Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Ion Responsive Near-IR BODIPY Dyes: Two Isomers, Two Different Signals

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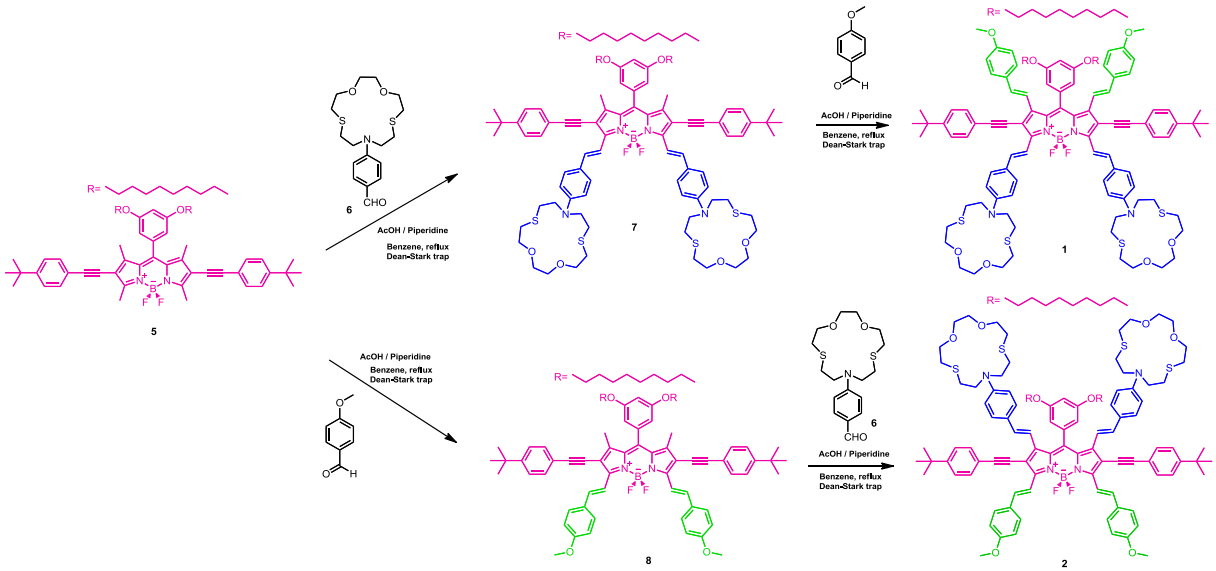
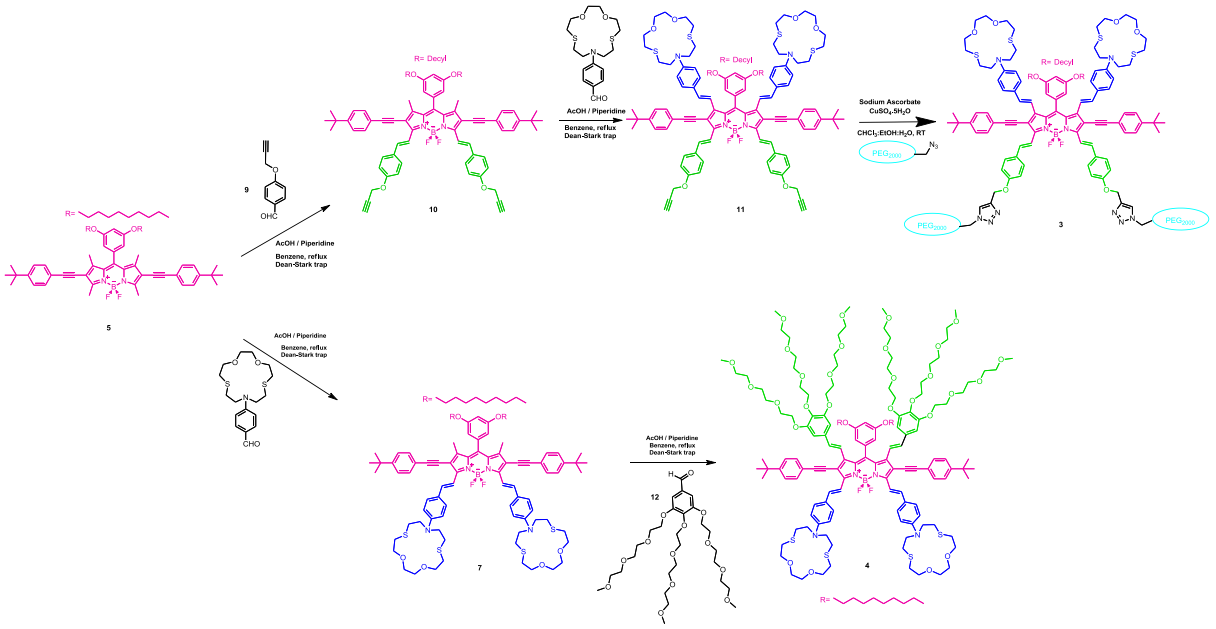
Supporting Information

EXPERIMENTAL PROCEDURES

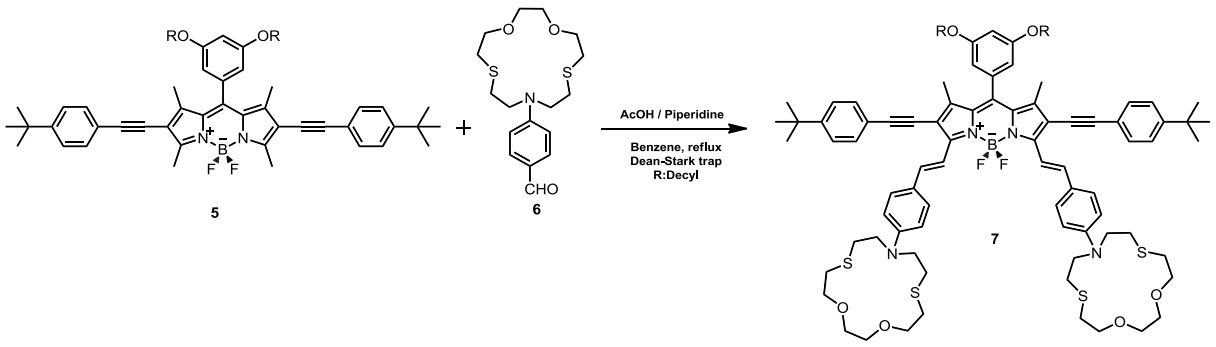
General: ^{1}H NMR and ^{1}3C NMR spectra were recorded on Bruker DPX-400 (operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) in $CDCl_3$ with tetramethylsilane as internal standard. All spectra were recorded at 25^{0}C and coupling constants (J values) are given in Hz. Chemical shifts are given in parts per million (ppm). Absorption spectra were performed by using a Varian Cary-100 spectrophotometer. Fluorescence measurements were conducted on a Varian Eclipse spectrofluorometer. Mass spectra were recorded on Agilent Technologies 6530 Accurate-Mass Q-TOF LC/MS. Reactions were monitored by thin layer chromatography using Merck TLC Silica gel 60 F254. Silica gel column chromatography was performed over Merck Silica gel 60 (particle size: 0.040-0.063 mm, 230-400 mesh ASTM). Compounds **5**[1], **6**[2], **9**[3] and PEG_{2000}-N_3[2] were synthesized according to literature. All other reagents and solvents were purchased from Aldrich and used without further purification.For a typical ITC run, the instrument chamber (200 µL) contained a solution of a ligand (0.125 mM) while a 2.5 mM solution of $Hg(ClO_4)_2$ was taken up in a 40 µL injection syringe. The syringe was assembled into the chamber for equilibration while stirring at 750 rpm. The chamber temperature was set to 25 °C. The injections were programmed at 0.5 µL each, added over 3 sec and spaced 2 min apart.[4]Association enthalpy (ΔH° in cal/mol), "number of sites" (N), and association constant (K in M-1) were obtained by fitting the titration data using the "Two Set of Sites model" algorithm provided in the S3 MicroCal Origin Software package (version 7.0). Association entropy (ΔS in cal/mol/K) is calculated from fitted values of ΔHº and K.





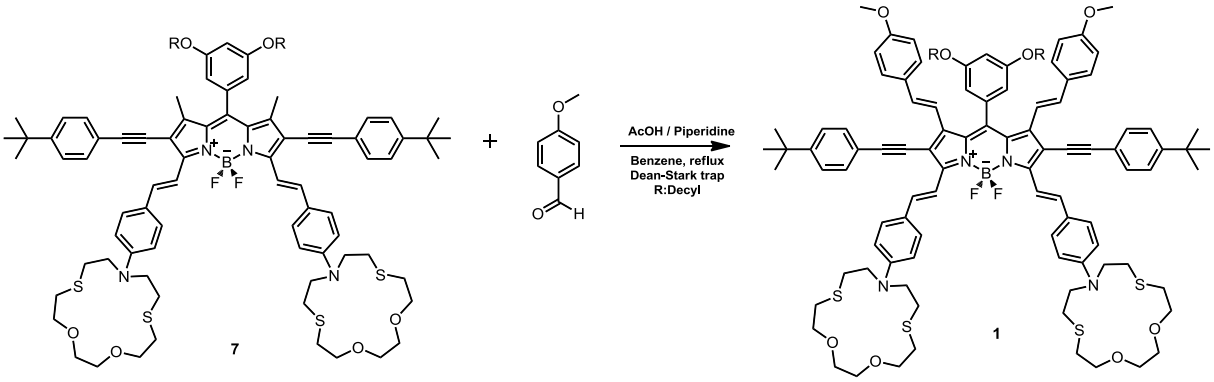
Scheme S1. Synthesis of target compounds.

Synthesis of Compound 7:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **5** (0.137 mmol, 130 mg) and compound **6** (0.342 mmol, 121 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC dichloromethane. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using dichloromethane as the eluant. (144 mg, 65%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 16.0 Hz, 2H), 7.69 (d, *J* = 16.1 Hz, 2H), 7.61 (d, *J* = 8.7 Hz, 4H), 7.48 (d, *J* = 8.4 Hz, 4H), 7.42 (d, *J* = 8.5 Hz, 4H), 6.73 (d, *J* = 8.5 Hz, 4H), 6.59 (s, 1H), 6.49 (s, 2H), 3.97 (t, *J* = 6.6 Hz, 4H), 3.84 (t, *J* = 8.0 Hz, 8H), 3.74 (m, 8H), 3.68 (s, 8H), 2.97 (m, 8H), 2.84 – 2.78 (m, 8H), 1.78 (m, 10H), 1.51 - 1.31 (m, 48H), 0.9 (t, 6H).

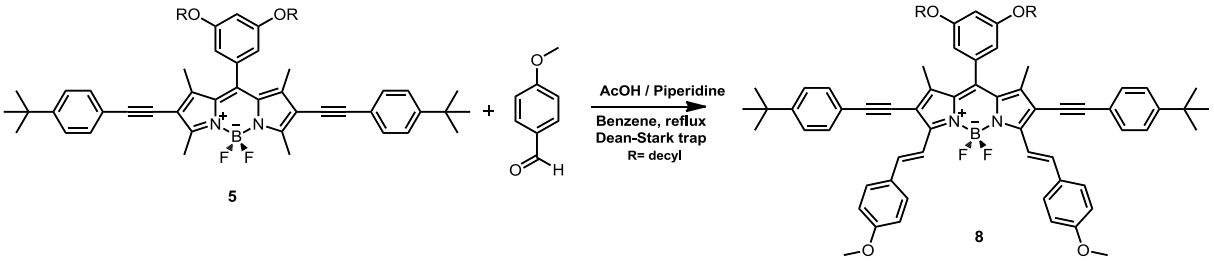
Synthesis of Compound 1:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **7** (0.023 mmol, 40 mg) and p-anisaldehyde (0.14 mmol, 18 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC chloroform. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using chloroform as the eluant. (15 mg, 34%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 16.2 Hz, 2H), 7.74 (d, *J* = 16.2 Hz, 4H), 7.65 (d, *J*= 8.5 Hz, 4H), 7.50 – 7.46 (m, 4H), 7.45 – 7.39 (m, 4H), 7.06 (d, *J* = 8.8 Hz, 4H), 6.81 (d, *J* = 8.8 Hz, 4H), 6.78 – 6.72 (m, 5H), 6.64 (d, *J* = 2.3 Hz, 2H), 6.08 (d, *J* = 16.3 Hz, 2H), 3.89 – 3.83 (m, 18H), 3.81 – 3.72 (m, 8H), 3.71 – 3.64 (m, 8H), 2.99 (m, 8H), 2.81 (m, 8H), 1.60 (s, 8H), 1.37 (s, 16H), 1.30 – 1.19 (m, 32H), 0.88 (t, *J* = 6.8 Hz, 6H).

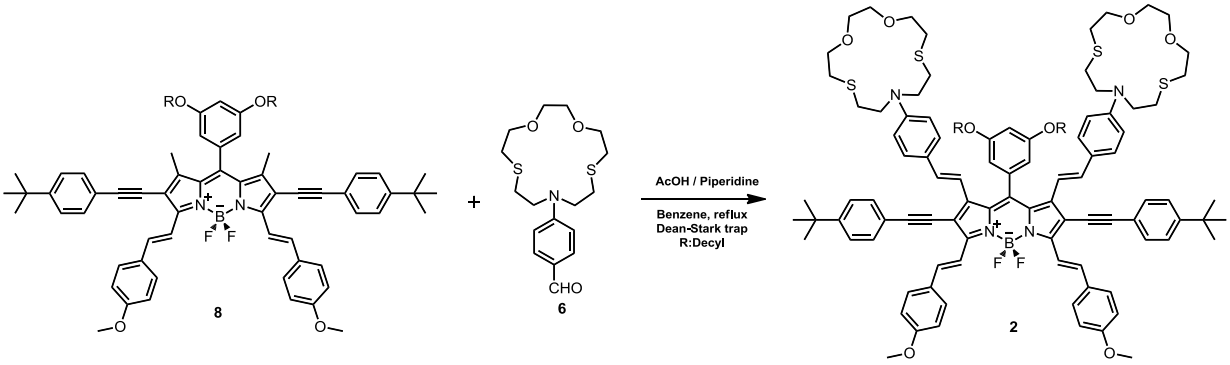
^{13}C NMR (400 MHz, $CDCl_3$) δ 161.41, 151.38, 149.74, 147.91, 139.36, 137.09, 133.35, 132.74, 130.48, 130.43, 129.77, 128.00, 125.72, 125.65, 120.96, 119.48, 113.88, 111.97, 111.47, 111.12, 108.51, 98.49, 74.22, 70.75, 69.56, 68.60, 55.28, 52.01, 34.87, 31.39, 31.23, 29.70, 29.56, 29.33, 28.98, 25.90, 14.12. Calcd: 1880.962 [M+Na]+ , Found: 1880.969 [M+Na]+, Δ=3.62 ppm.

Synthesis of Compound 8:



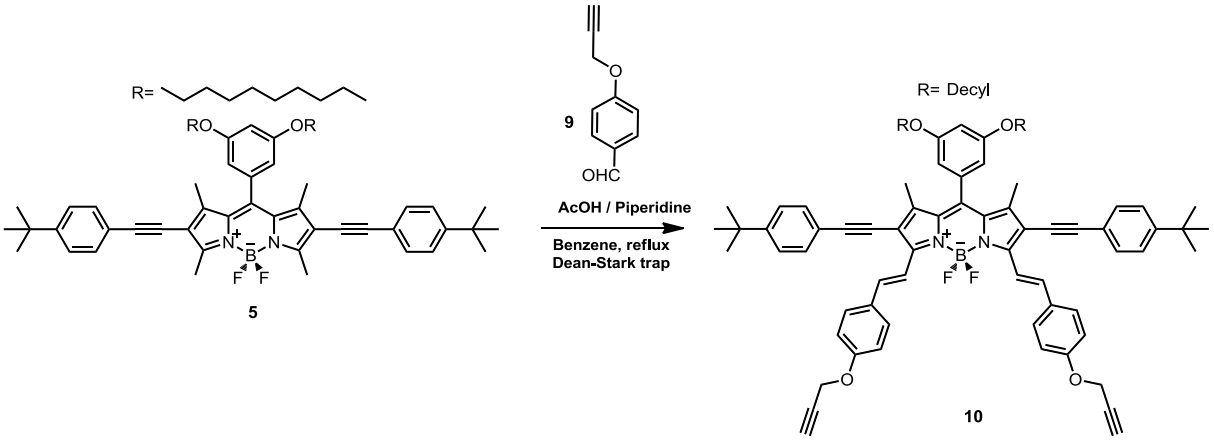
In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **5** (0.053 mmol, 50 mg) and p-anisaldehyde (0.080 mmol, 10.7 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC chloroform. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using chloroform as the eluant. (34 mg, 55%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 (d, *J* = 16.2 Hz, 2H), 7.77 (d, *J* = 16.3 Hz, 2H), 7.67 (d, *J* = 8.8 Hz, 4H), 7.51 – 7.45 (m, 4H), 7.45 – 7.38 (m, 4H), 7.00 (d, *J* = 8.7 Hz, 4H), 6.62 (t, *J* = 2.3 Hz, 1H), 6.50 (d, *J* = 2.2 Hz, 2H), 3.99 (t, *J* = 6.6 Hz, 4H), 3.90 (s, 6H), 1.81 (m, 10H), 1.54 – 1.28 (m, 46H), 0.91 (m, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 161.40, 161.23, 160.72, 152.38, 151.59, 144.61, 138.73, 138.70, 136.44, 132.46, 130.81, 130.49, 130.00, 129.31, 125.54, 116.97, 114.35, 113.78, 106.74, 102.64, 98.52, 98.26, 83.31, 68.51, 55.41, 34.85, 31.92, 31.20, 29.68, 29.65, 29.61, 29.58, 29.40, 29.36, 29.20, 22.69, 14.12, 13.13.

Synthesis of Compound 2:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **8** (0.021 mmol, 27 mg) and compound **6** (0.124 mmol, 44 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC chloroform. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using chloroform as the eluant. (11 mg, 29%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 (d, *J* = 16.3 Hz, 2H), 7.82 (m, *J* = 22.1, 16.4 Hz, 4H), 7.69 (d, *J* = 8.7 Hz, 4H), 7.49 (d, *J* = 8.4 Hz, 4H), 7.43 (d, *J* = 8.4 Hz, 4H), 7.01 (d, *J* = 8.8 Hz, 8H), 6.82 (s, 1H), 6.66 (d, *J* = 2.3 Hz, 2H), 6.57 (s, 4H), 6.05 (d, *J* = 16.1 Hz, 2H), 3.91-3.63 (m, 34H), 2.98 – 2.90 (m, 8H), 2.84 – 2.75 (m, 8H), 1.63-1.58 (m, 6H), 1.58- 1.18 (m, 44H), 0.91 – 0.80 (m, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 161.60, 161.40, 160.62, 160.58, 153.19, 151.39, 146.95, 142.58, 138.43, 136.97, 134.56, 132.76, 130.87, 130.43, 130.23, 129.22, 128.59, 127.80, 125.66, 125.61, 117.38, 117.13, 114.34, 114.11, 111.64, 108.27, 103.38, 98.47, 86.29, 74.34, 70.78, 70.50, 69.57, 68.71, 55.42, 51.93, 39.22, 34.88, 31.95, 31.27, 31.22, 31.15, 29.74, 29.70, 29.60, 29.40, 29.39, 29.04, 25.94, 22.70, 14.13, 10.96. Calcd: 951.9757 [M+2Na]+2 , Found: 951.9921 [M+2Na]+2, Δ=17.25 ppm.

