

Supporting Information

Effect of the Molecular Conformation on Excitation Energy Transfer in Conformationally Constrained Boryl-BODIPY Dyads

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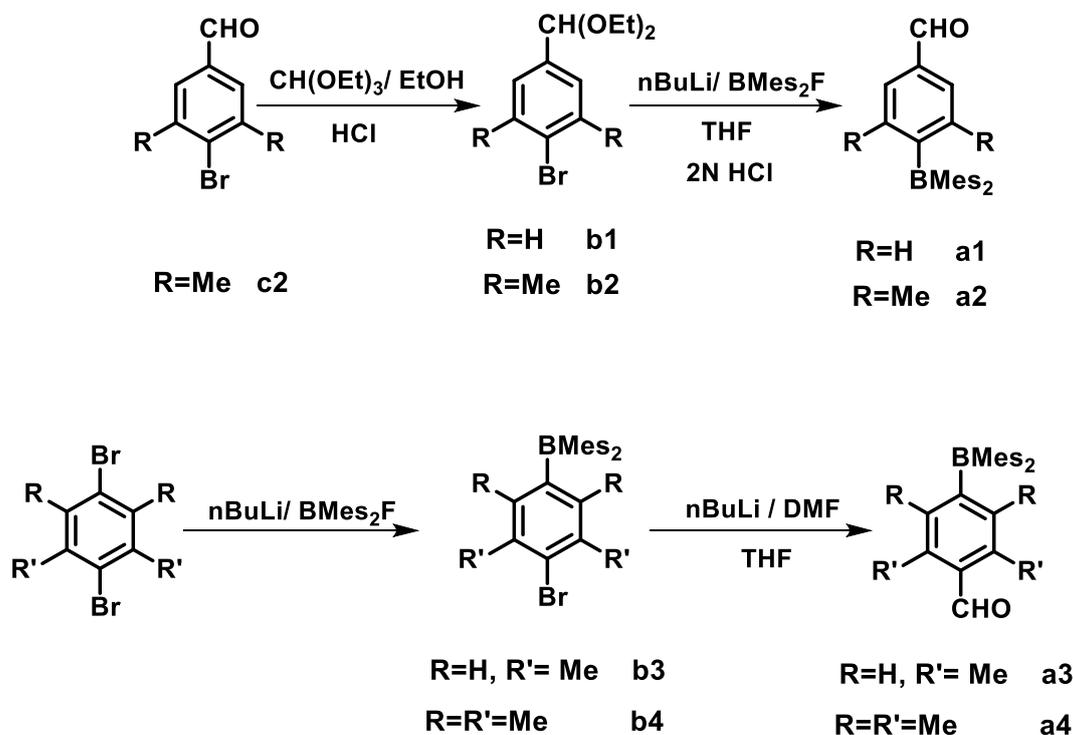
EXPERIMENTAL SECTION

Materials and methods

4-Bromobenzaldehyde, 2,5-dibromo-1,3-dimethylbenzene, 2,5-dibromo-1,3-dimethylbenzene, 1,4-dibromo-2,3,5,6-tetramethylbenzene, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), *n*-Butyllithium (1.6 M in hexane), triethylorthoformate, BF₃·Et₂O pyrrole and 2-methylpyrrole were purchased from commercial sources (Aldrich, USA; SRL, India; Spectrochem, India and Avra Syn. Pvt. Ltd., India). Mes₂BF was synthesized by following a reported procedure.¹ Model compounds **M1-M4** were also prepared according to the reported procedure in literature.²⁻⁶ Synthesis and characterization of model compounds **M5-M7** are described in supporting information. Synthesis and basic optical studies of **R1** and **R2** are described in our previous report.² All reactions were carried out under an atmosphere of purified nitrogen using Schleck techniques. THF, pyrrole, 2-methylpyrrole, triethylamine and diethylether were distilled over sodium. Chlorinated solvents were distilled over CaH₂ and subsequently stored over 3Å molecular sieves. The 400 MHz ¹H NMR, 376.5 MHz ¹⁹F NMR, 100 MHz ¹³C NMR were recorded on a Bruker Avance 400 MHz NMR spectrometer and 160.4 MHz ¹¹B NMR were recorded on a Bruker Avance 500 MHz NMR spectrometer. All solution state ¹H and ¹³C NMR spectra were referenced internally to the solvent signal. ¹¹B and ¹⁹F NMR spectra were referenced externally to BF₃.Et₂O in C₆D₆ and external standard fluorine signal of CFC₃, respectively. High resolution mass spectra (HRMS) were recorded on an Agilent Q-TOF LCMS by electrospray ionization (ESI) method. UV-visible absorption spectra were recorded on a Perkin Elmer LAMBDA 750 UV/visible spectrophotometer. A Horiba JOBIN YVON Fluoromax-4 spectrometer was used for steady state fluorescence measurements and time resolved fluorescence decay measurements were carried out using nanosecond diode laser-based time correlated single photon counting (TCSPC) techniques from IBH, UK. Quantum yields were calculated in reference method using Quinine Sulphate (0.1 M H₂SO₄, λ_{ex} = 350 nm, Φ_R = 57.7%) solution as reference and using the following formula (Φ = Φ_R × (I/I_R) × (A_R/A) × (η²/η_R²). Where Φ = Quantum Yield, I = Intensity of emission, A = absorbance at λ_{ex}, η = Refractive Index of Solvent. The radiative and non-radiative rates calculated with respect to the lifetime/average lifetime obtained at 510 nm emission band. Cyclic voltammetric measurements were performed using a three electrode CV cell with a Metrohm Autolab instrument. A Pt disk electrode was used as working electrode, a Pt wire was used as counter electrode and a Ag wire was used as reference electrode. Cyclic voltammograms were recorded in dichloromethane solution (for oxidation) and in THF (for reduction) at a voltage sweep rate of 100 mV/s, with [Bu₄N][PF₆] (0.1 M) as supporting electrolyte at 20 °C. The potential scale was referenced to the ferrocene/ferrocenium couple. Single-crystal X-ray diffraction studies were carried out with a Bruker SMART APEX diffractometer equipped with 3-axis goniometer. The data was integrated using SAINT,⁷ and an empirical absorption correction was applied with SADABS.⁸ The structures were solved by direct methods and refined by full matrix least-squares on F² using SHELXTL software.⁹ All the non-hydrogen atoms were refined with anisotropic displacement parameters, while the hydrogen atoms were refined isotropically on the positions calculated using a riding model.¹⁰ WinGX v2014.1. SQUEEZE/PLATON program was used to remove the solvents (/disordered solvent) (pentane for **1**; chloroform for **2** and **6**) by taking the corresponding scattering contribution into account.¹¹ For compound **6** overall data quality was not good because of poor quality crystal having disordered solvent molecules in crystal lattice. Density functional theory (DFT/TD-DFT) calculations were done using B3LYP functional with 6-31G(d) basis set as incorporated in Gaussian 09 package for all the atoms.¹² Frequency tests were performed

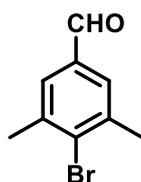
upon the ground state optimization to confirm the attainment of stationary points. TD-DFT calculations were performed on the ground state optimized structures to find the vertical transition energies. Gaussview 5.0.8. was used to analyze the findings of theoretical calculation.¹³

Synthesis



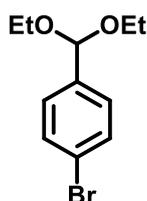
Scheme S1. Synthesis procedure for precursors **a1-a4**.

Synthesis of **4-bromo-3,5-dimethylbenzaldehyde (c2)**¹⁴



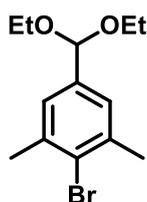
To a solution of 2,5-dibromo-1,3-dimethylbenzene (1.0 g, 3.22 mmol) in dry THF (20 mL), a hexane solution of *n*-BuLi (1.6 M, 2.4 mL, 3.75 mmol) was added dropwise at -78°C . After 30 min, stirring at -78°C , DMF (0.4 mL, 3.83 mmol) was added to the reaction mixture. The reaction mixture was allowed to warm to room temperature, followed by stirring for 12 h. After the addition of water, the product extracted with EtOAc. The combined extract was washed with 1N HCl and brine, dried over anhydrous MgSO_4 . Removal of all the volatiles under reduced pressure gave the crude product. The crude product purified through the silica gel column chromatography afforded **c2** (0.62g, 76% yield) as a colourless solid. ^1H NMR (400 MHz, CDCl_3 , δ ppm): 9.29 (s, 1H), 7.56 (s, 2H), 2.49 (s, 6H).

Synthesis of **1-bromo-4-(diethoxymethyl)benzene (b1)**²



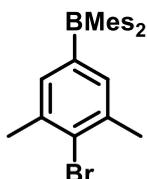
4-Bromobenzaldehyde (9.5 g, 51.41 mmol), triethylorthoformate (18.8ml, 113.24 mmol) and catalytic amount of conc. HCl was dissolved in ethanol, and the resultant solution was refluxed for 4 h. After all the 4-Bromobenzaldehyde consumed, the reaction temperature was brought to room temperature and extracted with a mixture of cold water/ethyl acetate. The combined organic layer was washed with brine and dried over anhydrous sodium sulfate. The volatiles were removed under reduced pressure afforded **b1** (13.98 g, 98% yield) as a colorless liquid. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.49 (d, *J* = 6.8 Hz, 2H), 7.35 (d, *J* = 8 Hz, 2H), 5.46 (s, 1H), 3.63-3.49 (m, 4H), 1.24 (t, *J* = 7.2 Hz, 6H).

Synthesis of **2-bromo-5-(diethoxymethyl)-1,3-dimethylbenzene (b2)**



Compound **b2** prepared following a procedure similar to that used for compound **b1**. The quantities involved and characterization data are as follows. 4-bromo-3,5-dimethylbenzaldehyde (2g 9.47 mmol), CH(OEt)₃ (4.7 mL, 32.2 mmol), HCl (one drop), EtOH (solvent). Yield: 2.65g (96%). ¹H NMR (400 MHz, CDCl₃, δ ppm) 7.02 (s, 2H), 5.41 (s, 1H), 3.65-3.40 (m, 4H), 2.32 (s, 6H), 1.23 (t, *J* = 7.0 Hz, 6H).

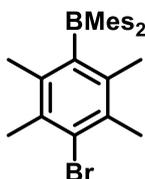
Synthesis of **(4-bromo-3,5-dimethylphenyl)dimesitylborane (b3)**



To a solution of 2,5-dibromo-1,3-dimethylbenzene (1.0 g, 3.22 mmol) in dry THF (20 mL); hexane solution of *n*-BuLi (1.6 M, 2.4 mL, 3.87 mmol) was added dropwise at -78°C. The reaction mixture was stirred for 30 min at -78°C. After that, Dimesitylfluoroborane (1.0 g, 3.87 mmol) at -78°C was added to it. The reaction mixture was allowed to warm to room temperature, followed by stirring for 12 h. After the addition of water, the mixture was extracted with EtOAc. The extract was washed with 1N HCl and brine, dried over anhydrous MgSO₄, and concentrated under reduced pressure. The resulting mixture was recrystallized from hexane to give **b3** (1.25 g, 75% yield) as white crystals. Mp: 120–122 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.19 (s, 2H), 6.82 (s, 4H),

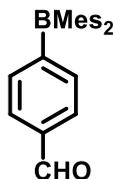
2.37 (s, 6H), 2.31 (s, 6H), 1.99 (s, 12H). ^{13}C NMR (100 MHz, CDCl_3 , δ ppm): 144.7, 141.2, 139.1, 138.3, 136.1, 133.1, 128.6, 24.2, 23.9, 21.7. ^{11}B NMR (160 MHz, CDCl_3 , δ ppm): 69. HRMS-QTOF ($\text{C}_{26}\text{H}_{30}\text{BBr}$): m/z calcd. for $[\text{M}]^+$ is 432.1624; found 432.1628.

Synthesis of **1-bromo-4-(dimesitylboryl)-2,3,5,6-tetramethylbenzene (b4)**¹⁵



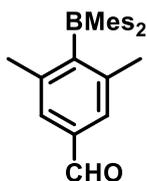
Compound **b4** was prepared following a procedure similar to that used for compound **b3**. The quantities involved and characterization data are as follows. 1,4-dibromodurene (5.0 g, 17.18 mmol), *n*-BuLi (1.6 M, 11.7 mL, 18.83 mmol), Dimesitylfluoroborane (4.8 g, 18.83 mmol). Yield: 8.08 g (44%). ^1H NMR (400 MHz, CDCl_3 , δ ppm): 6.74 (s, 4H), 2.34 (s, 6H), 2.26 (s, 6H), 2.05 (s, 6H), 1.95 (s, 12H). ^{13}C NMR (100 MHz, CDCl_3 , δ ppm): 141.3, 141.0, 137.0, 133.9, 130.8, 129.3, 129.2, 23.7, 23.2, 21.7, 20.1. ^{11}B NMR (160 MHz, CDCl_3 , δ ppm): 70. HRMS-QTOF ($\text{C}_{28}\text{H}_{34}\text{BBr}$): m/z calcd for $[\text{M}]^+$ is 460.1937; found 460.1927.

Synthesis of **4-dimesitylborylbenzaldehyde (a1)**²



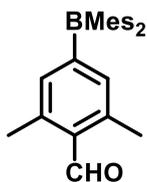
A solution of **b1** (2.5 g, 9.64 mmol) in dry THF was degassed by purging N_2 for 30 minutes, followed by cooling to -78°C . *n*-Butyllithium (6.6 mL of 1.6 M solution in hexane), 10.61 mmol) was added over 30 min. After one hour, a solution of dimesitylfluoroborane (2.9 g, 10.08 mmol) in 15 mL of dry THF was added over 10 min. The reaction mixture was allowed to warm to room temperature and stirring was continued for 12 h. After 12 h, 30 mL of 1N HCl was added, and stirring was continued for another 4 h and extracted with ether. The combined organic layers were washed with brine solution and dried over anhydrous Na_2SO_4 . Evaporation of the solvents under reduced pressure yielded crude product. Recrystallization of crude product in ethyl acetate gave pure **a1** (2.05 g, 59% yield) as a colourless solid. Mp: 115–117 $^\circ\text{C}$. ^1H NMR (399.99 MHz, CDCl_3 δ ppm) 10.07 (s, 1H), 7.85 (d, $J = 8$ Hz, 2H), 7.66 (d, $J = 8$ Hz, 2H), 6.83 (s, 4H), 2.32 (s, 6H), 1.98 (s, 12H). ^{13}C NMR (100.00 MHz, CDCl_3 , δ ppm) 193.3, 152.8, 141.3, 140.8, 139.9, 138.4, 136.4, 129.5, 128.9, 23.9, 21.8. ^{11}B NMR (160 MHz, CDCl_3 , δ ppm) 76.72. HRMS-QTOF ($\text{C}_{25}\text{H}_{27}\text{BO}$): m/z calcd for $[\text{M}]^+$ is 354.2155; found 354.2147.

Synthesis of **4-(dimesitylboryl)-3,5-dimethylbenzaldehyde (a2)**



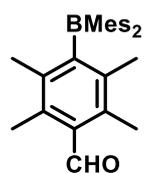
Compound **a2** was prepared following a procedure similar to that used for compound **a1**. The quantities involved and characterization data are as follows. **b2** (2.0g, 6.99 mmol), *n*-BuLi (1.6 M, 4.8 mL, 7.69 mmol), Dimesitylfluoroborane (2.0 g, 7.69 mmol). Yield: 1.4 g (80%). Mp: 134–136 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 9.93 (s, 1H), 7.42 (s, 2H), 6.77 (m, 4H), 2.28 (s, 12H), 2.11 (s, 6H), 1.95 (s, 6H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 193.4, 141.4, 141.3, 140.9, 140.4, 136.8, 129.3, 128.8, 128.0, 23.5, 23.1, 21.7. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 72.78. HRMS (positive ion mode): calcd. for C₂₇H₃₁BO [M]⁺ is 382.2468; found 382.2470.

Synthesis of 4-(dimesitylboryl)-2,6-dimethylbenzaldehyde (**a3**)



To a solution of **b3** (2.0 g, 4.62 mmol) in dry THF (100 mL), a hexane solution of *n*-BuLi (1.6 M, 3.2 mL, 5.07 mmol) was added dropwise at -78°C. The reaction mixture was stirred for 30 min at -78°C, and DMF (0.6 mL, 6.93 mmol) was added to the mixture. The reaction mixture was allowed to warm to room temperature, followed by stirring for 6 h. After the addition of water, the mixture was extracted with Et₂O. The extract was washed with 1 N HCl and brine, dried over anhydrous MgSO₄, and concentrated under reduced pressure. The resulting mixture was recrystallized from hexane and ethyl acetate to give **a3** (1.42g, 80% yield) as a colourless powder. Mp: 117–119 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm) 10.67 (s, 1H), 7.21 (s, 2H), 6.83 (s, 4H), 2.55 (s, 6H), 2.33 (s, 6H), 1.99 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm) 194.6, 141.2, 141.2, 140.4, 139.6, 136.8, 134.8, 128.7, 128.5, 23.9, 21.7, 20.8. ¹¹B NMR (160 MHz, CDCl₃, δ ppm) 76.92. HRMS (positive ion mode): calcd. for C₂₇H₃₁BO [M]⁺ is 382.2468; found 382.2471.

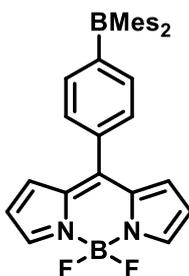
Synthesis of 4-(dimesitylboryl)-2,3,5,6-tetramethylbenzaldehyde (**a4**)¹⁶



Compound **a4** was prepared following a procedure similar to that used for compound **a3**. The quantities involved and characterization data are as follows. **b4** (1.0 g, 2.16 mmol), *n*-BuLi

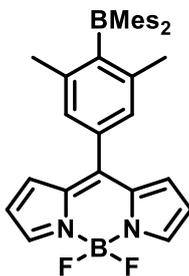
(1.6 M, 1.5 mL, 2.38 mmol), DMF (0.3 mL, 3.24 mmol), Yield: 0.75 g (84%). Mp: 117–119 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 10.67 (s, 1H), 6.75 (s, 4H), 2.31 (s, 6H), 2.27 (s, 6H), 2.03 (s, 6H), 1.97 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 197.6, 141.5, 141.1, 136.5, 135.7, 134.5, 129.4, 23.7, 23.2, 21.6, 20.4. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 74.60. HRMS (positive ion mode): calcd. for C₂₉H₃₅BO [M]⁺ is 410.2781; found 410.2771.

Synthesis of 1



Pyrrole (4.0 mL, 56.46 mmol) and *p*-dimesitylborylbenzaldehyde (**a1**) (0.50 g, 1.41 mmol) were stirred at room temperature under nitrogen atmosphere for 30 min then BF₃·Et₂O (one drop) was added. The resultant mixture was stirred for another 6 h at room temperature followed by the addition of DDQ (0.34 mg, 1.02 mmol) and stirring for 6 h at room temperature. The resultant product was treated with triethylamine (1.4 mL, 9.34 mmol) and then BF₃·Et₂O (1.6 mL, 9.34 mmol) was added. The reaction mixture was stirred for additional 5 h at RT and the solvent was removed in vacuo to give crude product which was further purified by alumina column chromatography (hexane:ethylacetate 98:2) to give compound **1** (0.30 g, 62 %) as a red colour solid. Mp: 118–120 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.95 (s, 2H), 7.67 (d, *J* = 8 Hz, 2H), 7.55 (d, *J* = 8 Hz, 2H), 6.95 (d, *J* = 4 Hz, 2H), 6.87 (s, 4H), 6.57–6.59 (m, 2H), 2.34 (s, 6H), 2.05 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 147.6, 144.7, 141.8, 141.2, 139.7, 137.0, 136.2, 135.2, 131.9, 130.5, 128.8, 119.1, 23.96, 21.71. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 1.27 (t, *J* = 36 Hz) and 66.2 (br). ¹⁹F NMR (376 MHz, CDCl₃, δ ppm): -146.3 (m). HRMS (ESI/Q-TOF) *m/z*: [M+Na]⁺ Calcd for C₃₃H₃₂B₂F₂N₂Na 539.2617; Found 539.2612.

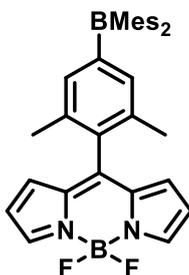
Synthesis of 2



Compound **2** was prepared following a procedure similar to that used for compound **1**. The quantities involved and characterization data are as follows. **a2** (500 mg, 1.31 mmol), pyrrole (3.5 mL, 52.32 mmol), BF₃·Et₂O (0.8 mL, 6.02), DDQ (150 mg, 0.66 mmol), Et₃N (0.8 mL, 6.02 mmol). Yield: 0.2 g (35%). Mp: 136–138 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.93 (s, 2H), 7.13 (s, 2H), 7.00 (d, *J* = 4.4 Hz, 2H), 6.80 (s, 4H), 6.65 (d, *J* = 4.4 Hz, 2H), 2.30 (s, 6H), 2.12 (s, 6H), 2.02–2.05 (m, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 151.3, 148.5, 144.2, 143.5, 141.4, 140.9, 140.3, 135.3, 134.7, 131.9, 130.0, 129.3, 118.7, 23.4, 23.3, 21.7. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 1.02 (t, *J* = 36 Hz) and 68.43 (br). ¹⁹F NMR (376 MHz,

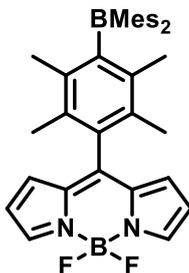
CDCl₃, δ ppm): -145.1 (m). HRMS (ESI/Q-TOF) m/z : [M+Na]⁺ Calcd for C₃₅H₃₆B₂F₂N₂Na 567.2930; Found 567.2935.

Synthesis of 3



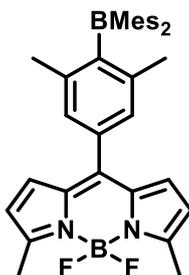
Compound **3** was prepared following a procedure similar to that used for compound **1**. The quantities involved and characterization data are as follows. **a3** (500 mg, 1.31 mmol), pyrrole (3.5 mL, 52.32 mmol), BF₃·Et₂O (0.8 mL, 6.02), DDQ (150 mg, 0.66 mmol), Et₃N (0.8 mL, 6.02 mmol). Yield: 0.3 g (45%). Mp: 120–122 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.94 (s, 2H), 7.27 (s, 2H), 6.85 (s, 4H), 6.65 (d, J = 4.4 Hz, 2H), 6.50 (d, J = 4.4 Hz, 2H), 2.33 (s, 6H), 2.11 (s, 6H), 2.05 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 147.7, 144.9, 141.2, 139.4, 137.4, 136.4, 136.2, 135.2, 134.9, 132.4, 130.3, 128.7, 127.1, 119.7, 23.8, 21.6, 20.3. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 0.85 (t, J = 36 Hz) and 66.56 (br). ¹⁹F NMR (376 MHz, CDCl₃, δ ppm): -148.1 (m). HRMS (ESI/Q-TOF) m/z : [M+Na]⁺ Calcd for C₃₅H₃₆B₂F₂N₂Na 567.2930; Found 567.2934.

Synthesis of 4



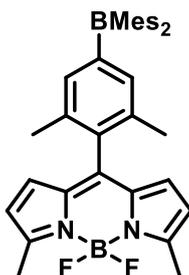
Compound **4** was prepared following a procedure similar to that used for compound **1**. The quantities involved and characterization data are as follows. Pyrrole (3.7 mL, 51.42 mmol), **a4** (0.50 g, 1.21 mmol), DDQ (0.09 g, 0.41 mmol), triethylamine (0.5 mL, 3.80 mmol), BF₃·Et₂O (0.5 mL, 3.80 mmol). Yield: 0.12 g (58%). Mp: 140–143 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.93 (s, 2H), 6.79 (s, 4H), 6.65 (d, J = 4 Hz 2H), 6.47–6.49 (m, 2H), 2.23 (s, 6H), 2.04 (s, 12H), 2.02 (s, 6H), 1.95 (s, 6H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 150.1, 144.5, 141.5, 140.9, 140.0, 136.0, 133.5, 132.1, 130.6, 129.4, 118.9, 23.7, 23.2, 21.7, 20.2, 18.1. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 0.57 (t, J = 36 Hz) and 65.30 (br). ¹⁹F NMR (376 MHz, CDCl₃, δ ppm): -145.1 (m). HRMS (ESI/Q-TOF) m/z : [M-BF₂+2H]⁺ Calcd for C₃₇H₄₁BN₂H 525.3441; Found 525.3442.

Synthesis of 5

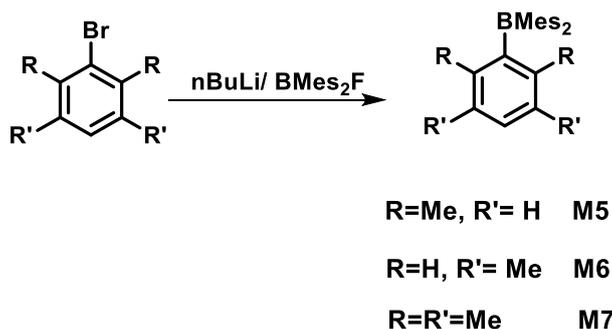


Compound **5** was prepared following a procedure similar to that used for compound **1**. The quantities involved and characterization data are as follows. **a2** (200 mg, 0.40 mmol), 2-methyl pyrrole (88 mg, 1.04 mmol), DDQ (100 mg, 0.44 mmol), Et₃N (0.6 mL, 4.01 mmol), BF₃·Et₂O (0.6 mL, 4.01 mmol). Yield: 59 mg (19%). Mp: 140–143 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.13 (s, 2H), 6.82 (s, 4H), 6.56 (d, *J* = 4.4 Hz, 2H), 6.28 (d, *J* = 4.4 Hz, 2H), 2.67 (s, 6H), 2.48 (s, 6H), 2.15 (s, 6H), 2.04 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 157.7, 141.3, 140.2, 138.2, 135.1, 134.9, 134.5, 132.0, 130.8, 129.9, 129.3, 128.6, 127.3, 119.5, 23.4, 23.2, 21.7, 15.3. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 1.06 (t, *J* = 36 Hz) and 69.16 (br). ¹⁹F NMR (376 MHz, CDCl₃, δ ppm): -147.9 (m). HRMS (ESI/Q-TOF) *m/z*: [M+Na]⁺ Calcd for C₃₇H₄₀B₂F₂N₂Na 595.3243; Found 595.3243.

Synthesis of 6

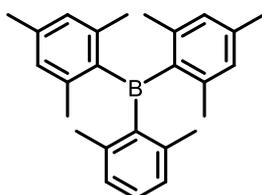


Compound **6** was prepared following a procedure similar to that used for compound **1**. The quantities involved and characterization data are as follows. **a3** (200 mg, 0.40 mmol), 2-methyl pyrrole (88 mg, 1.04 mmol), DDQ (100 mg, 0.44 mmol), Et₃N (0.6 mL, 4.01 mmol), BF₃·Et₂O (0.6 mL, 4.01 mmol). Yield: 0.1 g (20%). Mp: 126–129 °C. ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.24 (s, 2H), 6.84 (s, 4H), 6.43 (d, *J* = 4.4 Hz, 2H), 6.22 (d, *J* = 4.4 Hz, 2H), 2.65 (s, 6H), 2.32 (s, 6H), 2.09 (s, 6H), 2.03 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 158.2, 148.2, 142.3, 142.1, 141.2, 139.2, 136.7, 134.9, 134.4, 129.1, 128.7, 128.5, 119.9, 23.8, 21.7, 20.3, 15.4. ¹¹B NMR (160 MHz, CDCl₃, δ ppm): 0.81 (t, *J* = 36 Hz) and 66.33 (br). ¹⁹F NMR (376 MHz, CDCl₃, δ ppm): -146.2 (m). HRMS (ESI/Q-TOF) *m/z*: [M+Na]⁺ Calcd for C₃₇H₄₀B₂F₂N₂Na 595.3243; Found 595.3232.



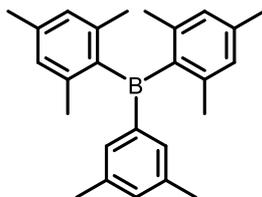
Scheme S2. Synthesis procedure for model compounds **M5-M7**.

Synthesis of **(2,6-dimethylphenyl)dimesitylborane (M5)**



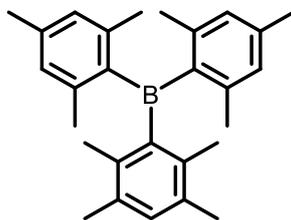
Compound **M5** was prepared following a procedure similar to that used for compound **b3**. The quantities involved and characterization data are as follows. 2-bromo-1,3-dimethylbenzene (1.0 g, 5.40 mmol), *n*-BuLi (1.6 M, 3.7 mL, 5.94 mmol), Mes₂BF (1.60 g, 5.94 mmol), Yield: 0.90 g (47%). ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.14 (d, *J* = 8 Hz, 1H), 6.92 (d, *J* = 8 Hz, 2H), 6.76 (s, 4H), 2.29 (s, 6H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 141.1, 141.0, 140.7, 139.7, 129.6, 129.1, 128.0, 23.3, 23.2, 21.7.

Synthesis of (3,5-dimethylphenyl)dimesitylborane (**M6**)



Compound **M6** was prepared following a procedure similar to that used for compound **b3**. The quantities involved and characterization data are as follows. 1-bromo-3,5-dimethylbenzene (1.0 g, 5.40 mmol), *n*-BuLi (1.6 M, 3.7 mL, 5.94 mmol), Mes₂BF (1.60 g, 5.94 mmol), Yield: 1.20 g (63%). ¹H NMR (400 MHz, CDCl₃, δ ppm): 7.20 (d, *J* = 14.2 Hz, 3H), 6.89 (s, 4H), 2.38 (s, 6H), 2.34 (s, 6H), 2.08 (s, 12H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 141.3, 138.9, 137.6, 134.5, 134.3, 128.6, 23.9, 21.8, 21.7.

Synthesis of dimesityl(2,3,5,6-tetramethylphenyl)borane (**M7**)



Compound **M7** was prepared following a procedure similar to that used for compound **b3**. The quantities involved and characterization data are as follows. 3-bromo-1,2,4,5-tetramethylbenzene (1.0 g, 4.69 mmol), *n*-BuLi (1.6 M, 3.2 mL, 5.16 mmol), Mes₂BF (1.38 g, 5.16 mmol), Yield: 0.74 g (42%). ¹H NMR (400 MHz, CDCl₃, δ ppm): 6.94 (s, 1H), 6.75 (s, 1H), 2.28 (s, 6H), 2.16 (s, 6H), 1.97 (s, 18H). ¹³C NMR (100 MHz, CDCl₃, δ ppm): 141.1, 139.5, 136.0, 133.5, 132.8, 129.2, 129.0, 128.8, 23.6, 23.1, 21.7, 20.5, 19.6.

