Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Synthesis and photophysical properties of novel butterfly-shaped blue emitters based on pyrene

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NMR spectrum

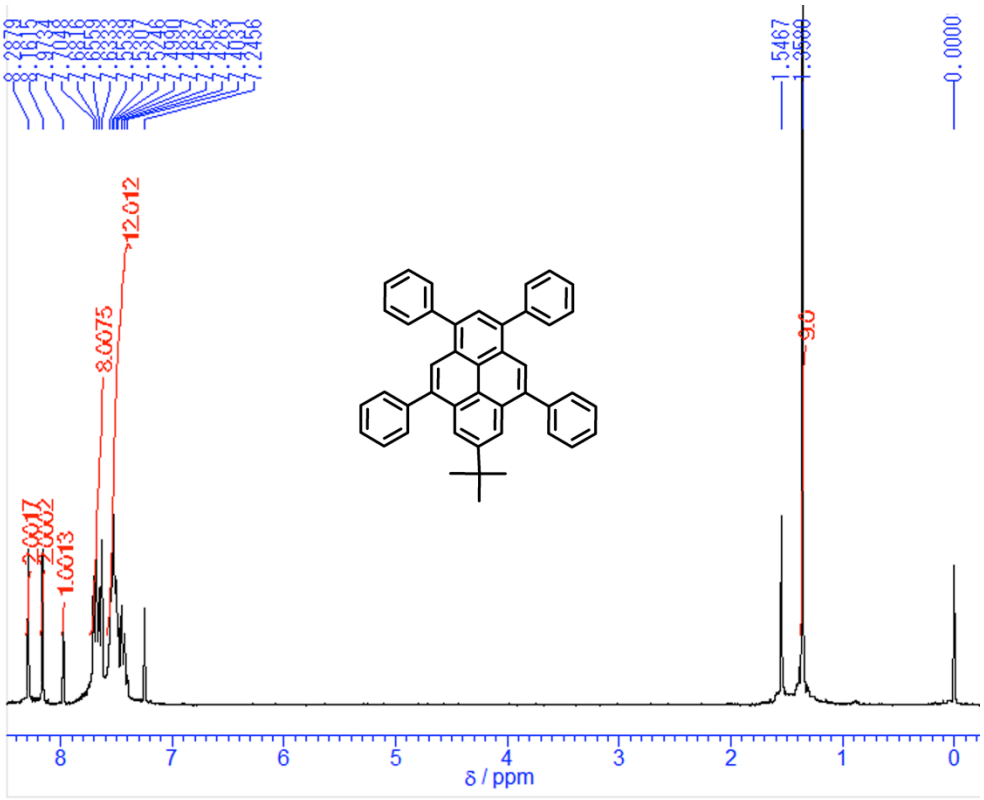

Figure S**1-1**. ^{1}H NMR spectrumof **4a** (300 MHz, $CDCl_3$, 293 K).

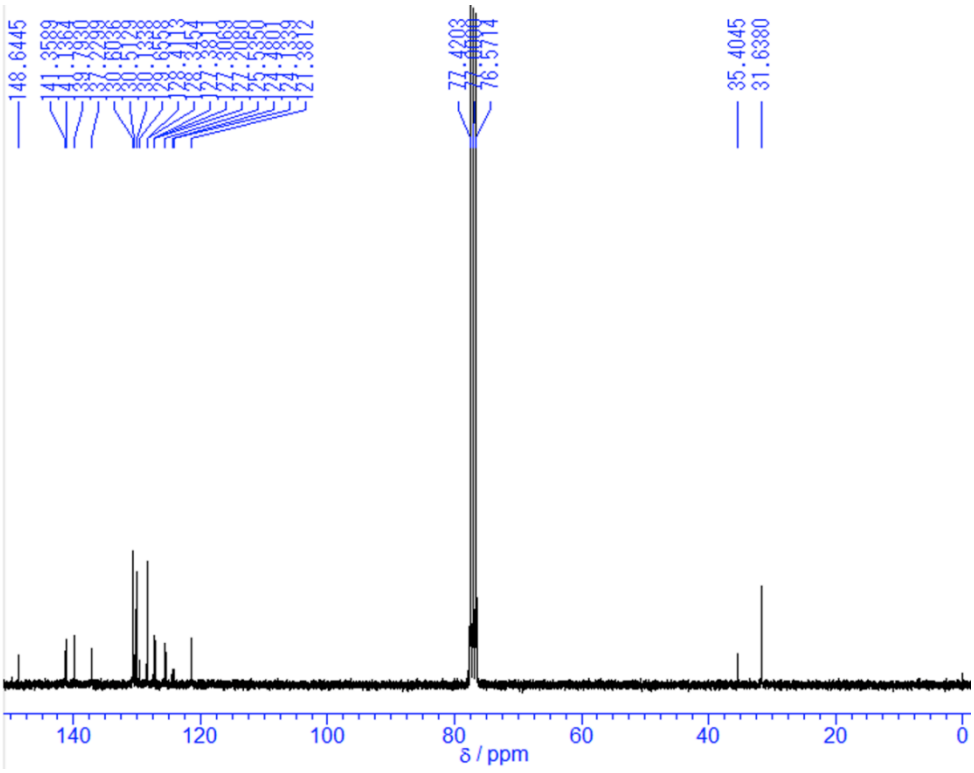

Figure S**1-2**. ^{13}C NMR spectrumof **4a** (75 MHz, $CDCl_3$, 293 K).

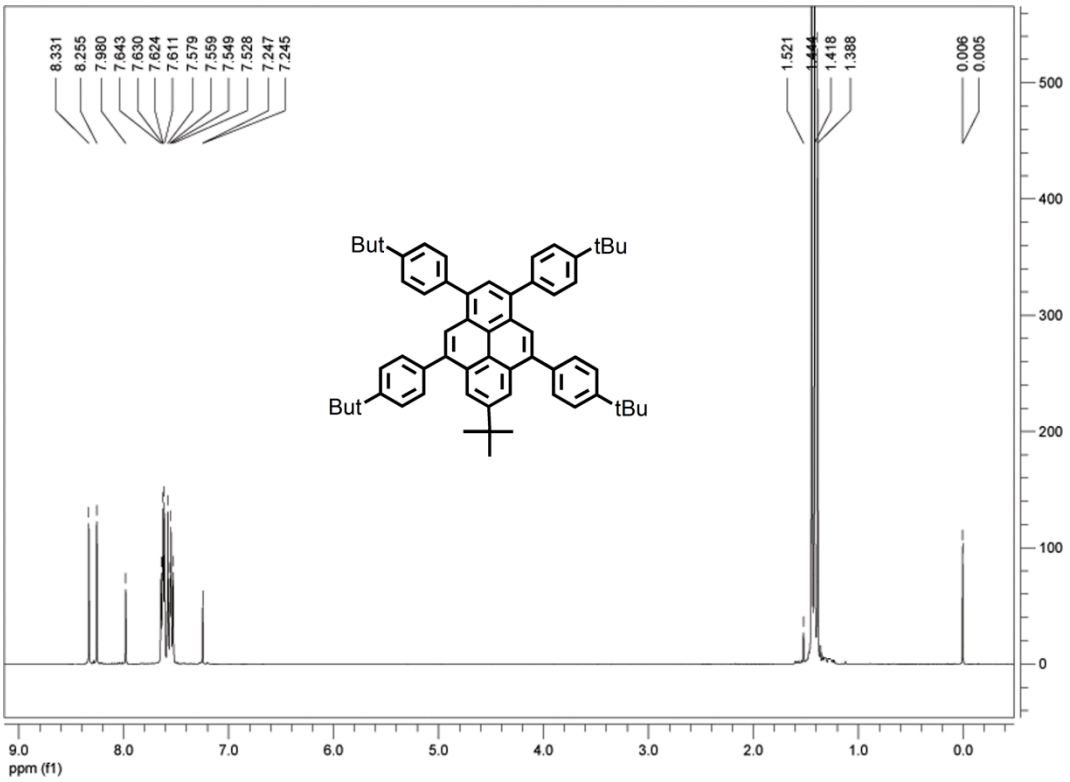

Figure S**1-3**. ^{1}H NMR spectrum of **4b** (400 MHz, $CDCl_3$, 293 K).

