Supporting Information

Synthesis and Spectroscopic Investigation of a Series of Push-Pull Boron Dipyrromethenes (BODIPYs)

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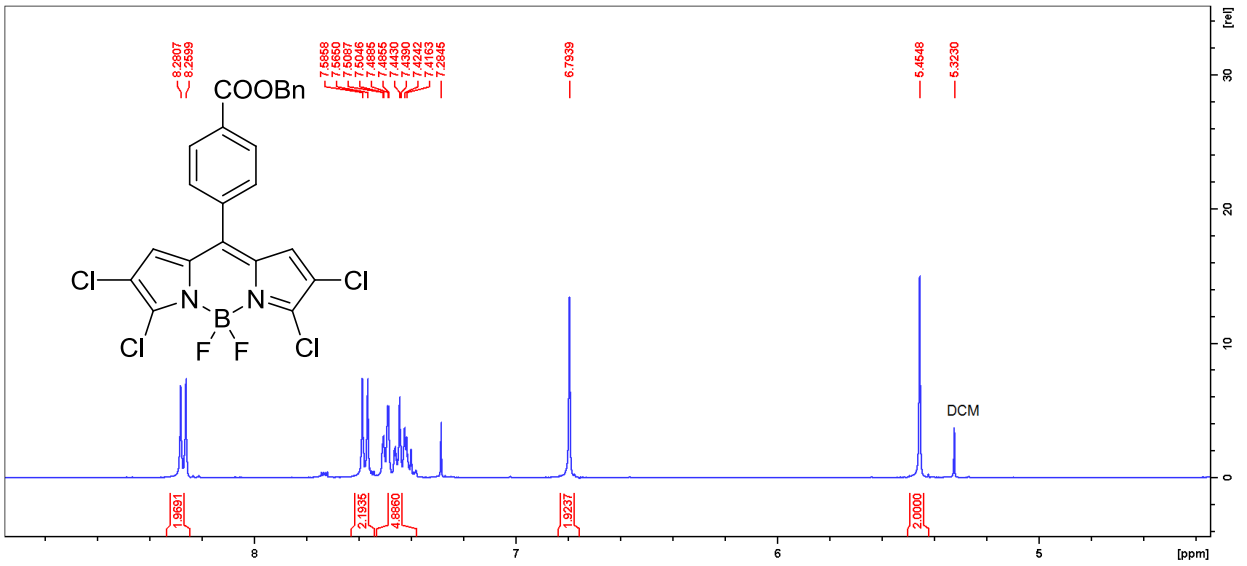


Figure S1. ^{1}H NMR spectrum of BODIPY **5a**.

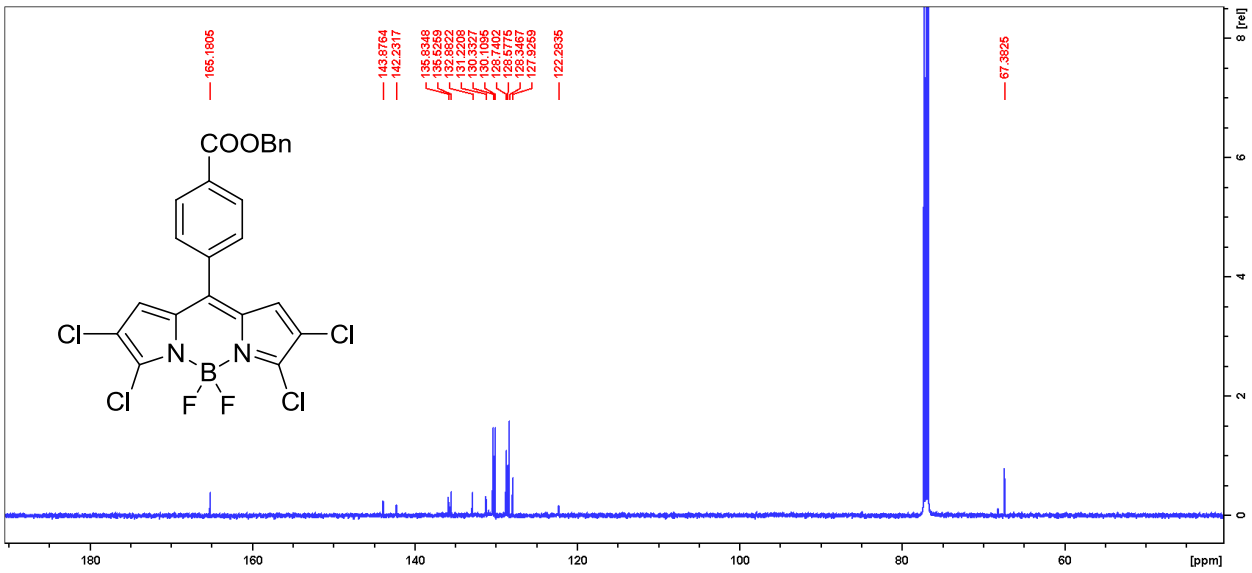


Figure S2. ^{13}C NMR spectrum of BODIPY **5a**.

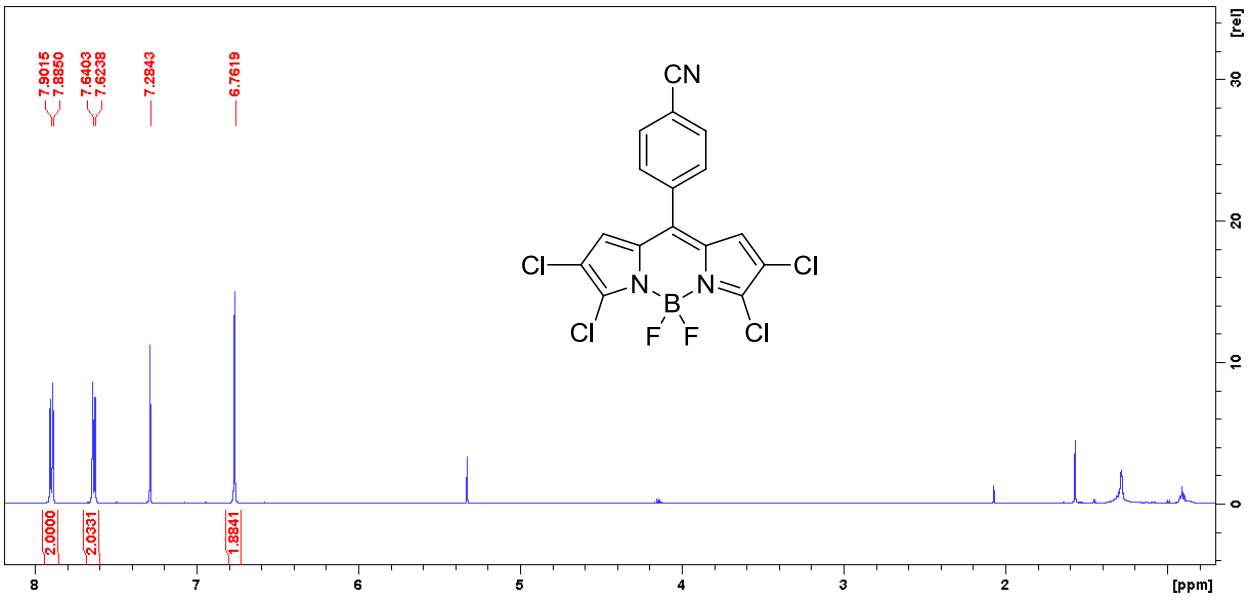


Figure S3. ^{1}H NMR spectrum of BODIPY **5b**.

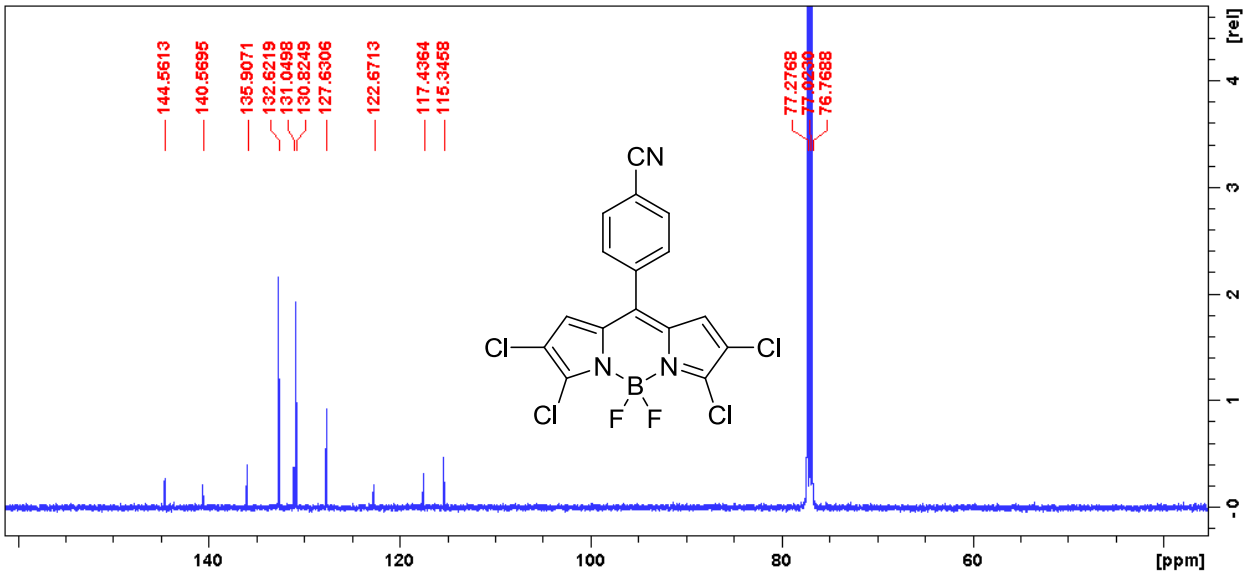


Figure S4. ^{13}C NMR spectrum of BODIPY **5b**.

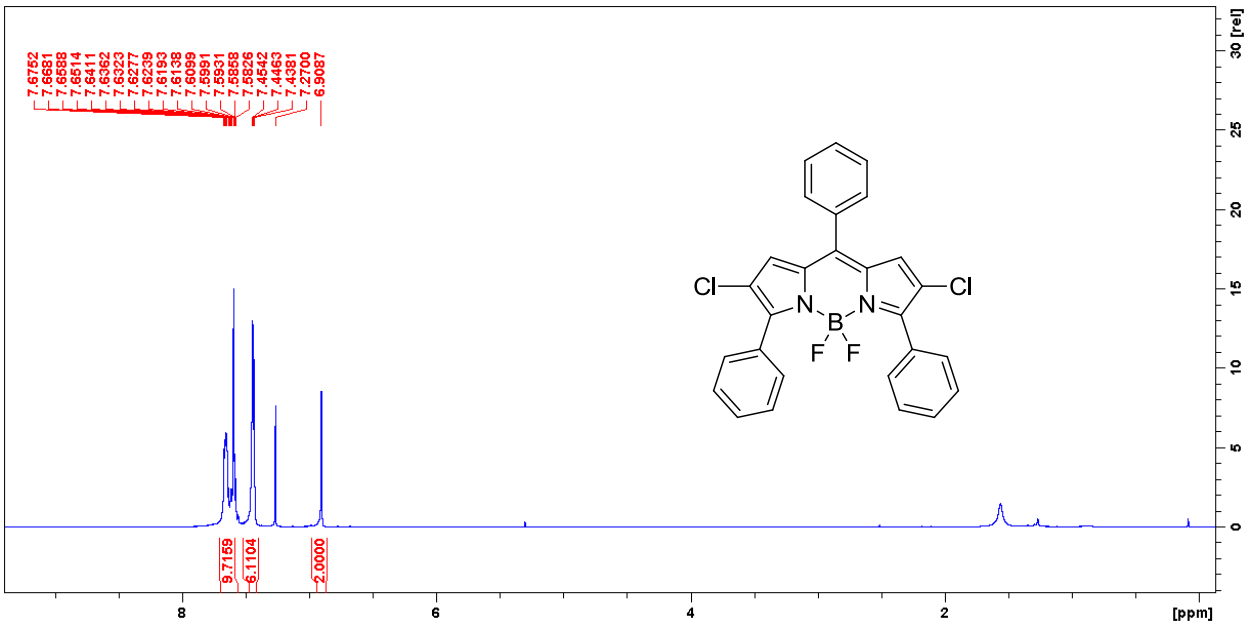


Figure S5. ^{1}H NMR spectrum of BODIPY **2**.

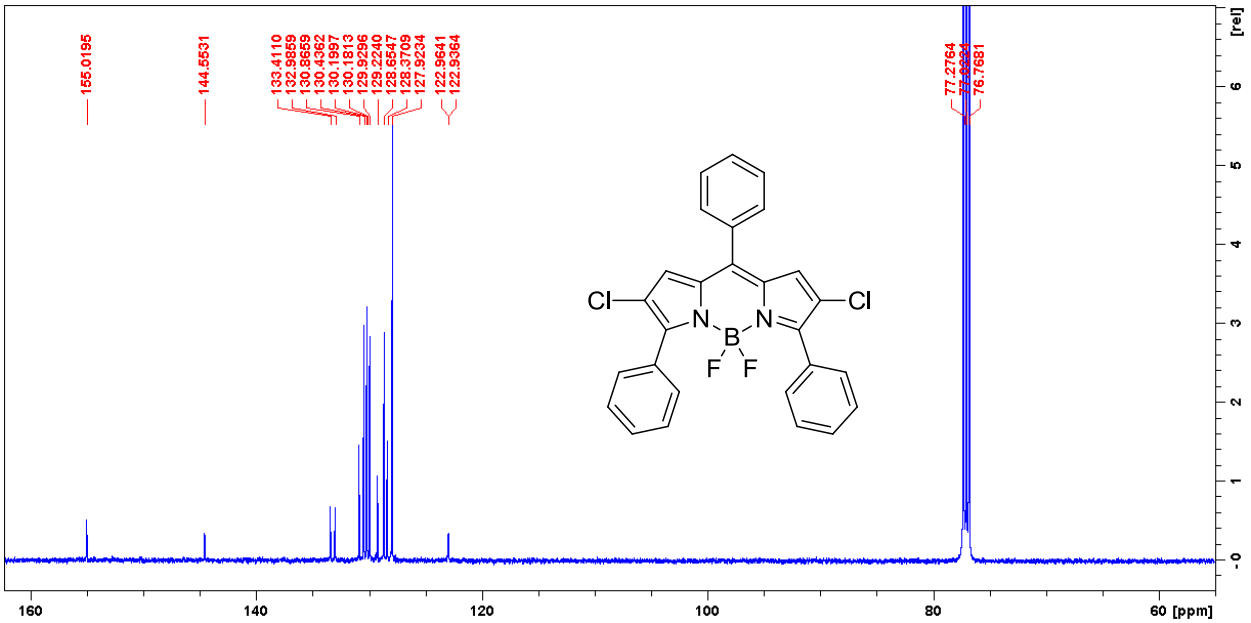


Figure S6. ^{13}C NMR spectrum of BODIPY **2**.

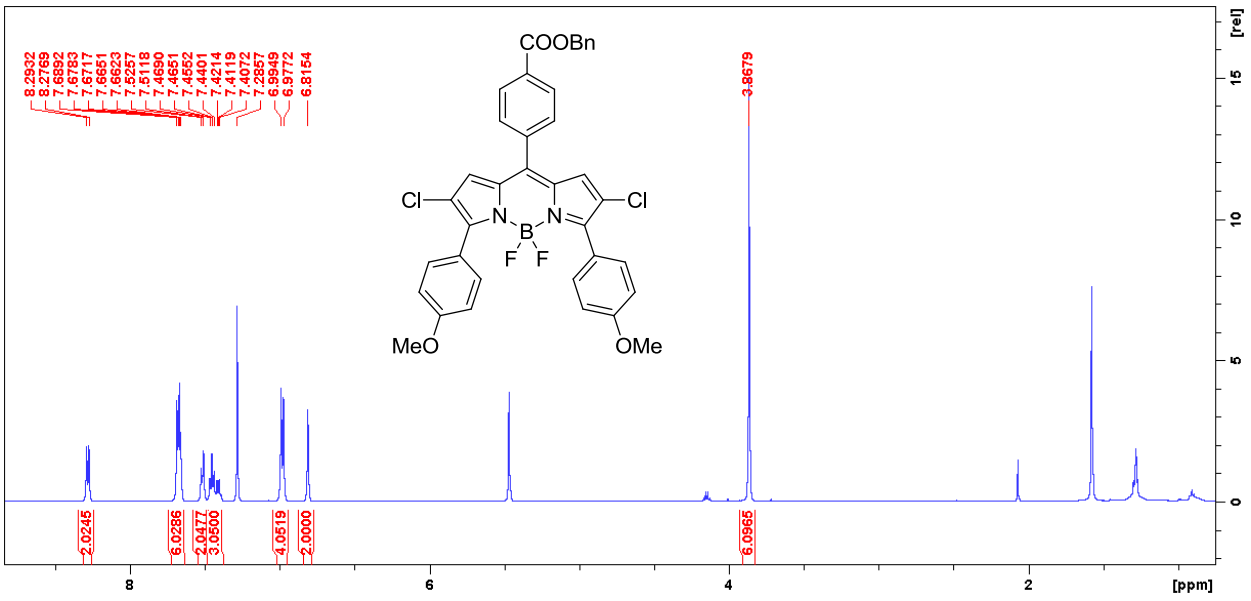


Figure S7. ^{1}H NMR spectrum of BODIPY **6a**.