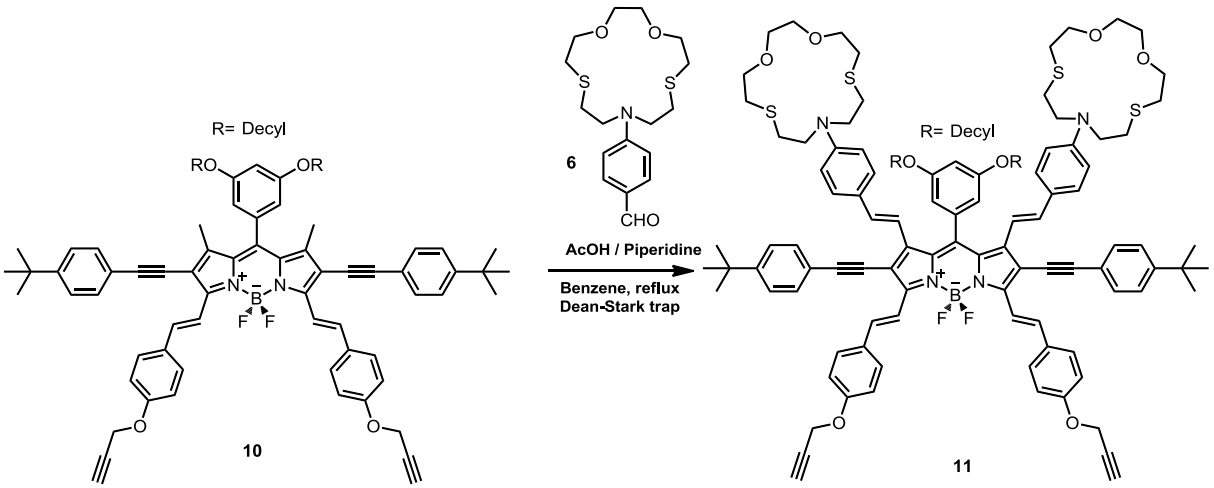
Synthesis of Compound 10:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **5** (0.12 mmol, 120 mg) and compound **9** (0.25 mmol, 40 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were

added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC chloroform. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was used without further purification.

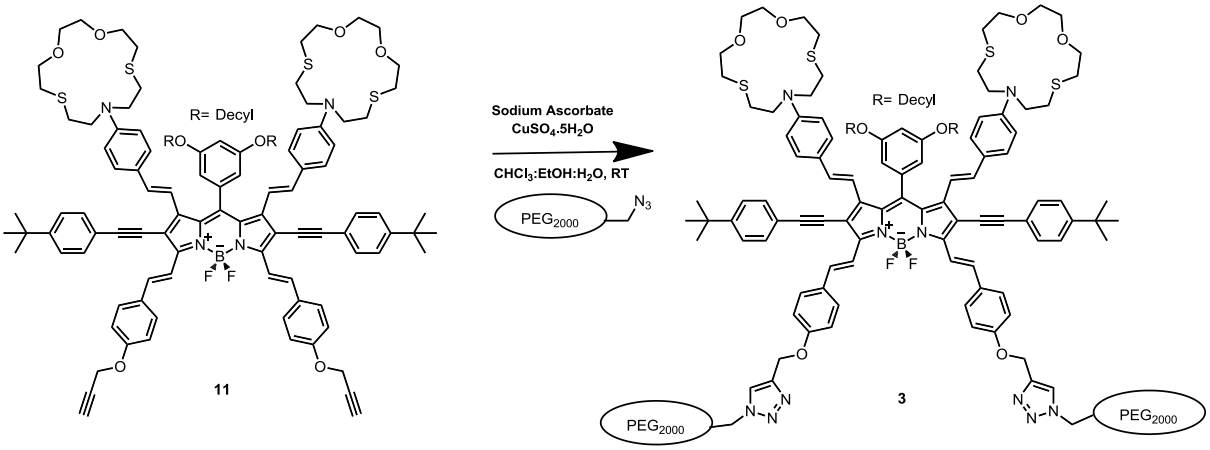
Synthesis of Compound 11:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **10** (0.081 mmol, 100 mg) and compound **6** (0.24mmol, 86 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC 3:1 Chloroform : Hexane. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using 3:1 $CHCl_3$: Hexanes as the eluant. (94mg, 60%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 (d, *J* = 15.9 Hz, 2H), 7.82 (t, *J* = 18.1 Hz, 4H), 7.76 – 7.62 (m, 6H), 7.55 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.52 – 7.46 (m, 2H), 7.43 (d, *J* = 8.5 Hz, 4H), 7.09 (d, *J* = 8.9 Hz, 4H), 7.01 (d, *J* = 8.3 Hz, 4H), 6.82 (s, 1H), 6.65 (d, *J* = 2.3 Hz, 2H), 6.57 (s, 4H), 6.06 (s, 2H), 4.80 (d, *J* = 2.5 Hz, 4H), 4.23 (m,4H), 3.87 (m, 8H), 3.69 (s, 16H), 2.94 (m, 8H), 2.81 (t, *J* = 5.1 Hz, 8H), 2.60 (t, *J* = 2.4 Hz, 2H), 1.78 (m, 4H), 1.51 - 1.31 (m, 46H), 0.9 (t, *J* = 6.8 Hz, 6H).^{13}C NMR (400 MHz, $CDCl_3$) δ 169.65, 167.77, 161.60, 158.43, 151.51, 132.82, 132.46, 131.00, 130.88, 130.43, 129.16, 128.80, 128.56,

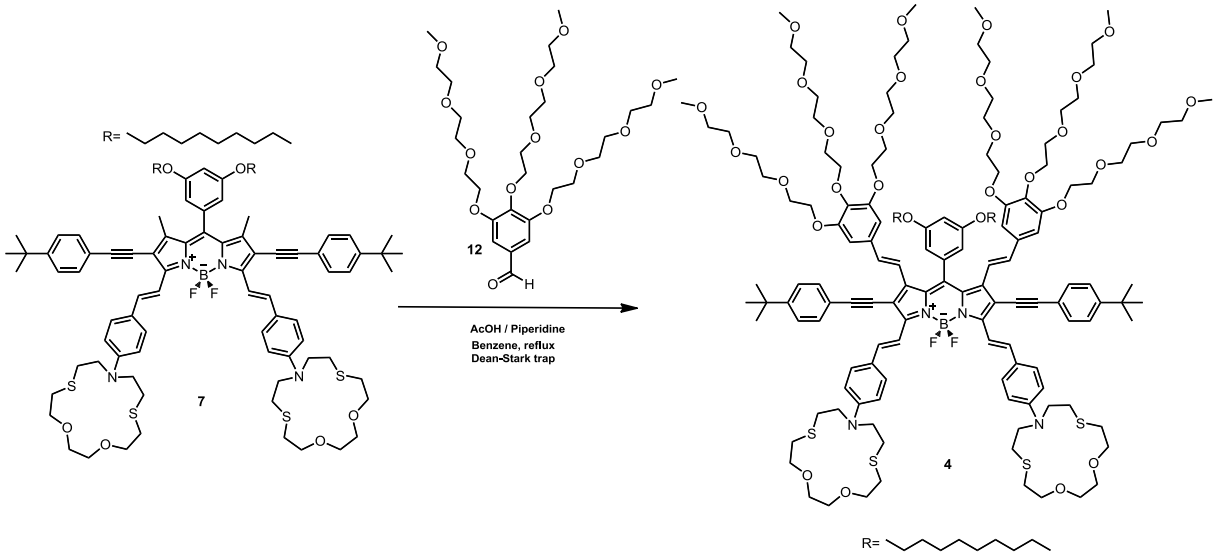
127.78, 125.70, 120.83, 117.58, 115.28, 115.08, 108.20, 103.42, 98.60, 86.08, 78.36, 75.80, 74.29, 70.78, 68.71, 68.16, 55.89, 52.38, 52.09, 38.73, 34.89, 31.94, 31.36, 31.22, 31.14, 29.70, 29.63, 29.58, 29.37, 29.01, 28.93, 25.92, 23.75, 22.99, 22.71. Calcd: 1928.962 [M+Na]+ , Found: 1928.968 [M+Na]+, Δ=3.07 ppm.

Synthesis of Compound 3:



To the solution of the compound **11** (0.017 mmol, 32 mg) in a 6:0.5:0.5 mixture of $CHCl_3$, EtOH and water; PEG_{2000}-N_3(0.033 mmol, 67 mg), 0.16 mg sodium ascorbate, 0.1 mg CuSO4 and 3-4 drop Et3N are added and it was stirred at room temperature for 24 h. Water (50 mL) was added to the residue and the product was extracted into the chloroform (3 x 50 mL). (76 mg, 75%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.53 (d, *J* = 16.3 Hz, 2H), 7.92 (s, 2H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.77 – 7.65 (m, 6H), 7.54 (m, 2H), 7.5-7.4 (m, 6H), 7.12 (m, 4H), 6.99 (d, *J* = 8.4 Hz, 4H), 6.81 (s, 1H), 6.64 (s, 2H), 6.54 (s, 2H), 6.04 (d, *J* = 15.9 Hz, 2H), 5.35 (s, 4H), 4.59 (t, *J*= 5.0 Hz, 4H), 4.31 – 4.11 (m, 6H), 3.97 –3.39 (s, 225H), 2.92 (s, 8H), 2.80 (s, 8H), 2.24 (s, 4H), 1.65 (m, 4H), 1.49 – 1.01 (m, 40H), 1.01 – 0.70 (m, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 167.73, 161.61, 159.22, 151.45, 147.03, 130.86, 130.61, 130.41, 129.19, 128.80, 128.58, 125.69, 120.88, 115.28, 115.16, 111.71, 108.26, 98.53, 86.22, 74.24, 71.95, 70.58, 68.15, 62.13, 59.03, 51.91, 50.70, 50.42, 38.74, 31.93, 31.92, 31.33, 31.23, 29.69, 29.62, 29.58, 29.36, 29.35, 29.02, 28.92, 25.92, 23.75, 22.97, 22.69, 14.14, 14.03, 10.95. MALDI: Distribution around 6000 with separation of 45 corresponding to ethyleneglycol unit.

Synthesis of Compound 4:



In a 100 mL round-bottomed flask containing 50 mL benzene, Compound **7** (0.092 mmol, 150 mg) and compound **12** (0.27 mmol, 164 mg) piperidine (0.3 mL) and acetic acid (0.3 mL) were added. The mixture was heated under reflux by using a Dean Stark trap and progress of the reaction was monitored by TLC 10% Methanol:Dichloromethane. When all the starting material had been consumed, the mixture was cooled to room temperature and solvent was evaporated. Water (100 mL) added to the residue and the product was extracted into the chloroform (3 x 100 mL). Organic phase dried over Na_2SO_4, evaporated and residue was purified by silica gel column chromatography using 10% Methanol:Dichloromethaneas the eluant. (87 mg, 34%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 16.1 Hz, 2H), 7.71 (d, *J* = 16.1 Hz, 2H), 7.63 (s, 4H), 7.46 (d, *J* = 8.2 Hz, 4H), 7.40 (d, *J* = 8.3 Hz, 4H), 6.74 (d, *J* = 8.4 Hz, 4H), 6.61 (s, 2H), 6.52 (s, 1H), 6.32 (s, 2H), 5.90 (d, *J* = 16.1 Hz, 2H), 5.66 (s, 4H), 4.16 (t, *J* = 5.2 Hz, 6H), 4.10 (s, 10H), 3.84-3.37 (m, 102H), 2.97 (t, *J* = 8.0 Hz, 8H), 2.80 (t, *J* = 5.2 Hz, 8H), 1.47-1.12 (m, 50H), 0.85 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 160.94, 153.47, 152.71, 151.57, 148.03, 141.34, 139.61, 138.59, 136.88, 135.26, 134.00, 132.83, 130.47, 129.83, 129.29, 128.44, 125.62, 124.03, 120.84, 120.29, 114.63, 112.00, 109.11, 108.12, 105.65, 98.61, 86.24, 74.24, 72.47, 71.98, 70.69, 70.58, 70.55, 69.82, 68.81, 59.00, 52.02, 34.87, 31.91, 31.41, 31.21, 29.61, 29.34, 29.00, 25.80, 22.66, 14.11. Calcd: 2793.4763 [M+Na]+ , Found: 2793.4909 [M+Na]+, Δ=5.23 ppm.

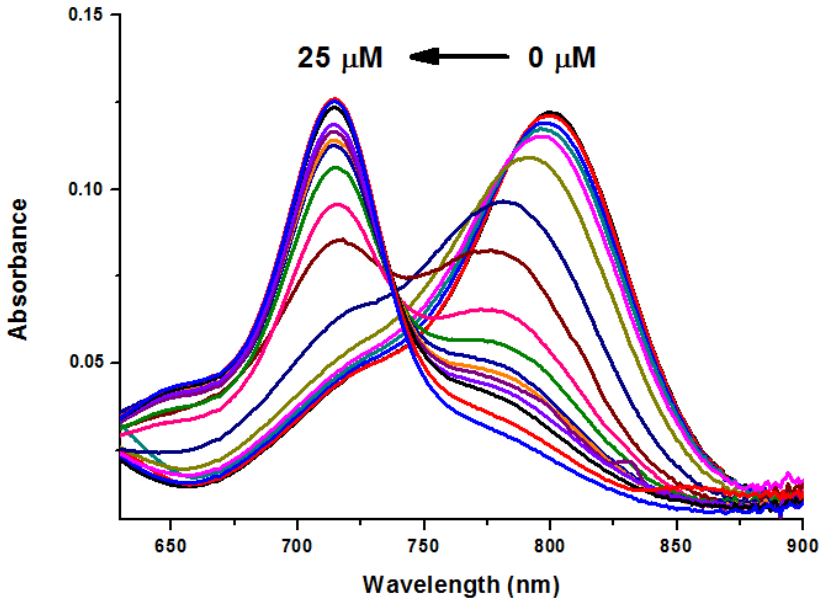


Figure S1. Electronic absorption spectra of **1** (0.5 μM) in the presence of an increasing concentration of Hg^{2+}in THF.

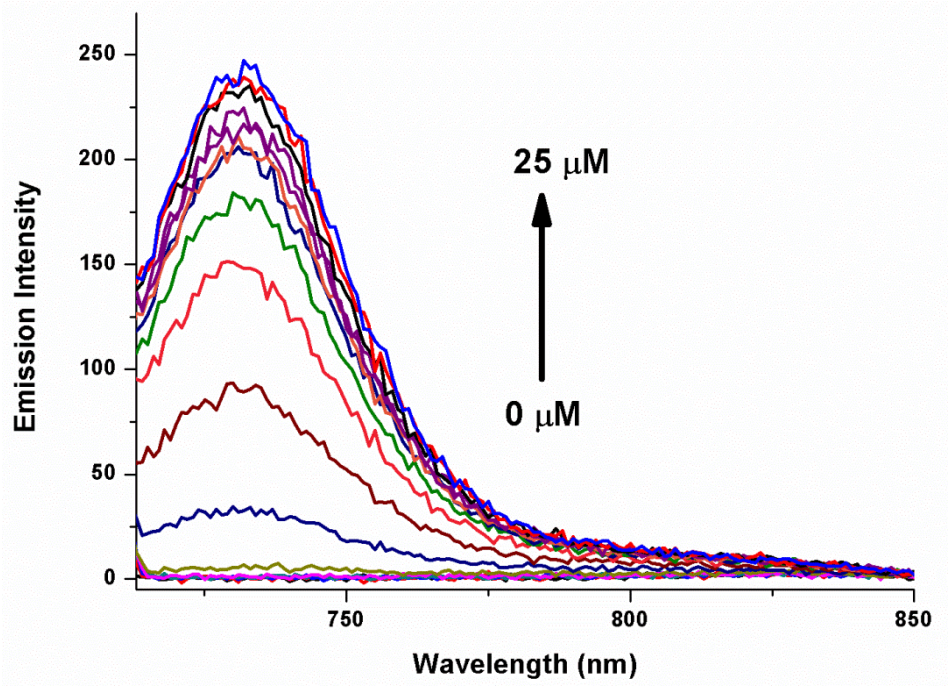


Figure S2.Emission spectra of **1** (0.5 μM) , at increasing concentrations of Hg^{2+}in THF. Excitation wavelength was 710 nm with a slit width of 5-2.5 nm.

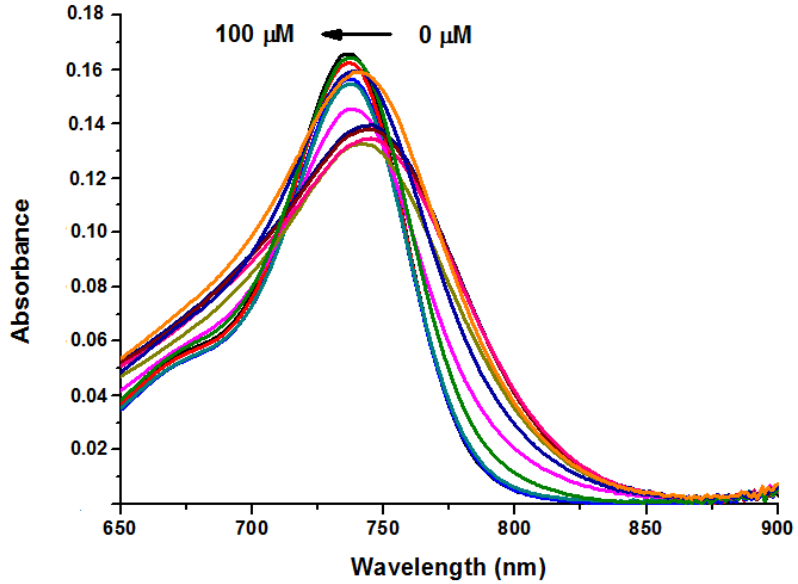


Figure S3.Electronic absorption spectra of **2** (1.0 μM) in the presence of an increasing concentration of Hg^{2+}in THF.