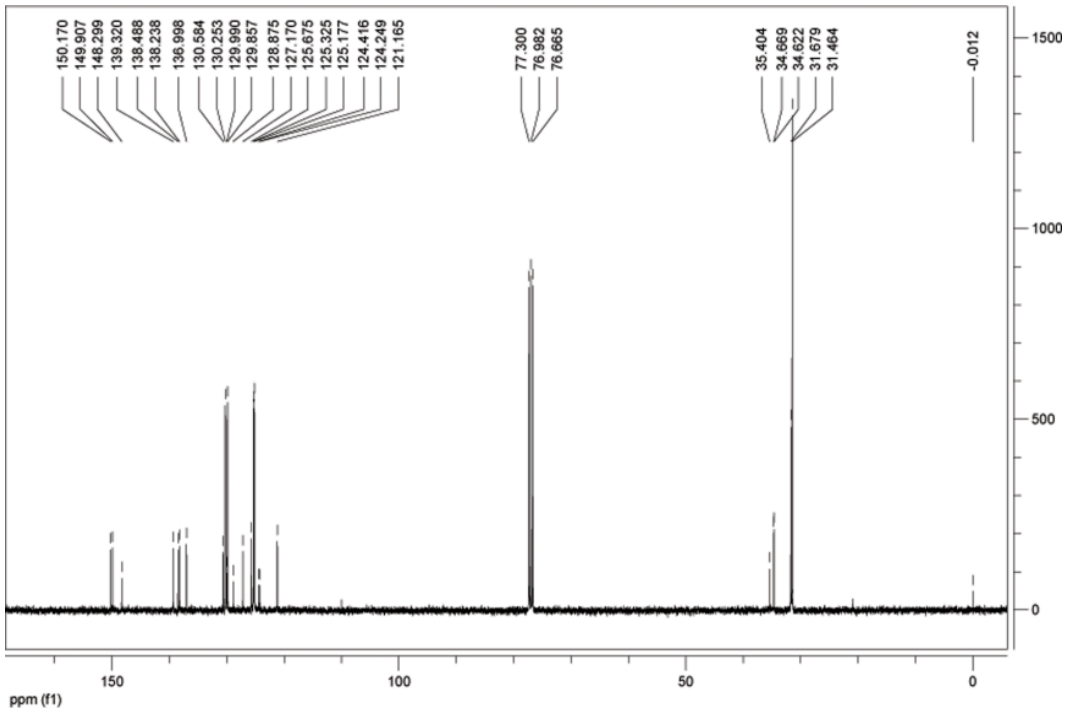

Figure S**1-4**. ^{13}C NMR spectrum of **4b** (100 MHz, $CDCl_3$, 293 K).

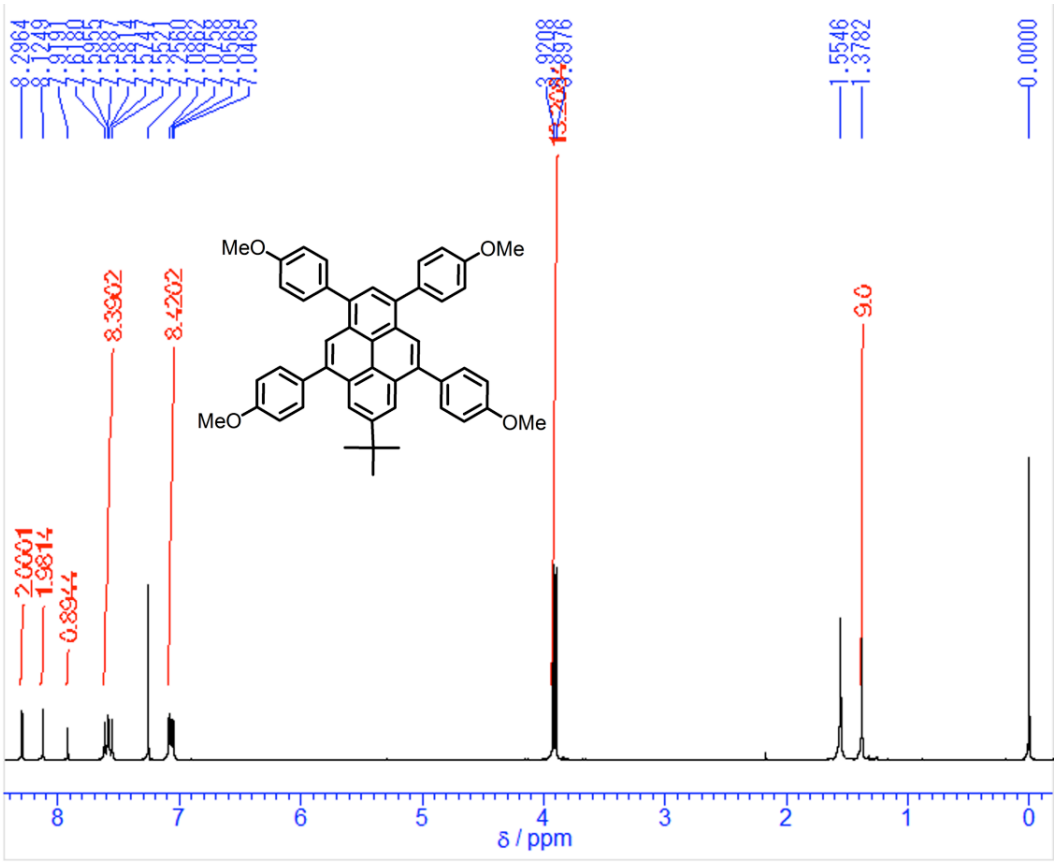

Figure S**1-5**. ^{1}H NMR spectrumof **4c** (300 MHz, $CDCl_3$, 293 K).

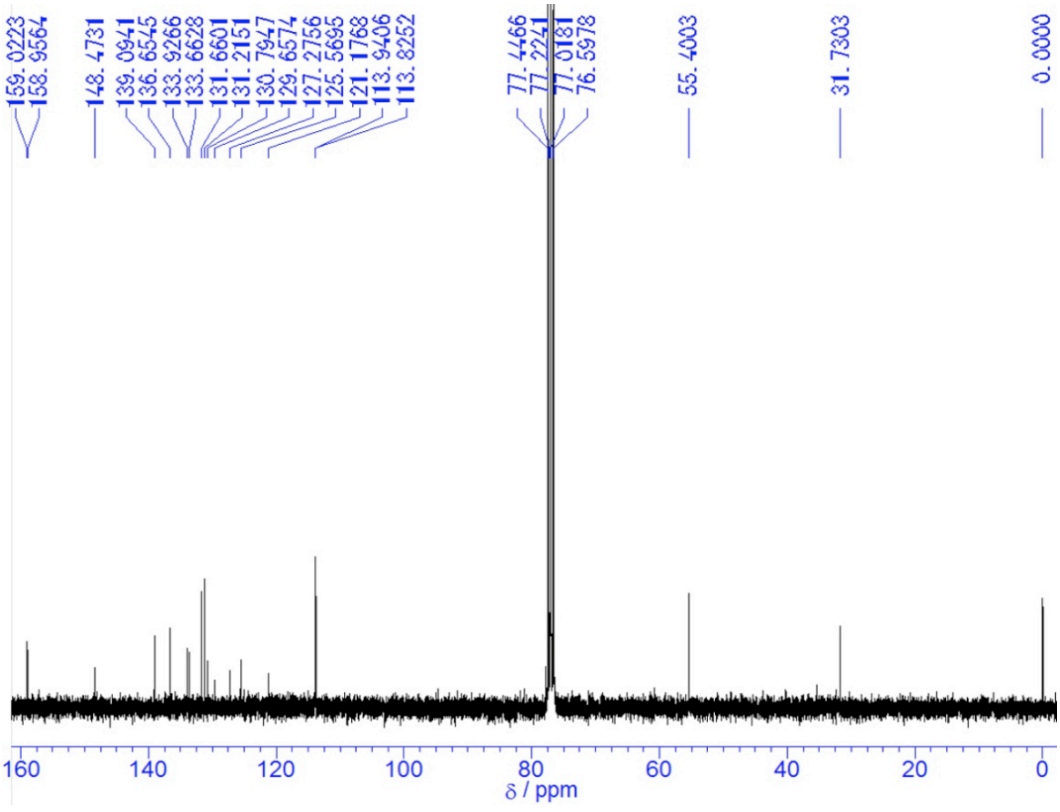

Figure S**1-6**. ^{13}C NMR spectrum of **4c** (75 MHz, $CDCl_3$, 293 K).

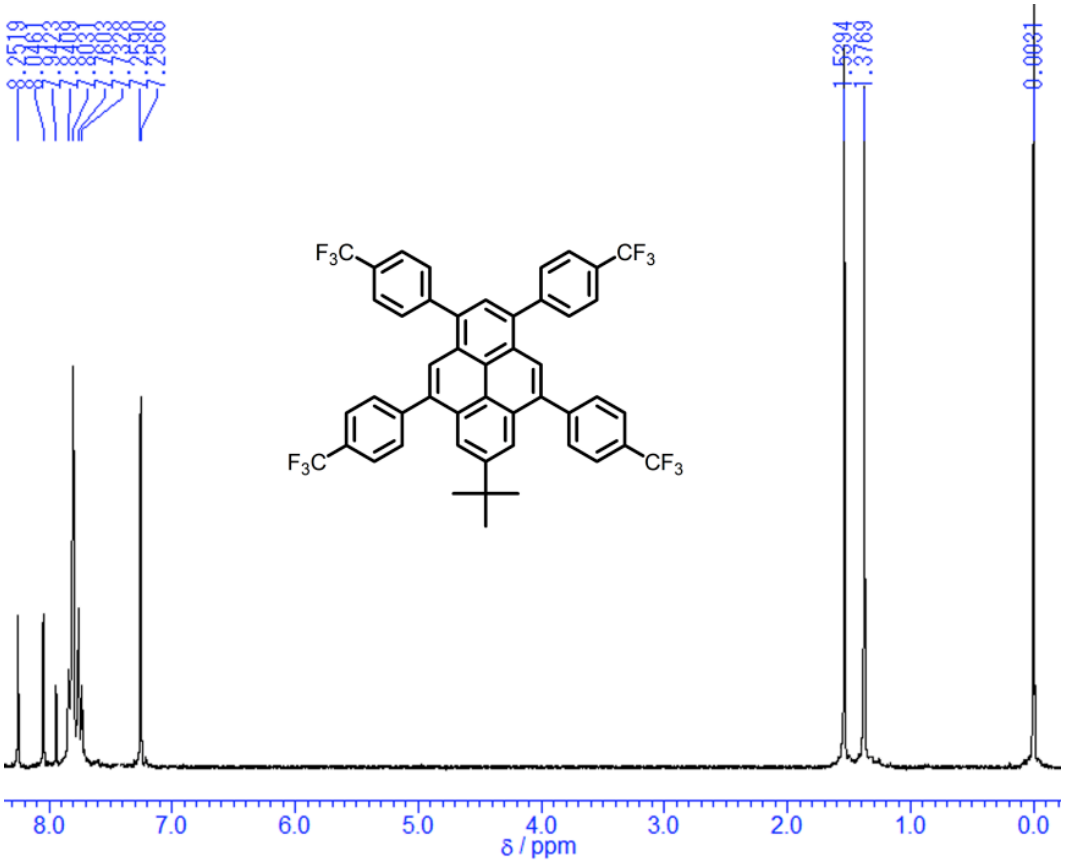

Figure S**1-7**. ^{1}H NMR spectrum of **4d** (300 MHz, $CDCl_3$, 293 K).

