971570	0.421814
34	6	0	-4.725082	2.749665	0.399621
35	7	0	-5.987992	0.897254	-0.007454
36	6	0	-3.074211	-2.086543	0.773163
37	7	0	-5.152262	-1.438508	0.105852
38	6	0	-6.038723	3.147140	0.176271
39	1	0	-3.873675	3.371377	0.637918
40	5	0	-6.354920	-0.571567	-0.415605
41	6	0	-6.781839	1.976409	-0.077631
42	1	0	-2.040299	-2.053228	1.083211
43	6	0	-3.880963	-3.214005	0.669167

44	6	0	-5.151438	-2.770541	0.255126
45	1	0	-6.432122	4.154094	0.197052
46	9	0	-6.434686	-0.664385	-1.793067
47	9	0	-7.522886	-0.968083	0.199830
48	1	0	-7.832293	1.866900	-0.311399
49	1	0	-3.601831	-4.238319	0.873876
50	1	0	-6.050810	-3.340273	0.064723
51	8	0	-2.466448	0.974106	0.800323
52	8	0	2.466458	-0.974104	-0.800360

Total Energy = -1743.0279511 HF

DFT Data for BODIPY dimer **3e**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.448826	-2.533066	-1.165405
2	1	0	3.538580	-3.038945	-1.454826
3	6	0	5.753029	-3.008142	-1.243164
4	1	0	6.079229	-3.974345	-1.602566
5	6	0	6.591525	-1.978765	-0.768148
6	1	0	7.667407	-1.966327	-0.656412
7	7	0	5.862469	-0.907993	-0.420403
8	5	0	6.366015	0.371139	0.335842

9	6	0	3.936718	3.266718	0.400041
10	6	0	3.059256	2.235340	0.086022
11	1	0	1.994286	2.312142	-0.077198
12	6	0	3.833372	1.051446	-0.009501
13	6	0	3.527864	-0.258880	-0.422759
14	6	0	4.526583	-1.216349	-0.651312
15	7	0	5.163032	1.379336	0.251588
16	9	0	6.619920	0.057004	1.658239
17	6	0	5.221191	2.696490	0.492995
18	1	0	6.168844	3.168043	0.715043
19	9	0	7.471207	0.902809	-0.293192
20	1	0	3.694945	4.311394	0.538633
21	6	0	1.160724	-0.288034	0.014130
22	6	0	-0.000018	0.000113	-0.700551
23	6	0	1.176926	-0.306267	1.409094
24	6	0	-1.160735	0.288292	0.014179
25	6	0	0.000038	0.000157	2.092739
26	1	0	2.087850	-0.549230	1.944719
27	6	0	-1.176892	0.306567	1.409126
28	1	0	0.000055	0.000174	3.178451
29	1	0	-2.087785	0.549543	1.944795
30	1	0	-0.000059	0.000097	-1.784460
31	6	0	-3.527870	0.259003	-0.422686
32	6	0	-4.526677	1.216399	-0.651173
33	6	0	-3.833266	-1.051360	-0.009490
34	6	0	-4.449035	2.533180	-1.165113
35	7	0	-5.862525	0.907925	-0.420228

36	6	0	-3.058967	-2.235110	0.086294
37	7	0	-5.162893	-1.379406	0.251553
38	6	0	-5.753285	3.008135	-1.242857
39	1	0	-3.538840	3.039179	-1.454484
40	5	0	-6.366086	-0.371448	0.335595
41	6	0	-6.591682	1.978662	-0.767877
42	1	0	-1.993969	-2.311707	-0.076837
43	6	0	-3.936273	-3.266563	0.400480
44	6	0	-5.220857	-2.696530	0.493176
45	1	0	-6.079570	3.974344	-1.602166
46	9	0	-7.470988	-0.903154	-0.293929
47	9	0	-6.620525	-0.057670	1.657978
48	1	0	-7.667563	1.966120	-0.656139
49	1	0	-3.694371	-4.311178	0.539313
50	1	0	-6.168449	-3.168217	0.715204
51	8	0	2.268550	-0.656615	-0.739851
52	8	0	-2.268588	0.656852	-0.739788

Total Energy = -1743.0282525 HF

DFT Data for BODIPY **3f**

Standard orientation:

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

1	6	0	2.077824	2.859575	-1.490047
2	1	0	2.606122	1.929298	-1.336088
3	6	0	2.438176	3.921568	-2.312024
4	1	0	3.319076	3.999945	-2.934100
5	6	0	1.422435	4.891918	-2.194585
6	1	0	1.343647	5.863866	-2.662809
7	7	0	0.466447	4.465177	-1.355673
8	5	0	-0.732833	5.299846	-0.788175
9	6	0	-3.415597	3.289785	0.955538
10	6	0	-2.373015	2.371195	1.001882
11	1	0	-2.399656	1.381688	1.433320
12	6	0	-1.267450	2.968636	0.344910
13	6	0	-0.000873	2.484777	-0.037939
14	6	0	0.840491	3.207532	-0.897258
15	7	0	-1.653539	4.238266	-0.083820
16	9	0	-0.266990	6.206659	0.146344
17	6	0	-2.930017	4.425093	0.279619

18	1	0	-3.434314	5.351274	0.039666
19	9	0	-1.422435	5.915770	-1.810493
20	1	0	-4.414471	3.164485	1.349989
21	6	0	0.192298	0.671988	1.528564
22	6	0	-0.192298	-0.671988	1.528564
23	6	0	0.401253	1.341974	2.734046
24	6	0	-0.401253	-1.341974	2.734046
25	6	0	0.199792	0.669195	3.937964
26	1	0	0.717548	2.379840	2.717260
27	6	0	-0.199792	-0.669195	3.937964
28	1	0	-0.717548	-2.379840	2.717260
29	1	0	0.360965	1.192064	4.875477
30	1	0	-0.360965	-1.192064	4.875477
31	6	0	0.000873	-2.484777	-0.037939
32	6	0	-0.840491	-3.207532	-0.897258
33	6	0	1.267450	-2.968636	0.344910
34	6	0	-2.077824	-2.859575	-1.490047
35	7	0	-0.466447	-4.465177	-1.355673

36	6	0	2.373015	-2.371195	1.001882
37	7	0	1.653539	-4.238266	-0.083820
38	6	0	-2.438176	-3.921568	-2.312024
39	1	0	-2.606122	-1.929298	-1.336088
40	5	0	0.732833	-5.299846	-0.788175
41	6	0	-1.422435	-4.891918	-2.194585
42	1	0	2.399656	-1.381688	1.433320
43	6	0	3.415597	-3.289785	0.955538
44	6	0	2.930017	-4.425093	0.279619
45	1	0	-3.319076	-3.999945	-2.934100
46	9	0	1.422435	-5.915770	-1.810493
47	9	0	0.266990	-6.206659	0.146344
48	1	0	-1.343647	-5.863866	-2.662809
49	1	0	4.414471	-3.164485	1.349989
50	1	0	3.434314	-5.351274	0.039666
51	8	0	-0.463432	-1.255921	0.300990
52	8	0	0.463432	1.255921	0.300990

Total energy = -1743.0216648 HF

DFT Data for BODIPY **2a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.956889	2.762731	0.302286
2	1	0	4.124555	3.438210	0.458503
3	6	0	6.293634	3.132766	0.153723
4	1	0	6.700803	4.134150	0.176335
5	6	0	7.021527	1.947167	-0.031018
6	1	0	8.079237	1.806517	-0.206200
7	7	0	6.196107	0.886657	0.015316
8	5	0	6.556933	-0.580437	-0.394410
9	6	0	4.077174	-3.183241	0.736635
10	6	0	3.261886	-2.054845	0.763520
11	1	0	2.225396	-2.014041	1.063375
12	6	0	4.059249	-0.955246	0.363739
13	6	0	3.819981	0.444542	0.359005
14	6	0	4.906800	1.352863	0.221000
15	7	0	5.341383	-1.430881	0.102830
16	9	0	6.664918	-0.664901	-1.771832
17	6	0	5.350038	-2.754343	0.324501
18	1	0	6.259826	-3.322449	0.187718
19	9	0	7.711995	-0.990009	0.239985

20	1	0	3.800276	-4.195703	0.996576
21	7	0	2.580405	0.981230	0.573510
22	1	0	2.580249	1.962336	0.818945
23	6	0	1.299787	0.445069	0.286830
24	6	0	0.229890	0.779581	1.128144
25	6	0	1.058620	-0.336058	-0.850726
26	6	0	-1.058644	0.336026	0.850650
27	1	0	0.414003	1.370192	2.021492
28	6	0	-0.229914	-0.779611	-1.128222
29	1	0	1.873677	-0.587361	-1.520028
30	6	0	-1.299809	-0.445107	-0.286901
31	1	0	-1.873703	0.587334	1.519949
32	1	0	-0.414029	-1.370217	-2.021573
33	7	0	-2.580431	-0.981256	-0.573583
34	6	0	-3.819996	-0.444562	-0.359037
35	6	0	-4.906839	-1.352863	-0.221087
36	6	0	-4.059221	0.955232	-0.363663
37	6	0	-4.956967	-2.762724	-0.302464
38	7	0	-6.196133	-0.886634	-0.015372
39	6	0	-3.261813	2.054835	-0.763340
40	7	0	-5.341340	1.430887	-0.102722
41	6	0	-6.293723	-3.132731	-0.153926
42	1	0	-4.124652	-3.438217	-0.458725
43	5	0	-6.556919	0.580444	0.394449
44	6	0	-7.021582	-1.947124	0.030895
45	1	0	-2.225318	2.014020	-1.063179
46	6	0	-4.077067	3.183254	-0.736385

47	6	0	-5.349950	2.754366	-0.324297
48	1	0	-6.700920	-4.134103	-0.176604
49	9	0	-6.664914	0.664818	1.771876
50	9	0	-7.711963	0.990093	-0.239928
51	1	0	-8.079289	-1.806456	0.206087
52	1	0	-3.800133	4.195727	-0.996246
53	1	0	-6.259721	3.322491	-0.187481
54	1	0	-2.580286	-1.962352	-0.819061

Total Energy ==-1703.31845

DFT Data for BODIPY **2b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.524764	-2.124129	1.874416
2	1	0	-3.605265	-2.578170	2.223527
3	6	0	-5.815798	-2.522936	2.220739
4	1	0	-6.094576	-3.329196	2.885038
5	6	0	-6.697197	-1.671187	1.537316
6	1	0	-7.778352	-1.667105	1.519452
7	7	0	-6.004410	-0.774497	0.813252
8	5	0	-6.595304	0.183235	-0.274674
9	6	0	-4.287401	2.957113	-1.361566
10	6	0	-3.352097	2.065797	-0.844055