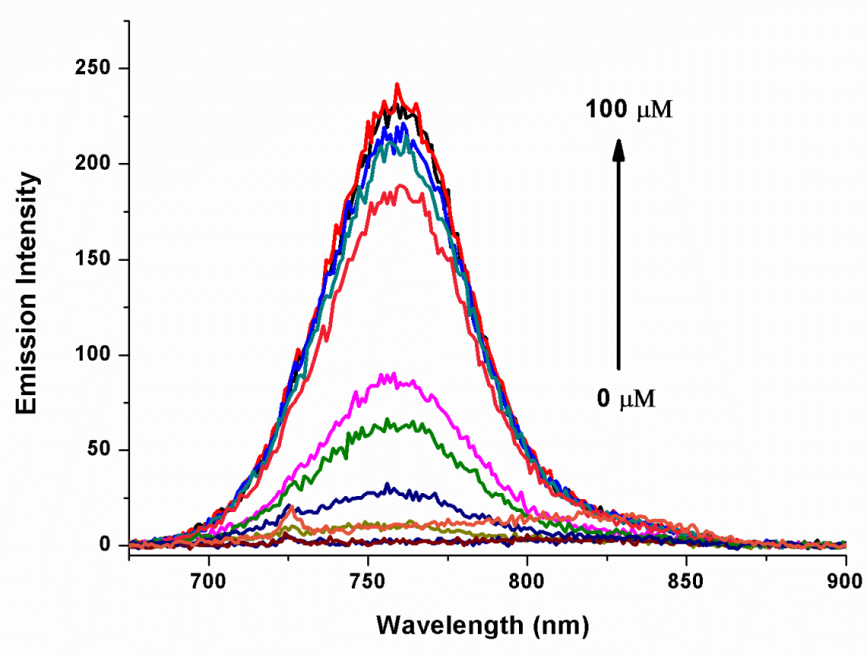


Figure S4.Emission spectra of **2** (1.0 μM) , at increasing concentrations of Hg^{2+}in THF. Excitation wavelength was 725 nm with a slit width of 5-2.5 nm.

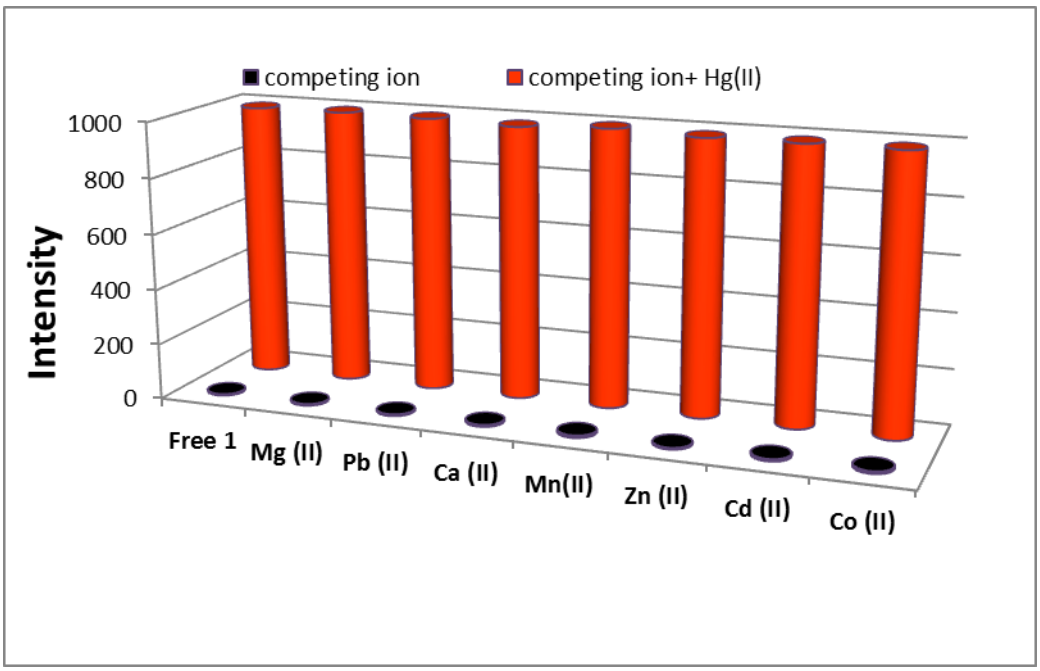


Figure S5.Emission intensityresponse of **1** (0.5 μM) , with 5 μM of a competing metal ion followed by addition of 5 μM Hg^{2+}in THF.Excitation wavelength was 710 nm with a slit width of 5-5 nm.

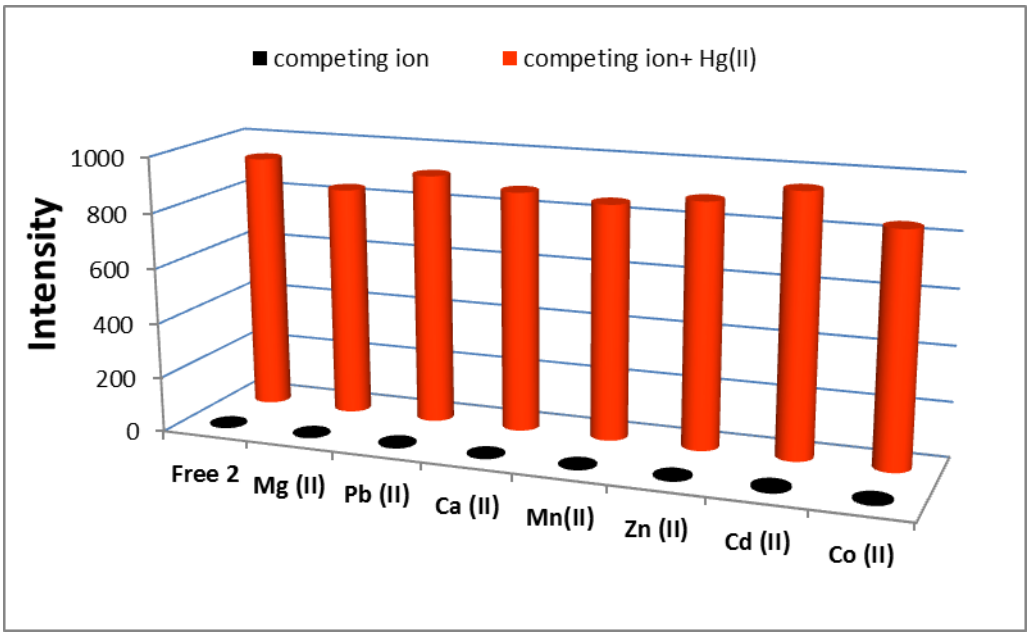


Figure S6. Emission intensityresponse of **2** (1.0 μM) with 10 μM of a competing metal ion followed by addition of 10 μM Hg^{2+}in THF. Excitation wavelength was 725 nm with a slit width of 5-5 nm.

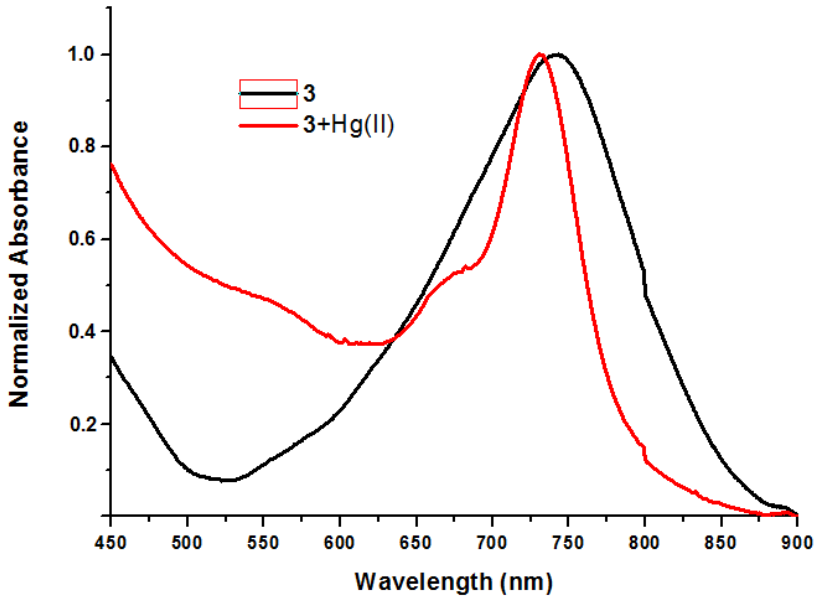


Figure S7. The electronic absorption of **3** (1.9 μM) in presence of excess Hg(II) in 10 mM HEPES:CH_3CN (50:50, v/v, pH=7.20, 25 °C).

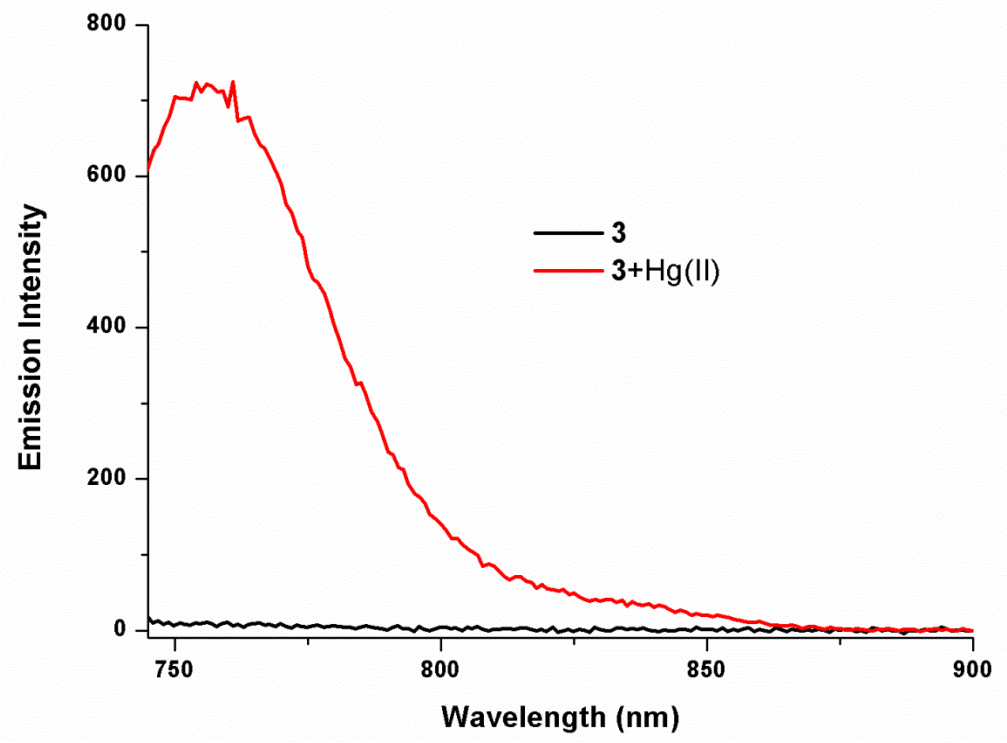


Figure S8. Emission spectra (excitation wavelength =730 nm) of **3** (1.9 μM) in 10 mM HEPES:CH_3CN (50:50, v/v, pH=7.20, 25 °C).

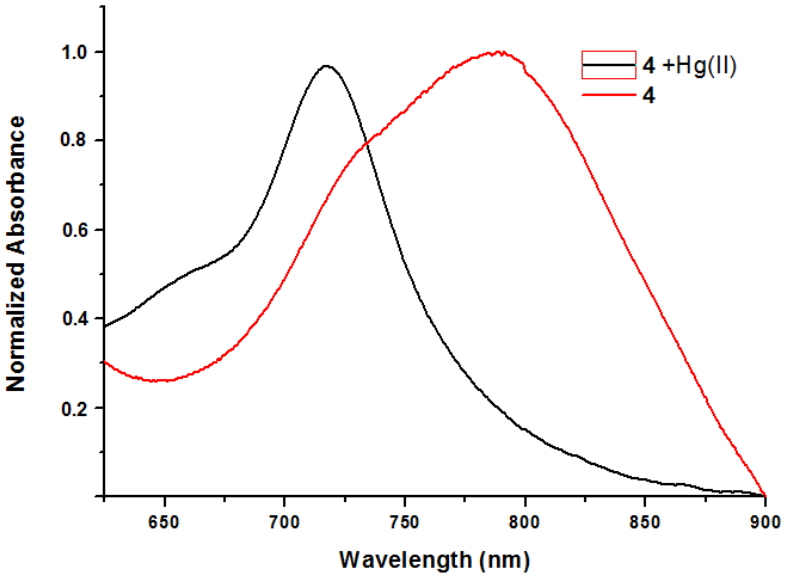


Figure S9. The electronic absorption of **4** (2.8 μM) in presence of excess Hg(II) in 10 mM HEPES:CH_3CN(50:50, v/v, pH=7.20,25°C).

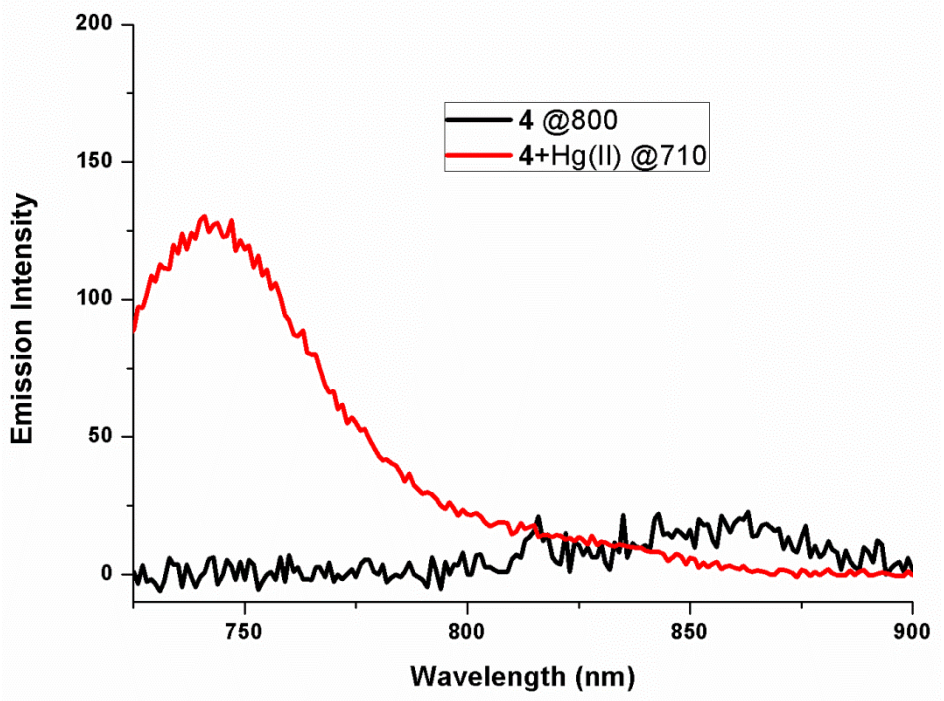


Figure S10. Emission spectra of **4** (2.8 μM) in presence of excess Hg(II) in 10 mM HEPES:CH_3CN (50:50, v/v, pH=7.20, 25 °C).

Table S1. Spectral data for **1**, **2**, **3**, **4**.

Compound	λ_{abs}(nm)	λ_{em} (nm)	Φ_f[c]	ε_{max}[d]
2[a]	785	745	0.012[f] (730 nm)	98900(THF)
1[a]	824	800	0.022[f] (730 nm)	222000(THF)
3[b]	740	-	-	50200(Acetonitrile)
4[b]	825	790	0.007[f]	42600(Acetonitrile)

[a] Data acquired in THF in dilute solutions. [b]Data acquired in acetonitrile in dilute solutions. [c]relative quantum yields. [d] unit: $cm^{-1}M^{-1}$. [f] Reference dye: tetrastyryl compound **2** in reference 3.

Table S2. Binding Constants Determined by Isothermal Titration Calorimetry (ITC) for compound**3** and **4**.

Compound	**K (M^{-1})**	**ΔH (kcal/mol)**	**ΔS cal/(mol · K)**	**model**
3 (1:1 binding)	$(7.15\pm1.95)\times10^5$	$-1.82\times10^4\pm1.03\times10^3$	-34.2	One set of sites
3 (1:2 binding)	$4.43\times10^4\pm6.90\times10^3$	-8288±514	-6.53	Two sets of sites
4 (1:1 binding)	$(7.23\pm1.41)\times10^6$	-2.64×10^4±682	-57.4	One set of sites
4 (1:2 binding)	$2.0\times10^5\pm2.5\times10^4$	-1.27×10^4±285	-18.6	Two sets of sites