CHARACTERIZATION DATA

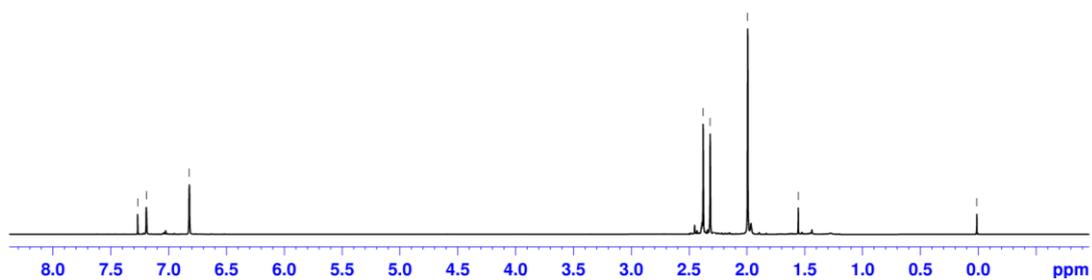


Figure S1. ^1H NMR of **b3** in CDCl_3

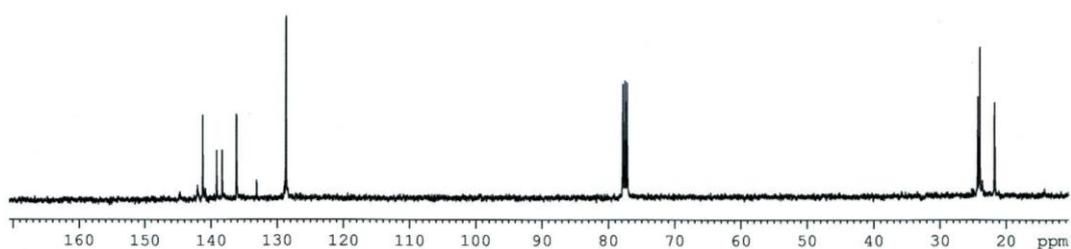


Figure S2. ^{13}C NMR of **b3** in CDCl_3

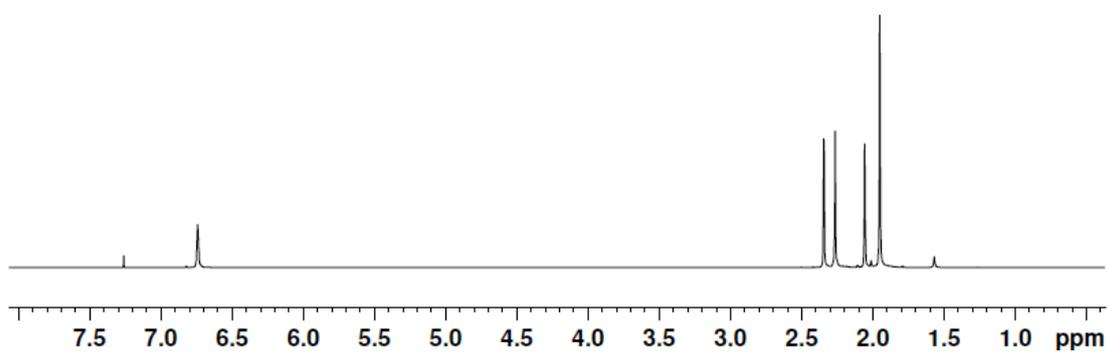


Figure S3. ^1H NMR of **b4** in CDCl_3

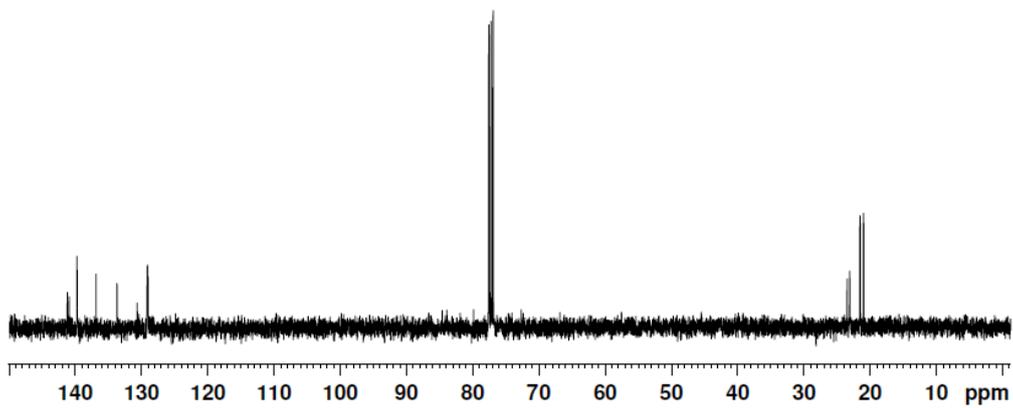


Figure S4. ^{13}C NMR of **b4** in CDCl_3

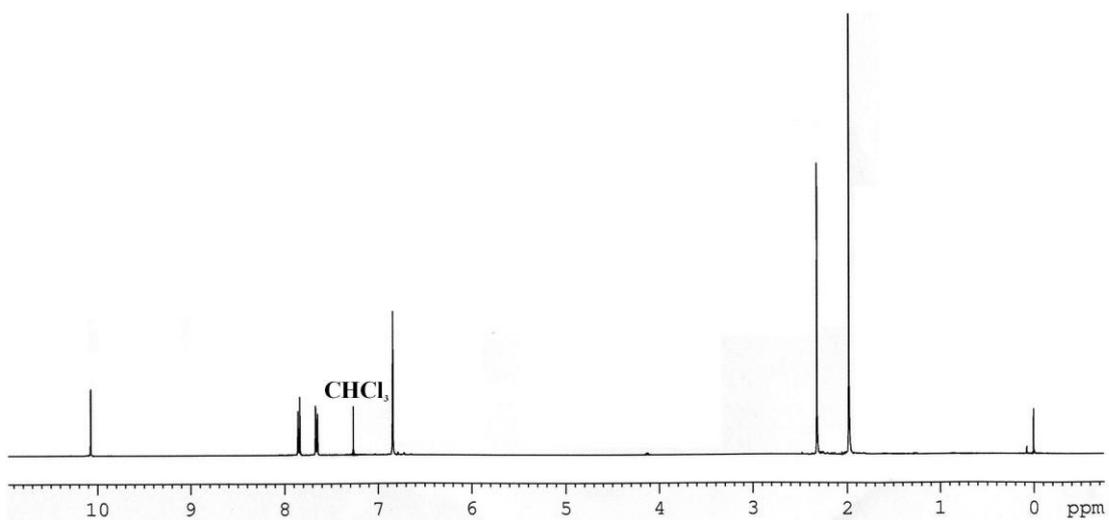


Figure S5. ^1H NMR of **a1** in CDCl_3

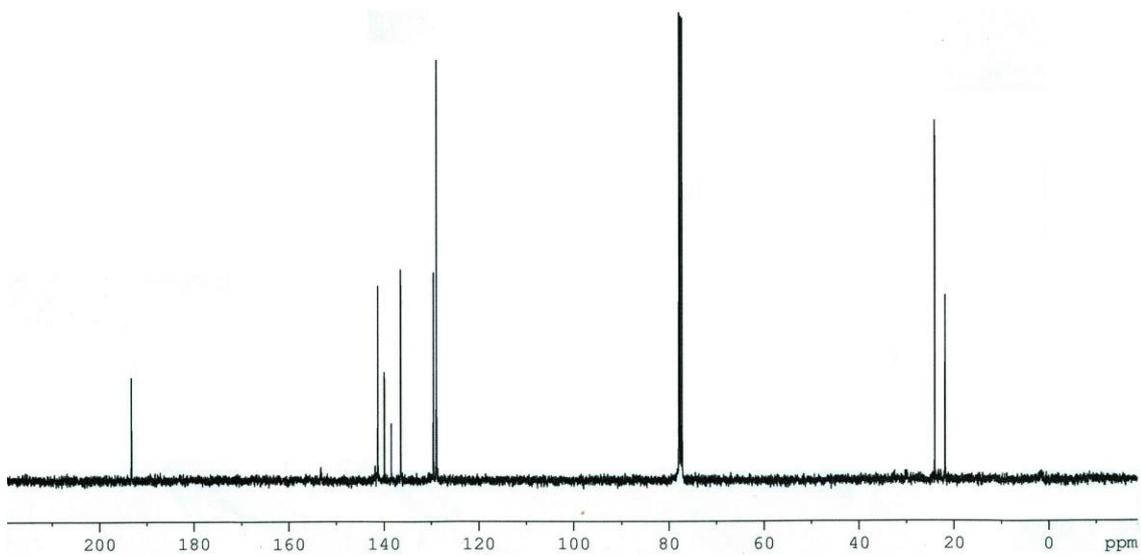


Figure S6. ^{13}C NMR of **a1** in CDCl_3

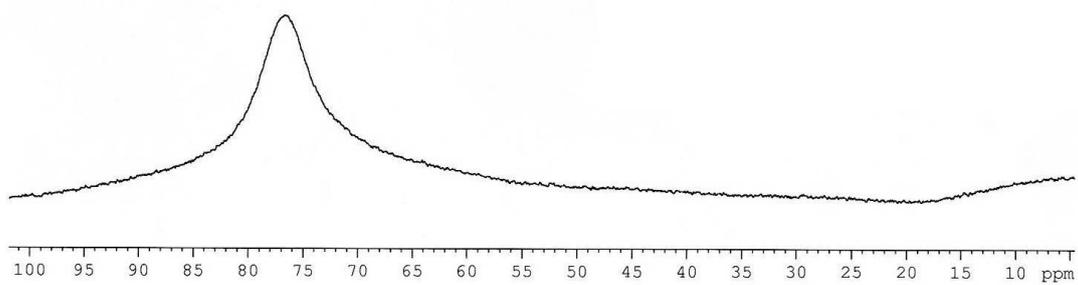


Figure S7. ^{11}B NMR of **a1** in CDCl_3

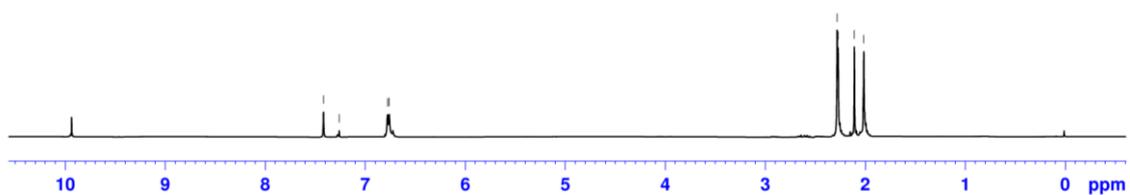


Figure S8. ^1H NMR of **a2** in CDCl_3

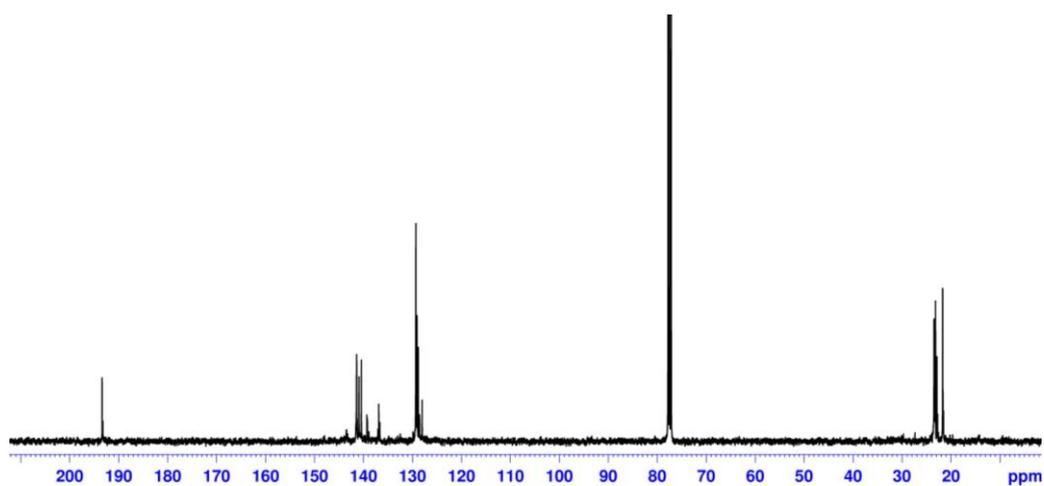


Figure S9. ^{13}C NMR of **a2** in CDCl_3

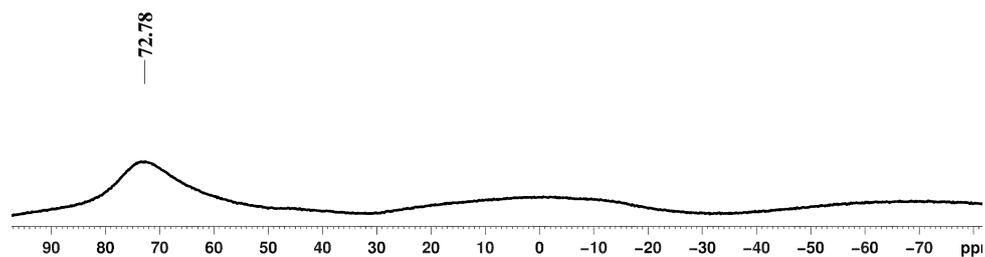


Figure S10. ^{11}B NMR of **a2** in CDCl_3

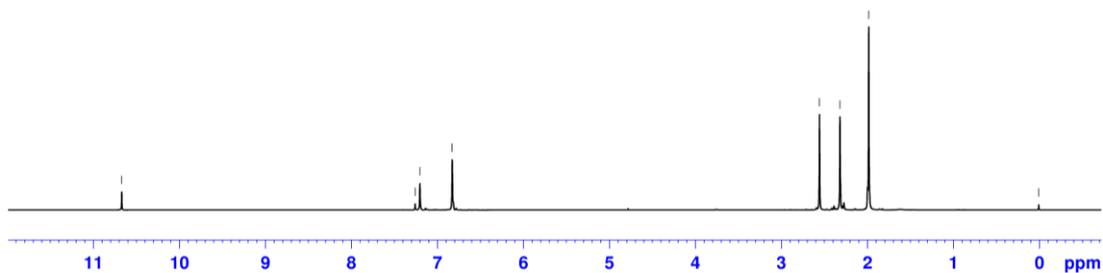


Figure S11. ^1H NMR of **a3** in CDCl_3

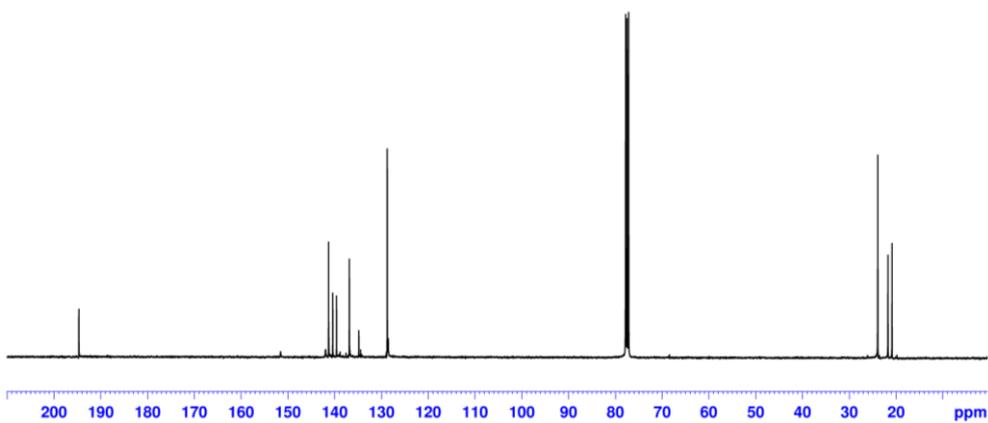


Figure S12. ^{13}C NMR of **a3** in CDCl_3

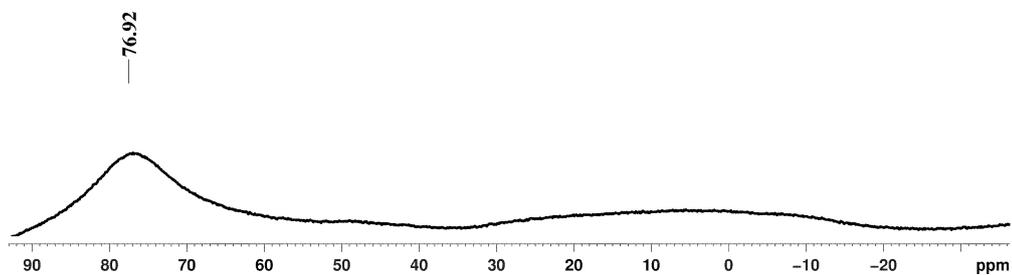


Figure S13. ^{11}B NMR of **a3** in CDCl_3

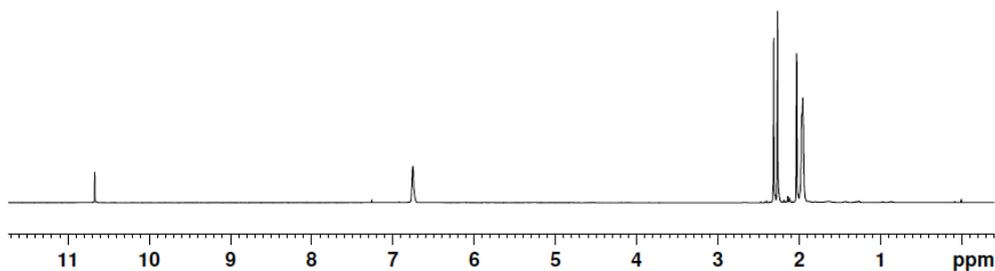


Figure S14. ^1H NMR of **a4** in CDCl_3

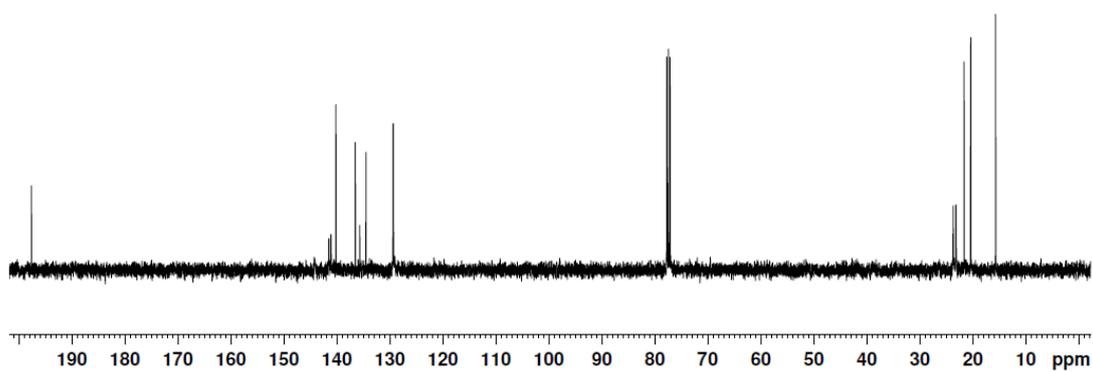


Figure S15. ^{13}C NMR of **a4** in CDCl_3

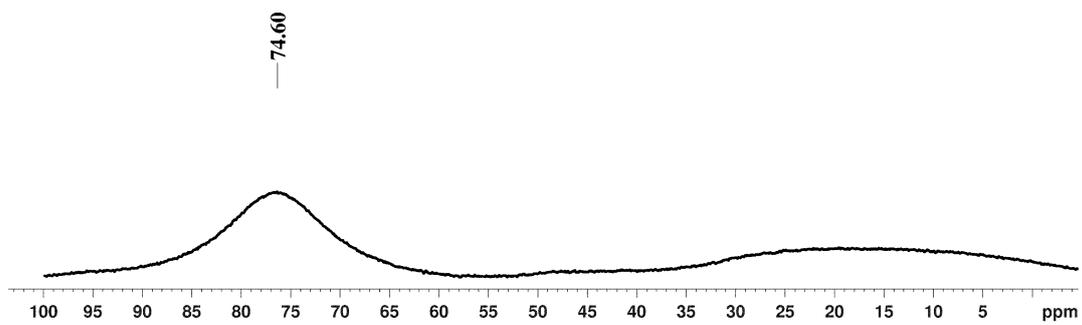


Figure S16. ^{11}B NMR of **a4** in CDCl_3

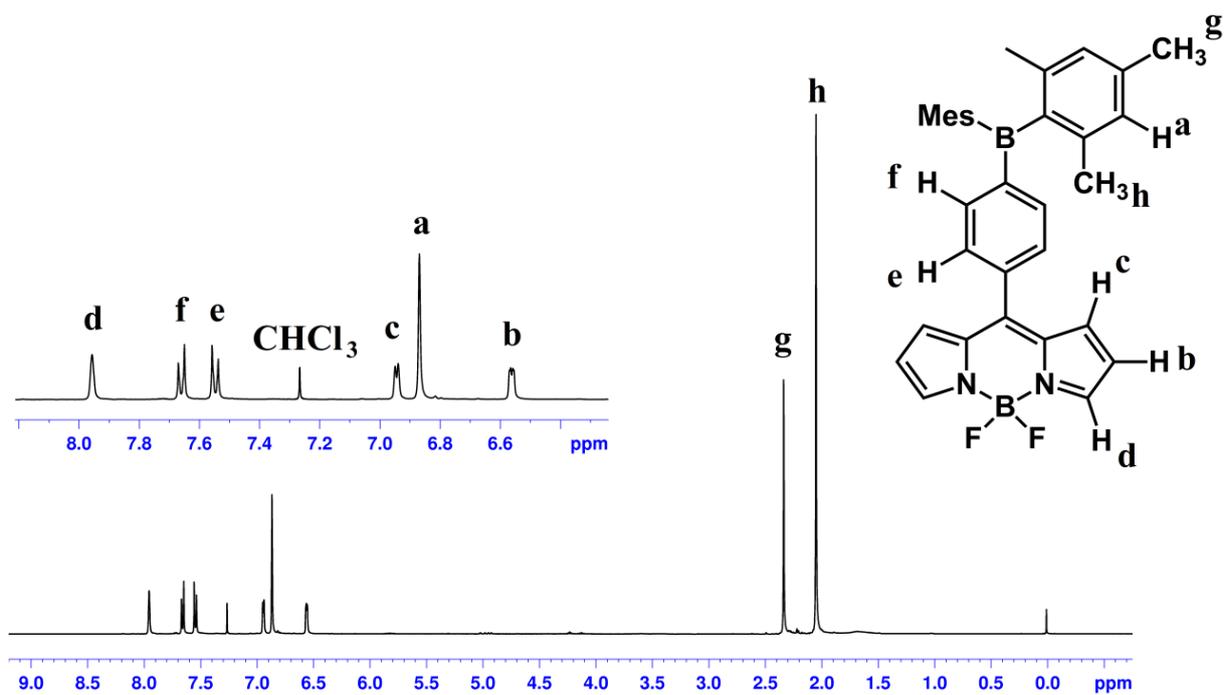


Figure S17. ^1H NMR of **1** in CDCl_3

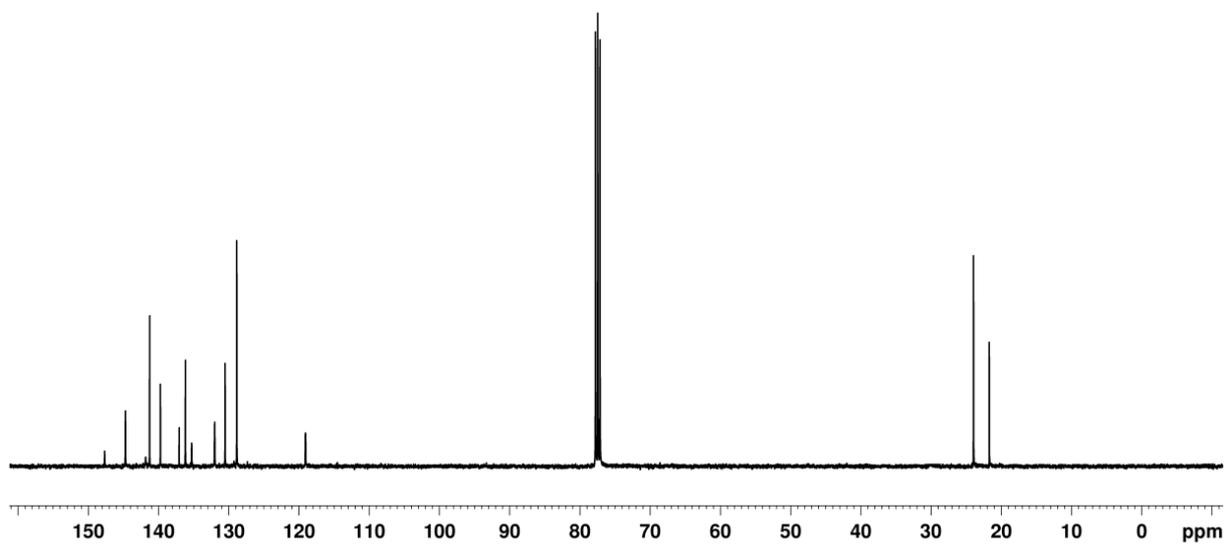


Figure S18. ^{13}C NMR of **1** in CDCl_3

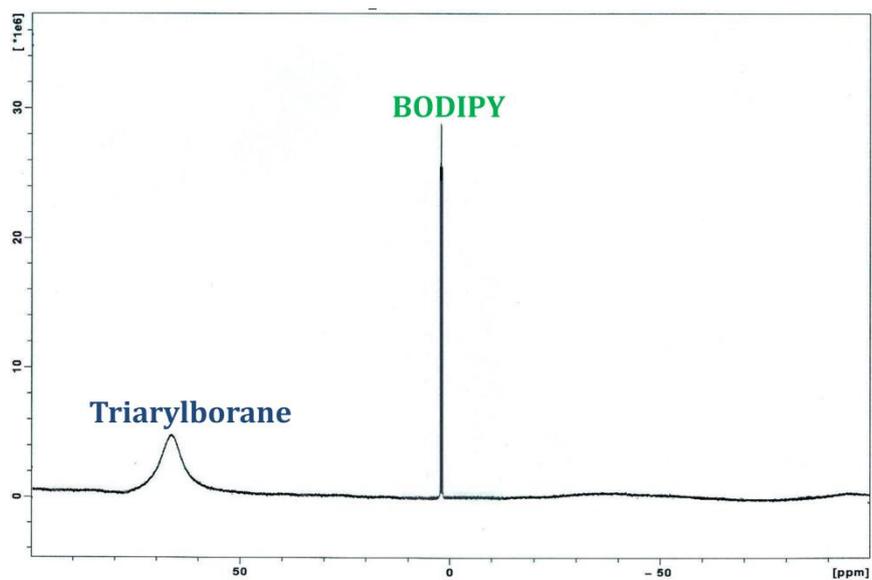


Figure S19. ^{11}B NMR of **1** in CDCl_3

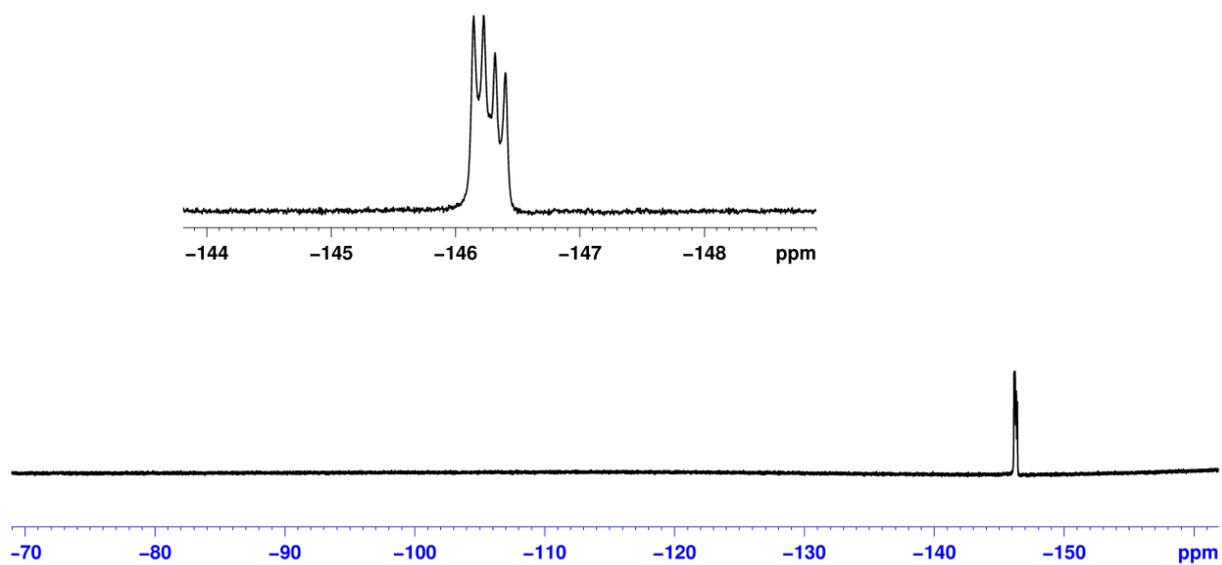


Figure S20. ^{19}F NMR of **1** in CDCl_3

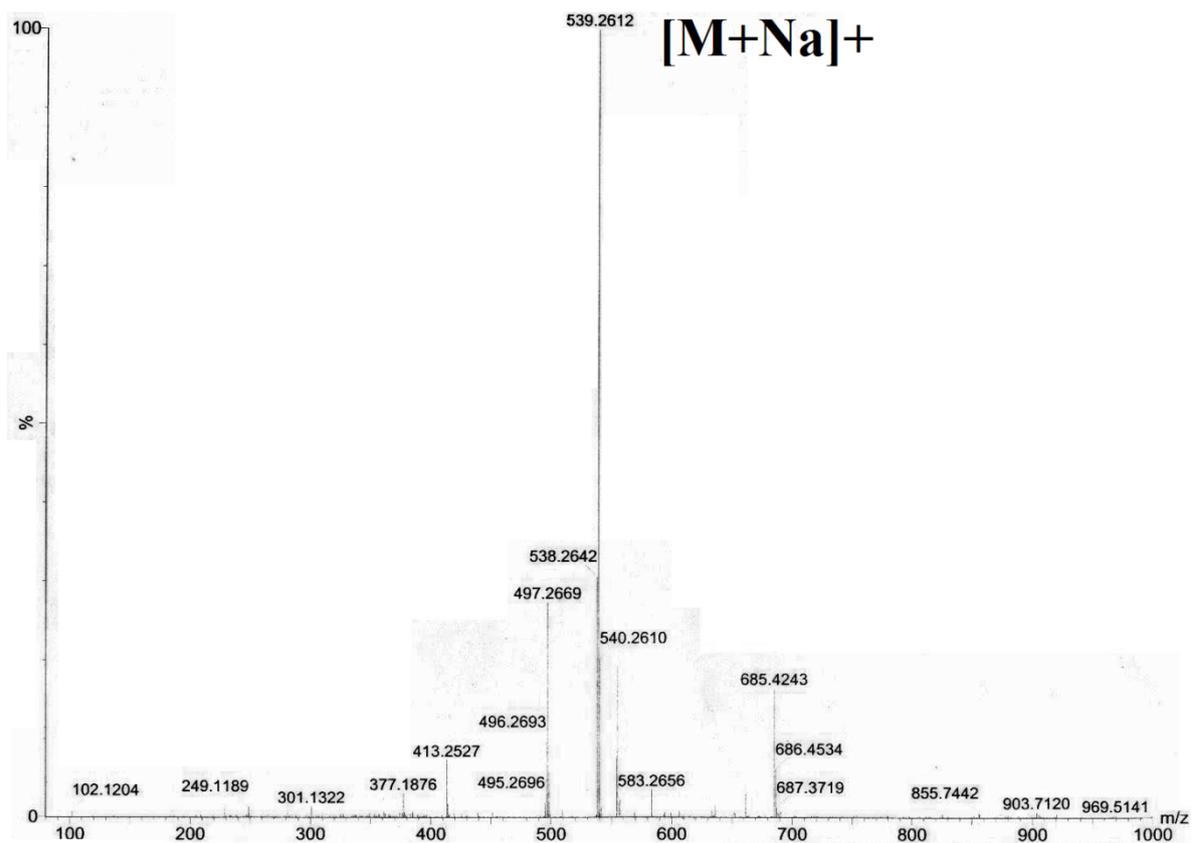


Figure S21. HRMS of **1**

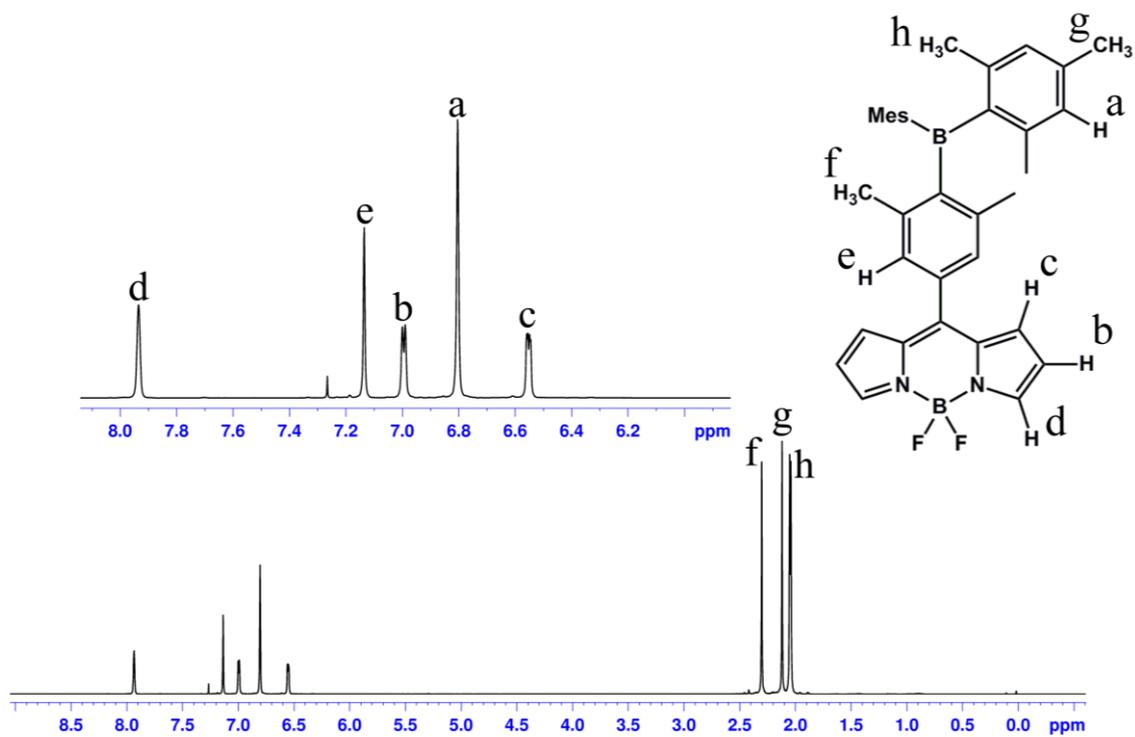


Figure S22. ^1H NMR of **2** in CDCl_3

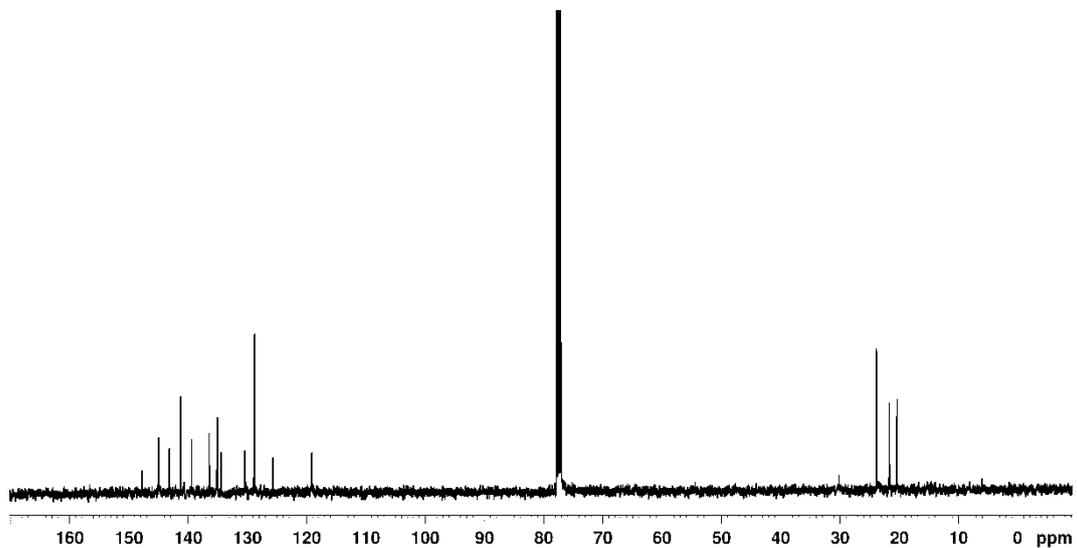


Figure S23. ^{13}C NMR of 2 in CDCl_3

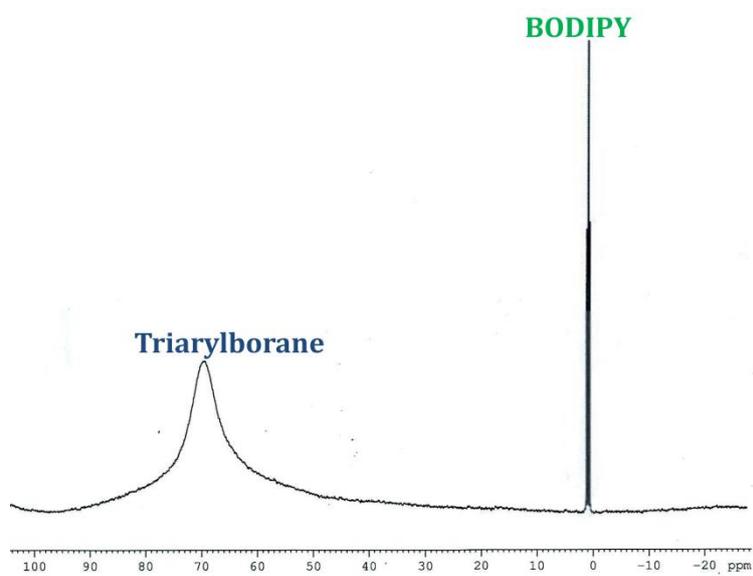


Figure S24. ^{11}B NMR of 2 in CDCl_3

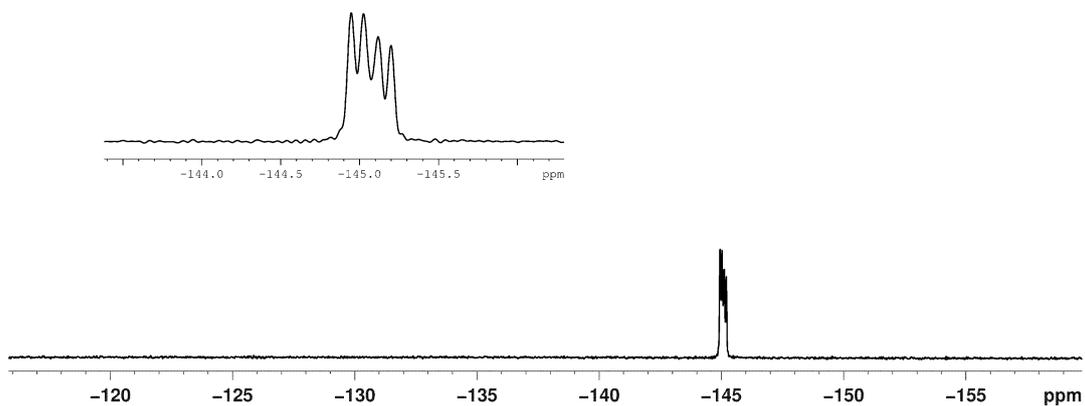


Figure S25. ^{19}F NMR of **2** in CDCl_3

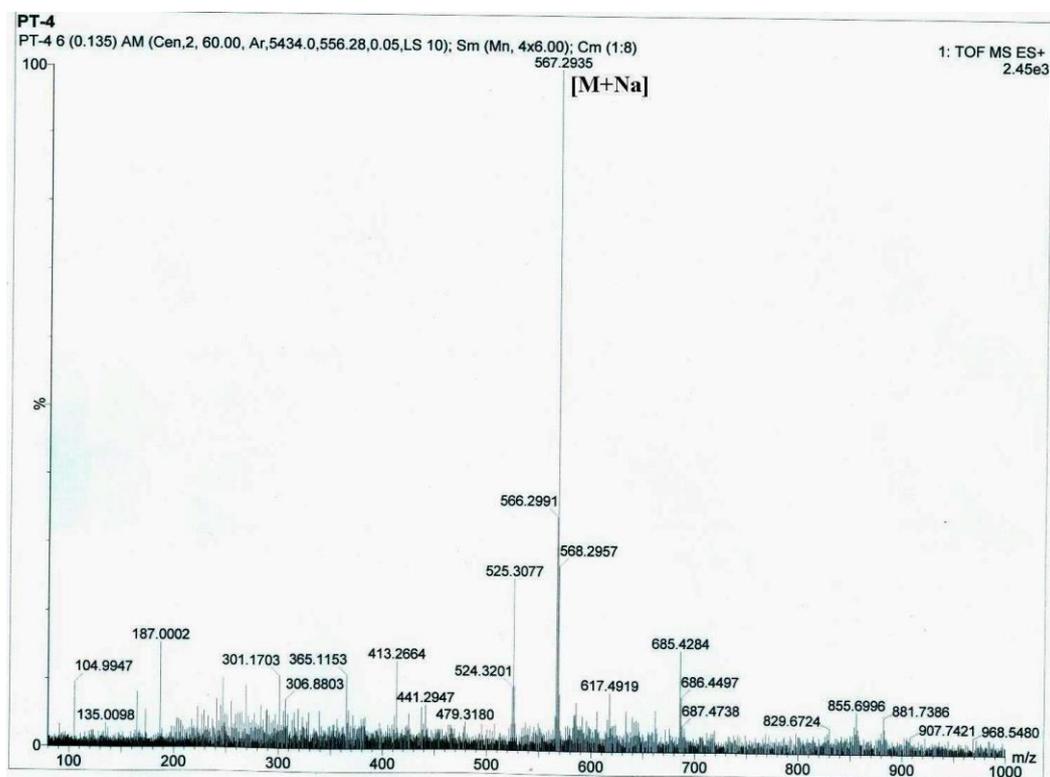


Figure S26. HRMS of **2**

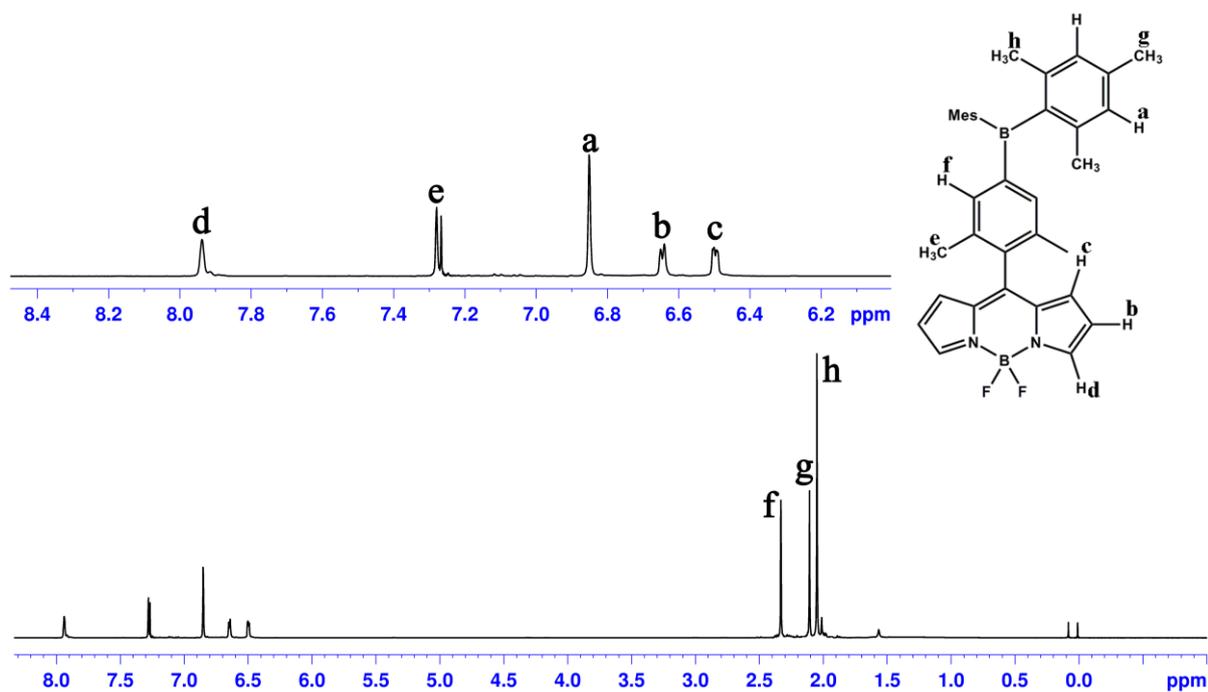


Figure S27. ^1H NMR of **3** in CDCl_3

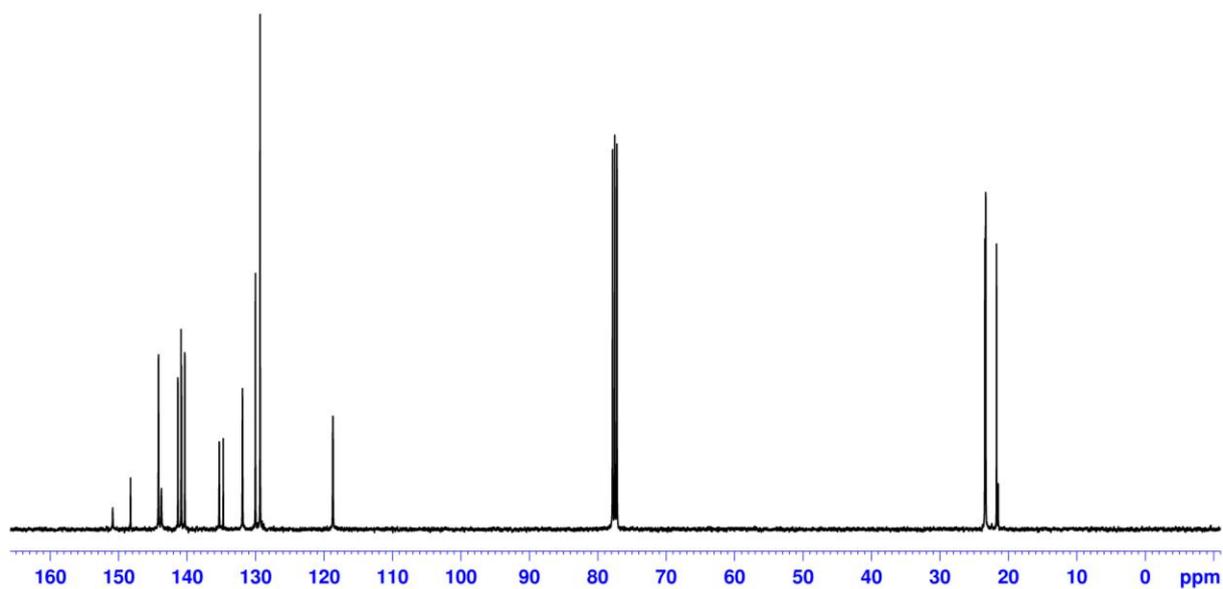


Figure S28. ^{13}C NMR of **3** in CDCl_3

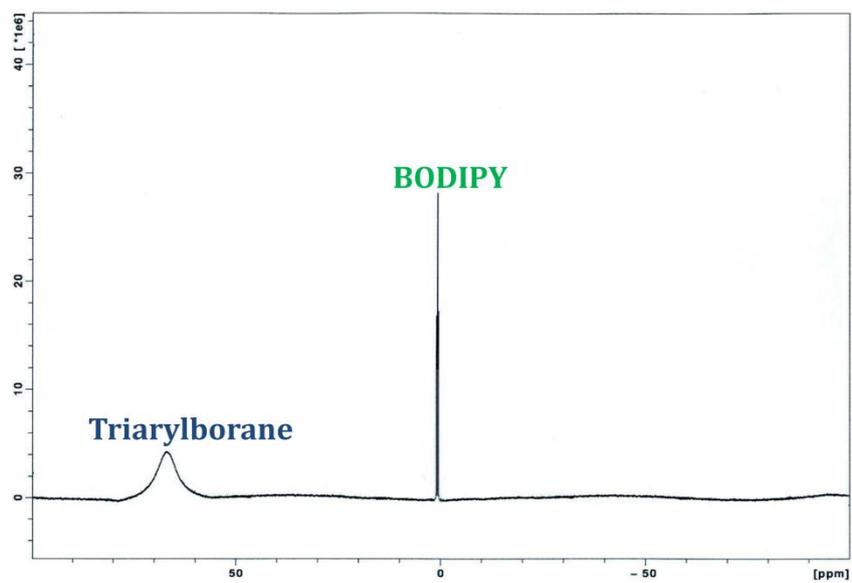


Figure S29. ^{11}B NMR of **3** in CDCl_3

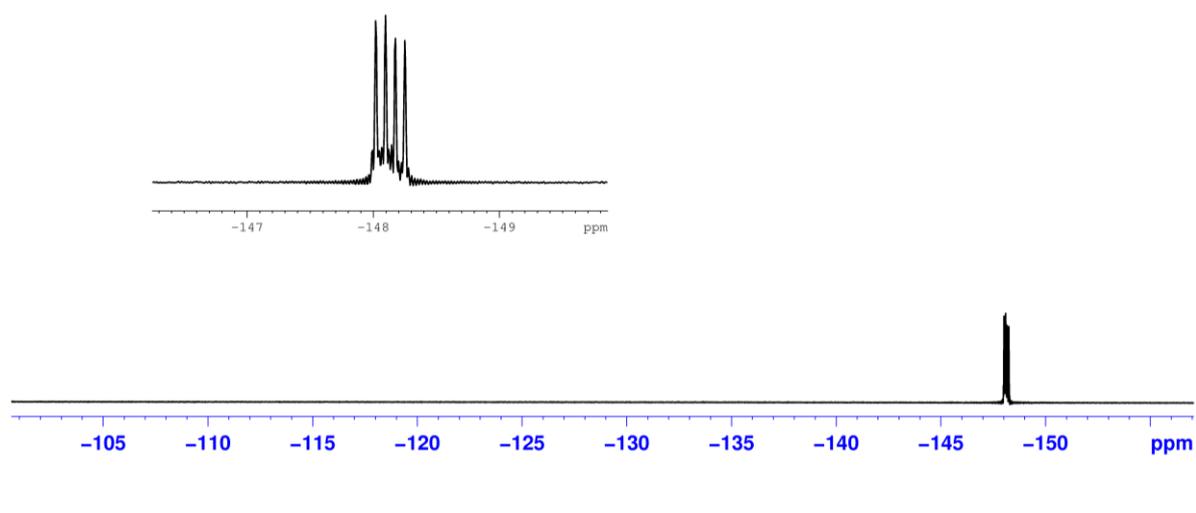
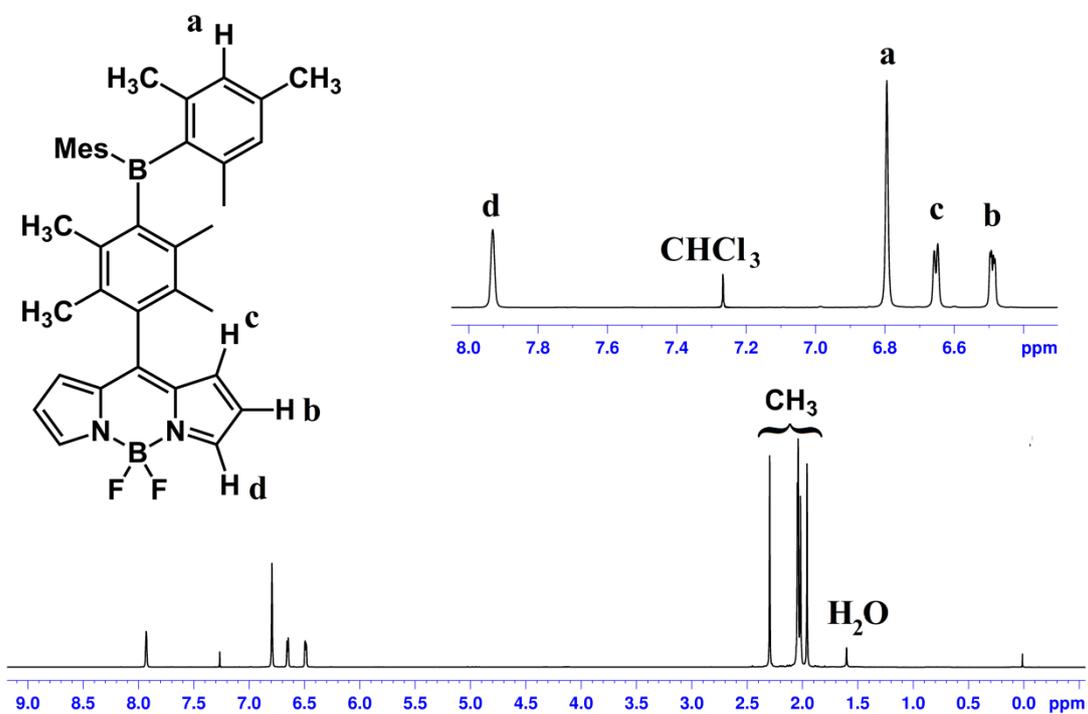
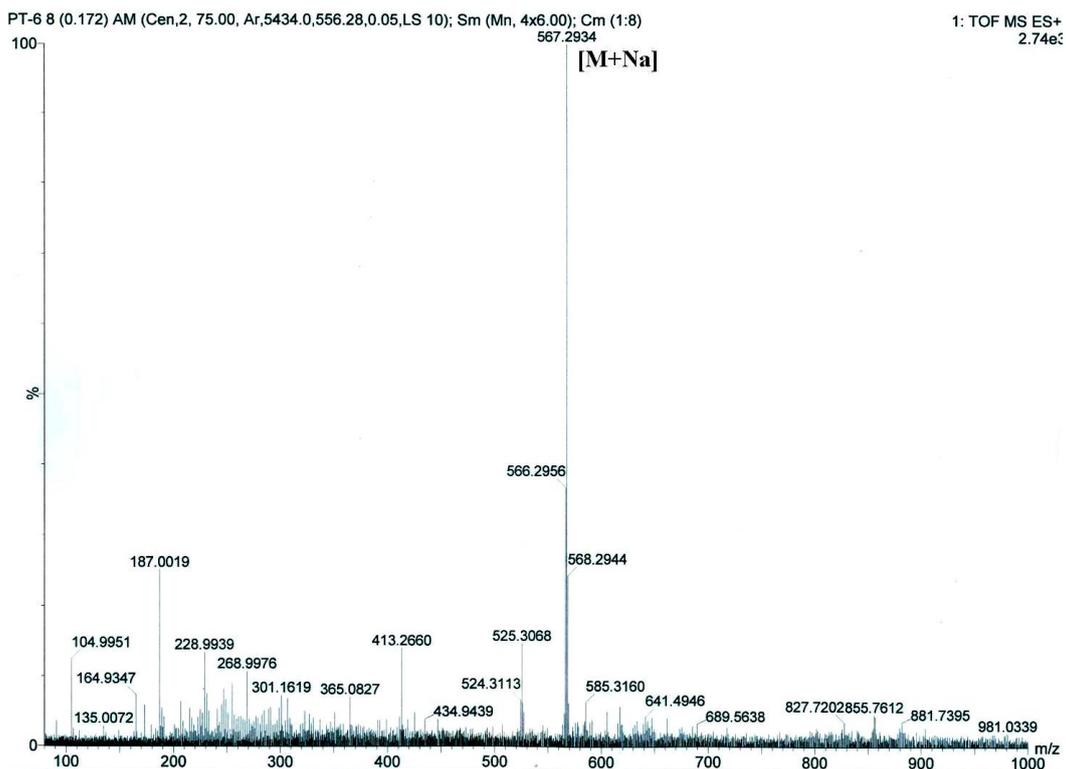


