Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

White Light Emissive Molecular Siblings

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Experimental Section

Materials and general methods:

$BF_3.Et_2O$, DDQ, Magnesium, anhydrous calcium hydride (CaH_2) were purchased from Sigma-Aldrich (USA).Pyrrole, 2-Bromothiophene, triethylamine, TFA, DMF were purchased from SD Fine Chemicals (India). $CDCl_3$ was purchased from Merck (Germany). Standard Schlenk technique was used for reactions requiring inert nitrogen atmosphere.CH_2Cl_2 was dried over CaH_2 and distilled under N_2 atmosphere. DMF was dried over Na_2SO_4 for overnight and distilled out at reduced pressure and stored over 3Å molecular sieves. THF and Et_2O were dried over sodium. Triethylamine was refluxed over sodium for 24 hours and distilled out at N_2 atmosphere and stored in an air tight stored round bottom flask.Bithiophene, 5-formyl-2,2´-bithiophene were synthesis according literature procedure[1,2]. All 400MHz ^1H NMR, 125.7 ^{13}C NMR Spectra were recorded by a Bruker Advance 400MHz NMR Spectrometer. Solution ^1H NMR and ^{13}C NMR Spectra were referenced internally to the solvent signals. High resolution mass spectra were obtained from Q-TOF instrument by electrospray ionization (ESI). Electronic absorption spectra were recorded on a Perkin Elmer LAMBDA 750 UV/visible spectrophotometer. Solution were prepared using a microbalance (± 0.1mg) and volumetric glassware and then charged in quartz cuvettes with sealing screw caps. Fluorescence emission studies were carried out on a Horiba JOBIN YVON Fluoromax-4 spectrometer.

Synthesis of 2

2-methyl-pyrrole (0.3 mL, 3.59 mmol) and borane-bithiophene-aldehyde (0.5 g, 1.13 mmol) were stirred at room temperature under nitrogen atmosphere for 30 min, then one drop $BF_3.OEt_2$ was added. The resultant mixture was stirred for another 6 h at room temperature and then DDQ (0.31 gm, 1.37 mmol) was added and stirred for additional 6 hours at room temperature. Then, Et_3N (1.6 ml, 11.46 mmol) was added and stirring was continued for another 1 hour. The resultant product was allowed to react with BF_3•OEt_2 (1.6 ml, 13 mmol) and the resultant mixture was stirred for 12 h. The crude product was extracted with dichloromethane and purified using column chromatography (ethyl acetate and petroleum ether (10:90)). Red color solid, Yield: 0.250 g, 35%. ^1H NMR (400 MHz, $CDCl_3$, δ in ppm) 7.39 (d, J = 8 Hz, 2H, thiophene C-H), 7.34 (2H, thiophene C-H), 7.10 (d, J = 4 Hz, 2H, BODIPY C-H), 6.85 (s, 4H,

Ar C-H), 6.31 (d, *J* = 4 Hz, 2H, BODIPY C-H), 2.65 (s, 6H, -CH_3), 2.32 (s, 6H, Mesitylene -CH_3), 2.15 (s, 12H, Mesityl -CH_3).^{13}CNMR (100.00 MHz, $CDCl_3$, δ in ppm) 158.2 (BODIPY-C), 148.4 (Thiophene-C), 142.2 (Ar-C), 141.7 (Ar-C), 141.3 (Ar-C), 139.3 (BODIPY-C), 138.2 4 (Thiophene-C), 134.9 4 (Thiophene-C), 134.2 4 (Thiophene-C), 133.1 (BODIPY-C), 130.5 (Thiophene-C), 128.7 (BODIPY-C), 127.3 (Ar-C), 127.2 (Thiophene-C), 125.7 (BODIPY-C), 119.9 (BODIPY-C),23.9 (Mesitylene-CH_3-C), 21.7 (Mesitylene-CH_3-C), 15.5 (BODIPY-CH_3-C).^{19}F NMR (376 MHz, $CDCl_3$, δ in ppm) -147.5 (q, *J* = 31.96 Hz). MALDI-Mass: M/Z= 631.282 [M] (28.2%), 613. 274 [M-F] (100%).

Synthesis of 3

Compound 3 was prepared following a procedure similar to that of 2. The quantities involved and characterization data are as follows: borane-bithiophene-aldehyde (1.0g, 2.26 mmol), 2,4-dimethyl-pyrrole (0.52 ml, 4.97 mmol), DDQ (0.62 g, 2.71 mmol), Et3N (3.2 ml, 22.6 mmol), BF3•OEt_2 (3.2 ml, 26 mmol. Red color solid. Yield: 550 mg, 37%. 1H NMR (400 MHz, CDCl3, δ in ppm) 7.38 (d, J = 3.6 Hz,2H, thiophene C-H), 7.33 (d, J = 3.6 Hz, 2H, thiophene C-H), 7.28 (d, J = 3.6 Hz, 2H, , thiophene C-H), 6.89 (d, J = 3.6 Hz, 2H, , thiophene C-H), 6.84 (s, 4H, Ar C-H), 6.01 (s, 2H, BODIPY C-H), 2.55 (s, 6H, -CH3), 2.31 (s, 6H, Mesitylene -CH3), 2.16 (s, 12H, Mesitylene -CH3), 1.72 (s, 6H, -CH3). 13CNMR (100.00 MHz, CDCl3, δ in ppm) 156.8, 150.1, 148.9, 143.8, 141.8, 141.2, 140.0, 139.1, 135.0, 133.2, 132.7, 129.4, 128.6, 126.8, 125.4, 122.0, 23.9, 21.6, 15.1, 14.4.19F NMR (376 MHz, CDCl3, δ in ppm) -146.2 (q, J = 32.33 Hz). MALDI-Mass: M/Z= 660.246 [M] (47.8%), 641.213 [M-F] (85.4%).