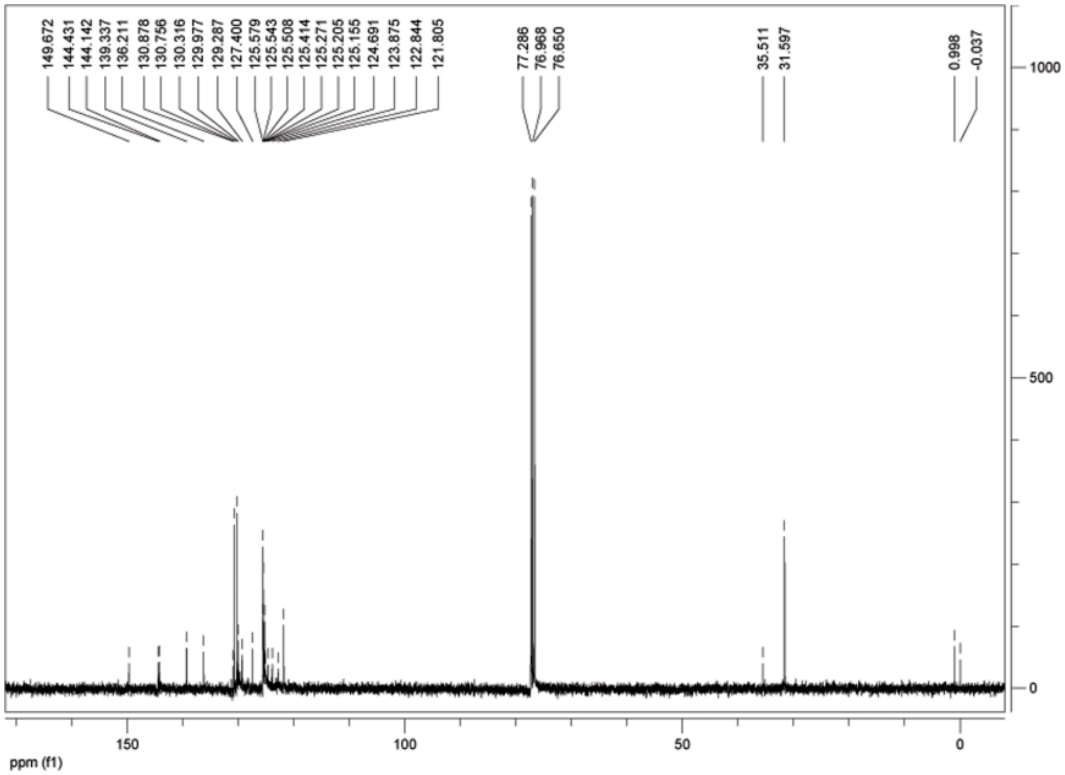

Figure S**1-8**. ^{13}C NMR spectrum of **4d** (100 MHz, $CDCl_3$, 293 K).

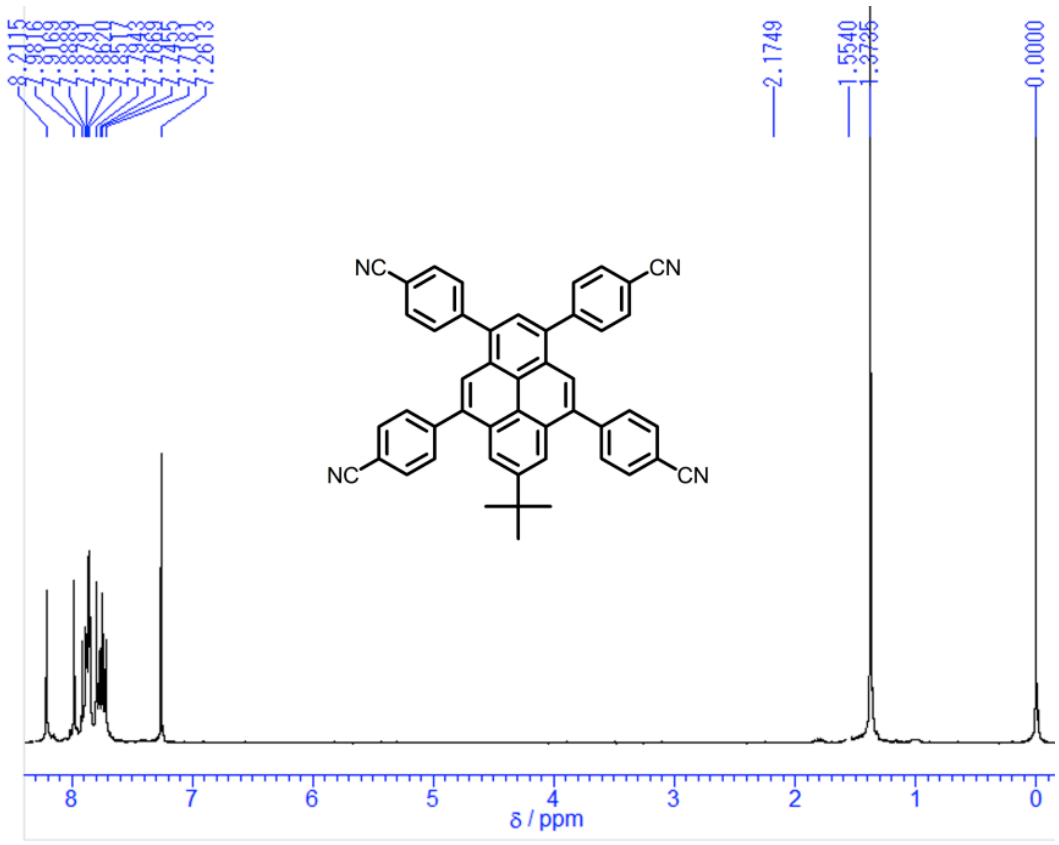

Figure S**1-9**. ^{1}H NMR spectrum of **4e** (300 MHz, $CDCl_3$, 293 K).

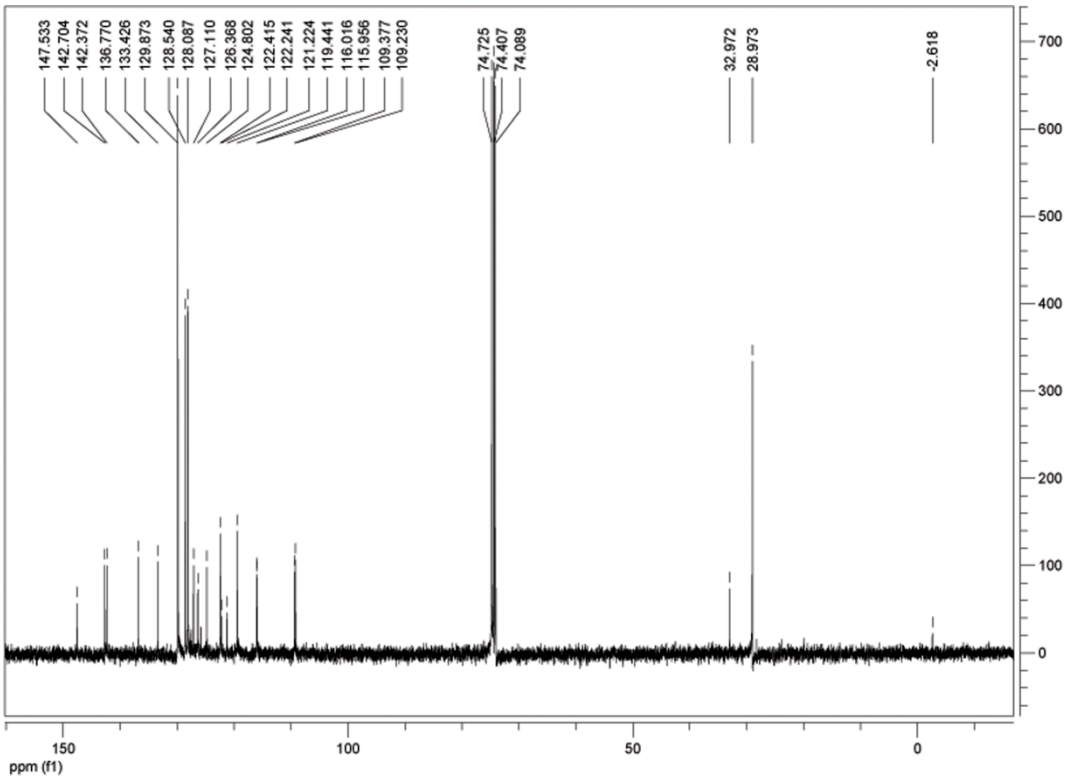

Figure S**1-10**. ^{13}C NMR spectrum of **4e** (100 MHz, $CDCl_3$, 293 K).