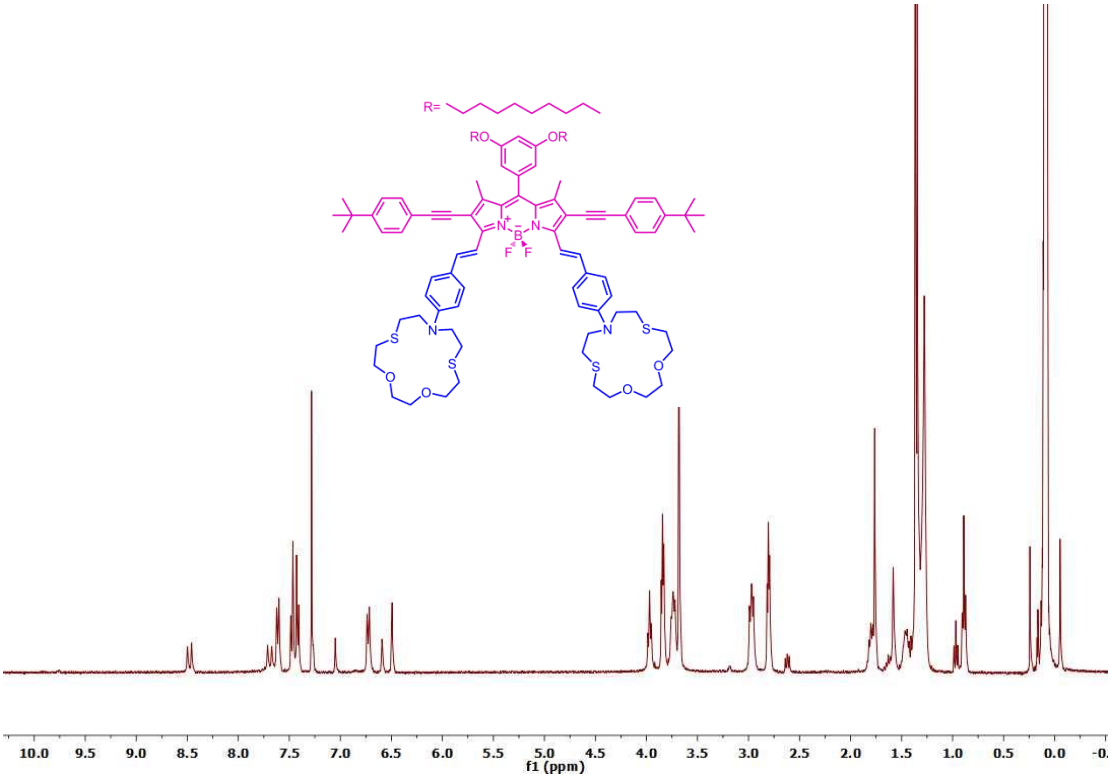


Figure S11. ^{1}H NMR spectrum of compound **7**

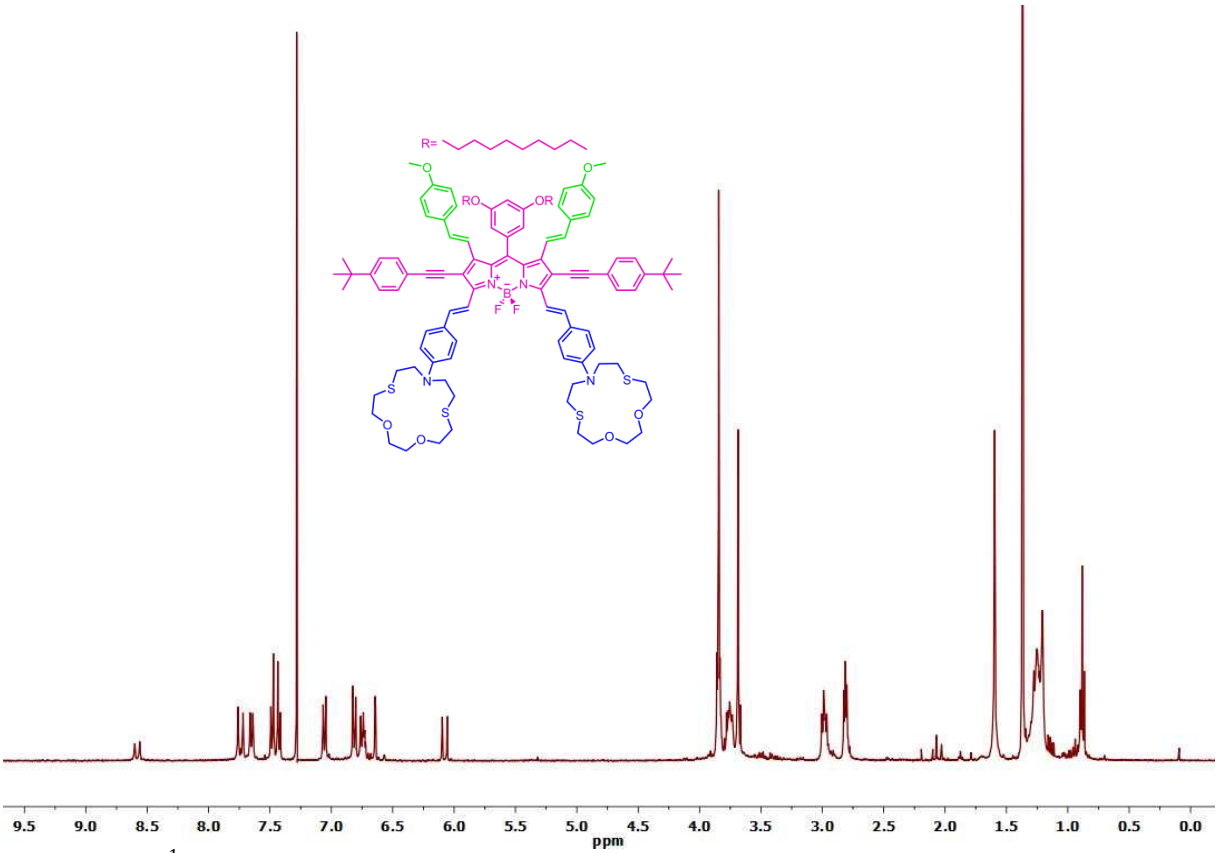


Figure S12. ^{1}H NMR spectrum of compound **1**

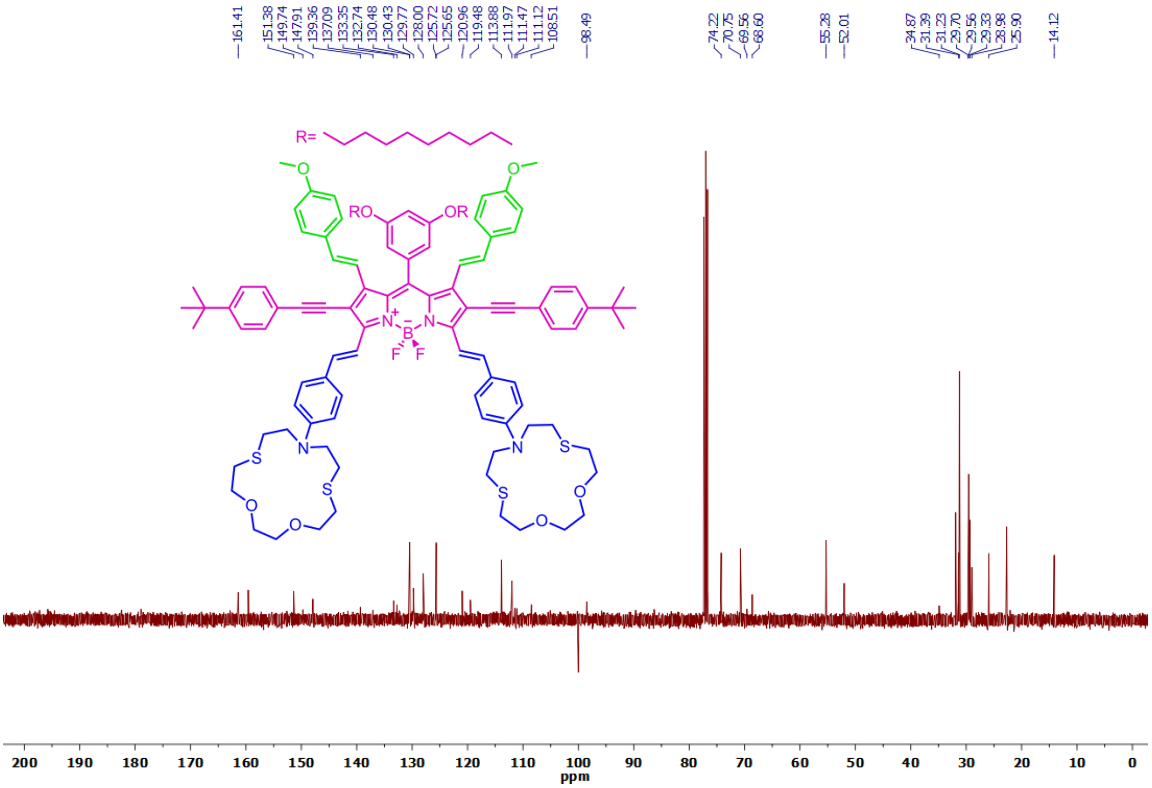


Figure S13. ^{13}C NMR spectrum of compound **1**

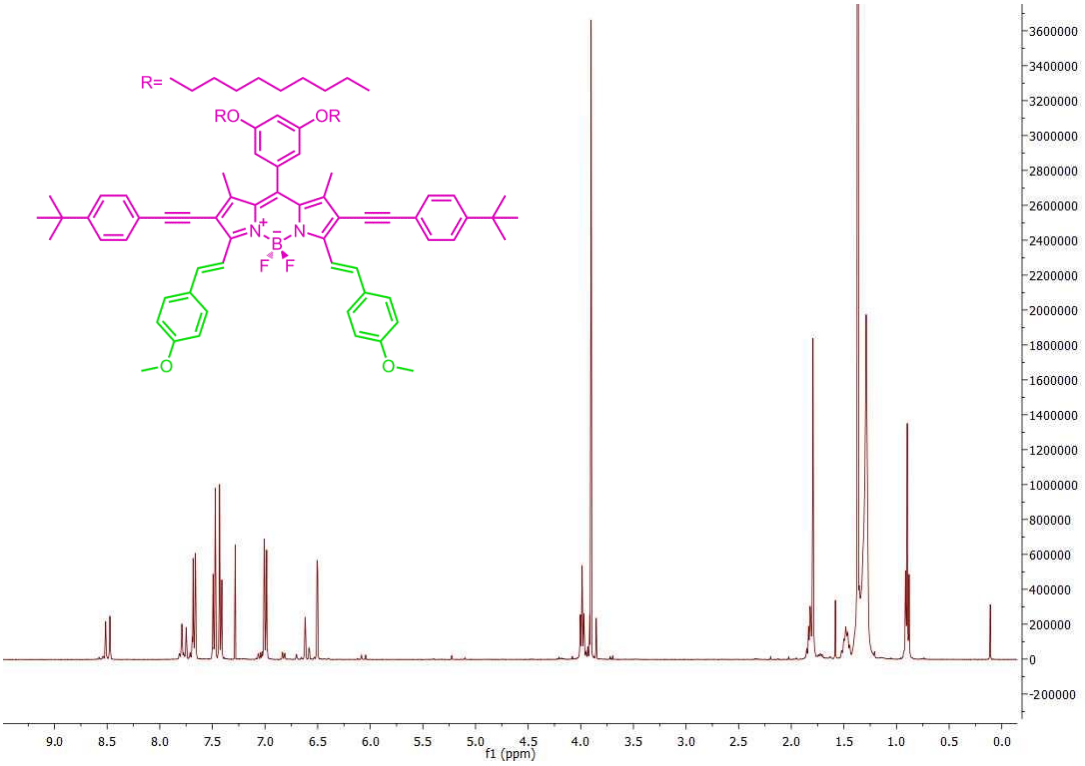


Figure S14 . ^{1}H NMR spectrum of compound **8**

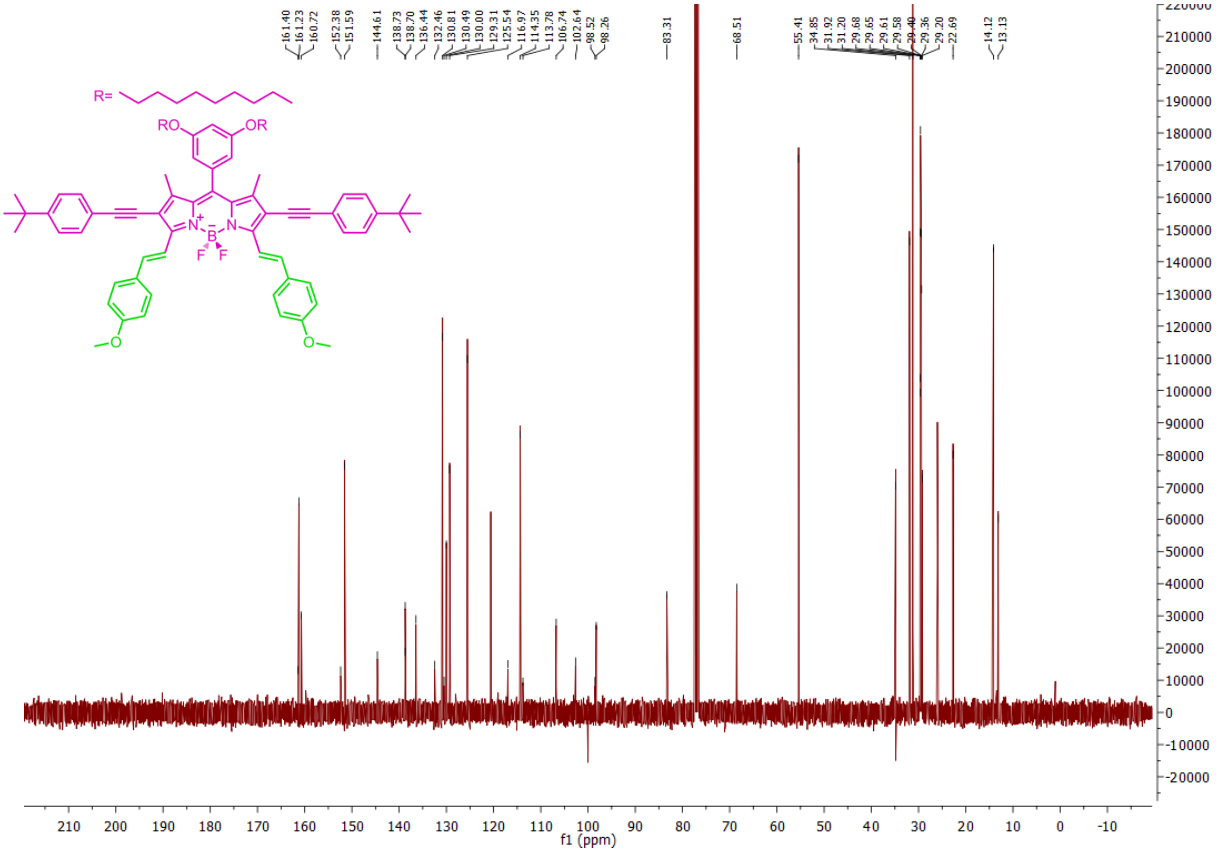


Figure S15. ^{13}C NMR spectrum of compound **8**

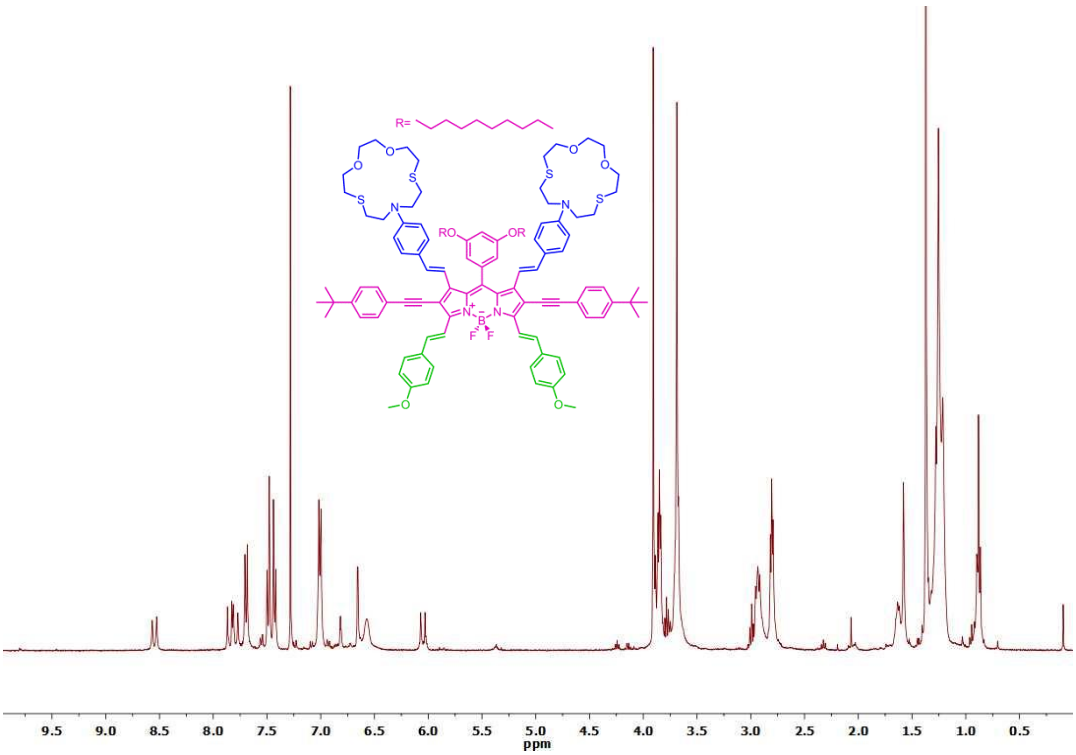


Figure S16. ^{1}H NMR spectrum of compound **2**

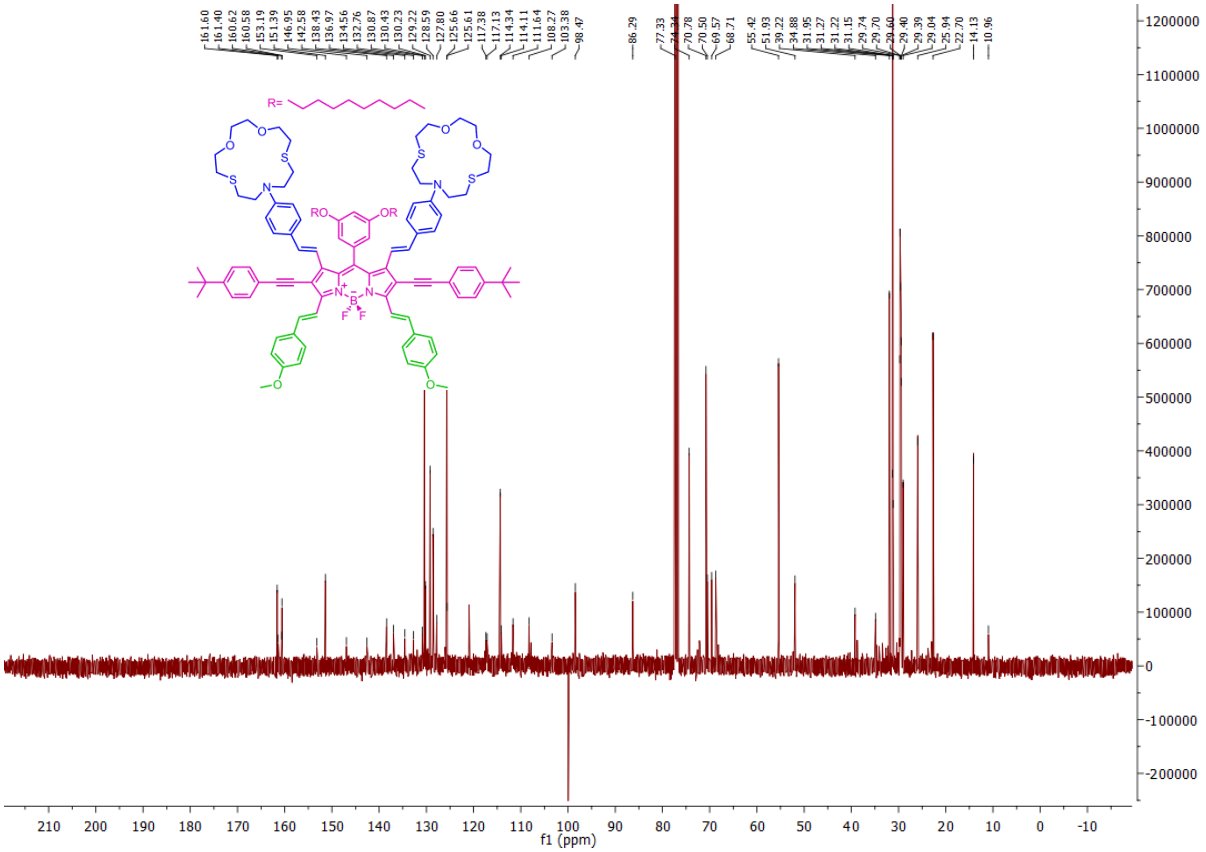


Figure S17. ^{13}C NMR spectrum of compound **2**

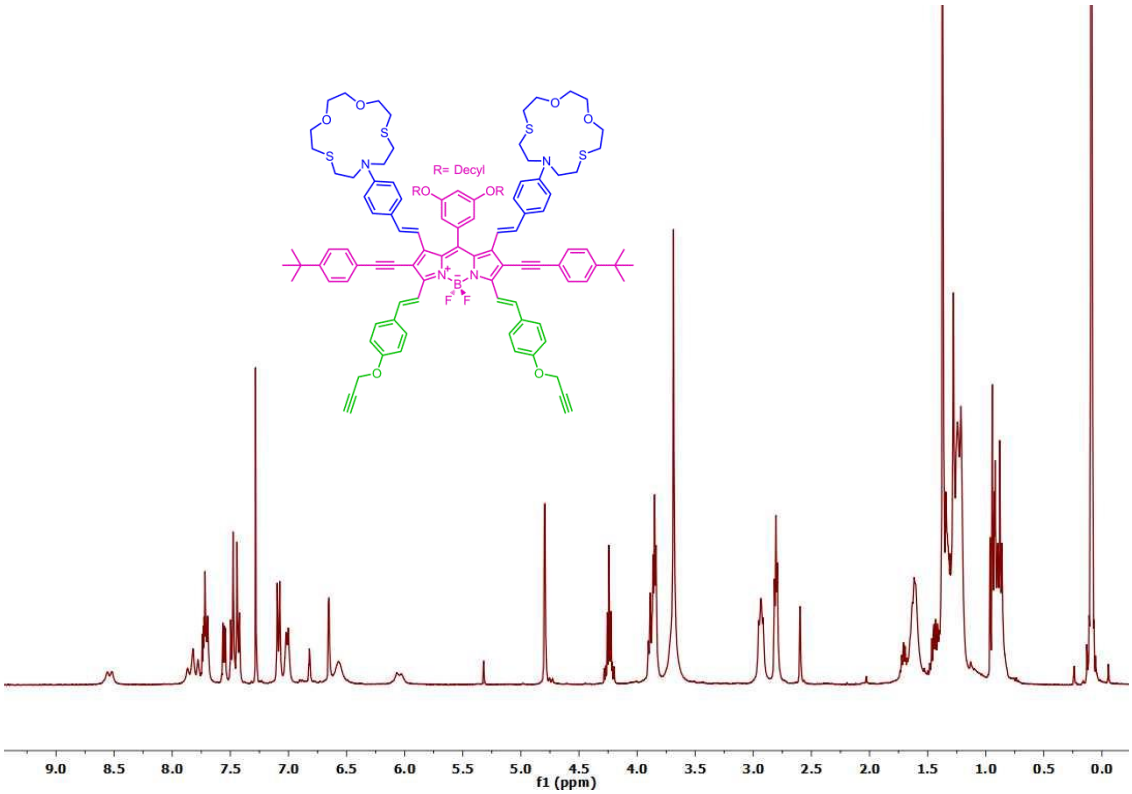


Figure S18. ^{1}H NMR spectrum of compound **11**

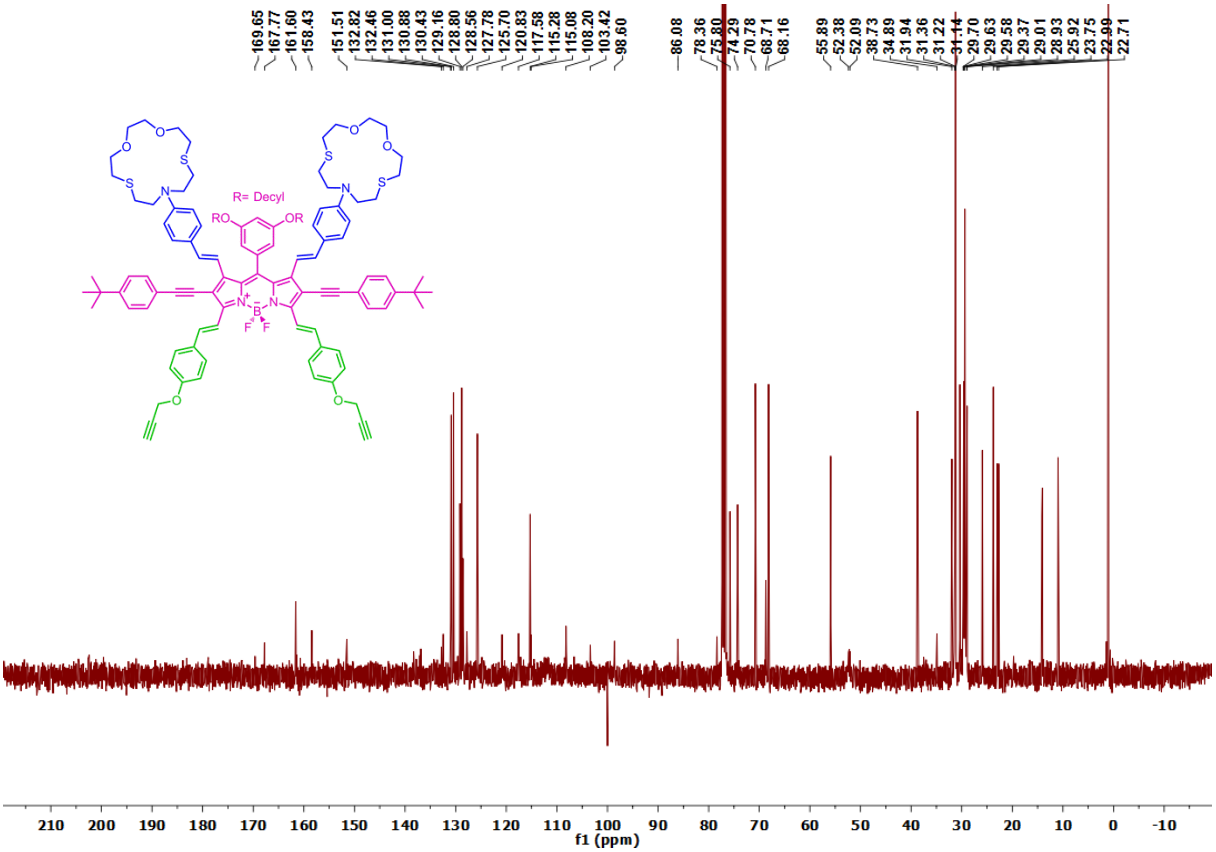


Figure S19. ^{13}C NMR spectrum of compound **11**

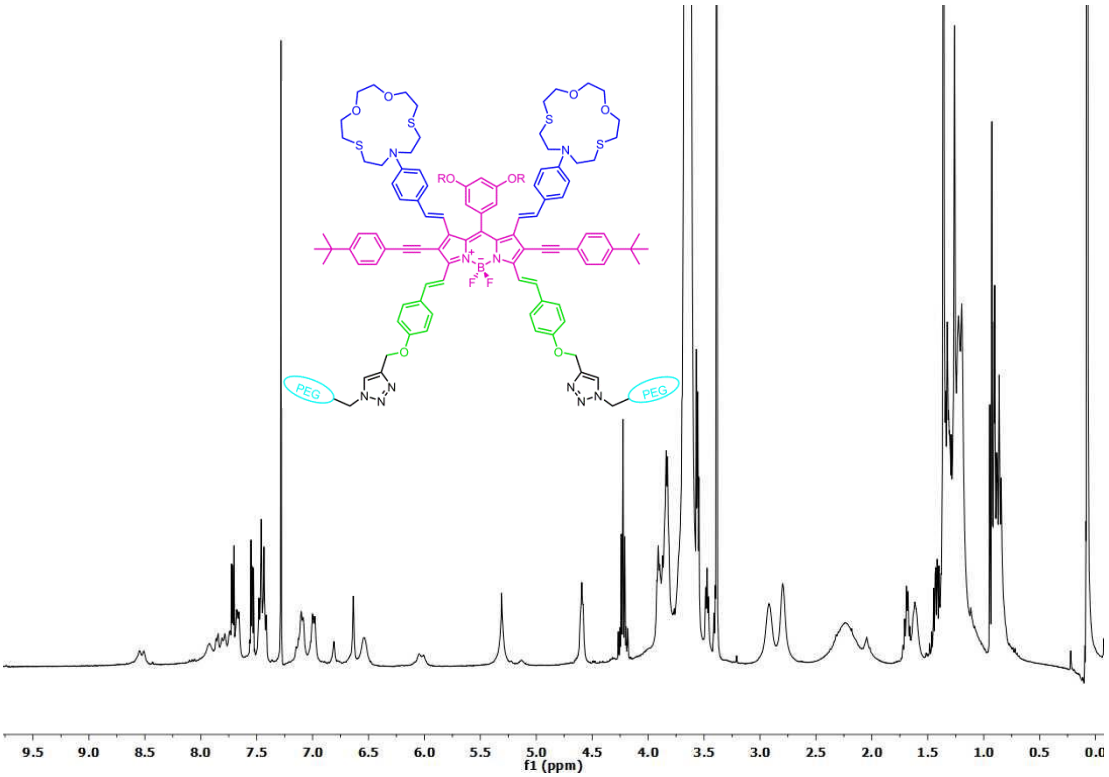


Figure S20. ^{1}H NMR spectrum of compound **3**

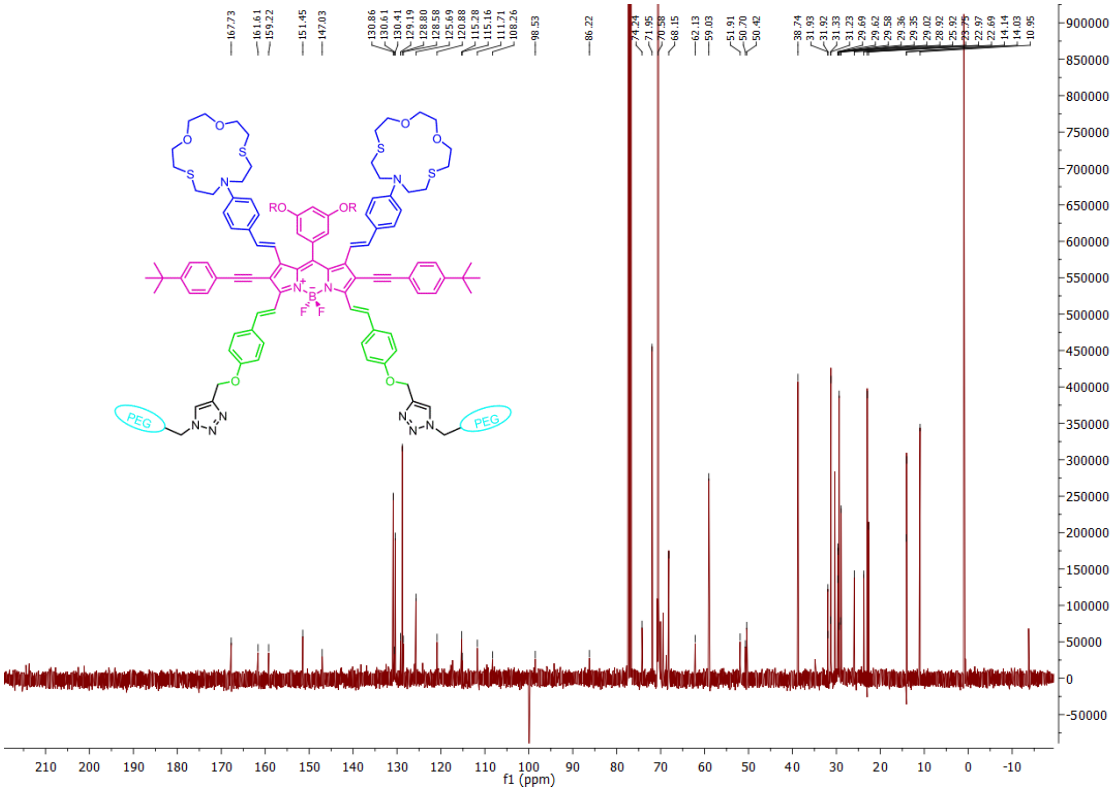


Figure S21. ^{13}C NMR spectrum of compound **3**

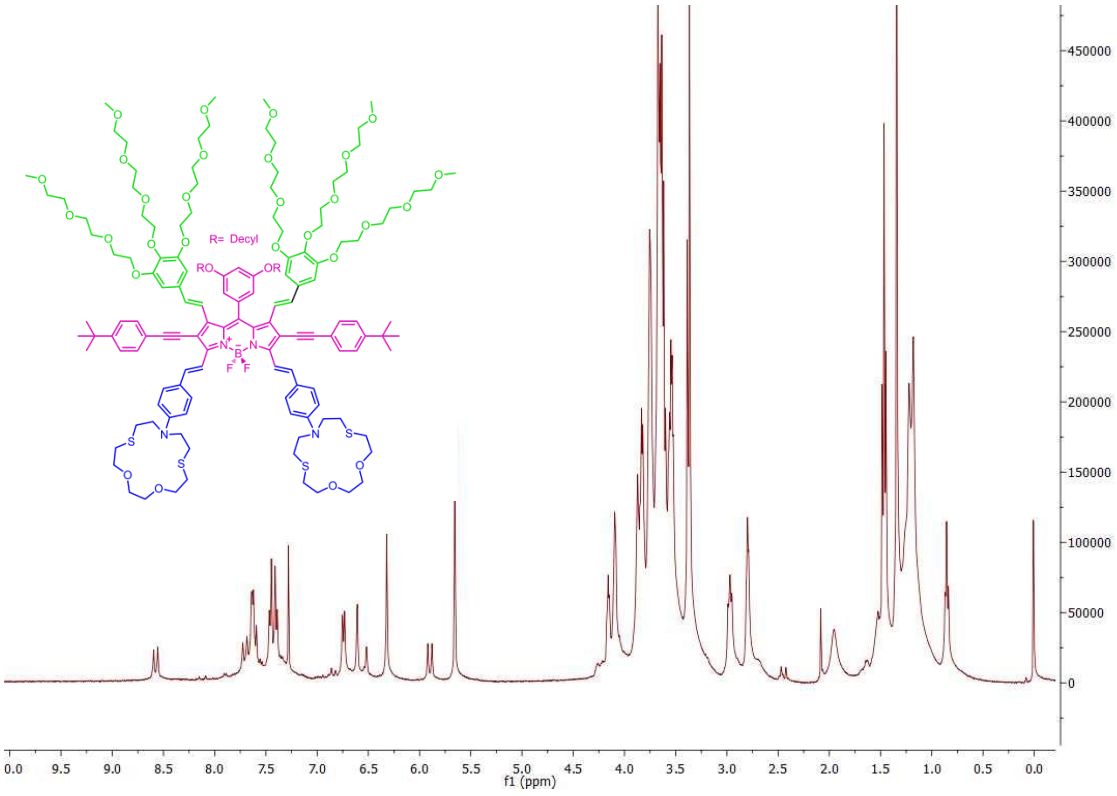


Figure S22. ^{1}H NMR spectrum of compound **4**

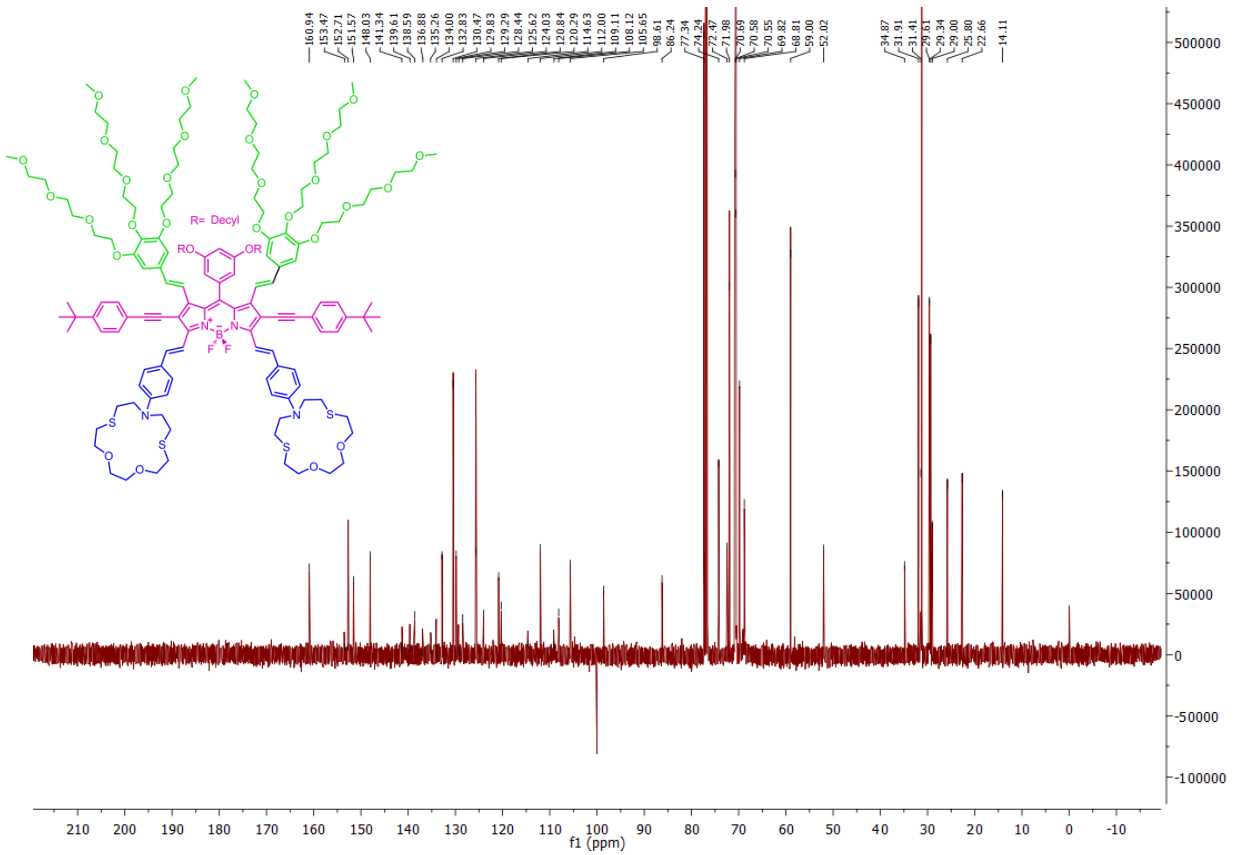


Figure S23. ^{13}C NMR spectrum of compound **4**

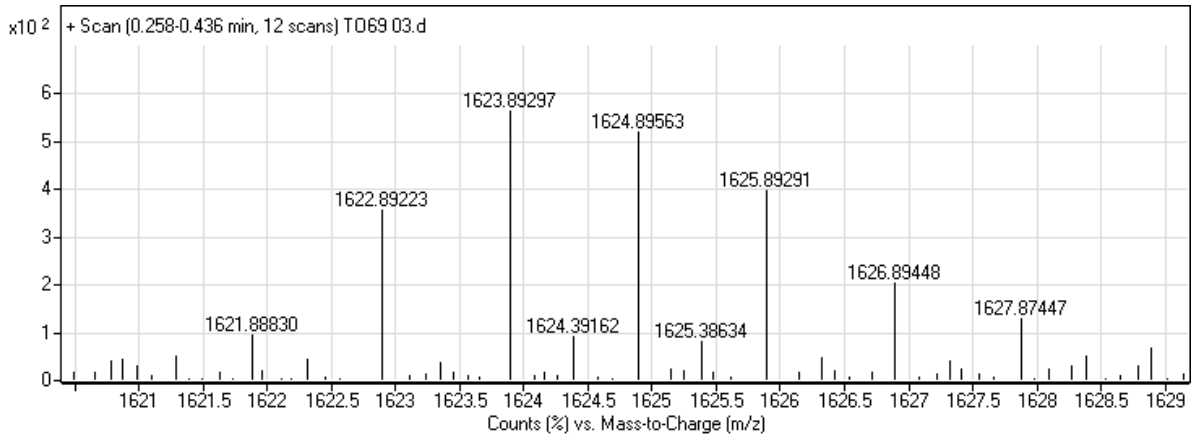