Spectral Characterization

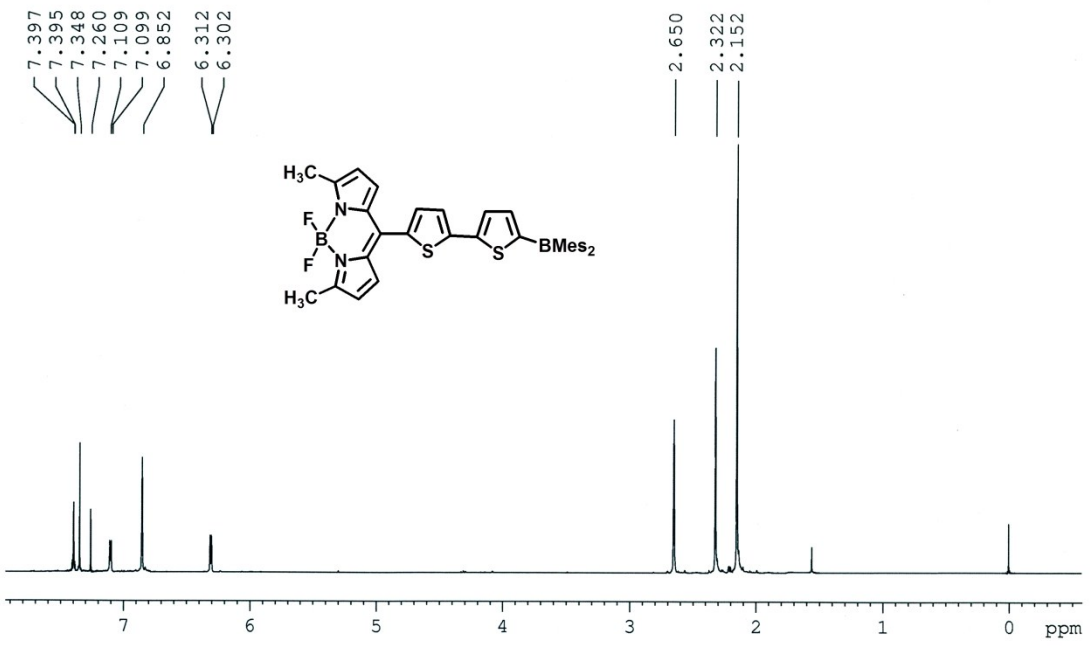

Figure S1: ^{1}H NMR of **2**

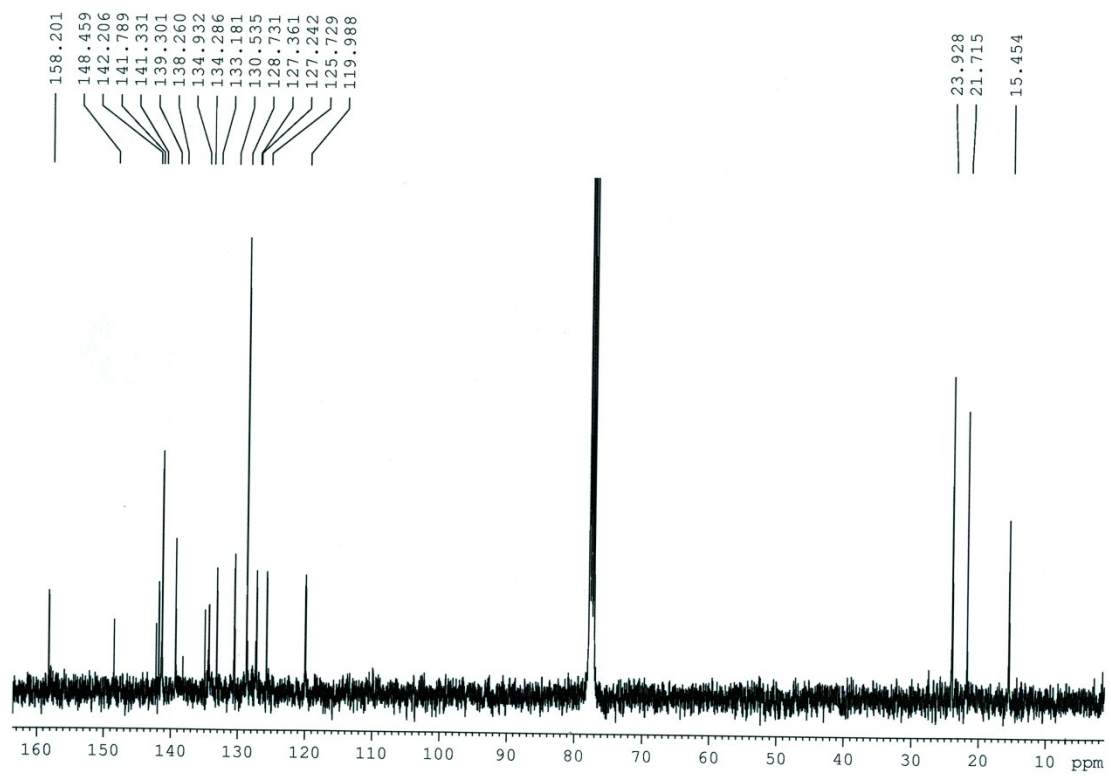

Figure S2: ^{13}C NMR of **2**

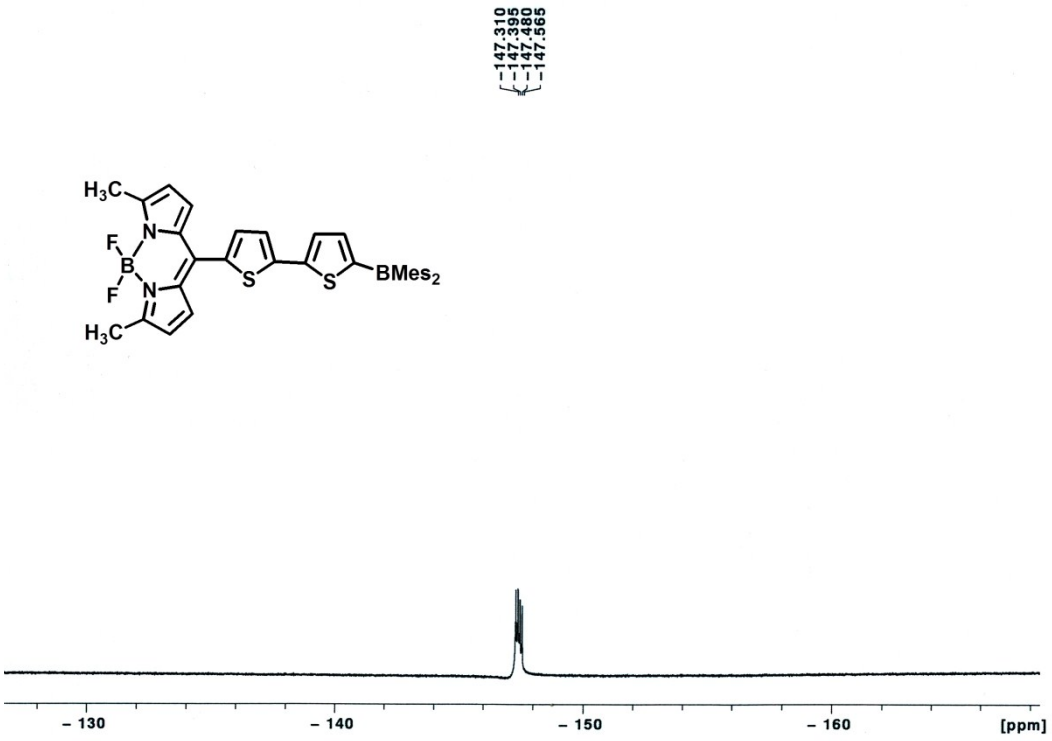

Figure S3: ^{11}B NMR of **2.** ^{11}B resonance of tricoordinated boron center could not be observed