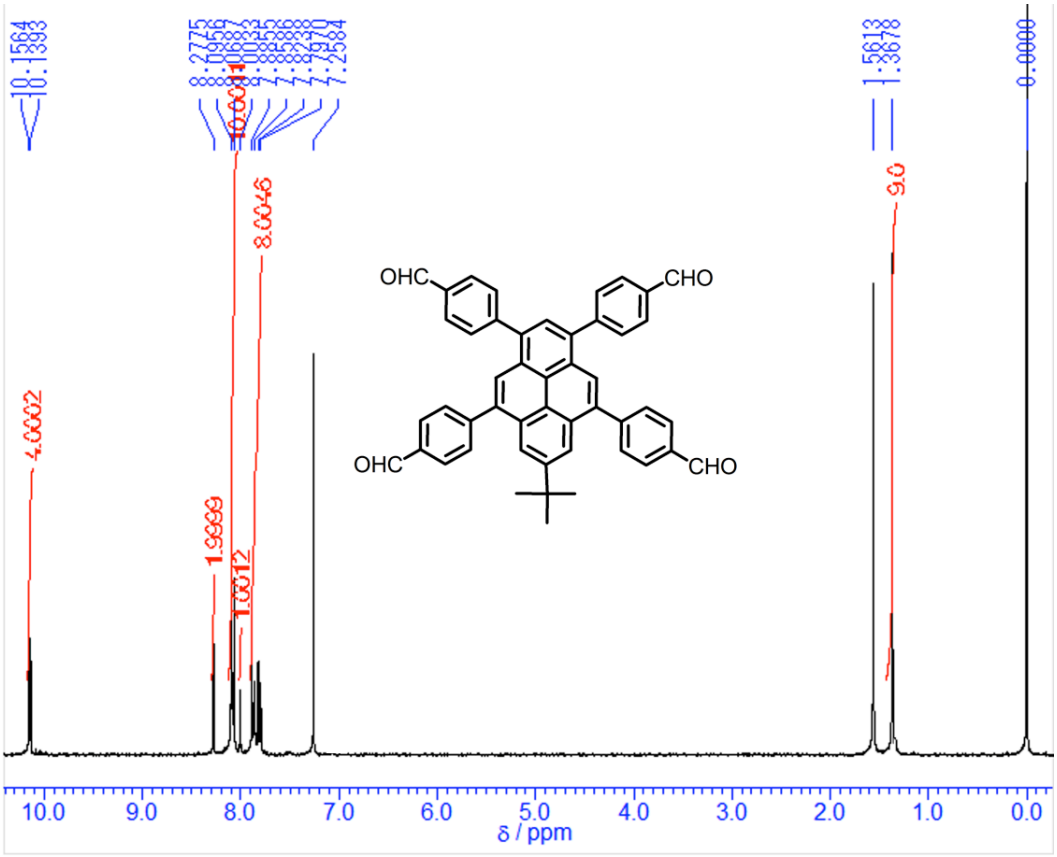

Figure S**1-11**. ^{1}H NMR spectrum of **4f** (300 MHz, $CDCl_3$, 293 K).

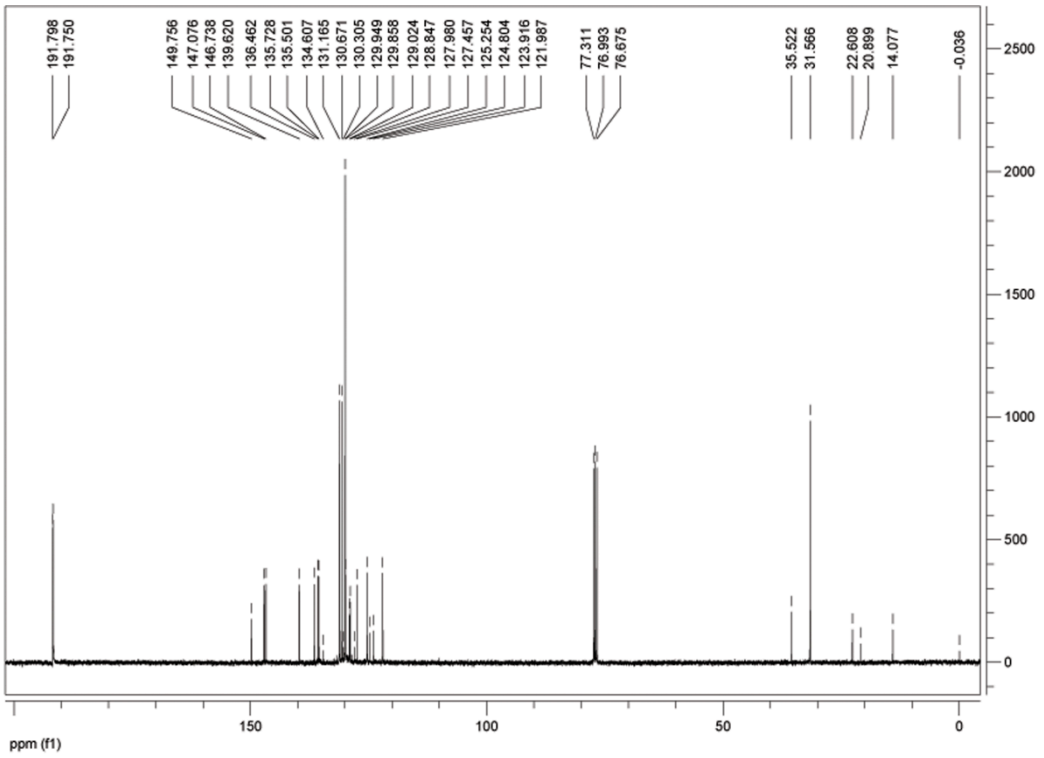

Figure S**1-12**. ^{13}C NMR spectrum of **4f** (100 MHz, $CDCl_3$, 293 K).

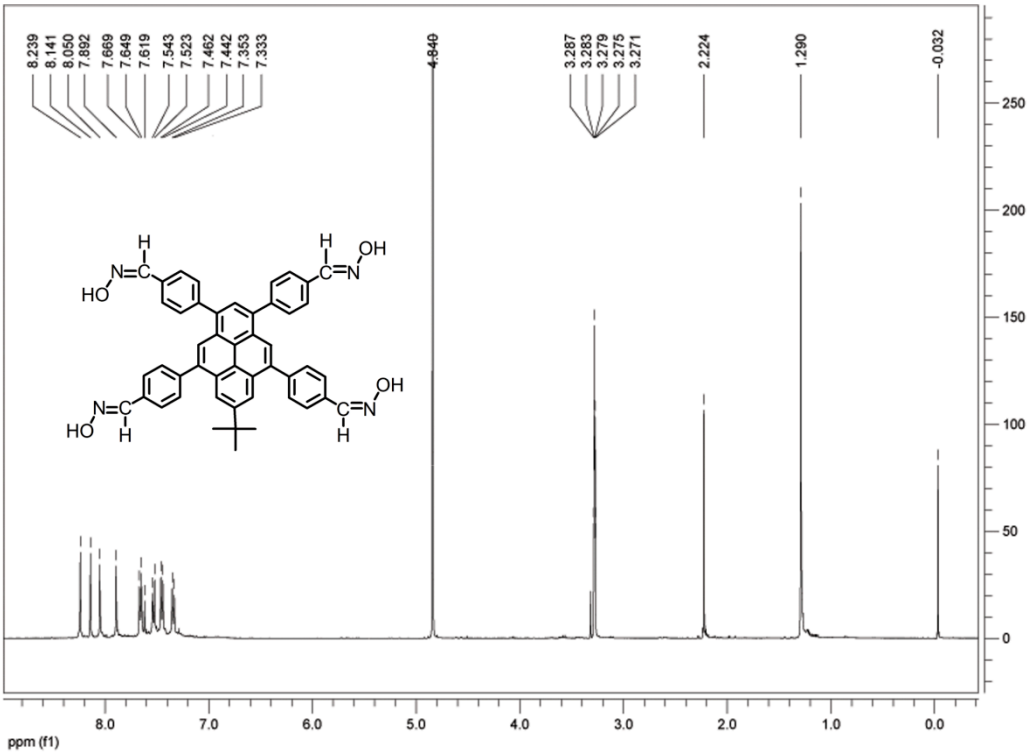

Figure S**1-13**. ^{1}H NMR spectrum of **5** (400 MHz, $CDCl_3$, 293 K).