Figure S30. ^{19}F NMR of **3** in CDCl_3



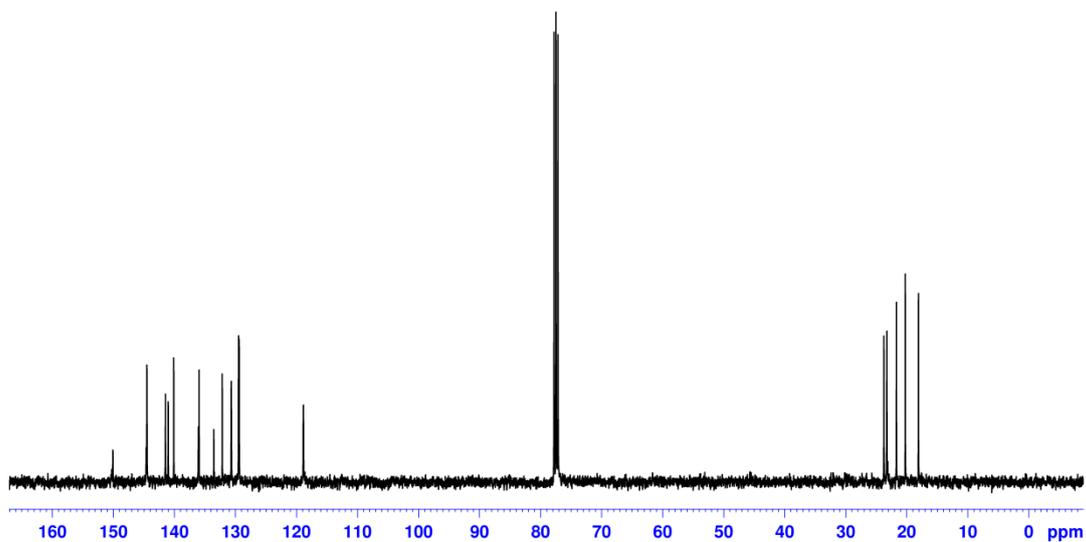


Figure S33. ^{13}C NMR of 4 in CDCl_3

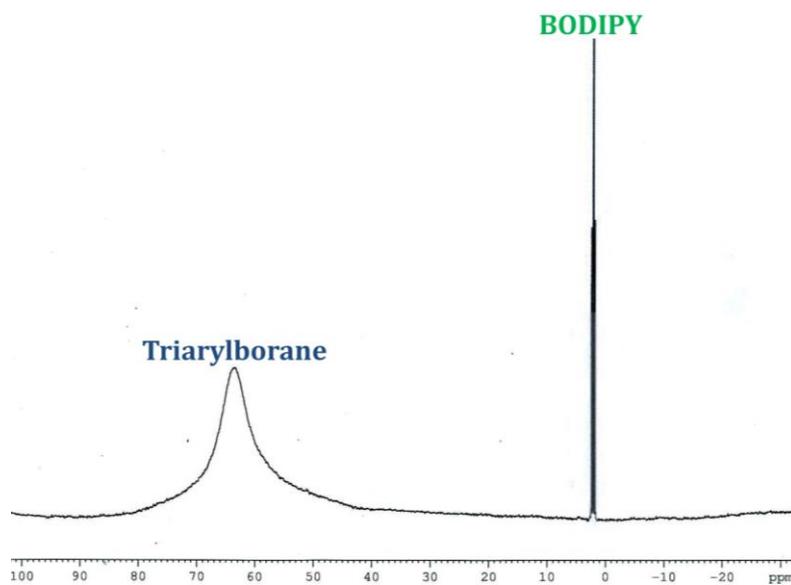


Figure S34. ^{11}B NMR of 4 in CDCl_3

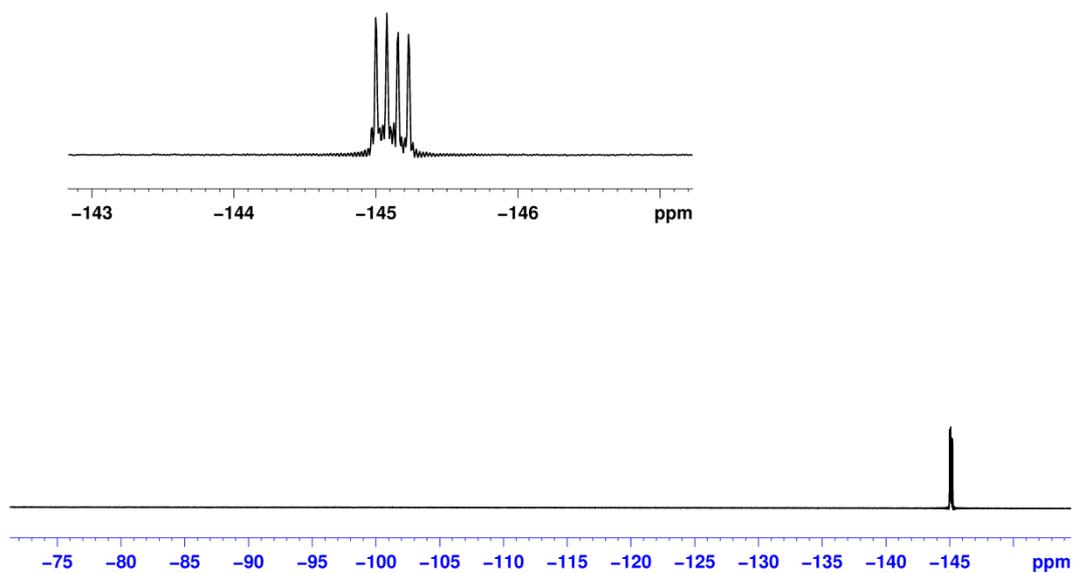


Figure S35. ^{19}F NMR of **4** in CDCl_3

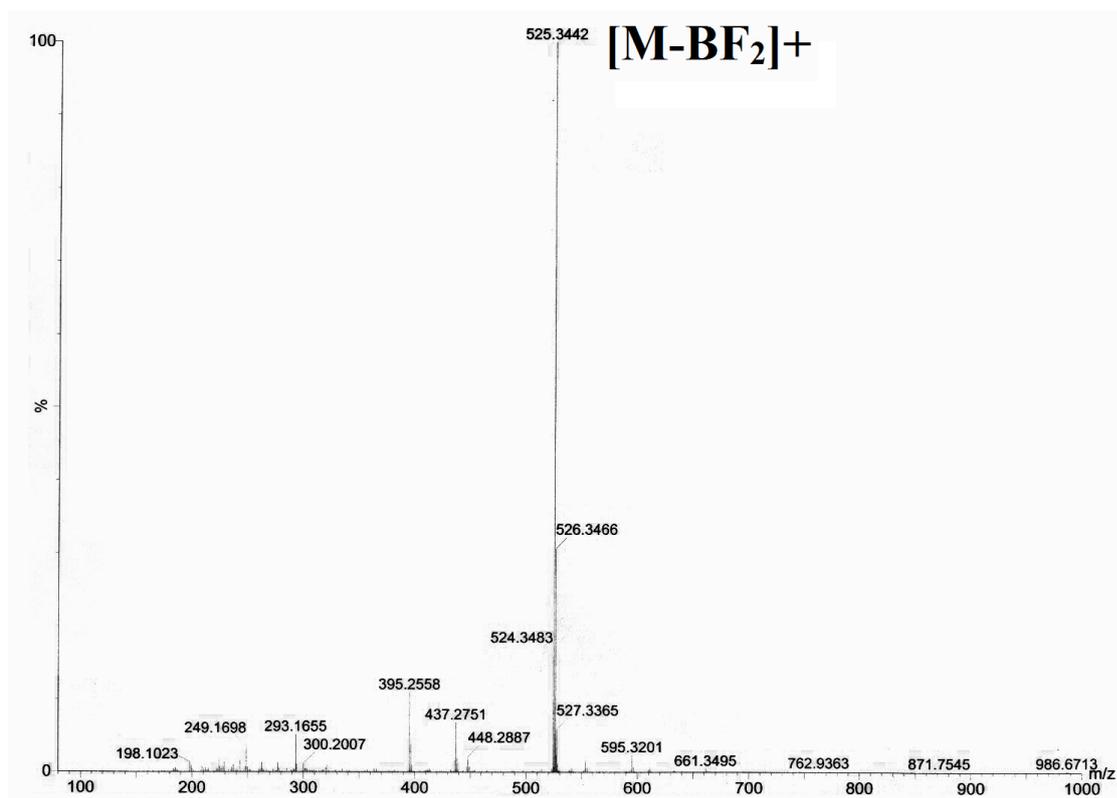


Figure S36. HRMS of **4**

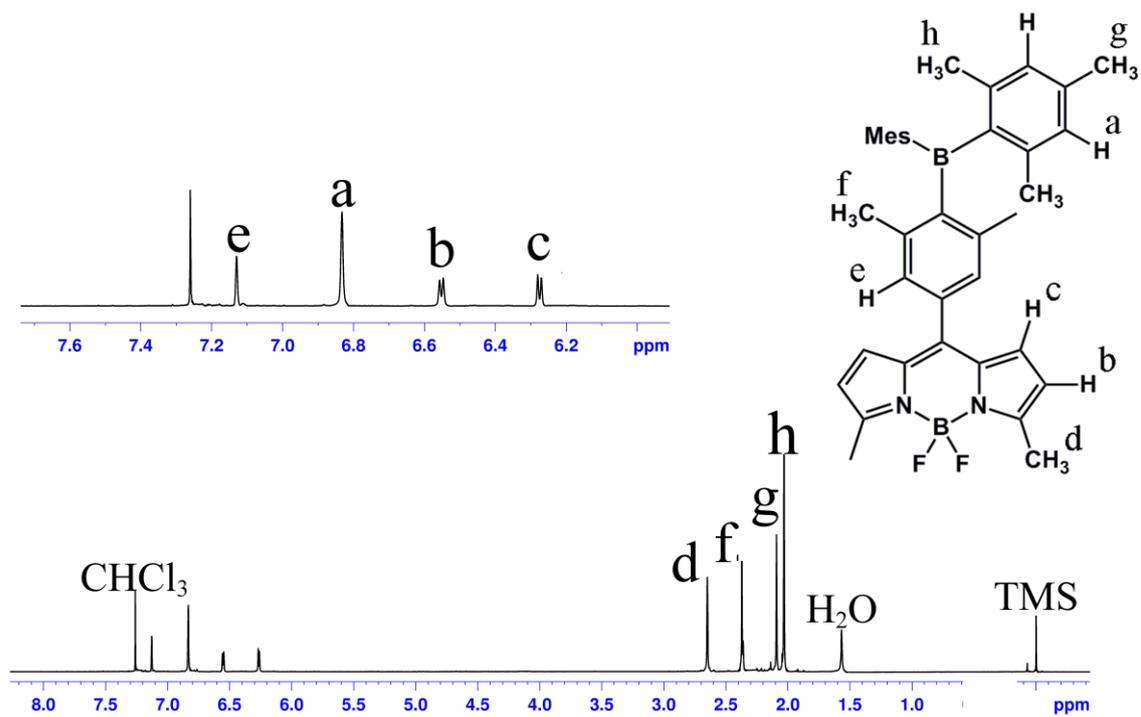


Figure S37. ^1H NMR of **5** in CDCl_3

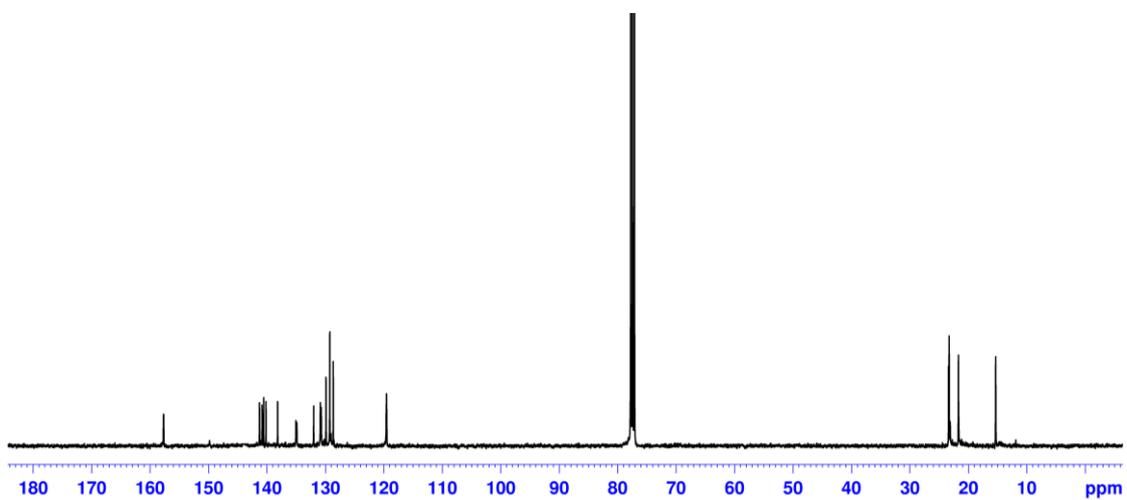


Figure S38. ^{13}C NMR of **5** in CDCl_3

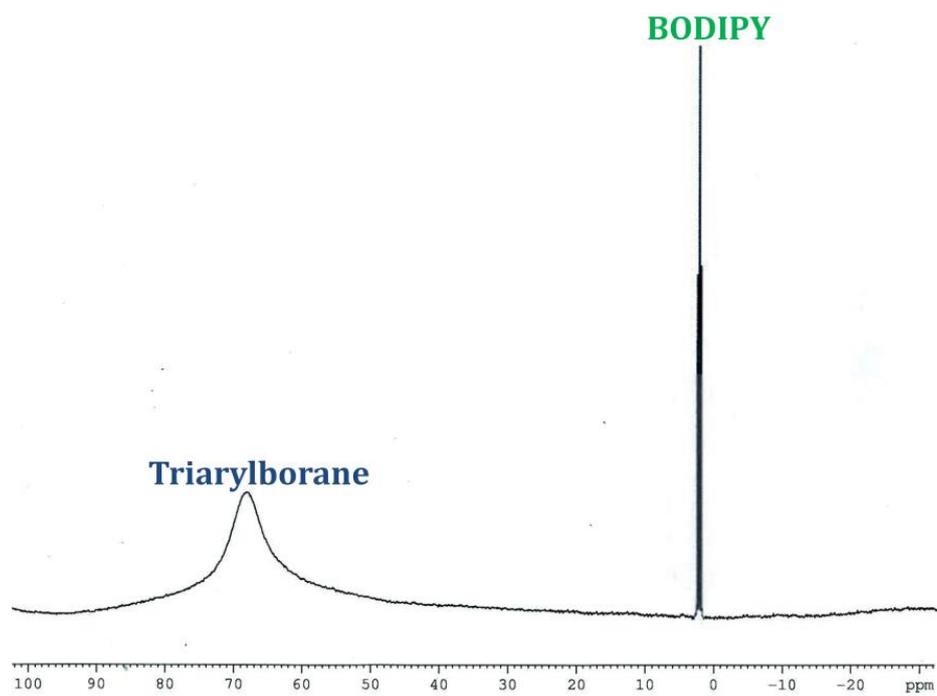


Figure S39. ^{11}B NMR of **5** in CDCl_3

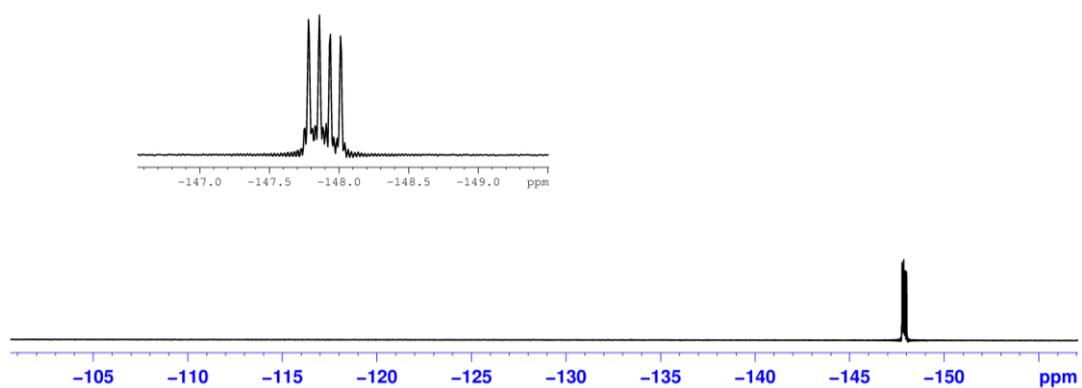


Figure S40. ^{19}F NMR of **5** in CDCl_3

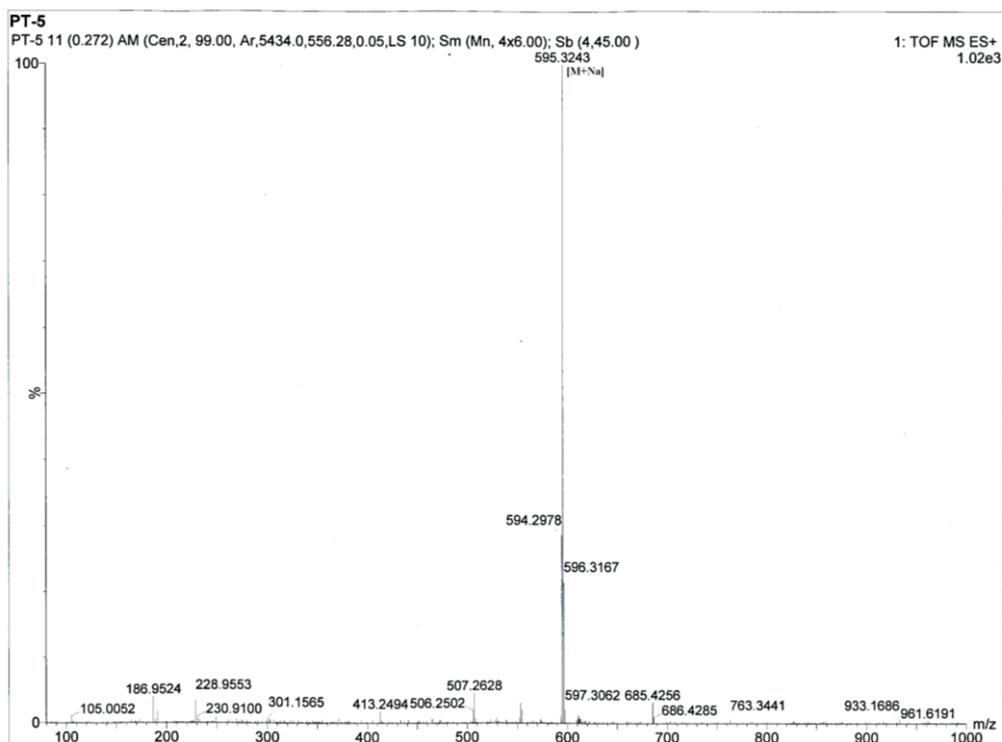


Figure S41. HRMS of 5

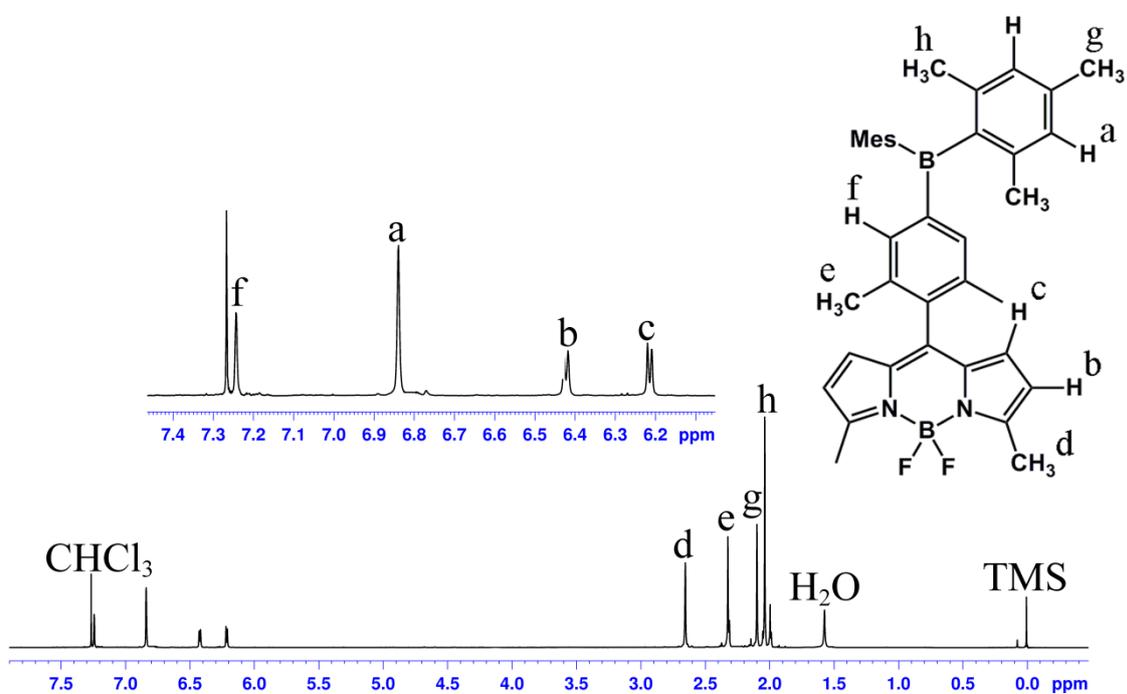


Figure S42. ¹H NMR of 6 in CDCl₃

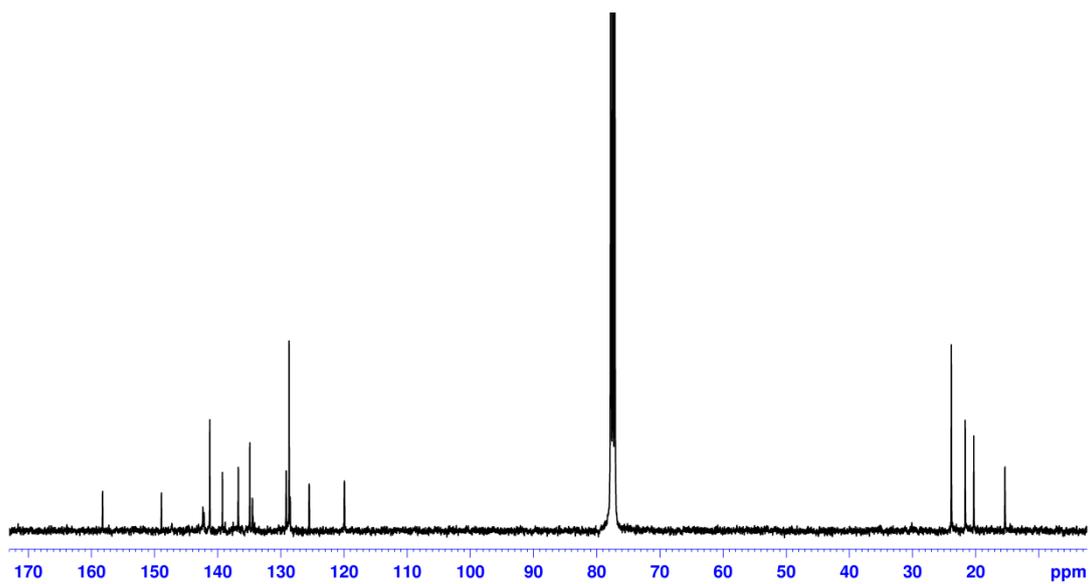


Figure S43. ^{13}C NMR of **6** in CDCl_3

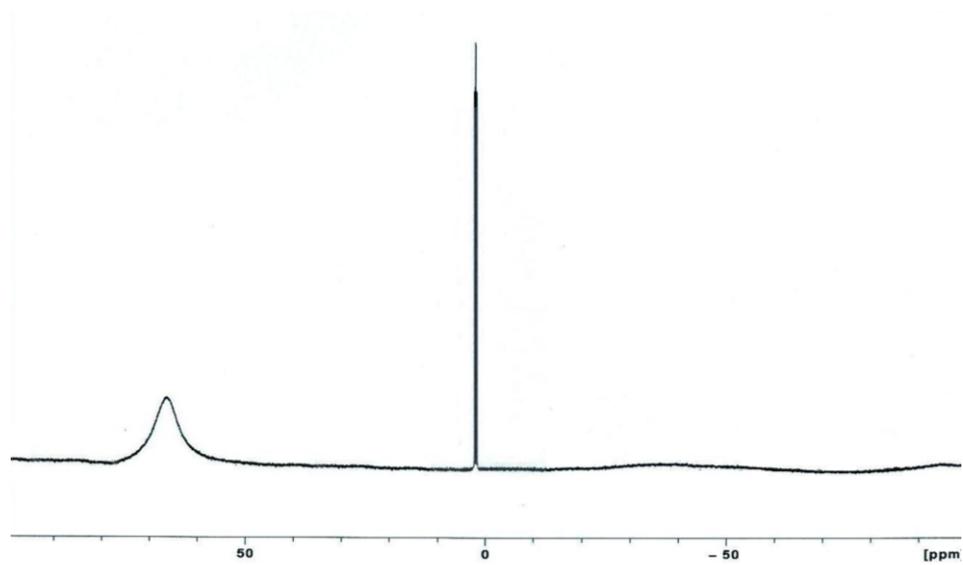


Figure S44. ^{11}B NMR of **6** in CDCl_3

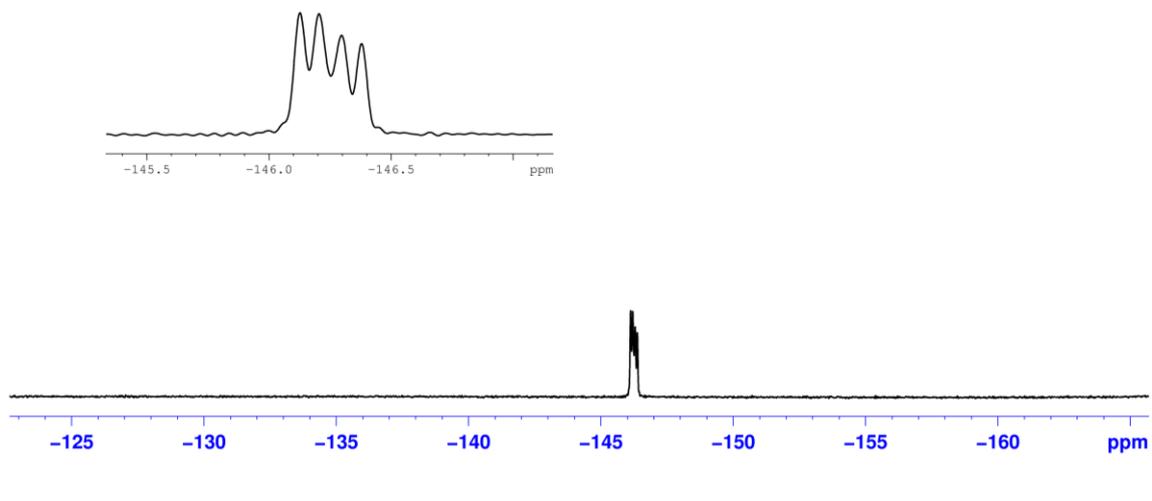


Figure S45. ^{19}F NMR of **6** in CDCl_3

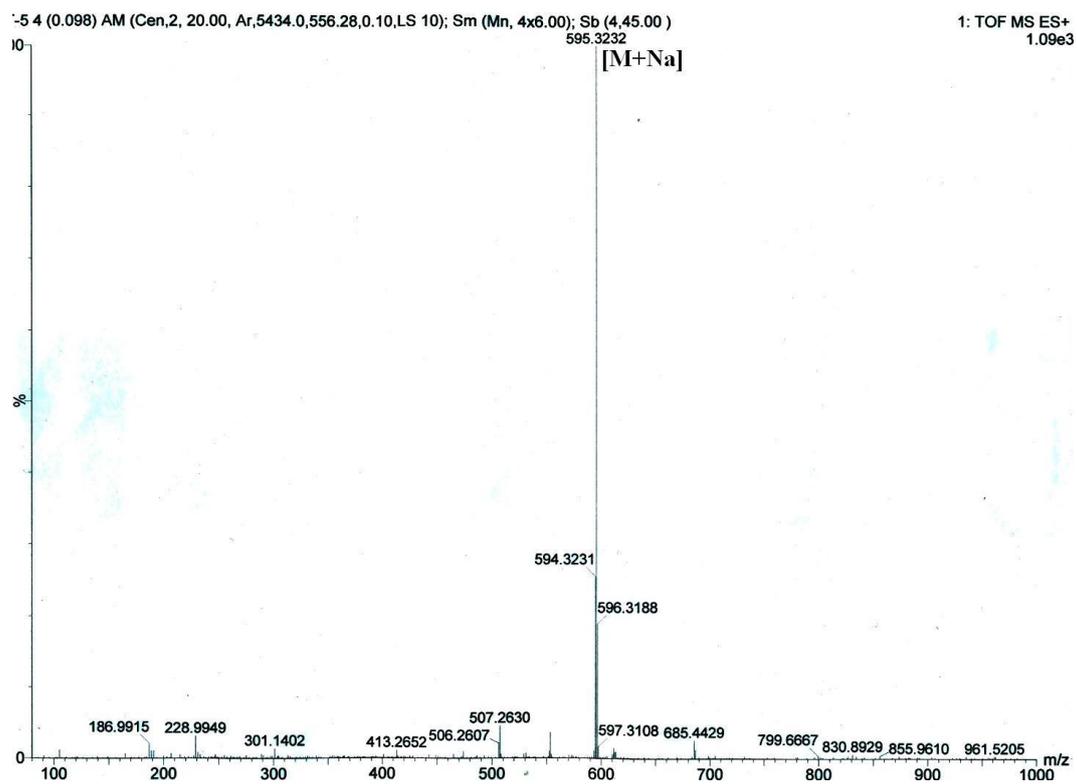


Figure S46. HRMS of **6**

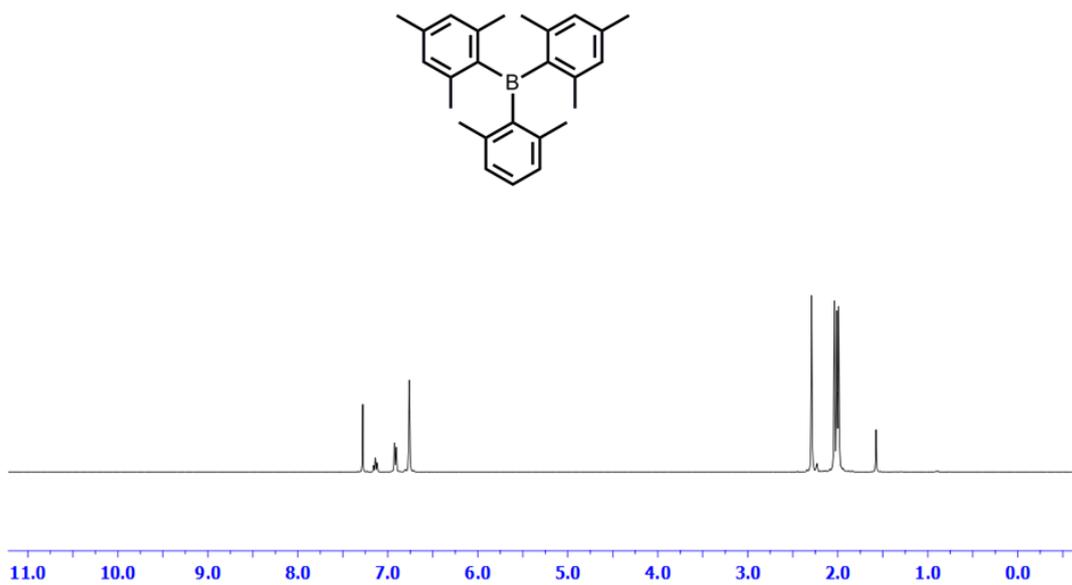


Figure S47. ¹H NMR of M5 in CDCl₃

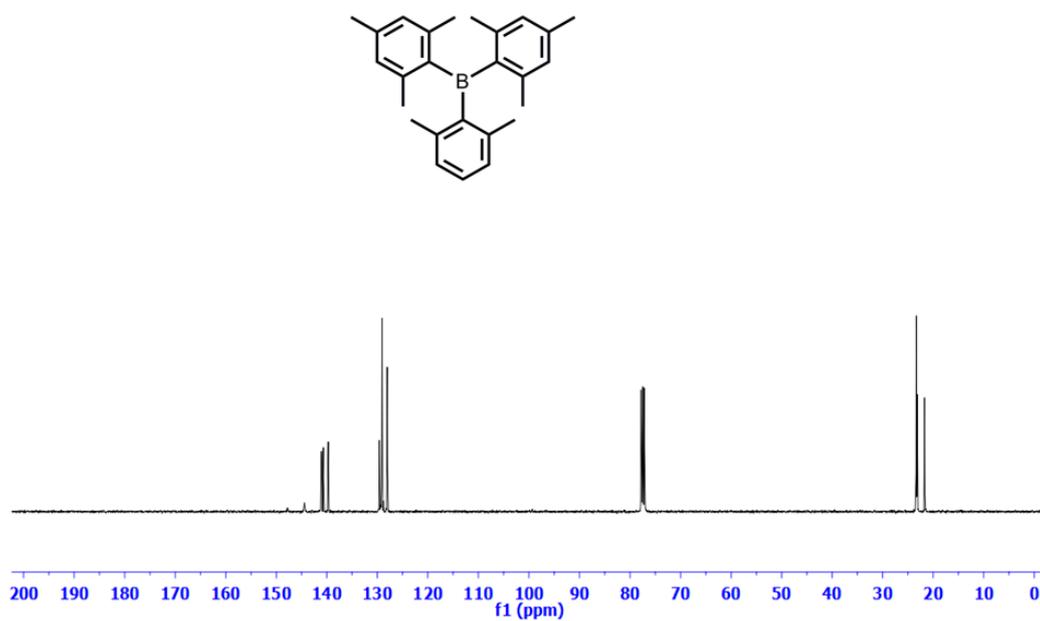


Figure S48. ¹³C NMR of M5 in CDCl₃

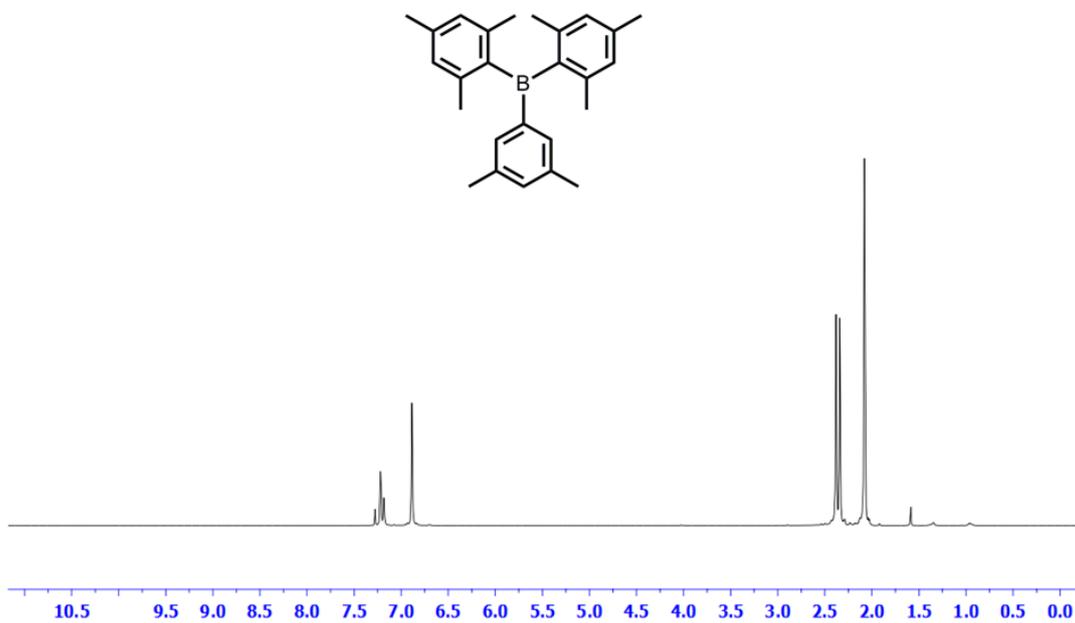


Figure S49. ¹H NMR of M6 in CDCl₃

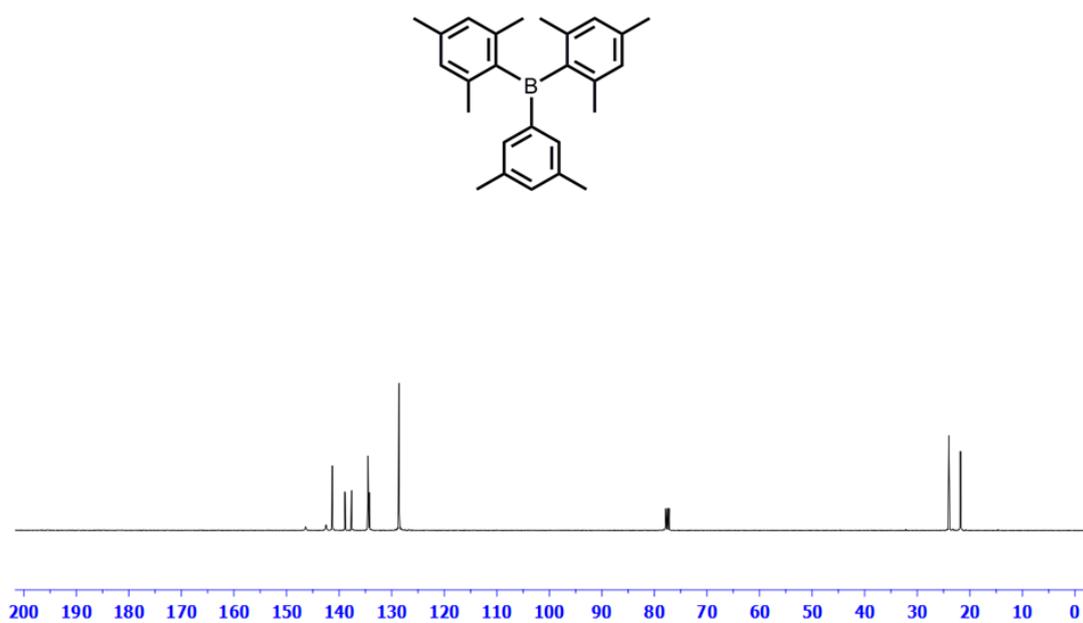


Figure S50. ¹³C NMR of M6 in CDCl₃

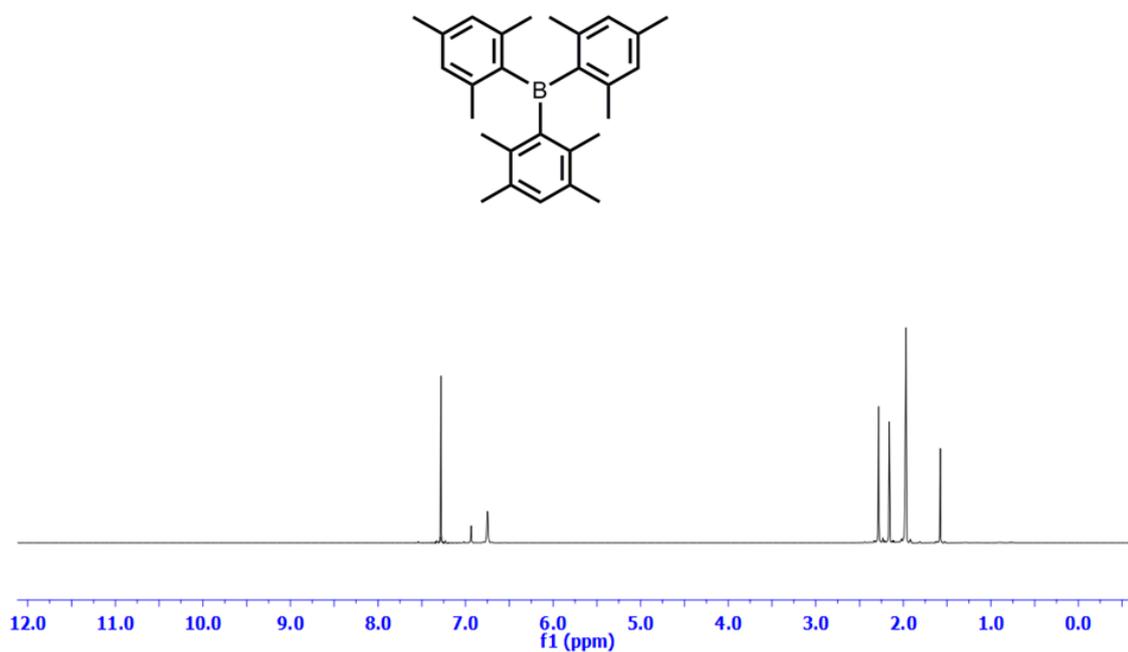


Figure S51. ¹H NMR of M7 in CDCl₃

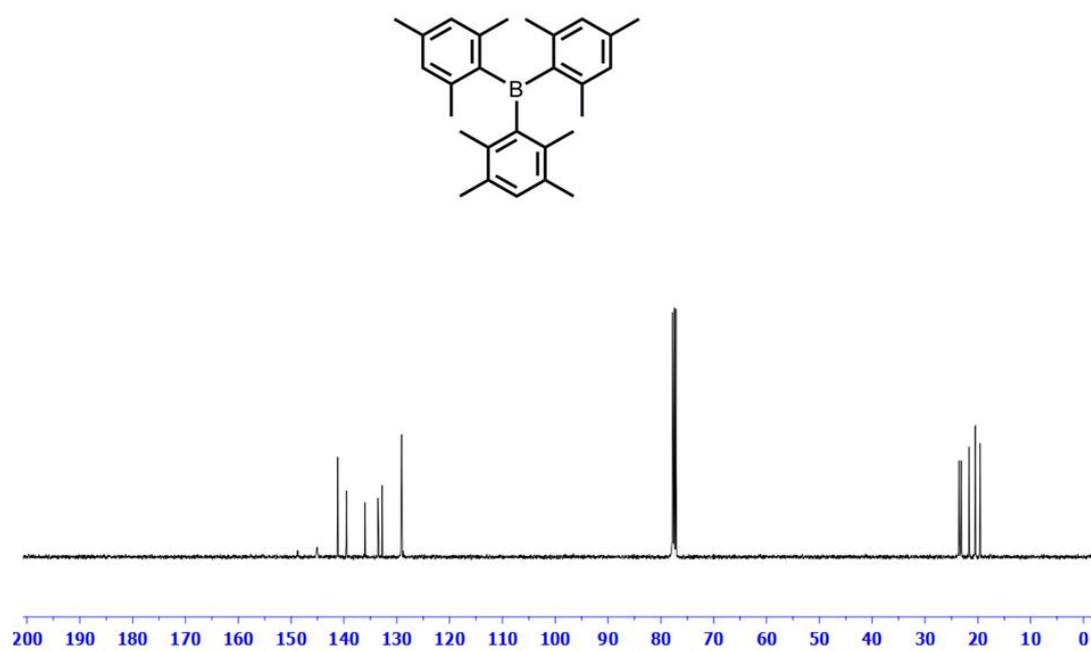


Figure S52. ¹³C NMR of M7 in CDCl₃

SINGLE CRYSTAL X-RAY DIFFRACTION ANALYSIS

Table S1. Crystallographic data and refinement parameters for structures of **1-3**.