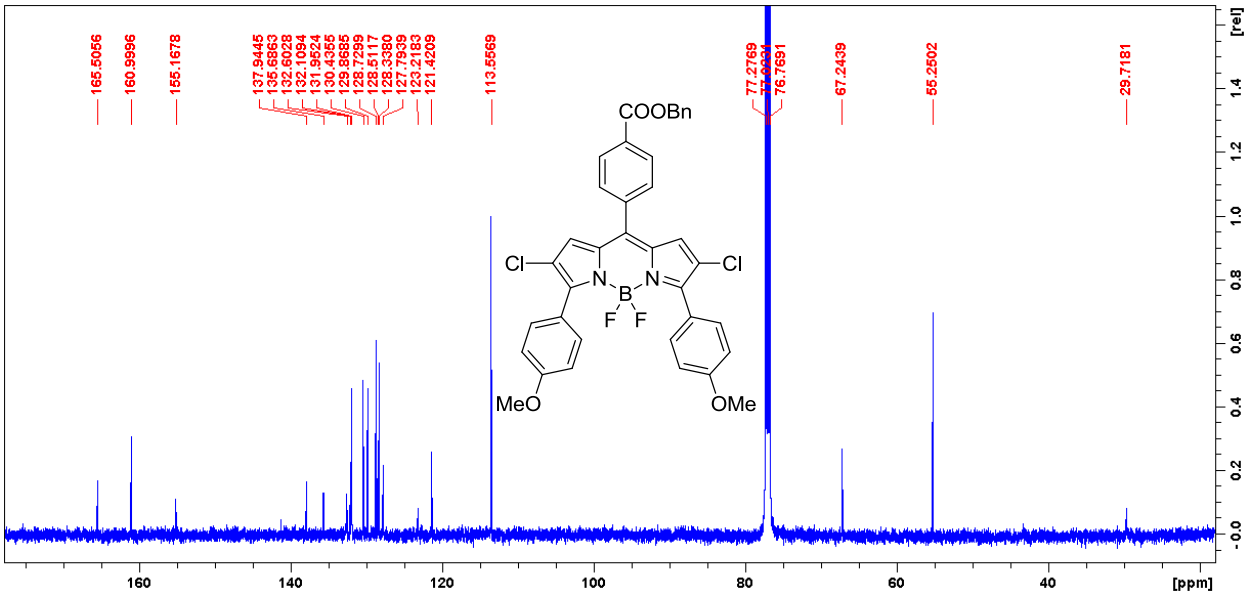
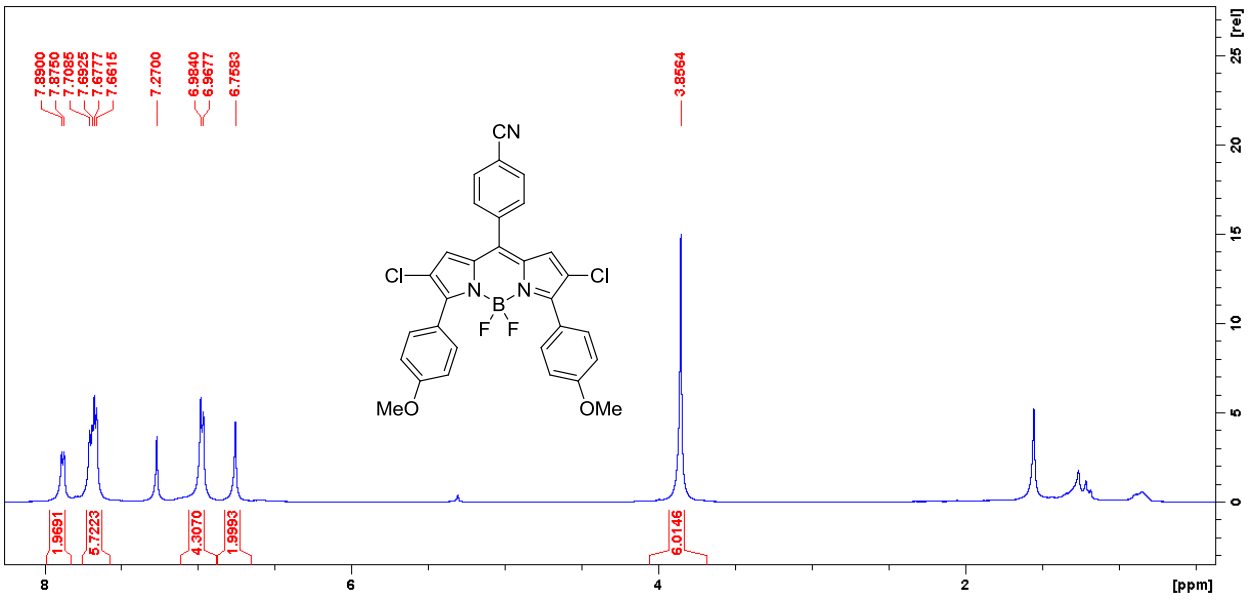


Figure S8. ^{13}C NMR spectrum of BODIPY **6a**.



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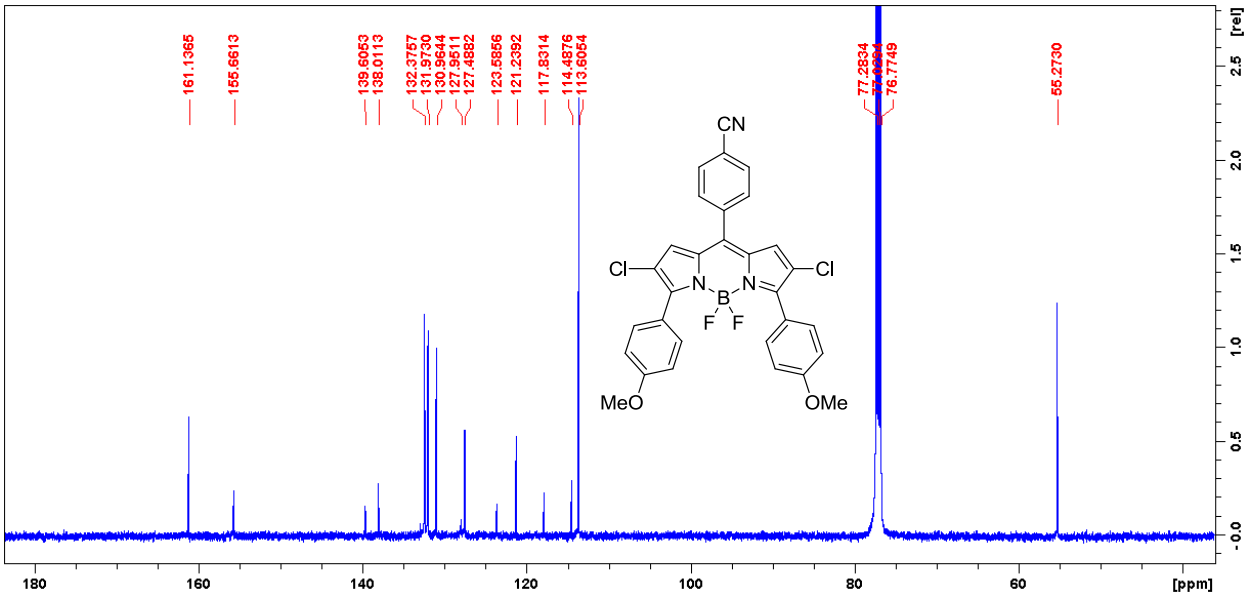


Figure S10. ^{13}C NMR spectrum of BODIPY **6b**.

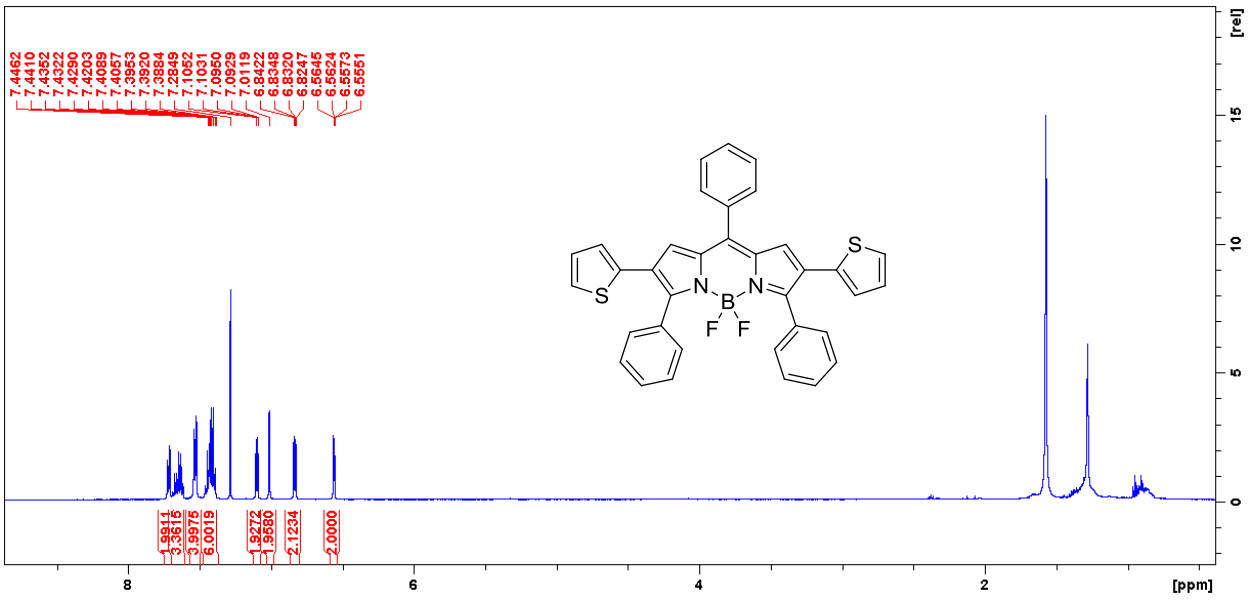


Figure S11. ^{1}H NMR spectrum of BODIPY **3**.

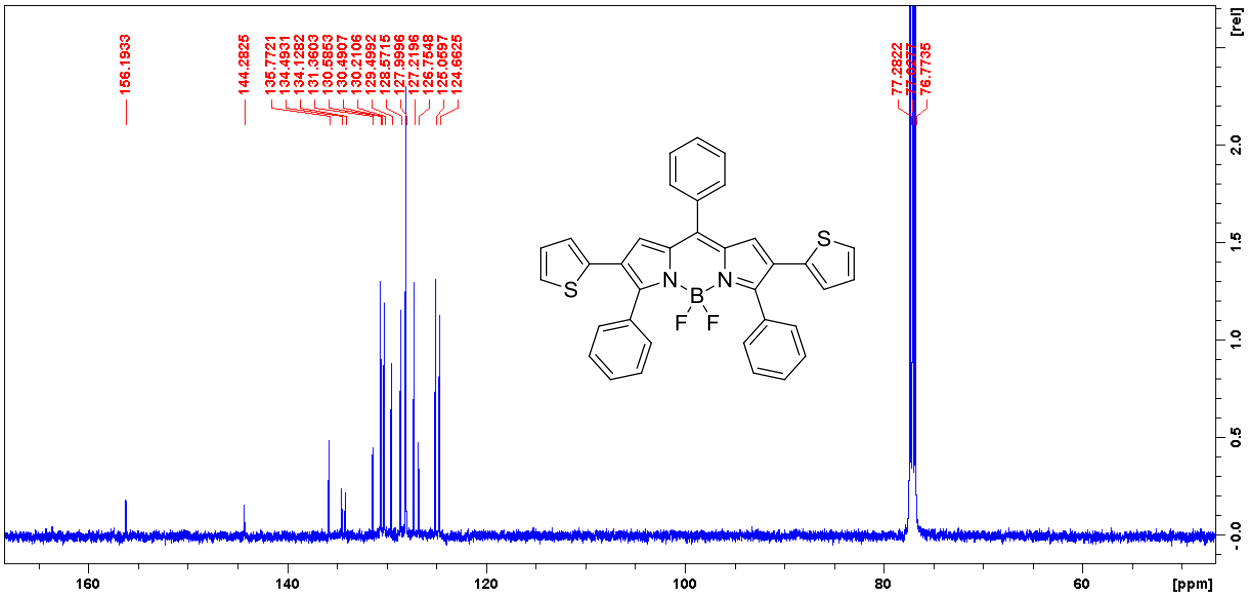


Figure S12. ^{13}C NMR spectrum of BODIPY **3**.

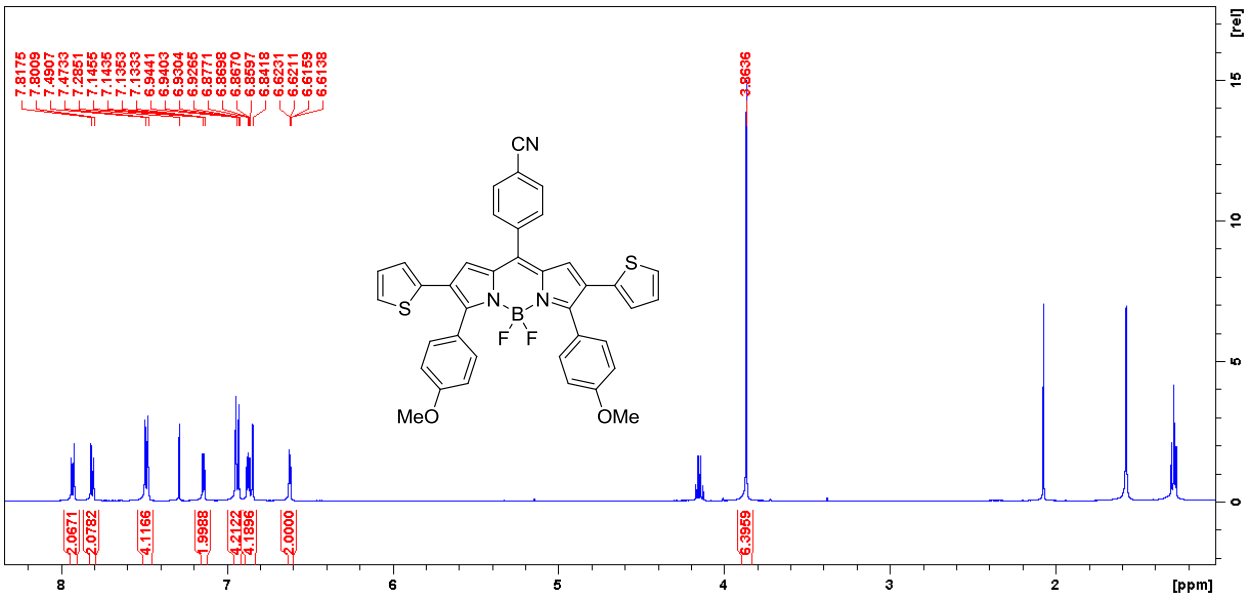


Figure S13. ^{1}H NMR spectrum of BODIPY **7**.

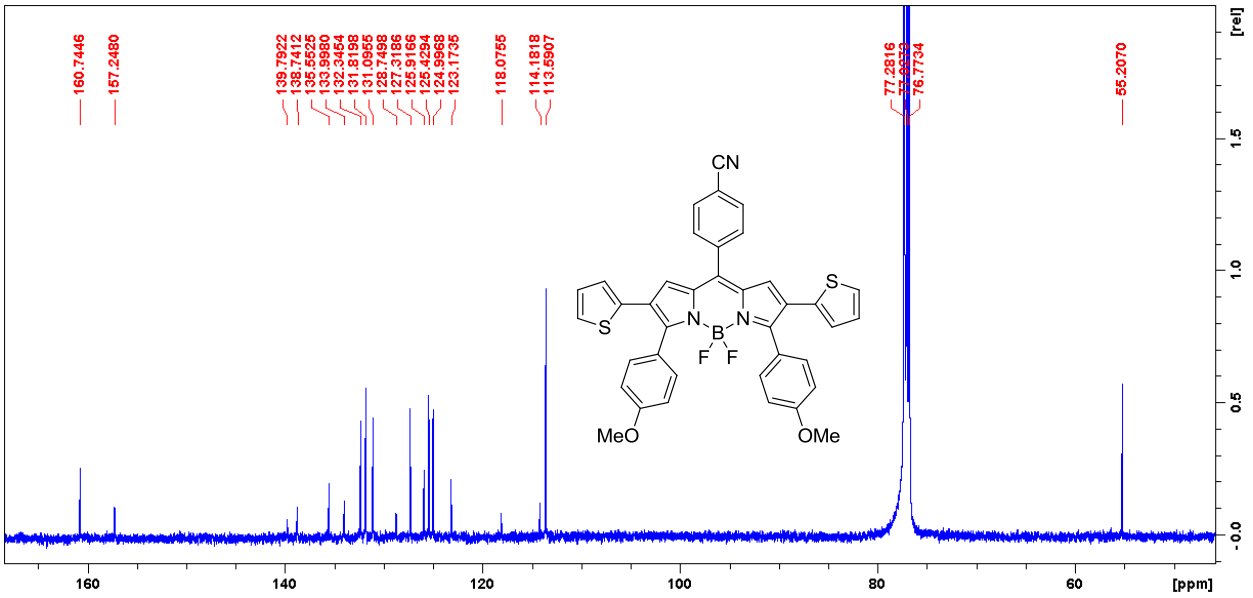


Figure S14. ^{13}C NMR spectrum of BODIPY **7**.