Figure S24. Mass Spectrum of **7**

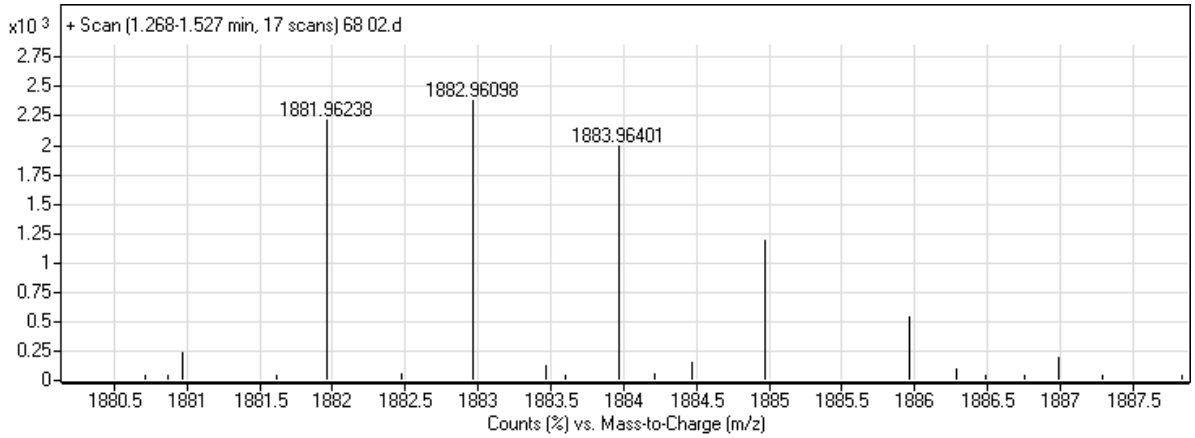


Figure S25. Mass Spectrum of **1**

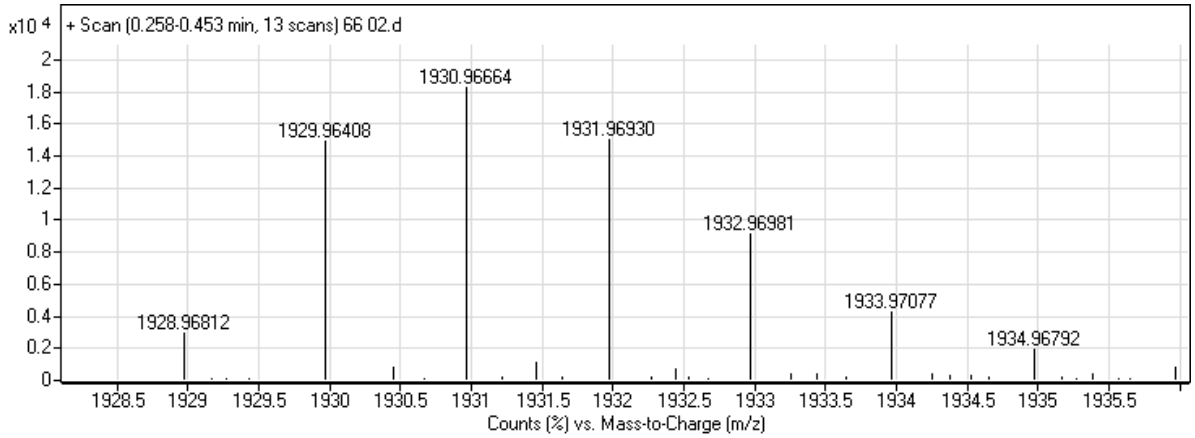


Figure S26. Mass Spectrum of **11**

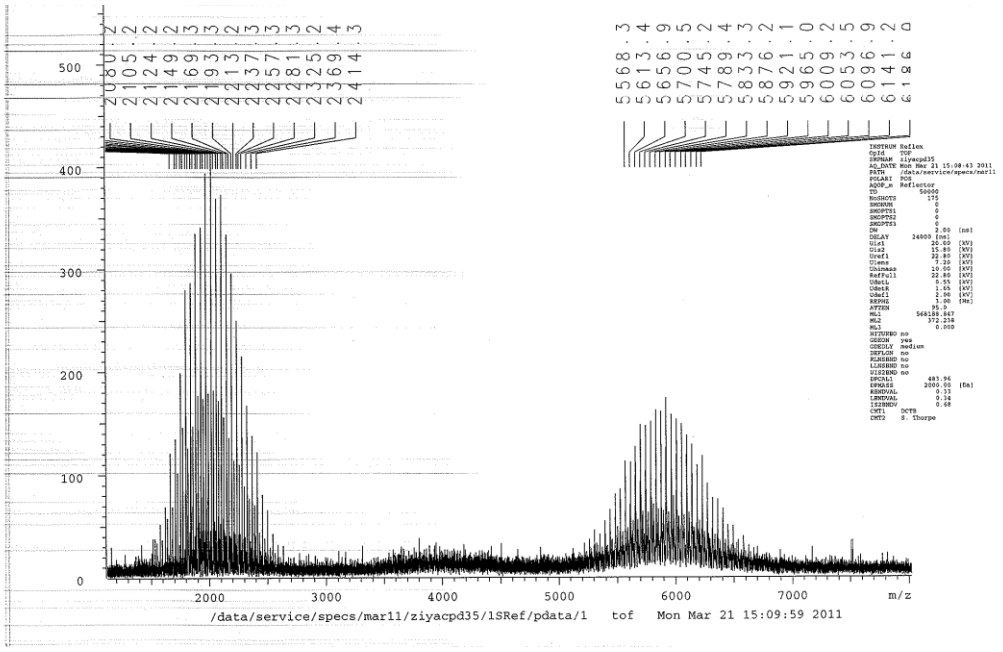


Figure S27. Mass Spectrum of **3**

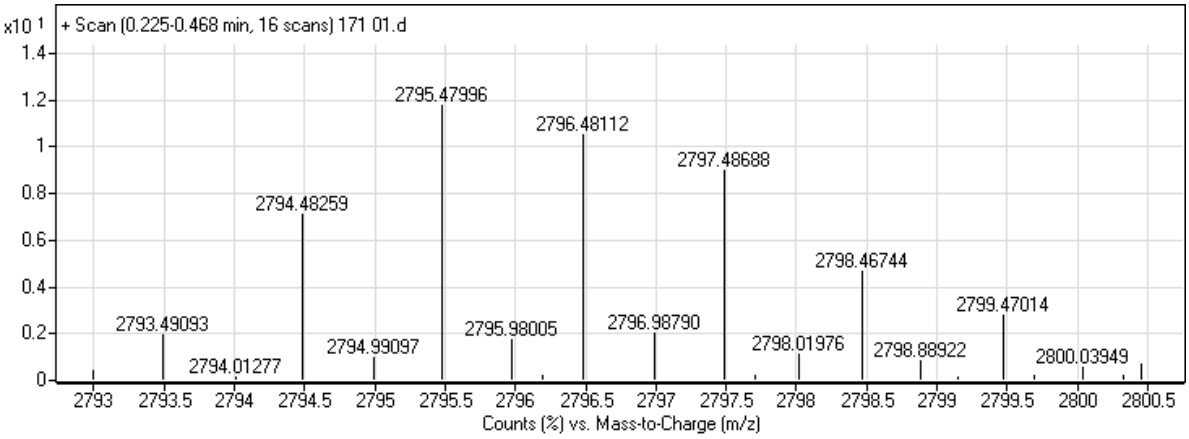


Figure S28. Mass Spectrum of **4**

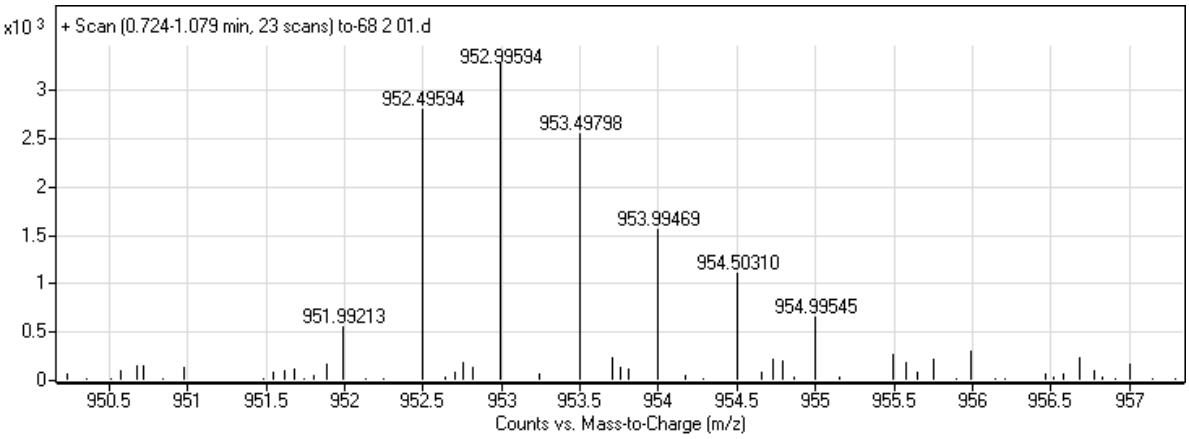


Figure S29. Mass Spectrum of **2**

Computational Details

Density Functional Theory employing the unrestricted B3LYP[5,6] hybrid functional is used throughout. Geometries were fully optimized with CEP-31G basis[7]. The choice of basis can be justified considering the system size and extensive benchmarking from literature[8]. Excitation energy and characteristics were probed via TDDFT. Solvent environment was treated as a dielectric medium (εTHF=7.43) using polarizable continuum model (PCM) as implemented in Gaussian03. No restrictions on symmetry were imposed.

Styryl derivatives of Bodipy were modelled to study the effect of position of charge injection on the HOMO-LUMO gap. These species were optimized using Pople'sall electron 6-31G[9] basis including d-type polarization functions. Vibrational frequencies (all positive) confirmed the species to be true minima. Single point