Identification code	1	2	3
Empirical formula	C ₃₃ H ₃₂ B ₂ F ₂ N ₂	C ₃₅ H ₃₆ B ₂ F ₂ N ₂	C ₃₅ H ₃₆ B ₂ F ₂ N ₂
Formula weight	516.22	544.28	544.28
Temperature	296(2) K	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> 21/n
Unit cell dimensions	a = 8.269(11) Å b = 12.335(19) Å c = 16.561(2) Å α = 102.030(4)° β = 101.141(4)° γ = 93.090(5)°	a = 8.473(5) Å b = 14.232(8) Å c = 15.185(9) Å α = 95.586(2)° β = 102.696(2)° γ = 93.870(2)°	a = 8.117(7) Å b = 13.259(11) Å c = 27.962(2) Å α = 90° β = 91.154(5)° γ = 90°
Volume (Å ³)	1613.4(4)	1770.77(18)	3008.9(4)
Z	2	2	4
Density (calculated)	1.063 Mg/m ³	1.021 Mg/m ³	1.202 Mg/m ³
Absorption coefficient	0.069 mm ⁻¹	0.066 mm ⁻¹	0.077 mm ⁻¹
F(000)	544	576	1152
Crystal size (mm ³)	0.07 x 0.05 x 0.05	0.13 x 0.11 x 0.10	0.15 x 0.12 x 0.11
Theta range for data collection	3.110 to 27.568°.	2.977 to 24.999°.	1.457 to 24.993°.
Index ranges	-9<=h<=9, -15<=k<=15, -19<=l<=18	-10<=h<=10, -16<=k<=16, -18<=l<=18	-9<=h<=9, -15<=k<=15, -32<=l<=33
Reflections collected	9000	56798	47159
Independent reflections	4874 [R(int) = 0.0359]	6211 [R(int) = 0.0697]	5298 [R(int) = 0.0977]
Completeness to theta = 25.000°	99 %	99.8 %	100.0 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.985 and 0.980	0.990 and 0.983	0.990 and 0.982
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	4874 / 0 / 358	6211 / 0 / 378	5298 / 0 / 378
Goodness-of-fit	1.002	1.074	1.028

on F ²			
Final R indices [I > 2σ(I)] ^[a,b]	R1 = 0.0636, wR2 = 0.1816	R1 = 0.0576, wR2 = 0.1785	R1 = 0.0517, wR2 = 0.1255
R indices (all data) ^[a,b]	R1 = 0.1196, wR2 = 0.2155	R1 = 0.1033, wR2 = 0.1995	R1 = 0.0998, wR2 = 0.1410
Extinction coefficient	n/a	n/a	n/a
Largest diff. peak and hole	0.235 and -0.206 e.Å ⁻³	0.322 and -0.191 e.Å ⁻³	0.222 and -0.199 e.Å ⁻³
CCDC No.	1994506	1994507	1994508

Table S2. Crystallographic data and refinement parameters for structures of **4** and **6**.

Identification code	4	6
Empirical formula	C ₃₇ H ₄₀ B ₂ F ₂ N ₂	C ₃₇ H ₄₀ B ₂ F ₂ N ₂
Formula weight	572.33	572.33
Temperature	100(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 21/c
Unit cell dimensions	a = 8.569(3) Å b = 13.515(6) Å c = 14.769(6) Å α = 106.796(2)° β = 103.405(2)° γ = 96.486(2)°	a = 26.581(4) Å b = 11.418(18) Å c = 14.125(2) Å α = 90° β = 105.243(4)° γ = 90°
Volume	1563.02(11) Å ³	4136.3(11) Å ³
Z	2	4
Density (calculated)	1.216 Mg/m ³	0.919 Mg/m ³
Absorption coefficient	0.078 mm ⁻¹	0.059 mm ⁻¹
F(000)	608	1216
Crystal size	0.100 x 0.080 x 0.080 mm ³	0.06 x 0.05 x 0.02 mm ³
Theta range for data collection	1.499 to 30.535°.	3.031 to 30.692°.
Index ranges	-12 ≤ h ≤ 12, -19 ≤ k ≤ 19, -21 ≤ l ≤ 21	-37 ≤ h ≤ 38, -16 ≤ k ≤ 14, - 20 ≤ l ≤ 20
Reflections collected	33700	145089
Independent reflections	9247 [R(int) = 0.0614]	11778 [R(int) = 0.4683]
Completeness to theta = 25.000°	98.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.998 and 0.985	0.988 and 0.983
Refinement method	Full-matrix least-squares on	Full-matrix least-squares on

	F ²	F ²
Data / restraints / parameters	9247 / 0 / 398	11778 / 0 / 398
Goodness-of-fit on F ²	1.058	1.055
Final R indices [I > 2σ(I)] ^[a,b]	R1 = 0.0673, wR2 = 0.1647	R1 = 0.1761, wR2 = 0.3400
R indices (all data) ^[a,b]	R1 = 0.1376, wR2 = 0.1965	R1 = 0.4152, wR2 = 0.4352
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	0.635 and -0.255 e.Å ⁻³	0.405 and -0.316 e.Å ⁻³
CCDC No.	1994509	1994510

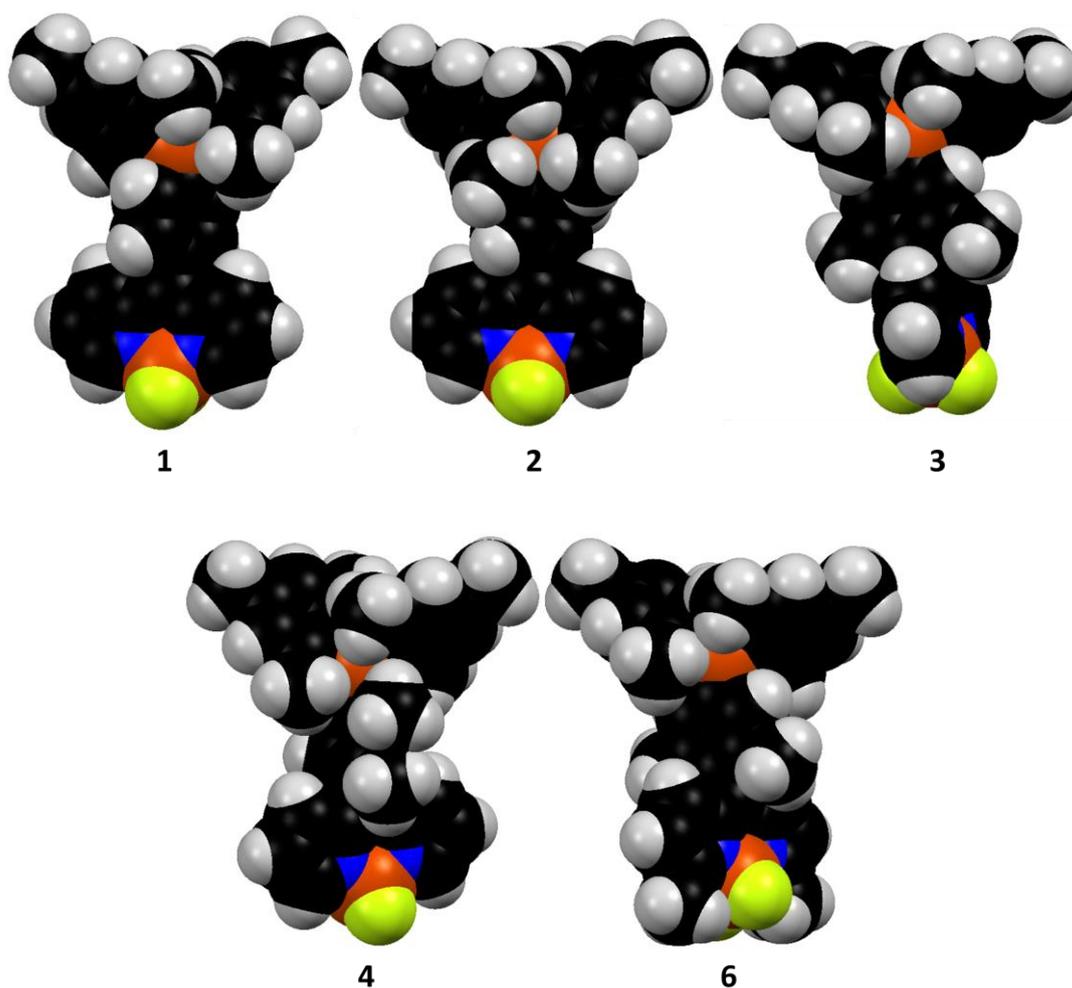


Figure S53. Space fill diagram for the molecular structure of 1-4 and 6.

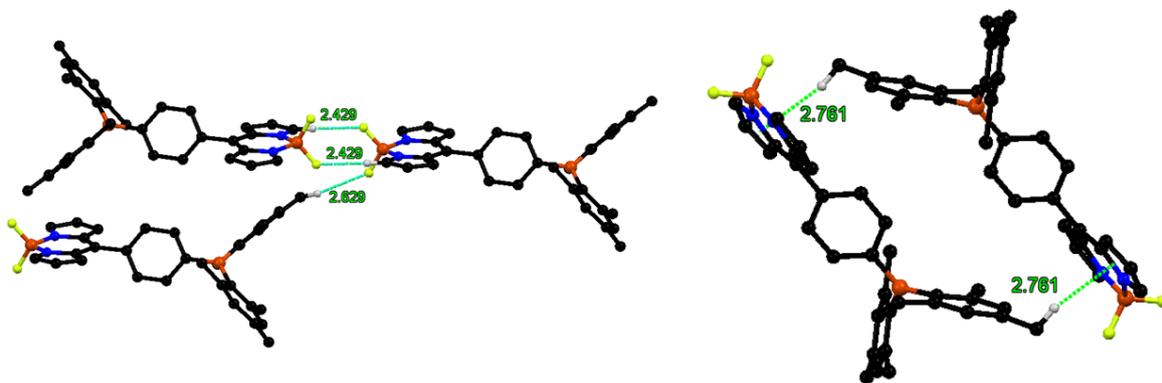


Figure S54. Intermolecular interactions in the crystal structure of 1.

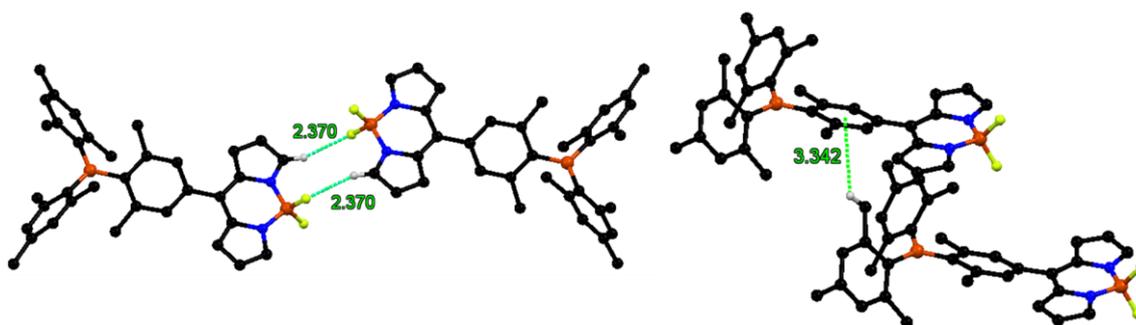


Figure S55. Intermolecular interactions in the crystal structure of 2.

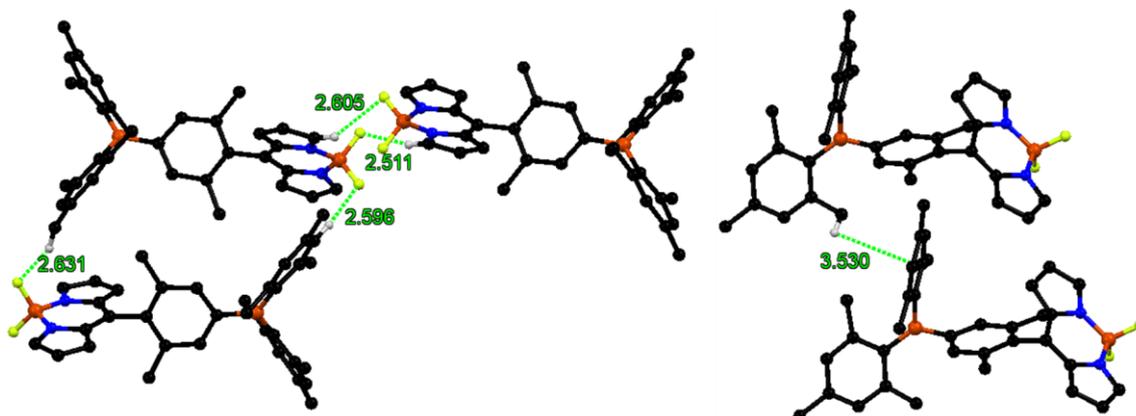


Figure S56. Intermolecular interactions in the crystal structure of 3.

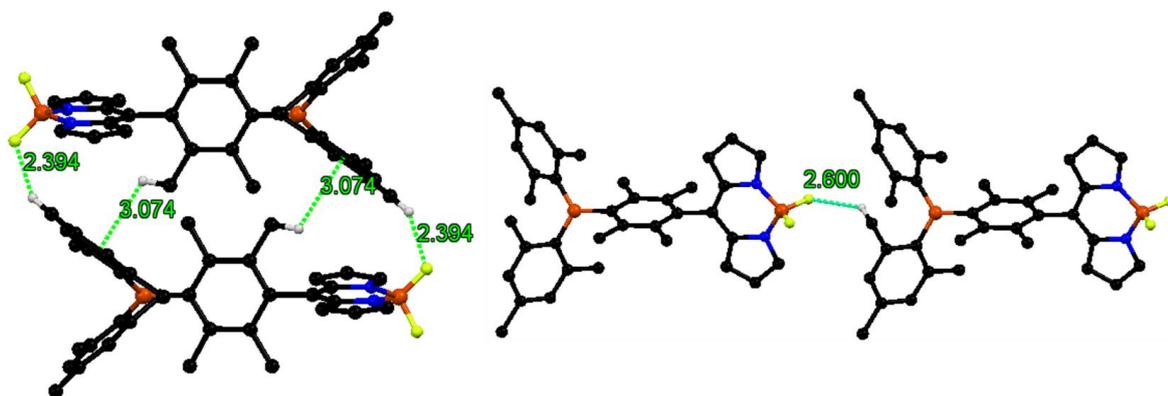


Figure S57. Intermolecular interactions in the crystal structure of **4**.

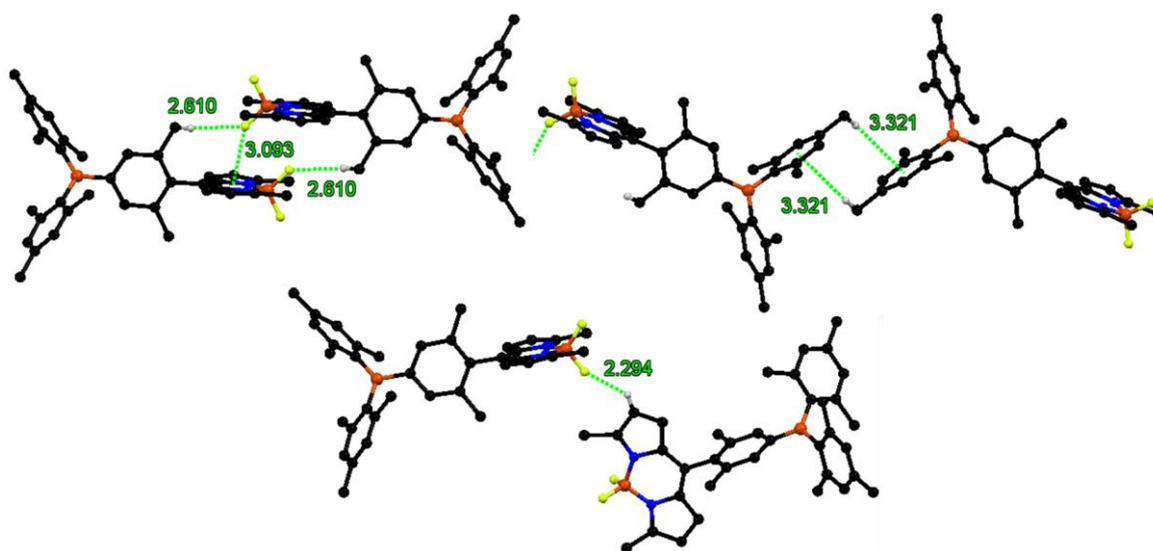


Figure S58. Intermolecular interactions in the crystal structure of **6**.

PHOTOPHYSICAL PROPERTIES

Chart S1. Chemical structures of the compounds used for optical studies.

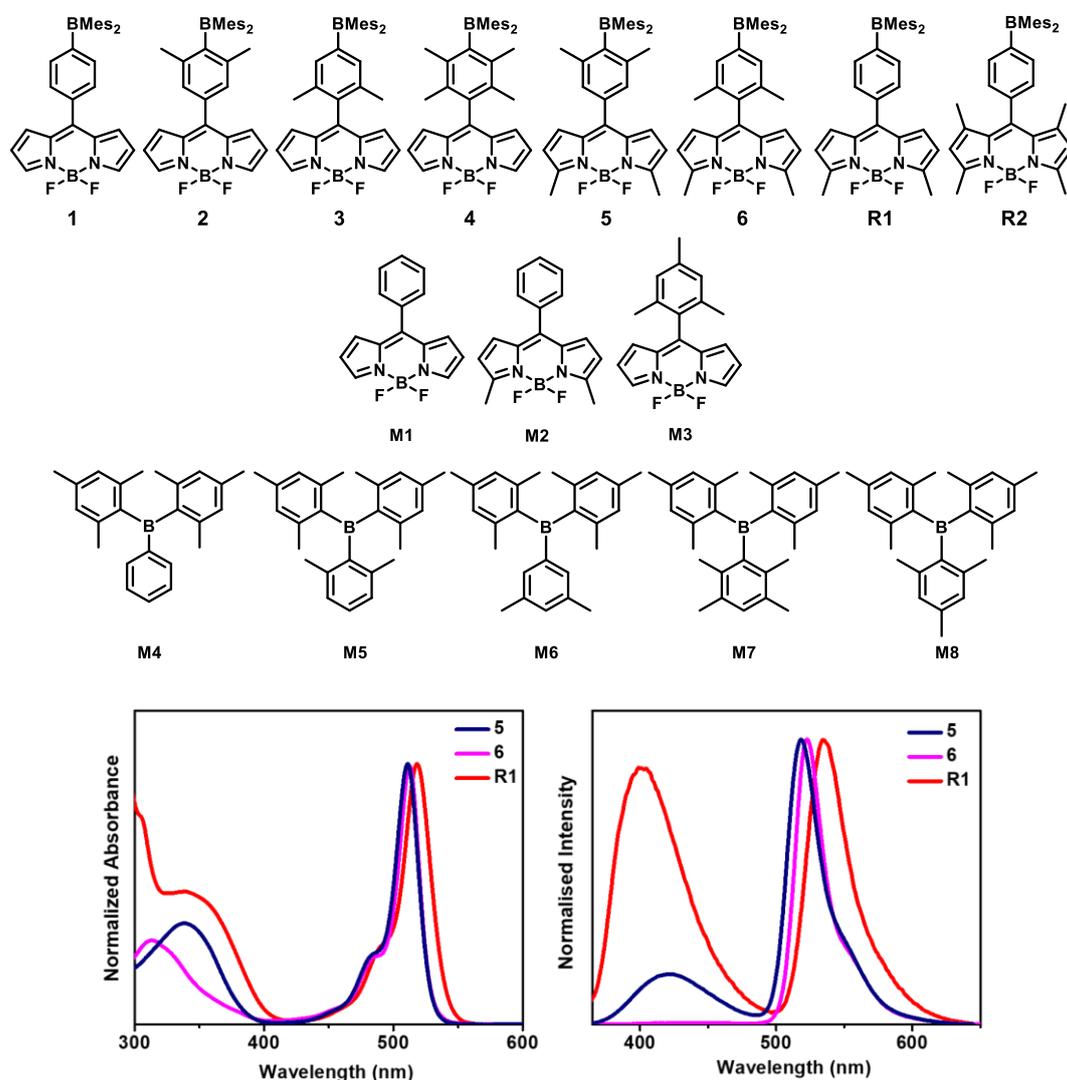


Figure S59. Comparison of UV-Visible (left) and emission (right) spectra of **R1**, **5**, and **6**. Compound **R1** showed more bathochromic shift compared to **5** and **6** in absorption as well as emission spectra.

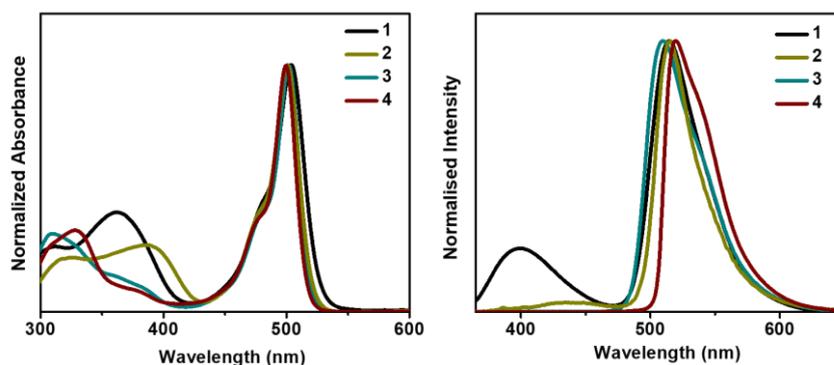


Figure S60: Comparison of UV-Visible (left) and emission (right) spectra of **1-4**. Absorption and emission bands of compounds **1-4** fall in the same region.

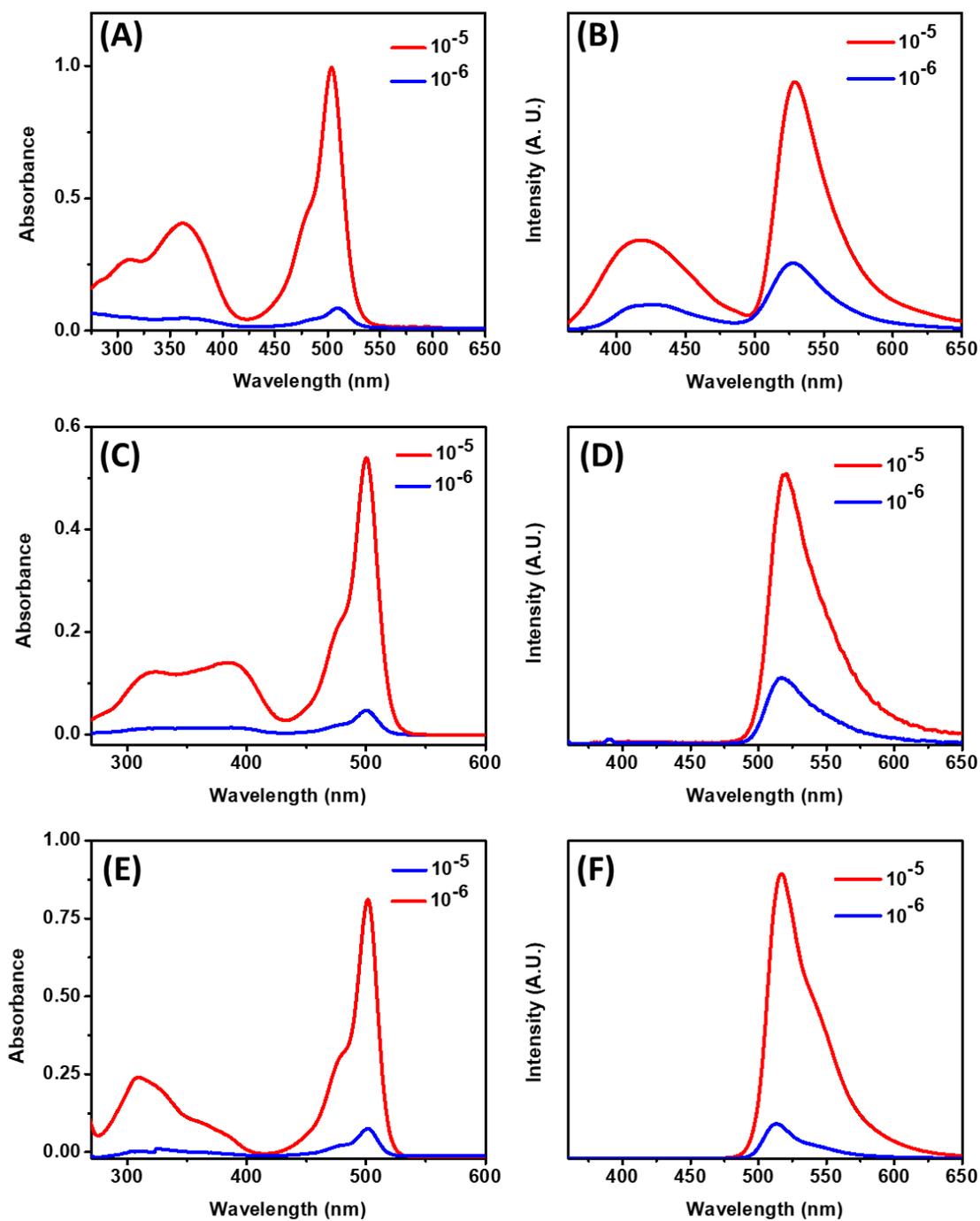


Figure S61. UV-Visible (left) and fluorescence (λ_{ex} at 350 nm) (right) spectra of **1** (A, B), **2** (C, D) and **3** (E, F) in dichloromethane at various concentrations (10^{-5} - 10^{-6} M). The intensity of absorption and emission bands is decreasing with decreasing the concentration of compounds. However, the ratio of dual emission bands remains the same throughout the concentration range.

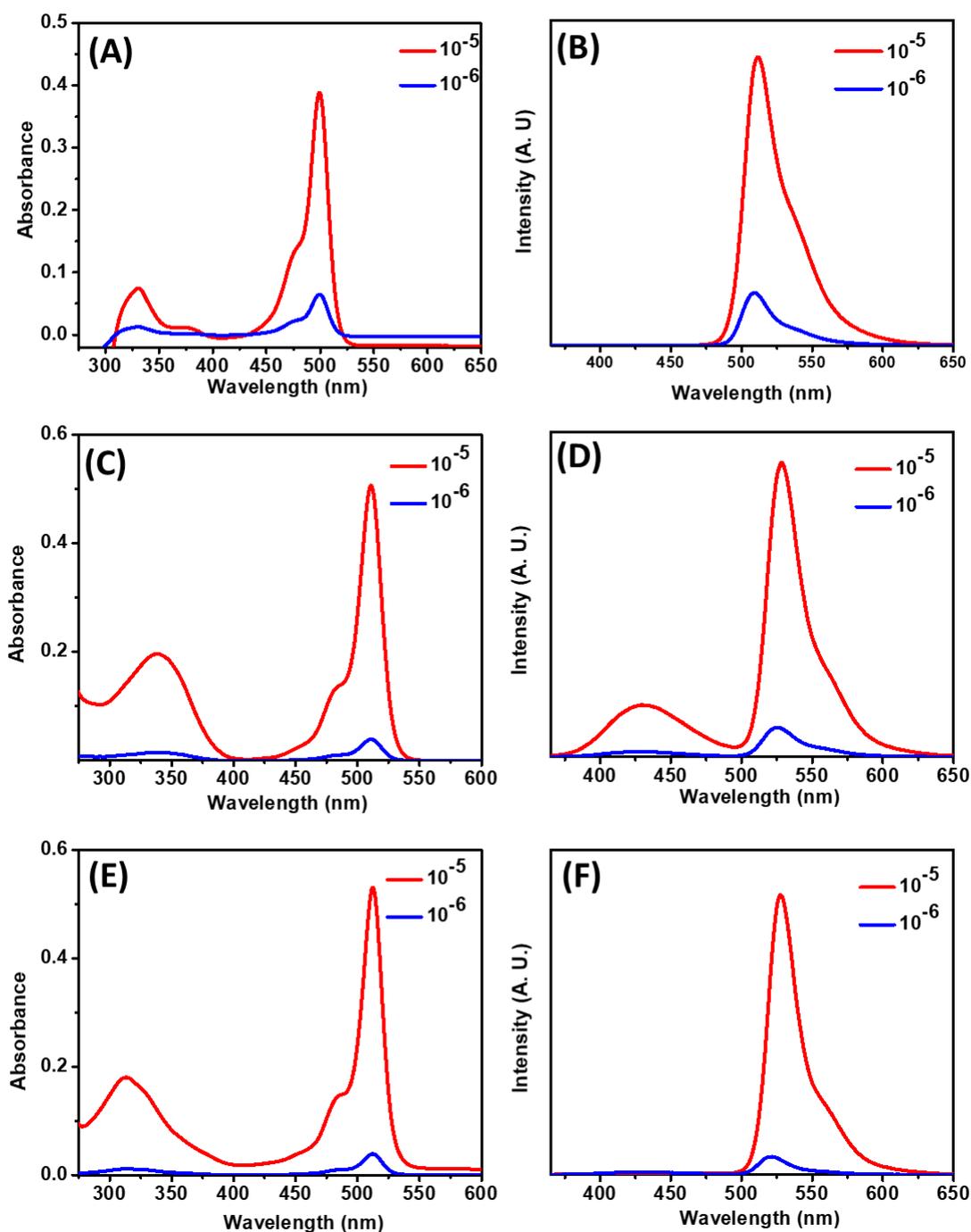


Figure S62. UV-Visible (left) and fluorescence (λ_{ex} at 350 nm) (right) spectra of **4** (A, B), **5** (C, D) and **6** (E, F) in dichloromethane at various concentrations (10^{-5} - 10^{-6} M). The intensity of absorption and emission bands is decreasing with decreasing the concentration of compounds. However, the ratio of dual emission bands remains the same throughout the concentration range.

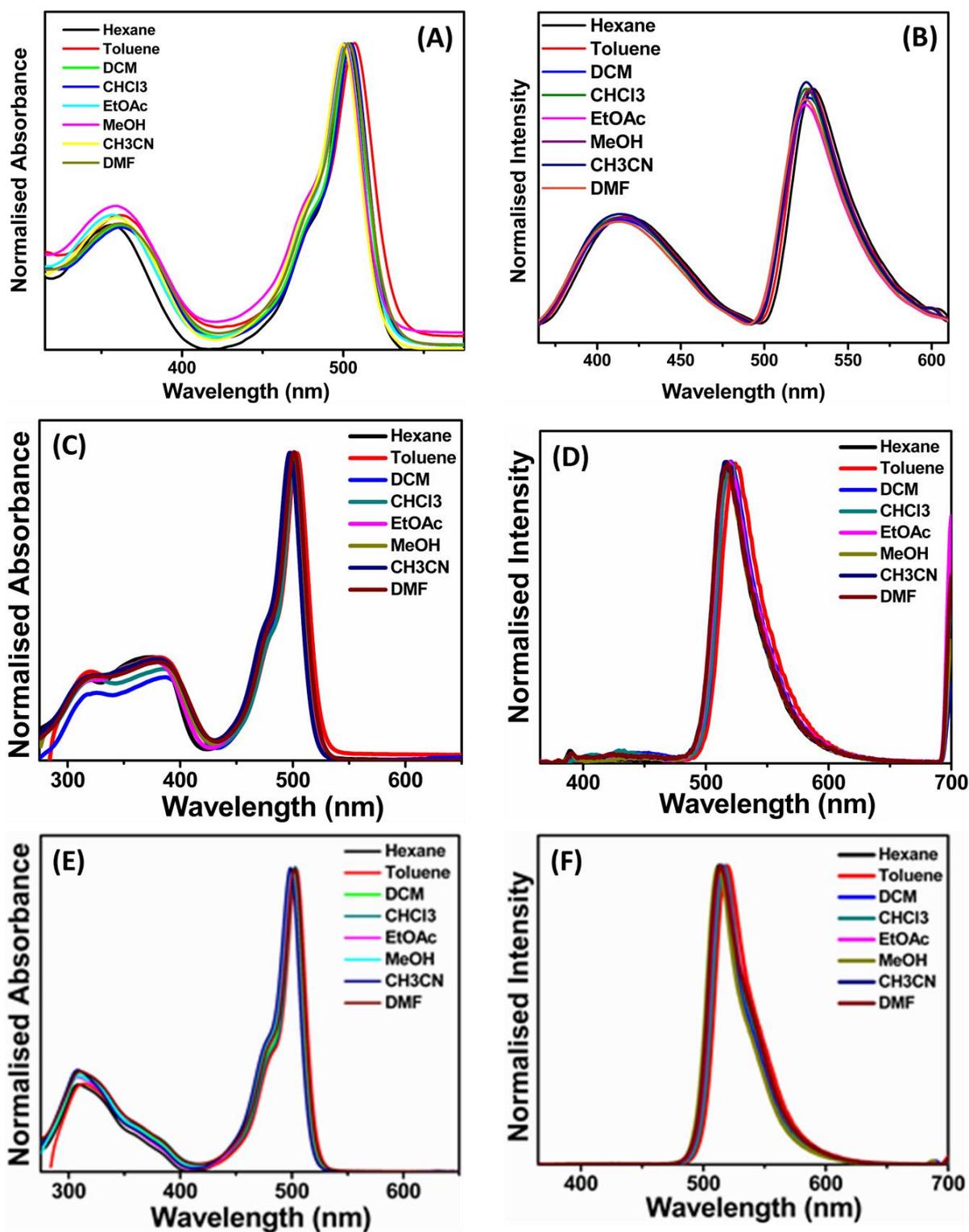


Figure S63. Normalized UV-Visible (left) and fluorescence (λ_{ex} at 350 nm) (right) spectra of **1** (A, B), **2** (C, D), and **3** (E, F) in solvents of different polarity (10 μM). With increasing polarity of solvents, absorption and emission bands have changed minimally.

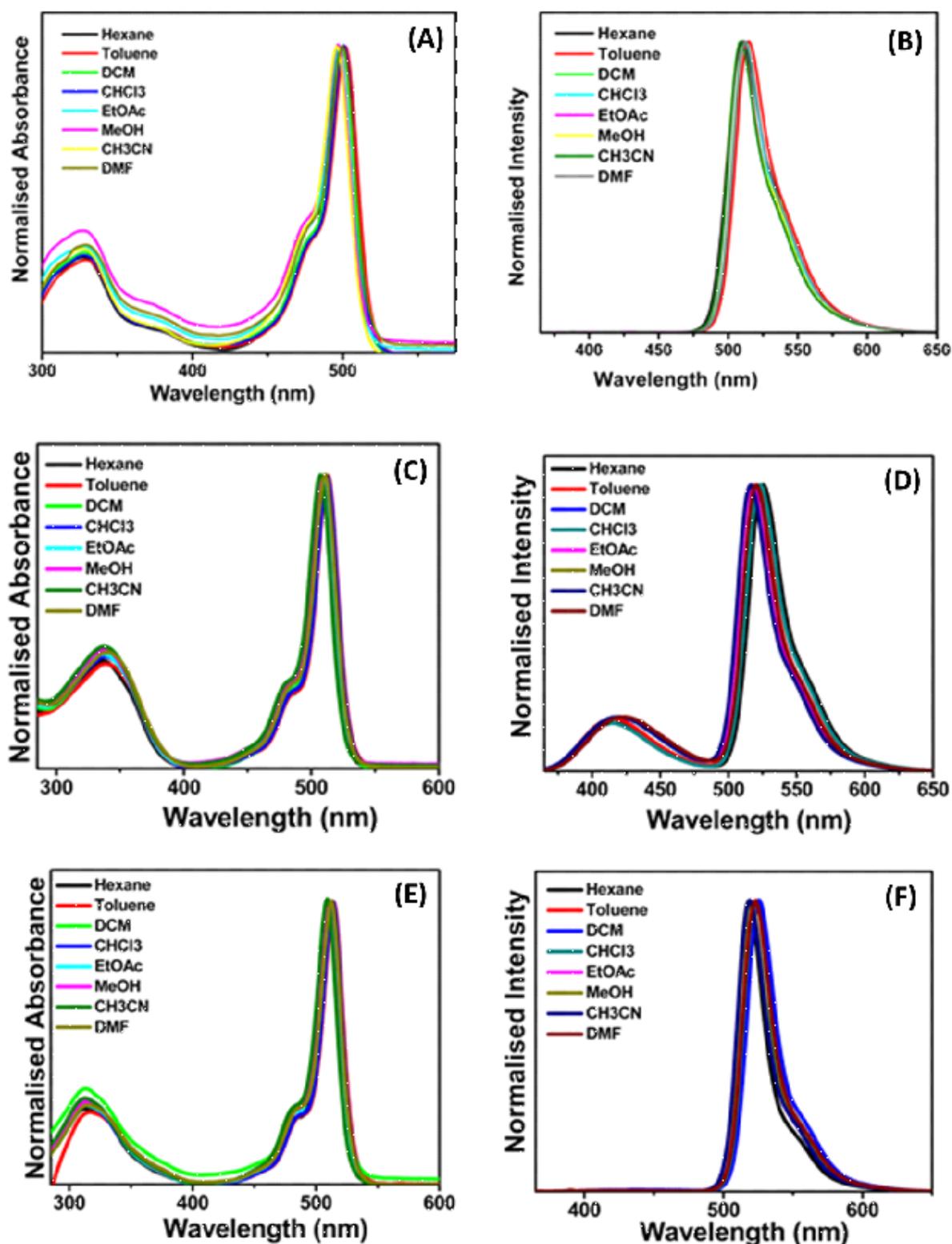


Figure S64. Normalized UV-Visible (left) and fluorescence (λ_{ex} at 350 nm) (right) spectra of **4** (A, B), **5** (C, D), and **6** (E, F) in solvents of different polarity (10 μ M). With increasing polarity of solvents, absorption and emission bands have changed minimally.