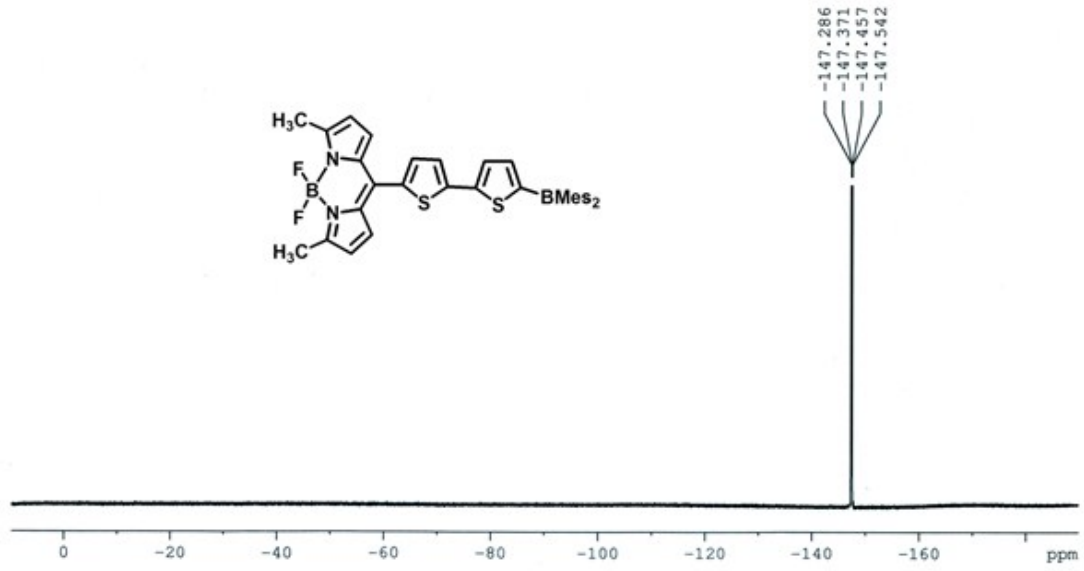

Figure S4: ^{19}F NMR of **2**

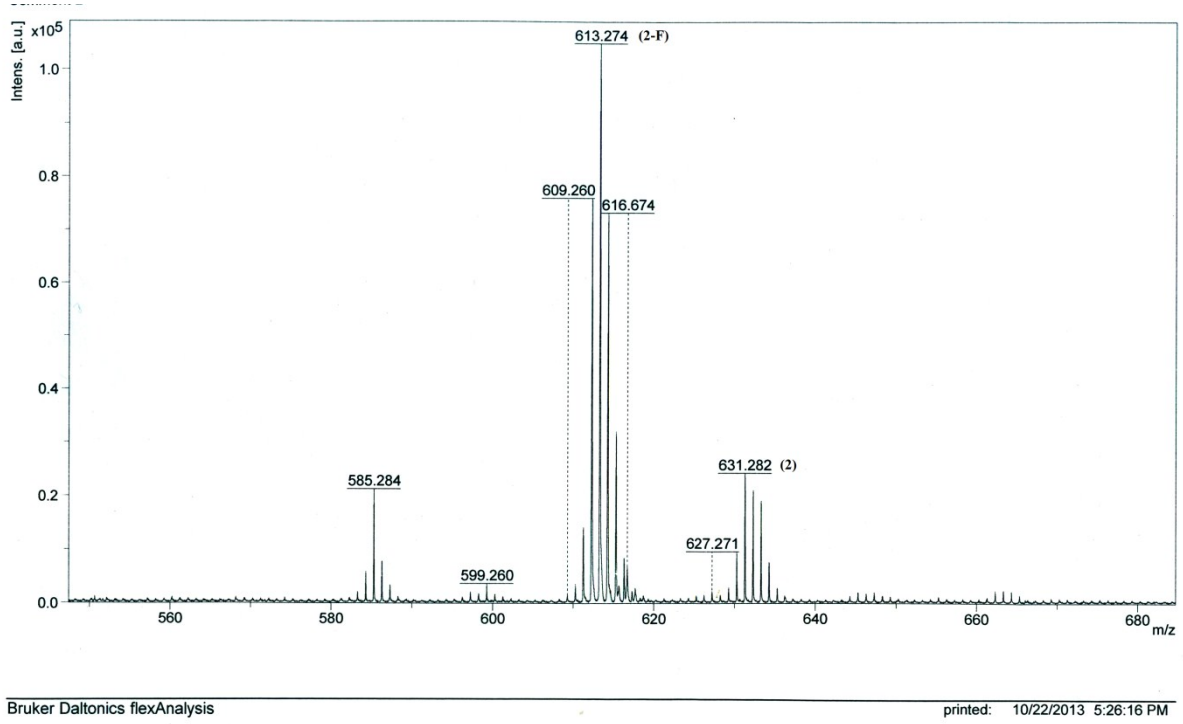

Figure S5:MALDI-Mass of spectrum of **2**