energy refinements were performed using Dunning type triple-ζ basis (cc-pVTZ)[10]. All molecular orbitals are plotted at an isosurface value of 0.04 A.U. All calculations were carried out with Gaussian 03 (D.01).[10]

We are grateful to TUBITAK ULAKBIM (TR-Grid infrastructure) and to Gazi University Physics Department (pizag cluster) for computing resources.

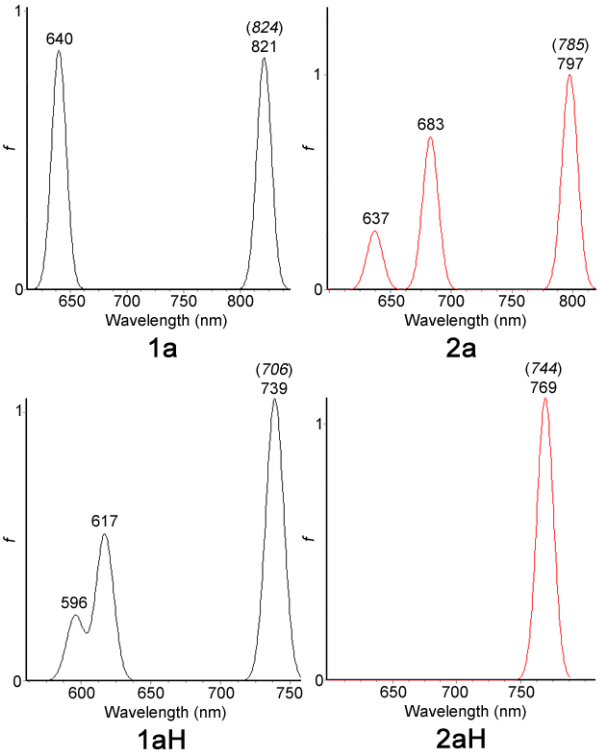


Figure S30. Computed absorption spectra. (Experimental values in parentheses)

Table S3. Summary of TDDFT Results [a]

Species	Major transitions & orbital contributions		ΔE (eV)	λ^{COMP} (nm)	λ^{EXP} (nm)	Oscillator strength
1a	237A→238A	0.625	1.51	821	798	1.103
	236A→238A	0.665	1.94	640	584	1.137
	237A→240A	0.675	2.85	436	470	1.325
1aH	237A→238A	0.621	1.68	739	706	1.185
2a	237A→238A	0.629	1.56	797	740	1.141
	236A→238A	0.670	1.82	683	-	0.811
	232A→238A	-0.369				
	237A→239A	0.466	2.90	427	403	0.820
	237A→240A	-0.274				
2aH	237A→238A	0.615	1.61	769	744	1.132
	236A→238A	0.662	2.22	558	-	0.911
	237A→239A	0.579	2.71	458	410	0.709
	234A→238A	0.329				
	237A→241A	0.616	3.24	382	-	0.918

[a] Experimental values belong to **1** and **2**.

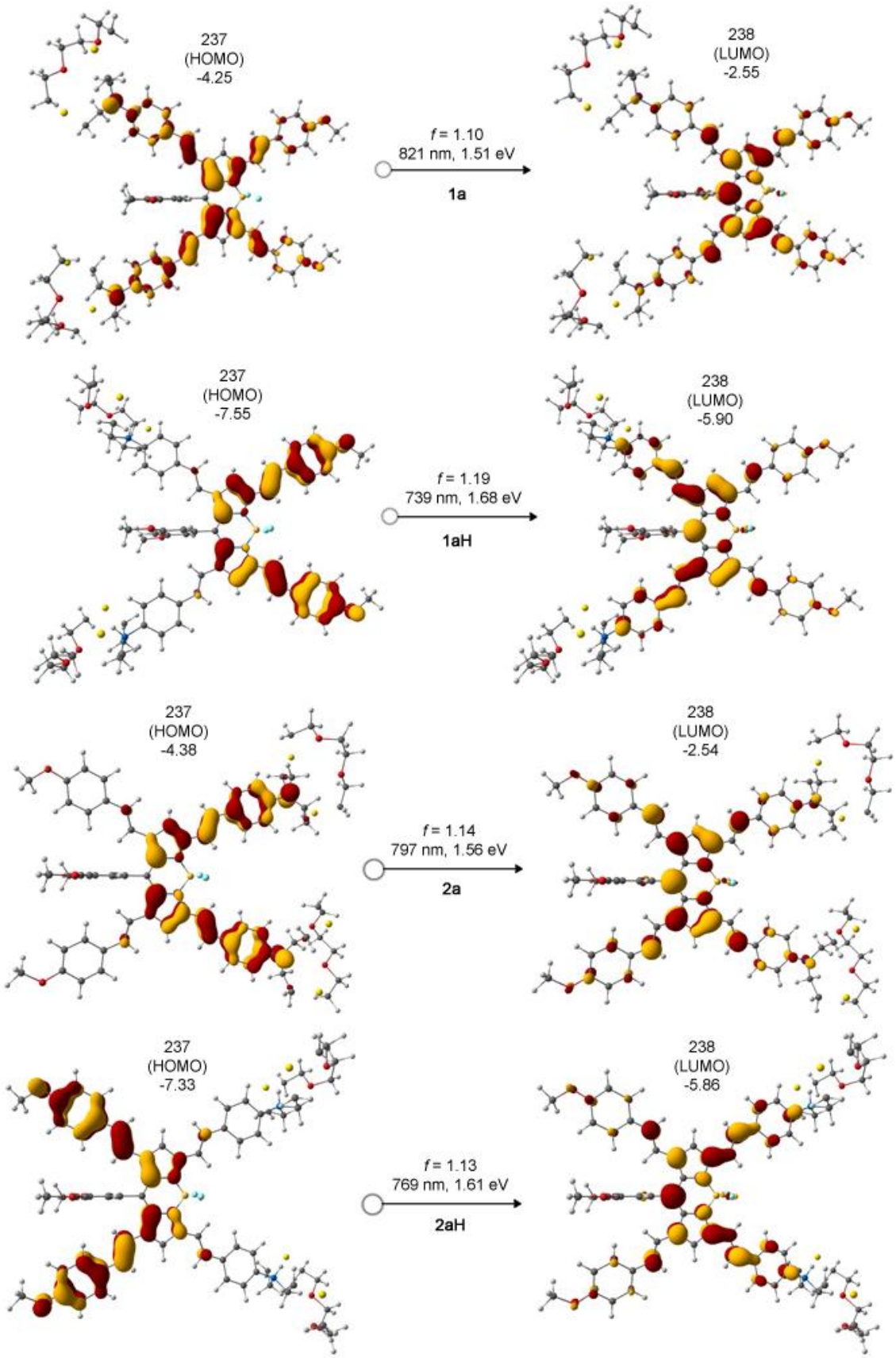


Figure S31.MO plots and energies (eV) for transitions with high oscillator strength.