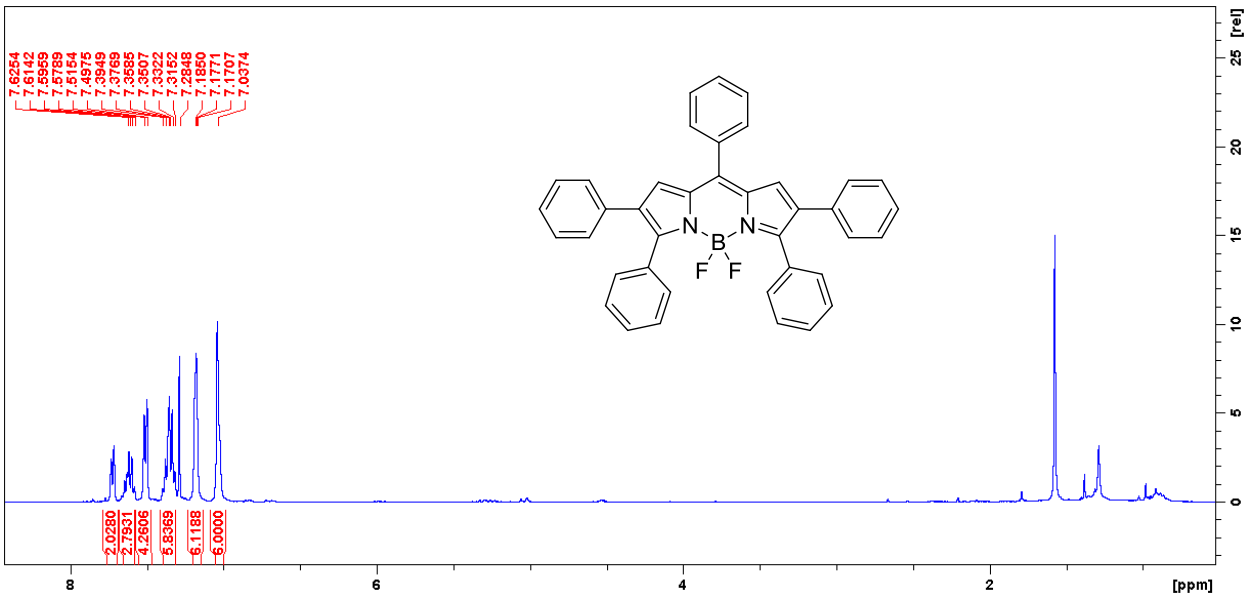
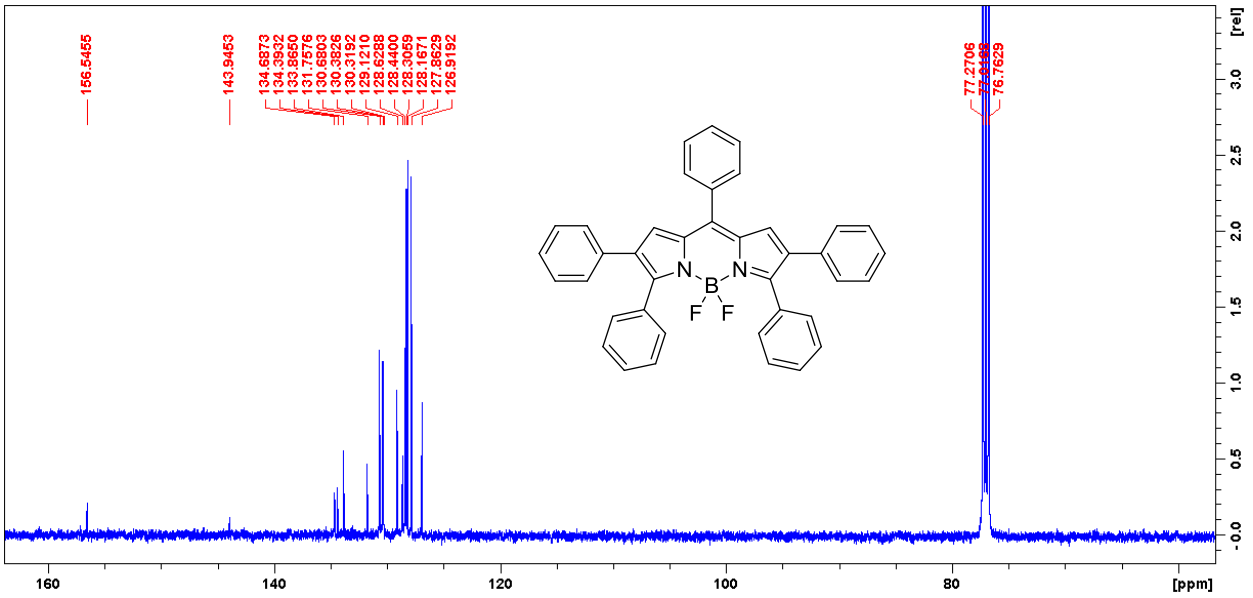


Figure S15. ^{1}H NMR spectrum of BODIPY **4**.



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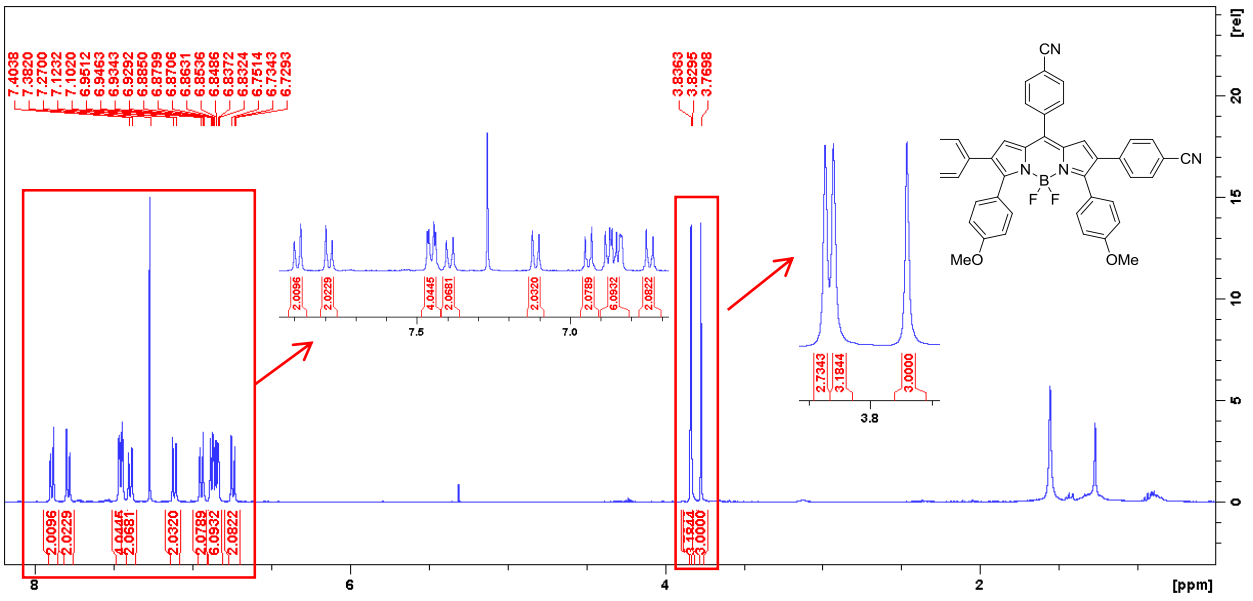


Figure S17. ^{1}H NMR spectrum of BODIPY **8**.

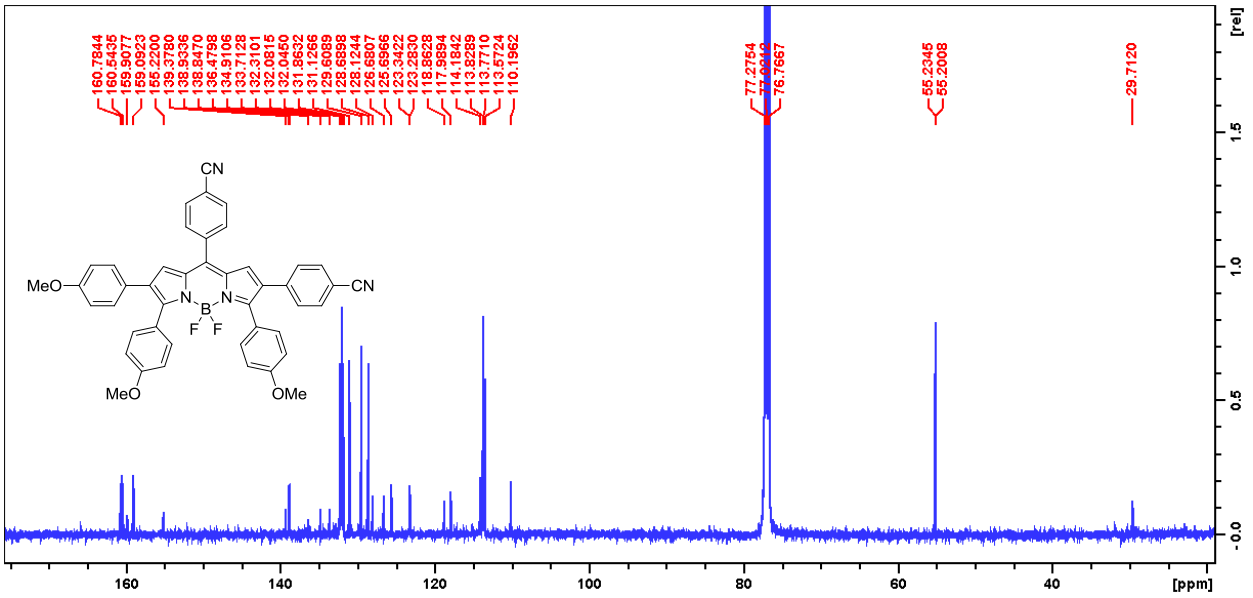
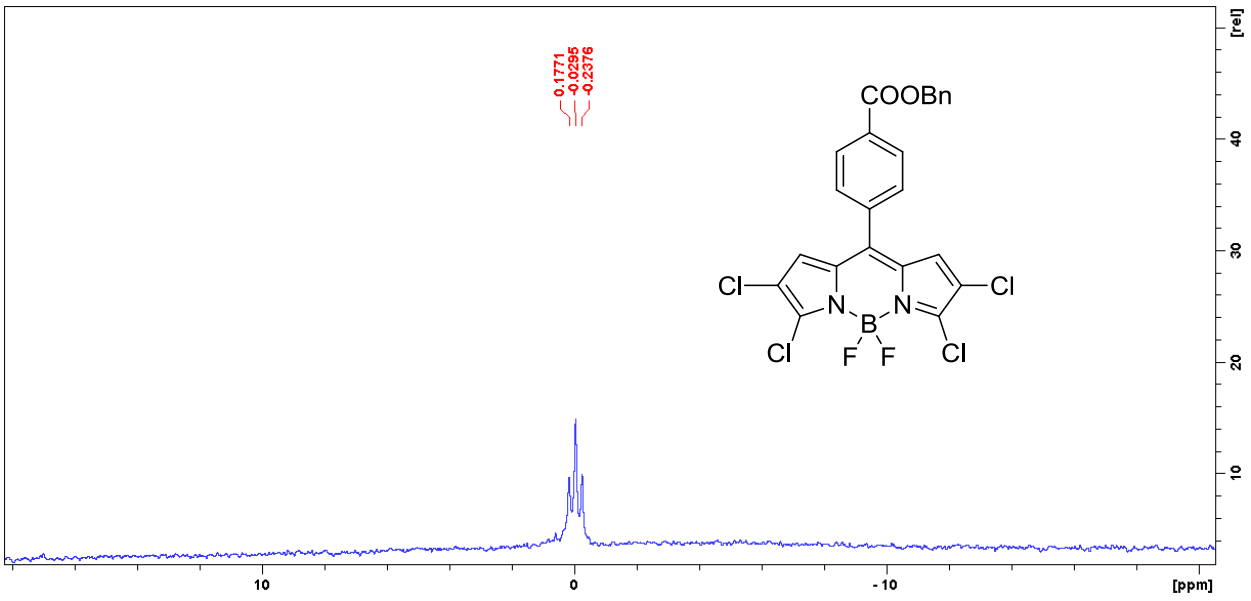


Figure S18. ^{13}C NMR spectrum of BODIPY **8**.



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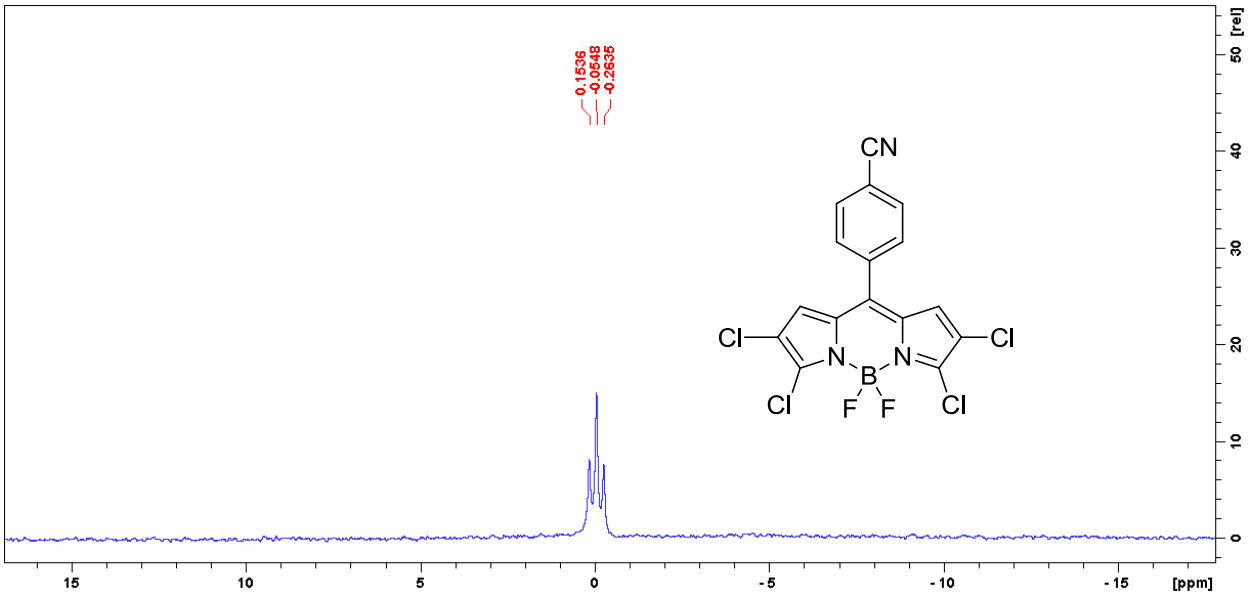

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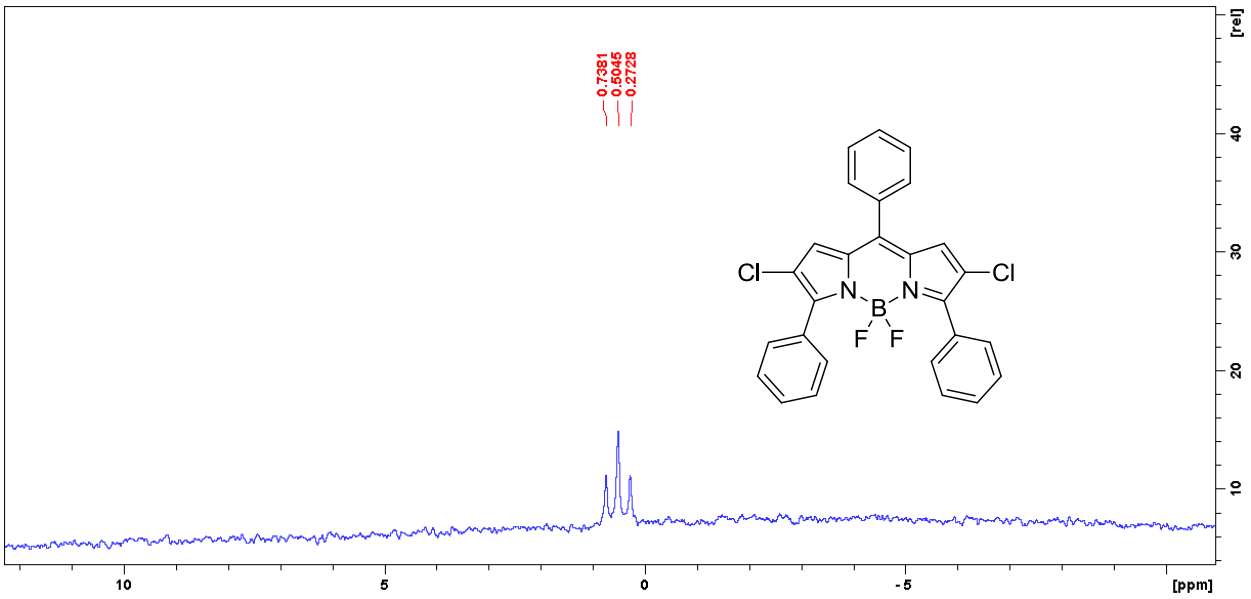


Figure S21. ^{11}B NMR spectrum of BODIPY **2**.