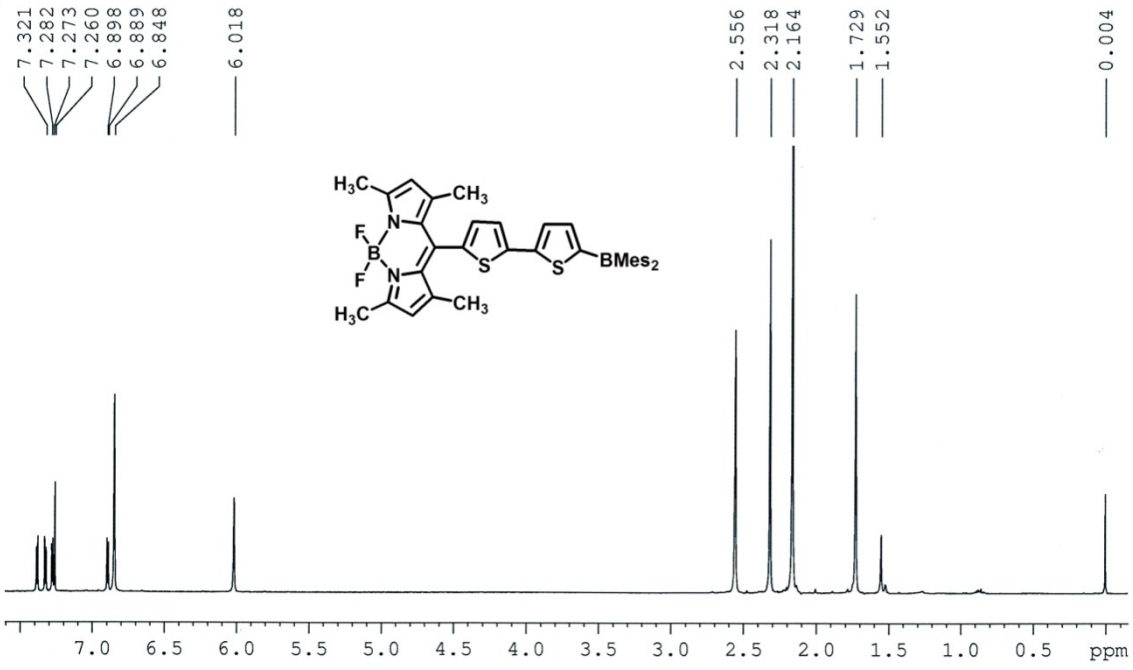

Figure S6:^{1}H NMR of **3**

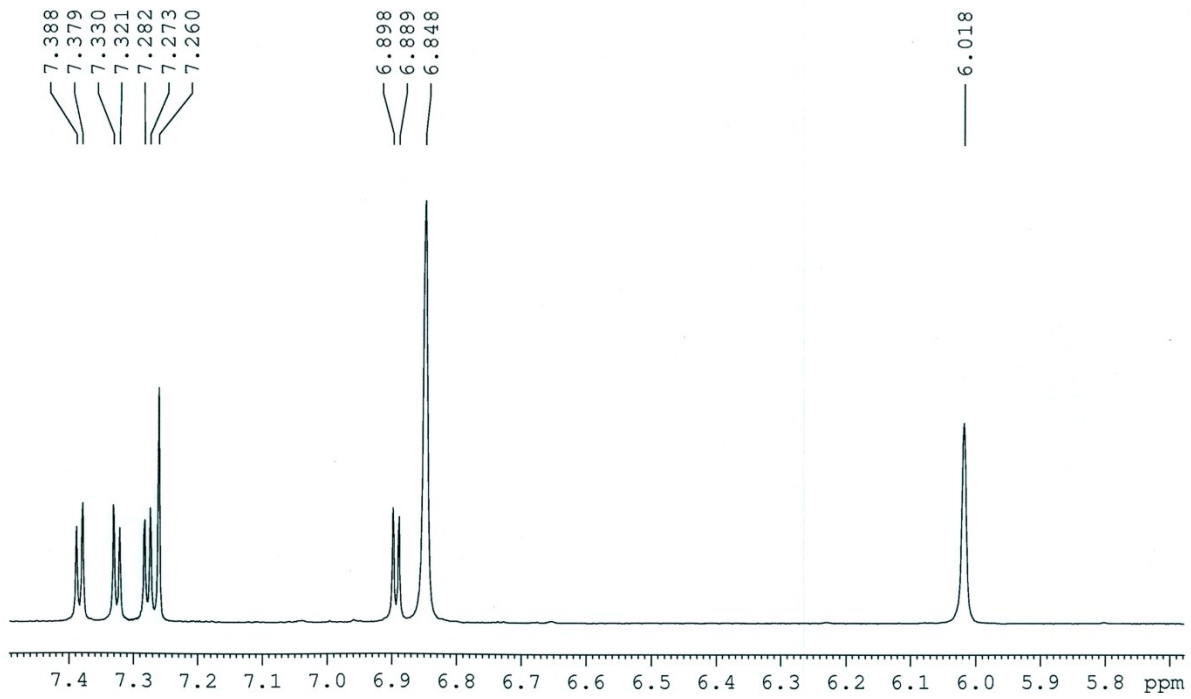

Figure S7: ^{1}H of **3** (enlarge view of aromatic region)