11	1	0	-2.283983	2.212621	-0.787528
12	6	0	-4.067263	0.938289	-0.371364
13	6	0	-3.671137	-0.195140	0.384957
14	6	0	-4.653225	-1.023551	0.997365
15	7	0	-5.421235	1.163331	-0.607371
16	9	0	-6.939822	-0.546490	-1.398925
17	6	0	-5.549721	2.362500	-1.195030
18	1	0	-6.529649	2.737197	-1.456820
19	9	0	-7.668709	0.887712	0.231645
20	1	0	-4.093658	3.927692	-1.797067
21	7	0	-2.360357	-0.493328	0.641676
22	1	0	-2.217221	-1.145848	1.400770
23	6	0	-1.195858	-0.208489	-0.115312
24	6	0	-0.000030	-0.000239	0.580853
25	6	0	-1.194248	-0.226326	-1.515722
26	6	0	1.195896	0.208398	-0.115019
27	6	0	0.000186	0.000540	-2.197546
28	1	0	-2.114152	-0.410932	-2.058235
29	6	0	1.194526	0.227012	-1.515414
30	1	0	0.000267	0.000838	-3.283484
31	1	0	2.114517	0.411900	-2.057682
32	1	0	-0.000091	-0.000550	1.668009
33	7	0	2.360304	0.492699	0.642364
34	6	0	3.671107	0.194821	0.385373
35	6	0	4.653182	1.023292	0.997711
36	6	0	4.067261	-0.938445	-0.371176
37	6	0	4.524752	2.123918	1.874712

38	7	0	6.004364	0.774370	0.813392
39	6	0	3.352091	-2.065776	-0.844273
40	7	0	5.421212	-1.163289	-0.607461
41	6	0	5.815796	2.522862	2.220819
42	1	0	3.605260	2.577835	2.224006
43	5	0	6.595222	-0.183191	-0.274710
44	6	0	6.697176	1.671169	1.537286
45	1	0	2.283991	-2.212683	-0.787671
46	6	0	4.287402	-2.956918	-1.362077
47	6	0	5.549709	-2.362304	-1.195445
48	1	0	6.094596	3.329191	2.885025
49	9	0	7.668727	-0.887663	0.231473
50	9	0	6.939660	0.546680	-1.398872
51	1	0	7.778328	1.667172	1.519262
52	1	0	4.093664	-3.927384	-1.797833
53	1	0	6.529642	-2.736890	-1.457370
54	1	0	2.217178	1.145303	1.401392

Total Energy = -1703.3178841

DFT Data for BODIPY **2c**

Standard orientation:

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

1	6	0	-2.448389	-1.843763	-2.077583
2	1	0	-1.431663	-1.735448	-2.435277
3	6	0	-3.374684	-2.786414	-2.521472
4	1	0	-3.222675	-3.547589	-3.274102
5	6	0	-4.557431	-2.560522	-1.799437
6	1	0	-5.512883	-3.062490	-1.866603
7	7	0	-4.385360	-1.543944	-0.936892
8	5	0	-5.513855	-0.821991	-0.126981
9	6	0	-4.296246	1.420868	2.646881
10	6	0	-3.140142	1.357715	1.874277
11	1	0	-2.196633	1.838759	2.085323
12	6	0	-3.424048	0.521508	0.766907
13	6	0	-2.602456	-0.023660	-0.253650
14	6	0	-3.088624	-1.073394	-1.079494
15	7	0	-4.743278	0.091796	0.884294
16	9	0	-6.275734	-0.046049	-0.982506
17	6	0	-5.259199	0.626295	2.001593

18	1	0	-6.279660	0.410281	2.286629
19	9	0	-6.281494	-1.741264	0.558398
20	1	0	-4.434888	1.963398	3.571892
21	7	0	-1.294332	0.350700	-0.425150
22	1	0	-0.745742	-0.273460	-1.004933
23	6	0	-0.679114	1.605628	-0.188639
24	6	0	0.679050	1.605416	0.188234
25	6	0	-1.345049	2.821839	-0.385355
26	6	0	1.345329	2.821405	0.385132
27	6	0	-0.672722	4.023759	-0.190744
28	1	0	-2.385091	2.813469	-0.692044
29	6	0	0.673340	4.023545	0.190719
30	1	0	2.385381	2.812687	0.691778
31	1	0	-1.196654	4.961436	-0.348721
32	1	0	1.197537	4.961053	0.348817
33	7	0	1.293977	0.350252	0.424415
34	6	0	2.602249	-0.023917	0.253324
35	6	0	3.088610	-1.073007	1.079810

36	6	0	3.423764	0.520851	-0.767496
37	6	0	2.448617	-1.842644	2.078633
38	7	0	4.385407	-1.543487	0.937425
39	6	0	3.139742	1.356611	-1.875165
40	7	0	4.743147	0.091552	-0.884513
41	6	0	3.375100	-2.784784	2.523178
42	1	0	1.431937	-1.734128	2.436399
43	5	0	5.513825	-0.821993	0.126900
44	6	0	4.557729	-2.559308	1.800794
45	1	0	2.196058	1.837158	-2.086566
46	6	0	4.295937	1.419876	-2.647628
47	6	0	5.259054	0.625840	-2.001937
48	1	0	3.223320	-3.545347	3.276472
49	9	0	6.281128	-1.741651	-0.558322
50	9	0	6.276042	-0.045900	0.981965
51	1	0	5.513257	-3.061093	1.868268
52	1	0	4.434547	1.962164	-3.572786
53	1	0	6.279608	0.410021	-2.286787

54	1	0	0.745485	-0.273728	1.004491

Total Energy = -1703.3190859

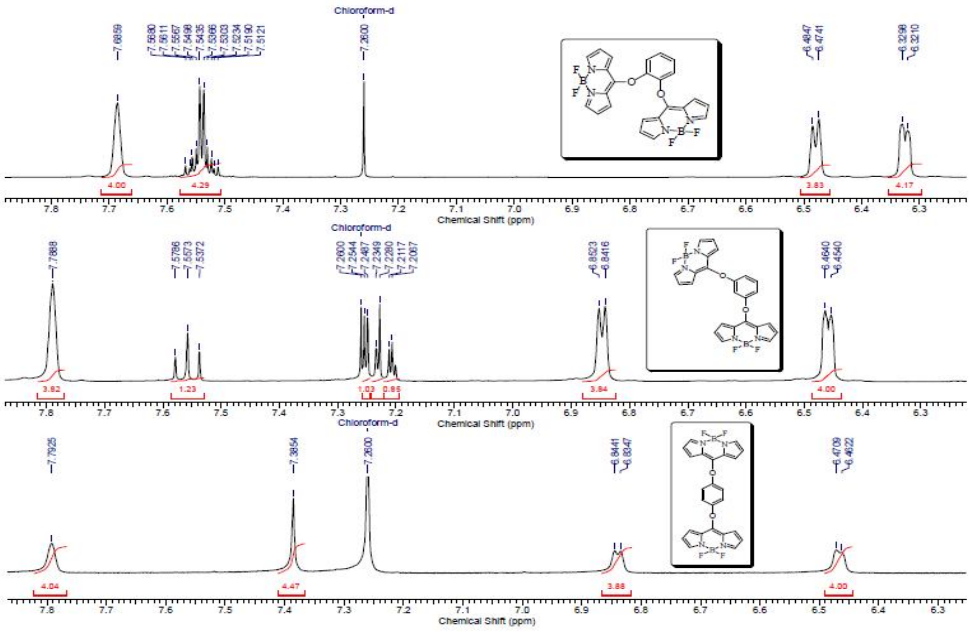


Figure S17. Comparison of ^{1}H NMR of aryloxy substituted BODIPYs (**3d-3f**).