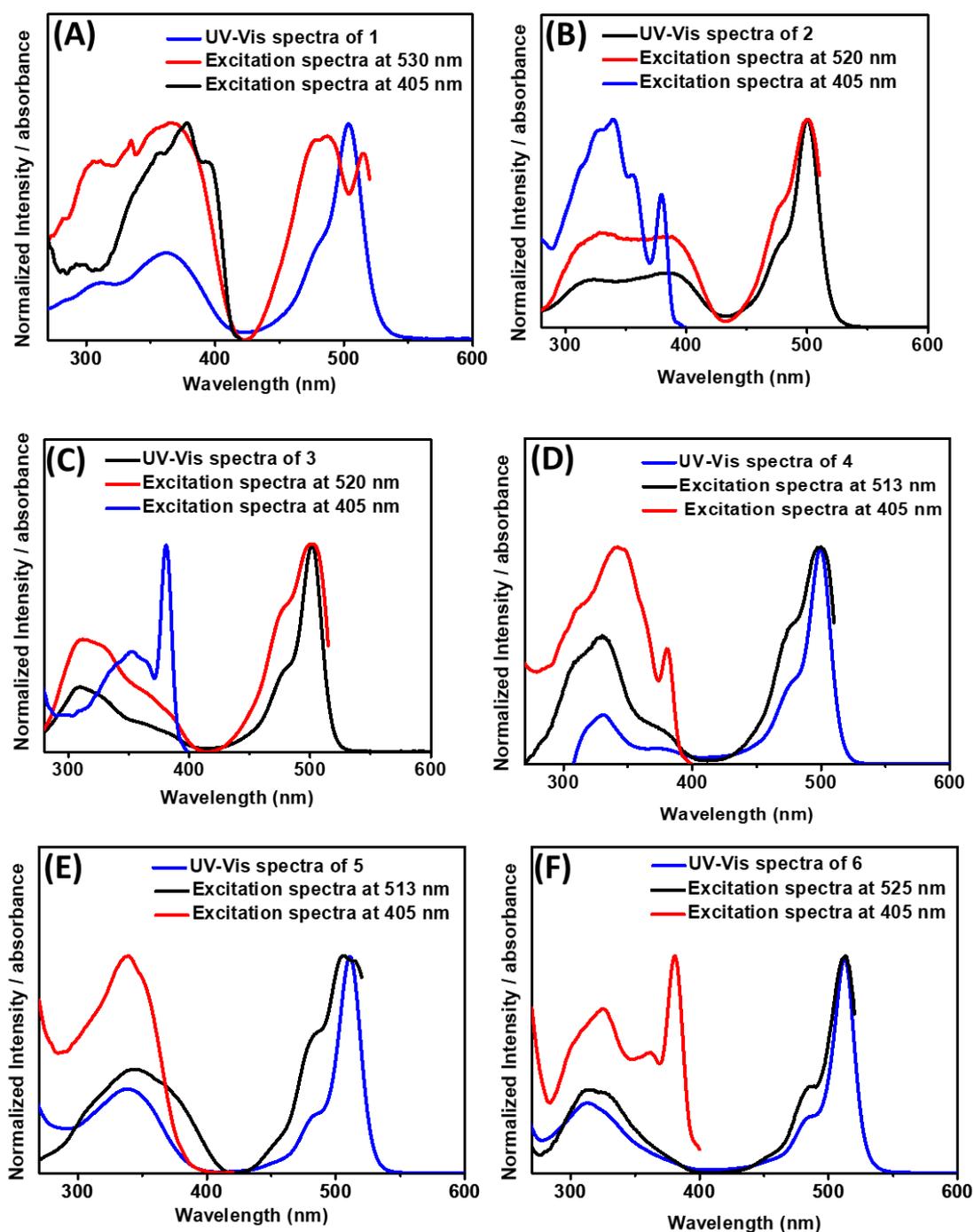


Figure S65. Comparison of normalized UV-visible absorption and excitation spectra of **1** (A), **2** (B) **3** (C), **4** (D) **5** (E) and **6** (F) in dichloromethane (10 μ M). The excitation spectra of parent compounds are duplicate of the absorption spectrum; these results indicate that dual emission bands are coming from a single molecular system.

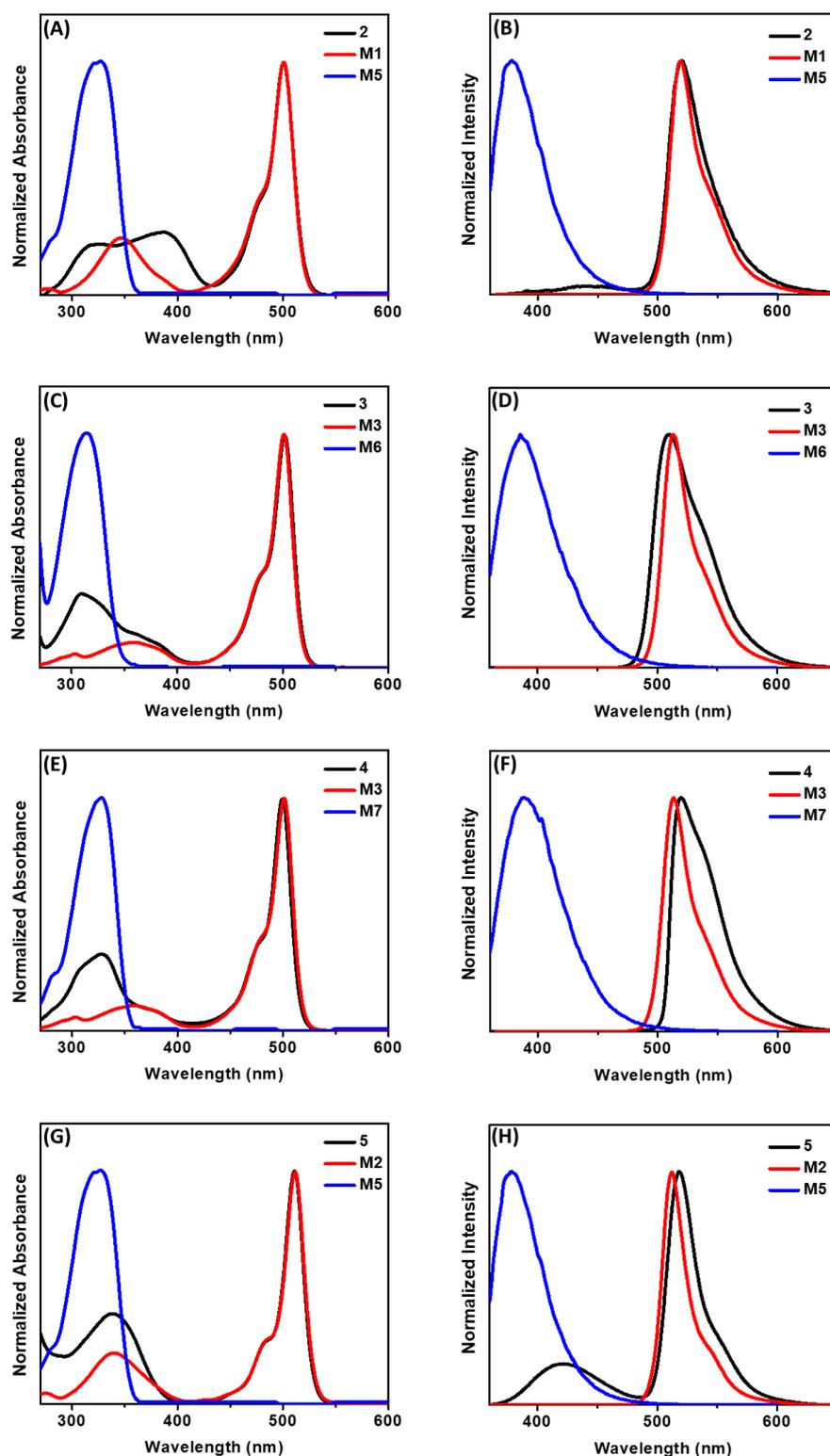


Figure S66. Normalized absorption and emission (λ_{ex} at 350 nm) spectra of **2-5** with respect to the model compounds (in DCM, conc. 10 μM). (A) absorption of **2**, **M1** and **M5**, (B) emission of **2**, **M1** and **M5**, (C) absorption of **3**, **M3** and **M6**, (D) emission of **3**, **M3**, and **M6**. (E) absorption of **4**, **M2** and **M3**, (F) emission of **4**, **M3** and **M7**, (G) absorption of **5**, **M1** and **M4**, (H) emission of **5**, **M2**, and **M5**.

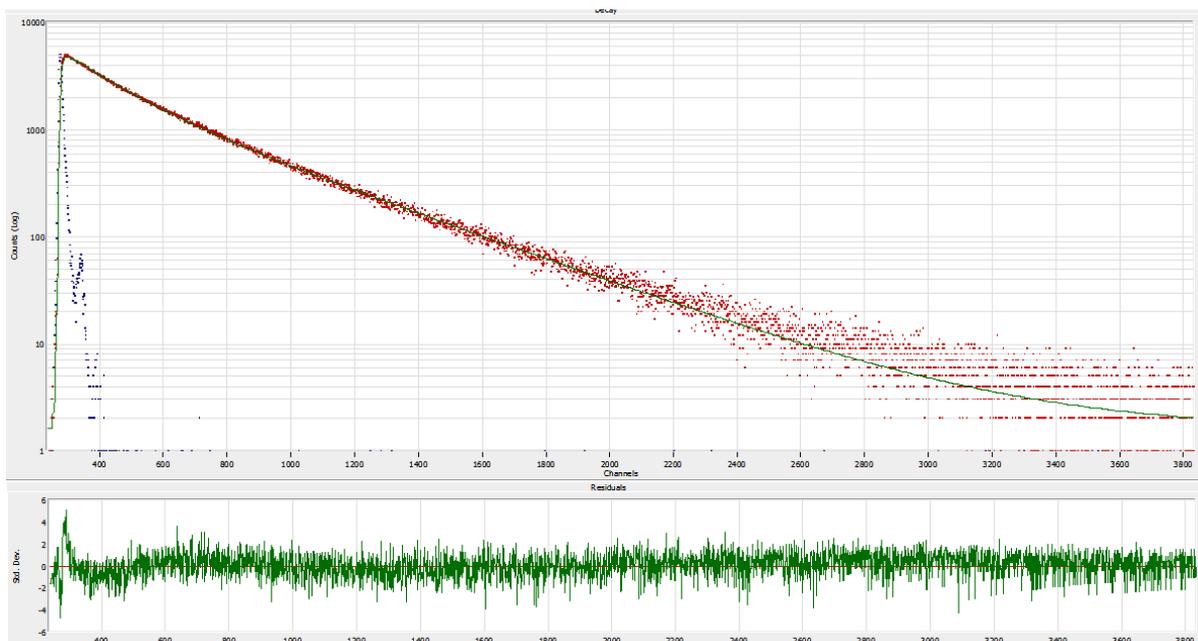


Figure S67. Fluorescence decay profile of **1** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

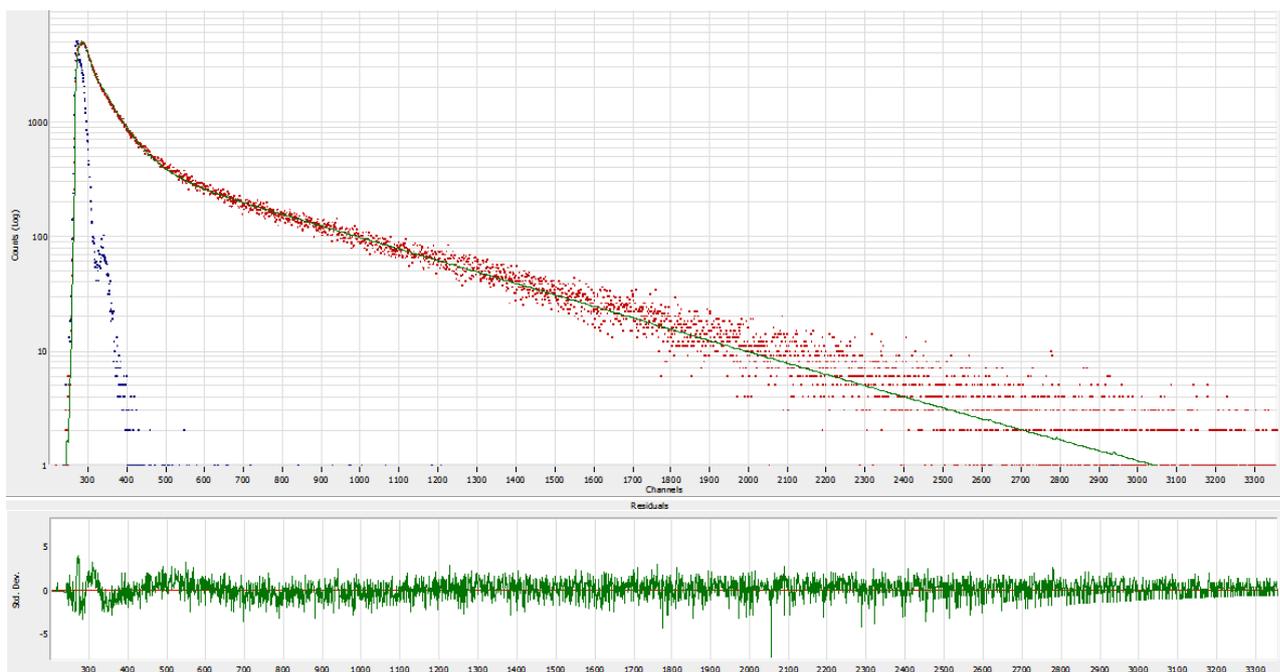


Figure S68. Fluorescence decay profile of **1** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

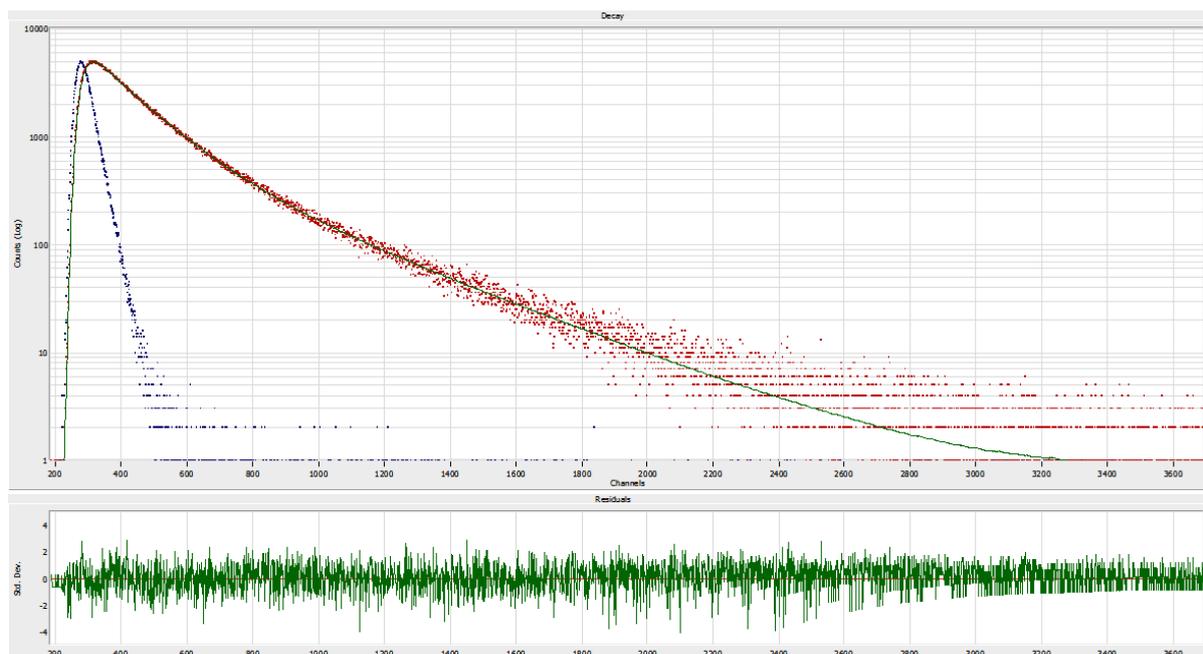


Figure S69. Fluorescence decay profile of **2** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

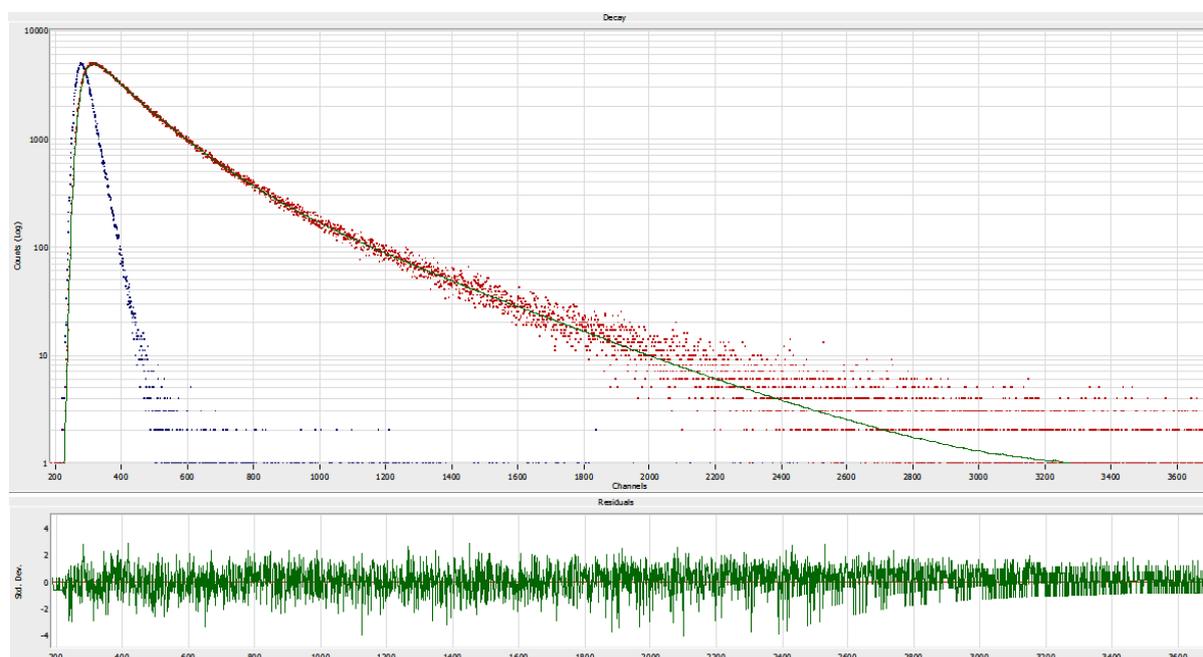


Figure S70. Fluorescence decay profile of **2** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

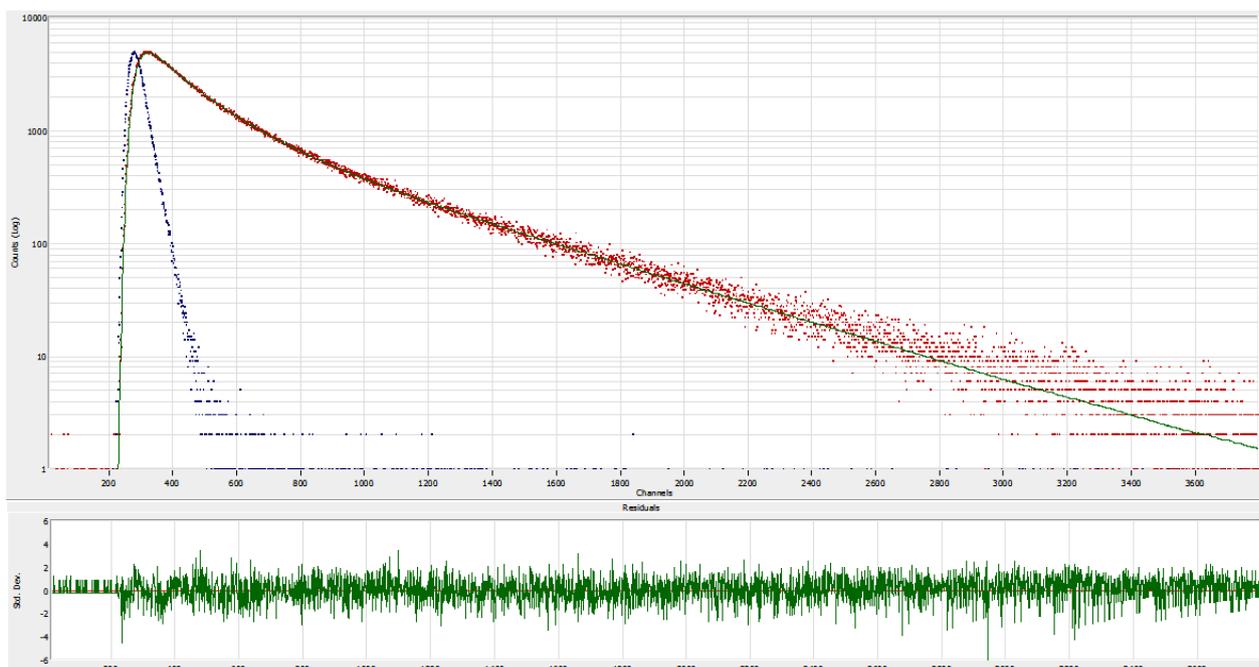


Figure S71. Fluorescence decay profile of **3** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

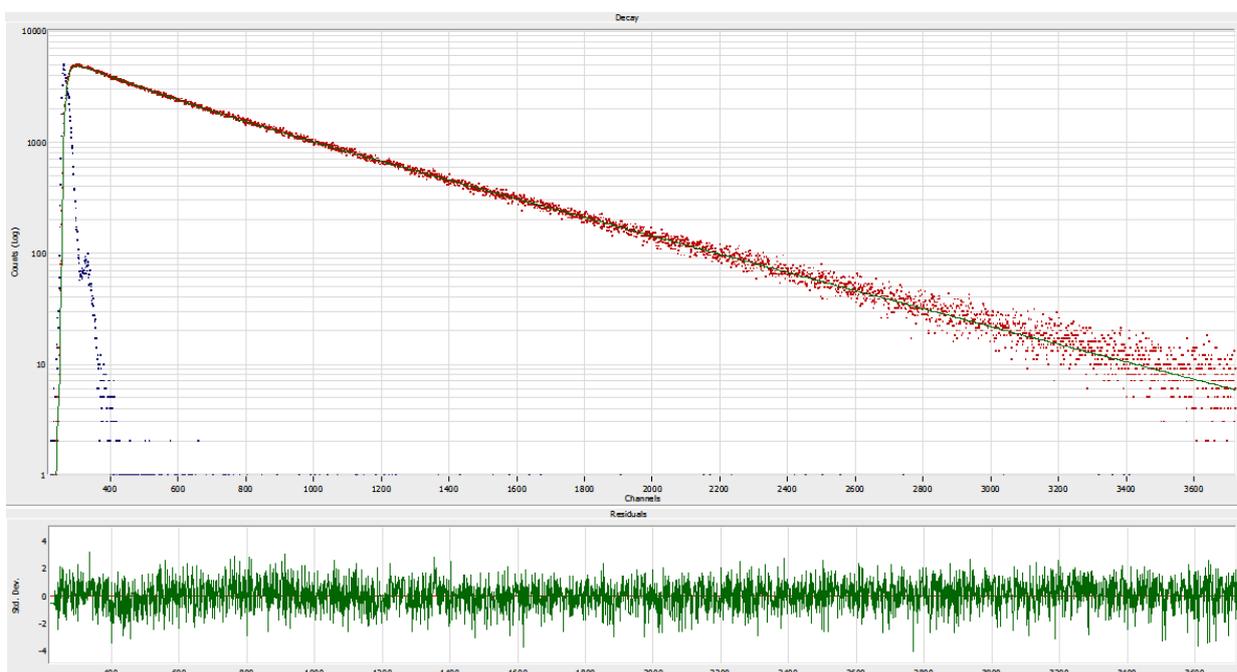


Figure S72. Fluorescence decay profile of **3** in dichloromethane. ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

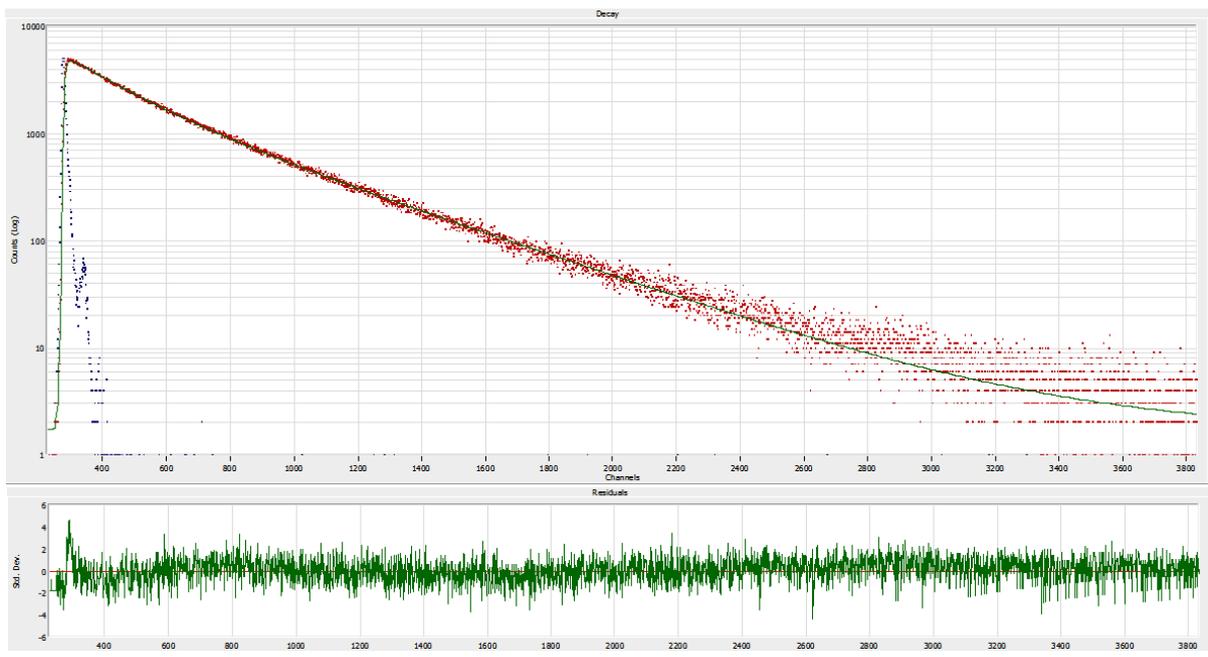


Figure S73. Fluorescence decay profile of **4** in dichloromethane ($\lambda_{ex} = 370$ nm, and $\lambda_{em} = 410$ nm).

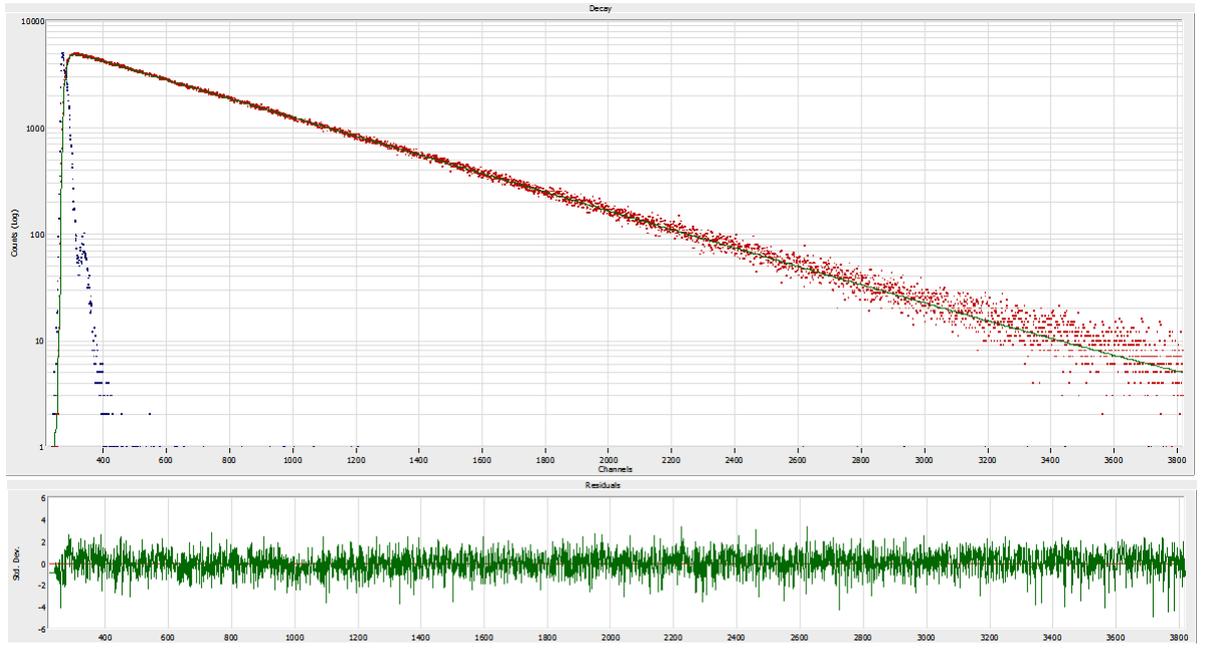


Figure S74. Fluorescence decay profile of **4** in dichloromethane ($\lambda_{ex} = 469$ nm, and $\lambda_{em} = 520$ nm).

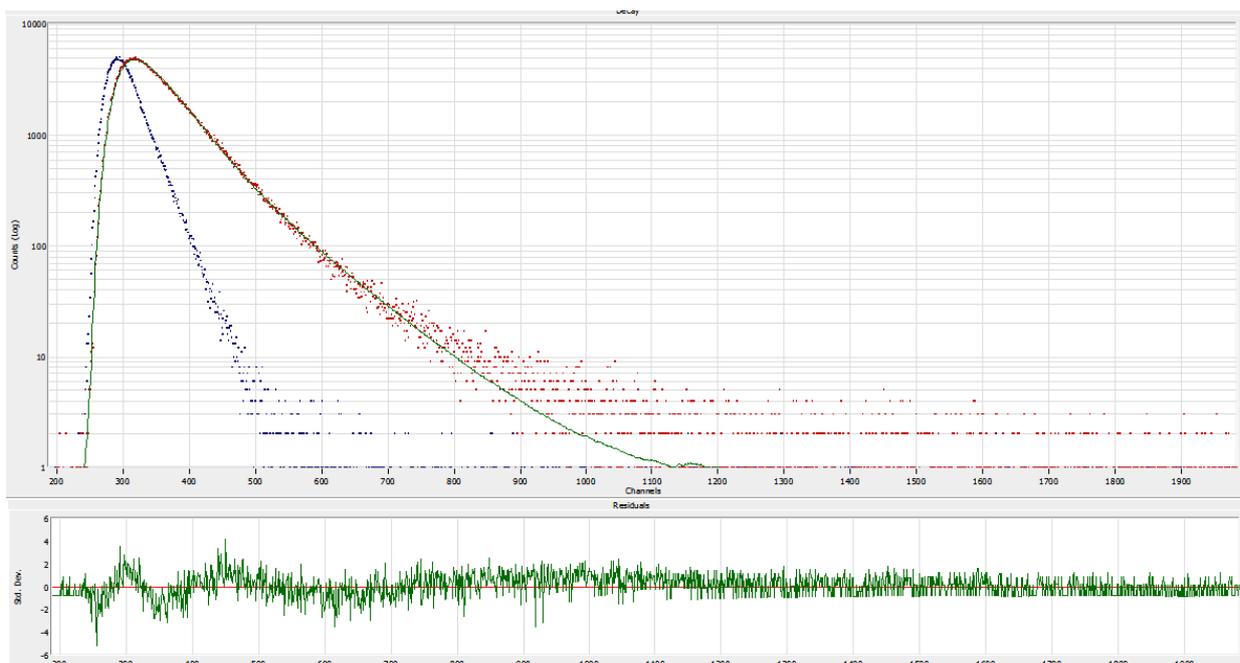


Figure S75. Fluorescence decay profile of **5** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

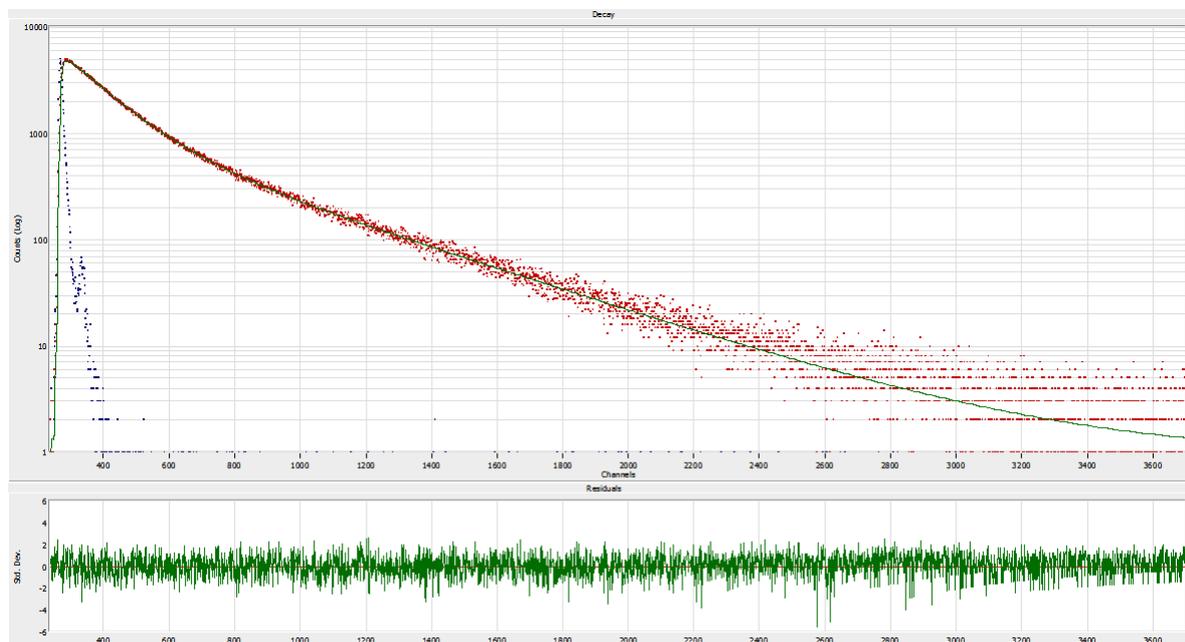


Figure S76. Fluorescence decay profile of **5** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

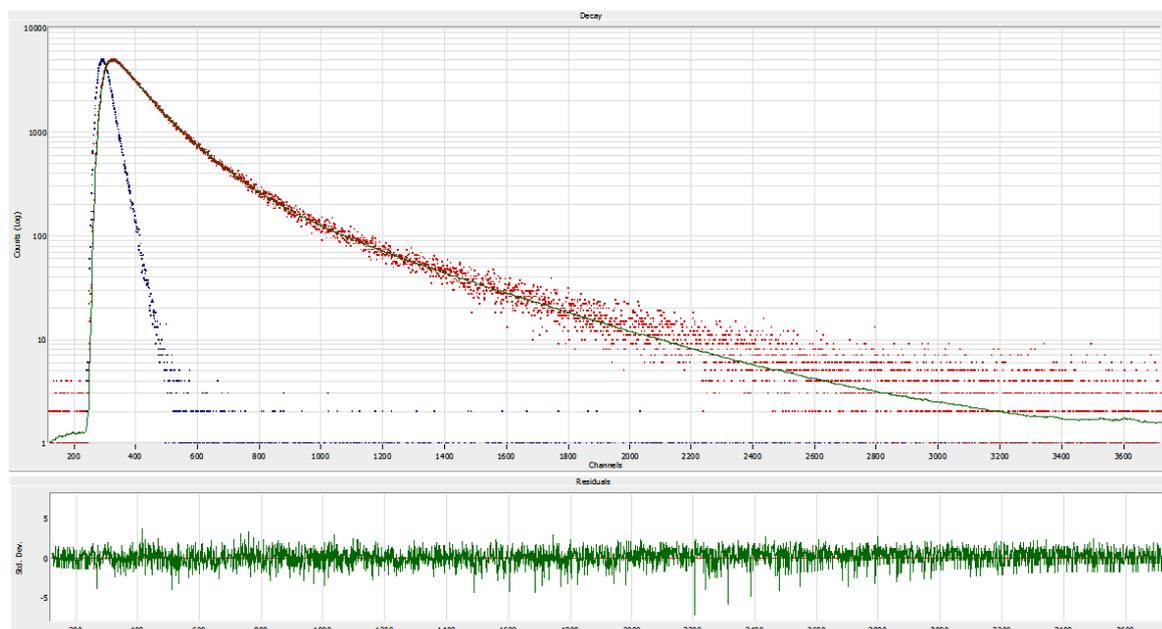


Figure S77. Fluorescence decay profile of **6** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

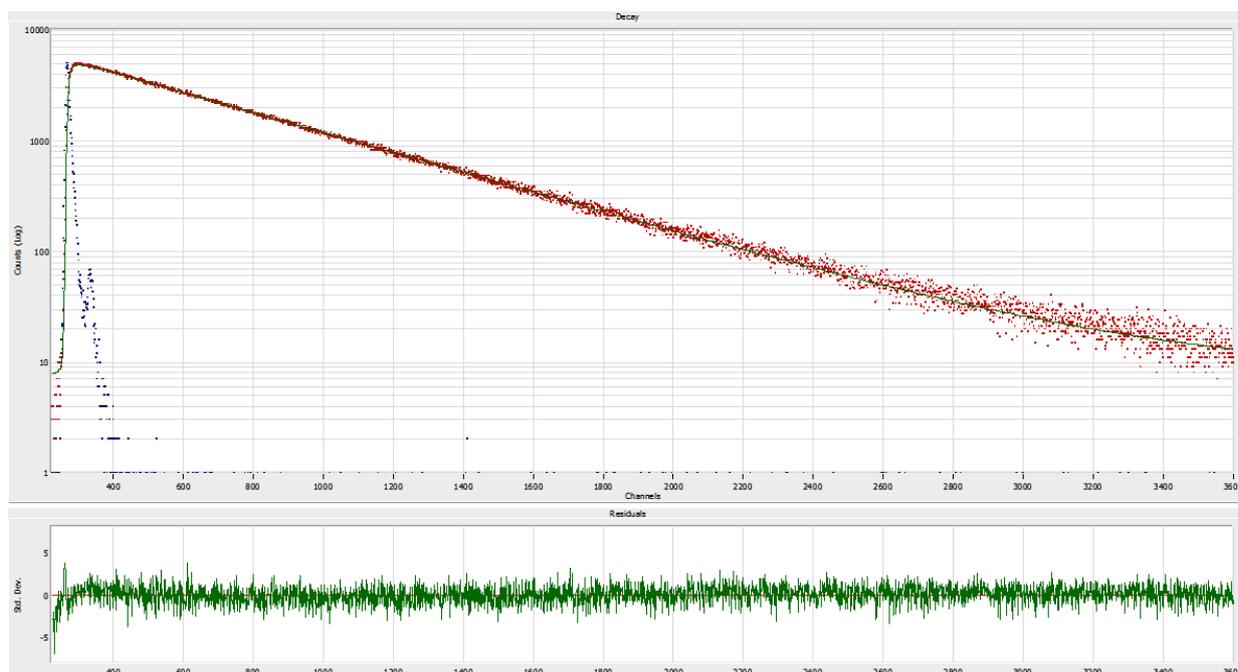


Figure S78. Fluorescence decay profile of **6** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