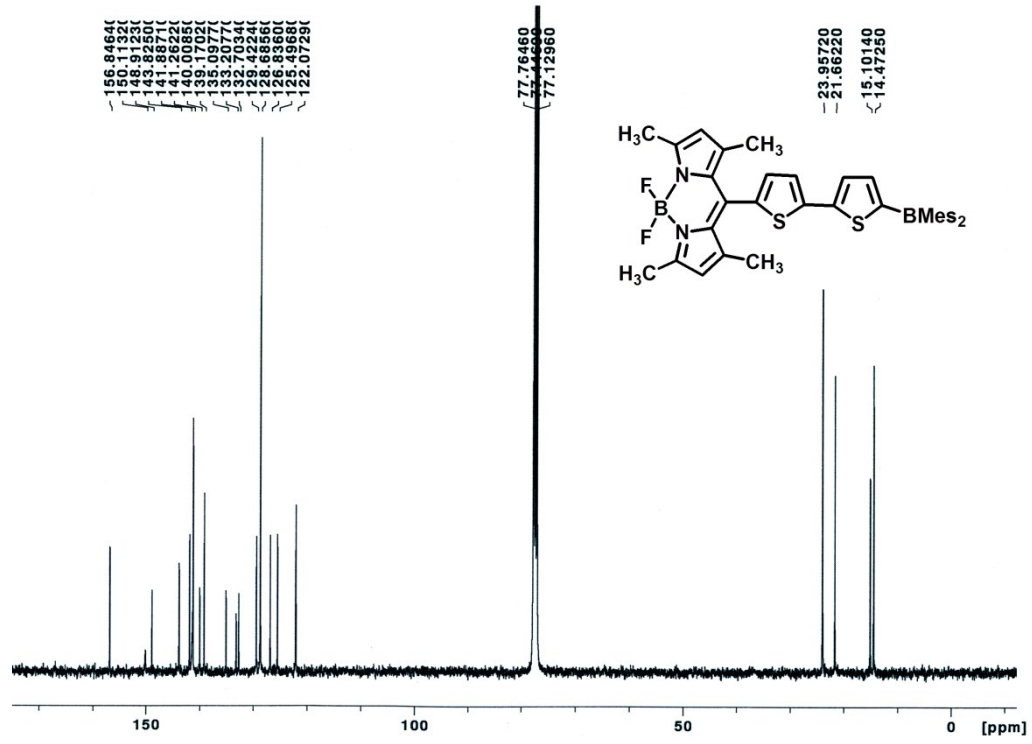

Figure S8: ^{13}C NMR of **3**

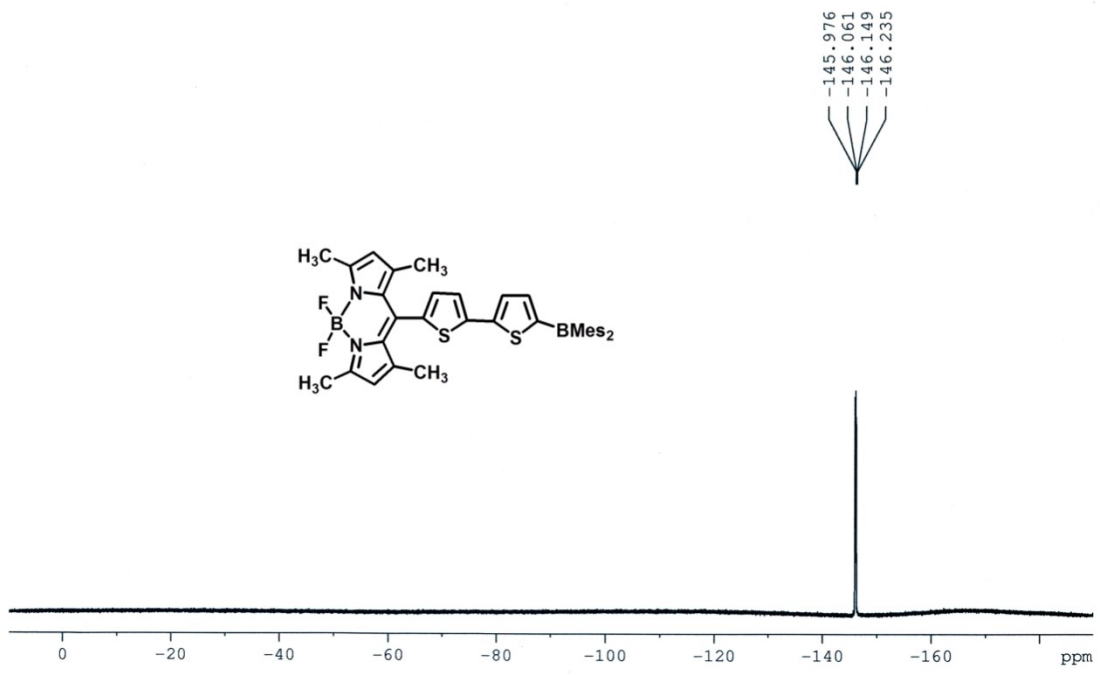

Figure S9: ^{11}F NMR of **3**

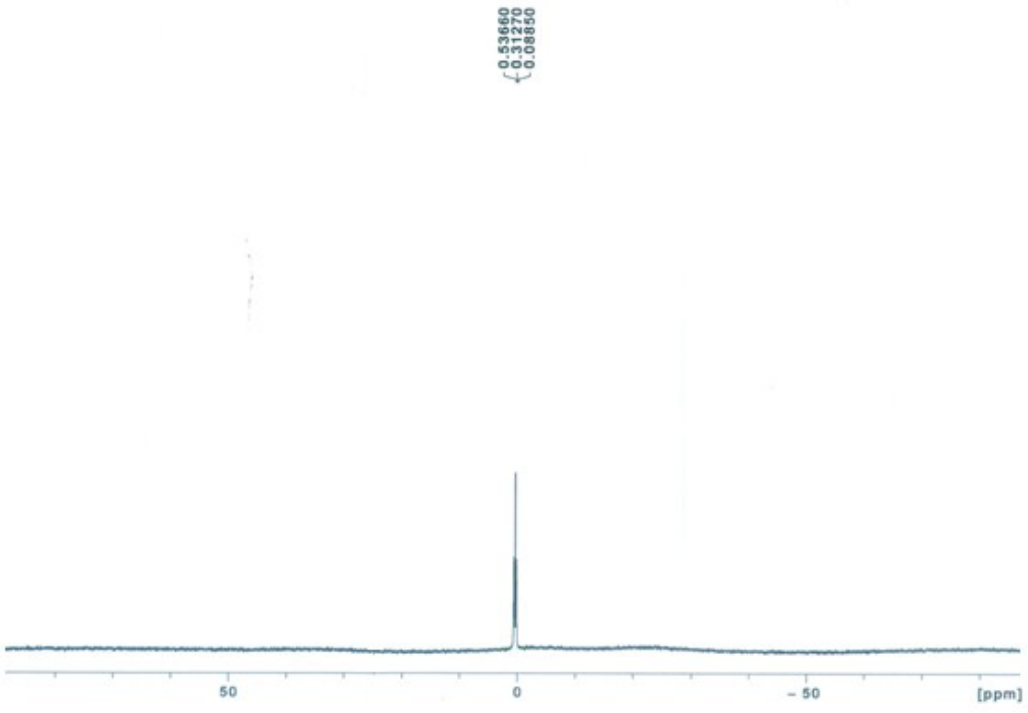

Figure S10: ^{11}B NMR of 3