Cartesian Coordinates and Total Energies

1a, UB3LYP/CEP-31G, Electronic State = S_0, E=-707.9093312 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.417031	0.852985	1.411775
C	-0.782050	-0.332418	2.127373
C	-0.977879	-1.387782	1.195506
C	-0.713944	-0.813766	-0.132423
N	-0.384896	0.551240	0.051734
B	-0.092105	1.554735	-1.078979
N	-0.159903	0.809316	-2.424539
C	-0.435839	-0.570974	-2.580198
C	-0.364671	-0.876418	-4.016878
C	-0.058351	0.350259	-4.666329
C	0.063663	1.378306	-3.676773
C	-1.375368	-2.766875	1.522571
C	-1.531985	-3.236671	2.809528
C	-1.950773	-4.600284	3.210853
C	-2.033452	-4.909838	4.611818
C	-2.430973	-6.187305	5.065970
C	-2.761433	-7.199103	4.119050
C	-2.688640	-6.923256	2.720103
C	-2.286792	-5.636146	2.279692
O	-3.149587	-8.437308	4.667004
C	-0.100253	2.183398	1.918511
C	-0.177970	2.535109	3.254164
C	0.156139	3.851148	3.825855
C	-0.027857	4.083319	5.229131
C	0.276284	5.324121	5.831673
C	0.803232	6.414419	5.051684
C	0.986096	6.184394	3.637036
C	0.672647	4.943200	3.048679
N	1.134748	7.651838	5.640242
C	0.357561	2.797307	-3.843037
C	0.609209	3.389403	-5.067740
C	0.892734	4.815564	-5.302873
C	0.902563	5.805507	-4.261245
C	1.180601	7.159303	-4.532008
C	1.462325	7.617045	-5.872691
C	1.456943	6.625656	-6.918934
C	1.174846	5.271090	-6.632381
N	1.720000	8.976310	-6.141329
C	-0.553092	-2.179485	-4.674934
C	-0.547597	-2.358276	-6.042163
C	-0.704067	-3.640171	-6.768864

C	-0.844053	-4.910137	-6.120481
C	-0.984558	-6.108660	-6.866023
C	-0.987961	-6.055538	-8.292703
C	-0.851365	-4.805437	-8.962240
C	-0.710744	-3.620437	-8.205815
O	-1.118469	-7.179809	-9.131182
H	-0.890585	-0.398201	3.203653
H	0.074708	0.495688	-5.731986
H	-1.562612	-3.439615	0.691369
H	-1.330467	-2.558911	3.646009
H	-1.782644	-4.136604	5.343069
H	-2.493998	-6.421533	6.129282
H	-2.941490	-7.686012	1.982722
H	-2.241090	-5.441755	1.206633
H	0.215116	2.914786	1.176902
H	-0.518743	1.786062	3.978522
H	-0.415741	3.273809	5.854763
H	0.125596	5.435305	6.904379
H	1.364607	6.977355	2.992531
H	0.830347	4.821132	1.975579
H	0.369682	3.394190	-2.933114
H	0.604966	2.762784	-5.967318
H	0.683550	5.514720	-3.232216
H	1.157953	7.866187	-3.704340
H	1.678286	6.901903	-7.949403
H	1.179667	4.546428	-7.452192
H	-0.692894	-3.043234	-4.032299
H	-0.422046	-1.482285	-6.687608
H	-0.838450	-4.969970	-5.030692
H	-1.083627	-7.057871	-6.338184
H	-0.856138	-4.789922	-10.052748
H	-0.604345	-2.664196	-8.725243
C	-1.241654	-8.498883	-8.511038
C	-0.727392	-1.382994	-1.442067
C	0.855658	7.932117	7.077769
C	-0.660049	8.139374	7.365066
S	-1.033230	8.914283	9.082366
C	-0.025246	7.856456	10.318523
C	1.228478	8.592738	10.838510
O	2.223537	8.660368	9.760843
C	3.102728	9.833860	9.781918
C	2.440601	11.105080	9.208495
O	2.407589	11.019390	7.740786
C	1.803403	12.216896	7.142116
C	1.770500	12.069195	5.607646
S	0.308960	11.007807	4.969052

C	1.241186	9.638238	4.016405
C	1.996193	8.615275	4.914567
C	1.773587	9.989942	-5.048561
C	3.066484	9.883622	-4.188923
S	3.384658	11.407839	-3.061629
C	1.709738	11.721867	-2.190195
C	0.967481	12.948887	-2.763355
O	0.460188	12.620236	-4.101736
C	0.383437	13.740598	-5.044860
C	1.742170	14.090541	-5.688711
O	2.067569	13.089704	-6.715923
C	3.354907	13.374410	-7.363275
C	3.647467	12.300315	-8.430662
S	4.364854	10.674850	-7.713907
C	1.697425	9.480649	-7.534239
C	3.056721	9.405969	-8.289053
H	1.387570	8.850258	7.347203
H	1.267850	7.127770	7.710216
H	-1.245440	7.213148	7.278329
H	-1.066944	8.891586	6.673345
H	0.254416	6.906479	9.839371
H	-0.707276	7.640150	11.157069
H	1.667436	8.032683	11.690660
H	0.949420	9.604759	11.189932
H	3.971702	9.560881	9.165019
H	3.445257	10.037502	10.817001
H	1.409153	11.221933	9.593847
H	3.038313	11.993669	9.507552
H	2.423756	13.101080	7.407574
H	0.784307	12.370210	7.547747
H	2.710715	11.617507	5.254231
H	1.656605	13.062810	5.145520
H	1.945373	10.136298	3.326724
H	0.456976	9.145932	3.422257
H	2.599268	9.159687	5.657656
H	2.701601	8.056409	4.272389
H	1.747745	10.981597	-5.511082
H	0.874216	9.910773	-4.415219
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H	1.084655	10.820087	-2.265995
H	1.653275	13.817160	-2.797463
H	0.106088	13.205245	-2.111922
H	-0.022419	14.640690	-4.539690
H	-0.322764	13.420091	-5.825151

H	2.545657	14.112423	-4.927339
H	1.672499	15.092324	-6.166168
H	4.160706	13.408704	-6.604494
H	3.294470	14.368762	-7.857911
H	4.400211	12.681904	-9.138835
H	2.726321	12.060862	-8.984818
H	1.350822	10.525160	-7.512759
H	0.953711	8.904770	-8.116156
H	2.904612	9.557273	-9.372416
H	3.546306	8.432461	-8.136691
C	-3.518225	-9.516778	3.751170
H	-2.149956	-8.560529	-7.883735
H	-0.349866	-8.736875	-7.902636
H	-1.320092	-9.205091	-9.347342
H	-2.667565	-9.795832	3.102475
H	-4.385447	-9.230420	3.128309
H	-3.786800	-10.363458	4.395566
C	-1.051973	-2.845478	-1.624487
C	-0.014059	-3.810793	-1.552524
C	-0.327625	-5.185972	-1.726844
C	-1.666647	-5.614925	-1.975899
C	-2.690259	-4.621476	-2.043083
C	-2.392520	-3.242895	-1.867892
O	-4.044195	-4.916670	-2.278695
O	0.765872	-6.065206	-1.639236
C	0.528079	-7.502759	-1.768868
C	-4.432126	-6.306284	-2.520869
H	1.018722	-3.521780	-1.364388
H	-1.900280	-6.668438	-2.110400
H	-3.199381	-2.514160	-1.926482
H	-0.151449	-7.866009	-0.976199
H	0.113772	-7.749987	-2.763893
H	1.514794	-7.967886	-1.653348
H	-4.213654	-6.940275	-1.641608
H	-5.514865	-6.275309	-2.694095
H	-3.921874	-6.710787	-3.414190
F	1.218694	2.164163	-0.897018
F	-1.052397	2.649173	-1.051463

2a, UB3LYP/CEP-31G, Electronic State = S_0, E=-707.9098288 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.178191	1.180741	1.541233
C	-0.545703	-0.028601	2.196031
C	-0.768030	-1.037584	1.206873
N	-0.552185	-0.479627	-0.050731
C	-0.196650	0.883311	0.102530
C	0.038577	1.703966	-1.041069
C	-0.048127	1.146947	-2.352304
N	-0.333076	-0.229923	-2.528626
C	-0.330128	-0.524111	-3.890071
C	-0.048217	0.675401	-4.614389
C	0.125054	1.740796	-3.685729
C	0.371775	3.164111	-0.859322
C	-0.677146	4.107790	-0.710080
C	-0.357847	5.481174	-0.534401
C	0.996830	5.930132	-0.513722
C	2.030952	4.958276	-0.668364
C	1.728545	3.579981	-0.837356
C	-1.145655	-2.439891	1.379516
C	-1.342975	-3.027776	2.612445
C	-1.725483	-4.434986	2.860814
C	-1.872100	-4.885802	4.217607
C	-2.234682	-6.217777	4.517725
C	-2.462551	-7.140918	3.455922
C	-2.325809	-6.722312	2.097199
C	-1.960738	-5.382979	1.811757
O	-2.818626	-8.443022	3.852835
O	3.400888	5.275102	-0.658726
O	-1.462363	6.339318	-0.394635
C	-1.223686	7.756030	-0.115843
C	3.798114	6.682830	-0.600274
C	0.176914	2.444633	2.203504
C	-0.099976	2.712889	3.530352
C	0.277752	3.923752	4.287254
C	-0.224357	4.102814	5.617905
C	0.094340	5.237488	6.396770
C	0.963781	6.264595	5.885398
C	1.472527	6.087350	4.545851
C	1.138218	4.952403	3.776498
N	1.311227	7.390900	6.662344
C	0.397081	3.145478	-4.019683
C	0.686409	3.590105	-5.295373
C	0.936684	4.985251	-5.708548

C	0.826476	6.114955	-4.829276
C	1.085545	7.427618	-5.274433
C	1.471509	7.698261	-6.638933
C	1.579147	6.566943	-7.523892
C	1.312502	5.257384	-7.064075
N	1.722095	9.013664	-7.084902
C	-0.591691	-1.872362	-4.393562
C	-0.600141	-2.193569	-5.735531
C	-0.856236	-3.530136	-6.315534
C	-1.132314	-4.692071	-5.522939
C	-1.372761	-5.953237	-6.123204
C	-1.340218	-6.073961	-7.546020
C	-1.067678	-4.933985	-8.356973
C	-0.829970	-3.683505	-7.744210
O	-1.563896	-7.274109	-8.245567
H	-0.602440	-0.180781	3.267588
H	-0.006107	0.755231	-5.694330
H	-1.722414	3.802935	-0.721882
H	1.234486	6.982657	-0.379816
H	2.543862	2.868134	-0.956870
H	-1.267731	-3.019395	0.465933
H	-1.208908	-2.419861	3.514282
H	-1.697605	-4.181022	5.035365
H	-2.345615	-6.562275	5.546537
H	-2.497515	-7.414851	1.272942
H	-1.861183	-5.078542	0.768634
H	-0.660104	7.884661	0.825999
H	-0.682668	8.240983	-0.949490
H	-2.221808	8.200046	-0.015526
H	3.469591	7.151590	0.345832
H	4.894057	6.673518	-0.646995
H	3.391730	7.245019	-1.460440
H	0.697455	3.191761	1.609932
H	-0.677450	1.976532	4.101073
H	-0.878485	3.336924	6.044893
H	-0.312341	5.309280	7.404257
H	2.129196	6.836115	4.102251
H	1.556054	4.862475	2.771685
H	0.354218	3.866967	-3.209511
H	0.759387	2.853754	-6.103699
H	0.524808	5.968123	-3.790279
H	0.964770	8.247113	-4.567291
H	1.874715	6.699085	-8.564039
H	1.406263	4.423616	-7.766124
H	-0.784504	-2.635922	-3.641885
H	-0.402268	-1.403028	-6.468145

H	-1.160198	-4.616504	-4.434697
H	-1.579458	-6.814819	-5.487966
H	-1.048636	-5.052475	-9.440961
H	-0.621684	-2.811357	-8.370179
C	-1.853714	-8.484488	-7.474229
B	-0.636693	-1.226457	-1.394669
F	-1.957561	-1.816687	-1.571457
F	0.304134	-2.338918	-1.423388
C	0.703869	7.622868	8.003998
C	-0.780314	8.082660	7.916094
S	-1.470195	8.826230	9.545940
C	-1.054940	7.517555	10.877691
C	0.114302	7.953715	11.787681
O	1.362126	7.909177	11.014876
C	2.380674	8.895814	11.389017
C	2.110004	10.305007	10.819242
O	2.449383	10.330190	9.388186
C	2.186021	11.646841	8.792667
C	2.565421	11.625858	7.297862
S	1.217889	10.859729	6.171003
C	2.181437	9.424021	5.356863
C	2.482668	8.220250	6.296951
C	1.637591	10.178923	-6.160575
C	2.837175	10.255538	-5.172380
S	2.992321	11.934200	-4.244923
C	1.214892	12.365132	-3.676519
C	0.568765	13.472506	-4.536947
O	0.208012	12.911079	-5.843908
C	0.222270	13.855743	-6.966197
C	1.639002	14.132329	-7.512347
O	2.091008	12.979059	-8.304528
C	3.439449	13.191867	-8.847483
C	3.859406	11.971675	-9.691137
S	4.493412	10.492603	-8.651535
C	1.822422	9.302014	-8.534807
C	3.245052	9.132373	-9.143788
H	1.280600	8.409455	8.500521
H	0.798717	6.718098	8.627712
H	-1.462028	7.281810	7.595823
H	-0.862284	8.928827	7.218173
H	-0.827123	6.560351	10.385433
H	-1.970616	7.394055	11.478907
H	0.204229	7.255047	12.645488
H	-0.077635	8.970182	12.181970
H	3.326692	8.508900	10.981936
H	2.464109	8.961075	12.493069

H	1.047632	10.586708	10.951083
H	2.745577	11.042791	11.355732
H	2.810079	12.406541	9.312559
H	1.120400	11.915679	8.928573
H	3.500984	11.062363	7.156035
H	2.712930	12.657886	6.941819
H	3.121464	9.843082	4.955729
H	1.542927	9.121799	4.512991
H	2.939038	8.595026	7.226434
H	3.237779	7.583352	5.799149
H	1.637010	11.088346	-6.769283
H	0.680256	10.159050	-5.612122
H	3.780812	10.209184	-5.734857
H	2.824232	9.456268	-4.418200
H	1.313456	12.713165	-2.635112
H	0.594529	11.456835	-3.687251
H	1.272653	14.319869	-4.644125
H	-0.354325	13.841379	-4.042364
H	-0.246493	14.815046	-6.666289
H	-0.391110	13.388319	-7.750645
H	2.352574	14.315894	-6.685708
H	1.608547	15.032482	-8.164138
H	4.155388	13.367320	-8.021080
H	3.424834	14.093346	-9.498649
H	4.689807	12.255555	-10.357115
H	3.012337	11.628271	-10.305365
H	1.475631	10.332899	-8.702735
H	1.134215	8.634175	-9.086563
H	3.194025	9.115433	-10.246753
H	3.717924	8.200313	-8.800563
C	-3.062630	-9.444404	2.812834
H	-2.778692	-8.364949	-6.881475
H	-1.011540	-8.740329	-6.806073
H	-1.989998	-9.276578	-8.221401
H	-2.158075	-9.607339	2.199314
H	-3.905899	-9.145465	2.164209
H	-3.316858	-10.365034	3.353262

1aH, UB3LYP/CEP-31G, Electronic State = S_0, E=-708.7013508 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.258037	0.911903	1.746006
C	-0.621447	-0.316383	2.368739
C	-0.786138	-1.310808	1.359980
C	-0.498023	-0.635428	0.085571
N	-0.188616	0.717458	0.367292
B	0.116715	1.796439	-0.686974
N	0.087235	1.139666	-2.078491
C	-0.167302	-0.231365	-2.330015
C	-0.065601	-0.453109	-3.781428
C	0.236409	0.820992	-4.345442
C	0.324373	1.778328	-3.294445
C	-1.177488	-2.706644	1.582244
C	-1.325340	-3.260701	2.840819
C	-1.743630	-4.637617	3.165380
C	-1.795466	-5.029083	4.548887
C	-2.193640	-6.325912	4.933440
C	-2.557908	-7.276588	3.932998
C	-2.515861	-6.916625	2.549065
C	-2.111565	-5.611134	2.178429
O	-2.942851	-8.531242	4.413463
C	0.026997	2.203738	2.374154
C	-0.122260	2.418101	3.729042
C	0.169596	3.668340	4.461628
C	-0.120109	3.712834	5.869097
C	0.140841	4.866448	6.644198
C	0.709134	6.001927	6.010895
C	1.005996	5.998195	4.621049
C	0.738558	4.839004	3.852971
N	0.987215	7.239687	6.814263
C	0.602297	3.213422	-3.388476
C	0.844521	3.843541	-4.591396
C	1.113461	5.282808	-4.796644
C	1.134710	6.252047	-3.733326
C	1.392773	7.617064	-3.998138
C	1.633979	8.033248	-5.336855
C	1.618186	7.107976	-6.409367
C	1.359716	5.743333	-6.133088
N	1.910745	9.482117	-5.637233
C	-0.223225	-1.707786	-4.523787
C	-0.179039	-1.781217	-5.904374
C	-0.300854	-2.992495	-6.736953
C	-0.453599	-4.314449	-6.201568

C	-0.556843	-5.443293	-7.050051
C	-0.509502	-5.266400	-8.468961
C	-0.360799	-3.960364	-9.025426
C	-0.257503	-2.846193	-8.167651
O	-0.597987	-6.305072	-9.399547
H	-0.754244	-0.461839	3.433999
H	0.386680	1.032691	-5.397133
H	-1.368146	-3.319853	0.707802
H	-1.108738	-2.637671	3.715662
H	-1.519082	-4.304366	5.319457
H	-2.234244	-6.626775	5.980502
H	-2.795881	-7.632325	1.775890
H	-2.089812	-5.350883	1.118610
H	0.371047	2.998335	1.711963
H	-0.495349	1.600188	4.352323
H	-0.555068	2.834571	6.350685
H	-0.098638	4.868525	7.709467
H	1.443315	6.877741	4.140045
H	0.978355	4.841470	2.789313
H	0.602389	3.768746	-2.450810
H	0.841815	3.246248	-5.507778
H	0.945739	5.939242	-2.705893
H	1.398901	8.329989	-3.170859
H	1.799049	7.434258	-7.435512
H	1.346442	5.027026	-6.956813
H	-0.371637	-2.616593	-3.950544
H	-0.045293	-0.854901	-6.473735
H	-0.486621	-4.466407	-5.121101
H	-0.667076	-6.436038	-6.613383
H	-0.328279	-3.854504	-10.109964
H	-0.141815	-1.848284	-8.598997
C	-0.735538	-7.685141	-8.919092
C	-0.474120	-1.120776	-1.257338
C	-0.268591	7.904539	7.456104
C	-1.406446	8.145940	6.436875
S	-2.451535	9.686666	6.863806
C	-3.170407	9.284384	8.595625
C	-2.387436	9.938547	9.751460
O	-1.101817	9.237042	9.894524
C	-0.098594	9.922733	10.722436
C	0.795088	10.878565	9.904498
O	1.737583	10.085102	9.082145
C	2.684065	10.933942	8.337566
C	3.911748	10.109876	7.899527
S	3.666507	8.920776	6.406881
C	3.482491	7.224930	7.270033

C	2.082298	7.048346	7.899212
C	3.212643	9.994151	-4.969082
C	4.445125	9.198639	-5.450776
S	4.719526	9.280904	-7.336542
C	5.633345	10.954829	-7.523302
C	4.732426	12.144108	-7.900112
O	3.829276	12.432648	-6.775516
C	3.090433	13.700095	-6.887741
C	2.022342	13.702413	-7.997632
O	0.988549	12.711825	-7.665325
C	0.074460	12.463558	-8.791273
C	-1.089265	11.575416	-8.322456
S	-0.587133	9.797954	-7.814535
C	0.725445	10.428129	-5.305526
C	-0.603692	9.930933	-5.913335
H	0.102706	8.841615	7.883033
H	-0.583267	7.261377	8.286465
H	-2.070680	7.276380	6.336712
H	-1.015077	8.395227	5.436710
H	-3.216811	8.191102	8.716587
H	-4.198431	9.677055	8.567632
H	-2.961309	9.835004	10.694253
H	-2.229151	11.014515	9.547680
H	0.518012	9.130741	11.173828
H	-0.591921	10.491331	11.533121
H	0.186811	11.530309	9.248609
H	1.379879	11.515408	10.597971
H	3.046070	11.741400	9.006248
H	2.175234	11.399666	7.472612
H	4.299482	9.511073	8.737809
H	4.704662	10.792068	7.556473
H	4.256810	7.137945	8.046502
H	3.689023	6.479939	6.487002
H	1.905190	7.815700	8.664054
H	1.954408	6.042189	8.321795
H	3.308446	11.051098	-5.251866
H	3.075863	9.883023	-3.882512
H	4.366698	8.127671	-5.217627
H	5.342835	9.596492	-4.953295
H	6.369760	10.777713	-8.322090
H	6.170680	11.147787	-6.582226
H	4.155256	11.918555	-8.814636
H	5.371091	13.031310	-8.090989
H	3.800433	14.531845	-7.064043
H	2.614332	13.841759	-5.906242
H	2.464653	13.465878	-8.984233