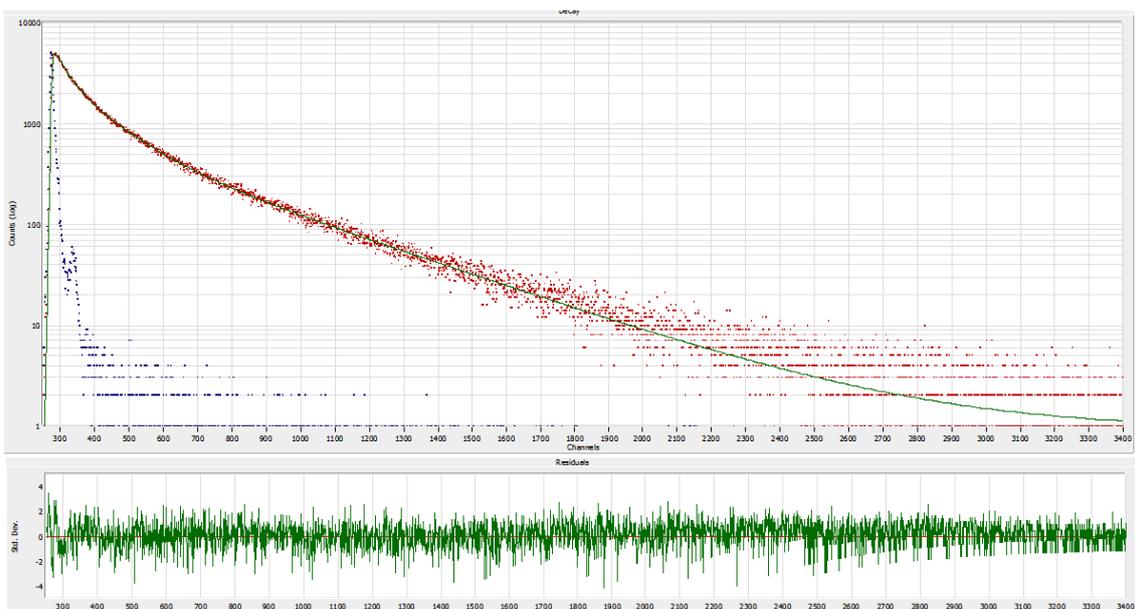


Figure S79. Fluorescence decay profile of **R1** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

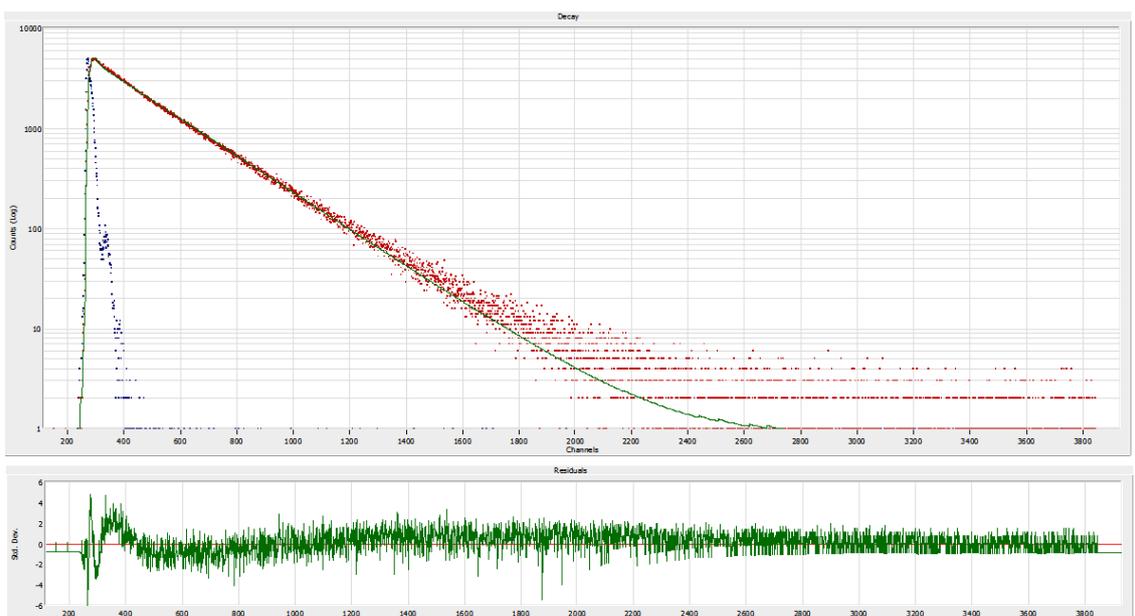


Figure S80. Fluorescence decay profile of **R1** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

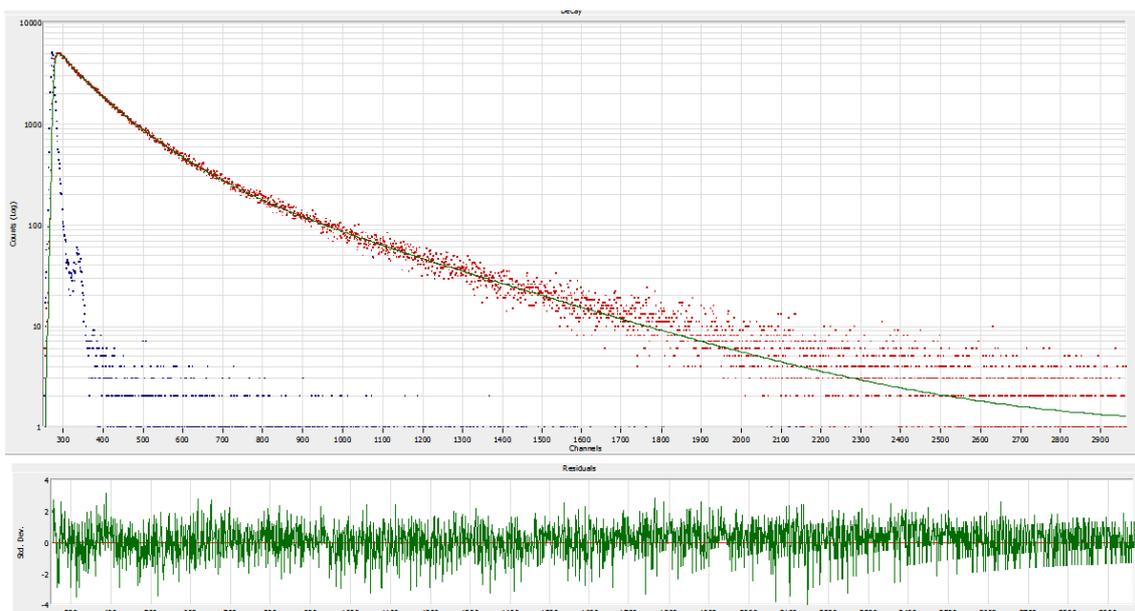


Figure S81. Fluorescence decay profile of **R2** in dichloromethane ($\lambda_{\text{ex}} = 370$ nm, and $\lambda_{\text{em}} = 410$ nm).

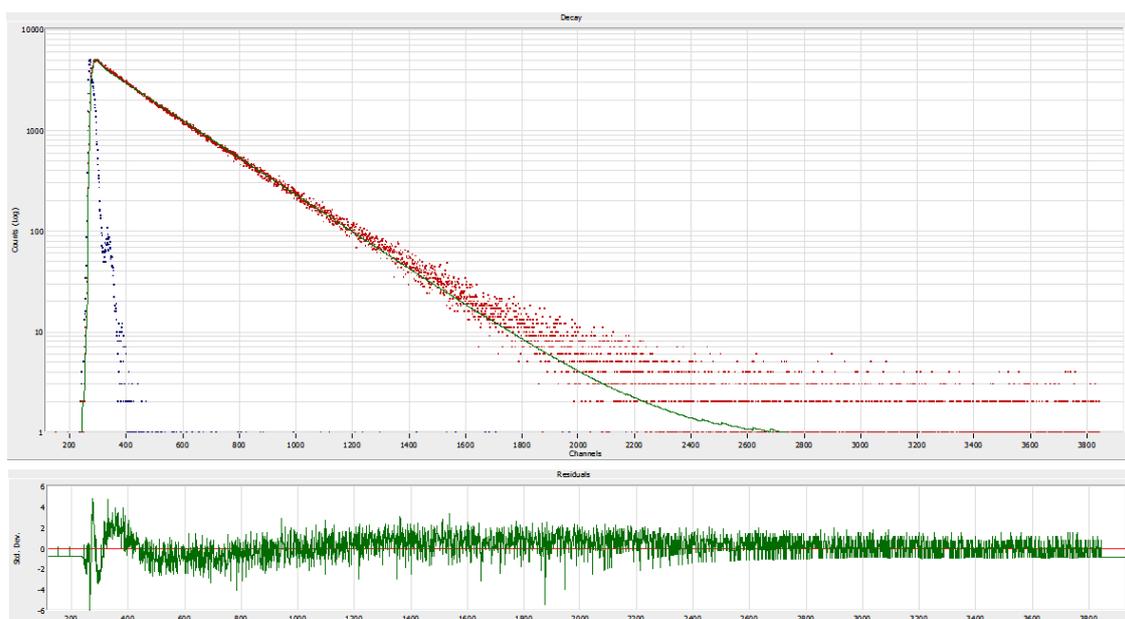


Figure S82. Fluorescence decay profile of **R2** in dichloromethane ($\lambda_{\text{ex}} = 469$ nm, and $\lambda_{\text{em}} = 520$ nm).

Table S3. Fluorescence lifetimes (τ), average lifetime $\langle\tau\rangle$ (in ns), radiative (k_r , 10^7 s^{-1}) and non-radiative (k_{nr} , 10^7 s^{-1}) rates for all compounds.

Dyads	Φ (λ_{em} = 510 nm)	τ (ns)		$\langle\tau\rangle$ (ns)		$\lambda_{em} = 510 \text{ nm}$	
		$\lambda_{em} = 410 \text{ nm}$	$\lambda_{em} = 510 \text{ nm}$	$\lambda_{em} = 410 \text{ nm}$	$\lambda_{em} = 510 \text{ nm}$	k_r (10^7 s^{-1})	k_{nr} (10^7 s^{-1})
1	0.38	0.8 (44%)	0.6 (51%)	5.94	5.30	7.2	11.7
		6.7 (56%)	6.0 (49%)				
2	0.34	1.9 (64%)	5.0 (9%)	3.70	0.59	57.6	111.9
		6.7 (37%)	0.1 (91%)				
3	0.86	1.7 (63%)	6.7 (100%)	2.96		12.8	2.1
		6.1 (37%)					
4	0.84	3.4 (44%)	7.5 (100%)	7.38		11.2	2.1
		8.9 (56%)					
5	0.76	0.55 (68%)	6.3 (100%)	0.79		12.1	3.8
		1.3 (32%)					
6	0.81	2.2 (46%)	2.8 (5%)	4.56	4.90	16.5	3.9
		6.9 (54%)	7.3 (95%)				
R1	0.49	2.5 (43%)	3.0 (100%)	4.04		16.3	17.0
		5.2 (57%)					
R2	0.42	2.4 (38%)	3.5 (100%)	4.28		12.0	16.6
		5.4 (62%)					

Excitation energy transfer rate calculation:

The energy transfer rate for **1**, **2**, **5**, **R1**, and **R2** was calculated using the following equation:

$$ETE = \frac{k_T}{k_T + \frac{1}{\tau_D}} \quad \text{i.e.,} \quad k_T = \frac{ETE}{(1-ETE)\tau_D} \quad \dots \text{Equation S1}$$

ETE is the energy transfer efficiency (calculated), k_T is the energy transfer rate, and τ_D is the donor's emission lifetime in the absence of an acceptor. Model complex **M4** is considered as

the donor for **1**, **R1**, and **R2**; **M5** for **2** and **5**; **M6** for **3** and **6** and **M7** for **4** (Chart S1, Figure S83).

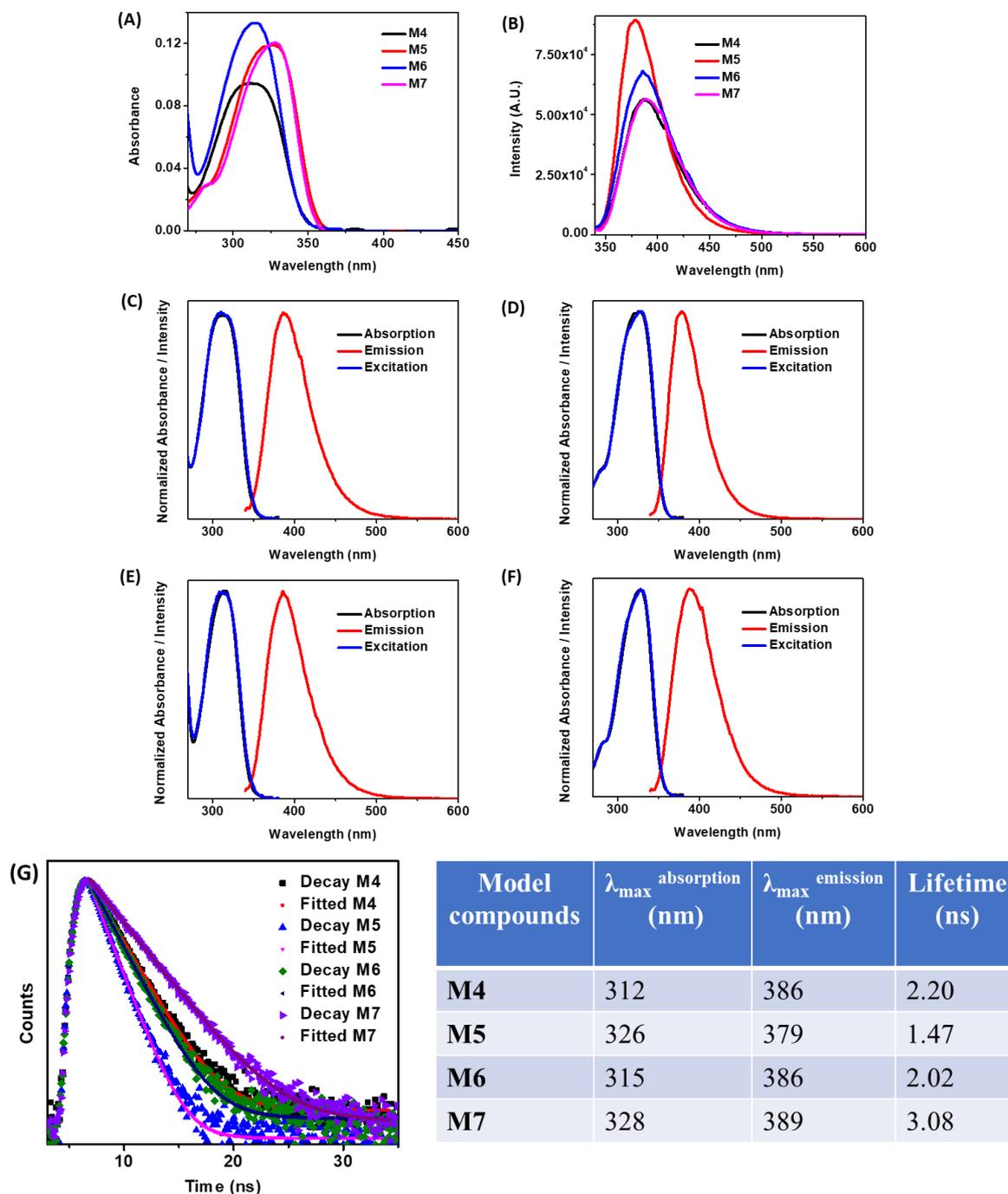


Figure S83. (A) Absorption spectra of **M4**, **M5**, **M6**, and **M7** (10 μM in dichloromethane). (B) Emission spectra ($\lambda_{\text{ex}} = 330 \text{ nm}$) of **M4**, **M5**, **M6**, and **M7** (10 μM in dichloromethane). (C), (D), (E) and (F) Normalized absorption, emission ($\lambda_{\text{ex}} = 330 \text{ nm}$) and excitation ($\lambda_{\text{em}} = 390 \text{ nm}$) spectra of **M4**, **M5**, **M6** and **M7**, respectively. (G) Time-resolved fluorescence decay profiles along with the fitted curves of **M4**, **M5**, **M6**, and **M7**; table include the absorption maxima, emission maxima, and corresponding fluorescence lifetime values ($\lambda_{\text{ex}} = 330 \text{ nm}$).

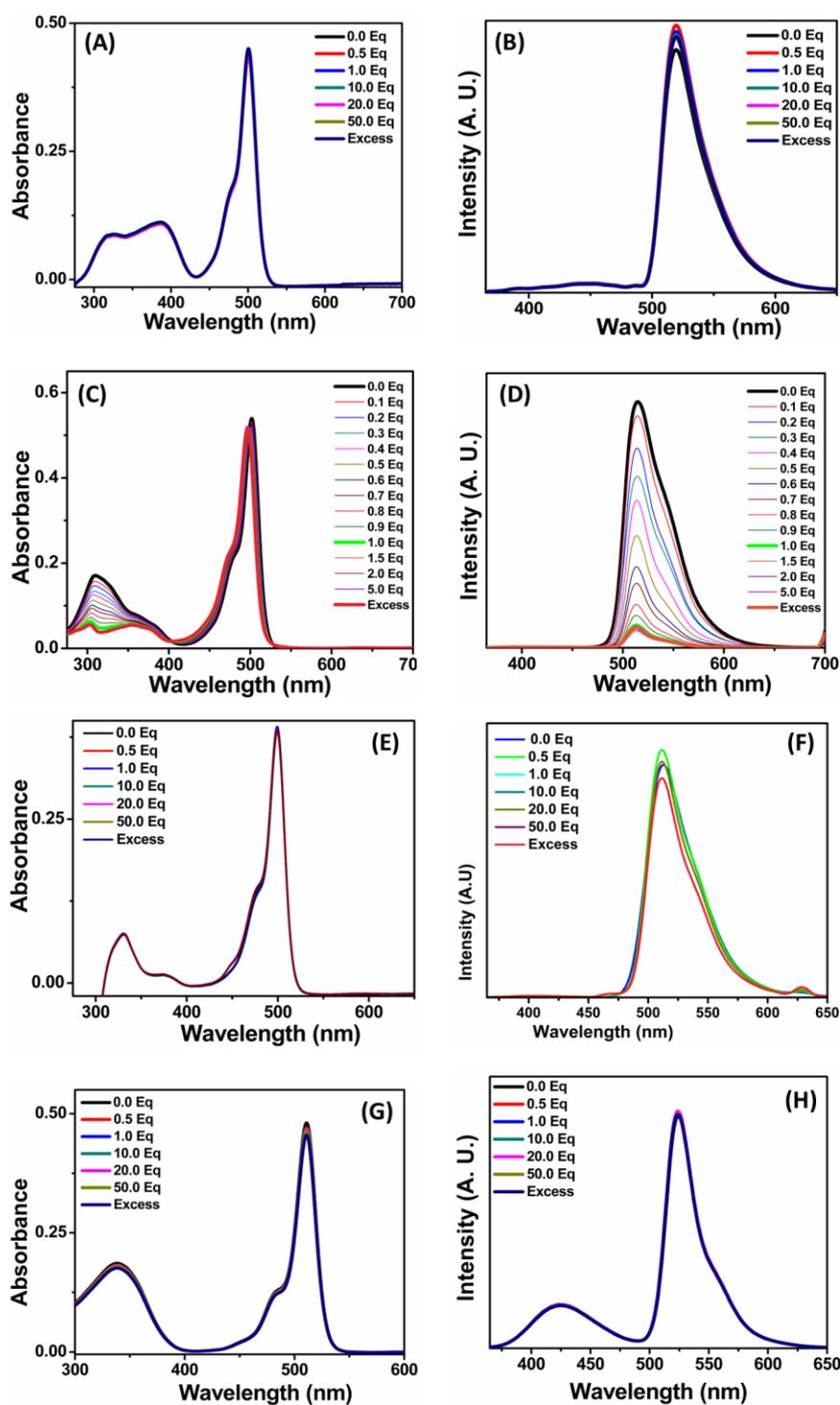


Figure S84. Changes in absorption and emission spectra of **2**, **3**, **4**, and **5** (in DCM, 1.0×10^{-5} M) upon incremental addition of TBAF (in DCM, 1.0×10^{-3} M). (A) absorption of **2**, (B) emission of **2**, (C) absorption of **3**, (D) emission of **3**, (E) absorption of **4**, (F) emission of **4**, (G) absorption of **5**, (H) emission of **5**.

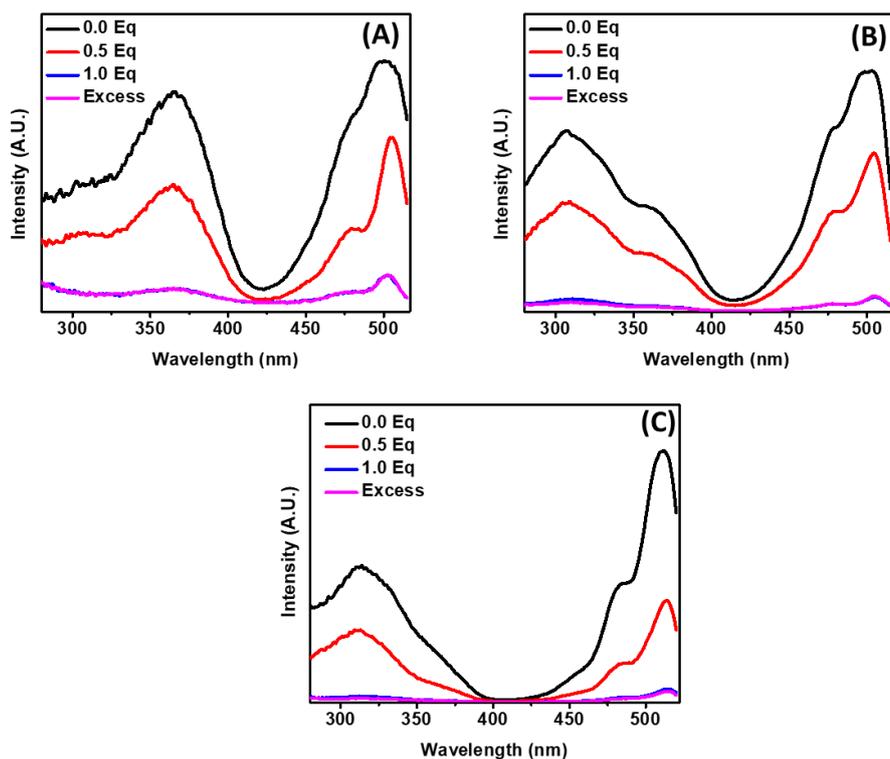


Figure S85. Changes in excitation spectra ($\lambda_{em} = 520$ nm) of **1** (A), **3** (B) and **6** (C) (in DCM, 1.0×10^{-5} M) upon incremental addition of TBAF (in DCM, 1.0×10^{-3} M).

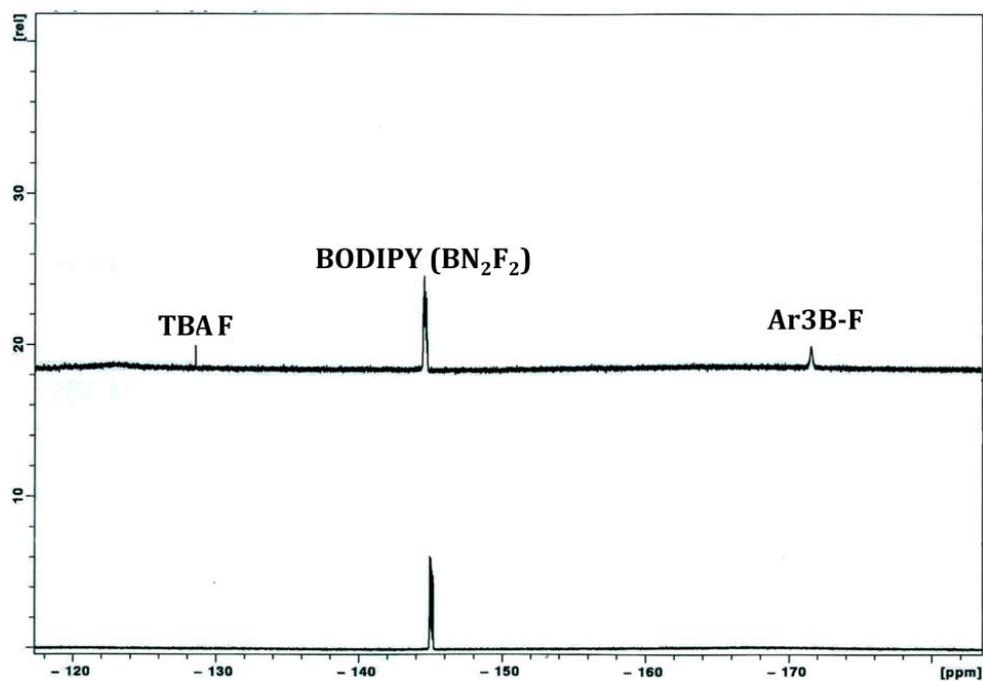


Figure S86. Changes in ^{19}F NMR of **1** upon addition of excess TBAF (tetrabutylammonium fluoride) in CDCl_3 . The ~ -172 ppm band arises from the borane bound fluoride atoms whereas the ~ -130 ppm band appears from the excess TBAF present in solution. Evidently, no observable degradation of the original compound can be followed from this data.

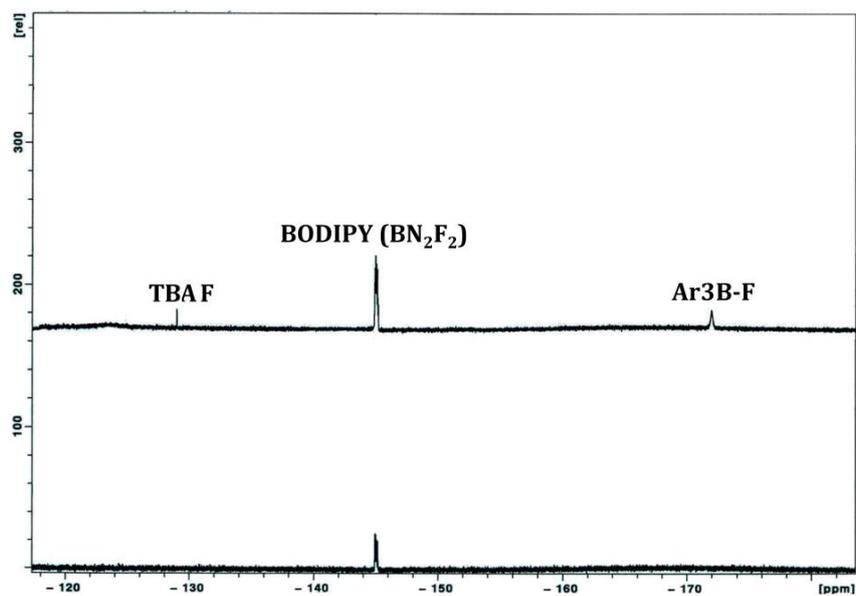


Figure S87. Changes in ^{19}F NMR of **3** upon addition of excess TBAF (tetrabutylammonium fluoride) in CDCl_3 . The ~ -172 ppm band arises from the borane bound fluoride atoms whereas the ~ -130 ppm band appears from the excess TBAF present in solution. Evidently, no observable degradation of the original compound can be followed from this data.

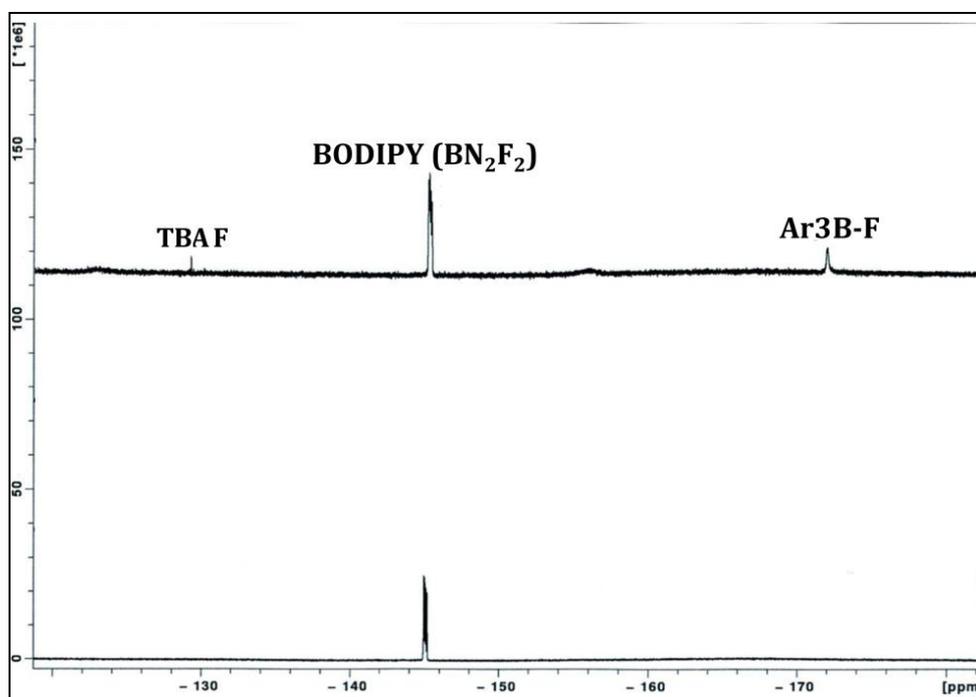


Figure S88. Changes in ^{19}F NMR of **6** upon addition of excess TBAF (tetrabutylammonium fluoride) in CDCl_3 . The ~ -172 ppm band arises from the borane bound fluoride atoms whereas the ~ -130 ppm band appears from the excess TBAF present in solution. Evidently, no observable degradation of the original compound can be followed from this data.

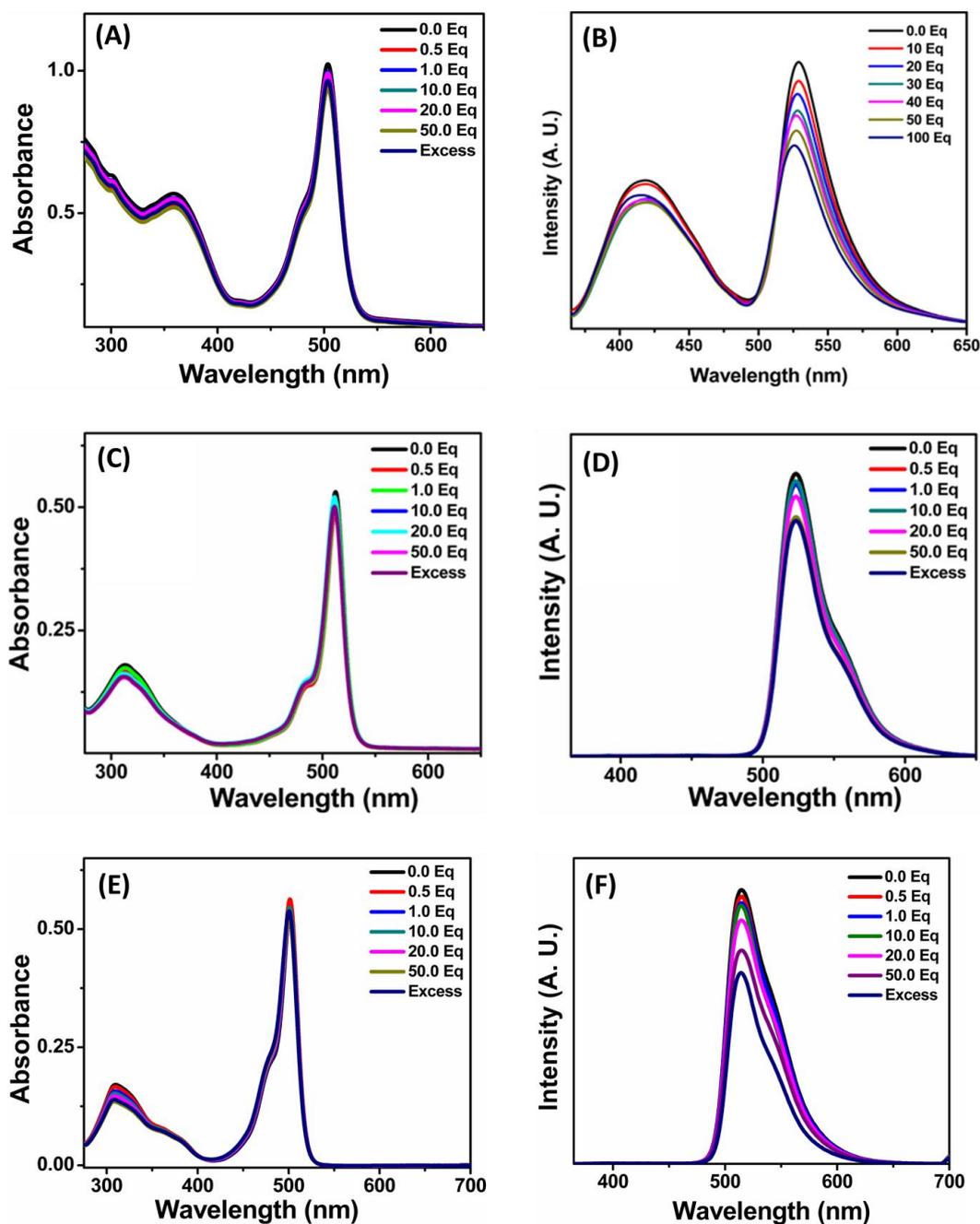


Figure S89. Changes in absorption and emission spectra (λ_{ex} at 350 nm) of **1**, **3** and **6** (in DCM, 1.0×10^{-5} M) upon incremental addition of TBA-CN (in DCM, 1.0×10^{-3} M). (A) absorption of **1**, (B) emission of **1**, (C) absorption of **3**, (D) emission of **3**, (E) absorption of **6**, (F) emission of **6**, There were minimal changes in absorption and emission spectra of the compounds upon addition of cyanide compared to fluoride ions.

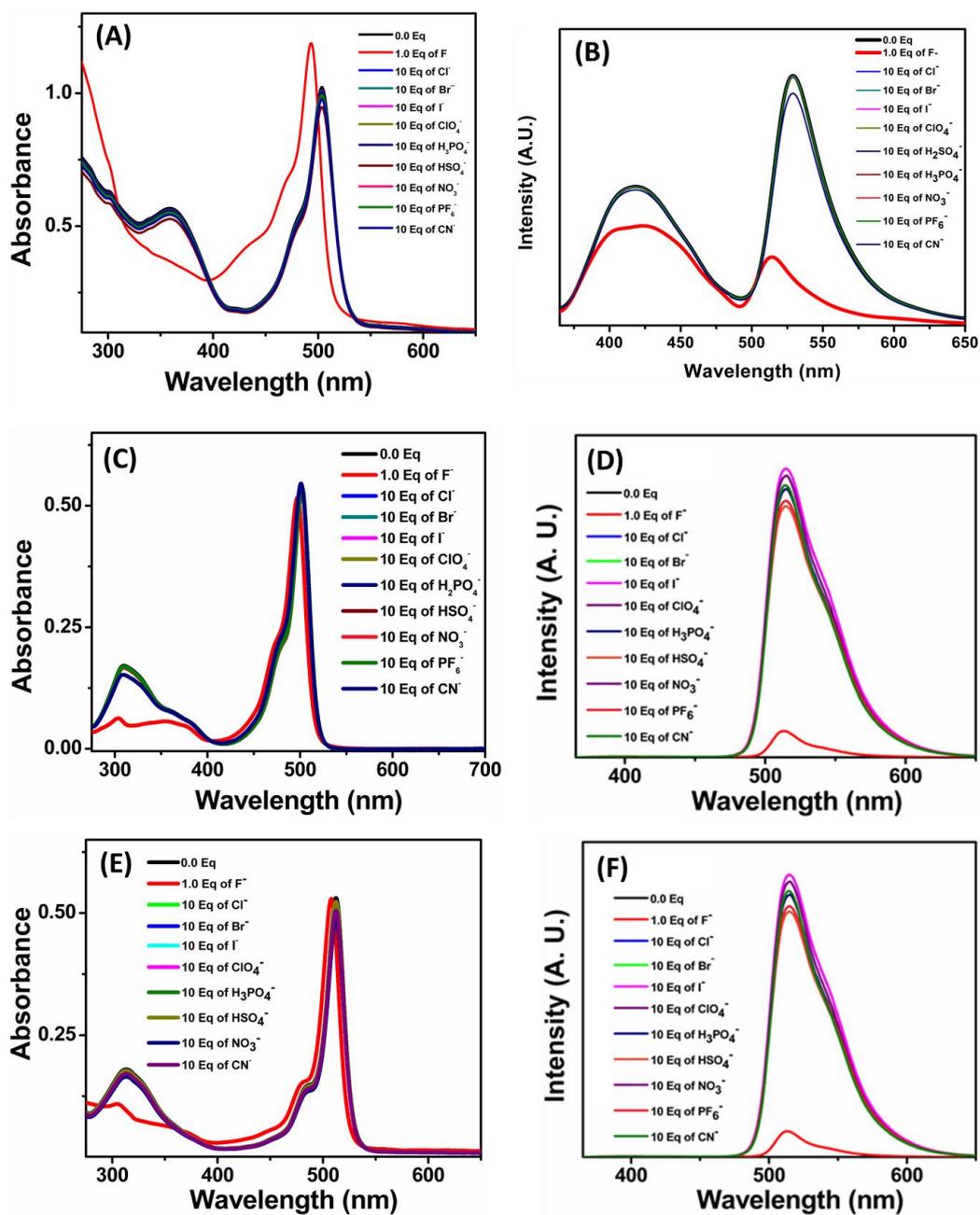


Figure S90. Absorption and emission spectra of **1**, **3** and **6** (in dichloromethane, 1.0×10^{-5} M) in presence of various anions (dichloromethane solution; 1.0×10^{-3} M, $\lambda_{\text{ex}} = 350$ nm). (A) absorption of **1**, (B) emission of **1**, (C) absorption of **3**, (D) emission of **3**, (E) absorption of **6**, (F) emission of **6**. No change in absorption and emission spectra upon the addition of various anions (10 equiv.), whereas upon the addition of 1.0 equivalent of fluoride to DCM solution of compounds, both absorptions as well as emission spectra changed.

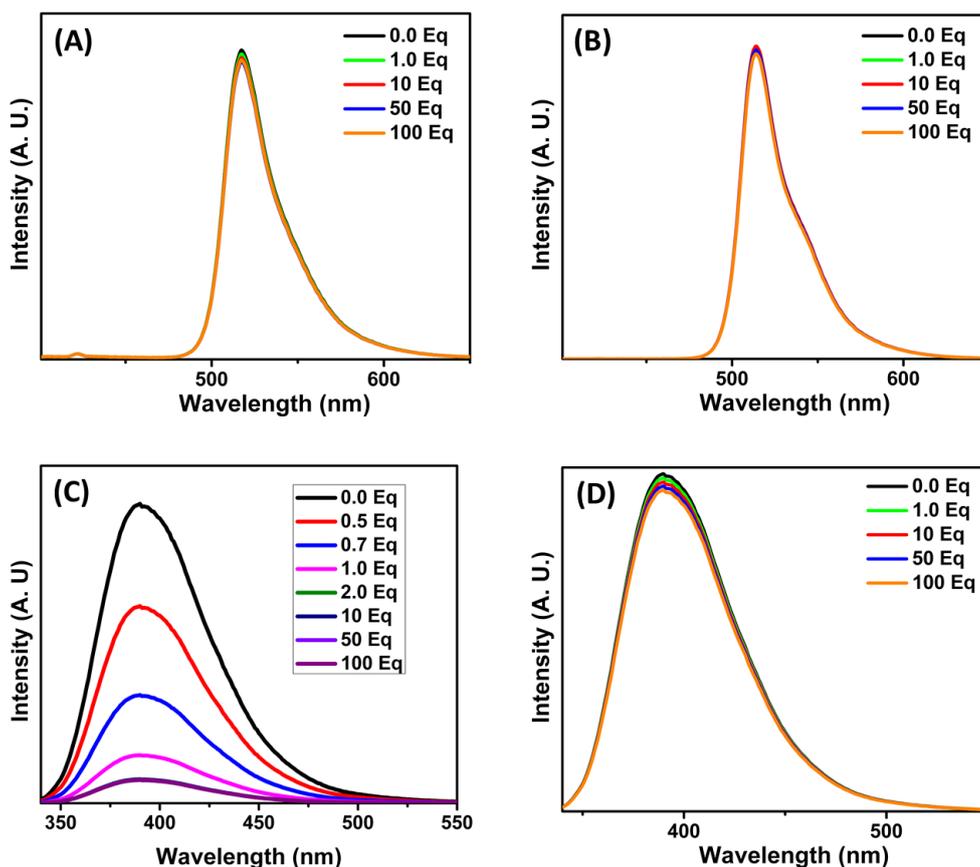


Figure S91. Fluorescence spectra ($\lambda_{\text{ex}} = 350 \text{ nm}$) of (A) **M1**, (B) **M3**, (C) **M4** and (D) **M8** (in dichloromethane, $1.0 \times 10^{-5} \text{ M}$) in presence of various amount of fluoride ions. (dichloromethane solutions, $1.0 \times 10^{-3} \text{ M}$). The emission band of **M4** at 400 nm was decreased gradually upon the addition of fluoride. Whereas, for **M1**, **M3**, and **M8**, there was no significant change in emission spectra upon the addition of 100 equivalent of fluoride ions.

Determination of Binding Constant and quenching constants¹⁷⁻¹⁸

Solution (in DCM) of compounds **1**, **3**, or **6** (2 mL, $1 \times 10^{-5} \text{ M}$) was placed in a septum screw-capped quartz cuvette and titrated against the incremental amount of fluoride ions. The change in absorbance of the band at 350 nm concerning fluoride concentration was used for calculations.