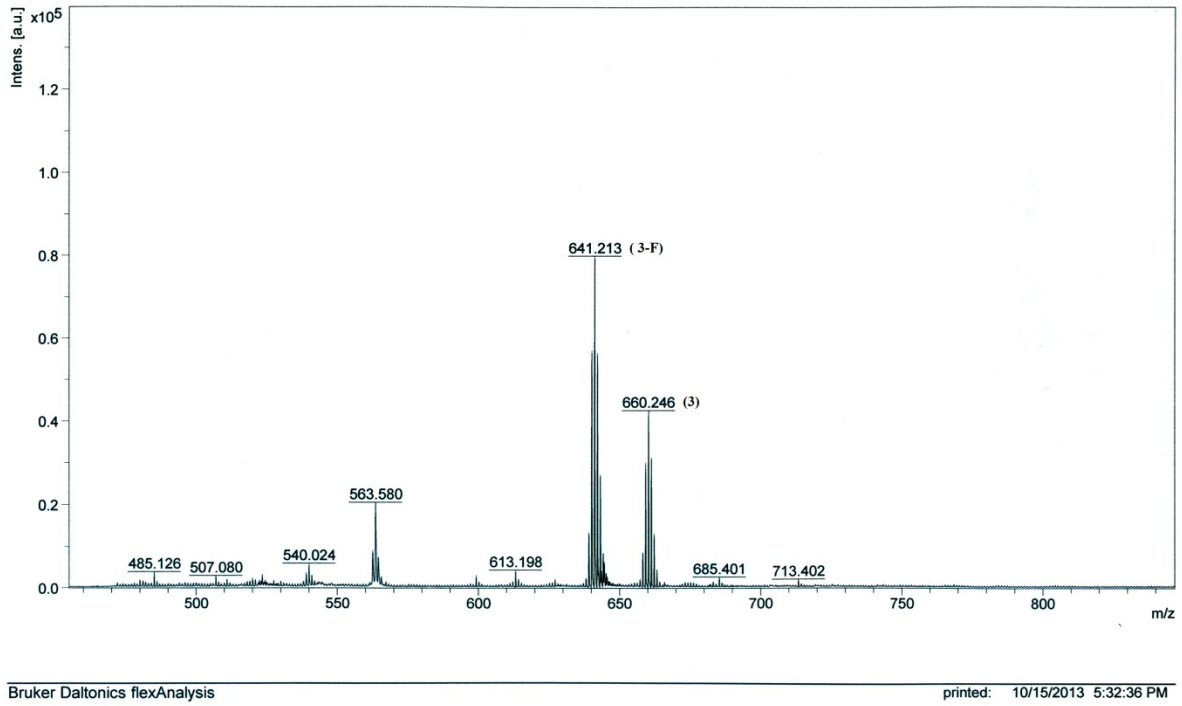

Figure S11:MALDI-Mass of spectra **3**

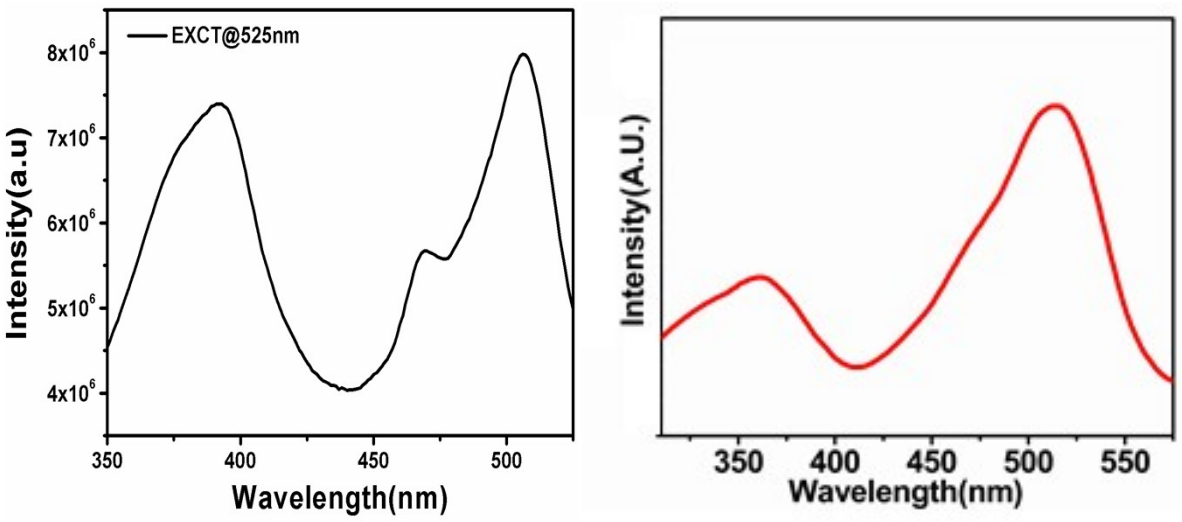

Figure S12: Excitation spectra of **2** (left) (λ_{em}525 nm) and **3** (right) (λ_{em}600 nm) in DCM