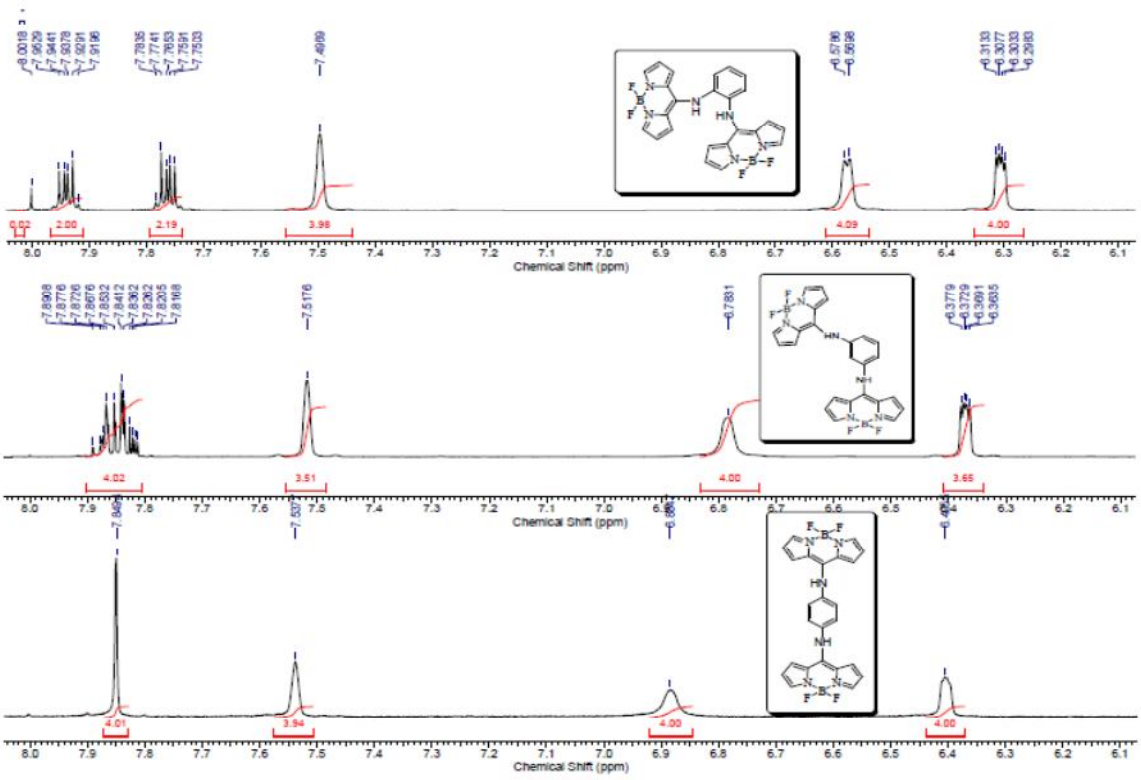
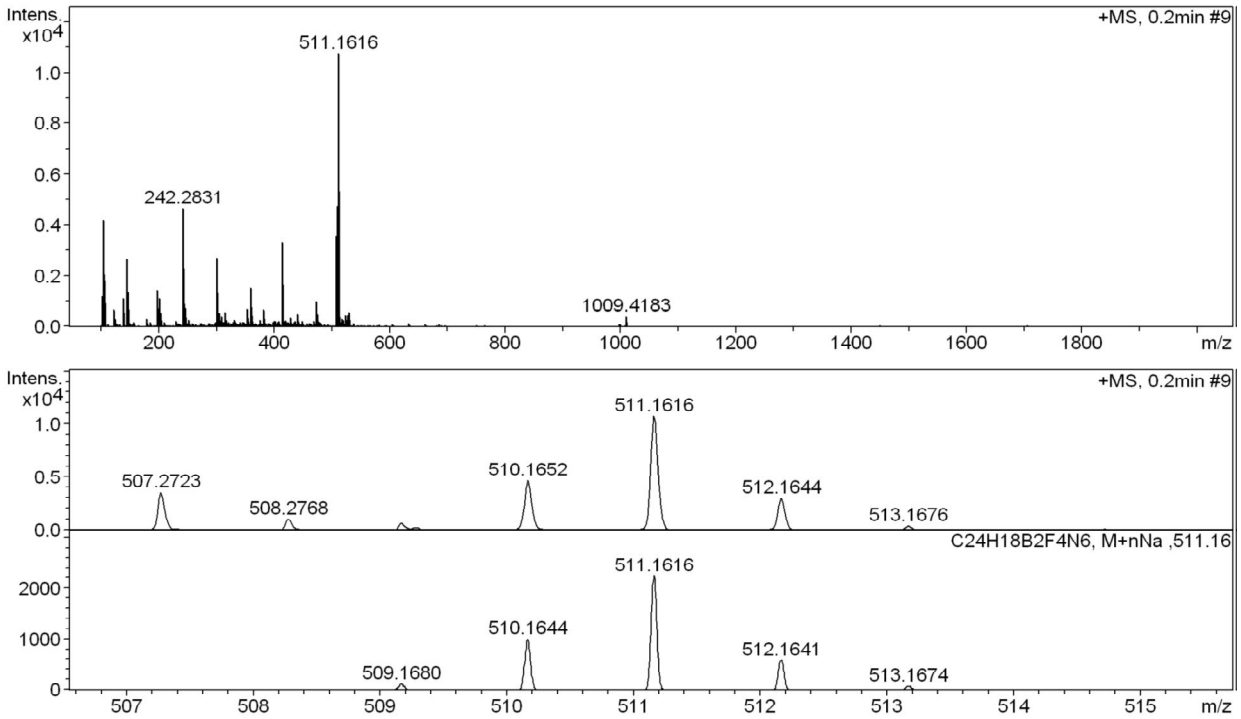
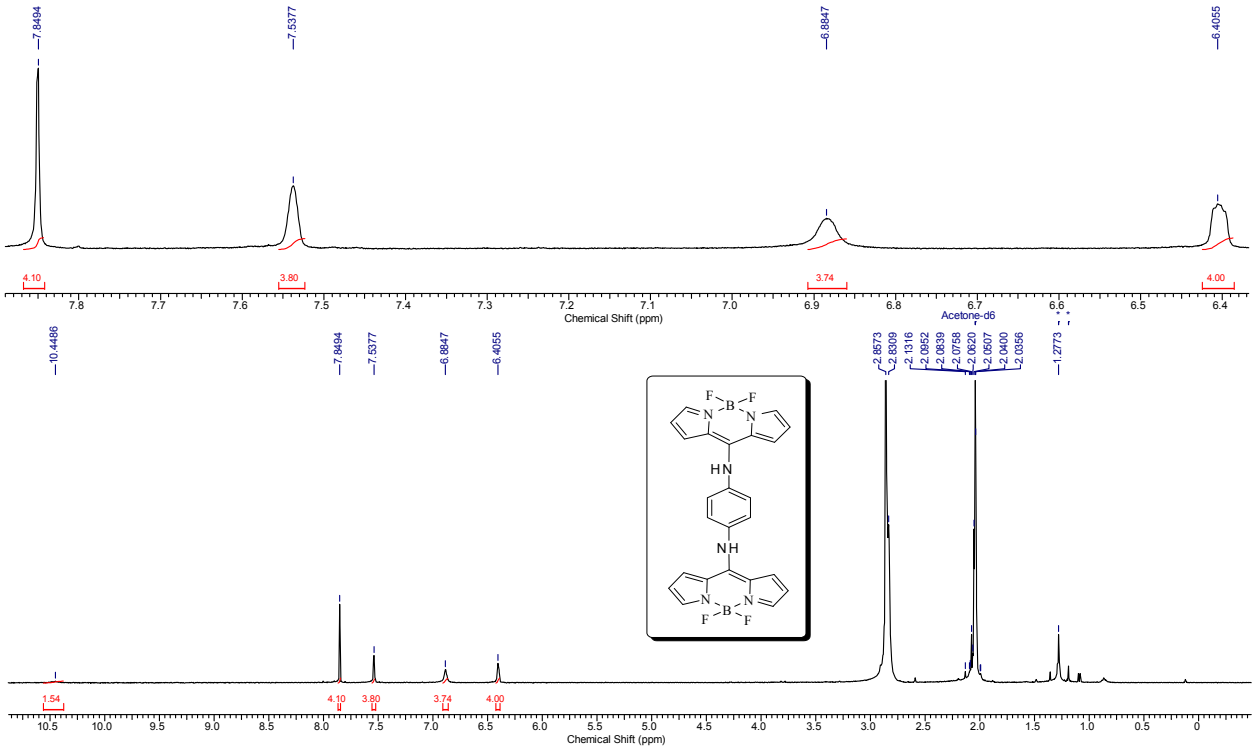


Figure S18. Comparison of ^{1}H NMR of arylaza substituted BODIPYs (**2a-2c**).