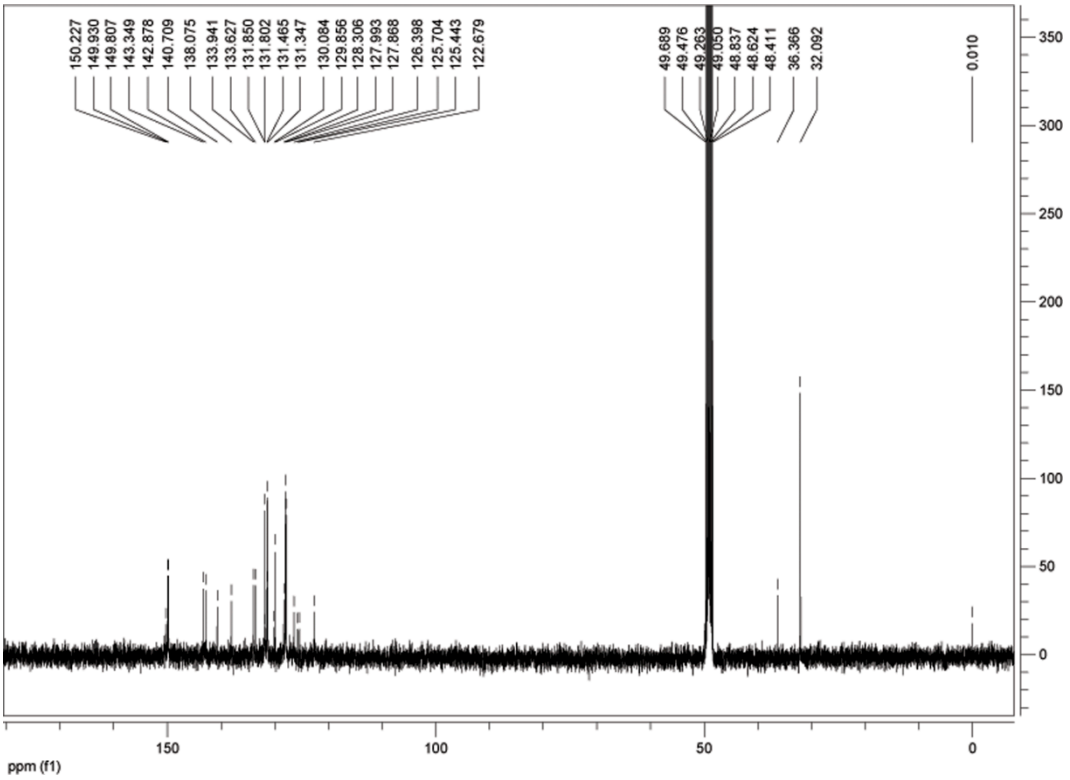

Figure S**1-14**. ^{13}CNMR spectrum of **5** (100 MHz, $CDCl_3$, 293 K).

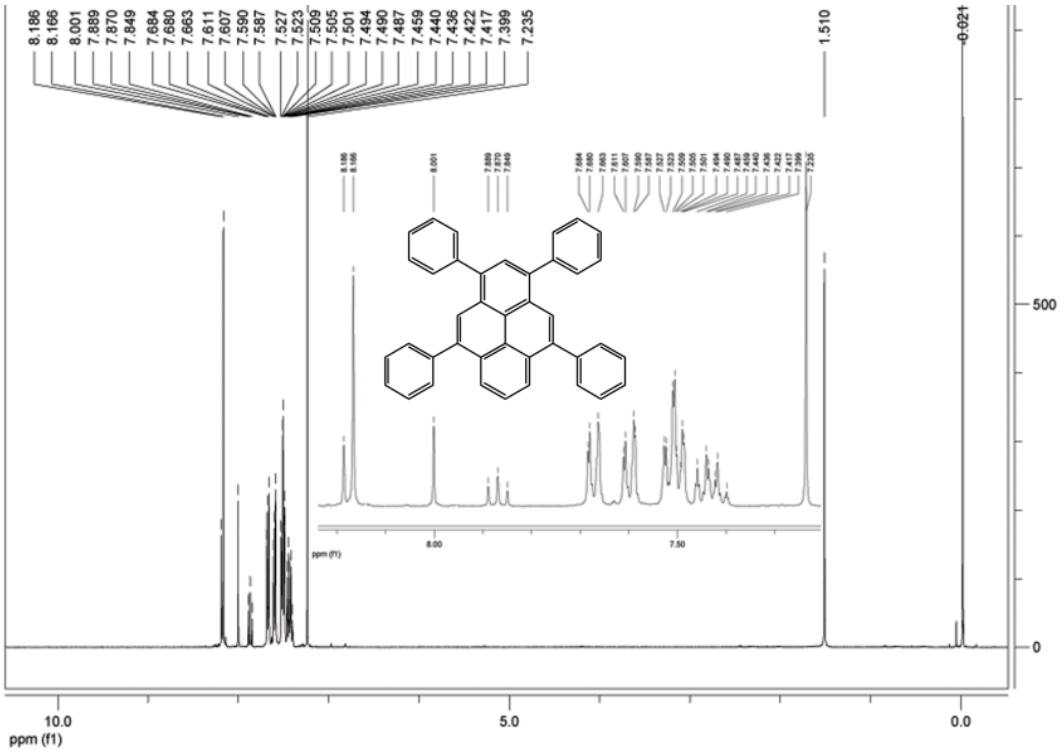

Figure S**1-15**. ^{1}H NMR spectrum of **6** (400 MHz, $CDCl_3$, 293 K).

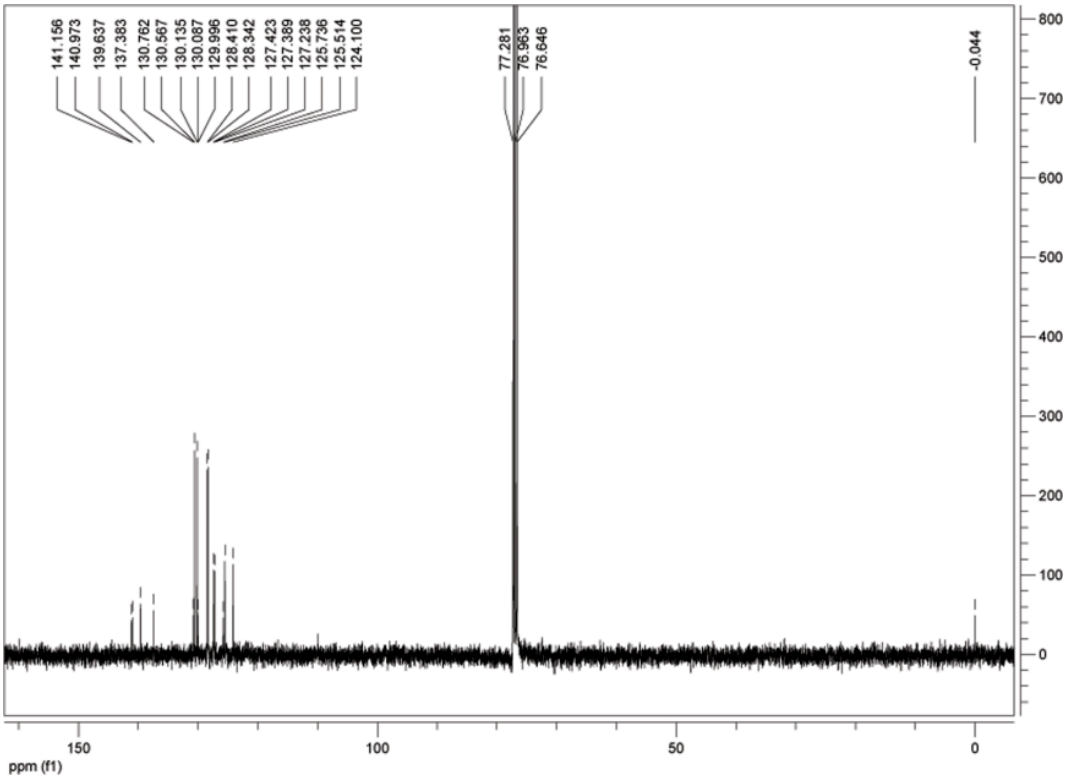

Figure S**1-16**. ^{13}CNMR spectrum of **6** (100 MHz, $CDCl_3$, 293 K).

PhotophyscalAnalysis

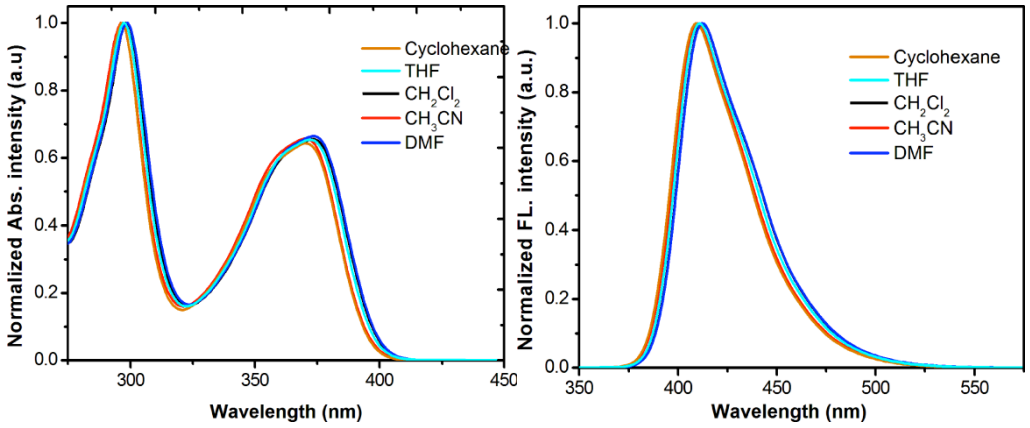

Figure S**2-1**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4a** recorded in different solvents at ~10^{-5} M and 25 °C.