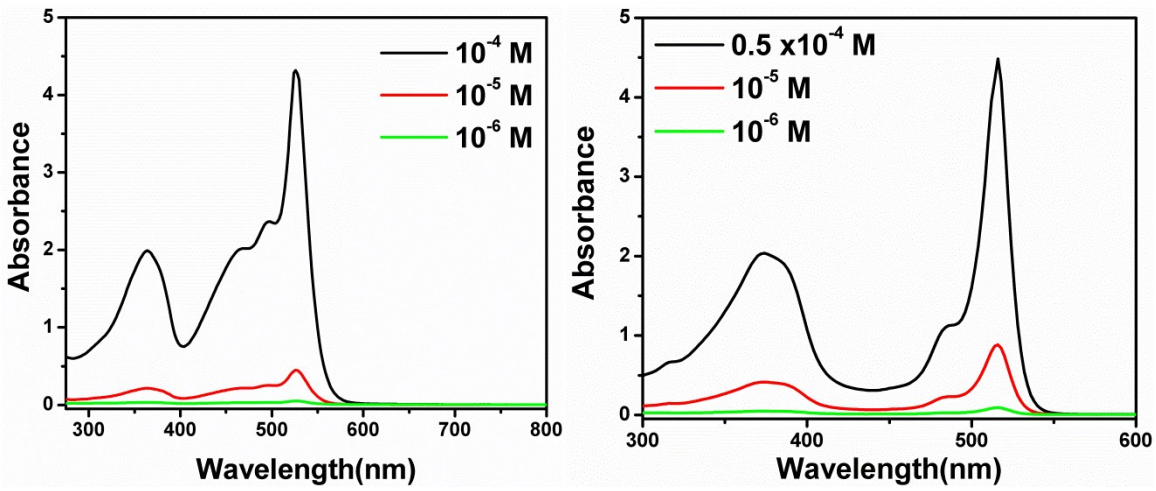

Figure S13: Concentration Variation UV-Vis Spectra of **2** (left) and **3** (right) in DCM

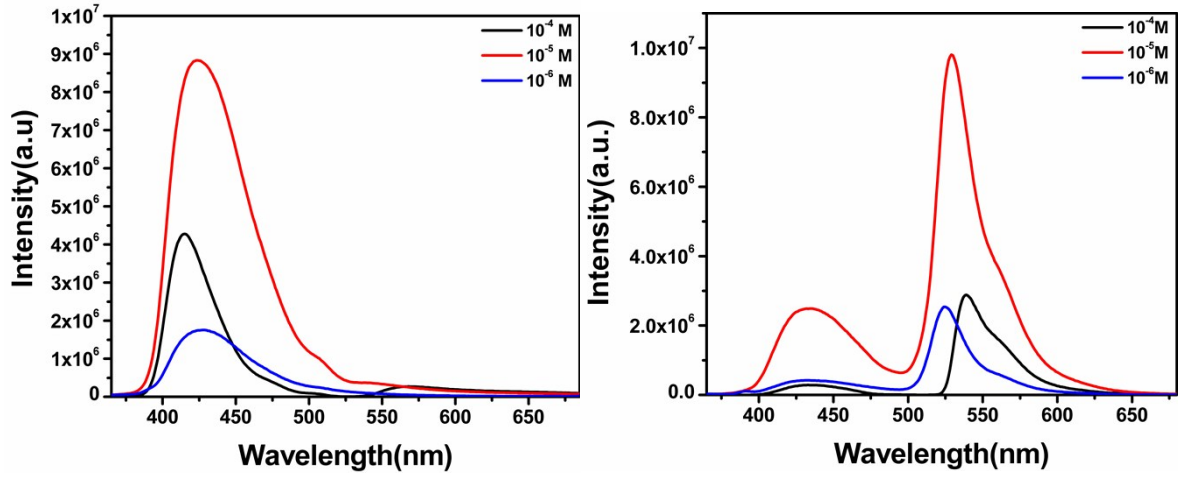

Figure S14: Concentration Variation Emission Spectra of **2** (left) and **3** (right) (λ_{ex} = 350 nm in DCM)

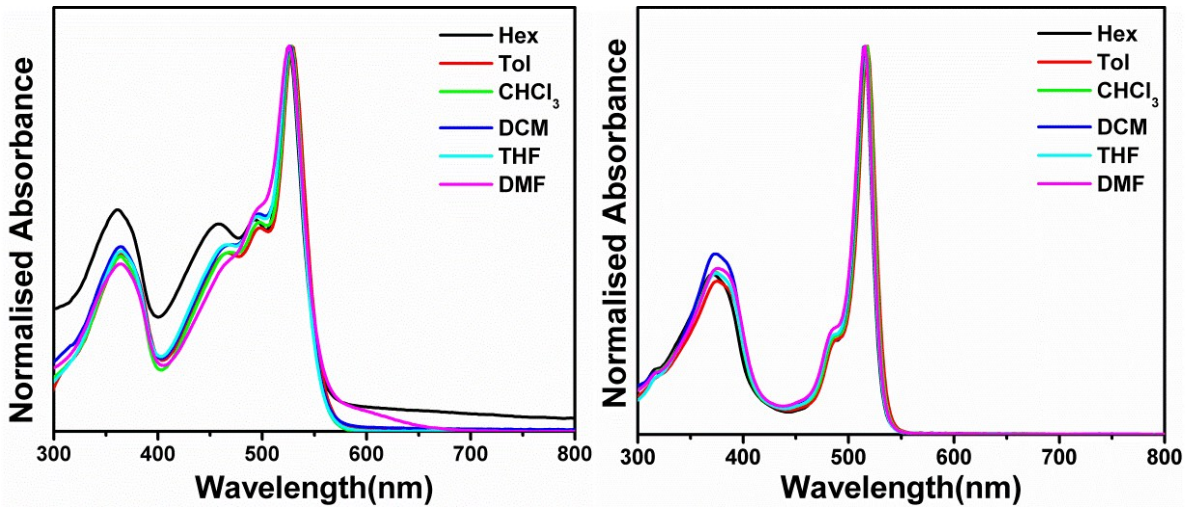

Figure S15: Absorption spectra of **2**(left) and **3** (right) in different solvents (10^{-5}M)