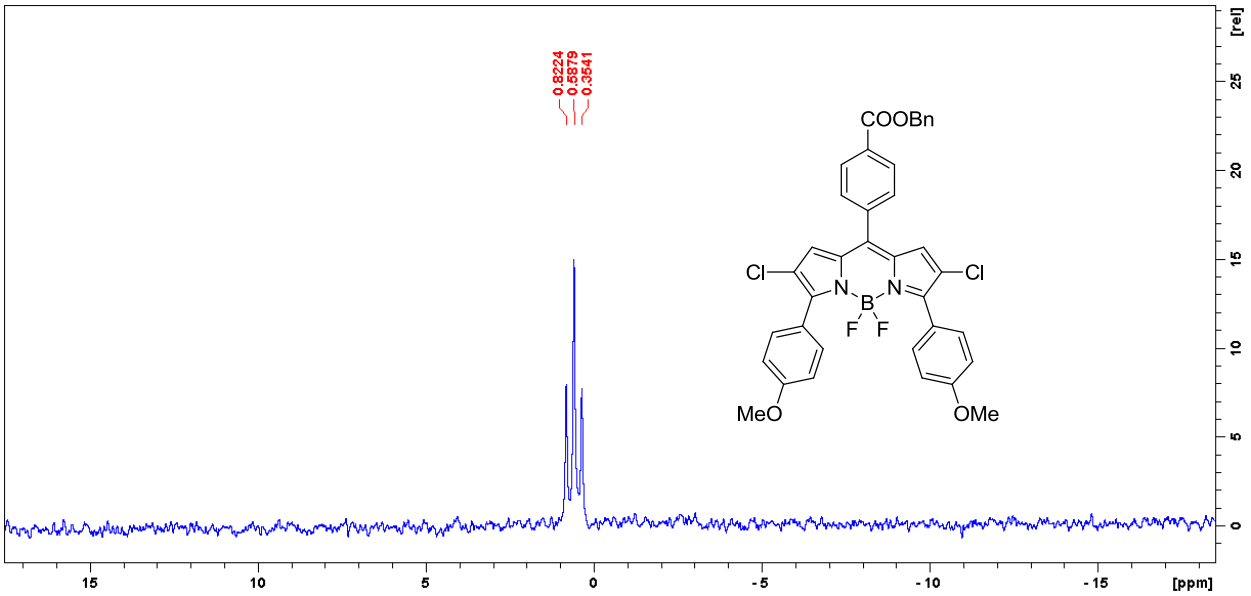
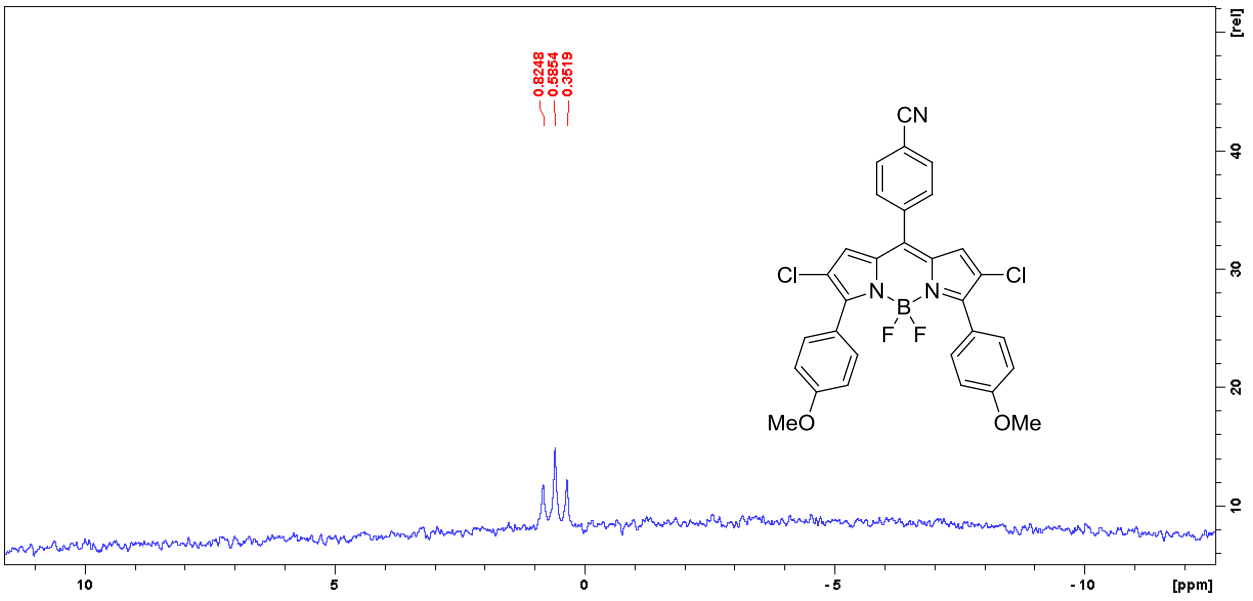


Figure S22. ^{11}B NMR spectrum of BODIPY **6a**.



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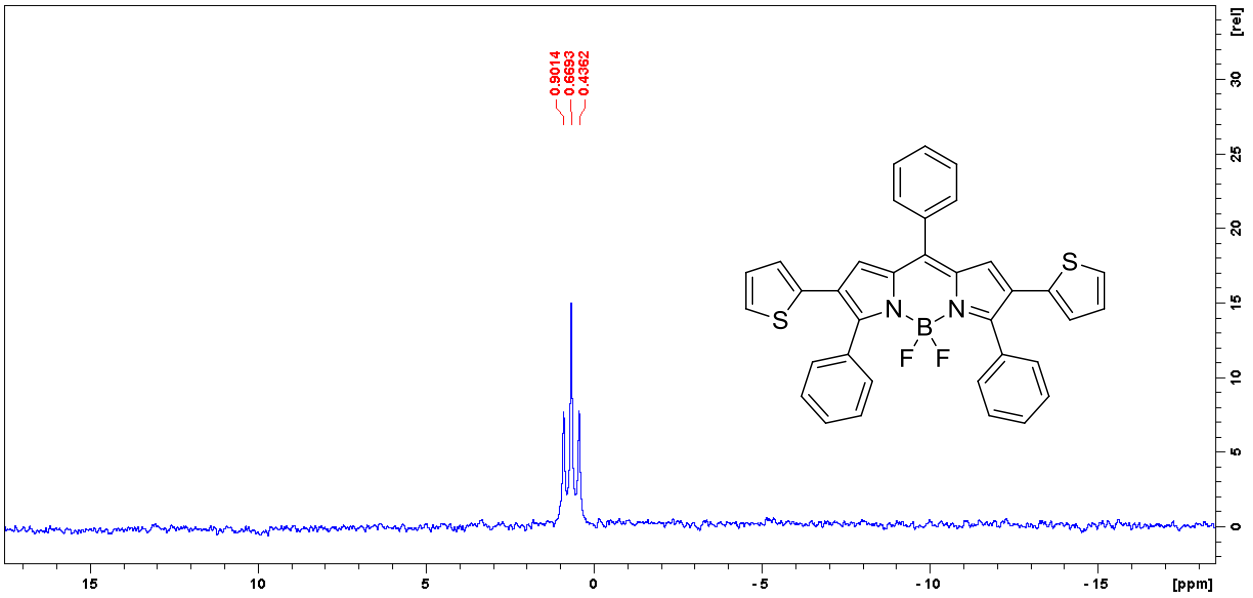


Figure S24. ^{11}B NMR spectrum of BODIPY **3**.

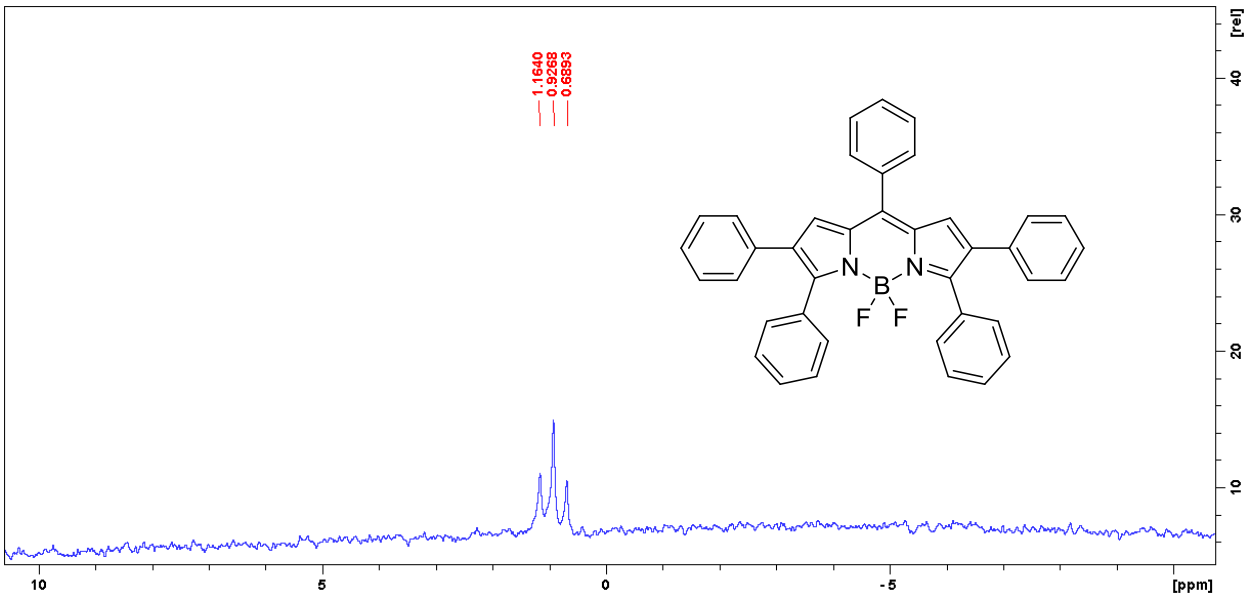


Figure S25. ^{11}B NMR spectrum of BODIPY **4**.

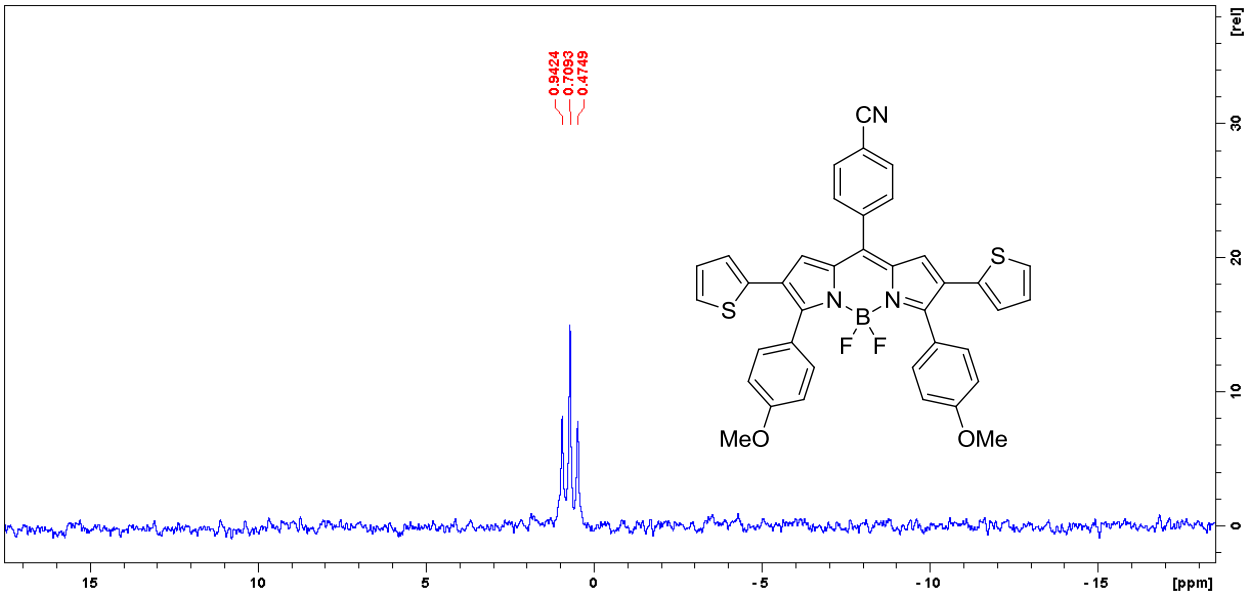


Figure S26. ^{11}B NMR spectrum of BODIPY **7**.

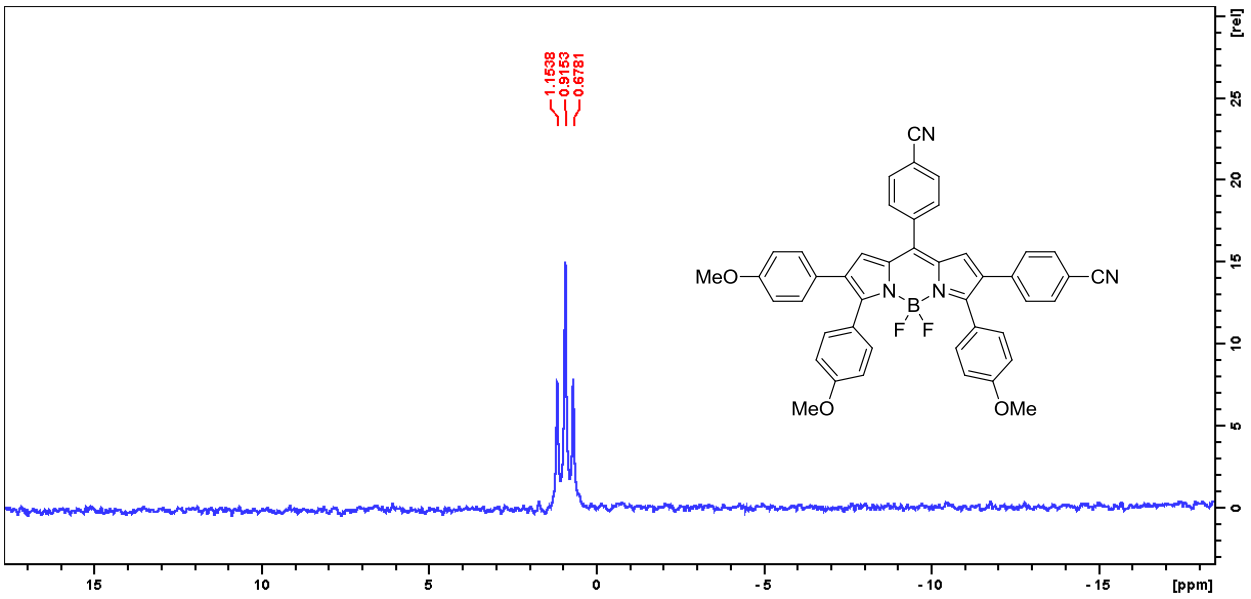
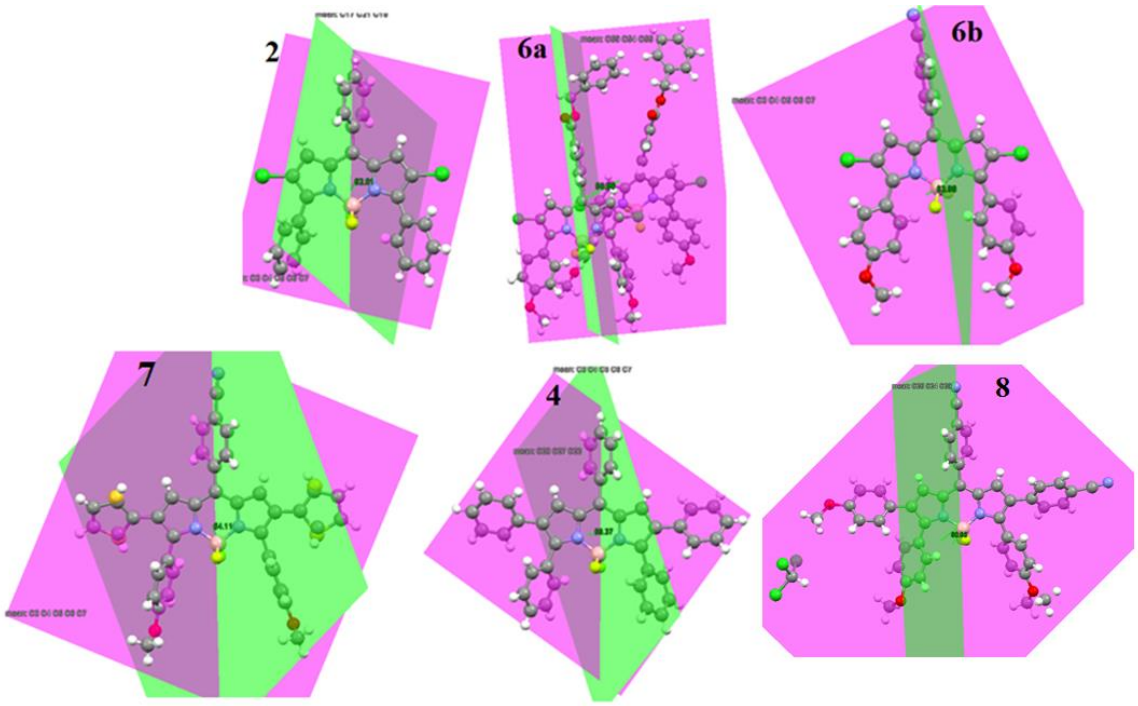
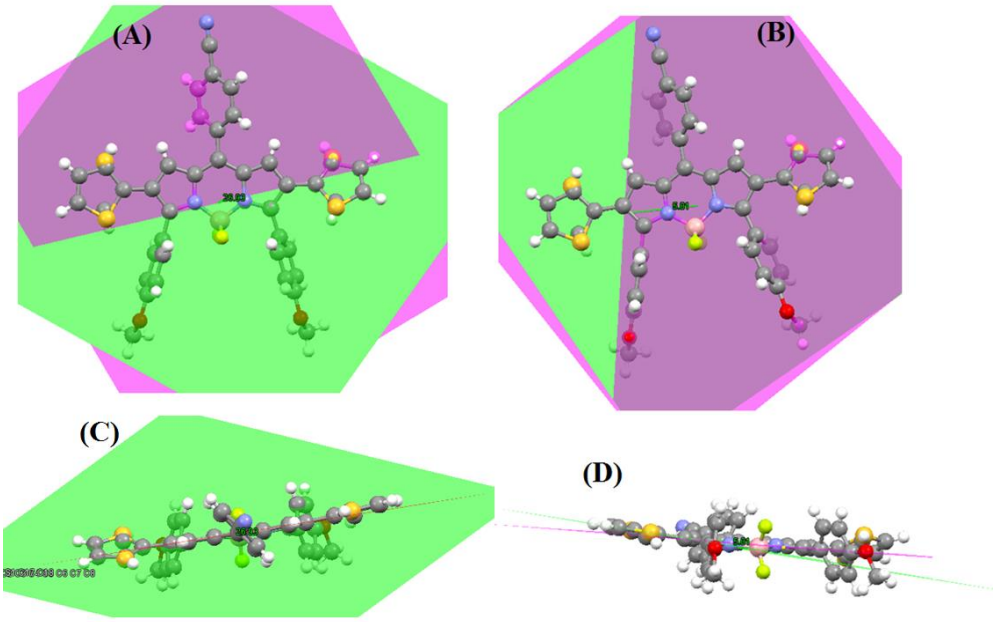