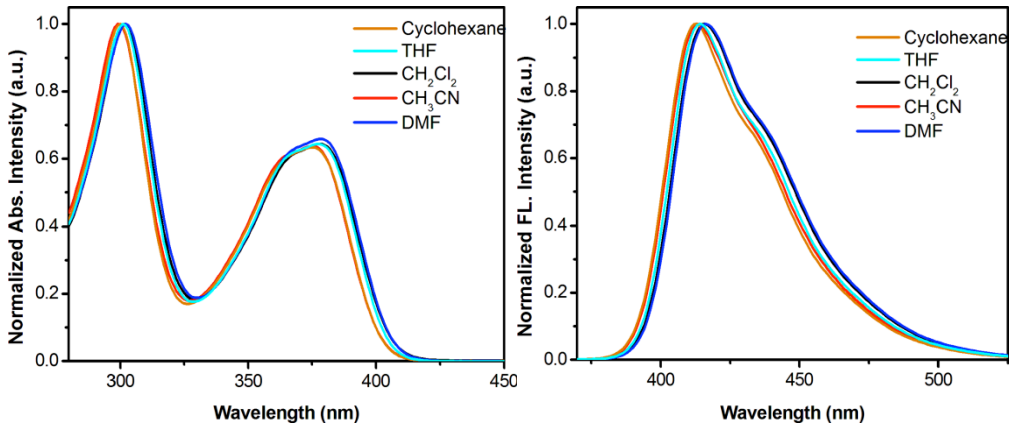

Figure S**2-2**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4b** recorded in different solvents at ~10^{-5} M and 25 °C.

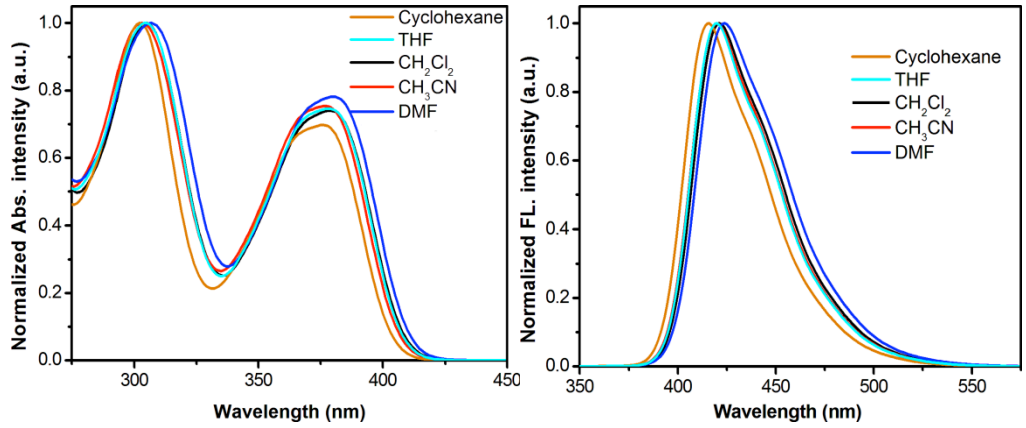

Figure S**2-3**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4c** recorded in different solvents at ~10^{-5} M and 25 °C.

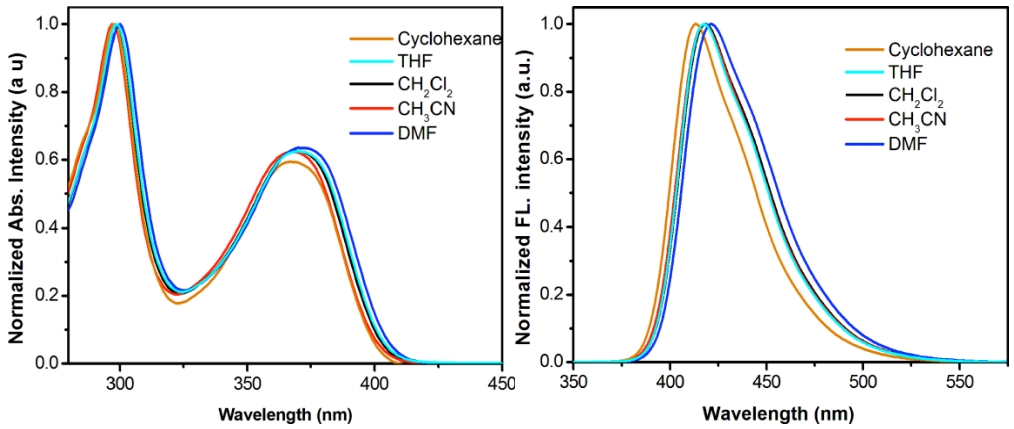

Figure S**2-4**.UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4d** recorded in different solvents at ~10^{-5} M and 25 °C.

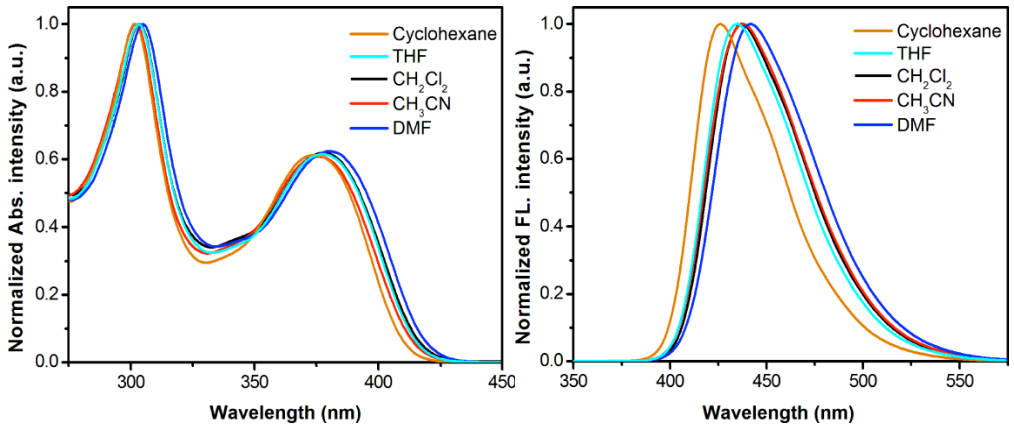

Figure S**2-5**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4e** recorded in different solvents at ~10^{-5} M and 25 °C.

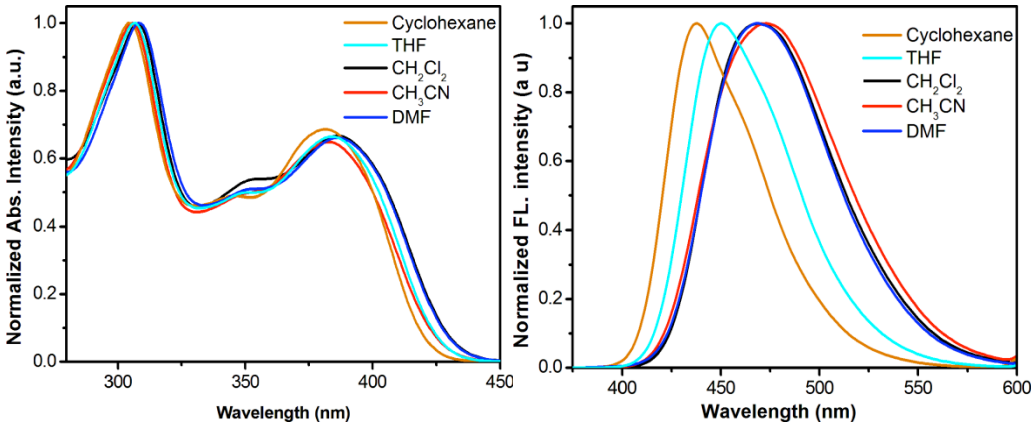

Figure S**2-6**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **4f** recorded in different solvents at ~10^{-5} M and 25 °C.

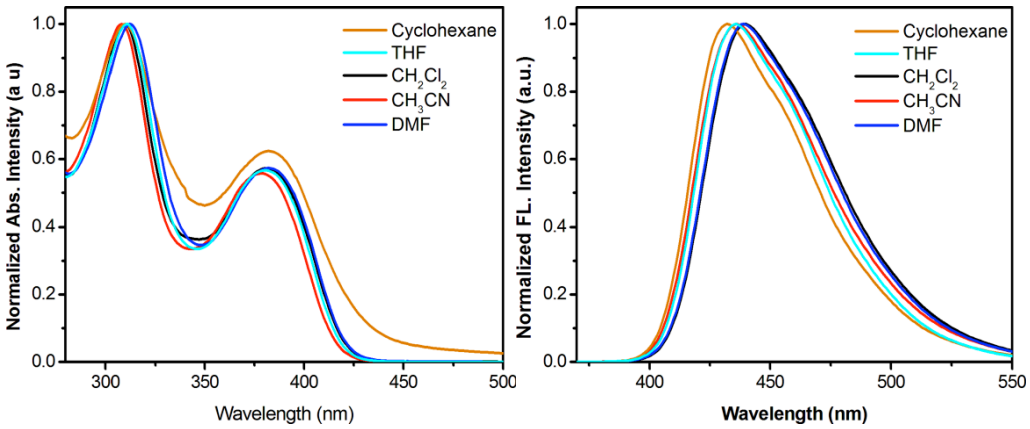

Figure S**2-7**. UV/Vis absorption (left) and fluorescence spectra (right) of the compound **5** recorded in different solvents at ~10^{-5} M and 25 °C.