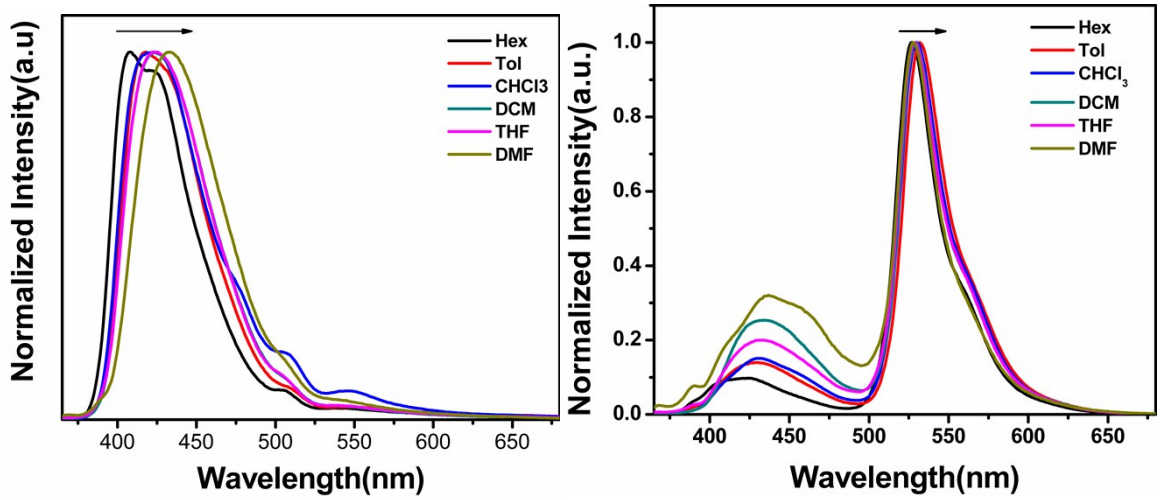

Figure S16: Emission spectra of **2** (left) and **3** (right) in different solvents (λ_{ex} = 350 nm, 10^{-5}M)

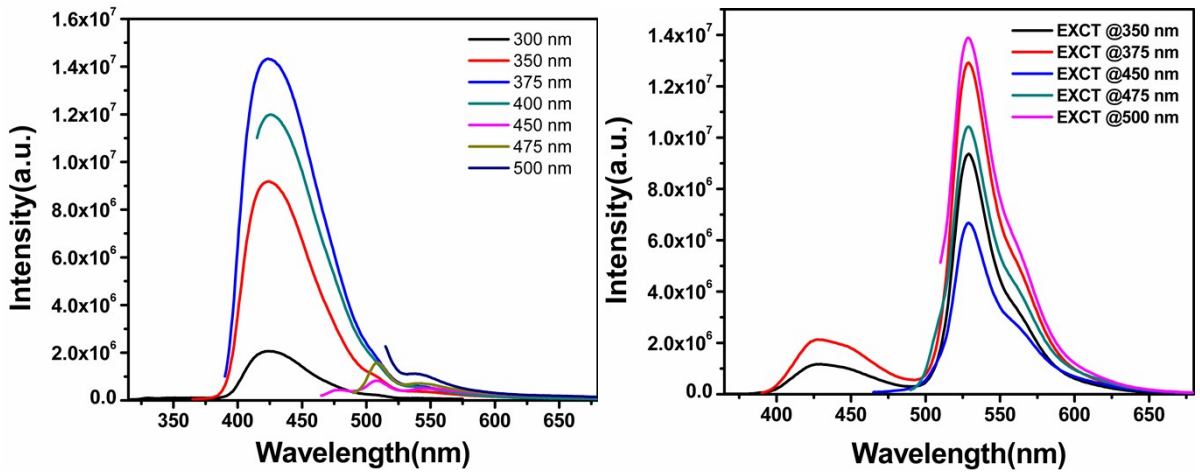

Figure S17: Emission spectra of **2** (left) and **3** (right) on different excitations (10^{-5}M in DCM)

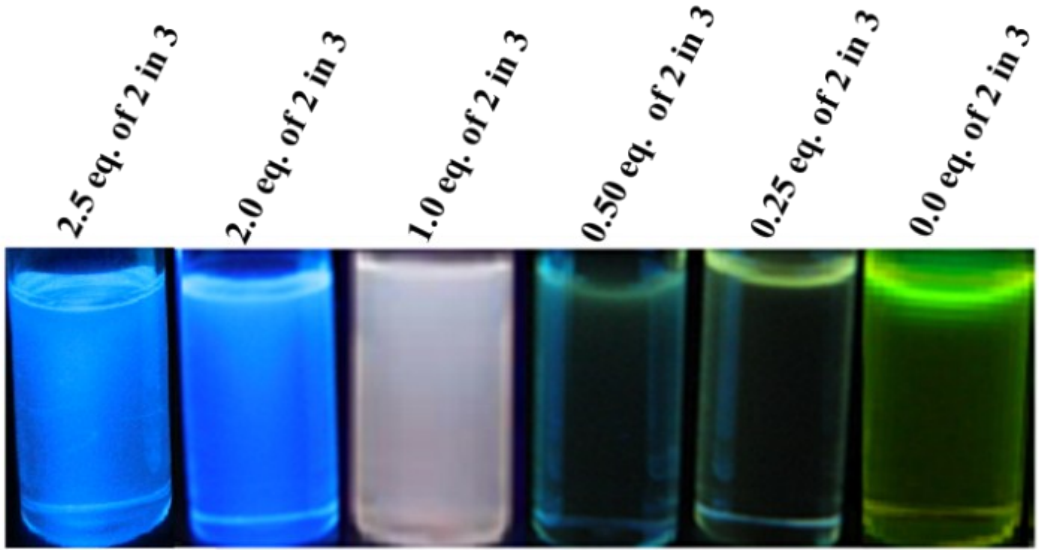

Figure 18. Photographs of different colour emission from different molar ratio of **2** and **3** in CH_2Cl_2 under UV light (365 nm).