Figure S27. ^{11}B NMR spectrum of BODIPY **8**.



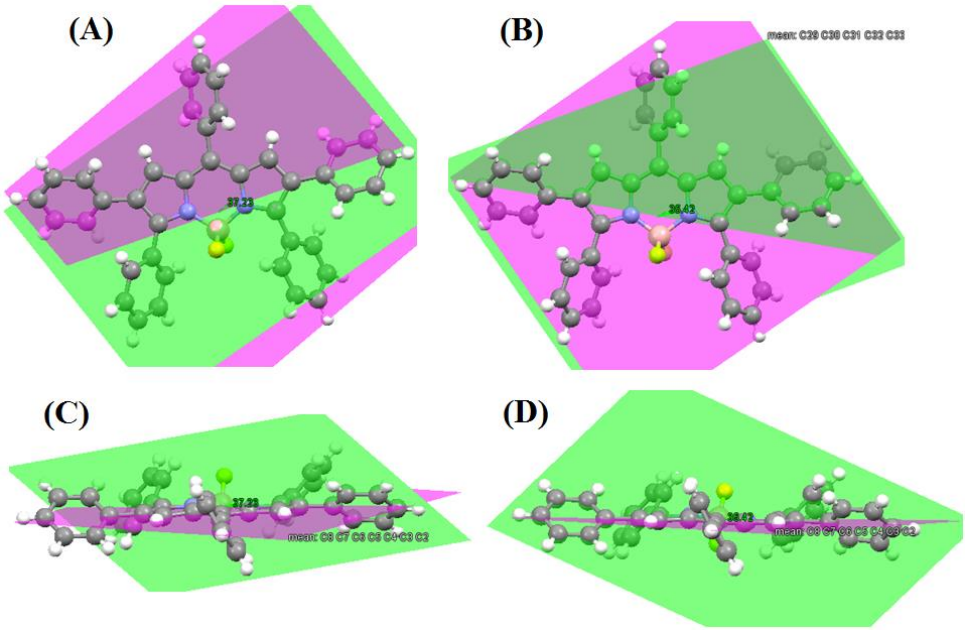
Cpds	**2**	**6a**	**6b**	**4**	**7**	**8**
Dihedral angle (^{o})	62.0	56.6	63.7	59.4	54.1	60.7

Figure S28. Dihedral angles of the meso substituent with the 12-atom BODIPY core for BODIPY **2**, **6a**, **6b**,**4**, **7**, and **8**: the purple and green plane corresponds to the 12-atom BODIPY and the meso substituent, respectively.



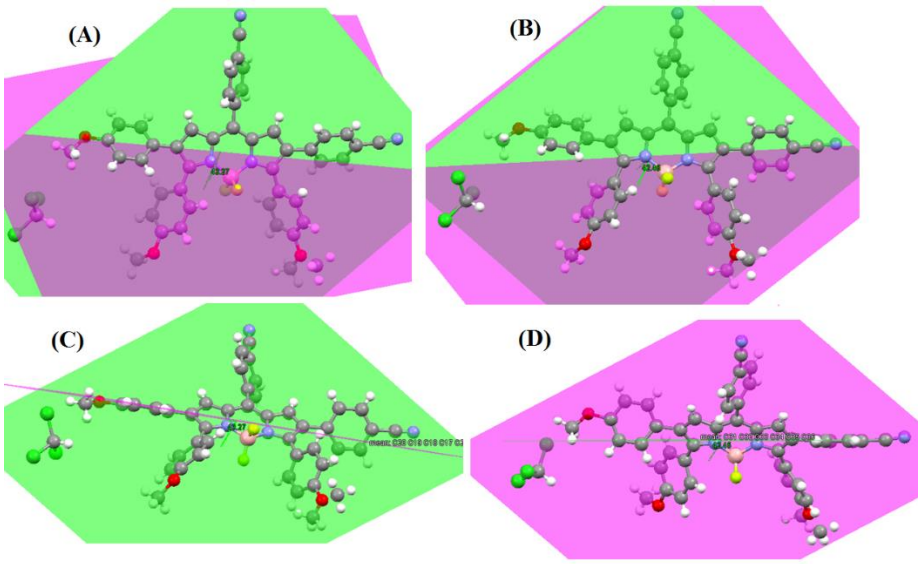
Cpds	Dihedral angle-2 position (°)	Dihedral angle-6position (°)
7	26.9	5.0

Figure S29. Dihedral angles of the 2,6 substituents with the 12-atom BODIPY core for BODIPY **7**: (A, B) is the front view and (C,D) is the side view. The purple and green plane corresponds to the 12-atom BODIPY and the 2,6 substituents, respectively.



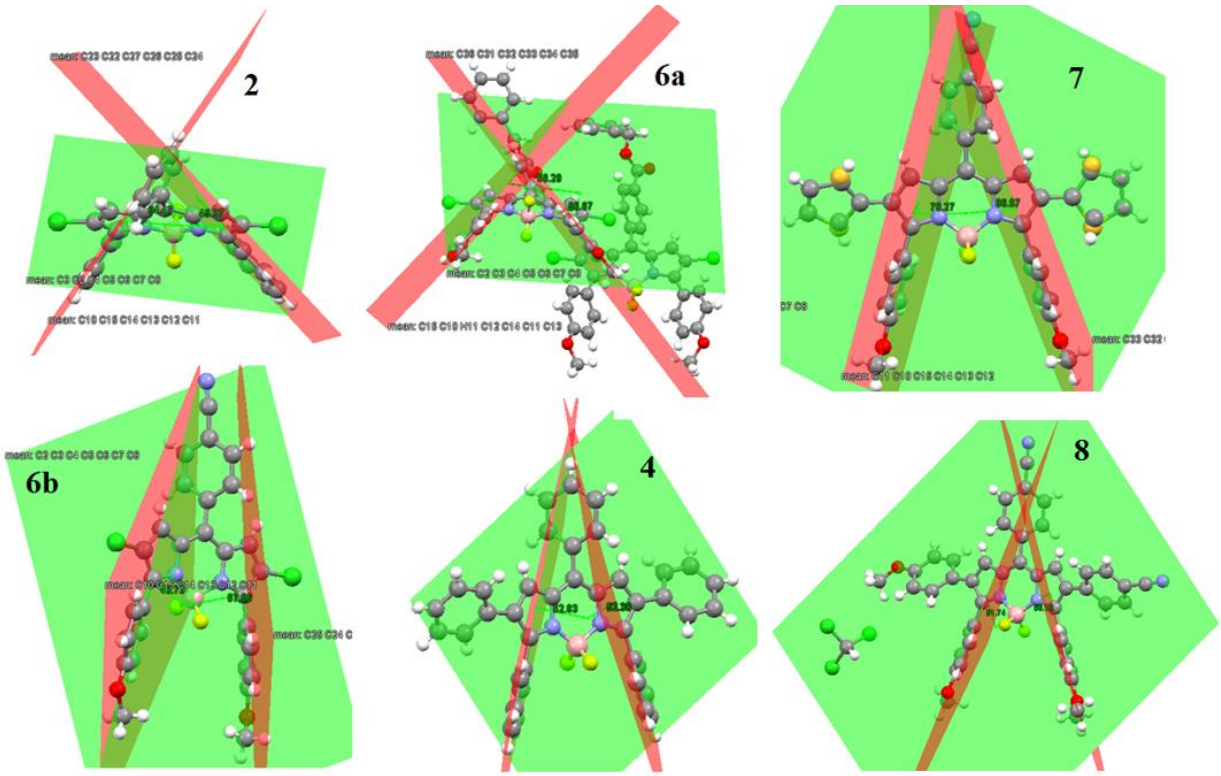
Cpds	Dihedral angle-2 position (°)	Dihedral angle-6position (°)
4	37.2	35.4

Figure S30. Dihedral angles of the 2,6 substituents with the 12-atom BODIPY core for BODIPY **4**: (A, B) is the front view and (C,D) is the side view. The purple and green plane corresponds to the 12-atom BODIPY and the 2,6 substituents, respectively.



Cpds	Dihedral angle-2 position (°)	Dihedral angle-6position (°)
8	43.3	42.5

Figure S31. Dihedral angles of the 2,6 substituents with the 12-atom BODIPY core for BODIPY **8**: (A, B) is the front view and (C,D) is the side view. The purple and green plane corresponds to the 12-atom BODIPY and the 2,6 substituents, respectively.



Cpds	**2**	**6a**	**6b**	**4**	**7**	**8**
Dihedral angle-3 position (°)	64.5	56.3	43.7	52.9	70.3	51.7
Dihedral angle-5 position (°)	45.4	56.7	57.6	52.4	86.1	56.1

Figure S32. Dihedral angles of the 3,5 substituents with the 12-atom BODIPY core for BODIPY **2**, **6a**, **6b**, **4**, **7**, and **8**: the green and red plane corresponds to the 12-atom BODIPY and the 2,6 substituents, respectively.

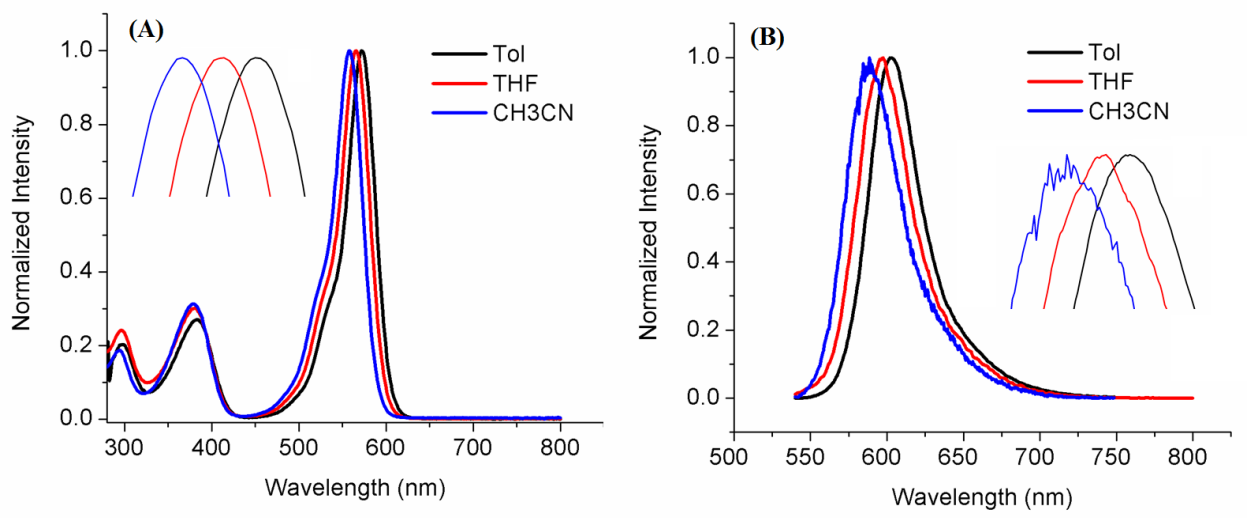


Figure S33. Absorbance (A) and fluorescence (B) spectra of BODIPY **2** in toluene, tetrahydrofuran and acetonitrile.

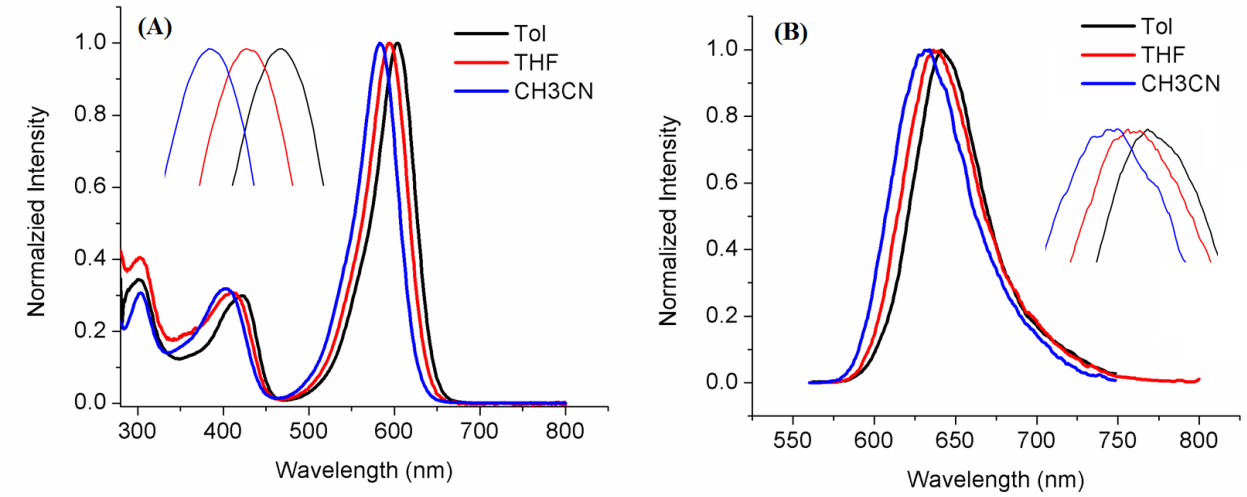


Figure S34. Absorbance (A) and fluorescence (B) spectra of BODIPY **6a** in toluene, tetrahydrofuran and acetonitrile.

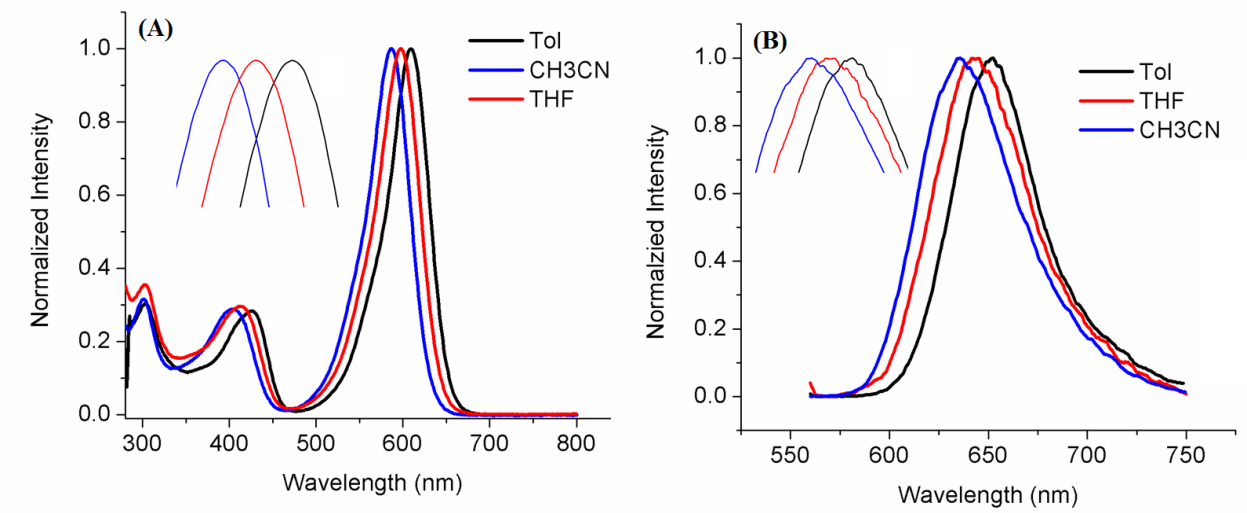


Figure S35. Absorbance (A) and fluorescence (B) spectra of BODIPY **6b** in toluene, tetrahydrofuran and acetonitrile.