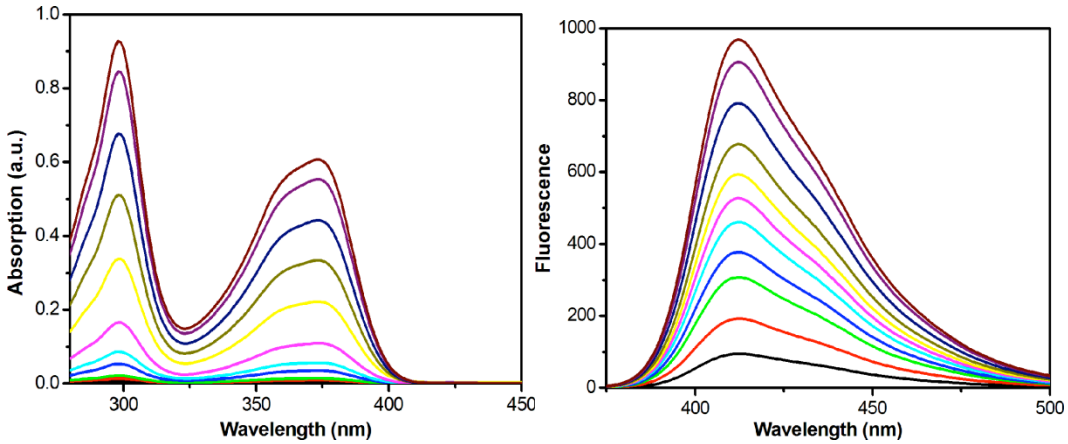

Figure S**2-8**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4a**in CH_2Cl_2 at 25 °C.

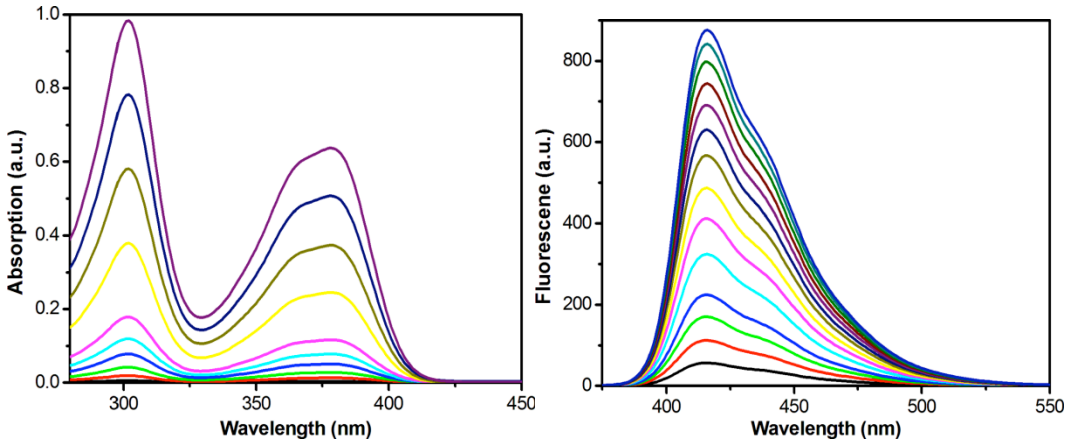

Figure S**2-9**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4b**in CH_2Cl_2 at 25 °C.

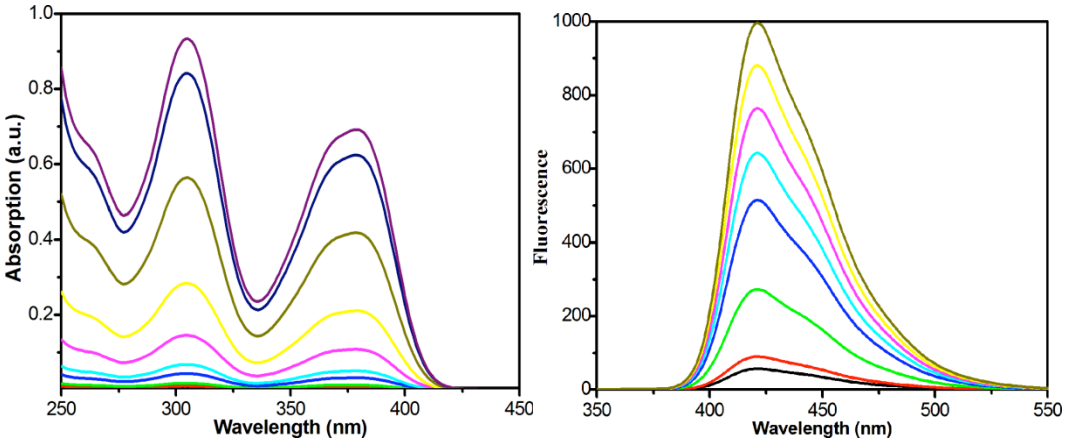

Figure S**2-10**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4c**in CH_2Cl_2 at 25 °C.

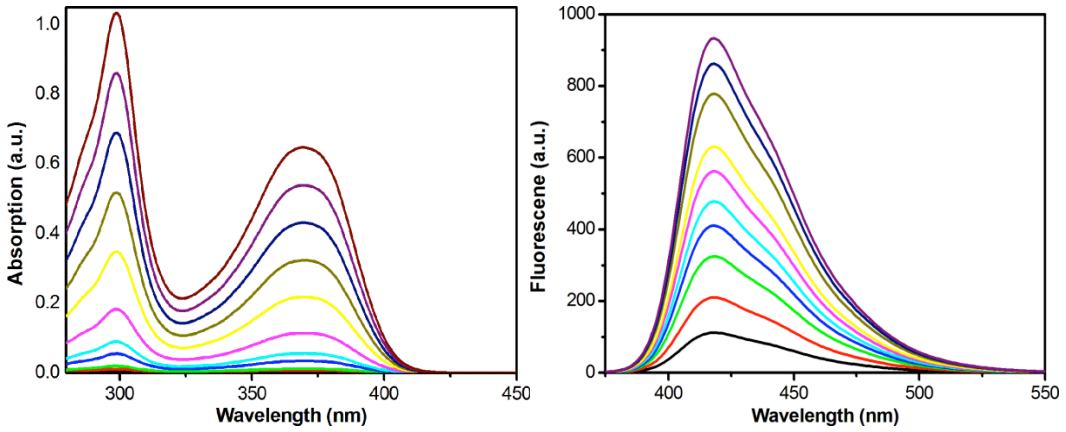

Figure S**2-11**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4d**in CH_2Cl_2 at 25 °C.

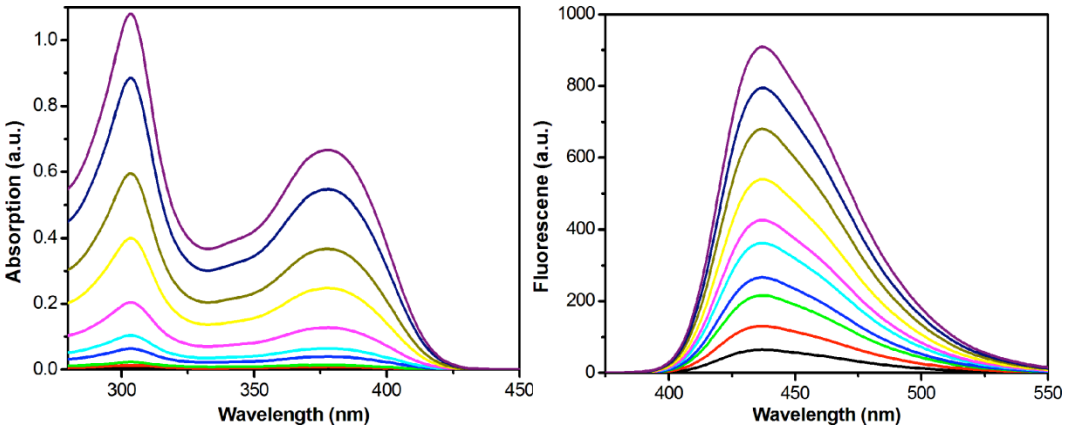

Figure S**2-12**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4e**in CH_2Cl_2 at 25 °C.