Sensor + $\text{F}^- \leftrightarrow \text{F} \cdot \text{sensor}$; here sensor is compound **1**, **3**, or **6**

$$I = K_s[\text{sensor}] + K_p[\text{F} \cdot \text{sensor}]$$

$$I_0 = K_s[\text{sensor}]_0$$

$$[\text{sensor}]_0 = [\text{sensor}] + [\text{F} \cdot \text{sensor}]$$

$$K = [\text{F} \cdot \text{sensor}] / [\text{sensor}][\text{F}]$$

$$I/I_0 = (1 + (K_p/K_s)K[\text{F}]) / (1 + K[\text{F}]) \quad (1 - I/I_0) / [\text{F}] \rightarrow K(I/I_0) - K(K_p/K_s)I/I_0 = 1 + K(1 - I/I_0) / [\text{F}]$$

Here, I_0 is initial absorbance of respective band (350 nm), I is absorbance of respective band upon addition of 1.0 equiv of Fluoride. The association constant was obtained from the slope of $(1 - I/I_0)/[F^-]$ Vs I/I_0 , which are given in Table S4.

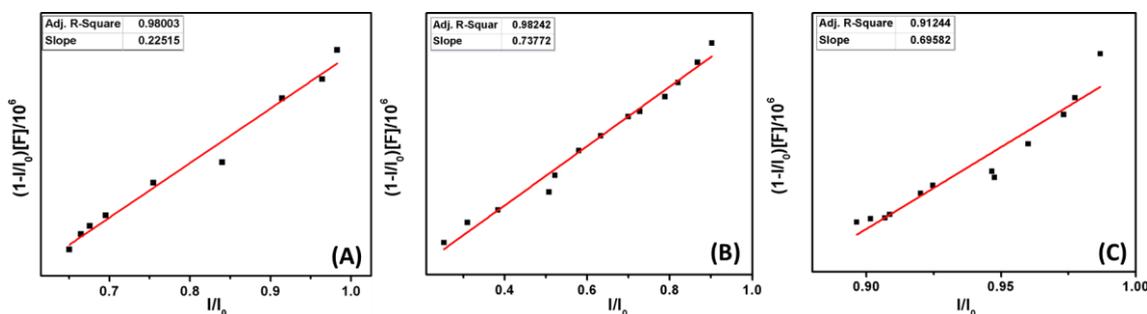


Figure S92. Binding constant measurement plots of **1** (A), **3** (B) and **6** (C). The absorbance at 350 nm band was monitored in the presence of fluoride (tetrabutylammonium fluoride).

Table S4. The association constants of **1**, **3**, and **6**.

Compounds	Association constants (10^5 M^{-1})	Quenching constants (10^6 M^{-1})
1	2.25	0.65
3	7.37	1.22
6	6.95	2.62

Calculation of Limit of Detection (LoD)

The limit of detection for **1**, **3**, and **6** calculated from the fluorescence quenching titration experiment (DCM solutions). The intercept to X-axis ($\log[F^-]$) was obtained by linear fitting of the $(I_{\max}-I)/(I_{\max}-I_{\min})$ vs $\log[F^-]$, where I_{\max} , I and I_{\min} are the initial fluorescence intensity, PL intensity at particular concentration and PL intensity at saturation point respectively. The limit of detection was calculated using the formula, $([F^-] \times \text{MWPA})/1000$ (multiplied by 10^9 to get the values in ppb), where MWPA is the molecular weight of F^- source.

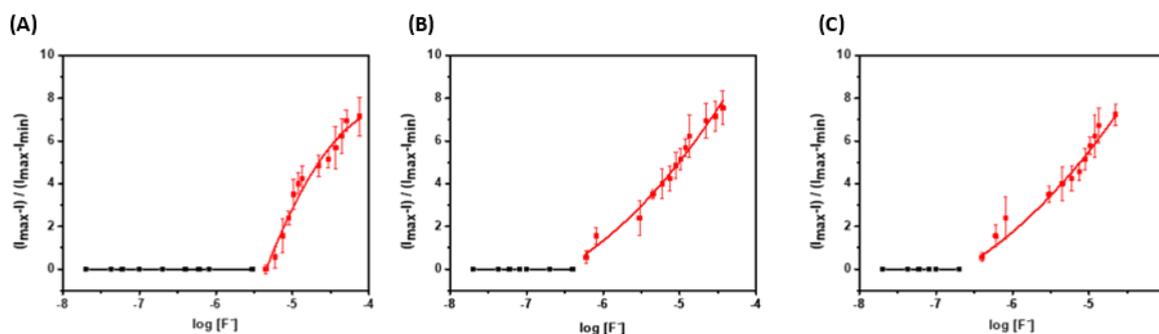


Figure S93. $(I_{\max}-I)/(I_{\max}-I_{\min})$ vs $\log[F^-]$ plots for PL data obtained for dichloromethane (CH_2Cl_2) solutions of **1** (A), **3** (B) and **6** (C). For **1**, **3**, and **6**, the lowest detection limit ($[F^-]$) was found to be $1.34 (\pm 0.06)$, $1.00 (\pm 0.05)$, and $0.07 (\pm 0.03)$, respectively.

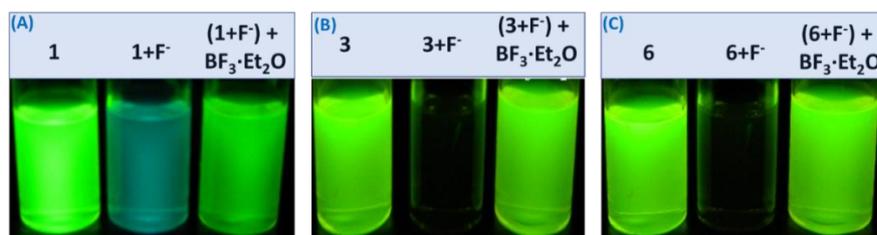


Figure S94. Digital photograph demonstrating the regeneration of sensors **1**, **3**, and **6**. The addition of fluoride quenched the fluorescence (sensor + F⁻), and the addition of BF₃·Et₂O to fluoride complexes restored the fluorescence of free Lewis acids **1**, **3**, and **6**.

Excited state dipole moment calculation:

Excited state dipole moments were calculated using the Lippert-Mataga equation:

$$\Delta\nu_s = [2(\mu_e - \mu_g)^2 / hca^3] \Delta f + \Delta\nu_s^\circ$$

where $\Delta\nu_s$ is the Stokes shift, the superscript “^o” indicates the absence of solvent, μ_g and μ_e are dipole moments in the ground state and the excited state, respectively, a is Onsager cavity radius. μ_g and a were obtained from DFT calculation.

The orientation polarizability Δf is defined as

$$\Delta f = [(\varepsilon - 1) / (2\varepsilon + 1)] - [(n^2 - 1) / (2n^2 + 1)]$$

where ε and n denote solvent dielectric constant and refractive index, respectively.

Table S6. Ground and excited state dipole moment values of **1-6**.

	μ_g (Debye)	μ_e (Debye)	$(\mu_e - \mu_g)$ (Debye)
1	5.47	6.97	1.50
2	6.83	8.67	1.84
3	4.38	7.75	3.37
4	5.76	7.72	1.96
5	5.20	6.95	1.75
6	2.90	6.00	3.10
R1	3.89	10.13	6.24
R2	4.50	7.77	3.27

Cyclic voltammetry studies:

Table S7. Summary of CV data of **1-6, R1** and **R2**.

Compound	1	2	3	4	5	6	R1	R2
E_{Red}	-1.18 ^c -1.79 ^c	-1.27 ^c -1.95 ^c	-1.33 ^c -2.38 ^c	-1.37 ^c -2.24 ^d	-1.48 ^c -2.07 ^c	-1.64 ^c -2.48 ^c	-1.34 ^c -2.34 ^d	-1.62 ^c -2.06 ^d
E_{Ox}	1.20 ^d	1.23 ^d	1.23 ^d	1.23 ^d	0.90 ^d	0.91 ^c	1.25 ^d	0.80 ^c
LUMO ^a (eV) (from CV)	-3.62	-3.53	-3.47	-3.43	-3.32	-3.16	-3.46	-3.18
HOMO ^a (eV) (from CV)	-6.00	-6.03	-6.03	-6.03	-5.70	-5.71	-6.05	-5.60
LUMO ^b (eV) (from DFT)	-2.85	-2.71	-2.79	-2.66	-2.50	-2.57	-2.63	-2.35
HOMO ^b (eV) (from DFT)	-5.87	-5.77	-5.92	-5.80	-5.43	-5.56	-5.52	-5.34
LUMO-HOMO (eV) (from CV)	2.38	2.50	2.56	2.60	2.38	2.55	2.59	2.42
LUMO-HOMO (eV) (from DFT)	3.02	3.06	3.13	3.14	2.93	2.99	2.89	2.99
LUMO-HOMO (eV) (from UV- Vis spectra)	2.46	2.48	2.47	2.48	2.43	2.42	2.42	2.47

[a] Determined from CV data using the equation $E_{LUMO} = -(E_{Red, 1/2} + 4.8)$ and $E_{HOMO} = -(E_{Ox, 1/2} + 4.8)$; [b] from DFT calculations at b3lyp/6-31g (d) level of theory; [c] quasi-reversible or reversible (E_{Red} or $E_{Ox} = 0.5 (E_{pc} + E_{pa})$); [d] Irreversible ($E_{Ox} = E_{pa}$; $E_{Red} = E_{pc}$); E_{pa} = Anodic peak potential, E_{pc} = Cathodic peak potential.

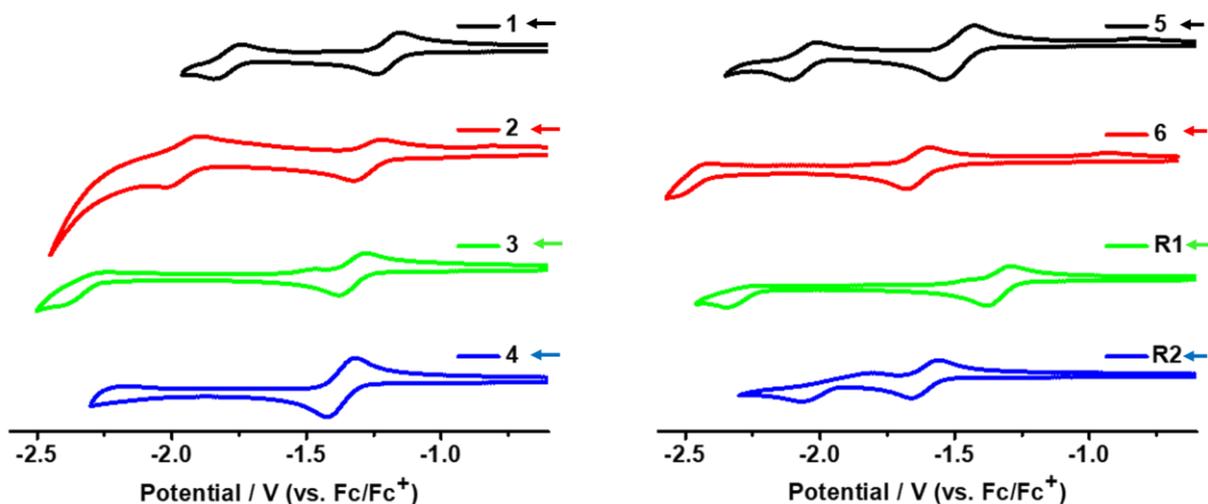


Figure S95. Cyclic voltammograms (cathodic scan) of **1-4** (left) and **5-6**, **R1** and **R2** (right) recorded in THF solution (1 mM) at a voltage sweep rate of 100 mV/s, with [Bu₄N][PF₆] (100 mM) as supporting electrolyte at 20 °C. A Pt disk electrode was used as working electrode, a Pt wire was used as counter electrode and a Ag wire was used as reference electrode. The potential scales are referenced to the ferrocene/ferrocenium couple.

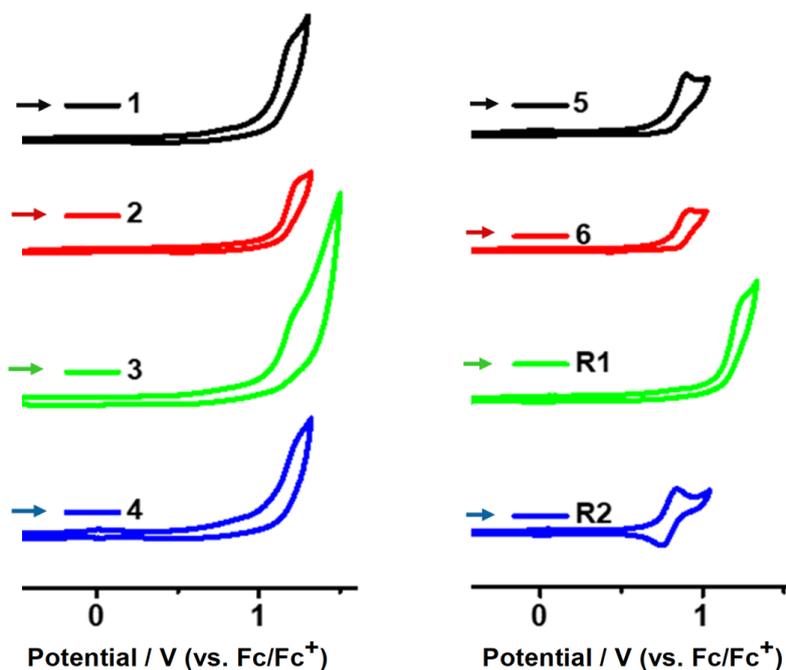


Figure S96. Cyclic voltammograms (anodic scan) of **1-4** (left) and **5-6**, **R1** and **R2** (right) recorded in dichloromethane solution (1 mM) at a voltage sweep rate of 100 mV/s, with [Bu₄N][PF₆] (100 mM) as supporting electrolyte at 20 °C. A Pt disk electrode was used as working electrode, a Pt wire was used as counter electrode and a Ag wire was used as reference electrode. The potential scales are referenced to the ferrocene/ferrocenium couple.

Theoretical calculations¹²

Table S8. Summary of dominant electronic transitions of **1-6** obtained from TD-DFT calculations (in gas phase).

Compound	Excited State	E/eV	E/nm	f	Dominant transitions (percentage contribution)
1	S1	2.9244	423.97	0.0344	HOMO-1 → LUMO (90%)
	S2	2.9937	414.15	0.2349	HOMO → LUMO (82%)
	S3	3.0371	408.23	0.0665	HOMO-2 → LUMO (95%)
	S8	3.6246	342.07	0.1038	HOMO-1 → LUMO+1 (39%) HOMO → LUMO+1 (40%)
	S9	3.6635	338.43	0.1456	HOMO-1 → LUMO+1 (56%) HOMO → LUMO+1 (29%)
	S10	3.6749	337.38	0.3219	HOMO-7 → LUMO (40%) HOMO-6 → LUMO (54%)
2	S1	3.0366	408.30	0.2429	HOMO → LUMO (84%)
	S3	3.1674	391.44	0.1923	HOMO-2 → LUMO (90%)
	S8	3.4916	355.09	0.1106	HOMO-5 → LUMO (92%)
	S9	3.5984	344.56	0.1922	HOMO-7 → LUMO (42%) HOMO → LUMO+1 (34%)
	S10	3.6209	342.41	0.0871	HOMO-1 → LUMO+1 (82%)
3	S1	2.9878	414.97	0.0003	HOMO-1 → LUMO (99%)
	S3	3.1356	395.40	0.3037	HOMO → LUMO (84%)
	S8	3.4898	355.28	0.0936	HOMO-1 → LUMO+1 (98%)
	S10	3.6116	343.29	0.1457	HOMO-7 → LUMO (84%)
	S11	3.6465	340.01	0.0617	HOMO-2 → LUMO+1 (98%)

	S12	3.7466	330.92	0.1111	HOMO-3 → LUMO+1 (84%)
4	S1	2.8646	432.81	0.0102	HOMO-2 → LUMO (77%)
	S4	3.1630	391.98	0.2824	HOMO → LUMO (74%)
	S8	3.6137	343.10	0.0852	HOMO-1 → LUMO+1 (84%)
	S10	3.6448	340.17	0.2052	HOMO-7 → LUMO (79%)
	S11	3.7328	332.14	0.1111	HOMO-3 → LUMO+1 (92%)
5	S1	2.9042	426.91	0.2835	HOMO → LUMO (92%)
	S3	3.2566	380.72	0.0717	HOMO → LUMO+1 (87%)
	S4	3.2601	380.31	0.2507	HOMO-2 → LUMO (79%)
	S8	3.5963	344.76	0.0932	HOMO-7 → LUMO (90%)
	S9	3.5988	344.52	0.0544	HOMO-5 → LUMO (87%)
	S10	3.6515	339.54	0.0936	HOMO-1 → LUMO+1 (90%)
	S11	3.7378	331.71	0.0753	HOMO-8 → LUMO (20%) HOMO-2 → LUMO+1 (70%)
6	S1	3.0126	411.55	0.3909	HOMO → LUMO (95%)
	S9	3.6034	344.07	0.0870	HOMO-1 → LUMO+1 (98%)
	S10	3.6321	341.35	0.0874	HOMO-7 → LUMO (92%)
	S11	3.7268	332.68	0.1162	HOMO-2 → LUMO+1 (98%)
	S12	3.7860	327.48	0.0514	HOMO-3 → LUMO+1 (98%)

Table S9. Summary of dominant electronic transitions of **1-6** obtained from TD-DFT calculations (in dichloromethane solvated state).

Compound	Excited State	E/eV	E/nm	f	Dominant transitions (percentage contribution)
1	S1	2.8153	440.40	0.0291	HOMO-1 → LUMO (92%)
	S2	2.9212	424.43	0.2571	HOMO → LUMO (54%) HOMO-2 → LUMO (39%)
	S3	2.9218	424.34	0.1964	HOMO → LUMO (35%) HOMO-2 → LUMO (58%)
	S7	3.5002	354.22	0.3137	HOMO-5 → LUMO (98%)
	S9	3.6217	342.34	0.1095	HOMO-1 → LUMO+1 (87%)
	S11	3.7422	331.31	0.1131	HOMO-1 → LUMO (87%)
2	S1	2.9586	419.06	0.3854	HOMO → LUMO (87%)
	S2	2.9778	416.36	0.2006	HOMO-2 → LUMO (90%)
	S7	3.2910	376.74	0.1574	HOMO-5 → LUMO (90%)
	S8	3.5252	351.71	0.0833	HOMO-7 → LUMO (87%)
	S9	3.5668	347.61	0.1623	HOMO-1 → LUMO+1 (92%)
3	S1	2.9143	425.43	0.0004	HOMO-1 → LUMO (98%)
	S3	3.0117	411.68	0.4187	HOMO → LUMO (92%)
	S8	3.5025	353.98	0.1180	HOMO-1 → LUMO+1 (98%)
	S9	3.5879	345.56	0.1351	HOMO-7 → LUMO (92%)
	S10	3.6634	338.44	0.0954	HOMO-2 → LUMO+1 (98%)
4	S1	2.6828	462.14	0.0102	HOMO-2 → LUMO (72%)
	S4	3.0438	407.34	0.4072	HOMO → LUMO (74%)
	S8	3.6067	343.76	0.0855	HOMO-1 → LUMO+1 (79%)

	S9	3.6204	342.46	0.2379	HOMO-7 → LUMO (77%)
	S11	3.7315	332.26	0.1362	HOMO-3 → LUMO+1 (92%)
5	S1	2.8374	436.97	0.4460	HOMO → LUMO (98%)
	S3	3.0977	400.25	0.2549	HOMO-2 → LUMO (87%)
	S7	3.4186	362.67	0.0986	HOMO-5 → LUMO (84%)
	S9	3.5863	345.71	0.1672	HOMO-1 → LUMO+1 (77%)
	S10	3.5947	344.91	0.0757	HOMO-7 → LUMO (70%)
	S11	3.7133	333.89	0.0619	HOMO-2 → LUMO+1 (92%)
6	S1	2.8878	429.34	0.4986	HOMO → LUMO (98%)
	S9	3.6049	343.93	0.1083	HOMO-1 → LUMO+1 (98%)
	S10	3.6215	342.36	0.0867	HOMO-7 → LUMO (98%)
	S11	3.7240	332.94	0.1594	HOMO-2 → LUMO+1 (95%)

Table S10. Comparison of metric parameters of the ground state optimized structures of all the molecules obtained from DFT calculation in the gas phase and solution phase (in dichloromethane).

Compounds	DFT optimized structure (gas phase)				DFT optimized structure (solution phase, in dichloromethane)			
	Bond distance (Å)		Dihedral angle (°)		Bond distance (Å)		Dihedral angle (°)	
	B(borane) - C(spacer)	C(BODIPY) -C(spacer)	BC2 - spacer	BODIPY - spacer	B(borane) - C(spacer)	C(BODIPY) -C(spacer)	BC2 - spacer	BODIPY - spacer
1	1.576	1.482	27.23	54.90	1.577	1.482	27.77	54.42
2	1.593	1.481	53.05	54.30	1.595	1.480	53.42	53.49
3	1.574	1.497	28.25	88.61	1.574	1.496	28.44	88.33
4	1.598	1.499	57.60	88.19	1.598	1.499	57.97	87.66
5	1.592	1.483	52.51	55.95	1.594	1.482	53.04	55.78
6	1.576	1.497	23.08	89.53	1.578	1.497	22.81	88.84
R1	1.575	1.484	27.03	55.81	1.575	1.484	27.35	55.45
R2	1.577	1.495	21.39	88.80	1.577	1.495	21.44	88.05

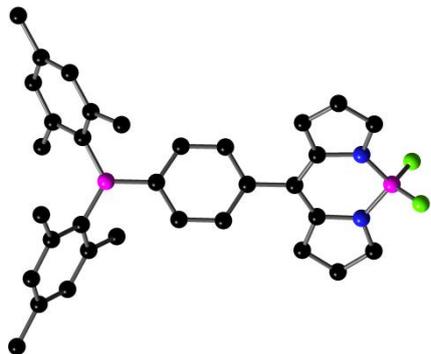
Table S11. The energy gap between frontier molecular orbitals of **1-6**, **R1**, and **R2** obtained from DFT calculation in the gas phase.

	1	2	3	4	5	6	R1	R2
LUMO+1 (eV)	-1.86	-1.87	-1.86	-1.75	-1.80	-1.72	-1.76	-1.88
LUMO (eV)	-2.85	-2.71	-2.79	-2.66	-2.50	-2.57	-2.63	-2.35
HOMO (eV)	-5.87	-5.77	-5.92	-5.80	-5.43	-5.56	-5.52	-5.34
HOMO-1 (eV)	-6.21	-6.21	-6.12	-6.13	-6.15	-6.10	-6.17	-6.18
LUMO-HOMO (eV)	3.02	3.06	3.13	3.14	2.93	2.99	2.89	2.99
LUMO+1 – HOMO-1 (eV)	4.35	4.34	4.26	4.38	4.35	4.38	4.41	4.30

Table S12. The energy gap between frontier molecular orbitals of **1-6**, **R1**, and **R2** obtained from DFT calculation in solution (in dichloromethane).

	1	2	3	4	5	6	R1	R2
LUMO+1 (eV)	-1.82	-1.82	-1.84	-1.72	-1.79	-1.76	-1.78	-1.83
LUMO (eV)	-2.95	-2.86	-2.88	-2.81	-2.69	-2.70	-2.77	-2.52
HOMO (eV)	-6.00	-5.95	-6.01	-5.95	-5.64	-5.69	-5.68	-5.53
HOMO-1 (eV)	-6.18	-6.15	-6.14	-6.12	-6.13	-6.16	-6.16	-6.19
LUMO – HOMO (eV)	3.05	3.09	3.13	3.14	2.95	2.99	2.91	3.01
LUMO+1 – HOMO-1 (eV)	4.36	4.33	4.30	4.40	4.34	4.40	4.38	4.36

Table S13. Cartesian coordinates of ground state optimized (gas phase) structure of **1**.



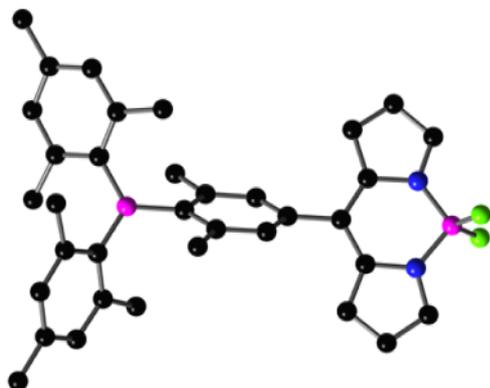
Total energy: -1635.89738801 a.u.

No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	5.488246	-1.177514	-0.417261
2	7	0	5.496457	1.184045	0.356052
3	5	0	6.439550	-0.041600	0.093272
4	9	0	7.045059	-0.424005	1.276529
5	9	0	7.371308	0.267554	-0.878486
6	6	0	-0.936129	-0.002271	0.005954
7	6	0	-0.190778	-0.993562	0.677726
8	1	0	-0.718787	-1.775492	1.217229
9	6	0	1.201043	-0.991647	0.679476
10	1	0	1.748384	-1.750415	1.230628
11	6	0	1.912026	0.005523	-0.011750
12	6	0	1.187074	0.997185	-0.695533
13	6	0	-0.204649	0.992675	-0.675380
14	6	0	3.395004	0.006777	-0.016382
15	6	0	4.094940	-1.144769	-0.419756
16	6	0	3.631868	-2.375933	-0.958917
17	1	0	2.595634	-2.639782	-1.114482
18	6	0	4.752161	-3.136890	-1.265059
19	1	0	4.777178	-4.127517	-1.697688
20	6	0	5.875581	-2.358842	-0.919041
21	6	0	4.102420	1.160566	0.366535
22	6	0	3.649442	2.430552	0.817183
23	1	0	2.615631	2.716083	0.948191
24	6	0	4.775641	3.207042	1.055064
25	1	0	4.808082	4.230876	1.401263
26	6	0	5.892690	2.398455	0.762922
27	1	0	1.722578	1.758274	-1.254930
28	1	0	-0.742841	1.774270	-1.204480
29	5	0	-2.514244	-0.002931	0.020493

30	6	0	-3.270072	-1.375475	0.237879
31	6	0	-4.222117	-1.525480	1.284070
32	6	0	-3.010354	-2.502801	-0.586641
33	6	0	-4.853490	-2.754919	1.489182
34	6	0	-3.687379	-3.707526	-0.365835
35	6	0	-4.608857	-3.860680	0.670361
36	1	0	-5.562696	-2.850263	2.309626
37	1	0	-3.486630	-4.551082	-1.024574
38	6	0	-3.269693	1.370316	-0.200642
39	6	0	-3.036876	2.494305	0.633628
40	6	0	-4.182824	1.529380	-1.283852
41	6	0	-3.680354	3.712657	0.375527
42	6	0	-4.791612	2.763691	-1.513257
43	6	0	-4.555245	3.874721	-0.695391
44	1	0	-3.491433	4.555399	1.038905
45	1	0	-5.471996	2.863930	-2.357390
46	6	0	-4.563951	-0.390524	2.229493
47	1	0	-5.012968	0.456407	1.700779
48	1	0	-5.273445	-0.725418	2.992724
49	1	0	-3.678807	-0.008993	2.752162
50	6	0	-2.027588	-2.468424	-1.743988
51	1	0	-1.017997	-2.752431	-1.422408
52	1	0	-2.331410	-3.174612	-2.524195
53	1	0	-1.944550	-1.481080	-2.205250
54	6	0	-5.341766	-5.164146	0.881311
55	1	0	-6.321022	-5.153937	0.383834
56	1	0	-4.779254	-6.011153	0.474657
57	1	0	-5.522841	-5.354961	1.944801
58	6	0	-2.180614	2.430892	1.883999
59	1	0	-2.813359	2.357363	2.778907
60	1	0	-1.500247	1.578048	1.895561
61	1	0	-1.579311	3.340629	1.995017
62	6	0	-4.499408	0.399129	-2.243307
63	1	0	-3.613680	0.077566	-2.805695
64	1	0	-4.885420	-0.482626	-1.723314
65	1	0	-5.248641	0.714705	-2.976151
66	6	0	-5.223964	5.199239	-0.976844
67	1	0	-6.307820	5.082802	-1.097085
68	1	0	-5.049686	5.916170	-0.168324
69	1	0	-4.845921	5.647222	-1.905077
70	1	0	6.927291	-2.593481	-1.015610
71	1	0	6.946209	2.633218	0.837210

Table S14. Cartesian coordinates of ground state optimized (gas phase) structure of **2**.

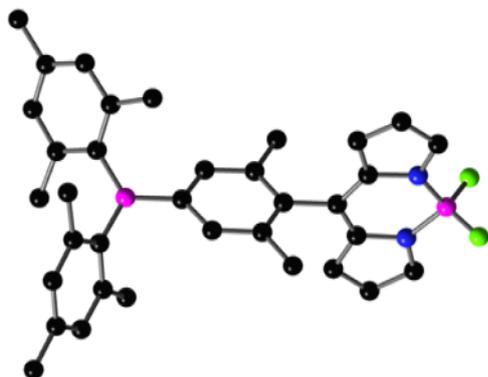


Total energy: -1714.52148634 a.u.

No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.593892	-1.239717	-0.038042
2	7	0	-5.583143	1.244017	-0.022865
3	5	0	-6.534274	0.006443	0.107193
4	9	0	-7.473237	0.022781	-0.906512
5	9	0	-7.133248	-0.005646	1.354397
6	6	0	0.843457	-0.002521	-0.007460
7	6	0	0.115707	-0.757514	-0.968042
8	6	0	-1.281947	-0.744188	-0.964091
9	6	0	-2.007579	-0.008290	-0.019094
10	6	0	-1.292515	0.732225	0.930364
11	6	0	0.105096	0.750591	0.946280
12	6	0	-3.489085	-0.007687	-0.021267
13	6	0	-4.199743	-1.222685	-0.020972
14	6	0	-3.749676	-2.570443	0.006090
15	1	0	-2.716410	-2.884142	0.040275
16	6	0	-4.877415	-3.380963	-0.013481
17	1	0	-4.911363	-4.461729	-0.008272
18	6	0	-5.992637	-2.520023	-0.035062
19	6	0	-4.189891	1.212922	-0.040708
20	6	0	-3.727563	2.550354	-0.172580
21	1	0	-2.691536	2.848594	-0.243873
22	6	0	-4.848057	3.369484	-0.222489
23	1	0	-4.872938	4.445526	-0.326185
24	6	0	-5.970990	2.523012	-0.131348
25	5	0	2.437167	-0.000497	-0.000285
26	6	0	3.223414	-1.374684	-0.005454
27	6	0	4.279486	-1.608951	-0.931462
28	6	0	2.896201	-2.420762	0.901083
29	6	0	4.945410	-2.838396	-0.940798
30	6	0	3.611038	-3.622599	0.878234

31	6	0	4.637812	-3.858212	-0.037637
32	1	0	5.732770	-3.003148	-1.674189
33	1	0	3.353433	-4.400358	1.595090
34	6	0	3.219155	1.376118	0.012926
35	6	0	2.899739	2.420184	-0.898045
36	6	0	4.267792	1.612206	0.947461
37	6	0	3.613819	3.622813	-0.870688
38	6	0	4.932780	2.841674	0.960786
39	6	0	4.627698	3.862845	0.057755
40	1	0	3.366981	4.396525	-1.595526
41	1	0	5.719121	3.004934	1.695745
42	6	0	4.713757	-0.580703	-1.960058
43	1	0	5.212037	0.275940	-1.495447
44	1	0	5.413423	-1.027957	-2.673445
45	1	0	3.872409	-0.180919	-2.536898
46	6	0	1.797229	-2.291738	1.939543
47	1	0	0.800912	-2.322476	1.485944
48	1	0	1.857191	-3.111406	2.662682
49	1	0	1.859266	-1.355369	2.504069
50	6	0	5.405906	-5.158150	-0.035520
51	1	0	6.307016	-5.084997	0.588388
52	1	0	4.802027	-5.980605	0.362294
53	1	0	5.733373	-5.432434	-1.044193
54	6	0	1.814431	2.286517	-1.950192
55	1	0	1.886779	1.350491	-2.514005
56	1	0	0.812685	2.313346	-1.508417
57	1	0	1.879726	3.106546	-2.672480
58	6	0	4.698742	0.582803	1.976246
59	1	0	3.854005	0.174122	2.541654
60	1	0	5.208756	-0.268071	1.513683
61	1	0	5.386850	1.032352	2.699393
62	6	0	5.354230	5.185690	0.102396
63	1	0	6.412440	5.053953	0.354184
64	1	0	5.295057	5.708710	-0.857731
65	1	0	4.922194	5.849663	0.863318
66	1	0	-7.046646	-2.764226	-0.037419
67	1	0	-7.022834	2.775654	-0.147535
68	1	0	-1.820387	-1.298424	-1.727249
69	1	0	-1.840022	1.287424	1.686447
70	6	0	0.795509	-1.583372	-2.043735
71	1	0	1.545623	-1.010072	-2.599687
72	1	0	1.311011	-2.451535	-1.621487
73	1	0	0.060721	-1.946956	-2.768930
74	6	0	0.772329	1.580061	2.027104
75	1	0	1.520206	1.010353	2.589767
76	1	0	1.287653	2.450158	1.608674
77	1	0	0.029775	1.940782	2.745713

Table S15. Cartesian coordinates of ground state optimized (gas phase) structure of **3**.

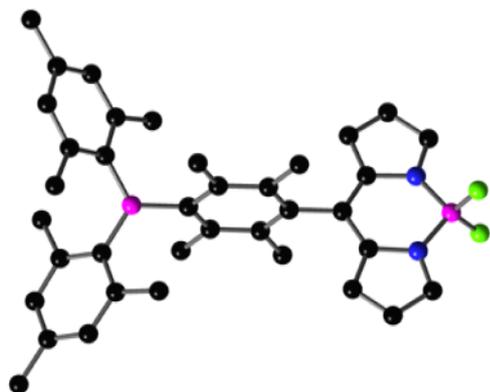
Total energy: - 1714.52926850 a.u.

No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.384146	-1.330912	-0.545416
2	7	0	-5.528827	1.013555	0.269563
3	5	0	-6.399607	-0.176417	-0.254496
4	9	0	-7.055035	0.187159	-1.422094
5	9	0	-7.307778	-0.568877	0.717965
6	6	0	0.962192	-0.004914	0.476019
7	6	0	0.307269	0.497632	-0.659002
8	1	0	0.901868	0.936193	-1.458827
9	6	0	-1.082094	0.480371	-0.820265
10	6	0	-1.875902	-0.061850	0.213716
11	6	0	-1.266097	-0.556647	1.387815
12	6	0	0.127465	-0.505244	1.489854
13	6	0	-3.360567	-0.101075	0.069176
14	6	0	-3.997803	-1.261747	-0.400381
15	6	0	-3.450833	-2.506294	-0.800296
16	1	0	-2.395851	-2.743486	-0.796920
17	6	0	-4.515092	-3.317546	-1.180199
18	1	0	-4.470872	-4.336495	-1.540341
19	6	0	-5.686242	-2.553846	-1.009171
20	6	0	-4.139419	1.019910	0.401171
21	6	0	-3.751409	2.284427	0.909764
22	1	0	-2.731375	2.577010	1.117466
23	6	0	-4.912784	3.031240	1.078525
24	1	0	-4.996743	4.043803	1.449443
25	6	0	-5.983336	2.210269	0.673562
26	1	0	0.594382	-0.860486	2.405512
27	6	0	-2.090605	-1.112252	2.530385
28	1	0	-2.812916	-0.378367	2.911071
29	1	0	-2.667678	-1.996908	2.232388
30	1	0	-1.440296	-1.402420	3.361277

31	6	0	-1.704512	1.028219	-2.087705
32	1	0	-2.325751	0.279614	-2.596226
33	1	0	-2.350444	1.893402	-1.891491
34	1	0	-0.925688	1.347205	-2.787142
35	5	0	2.597512	0.045662	0.726411
36	9	0	2.731383	0.137946	2.176968
37	6	0	3.159838	1.456548	0.024951
38	6	0	3.476415	-1.329013	0.351271
39	6	0	3.012887	2.696346	0.714716
40	6	0	3.720743	1.536032	-1.278890
41	6	0	3.018282	-2.483030	-0.337435
42	6	0	4.818040	-1.390944	0.838110
43	6	0	3.448977	3.900467	0.146188
44	6	0	2.360120	2.803524	2.082410
45	6	0	4.140979	2.761879	-1.819947
46	6	0	3.901855	0.323521	-2.176604
47	6	0	3.850983	-3.599860	-0.525783
48	6	0	1.625531	-2.610222	-0.931468
49	6	0	5.621512	-2.517618	0.626728
50	6	0	5.456776	-0.250415	1.610668
51	6	0	4.031068	3.960468	-1.119812
52	1	0	3.317214	4.824432	0.710963
53	1	0	2.200962	3.857732	2.343423
54	1	0	1.392964	2.292824	2.108632
55	1	0	2.967327	2.337301	2.861996
56	1	0	4.564117	2.774134	-2.825213
57	1	0	4.703736	-0.333929	-1.825785
58	1	0	3.000462	-0.293314	-2.232335
59	1	0	4.150223	0.641354	-3.197187
60	6	0	5.158480	-3.644806	-0.053086
61	1	0	3.457229	-4.461826	-1.065484
62	1	0	1.528329	-3.562541	-1.467428
63	1	0	0.845374	-2.574779	-0.164691
64	1	0	1.394180	-1.807511	-1.639010
65	1	0	6.643463	-2.512277	1.008199
66	1	0	5.367991	0.700751	1.077070
67	1	0	4.962382	-0.107385	2.574407
68	1	0	6.521895	-0.449865	1.782630
69	6	0	4.527609	5.265017	-1.700619
70	6	0	6.032397	-4.863052	-0.247917
71	1	0	3.910016	6.112102	-1.376728
72	1	0	5.559812	5.485755	-1.390545
73	1	0	4.520257	5.244753	-2.797267
74	1	0	6.131459	-5.449612	0.677230
75	1	0	5.620173	-5.532006	-1.012681
76	1	0	7.049016	-4.587720	-0.557808
77	1	0	-7.043621	2.426350	0.658143
78	1	0	-6.715796	-2.827511	-1.199578

Table S16. Cartesian coordinates of ground state optimized (gas phase) structure of **4**.



Total energy: -1793.14410737 a.u.

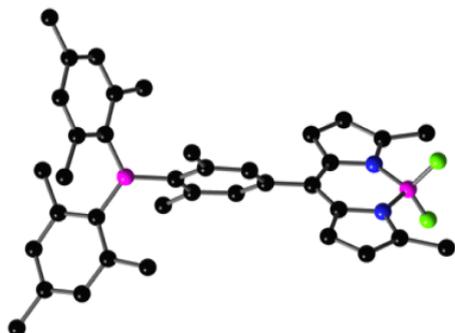
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	5.482876	1.120692	-0.547374
2	7	0	5.484101	-1.093962	0.589563
3	5	0	6.434516	-0.032232	-0.068759
4	9	0	7.080729	-0.590412	-1.156851
5	9	0	7.331879	0.447714	0.865563
6	6	0	-0.938280	0.000636	0.002923
7	6	0	-0.210631	-0.517663	-1.097773
8	6	0	1.198722	-0.520870	-1.098212
9	6	0	1.888407	0.005510	0.009901
10	6	0	1.191400	0.529493	1.114638
11	6	0	-0.217927	0.521385	1.107250
12	6	0	3.387129	0.007318	0.011969
13	6	0	4.088008	1.091743	-0.533858
14	6	0	3.617904	2.301227	-1.109698
15	6	0	4.734763	3.046984	-1.462136
16	1	0	4.756656	4.025530	-1.921755
17	6	0	5.863116	2.281759	-1.098362
18	6	0	4.089216	-1.069093	0.571849
19	6	0	3.620750	-2.244892	1.214983
20	6	0	4.738573	-2.964007	1.616247
21	1	0	4.761726	-3.909145	2.141084
22	6	0	5.865881	-2.218732	1.210340
23	5	0	-2.536055	-0.002076	-0.001316
24	6	0	-3.328122	1.361508	0.164888
25	6	0	-2.982069	2.523475	-0.581307
26	6	0	-4.413230	1.468558	1.081908
27	6	0	-3.707418	3.707793	-0.419194
28	6	0	-5.088209	2.683710	1.236836

29	6	0	-4.763540	3.815424	0.487191
30	1	0	-3.432903	4.576534	-1.015083
31	1	0	-5.896648	2.745507	1.963304
32	6	0	-3.322345	-1.368456	-0.171776
33	6	0	-4.402682	-1.479573	-1.095551
34	6	0	-2.976968	-2.528036	0.576425
35	6	0	-5.071953	-2.696248	-1.254221
36	6	0	-3.698069	-3.715586	0.410475
37	6	0	-4.747174	-3.827446	-0.501925
38	1	0	-5.876008	-2.760933	-1.985482
39	1	0	-3.424903	-4.582898	1.008805
40	6	0	-1.858739	2.542132	-1.601246
41	1	0	-1.943889	1.732383	-2.334533
42	1	0	-1.865459	3.485399	-2.156831
43	1	0	-0.877337	2.438936	-1.127923
44	6	0	-4.878618	0.312621	1.950316
45	1	0	-4.050953	-0.217004	2.433214
46	1	0	-5.541077	0.677053	2.742196
47	1	0	-5.431230	-0.434519	1.371088
48	6	0	-5.539523	5.102262	0.633850
49	1	0	-6.361687	5.154560	-0.092823
50	1	0	-5.982345	5.192650	1.631371
51	1	0	-4.902374	5.976884	0.463220
52	6	0	-4.866521	-0.324698	-1.966166
53	1	0	-5.422488	0.421806	-1.389398
54	1	0	-4.037606	0.205999	-2.445836
55	1	0	-5.525105	-0.690442	-2.760655
56	6	0	-1.859634	-2.543511	1.603017
57	1	0	-0.875713	-2.439377	1.135111
58	1	0	-1.950288	-1.733147	2.334929
59	1	0	-1.867947	-3.486207	2.159556
60	6	0	-5.517700	-5.116369	-0.659200
61	1	0	-6.470008	-5.078883	-0.113174
62	1	0	-5.757986	-5.314681	-1.709821
63	1	0	-4.952922	-5.970891	-0.272454
64	6	0	-0.919018	1.042362	2.346579
65	1	0	-2.001486	0.940155	2.292652
66	1	0	-0.578253	0.511619	3.244889
67	1	0	-0.708139	2.106516	2.514699
68	6	0	-0.903542	-1.041054	-2.340608
69	1	0	-0.687118	-2.104158	-2.508178
70	1	0	-1.986676	-0.943519	-2.291915
71	1	0	-0.560637	-0.508409	-3.236963
72	6	0	1.932254	1.092926	2.309678
73	1	0	1.599163	2.111599	2.541241
74	1	0	1.754125	0.493066	3.211755
75	1	0	3.010545	1.129143	2.149459
76	6	0	1.947443	-1.082427	-2.289215
77	1	0	1.622774	-2.104460	-2.518099
78	1	0	1.767103	-0.487022	-3.193753

79	1	0	3.025669	-1.110071	-2.126597
80	1	0	2.577012	2.568063	-1.229916
81	1	0	2.580263	-2.502388	1.357068
82	1	0	6.916356	-2.444888	1.337451
83	1	0	6.913265	2.517373	-1.210166

Table S17. Cartesian coordinates of ground state optimized (gas phase) structure of **5**.