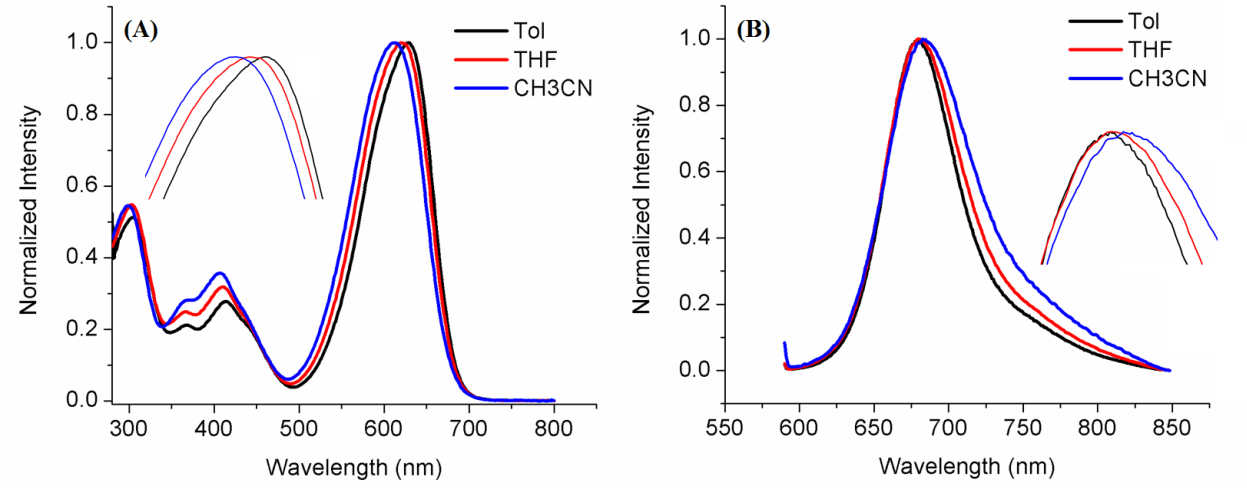


Figure S36. Absorbance (A) and fluorescence (B) spectra of BODIPY **3** in toluene, tetrahydrofuran and acetonitrile.

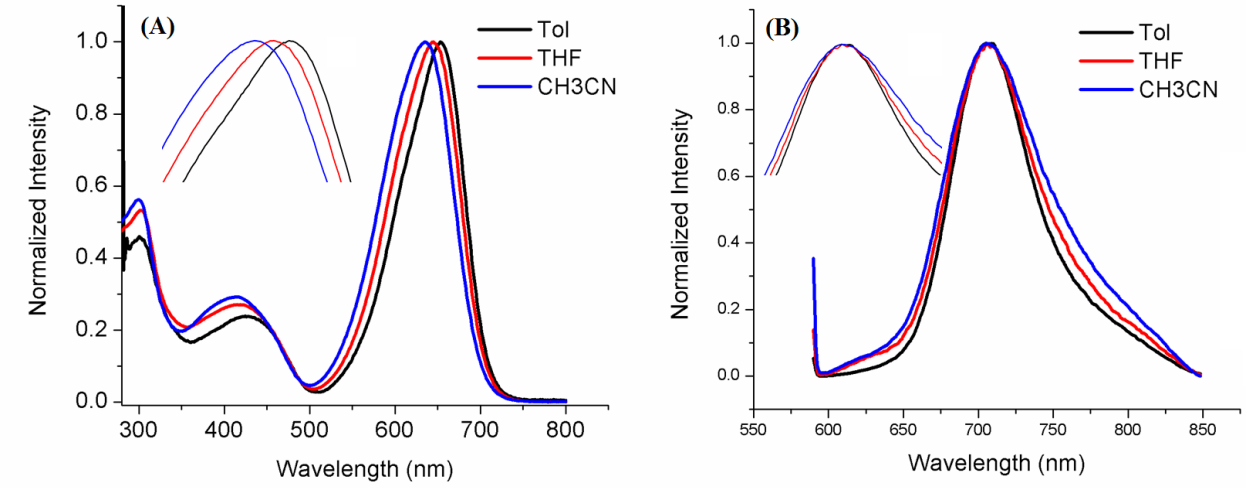


Figure S37. Absorbance (A) and fluorescence (B) spectra of BODIPY **7** in toluene, tetrahydrofuran and acetonitrile.

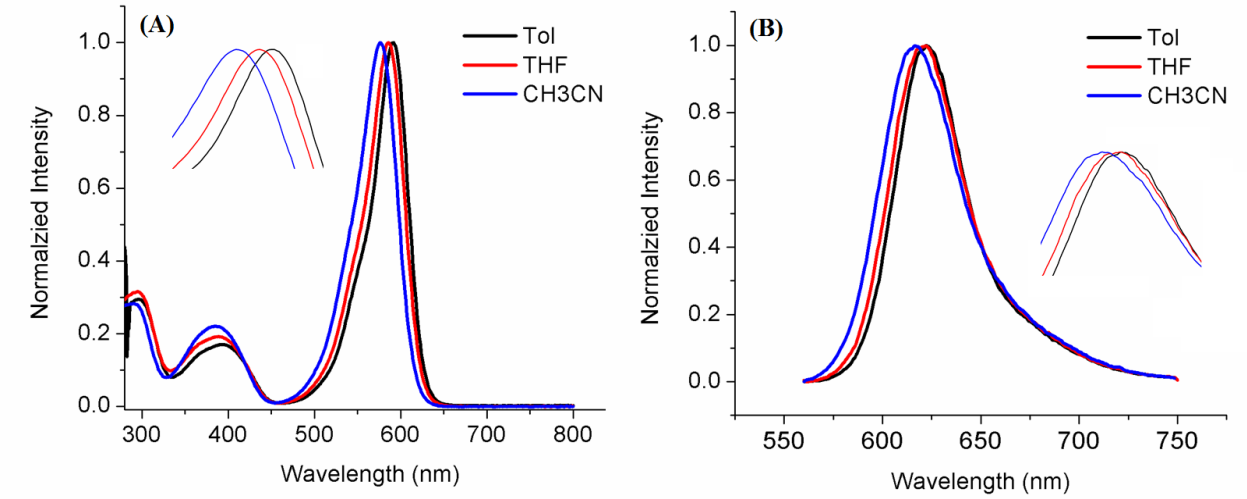


Figure S38. Absorbance (A) and fluorescence (B) spectra of BODIPY **4** in toluene, tetrahydrofuran and acetonitrile.

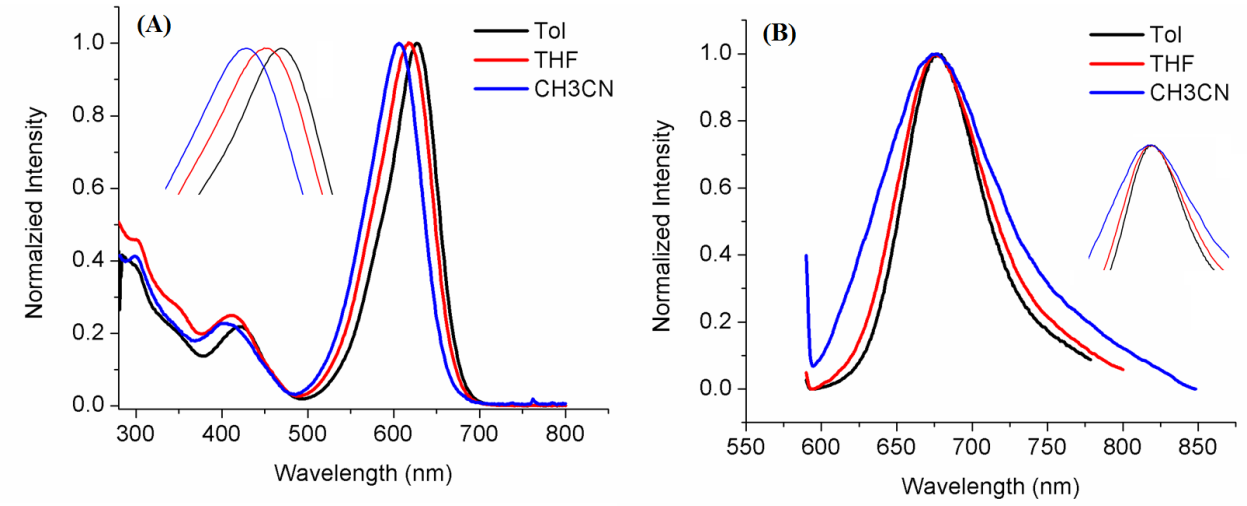


Figure S39. Absorbance (A) and fluorescence (B) spectra of BODIPY **8** in toluene, tetrahydrofuran and acetonitrile.

Table S1. Half-wave potentials (V vs. SCE) for the investigated BODIPYs in CH_3CN and THF, 0.1 M TBAP.

		Oxidation		Reduction				H-L
Solvent	Cpd.#	2nd	1st	1st	2nd	3rd	Δ (2-1) (Volt)	Gap[b]
CH_3CN	**2**		1.42[a]	-0.55	-1.54[a]		0.99	
	4		1.28[a]	-0.72	-1.68[a]		0.96	
	3		1.16[a]	-0.67	-1.66[a]		0.99	
	6a		1.32[a]	-0.53	-1.22		0.71	
	6b	1.60	1.31	-0.48	-1.20		0.72	1.79
	8	1.41	1.16	-0.62	-1.28	-2.05	0.66	1.78
	7		1.11[a]	-0.59	-1.27		0.68	
THF	**2**		N/A	-0.55	-1.56[a]		0.99	
	4		1.43	-0.74	-1.68[a]		0.94	2.17
	3		1.34[a]	-0.69	-1.64[a]		0.95	
	6a		1.56[a]	-0.53	-1.20		0.67	
	6b		1.56[a]	-0.49	-1.16		0.67	
	8		1.25	-0.84	-1.26	-2.60[a]	0.42	2.09
	7		1.30[a]	-0.61	-1.23		0.62	

[a]Peak potential, E_p at scan rate of 0.1 V/s; [b]HOMO - LUMO Gap calculated as $|E_{1/2}$ (1st Ox) - $E_{1/2}$ (1st Red)| for processes with reversible first oxidation and first reduction.

Table S2. The DFT calculated atom coordinates and their absolute energies for BODIPYs

BODIPY **2**: HF = -2293.7581247 a.u.

C	-1.16031	1.423793	0.088923
C	0.085864	2.070975	0.094194
C	1.273671	1.321284	0.070052
C	-3.33012	0.904537	-0.04917
C	-2.57491	-0.3056	-0.01134
C	3.379547	0.623832	-0.2071
C	2.537426	-0.51922	-0.06359
B	-0.03729	-0.93057	0.315303
F	-0.0706	-1.34354	1.653493
F	-0.07093	-1.98056	-0.56557
N	-1.26275	0.033796	0.076197
N	1.265381	-0.07108	0.10041
Cl	5.106388	0.606262	-0.38997
Cl	-5.0613	1.02592	-0.10406
C	2.95169	-1.93128	-0.06814
C	4.27036	-3.71243	-1.06403
H	4.945156	-4.05366	-1.84333
C	3.836505	-4.59522	-0.0739
H	4.178289	-5.62614	-0.07503
C	2.515533	-2.8286	0.922161
H	1.828433	-2.48838	1.686425
C	-3.10879	-1.67767	-0.04914
C	-3.2836	-3.92522	0.843777
H	-2.98081	-4.66694	1.576777
C	-4.22608	-4.25109	-0.13282
H	-4.65719	-5.24749	-0.16412
C	-4.06373	-2.0121	-1.02552
H	-4.36149	-1.27258	-1.76057
C	3.838272	-2.38872	-1.05886
H	4.172354	-1.71036	-1.83582
C	2.960059	-4.14794	0.916137
H	2.618886	-4.82953	1.689548
C	-4.61142	-3.29156	-1.07014
H	-5.33838	-3.53811	-1.83813
C	-2.72362	-2.65107	0.888588
H	-1.98809	-2.40433	1.643237
C	0.157871	3.553982	0.082943
C	-0.40666	5.694581	-0.91781
H	-0.8996	6.259469	-1.70321
C	0.308029	6.358803	0.080483
H	0.365397	7.443066	0.079664

C	0.882024	4.231975	1.078426
H	1.370962	3.662307	1.86203
C	0.950253	5.624081	1.078564
H	1.503148	6.134348	1.861397
C	-0.48623	4.302935	-0.91637
H	-1.02635	3.788151	-1.7041
C	2.60503	1.762603	-0.12102
H	2.935975	2.78602	-0.20137
C	-2.46327	1.974755	0.03437
H	-2.71935	3.022036	0.059208

BODIPY **6a**: HF = -2981.751587 a.u.

C	-1.12214	1.617352	0.340587
C	0.129745	2.25221	0.336976
C	1.311056	1.494242	0.304415
C	-3.29749	1.120398	0.215051
C	-2.55609	-0.10037	0.249208
C	3.408355	0.78192	0.004281
C	2.559333	-0.35834	0.148313
B	-0.01765	-0.74512	0.546607
F	-0.03984	-1.1709	1.88271
F	-0.06983	-1.79028	-0.34085
N	-1.23829	0.228553	0.329143
N	1.291211	0.101789	0.325942
Cl	5.135114	0.75781	-0.18704
Cl	-5.02831	1.26699	0.179415
C	2.962029	-1.76855	0.130922
C	4.30037	-3.54656	-0.8703
H	4.991968	-3.85993	-1.64257
C	3.827309	-4.44966	0.08971
C	2.490706	-2.69445	1.085086
H	1.786267	-2.37198	1.840859
C	-3.10344	-1.46183	0.214225
C	-3.25434	-3.73018	1.069542
H	-2.94202	-4.50542	1.760965
C	-4.2525	-4.03338	0.130459
C	-4.10758	-1.77737	-0.7144
H	-4.43862	-1.02664	-1.42304
C	3.873156	-2.22114	-0.83605
H	4.239736	-1.53544	-1.5913
C	2.920315	-4.00991	1.066695
H	2.567314	-4.72358	1.803339
C	-4.67571	-3.04803	-0.77001

H	-5.43648	-3.25569	-1.51241
C	-2.68554	-2.46885	1.10875
H	-1.91436	-2.25157	1.836043
C	0.213499	3.73517	0.318411
C	-0.33462	5.871944	-0.70211
H	-0.81793	6.442299	-1.48663
C	0.386219	6.540601	0.295455
C	0.940946	4.414821	1.311504
H	1.424164	3.847753	2.100251
C	1.021645	5.802678	1.301826
H	1.571145	6.336405	2.069517
C	-0.42181	4.483025	-0.68769
H	-0.96507	3.967873	-1.47272
C	2.644738	1.925722	0.104881
H	2.9853	2.946625	0.032392
C	-2.41982	2.181226	0.292171
H	-2.66666	3.230818	0.318822
O	-4.74236	-5.30228	0.176081
C	-5.75442	-5.66956	-0.75034
H	-5.40265	-5.58702	-1.78628
H	-5.99485	-6.71131	-0.53454
H	-6.65643	-5.05729	-0.62684
O	4.183227	-5.76116	0.16103
C	5.096243	-6.26795	-0.80182
H	5.236941	-7.32127	-0.55618
H	4.696702	-6.1849	-1.82024
H	6.063669	-5.75289	-0.75156
C	0.512529	8.027826	0.333017
O	1.134967	8.638895	1.180027
O	-0.14503	8.623308	-0.68478
C	-0.06191	10.07496	-0.7189
H	-0.48449	10.46976	0.209024
H	0.994469	10.35677	-0.75009
C	-0.81313	10.55601	-1.92908
C	-2.12762	11.02152	-1.81349
C	-0.21039	10.53138	-3.19332
C	-2.8287	11.45601	-2.93898
H	-2.60293	11.04547	-0.83625
C	-0.90894	10.96155	-4.32025
H	0.811242	10.17354	-3.29196
C	-2.2203	11.42567	-4.19435
H	-3.8471	11.81862	-2.83527
H	-0.43018	10.93984	-5.29481
H	-2.76367	11.76566	-5.07108

BODIPY **6b**: HF = -2615.0506235 a.u.