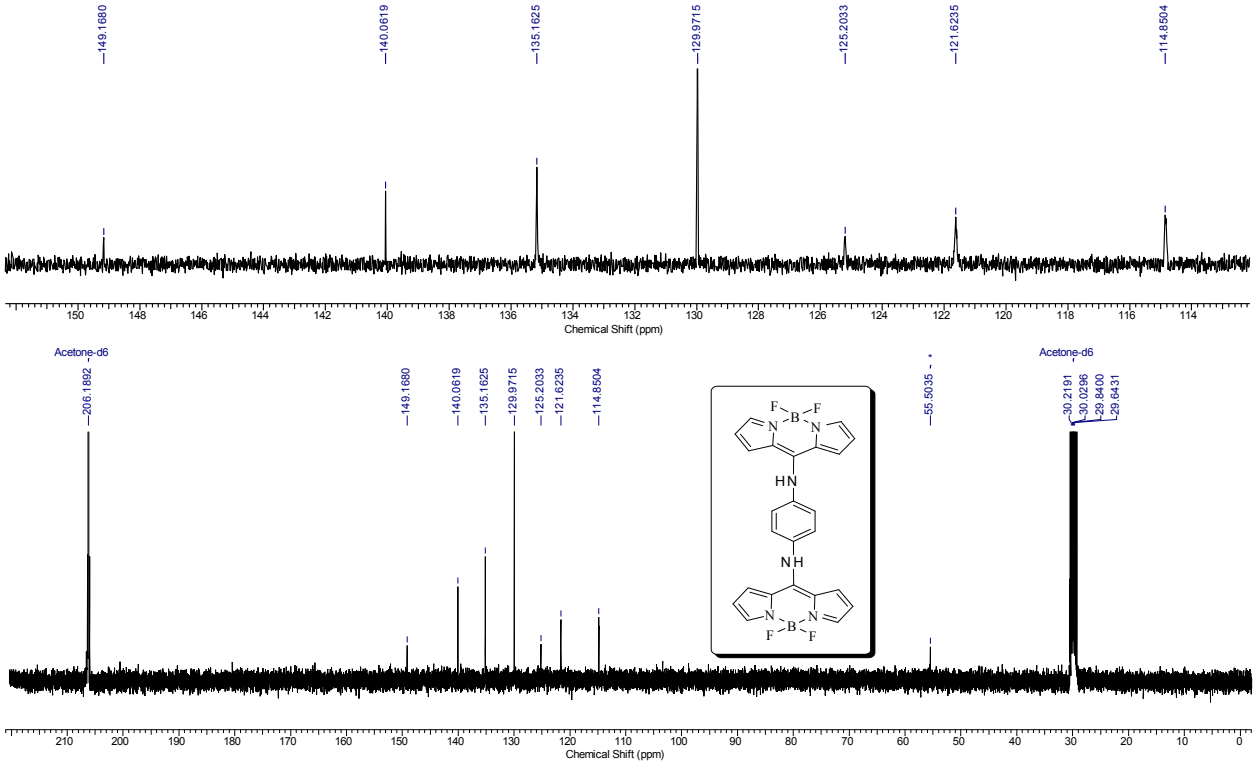
2a HRMS



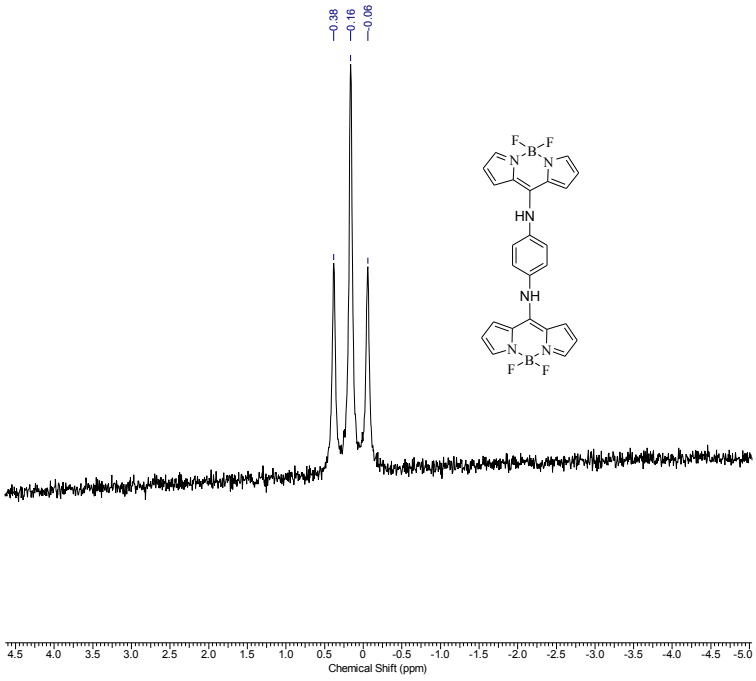
2a ^{1}H NMR



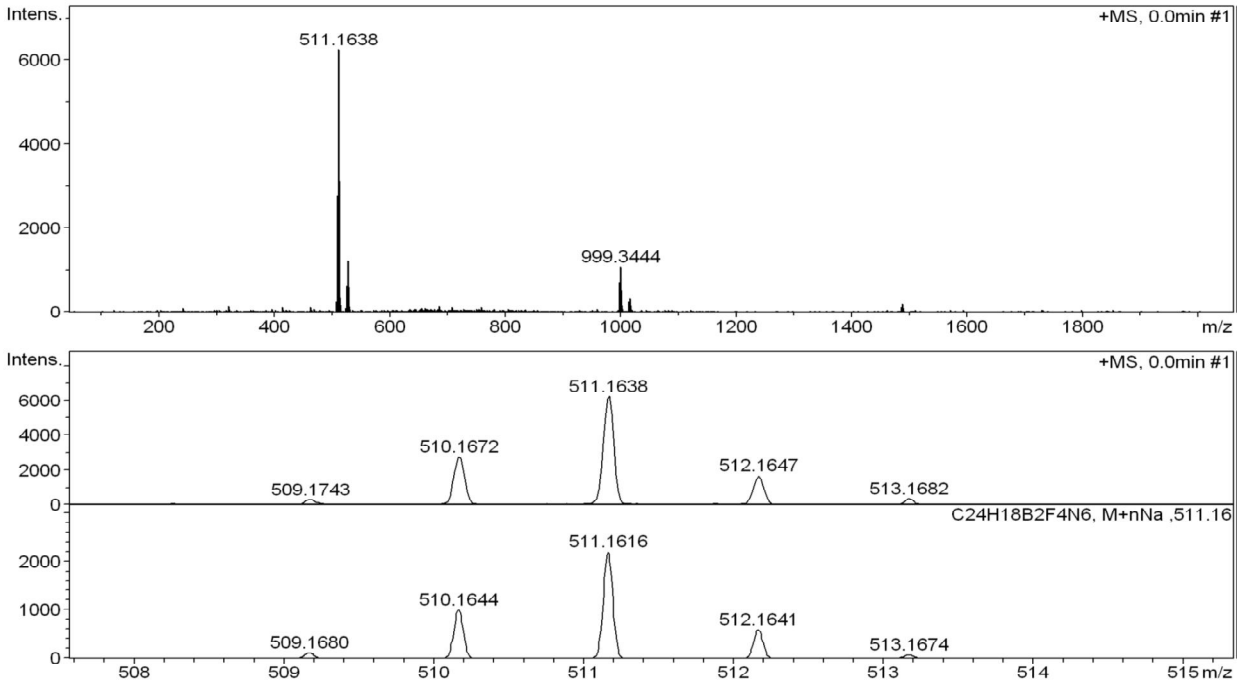
2a ^{13}C NMR



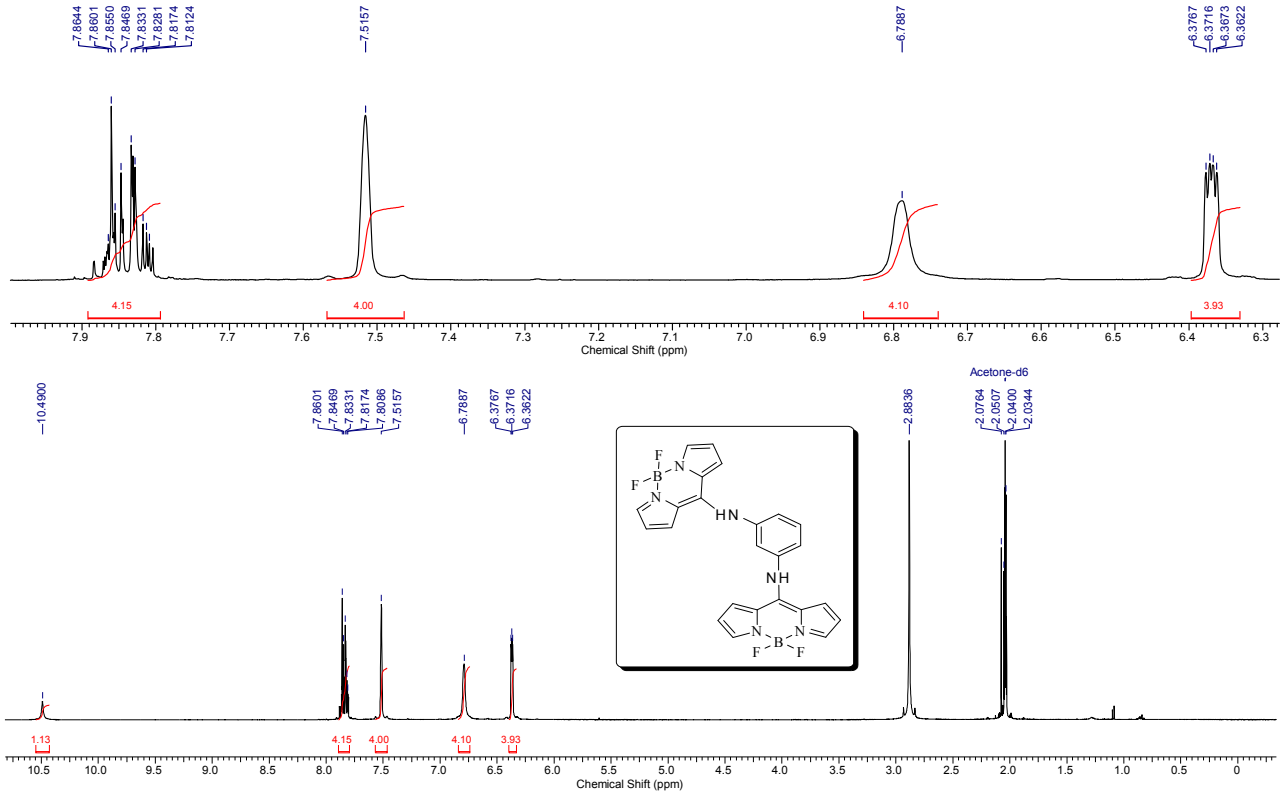
2a ^{11}B NMR



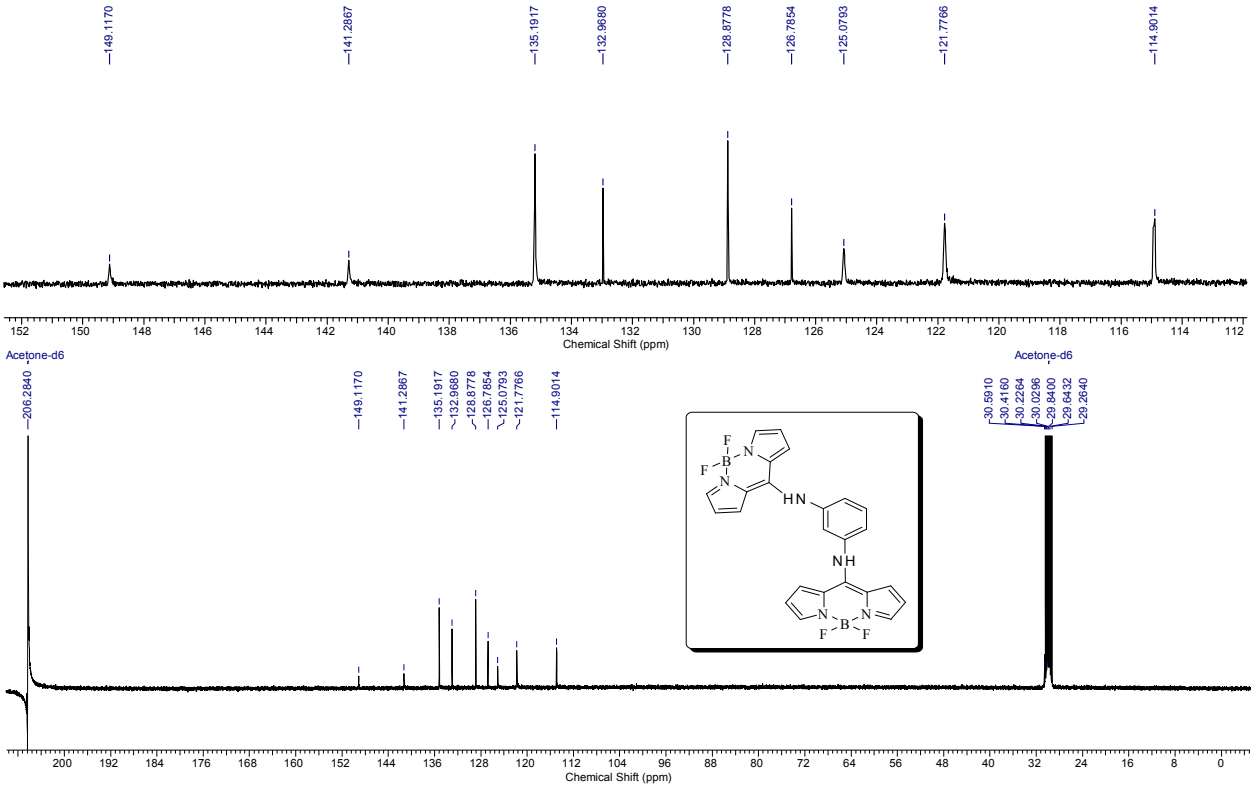