Total energy: -1793.16945365 a.u.

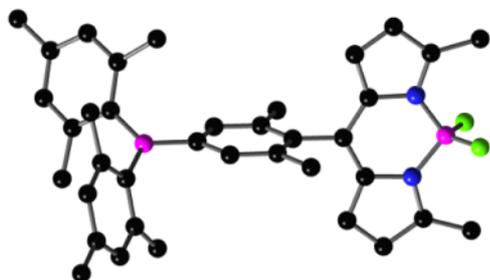
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.182567	-0.638912	-1.071699
2	7	0	-5.182646	0.638844	1.071639
3	5	0	-6.123588	-0.000054	-0.000053
4	9	0	-6.914617	0.984225	-0.585028
5	9	0	-6.914605	-0.984368	0.584884
6	6	0	1.250119	-0.000020	0.000054
7	6	0	0.517025	-0.497219	1.111998
8	6	0	-0.880541	-0.468977	1.105181
9	6	0	-1.600877	0.000038	0.000054
10	6	0	-0.880520	0.469070	-1.105035
11	6	0	0.517054	0.497265	-1.111847
12	6	0	-3.083732	0.000009	0.000025
13	6	0	-3.787726	-0.635557	-1.037041
14	6	0	-3.323857	-1.387904	-2.147431
15	6	0	-4.442955	-1.820271	-2.842819
16	1	0	-4.468649	-2.418813	-3.743732
17	6	0	-5.581367	-1.345228	-2.151193
18	6	0	-3.787804	0.635546	1.037053
19	6	0	-3.324021	1.387919	2.147462
20	6	0	-4.443171	1.820198	2.842822
21	1	0	-4.468935	2.418716	3.743748
22	6	0	-5.581529	1.345128	2.151124

23	5	0	2.842176	-0.000016	0.000080
24	6	0	3.624020	1.335625	-0.332040
25	6	0	3.290579	2.568681	0.295110
26	6	0	4.675955	1.346948	-1.290668
27	6	0	3.992749	3.734871	-0.024147
28	6	0	5.328915	2.543296	-1.604356
29	6	0	5.013133	3.749744	-0.976949
30	1	0	3.729344	4.661860	0.482202
31	1	0	6.112401	2.530798	-2.359997
32	6	0	3.624061	-1.335618	0.332137
33	6	0	4.676049	-1.346980	1.290714
34	6	0	3.290648	-2.568626	-0.295110
35	6	0	5.329083	-2.543310	1.604265
36	6	0	3.992894	-3.734817	0.024023
37	6	0	5.013317	-3.749729	0.976770
38	1	0	6.112609	-2.530830	2.359865
39	1	0	3.729522	-4.661774	-0.482402
40	6	0	2.197423	2.687165	1.341187
41	1	0	2.273155	1.917889	2.117235
42	1	0	2.251496	3.659888	1.840528
43	1	0	1.199504	2.595523	0.899698
44	6	0	5.124268	0.102913	-2.036370
45	1	0	4.289181	-0.447600	-2.483382
46	1	0	5.807779	0.372556	-2.847952
47	1	0	5.647297	-0.599447	-1.379267
48	6	0	5.765493	5.018934	-1.297863
49	1	0	6.636695	5.140558	-0.639925
50	1	0	6.136264	5.015732	-2.328420
51	1	0	5.134193	5.904187	-1.165496
52	6	0	5.124238	-0.102971	2.036528
53	1	0	5.646862	0.599691	1.379434
54	1	0	4.289076	0.447160	2.483885
55	1	0	5.808044	-0.372578	2.847872
56	6	0	2.197407	-2.687136	-1.341100
57	1	0	1.199508	-2.596358	-0.899360
58	1	0	2.272497	-1.917383	-2.116722
59	1	0	2.251971	-3.659555	-1.840981
60	6	0	5.765782	-5.018893	1.297538
61	1	0	6.637540	-5.139884	0.640220
62	1	0	6.135754	-5.016176	2.328387
63	1	0	5.134835	-5.904244	1.164174
64	6	0	-7.022712	-1.555279	-2.483331
65	1	0	-7.525506	-2.106591	-1.681206
66	1	0	-7.540058	-0.594587	-2.576629
67	1	0	-7.124037	-2.111626	-3.418676
68	6	0	-7.022901	1.555085	2.483205
69	1	0	-7.525729	2.106250	1.681003
70	1	0	-7.540156	0.594352	2.576604
71	1	0	-7.124301	2.111528	3.418485
72	6	0	1.189266	1.061443	-2.349775

73	1	0	1.985993	0.412328	-2.728207
74	1	0	0.459828	1.188483	-3.156118
75	1	0	1.644386	2.037904	-2.153714
76	6	0	1.189263	-1.061122	2.350035
77	1	0	1.645327	-2.037128	2.153969
78	1	0	1.985264	-0.411324	2.728878
79	1	0	0.459656	-1.188935	3.156100
80	1	0	-2.286914	-1.583660	-2.379617
81	1	0	-2.287098	1.583731	2.379688
82	1	0	-1.424122	-0.850747	1.964795
83	1	0	-1.424077	0.850878	-1.964649

Table S18. Cartesian coordinates of ground state optimized (gas phase) structure of **6**.



Total energy: -1793.17737716 a.u.

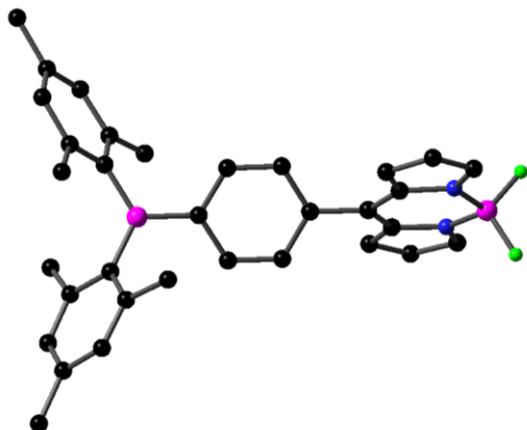
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	4.999339	-0.826778	-0.936539
2	7	0	4.986133	0.816651	0.947313
3	5	0	5.934644	-0.003304	0.010514
4	9	0	6.720804	-0.865154	0.767556
5	9	0	6.725919	0.861366	-0.737917
6	6	0	-1.429090	-0.014128	-0.005459
7	6	0	-0.693296	-0.935658	0.762351
8	1	0	-1.230041	-1.663435	1.366566
9	6	0	0.703721	-0.947309	0.791622
10	6	0	1.400995	-0.015675	-0.008466
11	6	0	0.702884	0.915227	-0.808061
12	6	0	-0.694165	0.905807	-0.775505
13	6	0	2.897964	-0.011572	-0.003905
14	6	0	3.603962	-0.805975	-0.915777
15	6	0	3.136804	-1.683897	-1.927560
16	1	0	2.096428	-1.876145	-2.151992
17	6	0	4.255514	-2.222524	-2.544225

18	1	0	4.281871	-2.931826	-3.360745
19	6	0	5.396372	-1.672864	-1.909599
20	6	0	3.591187	0.787463	0.913848
21	6	0	3.109533	1.663384	1.920608
22	1	0	2.066027	1.850165	2.134820
23	6	0	4.219315	2.209115	2.547034
24	1	0	4.233972	2.919326	3.363063
25	6	0	5.369195	1.665705	1.923404
26	1	0	-1.230570	1.639092	-1.372688
27	5	0	-3.003321	-0.003130	0.009966
28	6	0	-3.773845	-1.344514	0.348447
29	6	0	-4.723818	-1.397388	1.405800
30	6	0	-3.532493	-2.538064	-0.382481
31	6	0	-5.374666	-2.596354	1.707962
32	6	0	-4.228716	-3.710728	-0.067127
33	6	0	-5.150920	-3.766732	0.977843
34	1	0	-6.083231	-2.615669	2.534277
35	1	0	-4.041654	-4.607023	-0.656643
36	6	0	-3.755573	1.350363	-0.326589
37	6	0	-3.521592	2.537230	0.414611
38	6	0	-4.669258	1.423161	-1.418050
39	6	0	-4.168284	3.730416	0.063410
40	6	0	-5.280799	2.634734	-1.742946
41	6	0	-5.045624	3.806622	-1.014974
42	1	0	-3.979146	4.623080	0.658026
43	1	0	-5.963242	2.667516	-2.590753
44	6	0	-5.042826	-0.187103	2.261378
45	1	0	-5.468834	0.628442	1.668336
46	1	0	-5.763488	-0.446767	3.043375
47	1	0	-4.150694	0.210890	2.759672
48	6	0	-2.546241	-2.613574	-1.535094
49	1	0	-1.536407	-2.855902	-1.182264
50	1	0	-2.843161	-3.396910	-2.240819
51	1	0	-2.467413	-1.676741	-2.092781
52	6	0	-5.905238	-5.037022	1.291529
53	1	0	-6.900246	-5.033748	0.826223
54	1	0	-5.375059	-5.920457	0.920522
55	1	0	-6.055336	-5.158664	2.370110
56	6	0	-2.657793	2.575757	1.661114
57	1	0	-3.285130	2.593435	2.562673
58	1	0	-1.988909	1.718029	1.744219
59	1	0	-2.043276	3.483312	1.684270
60	6	0	-4.985379	0.220320	-2.284899
61	1	0	-4.097450	-0.148791	-2.813557
62	1	0	-5.378476	-0.615311	-1.698022
63	1	0	-5.728989	0.478282	-3.045627
64	6	0	-5.713954	5.105338	-1.399442
65	1	0	-6.787514	4.967147	-1.574579
66	1	0	-5.594122	5.864063	-0.619447
67	1	0	-5.288765	5.513807	-2.325833

68	6	0	1.436493	1.913911	-1.675541
69	1	0	2.086771	2.565541	-1.080446
70	1	0	2.076891	1.414706	-2.411926
71	1	0	0.728578	2.547612	-2.217578
72	6	0	1.438204	-1.944146	1.660583
73	1	0	2.093001	-2.592850	1.067292
74	1	0	2.074313	-1.443092	2.399449
75	1	0	0.730960	-2.580791	2.200121
76	6	0	6.805628	1.931661	2.235416
77	1	0	7.308244	1.010018	2.549145
78	1	0	7.332045	2.288958	1.344116
79	1	0	6.895135	2.676394	3.030265
80	6	0	6.837183	-1.930092	-2.208440
81	1	0	7.336972	-1.005491	-2.517930
82	1	0	7.357669	-2.283881	-1.312263
83	1	0	6.938525	-2.674527	-3.002139

Table S19. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **1**.



Total energy: -1635.908401 a.u.

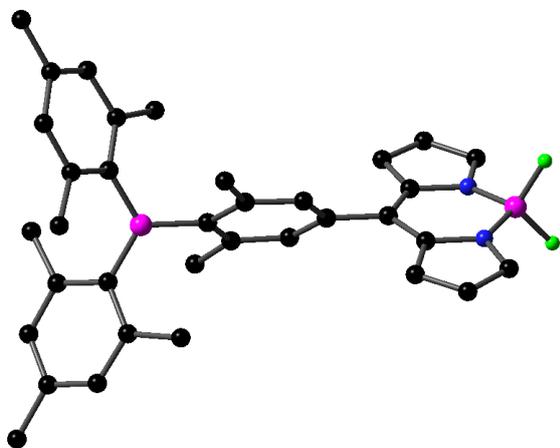
No of imaginary frequency: 0

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.202912	-1.078791	-0.552140
2	6	0	1.188758	-1.083833	-0.574662

3	6	0	1.911450	-0.020085	-0.004934
4	6	0	1.199850	1.050231	0.566531
5	6	0	-0.191773	1.060062	0.544131
6	6	0	-0.935509	-0.005322	-0.004277
7	6	0	3.393035	-0.024090	-0.002141
8	6	0	4.093334	0.156817	1.205064
9	7	0	5.488529	0.176680	1.232827
10	5	0	6.431141	0.074139	-0.003581
11	7	0	5.500127	-0.242472	-1.213701
12	6	0	4.104137	-0.220776	-1.200541
13	6	0	3.631325	0.259686	2.544256
14	6	0	4.752019	0.351337	3.361353
15	6	0	5.875308	0.292415	2.515146
16	6	0	5.898322	-0.438924	-2.482830
17	6	0	4.783076	-0.548479	-3.334358
18	6	0	3.654921	-0.402094	-2.535620
19	9	0	7.085207	1.285277	-0.214103
20	9	0	7.355495	-0.946973	0.181727
21	5	0	-2.512069	0.003355	-0.003322
22	6	0	-3.277001	-1.382554	0.000636
23	6	0	-4.237406	-1.694746	-1.001898
24	6	0	-4.878806	-2.937358	-0.998287
25	6	0	-4.632075	-3.898044	-0.013181
26	6	0	-3.707129	-3.580586	0.983382
27	6	0	-3.019450	-2.361285	0.998011
28	6	0	-2.029731	-2.141358	2.128871
29	6	0	-4.584115	-0.727566	-2.117131
30	6	0	-5.329281	-5.237591	-0.038009
31	6	0	-3.260552	1.398284	-0.005558
32	6	0	-2.992742	2.374460	-1.002531
33	6	0	-3.664665	3.602595	-0.985204
34	6	0	-4.583203	3.930934	0.013563
35	6	0	-4.840626	2.972252	0.998041
36	6	0	-4.215302	1.721580	0.999049
37	6	0	-4.572924	0.757510	2.113580
38	6	0	-2.008507	2.143127	-2.135881
39	6	0	-5.263069	5.279297	0.041751
40	1	0	-0.737830	-1.926316	-0.972078
41	1	0	1.723053	-1.927860	-0.999549
42	1	0	1.743694	1.886705	0.994365
43	1	0	-0.717702	1.912520	0.965393
44	1	0	2.595680	0.247122	2.852154
45	1	0	4.775935	0.437662	4.438782
46	1	0	6.925481	0.320280	2.773919

47	1	0	6.950735	-0.482970	-2.730215
48	1	0	4.816535	-0.710151	-4.402824
49	1	0	2.622396	-0.414796	-2.853477
50	1	0	-5.600197	-3.158476	-1.782883
51	1	0	-3.512651	-4.302228	1.775131
52	1	0	-2.301973	-2.749079	2.998221
53	1	0	-1.013888	-2.430774	1.833759
54	1	0	-1.978868	-1.099135	2.455823
55	1	0	-3.707442	-0.465297	-2.721609
56	1	0	-5.324153	-1.167569	-2.792928
57	1	0	-4.996018	0.209590	-1.730184
58	1	0	-6.339760	-5.155973	-0.452939
59	1	0	-4.781468	-5.957107	-0.661509
60	1	0	-5.404280	-5.669431	0.965456
61	1	0	-3.462565	4.322518	-1.776577
62	1	0	-5.557667	3.201775	1.784220
63	1	0	-5.304237	1.207295	2.792427
64	1	0	-5.000132	-0.172600	1.726179
65	1	0	-3.698537	0.480780	2.714876
66	1	0	-1.970303	1.100316	-2.462611
67	1	0	-2.276247	2.753631	-3.004687
68	1	0	-0.988712	2.421296	-1.843608
69	1	0	-5.310739	5.725406	-0.957069
70	1	0	-6.283303	5.205821	0.433941
71	1	0	-4.719655	5.982754	0.687015

Table S20. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **2**.



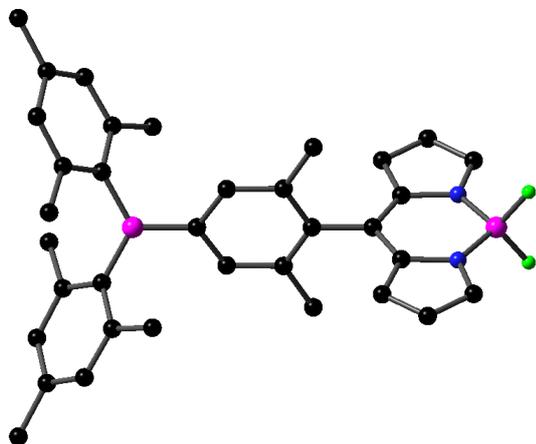
Total energy: -1714.532453 a.u.

No of imaginary frequency: 0

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.119007	-0.593081	1.074912
2	6	0	-1.278341	-0.570490	1.075801
3	6	0	-2.003308	-0.017060	0.012074
4	6	0	-1.289013	0.540237	-1.056911
5	6	0	0.108134	0.575532	-1.063832
6	6	0	0.845434	-0.004761	0.003899
7	6	0	-3.482838	-0.020825	0.012542
8	6	0	-4.186595	-0.532103	-1.095385
9	7	0	-5.581734	-0.526621	-1.130100
10	5	0	-6.522561	0.068396	-0.041119
11	7	0	-5.591903	0.461056	1.145694
12	6	0	-4.195968	0.472787	1.122532
13	6	0	-3.726842	-1.188025	-2.267671
14	6	0	-4.848741	-1.559330	-3.000470
15	6	0	-5.970482	-1.137851	-2.263207
16	6	0	-5.990933	0.993751	2.314416
17	6	0	-4.876405	1.370055	3.086017
18	6	0	-3.747682	1.055030	2.337326
19	9	0	-7.171798	1.200709	-0.528065
20	9	0	-7.452694	-0.883345	0.361109
21	5	0	2.439997	0.003866	0.000369
22	6	0	3.229111	-1.353643	0.201805
23	6	0	4.290910	-1.446199	1.145342
24	6	0	4.965074	-2.658482	1.330580
25	6	0	4.656418	-3.802007	0.590914
26	6	0	3.627290	-3.705183	-0.349302
27	6	0	2.904559	-2.523510	-0.542236
28	6	0	1.807579	-2.550687	-1.590590
29	6	0	4.735248	-0.275774	2.004197
30	6	0	5.390416	-5.102493	0.814769
31	6	0	3.212380	1.370378	-0.204708
32	6	0	2.877061	2.536595	0.540246
33	6	0	3.583855	3.727111	0.342662
34	6	0	4.606804	3.836045	-0.602948

35	6	0	4.926326	2.695765	-1.343056
36	6	0	4.268439	1.475254	-1.153464
37	6	0	4.722836	0.309631	-2.013545
38	6	0	1.785397	2.550657	1.594385
39	6	0	5.322986	5.145564	-0.831853
40	6	0	0.799862	-1.254598	2.258248
41	6	0	0.776136	1.241178	-2.252207
42	1	0	-1.814904	-1.028028	1.901704
43	1	0	-1.834650	0.989359	-1.881612
44	1	0	-2.691654	-1.373551	-2.514944
45	1	0	-4.873805	-2.083067	-3.946021
46	1	0	-7.021036	-1.255190	-2.493821
47	1	0	-7.043575	1.092909	2.544284
48	1	0	-4.910014	1.821397	4.067936
49	1	0	-2.715196	1.220069	2.608913
50	1	0	5.761058	-2.707922	2.071413
51	1	0	3.375912	-4.578108	-0.948973
52	1	0	0.812823	-2.470649	-1.140381
53	1	0	1.896540	-1.732828	-2.314399
54	1	0	1.842155	-3.488198	-2.154371
55	1	0	3.896687	0.237296	2.486677
56	1	0	5.407591	-0.620275	2.796312
57	1	0	5.270286	0.477871	1.416950
58	1	0	6.387707	-4.932732	1.233583
59	1	0	4.846812	-5.747470	1.518288
60	1	0	5.500988	-5.665872	-0.118133
61	1	0	3.324519	4.597346	0.942864
62	1	0	5.717883	2.754604	-2.087940
63	1	0	5.389030	0.661249	-2.807721
64	1	0	5.267523	-0.438224	-1.427801
65	1	0	3.888257	-0.212321	-2.493483
66	1	0	1.887077	1.732955	2.316681
67	1	0	1.812811	3.487819	2.159147
68	1	0	0.789137	2.460394	1.149467
69	1	0	5.430718	5.711535	0.099808
70	1	0	6.320394	4.988110	-1.255176
71	1	0	4.767841	5.782623	-1.533579
72	1	0	0.080057	-1.434803	3.062686
73	1	0	1.239806	-2.218269	1.980779
74	1	0	1.608727	-0.643444	2.671009
75	1	0	0.051320	1.407589	-3.055137
76	1	0	1.202897	2.212507	-1.980591
77	1	0	1.592326	0.639880	-2.664899

Table S21. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **3**.



Total energy: -1714.539878 a.u.

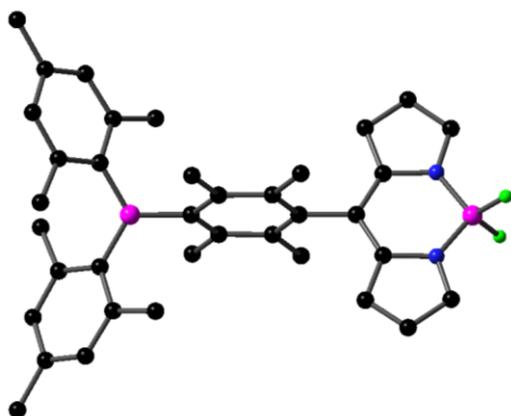
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.306121	-0.940796	-0.744316
2	6	0	1.091173	-0.953229	-0.775670
3	6	0	1.786785	-0.000018	-0.000009
4	6	0	1.091172	0.953196	0.775648
5	6	0	-0.306121	0.940767	0.744286
6	6	0	-1.040394	-0.000013	-0.000016
7	6	0	3.283184	-0.000019	-0.000006
8	6	0	3.984743	-0.787312	0.923558
9	7	0	5.380925	-0.809355	0.945192
10	5	0	6.324213	-0.000035	-0.000014
11	7	0	5.380929	0.809335	-0.945179
12	6	0	3.984746	0.787282	-0.923560
13	6	0	3.516352	-1.653801	1.945612
14	6	0	4.634303	-2.190101	2.572657
15	6	0	5.761827	-1.644177	1.926658
16	6	0	5.761836	1.644183	-1.926623
17	6	0	4.634314	2.190110	-2.572623
18	6	0	3.516360	1.653793	-1.945598
19	9	0	7.117997	0.866942	0.742650

20	9	0	7.117917	-0.867057	-0.742713
21	5	0	-2.614293	-0.000004	-0.000023
22	6	0	-3.374145	-1.367786	-0.248973
23	6	0	-4.331011	-1.505734	-1.292578
24	6	0	-4.972273	-2.730701	-1.502704
25	6	0	-4.725843	-3.846008	-0.696762
26	6	0	-3.801787	-3.703445	0.339967
27	6	0	-3.116540	-2.503501	0.565813
28	6	0	-2.130502	-2.478114	1.720544
29	6	0	-4.671523	-0.364454	-2.230961
30	6	0	-5.424669	-5.160817	-0.950624
31	6	0	-3.374124	1.367787	0.248940
32	6	0	-3.116511	2.503504	-0.565857
33	6	0	-3.801707	3.703462	-0.339984
34	6	0	-4.725710	3.846057	0.696799
35	6	0	-4.972136	2.730767	1.502748
36	6	0	-4.330922	1.505769	1.292591
37	6	0	-4.671410	0.364520	2.231021
38	6	0	-2.130499	2.478081	-1.720610
39	6	0	-5.424403	5.160929	0.950703
40	6	0	1.824293	-1.974028	-1.617395
41	6	0	1.824291	1.973990	1.617380
42	1	0	-0.842025	-1.686711	-1.326448
43	1	0	-0.842026	1.686685	1.326414
44	1	0	2.476181	-1.842860	2.172892
45	1	0	4.656600	-2.889758	3.396599
46	1	0	6.810583	-1.817921	2.128730
47	1	0	6.810592	1.817938	-2.128679
48	1	0	4.656614	2.889786	-3.396549
49	1	0	2.476190	1.842855	-2.172880
50	1	0	-5.692306	-2.813676	-2.315077
51	1	0	-3.607600	-4.550484	0.995905
52	1	0	-2.379552	-3.253295	2.452771
53	1	0	-1.106642	-2.667778	1.376774
54	1	0	-2.114158	-1.518815	2.245541
55	1	0	-5.041646	0.512173	-1.690815
56	1	0	-3.799698	-0.038118	-2.811432
57	1	0	-5.440849	-0.670265	-2.946888
58	1	0	-6.456631	-5.008159	-1.285386
59	1	0	-4.914123	-5.736362	-1.734560
60	1	0	-5.445482	-5.784148	-0.050716
61	1	0	-3.607524	4.550495	-0.995932
62	1	0	-5.692120	2.813767	2.315160
63	1	0	-5.440681	0.670371	2.946991

64	1	0	-5.041597	-0.512106	1.690918
65	1	0	-3.799559	0.038167	2.811443
66	1	0	-2.114307	1.518826	-2.245692
67	1	0	-2.379452	3.253363	-2.452762
68	1	0	-1.106604	2.667562	-1.376844
69	1	0	-5.446921	5.783456	0.050274
70	1	0	-6.455736	5.008336	1.287405
71	1	0	-4.912594	5.737314	1.733200
72	1	0	1.115787	-2.613897	-2.150784
73	1	0	2.471482	-1.494201	-2.360770
74	1	0	2.465285	-2.618667	-1.004781
75	1	0	2.465297	2.618621	1.004772
76	1	0	1.115784	2.613867	2.150758
77	1	0	2.471466	1.494160	2.360765

Table S22. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **4**.



Total energy: -1793.154900 a.u.

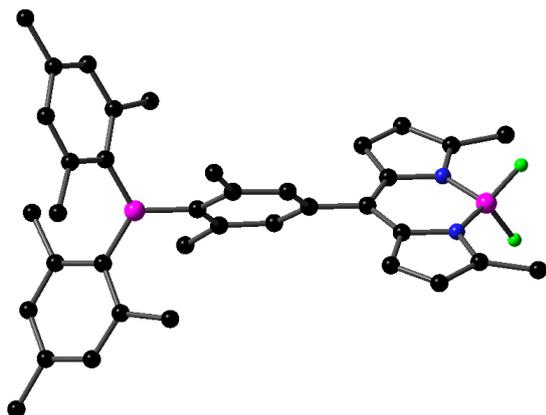
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.220254	0.515705	1.108834
2	6	0	1.189214	0.523519	1.115197

3	6	0	1.884086	0.002499	0.007647
4	6	0	1.194090	-0.520295	-1.102108
5	6	0	-0.215361	-0.515461	-1.100701
6	6	0	-0.941381	-0.000443	0.002730
7	6	0	3.382610	0.004364	0.008629
8	6	0	4.084475	1.083948	-0.546119
9	7	0	5.481073	1.111630	-0.562158
10	5	0	6.423659	-0.019451	-0.044040
11	7	0	5.483678	-1.093459	0.587949
12	6	0	4.086988	-1.069380	0.571456
13	6	0	3.615338	2.283660	-1.140310
14	6	0	4.732587	3.023873	-1.508054
15	6	0	5.860835	2.266509	-1.134778
16	6	0	5.866087	-2.224808	1.204160
17	6	0	4.739613	-2.970076	1.605971
18	6	0	3.620671	-2.247763	1.208998
19	9	0	7.136163	-0.571930	-1.104347
20	9	0	7.296306	0.482057	0.914765
21	5	0	-2.539729	-0.001512	-0.000472
22	6	0	-3.328984	1.364780	0.163504
23	6	0	-4.413046	1.476524	1.081548
24	6	0	-5.087128	2.693375	1.233305
25	6	0	-4.758924	3.824351	0.482833
26	6	0	-3.708946	3.709625	-0.431150
27	6	0	-2.984611	2.523331	-0.589800
28	6	0	-1.869159	2.534898	-1.618744
29	6	0	-4.884282	0.322523	1.949380
30	6	0	-5.493598	5.130244	0.670347
31	6	0	-3.326590	-1.368744	-0.167959
32	6	0	-2.983466	-2.527140	0.586115
33	6	0	-3.704911	-3.714666	0.423517
34	6	0	-4.750659	-3.830702	-0.495129
35	6	0	-5.077792	-2.699755	-1.246120
36	6	0	-4.406600	-1.481785	-1.090644
37	6	0	-4.876216	-0.328104	-1.959781
38	6	0	-1.872434	-2.537286	1.619837
39	6	0	-5.481935	-5.137863	-0.687007
40	6	0	-0.919321	1.030670	2.351670
41	6	0	-0.908920	-1.032176	-2.345887
42	6	0	1.929914	1.084411	2.311393
43	6	0	1.940106	-1.080169	-2.295490
44	1	0	2.574907	2.549781	-1.265755
45	1	0	4.753877	3.993852	-1.985238
46	1	0	6.909374	2.505553	-1.254766

47	1	0	6.915186	-2.457031	1.332314
48	1	0	4.763096	-3.918438	2.124690
49	1	0	2.580867	-2.508380	1.350181
50	1	0	-5.899174	2.756513	1.955505
51	1	0	-3.440589	4.572764	-1.037661
52	1	0	-0.884464	2.433326	-1.151761
53	1	0	-1.960680	1.721546	-2.347089
54	1	0	-1.878325	3.475622	-2.178291
55	1	0	-4.058979	-0.211557	2.431142
56	1	0	-5.544833	0.689861	2.741272
57	1	0	-5.441794	-0.419887	1.368508
58	1	0	-6.504345	4.969097	1.059379
59	1	0	-4.969541	5.780046	1.384221
60	1	0	-5.572492	5.684496	-0.271156
61	1	0	-3.437555	-4.577749	1.030544
62	1	0	-5.886590	-2.763864	-1.971872
63	1	0	-5.533260	-0.696085	-2.754282
64	1	0	-5.436911	0.413300	-1.380699
65	1	0	-4.049854	0.207321	-2.438221
66	1	0	-1.968053	-1.723911	2.347621
67	1	0	-1.882893	-3.477942	2.179475
68	1	0	-0.885873	-2.434645	1.157039
69	1	0	-5.562398	-5.693905	0.253302
70	1	0	-6.491873	-4.978259	-1.078780
71	1	0	-4.954371	-5.785280	-1.400469
72	1	0	-0.583998	0.488823	3.245149
73	1	0	-0.699758	2.091349	2.530003
74	1	0	-2.002295	0.934534	2.295534
75	1	0	-0.570636	-0.490666	-3.238434
76	1	0	-0.687421	-2.092750	-2.522499
77	1	0	-1.992213	-0.937235	-2.294137
78	1	0	1.601632	2.105259	2.539838
79	1	0	1.744864	0.486911	3.213337
80	1	0	3.009113	1.114575	2.154487
81	1	0	3.018930	-1.107604	-2.135335
82	1	0	1.615177	-2.102078	-2.524000
83	1	0	1.756438	-0.483946	-3.198555

Table S23. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **5**.



Total energy: -1793.178737 a.u.

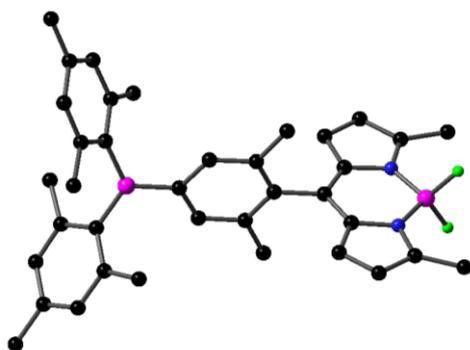
No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.518120	0.480603	-1.119243
2	6	0	-0.879623	0.450996	-1.112995
3	6	0	-1.598776	-0.005860	-0.001456
4	6	0	-0.878880	-0.463258	1.109357
5	6	0	0.518885	-0.492019	1.115083
6	6	0	1.251047	-0.004755	-0.001920
7	6	0	-3.080940	-0.004926	-0.000489
8	6	0	-3.785379	0.638825	1.031986
9	7	0	-5.182199	0.643741	1.067340
10	5	0	-6.115414	-0.002257	0.001687
11	7	0	-5.184807	-0.649845	-1.065318
12	6	0	-3.787934	-0.647434	-1.031954
13	6	0	-3.320708	1.399071	2.135328
14	6	0	-4.439106	1.839114	2.829260
15	6	0	-5.578670	1.361372	2.144451
16	6	0	-5.584087	-1.366709	-2.141890
17	6	0	-4.446352	-1.846471	-2.828339
18	6	0	-3.326178	-1.408455	-2.135979
19	9	0	-6.918892	-0.980640	0.594784
20	9	0	-6.918098	0.977466	-0.590282
21	5	0	2.844620	-0.000754	-0.000464
22	6	0	3.620605	1.338685	-0.333163
23	6	0	4.676187	1.353497	-1.288455

24	6	0	5.327143	2.552127	-1.600255
25	6	0	5.001242	3.759699	-0.978605
26	6	0	3.982323	3.739975	-0.023263
27	6	0	3.282418	2.570969	0.293860
28	6	0	2.192600	2.685389	1.344007
29	6	0	5.137124	0.110081	-2.027673
30	6	0	5.708365	5.043167	-1.342953
31	6	0	3.629239	-1.334555	0.333917
32	6	0	3.298644	-2.570345	-0.290448
33	6	0	4.003610	-3.734890	0.031529
34	6	0	5.024740	-3.745477	0.984654
35	6	0	5.337343	-2.536284	1.609904
36	6	0	4.681227	-1.341700	1.293202
37	6	0	5.127993	-0.095676	2.036751
38	6	0	2.207021	-2.694306	-1.337583
39	6	0	5.780104	-5.012314	1.308438
40	6	0	-7.023271	-1.584220	-2.479185
41	6	0	-7.016962	1.581572	2.483793
42	6	0	1.191329	-1.046497	2.356930
43	6	0	1.189954	1.033727	-2.362023
44	1	0	-1.421735	0.823684	-1.977367
45	1	0	-1.420429	-0.836565	1.973810
46	1	0	-2.283722	1.594665	2.367374
47	1	0	-4.462401	2.444469	3.725572
48	1	0	-4.472020	-2.451747	-3.724642
49	1	0	-2.289860	-1.605877	-2.369494
50	1	0	6.118782	2.540362	-2.347335
51	1	0	3.720409	4.664092	0.488872
52	1	0	1.194078	2.585925	0.905479
53	1	0	2.276388	1.919758	2.122721
54	1	0	2.241428	3.660432	1.838984
55	1	0	4.307483	-0.451958	-2.469941
56	1	0	5.816891	0.382674	-2.841214
57	1	0	5.669504	-0.581406	-1.366287
58	1	0	6.733344	4.854422	-1.679283
59	1	0	5.189272	5.561934	-2.160263
60	1	0	5.746758	5.734541	-0.494497
61	1	0	3.742417	-4.663532	-0.472790
62	1	0	6.120560	-2.520323	2.365650
63	1	0	5.809541	-0.363500	2.850380
64	1	0	5.654179	0.602889	1.377891
65	1	0	4.292286	0.456877	2.479668
66	1	0	2.285469	-1.930557	-2.118701
67	1	0	2.260282	-3.670533	-1.829754

68	1	0	1.208776	-2.598740	-0.897566
69	1	0	5.150013	-5.898781	1.179477
70	1	0	6.649393	-5.133891	0.648084
71	1	0	6.154419	-5.003593	2.337530
72	1	0	-7.115605	-2.142517	-3.413667
73	1	0	-7.528822	-2.140564	-1.682108
74	1	0	-7.547309	-0.627987	-2.580887
75	1	0	-7.522654	2.138699	1.687352
76	1	0	-7.542625	0.626336	2.586485
77	1	0	-7.106907	2.140223	3.418301
78	1	0	0.463160	-1.164206	3.165462
79	1	0	1.641390	-2.026586	2.166879
80	1	0	1.990692	-0.396591	2.727619
81	1	0	0.461594	1.149669	-3.170642
82	1	0	1.639546	2.014304	-2.173603
83	1	0	1.989577	0.383534	-2.731798

Table S24. Cartesian coordinates of ground state optimized (solvated in dichloromethane) structure of **6**.



Total energy: -1793.186348 a.u.

No of imaginary frequency: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.694426	0.978019	-0.694955
2	6	0	-0.702702	0.992366	-0.722942

3	6	0	-1.399281	-0.001635	-0.001038
4	6	0	-0.702139	-0.995488	0.720510
5	6	0	0.694997	-0.980537	0.692268
6	6	0	1.430377	-0.000994	-0.001269
7	6	0	-2.896428	-0.001534	-0.000453
8	6	0	-3.596408	0.684922	0.999603
9	7	0	-4.993504	0.706283	1.030004
10	5	0	-5.927410	-0.000750	0.000724
11	7	0	-4.994638	-0.708322	-1.029233
12	6	0	-3.597507	-0.687673	-0.999939
13	6	0	-3.122129	1.442271	2.100589
14	6	0	-4.235959	1.910763	2.781628
15	6	0	-5.381846	1.440577	2.097251
16	6	0	-5.384197	-1.442366	-2.096200
17	6	0	-4.239092	-1.913133	-2.781493
18	6	0	-3.124484	-1.445221	-2.101329
19	9	0	-6.728769	-0.943651	0.649084
20	9	0	-6.728693	0.942603	-0.647088
21	5	0	3.006369	-0.000051	-0.000519
22	6	0	3.768512	1.355641	-0.309020
23	6	0	4.661292	1.445820	-1.416871
24	6	0	5.287046	2.656105	-1.720095
25	6	0	5.085220	3.811148	-0.953998
26	6	0	4.224794	3.718436	0.137333
27	6	0	3.564713	2.525150	0.467507
28	6	0	2.712506	2.548103	1.722592
29	6	0	4.935787	0.262653	-2.324129
30	6	0	5.771405	5.108334	-1.312263
31	6	0	3.770426	-1.354447	0.308983
32	6	0	3.569783	-2.524330	-0.467583
33	6	0	4.230328	-3.716880	-0.135301
34	6	0	5.090002	-3.807636	0.956696
35	6	0	5.286195	-2.652882	1.724871
36	6	0	4.659813	-1.443504	1.419733
37	6	0	4.927299	-0.260721	2.329569
38	6	0	2.718501	-2.549167	-1.723204
39	6	0	5.795745	-5.097607	1.302783
40	6	0	-1.435980	2.058809	-1.505649
41	6	0	-1.434825	-2.062235	1.503353
42	6	0	-6.820344	-1.677257	-2.433681
43	6	0	-6.817595	1.676309	2.435835
44	1	0	1.229958	1.753698	-1.236235
45	1	0	1.230995	-1.755931	1.233502
46	1	0	-2.080654	1.607378	2.340635

47	1	0	-4.255094	2.523893	3.672665
48	1	0	-4.259249	-2.526226	-3.672534
49	1	0	-2.083281	-1.610839	-2.342204
50	1	0	5.952478	2.702508	-2.580607
51	1	0	4.058457	4.597465	0.758355
52	1	0	3.347651	2.572445	2.618021
53	1	0	2.085875	3.447077	1.753613
54	1	0	2.056867	1.680606	1.810000
55	1	0	4.022868	-0.097960	-2.813479
56	1	0	5.641924	0.537335	-3.113970
57	1	0	5.358380	-0.583741	-1.773203
58	1	0	6.848771	4.964173	-1.457292
59	1	0	5.376684	5.521998	-2.249470
60	1	0	5.632542	5.863334	-0.532090
61	1	0	4.064368	-4.597166	-0.754682
62	1	0	5.946430	-2.699105	2.589374
63	1	0	5.632129	-0.533920	3.121092
64	1	0	5.348519	0.587896	1.781005
65	1	0	4.011675	0.095997	2.816710
66	1	0	2.061879	-1.682495	-1.811619
67	1	0	3.354282	-2.573332	-2.618193
68	1	0	2.092987	-3.448936	-1.754107
69	1	0	5.458938	-5.921140	0.665377
70	1	0	6.882273	-5.002570	1.179400
71	1	0	5.618281	-5.383151	2.346801
72	1	0	-0.728884	2.757387	-1.961823
73	1	0	-2.044807	1.623832	-2.306854
74	1	0	-2.115090	2.633856	-0.865757
75	1	0	-2.114232	-2.637197	0.863704
76	1	0	-0.727379	-2.760835	1.958948
77	1	0	-2.043245	-1.627538	2.305024
78	1	0	-6.906092	-2.289065	-3.334566
79	1	0	-7.334180	-2.183526	-1.609214
80	1	0	-7.340713	-0.727290	-2.596949
81	1	0	-7.331812	2.182707	1.611684
82	1	0	-7.338372	0.726671	2.599726
83	1	0	-6.902280	2.288344	3.336668

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