C	-1.15507	1.501302	0.162285
C	0.090893	2.145239	0.12947
C	1.280477	1.400881	0.144904
C	-3.32507	0.97747	0.051567
C	-2.57191	-0.23303	0.161073
C	3.387239	0.696561	-0.10379
C	2.549276	-0.44386	0.10103
B	-0.02747	-0.83373	0.508765
F	-0.05219	-1.18073	1.867178
F	-0.06518	-1.92741	-0.31791
N	-1.25777	0.113259	0.230369
N	1.27515	0.012108	0.245793
Cl	5.114598	0.683003	-0.28304
Cl	-5.0559	1.106254	-0.00186
C	2.967939	-1.84709	0.168032
C	4.339442	-3.66262	-0.71409
H	5.045103	-4.01086	-1.4583
C	3.862259	-4.51651	0.288332
C	2.493814	-2.72376	1.166714
H	1.777133	-2.36753	1.895265
C	-3.1064	-1.5985	0.202745
C	-3.23316	-3.81767	1.182072
H	-2.9125	-4.55046	1.914701
C	-4.22999	-4.18217	0.263284
C	-4.11022	-1.97443	-0.70414
H	-4.45043	-1.26771	-1.45246
C	3.897788	-2.34258	-0.75986
H	4.267355	-1.69665	-1.54789
C	2.937766	-4.03286	1.227772
H	2.582875	-4.7082	1.998815
C	-4.6656	-3.25153	-0.68841
H	-5.42644	-3.50709	-1.41571
C	-2.67682	-2.55093	1.150482
H	-1.90836	-2.2865	1.864821
C	0.160336	3.62624	0.030482
C	-0.3974	5.697474	-1.11202
H	-0.87621	6.219347	-1.93336
C	0.303962	6.427696	-0.1388
C	0.865669	4.365788	0.99536
H	1.344431	3.84702	1.818912
C	0.935772	5.752045	0.918054
H	1.47271	6.316961	1.672211
C	-0.46816	4.311845	-1.02294

H	-0.99606	3.750236	-1.7859
C	2.610807	1.835242	-0.07204
H	2.942047	2.853493	-0.20252
C	-2.45805	2.049003	0.073342
H	-2.71647	3.095693	0.039021
C	0.376522	7.857297	-0.22529
N	0.435386	9.016844	-0.29594
O	-4.70559	-5.45097	0.379342
C	-5.71601	-5.88066	-0.52238
H	-5.3686	-5.84877	-1.56247
H	-5.94129	-6.91248	-0.25031
H	-6.62568	-5.27483	-0.42749
O	4.229324	-5.81754	0.436402
C	5.160065	-6.36813	-0.48526
H	5.305203	-7.40528	-0.18082
H	4.773879	-6.34343	-1.51176
H	6.122433	-5.84274	-0.44937

BODIPY **3**: HF = -2478.2095903 a.u.

C	-1.21918	1.127465	0.20941
C	-0.00099	1.825507	0.246337
C	1.218458	1.127839	0.231493
C	-3.39517	0.513299	0.065229
C	-2.55576	-0.65166	0.062876
C	3.390773	0.517407	0.026224
C	2.558317	-0.65013	0.101395
B	-0.00102	-1.18665	0.379589
F	-0.03862	-1.66945	1.695025
F	0.024691	-2.195	-0.55122
N	-1.2614	-0.26569	0.165047
N	1.26611	-0.2651	0.231931
C	2.998539	-2.05683	0.023117
C	4.285523	-3.77186	-1.11901
H	4.921424	-4.06914	-1.94762
C	3.918747	-4.70323	-0.14553
H	4.27355	-5.72778	-0.21043
C	2.627655	-3.00188	0.993895
H	1.967425	-2.70648	1.799831
C	-2.99842	-2.05482	-0.06751
C	-3.09928	-4.34783	0.716108
H	-2.80881	-5.10231	1.441205
C	-3.93146	-4.68731	-0.35139
H	-4.29066	-5.70651	-0.46083
C	-3.84223	-2.40386	-1.13646

H	-4.12998	-1.64696	-1.85836
C	3.836494	-2.45672	-1.0323
H	4.12362	-1.73458	-1.78903
C	3.090908	-4.31334	0.908091
H	2.799228	-5.03372	1.666614
C	-4.29745	-3.71176	-1.2808
H	-4.93784	-3.96856	-2.11945
C	-2.62963	-3.04346	0.85932
H	-1.96789	-2.7867	1.67687
C	0.005656	3.310414	0.256896
C	-0.64677	5.437091	-0.72089
H	-1.15873	5.989428	-1.50315
C	0.028525	6.119795	0.292211
H	0.036968	7.205537	0.305865
C	0.688531	4.007642	1.268045
H	1.195781	3.450009	2.0486
C	0.694084	5.401318	1.286788
H	1.216547	5.925482	2.081376
C	-0.66305	4.043421	-0.738
H	-1.1747	3.514826	-1.53545
C	2.537523	1.614642	0.101164
H	2.822447	2.655818	0.075605
C	-2.54514	1.611032	0.166578
H	-2.8381	2.648002	0.234964
C	4.846414	0.566104	-0.07051
C	5.797017	-0.2614	0.482757
S	5.624833	1.868922	-0.95557
C	7.135178	0.143612	0.207565
H	5.540787	-1.12642	1.081251
C	7.204775	1.278534	-0.55195
H	8.009261	-0.38683	0.567821
H	8.083675	1.80079	-0.90298
C	-4.85314	0.557486	0.022948
C	-5.78113	-0.30808	0.55623
S	-5.66682	1.907099	-0.75379
C	-7.12936	0.105019	0.351802
H	-5.50147	-1.20613	1.092207
C	-7.22974	1.283596	-0.33429
H	-7.98847	-0.45158	0.708596
H	-8.12226	1.821139	-0.62216

BODIPY **7**: HF = -2799.5020354 a.u.

C	-1.21793	1.432487	0.232958
C	0.001656	2.126629	0.231225
C	1.221546	1.432406	0.246765
C	-3.39531	0.81838	0.123435
C	2.55961	0.351119	0.179369
C	3.393277	0.816202	0.060023
C	2.563227	-0.35121	0.191942
B	0.000902	-0.86853	0.509332
F	-0.02806	-1.28766	1.848166
F	0.019945	-1.92149	-0.37123
N	-1.26281	0.039251	0.261287
N	1.269826	0.041134	0.311139
C	3.007868	-1.75319	0.174147
C	4.352915	-3.49923	-0.87278
H	5.024417	-3.79704	-1.66873
C	3.934772	-4.41283	0.10329
C	2.591891	-2.68827	1.143224
H	1.897857	-2.38313	1.916031
C	-3.0087	-1.75151	0.119321
C	-3.05599	-4.02753	0.966673
H	-2.7383	-4.7805	1.679978
C	-3.9525	-4.40119	-0.04599
C	-3.91325	-2.13731	-0.88192
H	-4.24908	-1.4059	-1.60896
C	3.895569	-2.18425	-0.82352
H	4.223924	-1.48537	-1.58498
C	3.053551	-3.99393	1.111743
H	2.741086	-4.71599	1.858525
C	-4.37906	-3.44673	-0.97828
H	-5.06369	-3.70836	-1.77571
C	-2.586	-2.72663	1.044831
H	-1.88272	-2.45577	1.821713
C	0.008549	3.610857	0.163459
C	-0.63905	5.679275	-0.9368
H	1.140867	6.196379	1.747394
C	0.030207	6.419586	0.051378
C	0.680272	4.361232	1.143937
H	1.181109	3.847058	1.957077
C	0.690471	5.750426	1.094896
H	1.202435	6.322602	1.860899
C	-0.64946	4.2905	-0.87581
H	1.154463	3.721758	1.648791
C	2.540147	1.913924	0.08783

H	2.82739	2.952355	0.015581
C	-2.54337	1.916722	0.165376
H	-2.83694	2.955758	0.1837
C	4.849127	0.868067	0.036882
C	5.804315	0.091628	0.579116
S	5.620353	2.112605	-1.00798
C	7.140069	0.489901	0.283451
H	5.552409	-0.73065	1.236828
C	7.2033	1.568401	-0.55505
H	8.017099	-0.00367	0.686377
H	8.079207	2.073564	-0.93719
C	-4.85359	0.869903	0.089275
C	-5.78292	0.058385	0.699776
S	-5.66415	2.161901	-0.78261
C	-7.12963	0.467489	0.478331
H	-5.50419	-0.79684	1.302227
C	-7.22748	1.588879	-0.29837
H	-7.9895	-0.04971	0.88851
H	-8.11843	2.111028	-0.6177
O	4.323357	-5.71656	0.160957
O	-4.34698	-5.70446	-0.03597
C	-5.24043	-6.14829	-1.04661
H	-4.8097	-6.02721	-2.04834
H	-5.4086	-7.20861	-0.85387
H	-6.19942	-5.61688	-1.00104
C	5.200614	-6.20576	-0.84297
H	5.367024	-7.25807	-0.60917
H	4.756289	-6.12376	-1.84271
H	6.162328	-5.67745	-0.83257
C	0.040663	7.852397	-0.00591
N	0.04915	9.014712	-0.05271

BODIPY **4**: HF = -1836.7043286 a.u.

C	-1.19127	1.37558	0.155742
C	0.040427	2.048522	0.188045
C	1.245351	1.328076	0.150875
C	-3.38271	0.811432	0.028086
C	-2.57003	-0.37047	0.011465
C	3.404852	0.683719	-0.09174
C	2.554196	-0.46882	-0.01638
B	-0.01695	-0.96096	0.280224
F	-0.04646	-1.46554	1.589879
F	-0.023	-1.95683	-0.66537
N	-1.26316	-0.01517	0.09906

N	1.267208	-0.06459	0.132439
C	2.974471	-1.87904	-0.12696
C	4.284452	-3.56955	-1.28251
H	4.947777	-3.84429	-2.09729
C	3.872035	-4.53048	-0.35759
H	4.217574	-5.55642	-0.44623
C	2.559876	-2.85424	0.795941
H	1.878364	-2.57953	1.591149
C	-3.05121	-1.75891	-0.13402
C	-3.1637	-4.07567	0.576969
H	-2.84835	-4.86165	1.256875
C	-4.0712	-4.3579	-0.44508
H	-4.46354	-5.36365	-0.56484
C	-3.97184	-2.05109	-1.15631
H	-4.28497	-1.26351	-1.83332
C	3.846492	-2.25308	-1.16476
H	4.168765	-1.50918	-1.88529
C	3.011191	-4.16714	0.679194
H	2.685206	-4.90991	1.401347
C	-4.47049	-3.34141	-1.31461
H	-5.17102	-3.5521	-2.11726
C	-2.65164	-2.7893	0.73367
H	-1.93691	-2.5778	1.518632
C	0.076951	3.533308	0.216136
C	-0.53429	5.684437	-0.73503
H	-1.03672	6.256421	-1.50941
C	0.157422	6.34146	0.283954
H	0.187996	7.426586	0.310315
C	0.776662	4.204692	1.233015
H	1.275228	3.627422	2.004845
C	0.810857	5.59777	1.268002
H	1.346124	6.101817	2.067104
C	-0.57891	4.291544	-0.76812
H	1.103309	3.782108	1.569816
C	2.572513	1.792338	0.006397
H	2.876247	2.828398	-0.00641
C	-2.50852	1.887381	0.126828
H	-2.7788	2.929529	0.208614
C	4.876442	0.732454	-0.20621
C	5.706691	-0.1149	0.548122
C	5.481906	1.684175	-1.04483
C	7.09368	-0.0137	0.461415
H	5.259618	-0.84692	1.212023
C	6.869727	1.786657	-1.12762
H	4.854303	2.336304	-1.64544

C	7.681867	0.936555	-0.37569
H	7.717125	-0.67548	1.055773
H	7.316245	2.526831	-1.78552
H	8.763212	1.013306	-0.44126
C	-4.8557	0.912357	0.005672
C	-5.66999	0.058948	0.770517
C	-5.47574	1.920793	-0.75213
C	-7.05515	0.209572	0.772045
H	-5.21154	-0.71631	1.374793
C	-6.86145	2.07263	-0.74687
H	-4.8617	2.579264	-1.35983
C	-7.65764	1.215944	0.01441
H	-7.66553	-0.45782	1.373621
H	-7.31922	2.856693	-1.34333
H	-8.73756	1.331005	0.017664

BODIPY **8**: HF = -2364.7647973 a.u.

C	-1.25031	1.259546	0.248795
C	-0.02955	1.959223	0.282719
C	1.186728	1.270918	0.344006
C	-3.42087	0.636805	0.087517
C	2.587958	0.526428	0.182342
C	3.370788	0.670157	0.236098
C	2.540676	-0.50278	0.345706
B	-0.03299	-1.03395	0.570456
F	-0.10252	-1.45759	1.907524
F	0.016143	-2.08566	-0.31099
N	-1.29171	-0.13153	0.288411
N	1.239858	-0.12087	0.415887
C	3.002903	-1.89742	0.34074
C	4.469507	-3.59765	-0.61791
H	5.215958	-3.86553	-1.35565
C	3.983301	-4.54008	0.297375
C	2.52015	-2.86241	1.248969
H	1.759726	-2.58644	1.96801
C	-3.03457	-1.92787	0.11369
C	-3.10902	-4.20274	0.96294
H	-2.80539	-4.95703	1.680997
C	-3.99867	-4.57137	-0.05809
C	-3.9301	-2.30966	-0.8973
H	-4.24928	-1.57824	-1.6323
C	3.985952	-2.29218	-0.58133
H	4.369182	-1.57182	-1.2954

C	3.00744	-4.15831	1.231277
H	2.644953	-4.90145	1.933417
C	-4.40707	-3.61506	-0.9964
H	-5.08529	-3.87231	-1.80066
C	-2.62999	-2.90553	1.045155
H	-1.93483	-2.63879	1.830659
C	-0.02625	3.443116	0.202688
C	-0.62894	5.498315	-0.94708
H	-1.09449	6.005997	-1.78488
C	-0.0052	6.250675	0.061673
C	0.59864	4.205395	1.20447
H	1.063672	3.700882	2.044494
C	0.608375	5.594152	1.141048
H	1.08423	6.175688	1.923128
C	-0.63972	4.110222	-0.87136
H	-1.10836	3.531492	-1.65981
C	2.51255	1.757925	0.229347
H	2.79679	2.798022	0.169849
C	-2.57156	1.73962	0.133837
H	-2.86624	2.778548	0.135948
C	4.843785	0.747153	0.187878
C	5.659698	-0.00835	1.053817
C	5.476721	1.637679	-0.68942
C	7.039503	0.123434	1.0368
H	5.200953	-0.69738	1.754707
C	6.86537	1.78194	-0.71728
H	4.873718	2.22307	-1.37773
C	7.65582	1.019961	0.150047
H	7.666736	-0.45275	1.708894
H	7.312472	2.478334	-1.41653
C	-4.8913	0.707342	0.029356
C	-5.70857	-0.13681	0.80507
C	-5.5154	1.680031	-0.77371
C	-7.0917	-0.01858	0.77586
H	-5.25116	-0.88238	1.444887
C	-6.89822	1.809583	-0.80785
H	-4.90343	2.330727	-1.39039
C	-7.70086	0.95647	-0.03295
H	-7.70896	-0.67151	1.383651
H	-7.36446	2.560979	-1.43618
C	0.007602	7.682688	-0.0124
C	-9.12805	1.078229	-0.06797
N	-10.2873	1.175981	-0.09823
N	0.019149	8.844245	-0.07419
O	-4.40408	-5.87053	-0.04928

O	4.389989	-5.83676	0.363101
O	9.017392	1.071949	0.211289
C	9.69579	1.970937	-0.65262
H	10.75814	1.853595	-0.4348
H	9.515873	1.731932	-1.70855
H	9.402117	3.01167	-0.46576
C	5.371765	-6.28577	-0.56028
H	5.540998	-7.33824	-0.32968
H	5.02304	-6.19442	-1.59641
H	6.313917	-5.73497	-0.44755
C	-5.29764	-6.30739	-1.06362
H	-4.8594	-6.19529	-2.06309
H	-5.47961	-7.36474	-0.86768
H	-6.25001	-5.76397	-1.02496

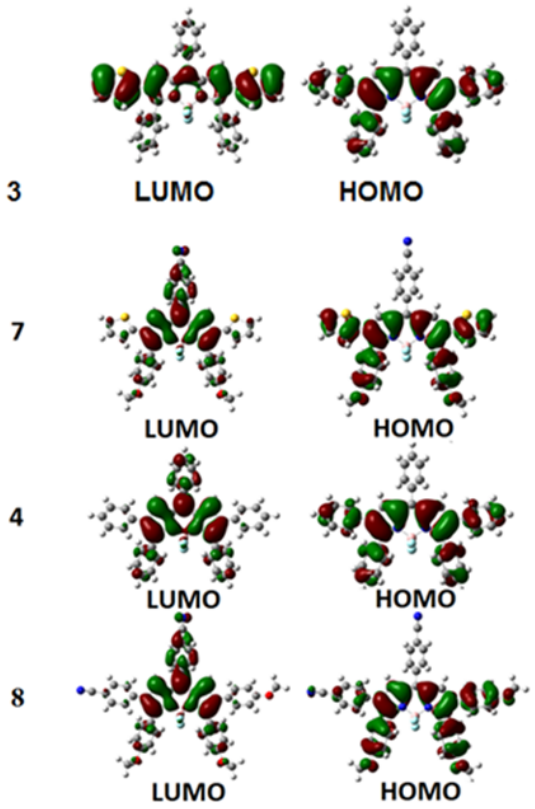


Figure S40. DFT calculated HOMO and LUMO orbitals for BODIPY **3**, **4**, **7** and **8** (B3LYP/6-31G(d)).