2b HRMS



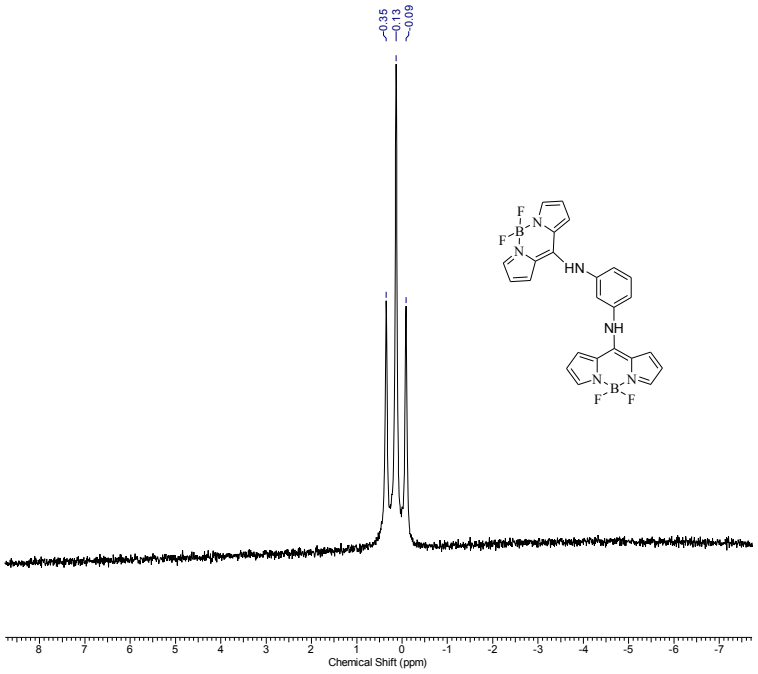
2b ^{1}H NMR



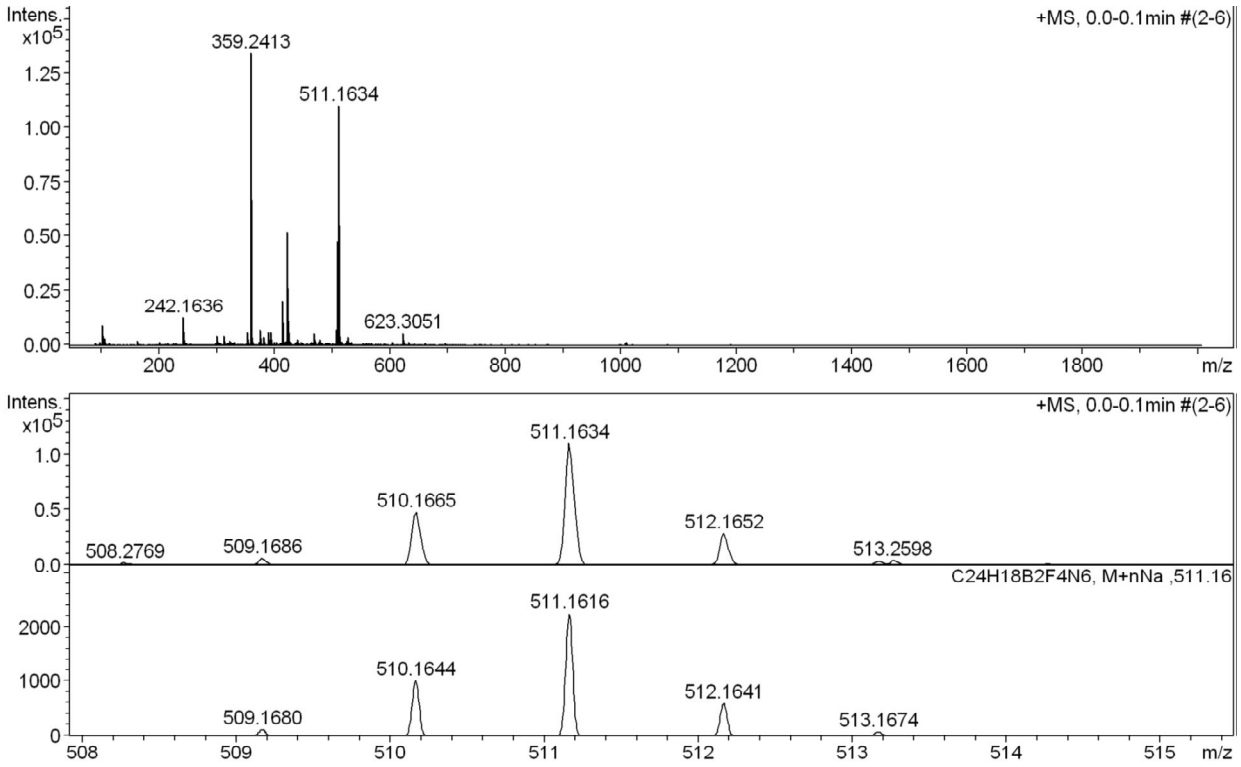
2b ^{13}C NMR



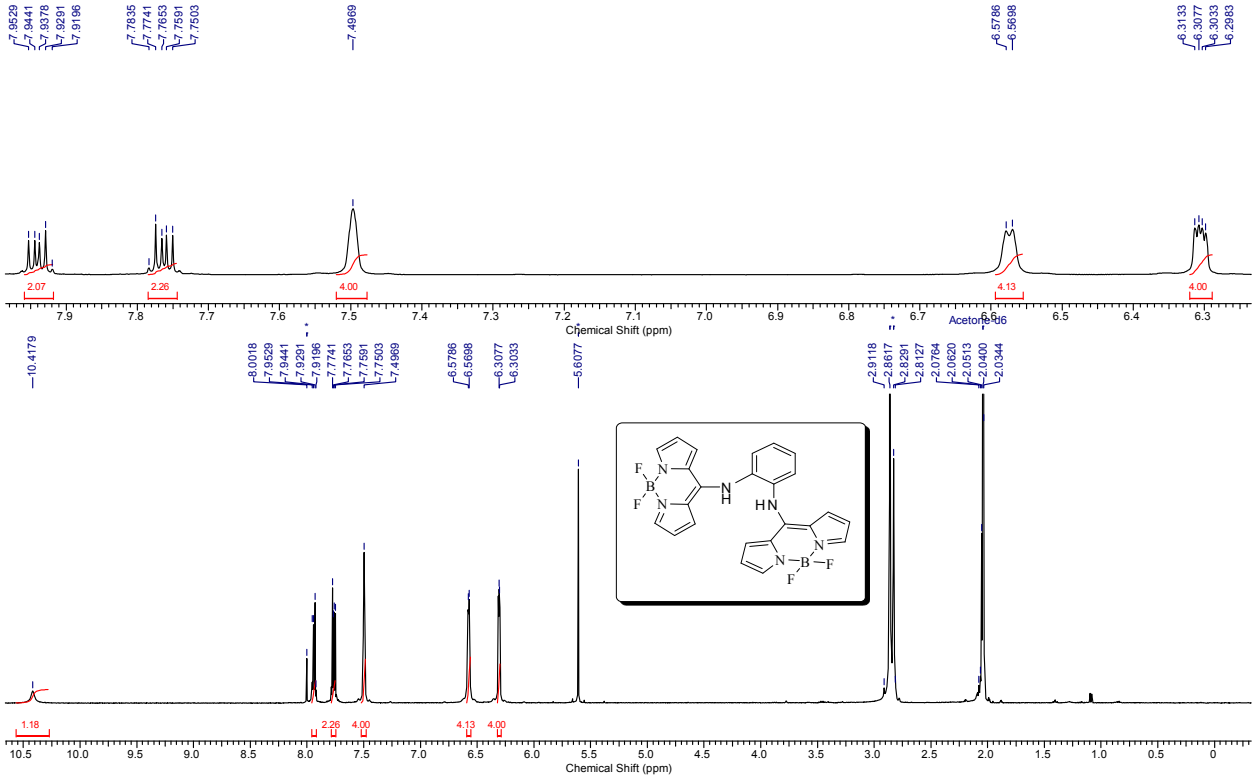
2b ^{11}B NMR



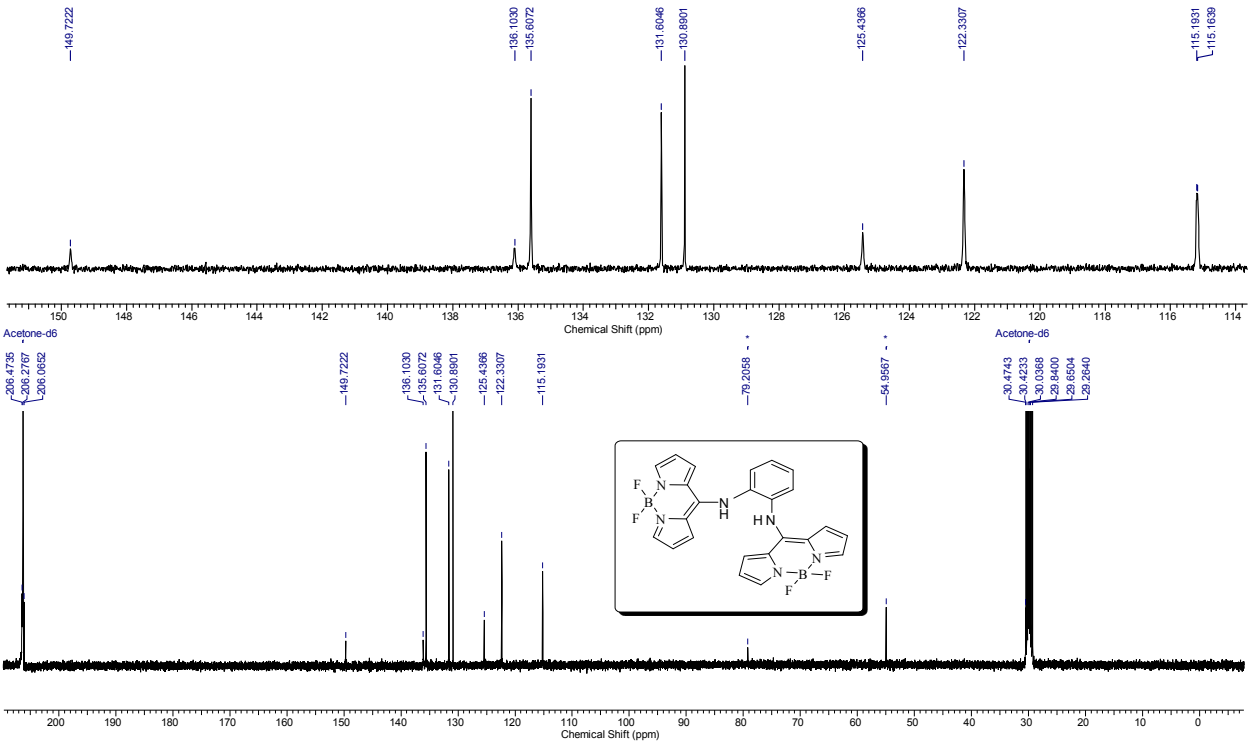
2c HRMS



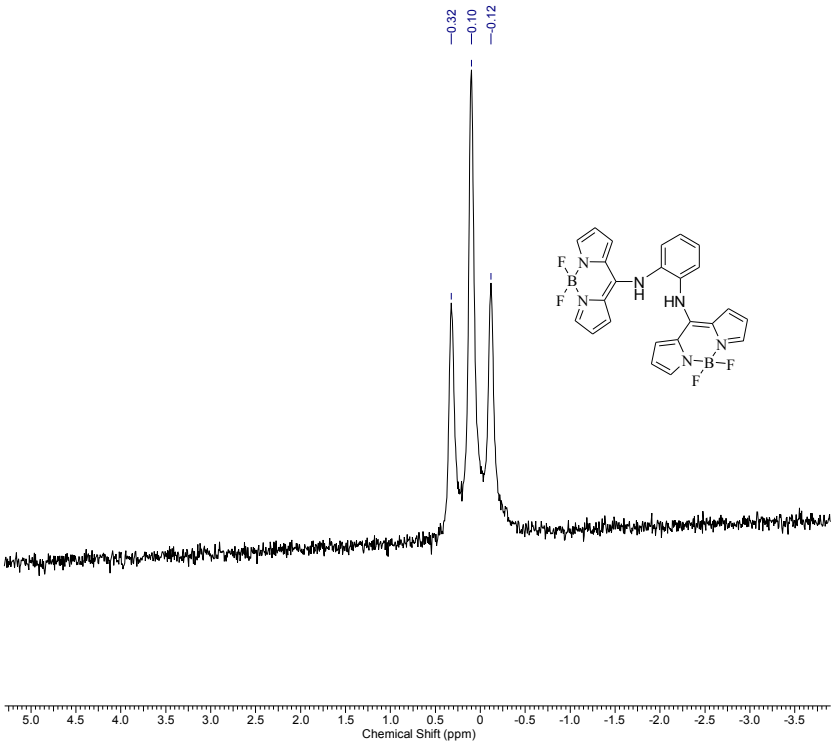