H	1.567272	14.711276	-8.059275
H	0.630130	11.987761	-9.621851
H	-0.340289	13.428107	-9.149845
H	-1.807260	11.441195	-9.145894
H	-1.612504	12.030414	-7.467620
H	0.999396	11.408966	-5.718989
H	0.656611	10.473359	-4.207040
H	-1.404821	10.629112	-5.625347
H	-0.874344	8.929873	-5.551318
C	-3.349287	-9.567943	3.457273
H	-1.667902	-7.808806	-8.339864
H	0.135970	-7.976327	-8.306230
H	-0.776104	-8.299654	-9.826139
H	-2.517836	-9.822059	2.775913
H	-4.231812	-9.243556	2.877770
H	-3.606004	-10.438173	4.072747
C	-0.768892	-2.572352	-1.540424
C	0.287727	-3.517875	-1.503234
C	0.004881	-4.886445	-1.771052
C	-1.321000	-5.320656	-2.077647
C	-2.363514	-4.344578	-2.108058
C	-2.096198	-2.972755	-1.840434
O	-3.701996	-4.644038	-2.391445
O	1.110807	-5.743157	-1.712191
C	0.916339	-7.179624	-1.936058
C	-4.071937	-6.024436	-2.721560
H	1.311310	-3.226106	-1.273101
H	-1.531645	-6.367881	-2.281440
H	-2.917581	-2.258633	-1.874442
H	0.231160	-7.606925	-1.182167
H	0.531908	-7.372808	-2.953865
H	1.913283	-7.622186	-1.826022
H	-3.860686	-6.703842	-1.876034
H	-5.151299	-5.992233	-2.910815
H	-3.542335	-6.368538	-3.627948
F	1.413614	2.416097	-0.431394
F	-0.849177	2.886174	-0.608744
H	2.065259	9.567601	-6.662213
H	1.388979	7.959966	6.178835

2aH, UB3LYP/CEP-31G, Electronic State = S_0, E=-708.7054738 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.288345	1.156786	1.882772
C	-0.602624	-0.134184	2.382568
C	-0.623942	-1.060484	1.288133
N	-0.332817	-0.355195	0.122257
C	-0.124780	1.007989	0.427949
C	0.163557	1.948997	-0.608863
C	0.264605	1.509340	-1.964055
N	0.112719	0.141847	-2.286152
C	0.274587	-0.039189	-3.657893
C	0.528150	1.243294	-4.246672
C	0.522202	2.226695	-3.223224
C	0.367733	3.404630	-0.264025
C	-0.750915	4.275211	-0.176913
C	-0.548571	5.638870	0.173585
C	0.759348	6.150988	0.436914
C	1.866766	5.253508	0.335520
C	1.679567	3.886996	-0.012204
C	-0.882726	-2.492960	1.296018
C	-1.166776	-3.202281	2.451120
C	-1.437221	-4.645422	2.551749
C	-1.717398	-5.207769	3.846666
C	-1.983731	-6.582441	4.008252
C	-1.976557	-7.440338	2.866245
C	-1.700747	-6.909400	1.566026
C	-1.435290	-5.527724	1.419343
O	-2.251225	-8.783589	3.127897
O	3.198533	5.632081	0.568757
O	-1.714735	6.419005	0.234741
C	-1.616663	7.815386	0.664598
C	3.492500	7.018163	0.937080
C	-0.136624	2.366955	2.706035
C	-0.462406	2.406333	4.046912
C	-0.291337	3.546057	4.972657
C	-0.731568	3.381441	6.331785
C	-0.589522	4.412336	7.289658
C	0.005289	5.637935	6.892954
C	0.452350	5.840499	5.560041
C	0.302154	4.803369	4.608192
N	0.176490	6.745123	7.898536
C	0.710180	3.671143	-3.437858
C	0.983765	4.206974	-4.680123
C	1.143327	5.633032	-5.034520

C	1.035160	6.721649	-4.098993
C	1.178295	8.064105	-4.523163
C	1.432834	8.339036	-5.895452
C	1.550204	7.293135	-6.843743
C	1.408430	5.953989	-6.408587
N	1.572252	9.759804	-6.372676
C	0.183711	-1.344402	-4.295777
C	0.346242	-1.530076	-5.658797
C	0.277456	-2.806853	-6.386975
C	0.033694	-4.067972	-5.745788
C	-0.021168	-5.269802	-6.489763
C	0.168985	-5.230794	-7.907880
C	0.412283	-3.987997	-8.568546
C	0.465027	-2.798661	-7.814155
O	0.136847	-6.351364	-8.739218
H	-0.767886	-0.400296	3.419739
H	0.679166	1.415056	-5.305491
H	-1.763445	3.921167	-0.365181
H	0.907853	7.193919	0.707637
H	2.548026	3.232810	-0.074528
H	-0.844865	-2.998911	0.333529
H	-1.199995	-2.661581	3.404040
H	-1.723706	-4.554381	4.723400
H	-2.196989	-7.015188	4.985844
H	-1.691369	-7.552716	0.686467
H	-1.225857	-5.137757	0.421949
H	-1.201348	7.888850	1.686230
H	-0.997746	8.406409	-0.035932
H	-2.647095	8.190320	0.654776
H	2.995175	7.292818	1.885594
H	4.580840	7.054791	1.065443
H	3.185964	7.716154	0.136153
H	0.272147	3.253062	2.225524
H	-0.899987	1.515063	4.505116
H	-1.185094	2.434799	6.632500
H	-0.933510	4.245767	8.312380
H	0.916699	6.785499	5.268839
H	0.655152	4.966761	3.589524
H	0.605207	4.327088	-2.576294
H	1.094215	3.524977	-5.527404
H	0.834354	6.518058	-3.046261
H	1.084805	8.870018	-3.791790
H	1.742003	7.509422	-7.896768
H	1.496448	5.146398	-7.137686
H	-0.021168	-2.191341	-3.644284
H	0.549026	-0.655035	-6.286974

H	-0.111797	-4.113811	-4.665292
H	-0.206913	-6.211428	-5.973572
H	0.553167	-3.989284	-9.649551
H	0.652261	-1.849264	-8.323306
C	-0.102693	-7.674795	-8.147697
B	-0.209042	-0.983339	-1.281186
F	-1.442006	-1.651556	-1.648415
F	0.834686	-1.989167	-1.294349
C	-1.178230	7.280862	8.430735
C	-2.035060	7.871705	7.290790
S	-1.194434	9.324933	6.383610
C	-1.591715	10.792696	7.550724
C	-0.470849	11.153440	8.542121
O	-0.325696	10.059198	9.511112
C	0.522554	10.365988	10.674113
C	2.015977	10.524386	10.331543
O	2.531655	9.242295	9.829528
C	3.874051	9.375782	9.244462
C	4.434785	7.982992	8.914715
S	3.481193	7.033018	7.551041
C	2.462172	5.807909	8.598161
C	1.109957	6.372511	9.082682
C	2.793482	10.486081	-5.754127
C	4.115521	9.787251	-6.139053
S	4.406737	9.696326	-8.021989
C	5.104032	11.442810	-8.392014
C	4.068465	12.457430	-8.908887
O	3.119725	12.767037	-7.827916
C	2.242987	13.920059	-8.090308
C	1.210680	13.678518	-9.208116
O	0.290801	12.613053	-8.785170
C	-0.545460	12.125849	-9.893735
C	-1.598964	11.147058	-9.350358
S	-0.889093	9.528935	-8.612740
C	0.287712	10.613319	-6.192597
C	-0.966886	9.904399	-6.745600
H	-0.936438	8.056262	9.169738
H	-1.692377	6.430223	8.902909
H	-2.988223	8.230893	7.707331
H	-2.254861	7.130860	6.509553
H	-2.524377	10.549480	8.081929
H	-1.779228	11.640724	6.874256
H	-0.754734	12.082534	9.078721
H	0.479921	11.328442	8.006658
H	0.379361	9.520298	11.362415
H	0.162107	11.290989	11.165128

H	2.173567	11.313798	9.571387
H	2.567015	10.816012	11.247819
H	4.550067	9.862548	9.977307
H	3.821917	10.009900	8.338124
H	4.454377	7.343682	9.810334
H	5.461077	8.079741	8.528506
H	3.062913	5.528957	9.477264
H	2.338151	4.914667	7.971297
H	1.257283	7.299752	9.654486
H	0.571286	5.624425	9.685065
H	2.775456	11.510417	-6.150621
H	2.648123	10.478247	-4.662950
H	4.152382	8.744919	-5.792238
H	4.955694	10.334946	-5.685151
H	5.873447	11.272744	-9.160618
H	5.592762	11.807607	-7.475723
H	3.536189	12.053530	-9.788472
H	4.596554	13.386858	-9.206608
H	2.857987	14.804371	-8.348578
H	1.728905	14.111207	-7.136753
H	1.703044	13.393779	-10.157555
H	0.643570	14.614434	-9.384011
H	0.094518	11.640948	-10.655616
H	-1.069212	12.982503	-10.365634
H	-2.255579	10.818584	-10.170494
H	-2.216021	11.623039	-8.573073
H	0.471688	11.552330	-6.733928
H	0.183453	10.799314	-5.111560
H	-1.841392	10.548083	-6.563139
H	-1.144948	8.936817	-6.257211
C	-2.269504	-9.740189	2.012903
H	-1.091265	-7.712020	-7.657406
H	0.691747	-7.930604	-7.424913
H	-0.077984	-8.372195	-8.993271
H	-1.282113	-9.788098	1.521109
H	-3.048989	-9.471153	1.278729
H	-2.505849	-10.707159	2.472346
H	1.753634	9.728135	-7.396463
H	0.632614	7.546256	7.417863

BODIPY, UB3LYP/6-31G(d), Electronic State = S_0, E=-681.3758523 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.444826	0.820165	1.369274
C	-0.769912	-0.362821	2.069884
C	-0.919236	-1.360607	1.117215
C	-0.680963	-0.764755	-0.149347
N	-0.390874	0.584416	0.051666
B	-0.063622	1.636997	-1.073523
N	-0.133451	0.833897	-2.426779
C	-0.430906	-0.522338	-2.558236
C	-0.393571	-0.852770	-3.938586
C	-0.073592	0.309453	-4.625819
C	0.078522	1.324672	-3.655162
H	-0.877000	-0.451933	3.142114
H	0.041876	0.434865	-5.693539
C	-0.698445	-1.298325	-1.434445
F	1.209272	2.139524	-0.890948
F	-1.015579	2.636918	-1.070925
H	-1.168710	-2.400795	1.281538
H	-0.251961	1.811233	1.758237
H	-0.582892	-1.835142	-4.351316
H	0.327290	2.368429	-3.794614
H	-0.927526	-2.351928	-1.564397

3,5-distyryl BODIPY, UB3LYP/6-31G(d), Electronic State = S_0, E=-1298.3156341 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.363821	1.017520	1.423870
C	-0.644529	-0.208195	2.101345
C	-0.816100	-1.183711	1.142761
C	-0.638040	-0.562933	-0.123542
N	-0.360647	0.782560	0.082739
B	-0.277649	1.844234	-1.073774
N	-0.104035	1.030483	-2.407771
C	-0.393618	-0.322700	-2.529080
C	-0.304680	-0.679341	-3.902233
C	0.037037	0.461109	-4.597067
C	0.155997	1.523534	-3.650058
C	-0.096723	2.320384	1.979002
C	-0.207809	2.617921	3.296042
C	0.053911	3.907193	3.928726
C	-0.097868	4.019425	5.324718
C	0.139569	5.223507	5.982927
C	0.534801	6.348989	5.258340
C	0.688898	6.256984	3.870826
C	0.452427	5.055289	3.212986
C	0.509902	2.902614	-3.872491
C	0.648691	3.460136	-5.099460
C	1.016250	4.841227	-5.397174
C	1.273131	5.806320	-4.401247
C	1.622029	7.107426	-4.744794
C	1.724500	7.483675	-6.088429
C	1.472574	6.542398	-7.087661
C	1.122713	5.238824	-6.744391
H	-0.688119	-0.334110	3.174156
H	0.211728	0.548792	-5.660290
H	0.217063	3.076427	1.268577
H	-0.527111	1.833558	3.981123
H	-0.406213	3.145248	5.893806
H	0.015731	5.283247	7.060918
H	0.994394	7.129614	3.299670
H	0.574270	5.006122	2.135344
H	0.674841	3.492078	-2.977970
H	0.470682	2.839021	-5.976524
H	1.197042	5.535404	-3.352770
H	1.815204	7.835207	-3.961175
H	1.548151	6.823286	-8.134728
H	0.927132	4.509117	-7.526940
C	-0.666161	-1.099560	-1.407157

F	0.826761	2.674173	-0.876887
F	-1.446989	2.583353	-1.120830
H	0.720529	7.290748	5.767411
H	1.997329	8.502021	-6.351303
H	-0.884823	-2.154993	-1.534787
H	-0.461628	-1.673823	-4.299558
H	-1.027652	-2.233752	1.298152

1,7-distyryl BODIPY, UB3LYP/6-31G(d), Electronic State = S_0, E=-1298.3064841 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.468463	0.894843	1.377254
C	-0.791835	-0.269435	2.081134
C	-0.898252	-1.310087	1.141946
C	-0.627430	-0.706119	-0.134508
N	-0.366984	0.644129	0.058653
B	0.043278	1.672630	-1.054913
N	-0.118862	0.894550	-2.409385
C	-0.389879	-0.460812	-2.543386
C	-0.393475	-0.793585	-3.942250
C	-0.118891	0.409263	-4.616213
C	0.039849	1.403232	-3.645506
C	-1.212157	-2.704550	1.346168
C	-1.510266	-3.269785	2.539655
C	-1.827919	-4.671358	2.804231
C	-2.178419	-5.047588	4.115634
C	-2.496302	-6.366723	4.429680
C	-2.469434	-7.347511	3.437268
C	-2.119896	-6.994277	2.129724
C	-1.802896	-5.677201	1.816333
C	-0.643605	-2.111131	-4.477135
C	-0.653576	-2.429591	-5.792929
C	-0.901554	-3.741213	-6.387420
C	-1.192699	-4.896942	-5.633855
C	-1.420049	-6.118353	-6.258094
C	-1.364057	-6.223531	-7.651819
C	-1.077974	-5.090711	-8.414963
C	-0.850466	-3.867271	-7.789446
H	-0.928733	-0.336814	3.151315
H	-0.044697	0.559234	-5.684181
H	-1.203179	-3.330265	0.456065
H	-1.528208	-2.626922	3.418803
H	-2.201606	-4.287739	4.893374
H	-2.764475	-6.628762	5.449604
H	-2.092599	-7.752575	1.351653
H	-1.527896	-5.428371	0.795585
H	-0.835197	-2.893744	-3.745878
H	-0.456572	-1.635563	-6.512062
H	-1.243274	-4.839773	-4.550513
H	-1.643062	-6.995402	-5.656246
H	-1.032054	-5.159250	-9.498482
H	-0.628114	-2.988084	-8.389775
C	-0.631325	-1.243731	-1.418255

F	1.362957	2.050557	-0.884206
F	-0.804134	2.763882	-1.028554
H	-2.715632	-8.377969	3.677840
H	-1.542604	-7.179857	-8.135442
H	-0.845332	-2.299452	-1.547084
H	0.259942	2.454141	-3.778959
H	-0.303320	1.894549	1.756662

1,3,5,7-tetrastyryl BODIPY, UB3LYP/6-31G(d), Electronic State = S_0, E=-1915.2445276 A.U.

	x(Å)	y(Å)	z(Å)
C	-0.436912	0.978962	1.416571
C	-0.746916	-0.223895	2.093511
C	-0.943993	-1.224247	1.141544
C	-0.740093	-0.591588	-0.134435
N	-0.431001	0.741556	0.070467
B	-0.314863	1.801507	-1.080883
N	-0.161106	0.985954	-2.412701
C	-0.481075	-0.354318	-2.539582
C	-0.403148	-0.722653	-3.928146
C	-0.030628	0.438651	-4.605404
C	0.109524	1.479746	-3.658251
C	-1.267219	-2.621793	1.325366
C	-1.438501	-3.234934	2.519069
C	-1.770141	-4.639182	2.755726
C	-1.867004	-5.096246	4.084434
C	-2.177657	-6.423031	4.373261
C	-2.401549	-7.330391	3.336987
C	-2.312011	-6.895019	2.010728
C	-2.001786	-5.570484	1.722831
C	-0.140465	2.280924	1.964350
C	-0.269983	2.597783	3.274292
C	0.020540	3.886123	3.897488
C	-0.153514	4.019678	5.288846
C	0.109941	5.223391	5.937952
C	0.553940	6.327182	5.208373
C	0.730389	6.213917	3.825103
C	0.468202	5.012475	3.176502
C	0.495619	2.854381	-3.867754
C	0.624174	3.426691	-5.088068
C	1.024243	4.801973	-5.372910
C	1.337921	5.741122	-4.368658
C	1.715306	7.037465	-4.700053
C	1.790677	7.434492	-6.039481
C	1.482781	6.518873	-7.046773
C	1.104393	5.220086	-6.715561
C	-0.654509	-2.049962	-4.444559
C	-0.608024	-2.401805	-5.749989
C	-0.855367	-3.723879	-6.323270
C	-1.167749	-4.862576	-5.552778
C	-1.394617	-6.094294	-6.156941
C	-1.316031	-6.227664	-7.547092
C	-1.006752	-5.112384	-8.326700

C	-0.779550	-3.878760	-7.721102
H	-0.795570	-0.335820	3.167393
H	0.154350	0.536773	-5.665713
H	-1.376903	-3.206793	0.414779
H	-1.318738	-2.639115	3.423162
H	-1.693442	-4.394412	4.897013
H	-2.245034	-6.748030	5.408065
H	-2.487182	-7.594021	1.197096
H	-1.942355	-5.255287	0.685261
H	0.211046	3.017894	1.251736
H	-0.630222	1.833107	3.961455
H	-0.500031	3.162498	5.861840
H	-0.031894	5.299737	7.012690
H	1.073684	7.069681	3.249891
H	0.607944	4.946695	2.101926
H	0.691900	3.425175	-2.967640
H	0.408774	2.825079	-5.970417
H	1.284191	5.453649	-3.323203
H	1.952320	7.745148	-3.910078
H	1.536924	6.815950	-8.090716
H	0.865153	4.510396	-7.504385
H	-0.903348	-2.808020	-3.705068
H	-0.364428	-1.630313	-6.479490
H	-1.232340	-4.784608	-4.471461
H	-1.633661	-6.957721	-5.541600
H	-0.942084	-5.202453	-9.407757
H	-0.539192	-3.013510	-8.334708
C	-0.777517	-1.124702	-1.419285
F	0.814241	2.599073	-0.879127
F	-1.459871	2.579025	-1.129100
H	-2.644756	-8.366077	3.557428
H	-1.493790	-7.191990	-8.014927
H	0.759995	7.268628	5.710181
H	2.086088	8.448954	-6.292831
H	-1.023623	-2.172355	-1.549493

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