Table S3. DFT calculated molecular orbital energy levels for the BODIPYs.

Cpd.#	E_{HOMO} (ev)	E_{LUMO} (ev)	[a]ΔE (ev)
2	-5.83	-3.25	2.61
6a	-5.32	-2.94	2.37
6b	-5.45	-3.13	2.32
3	-5.18	-2.78	2.40
7	-5.13	-2.92	2.21
4	-5.26	-2.71	2.55
8	-5.29	-2.71	2.27

[a]$\Delta E = E_{LUMO} - E_{HOMO}$

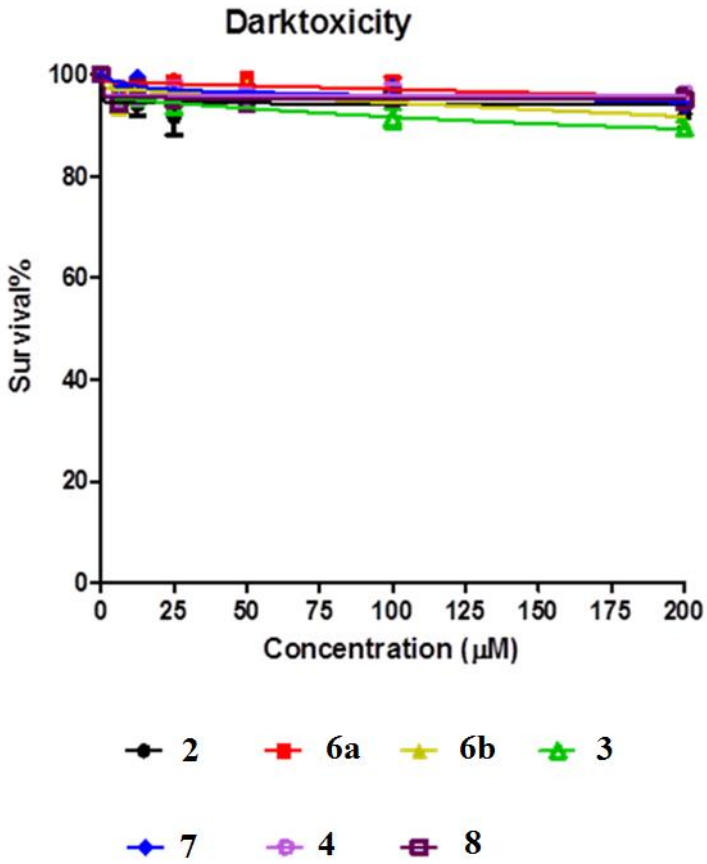


Figure S41. Concentration dependent dark toxicity of BODIPYs in HEp 2 cells.

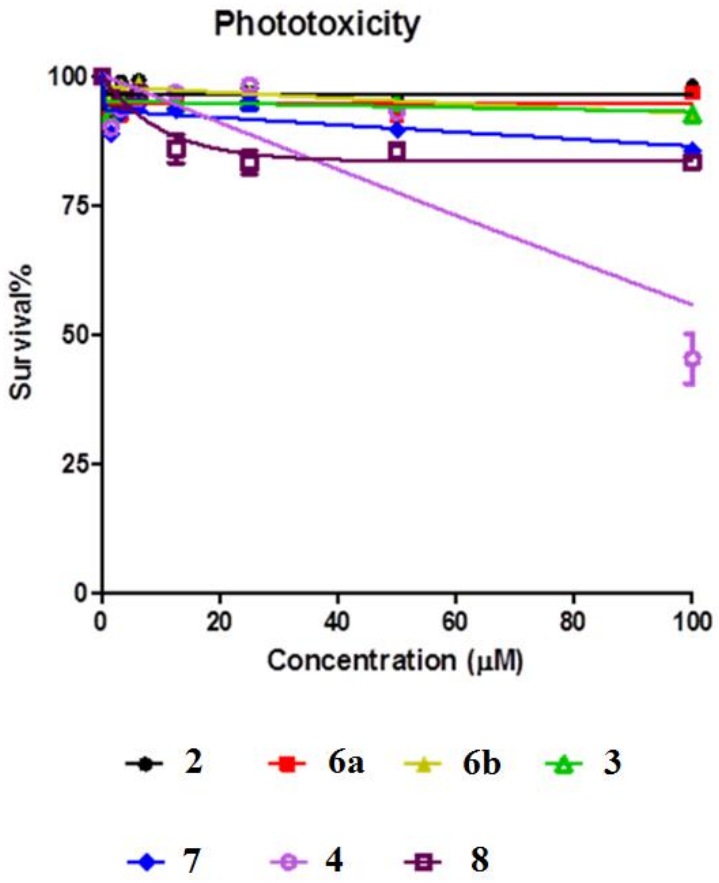


Figure S42. Concentration dependent phototoxicity (1.5 J/cm^2 light dose) of BODIPYs in HEp 2 cells.

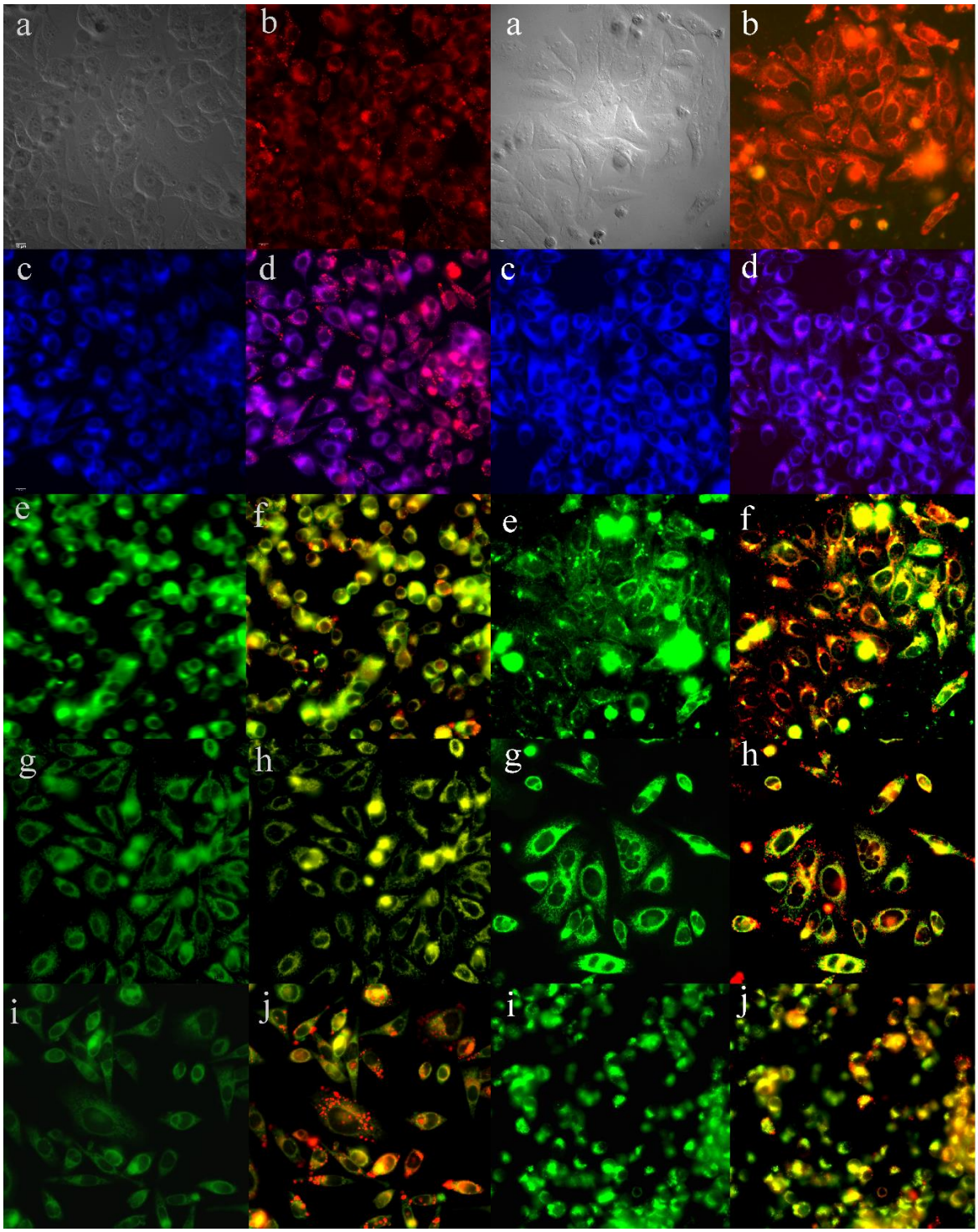


Figure S43. Subcellular localization of **2** (left) and **3** (right) in HEp2 cells at 10 µM for 6 h. (a) phase contrast, (b) overlay of BODIPY and phase contrast, (c) ER Tracker Blue/White, (d) overlay of BODIPY and ER Tracker, (e) BODIPY Ceramide, (f) overlay of BODIPY and BODIPY Ceramide, (g) MitoTracker Green, (h) overlay of BODIPY and MitoTracker, (i) LysoSensor Green, (j) overlay of BODIPY and LysoSensor Green. Scale bar: 10 µm.

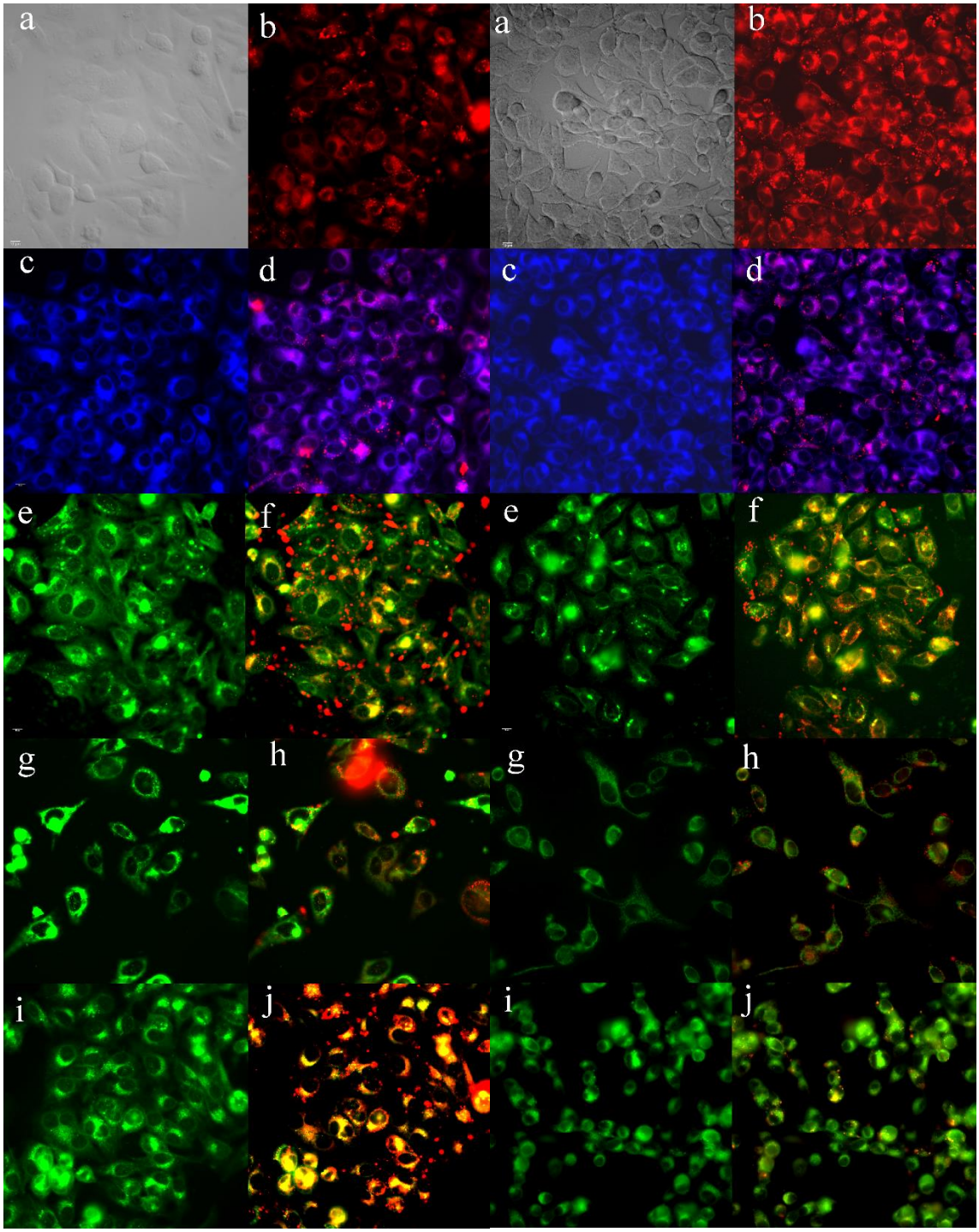


Figure S44. Subcellular localization of **4** (left) and **6a** (right) in HEp2 cells at 10 µM for 6 h. (a) phase contrast, (b) overlay of BODIPY and phase contrast, (c) ER Tracker Blue/White, (d) overlay of BODIPY and ER Tracker, (e) BODIPY Ceramide, (f) overlay of BODIPY and BODIPY Ceramide, (g) MitoTracker Green, (h) overlay of BODIPY and MitoTracker, (i) LysoSensor Green, (j) overlay of BODIPY and LysoSensor Green. Scale bar: 10 µm.

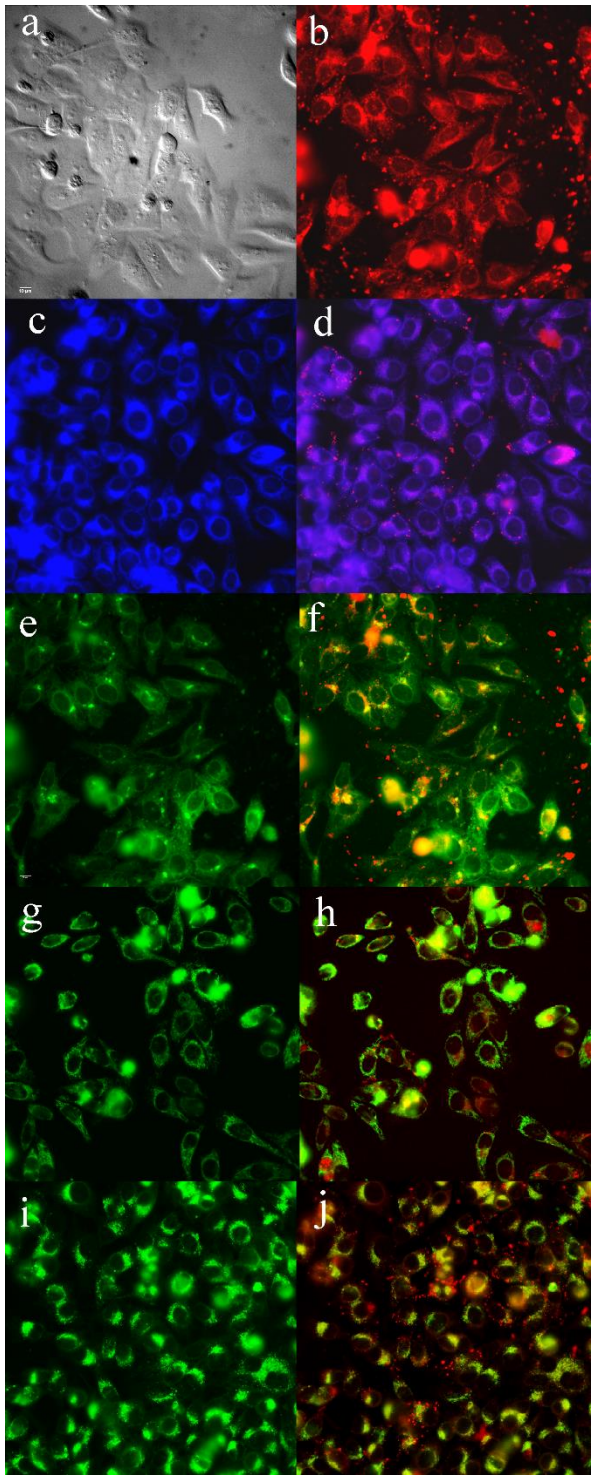


Figure S45. Subcellular localization of **7** in HEp2 cells at 10 μM for 6 h. (a) phase contrast, (b) overlay of BODIPY and phase contrast, (c) ER Tracker Blue/White, (d) overlay of BODIPY and ER Tracker, (e) BODIPY Ceramide, (f) overlay of BODIPY and BODIPY Ceramide, (g) MitoTracker Green, (h) overlay of BODIPY and MitoTracker, (i) LysoSensor Green, (j) overlay of BODIPY and LysoSensor Green. Scale bar: 10 μm.

Table S3. Major (+++) and Minor (+) Subcellular Sites of Localization in HEp2 Cells

compd.	Er	Golgi	Mito	Lys
2	+++	+++	++	+++
6a	++	++	+	+
6b	+++	+++	++	++
3	++	+++	+++	+++
7	+++	++	+	++
4	++	++	+	+++
8	++	++	+	+