2c ^{1}H NMR



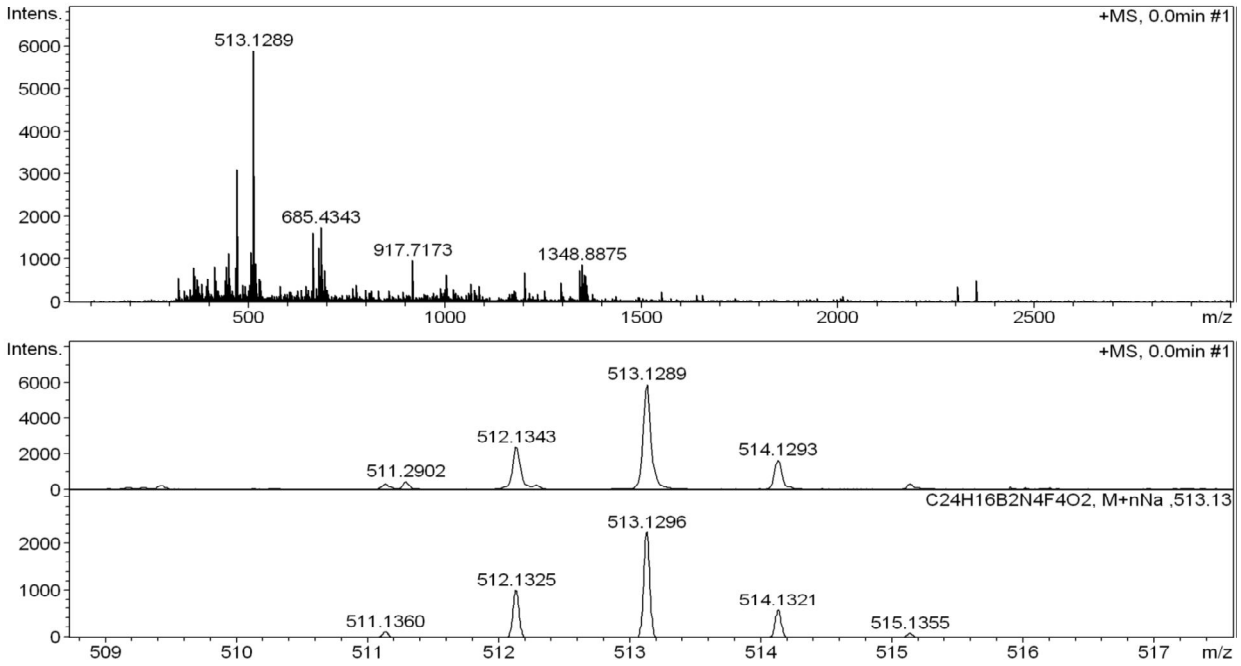
2c ^{13}C NMR



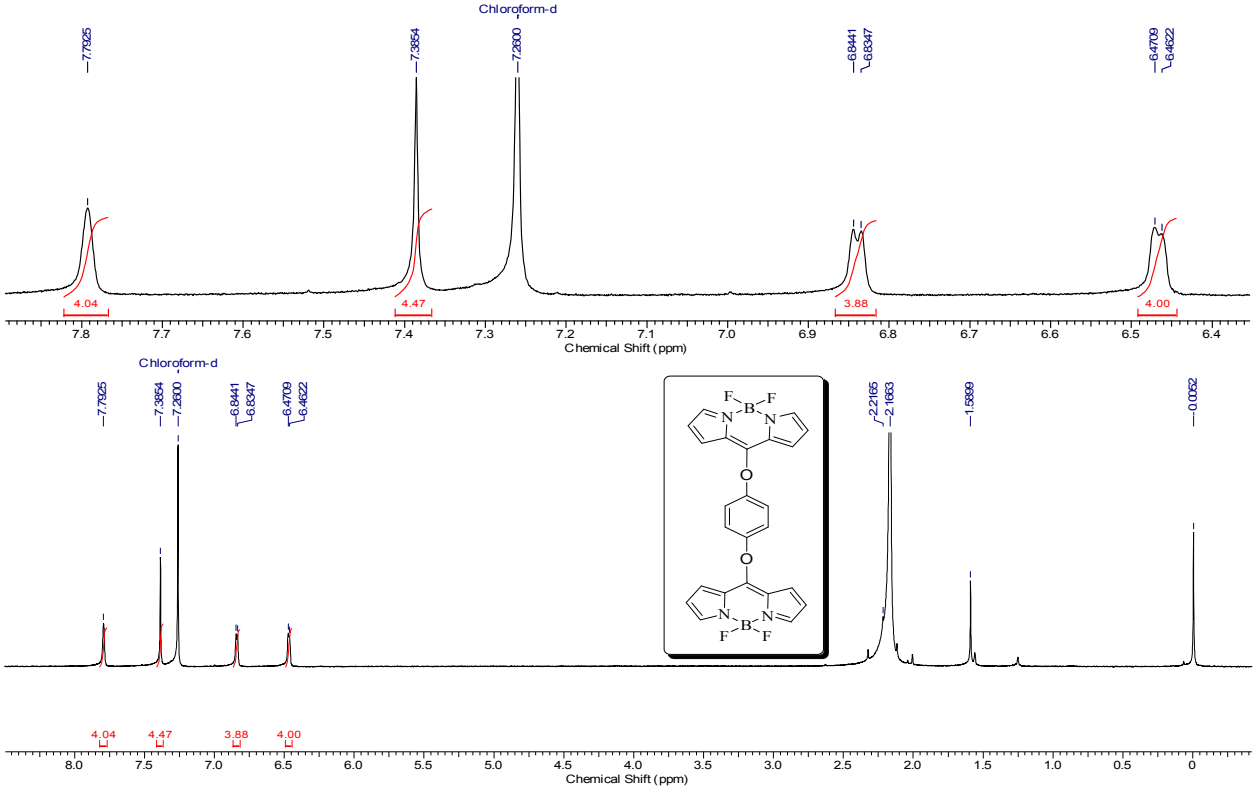
2c ^{11}B NMR



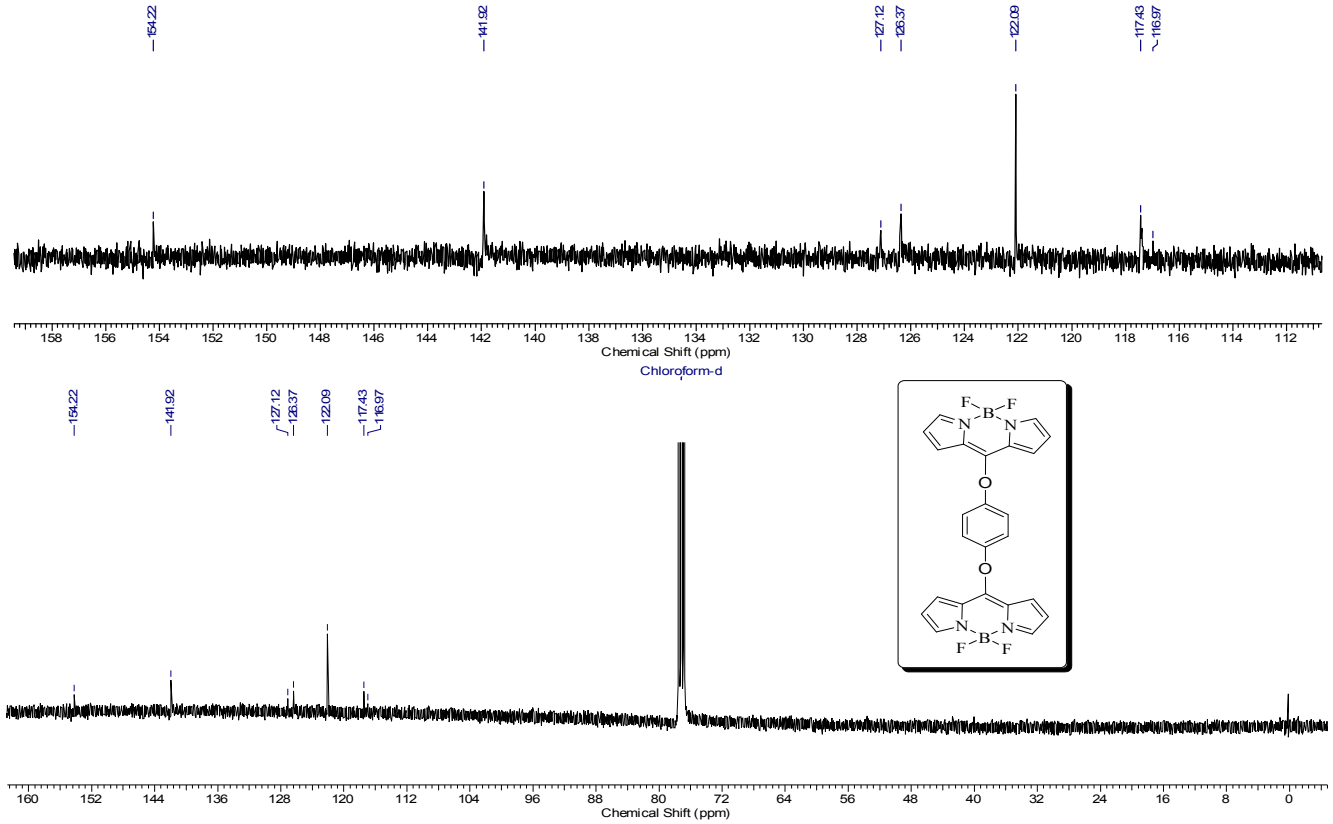
3d HRMS



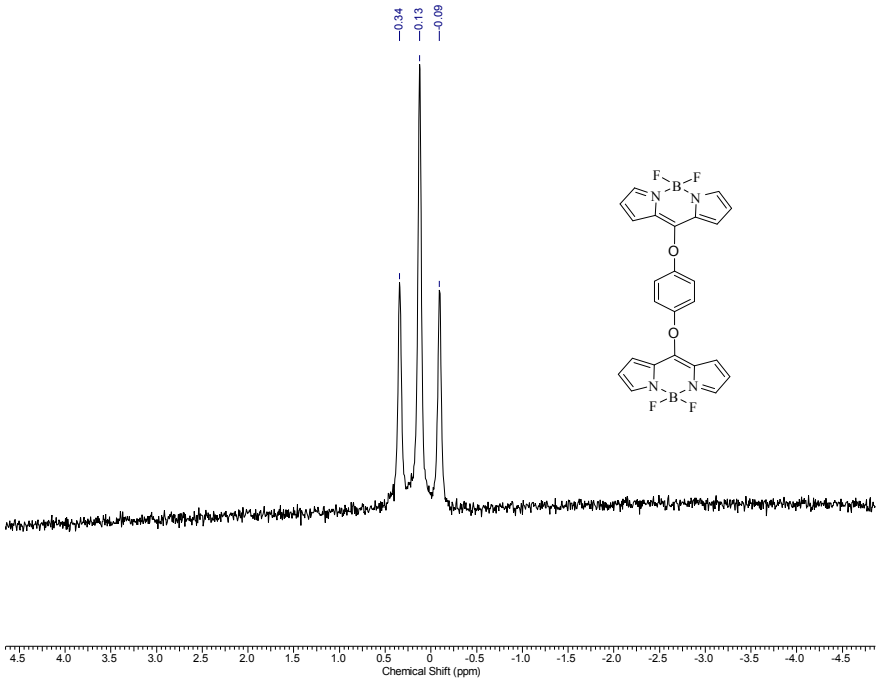
3d ^{1}H NMR



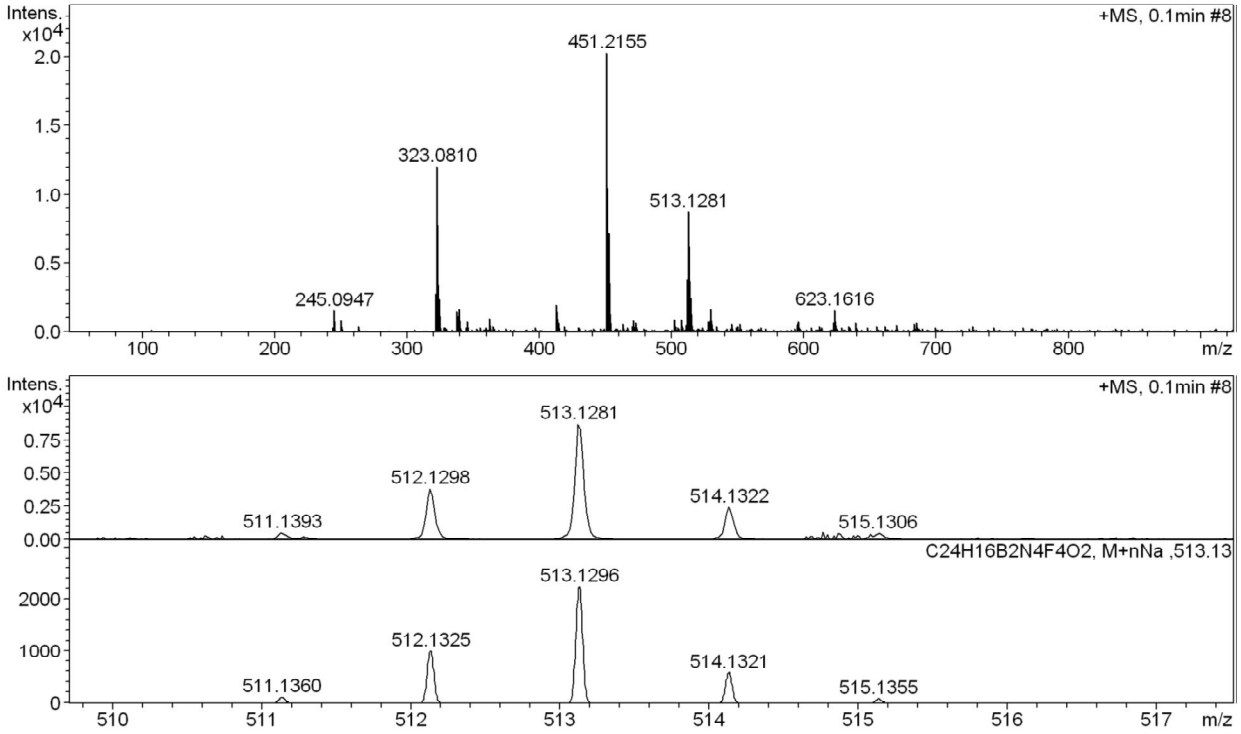
3d ^{13}C NMR



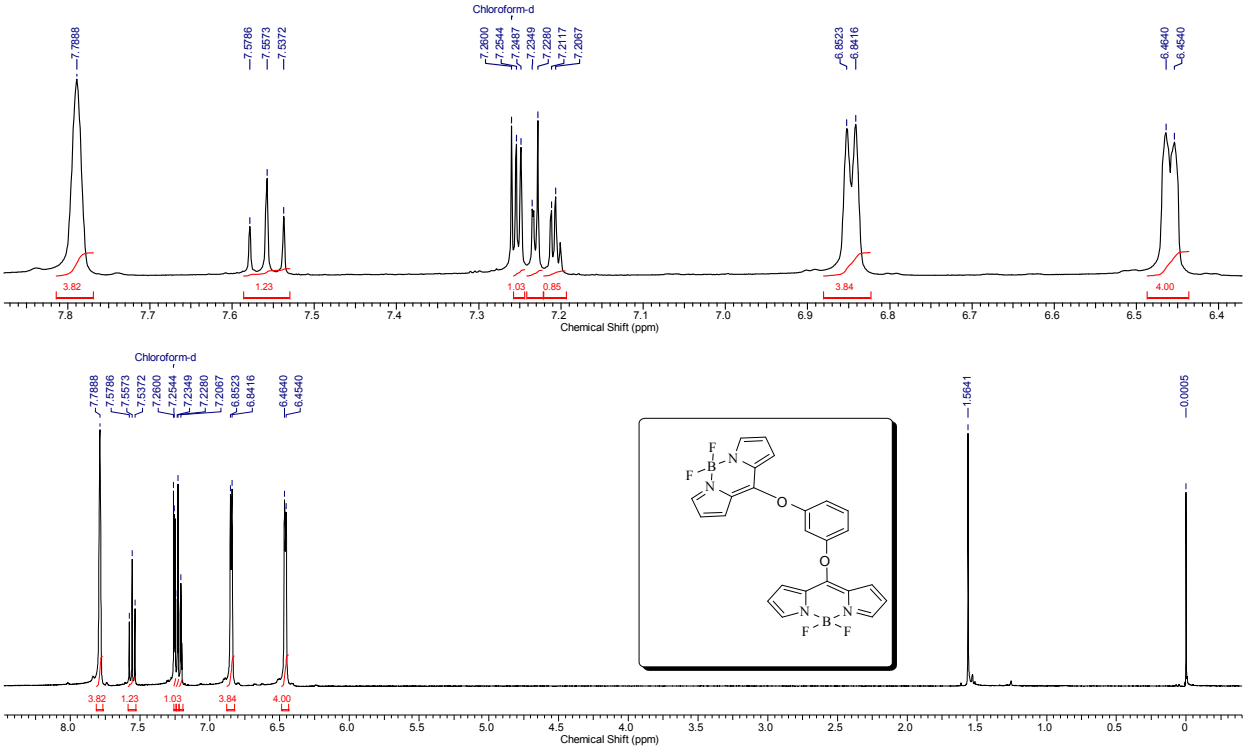
3d ^{11}B NMR



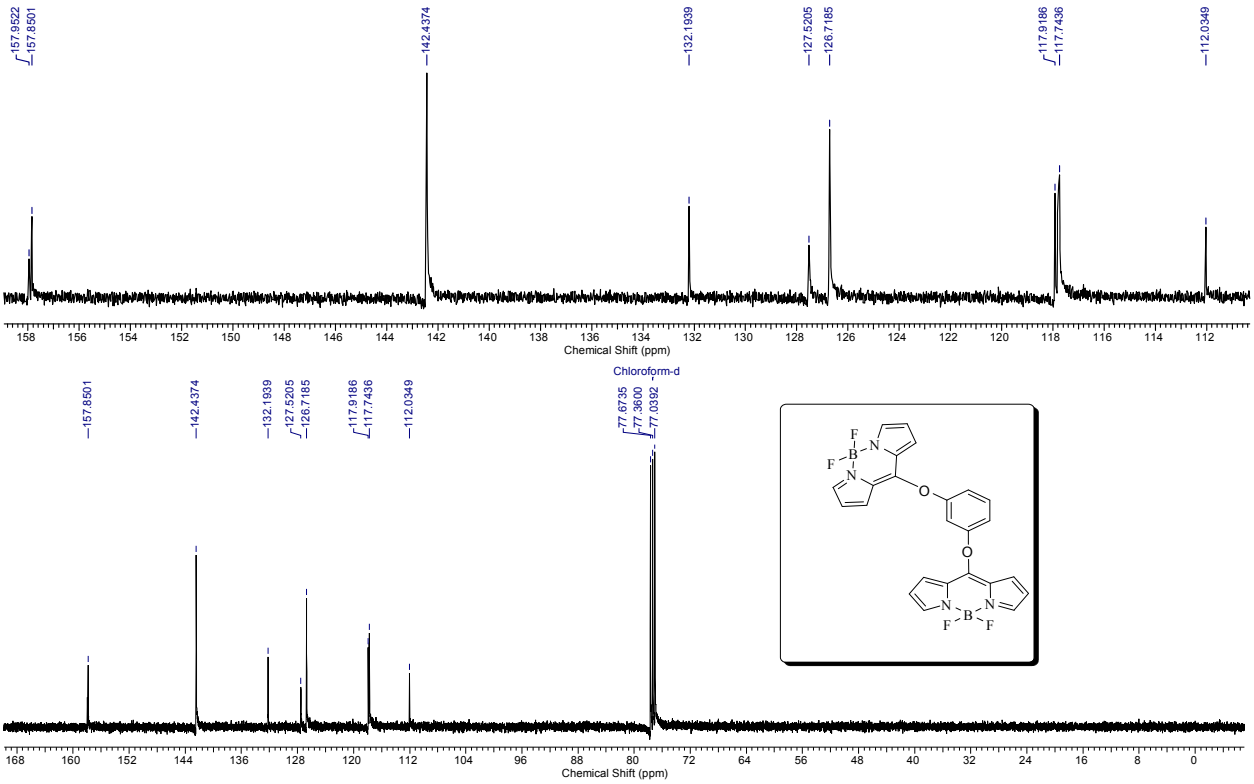
3e HRMS



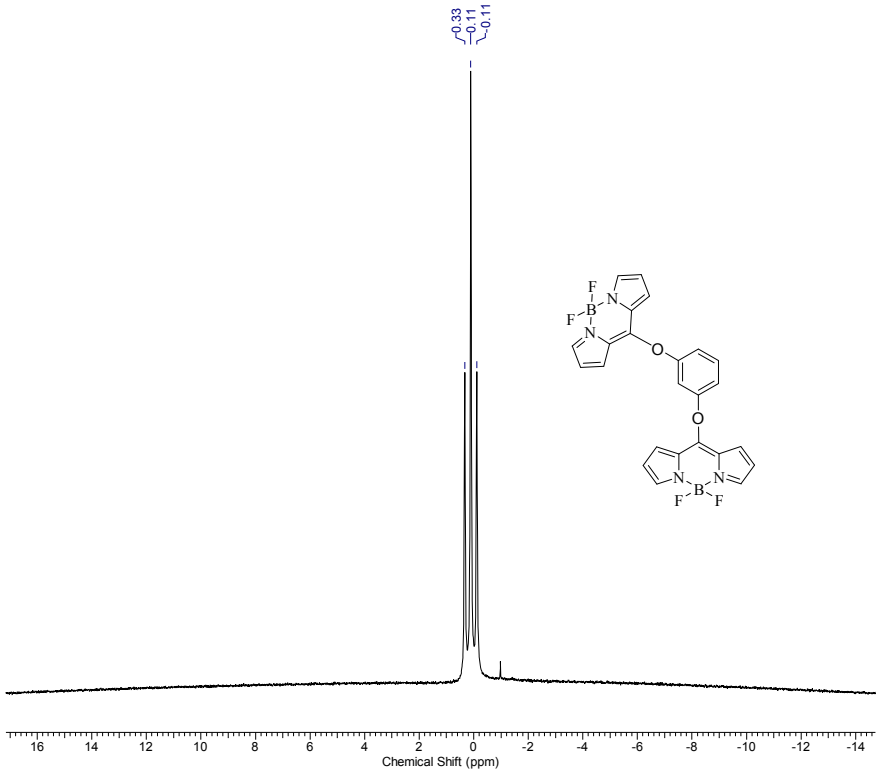
3e ^{1}H NMR



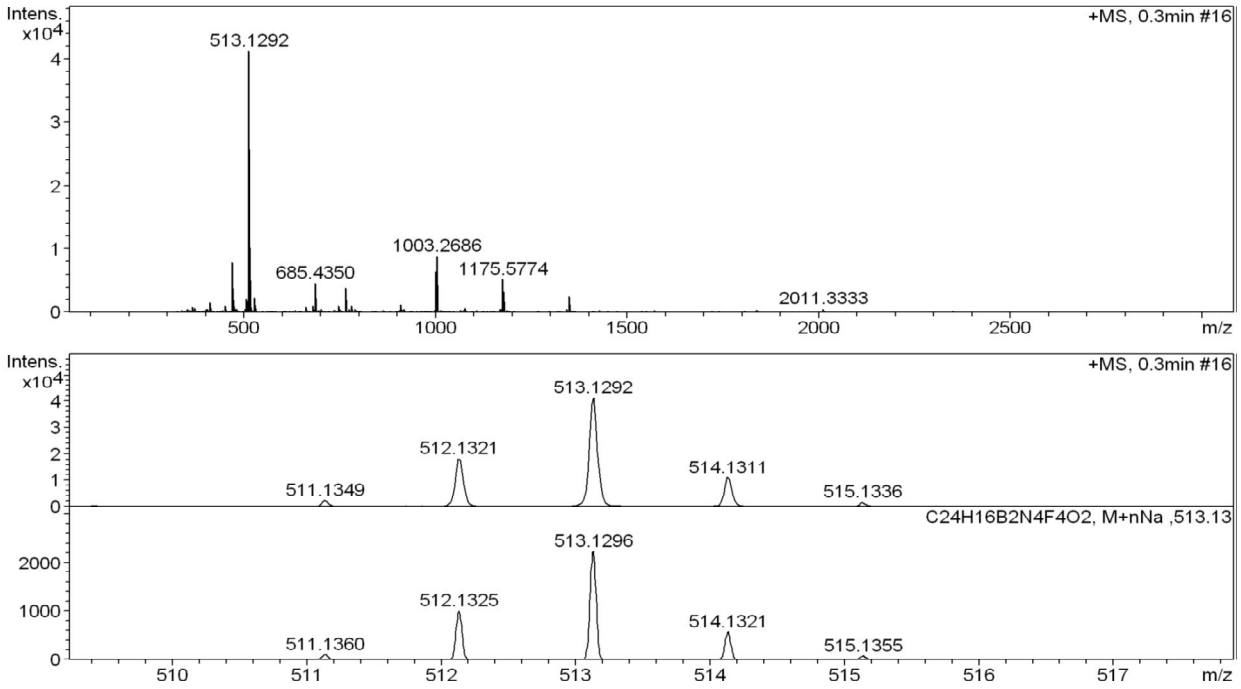
3e ^{13}C NMR



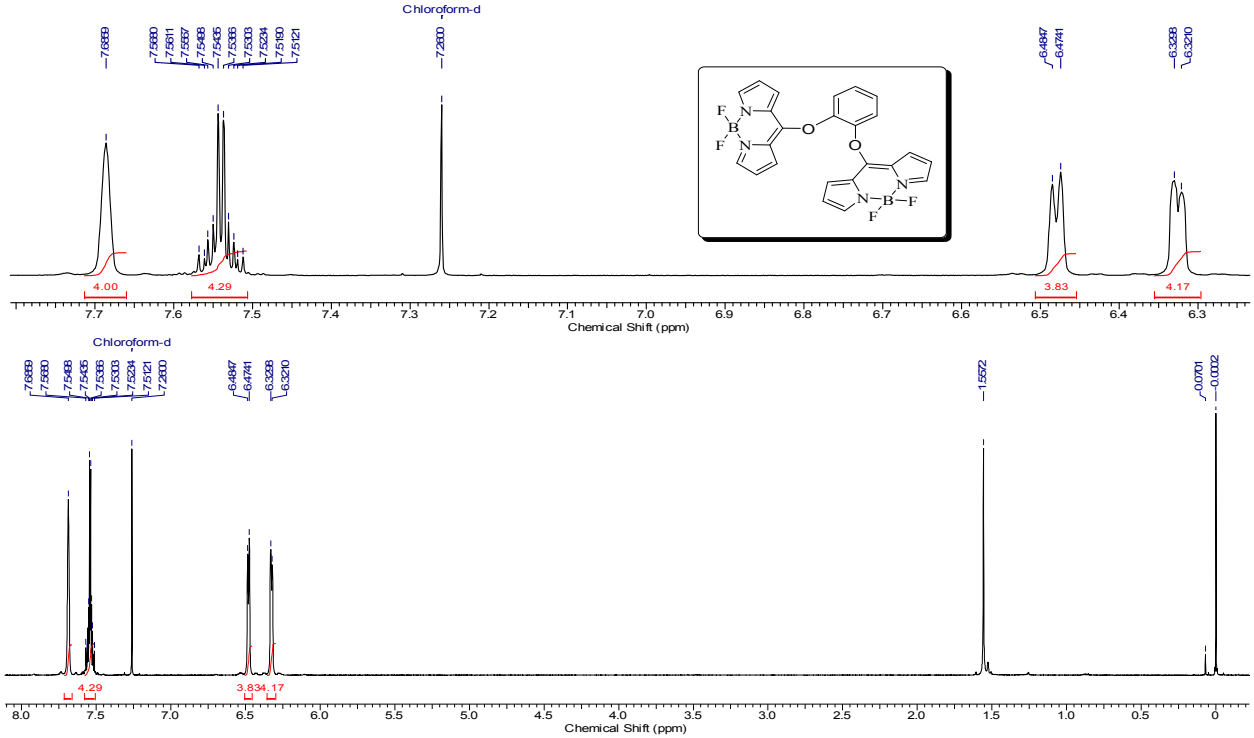
3e ^{11}B NMR



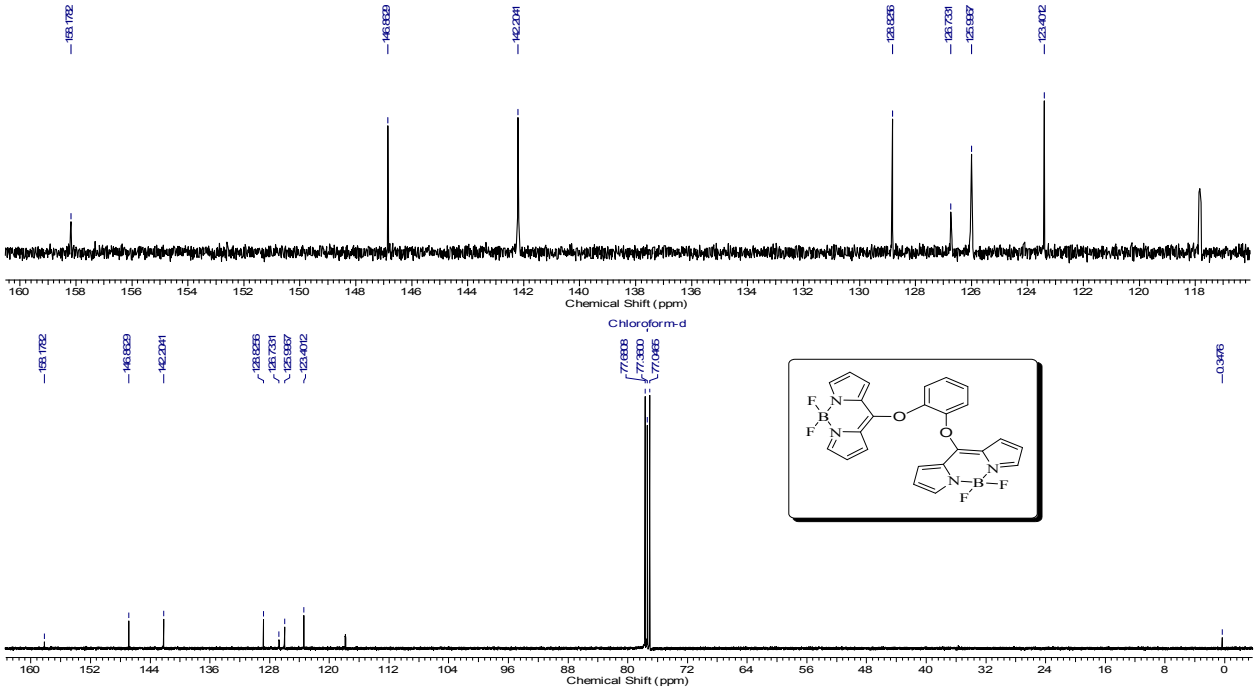
3f HRMS



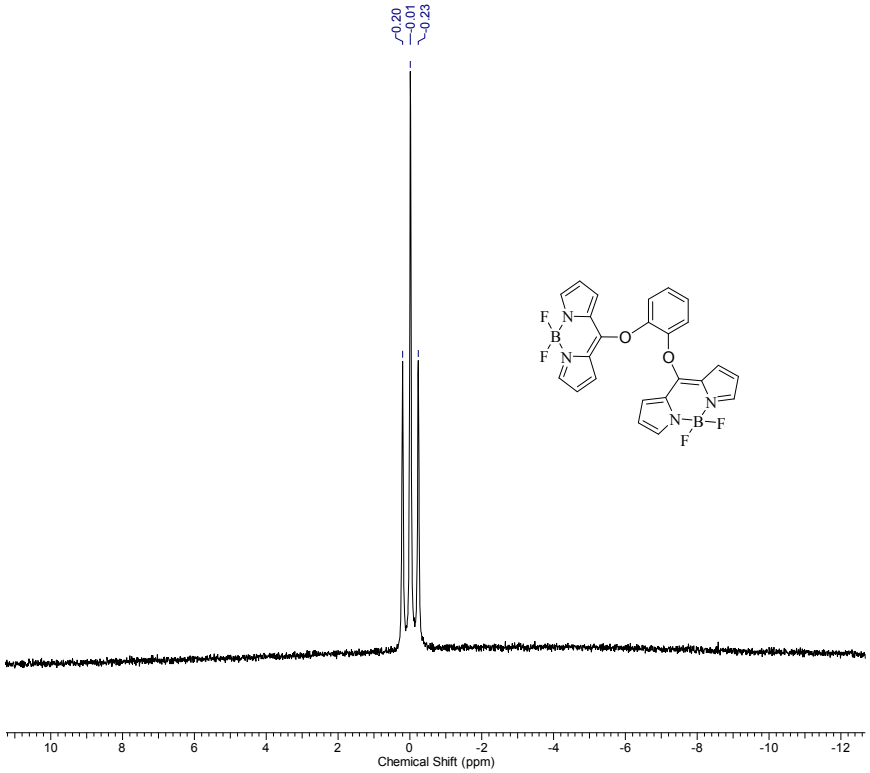
3f ^{1}H NMR



3f ^{13}C NMR



3f ^{11}B NMR



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