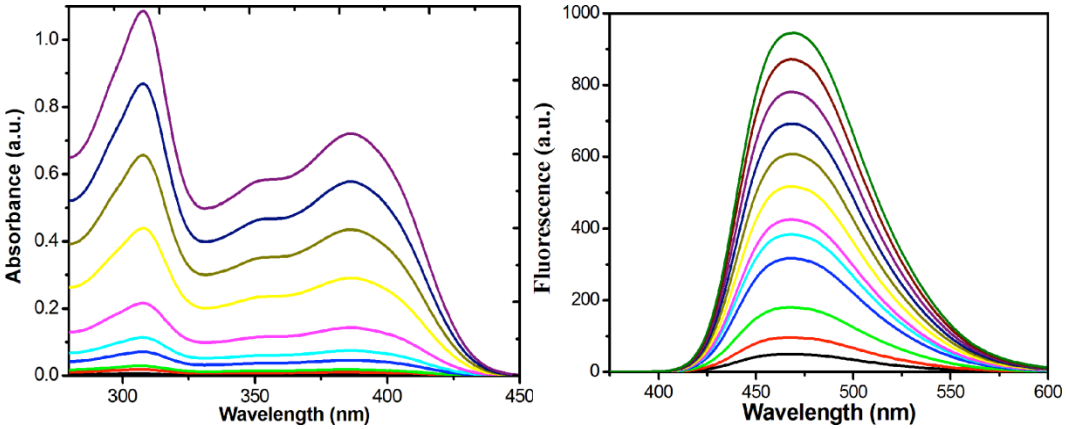

Figure S**2-13**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **4f**in CH_2Cl_2 at 25 °C.

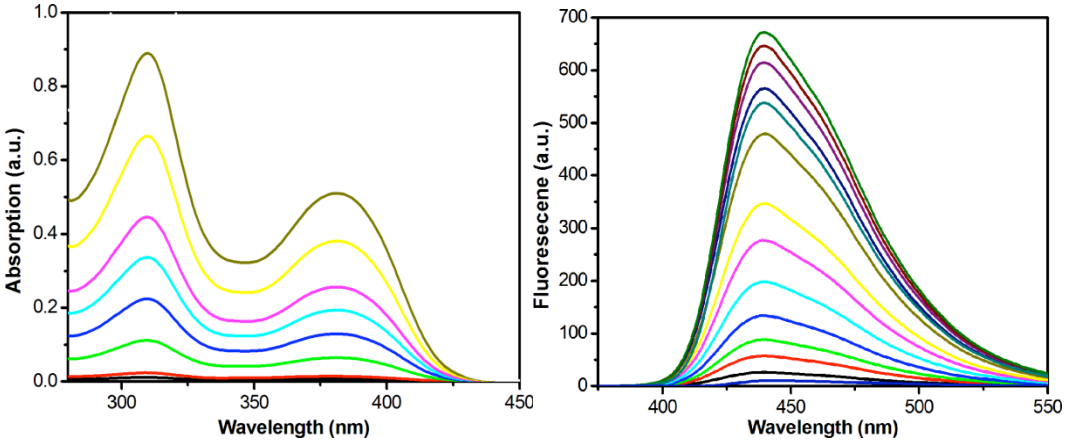

Figure S**2-14**Effect of concentration on the UV/Vis (left) and fluorescence emission (right) of **5**in CH_2Cl_2 at 25 °C.

DSC analysis

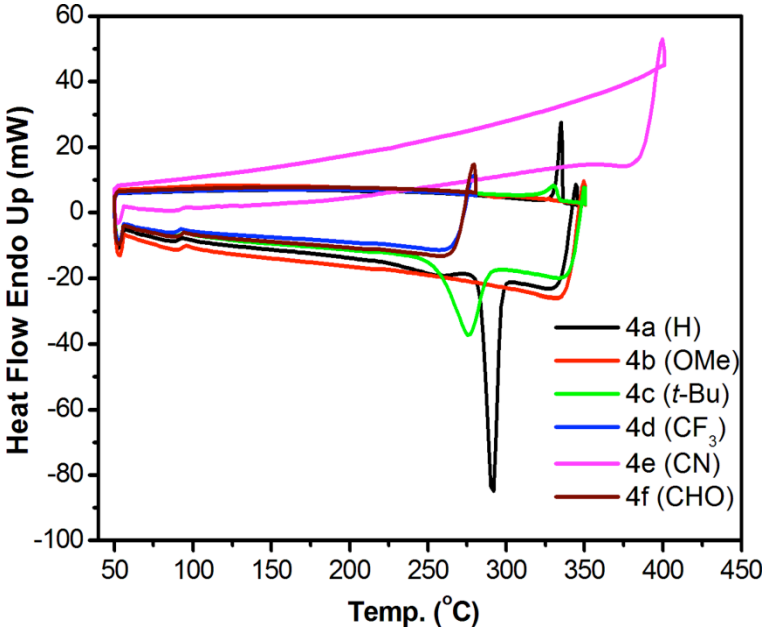

Figure S**3-1**The DSC curve of compounds **4a–f**

Electrochemistry Analysis

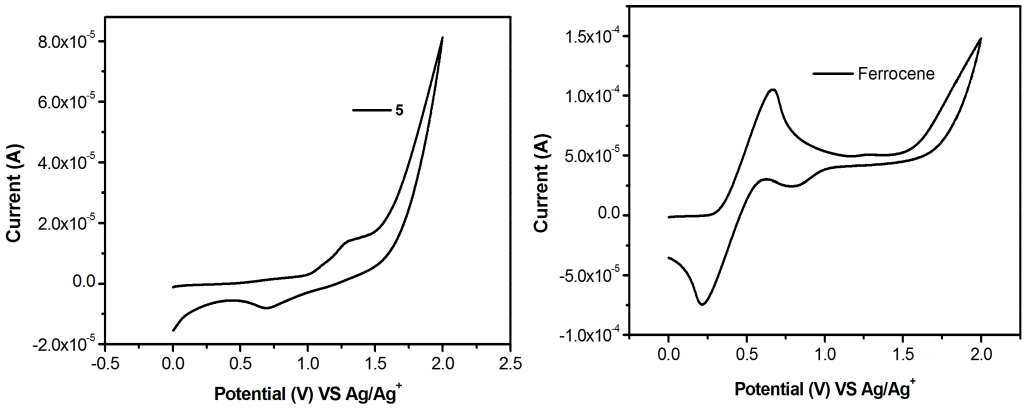

Figure S**4-1** Cyclic voltammogramscu for compound**5**.

Quantum Chemistry Computation

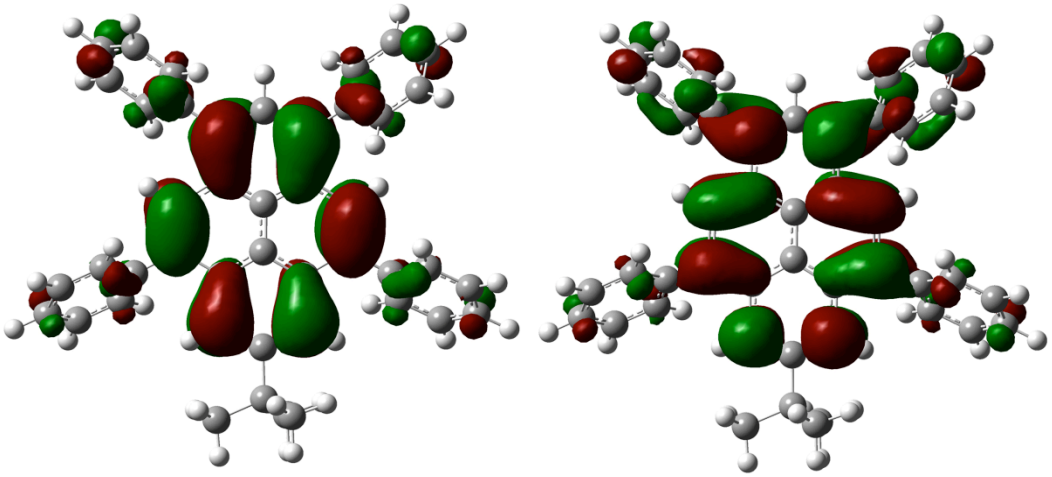

Figure S**4-1**. Computed molecular orbital plots (B3LYP/6–31G*) of the compound **4a**. The left plots represent the HOMOs, and the right plots represent the LUMOs.

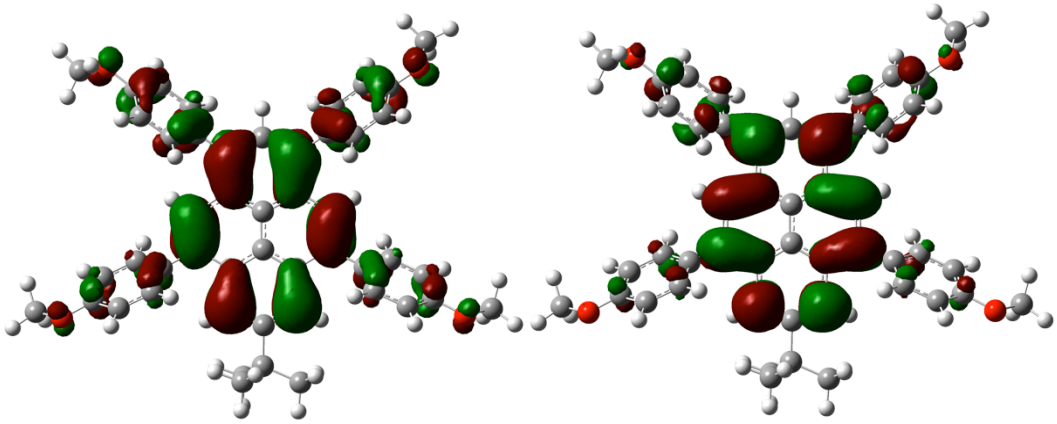

Figure S**4-2**. Computed molecular orbital plots (B3LYP/6–31G*) of the compound **4c**. The left plots represent the HOMOs, and the right plots represent the LUMOs.

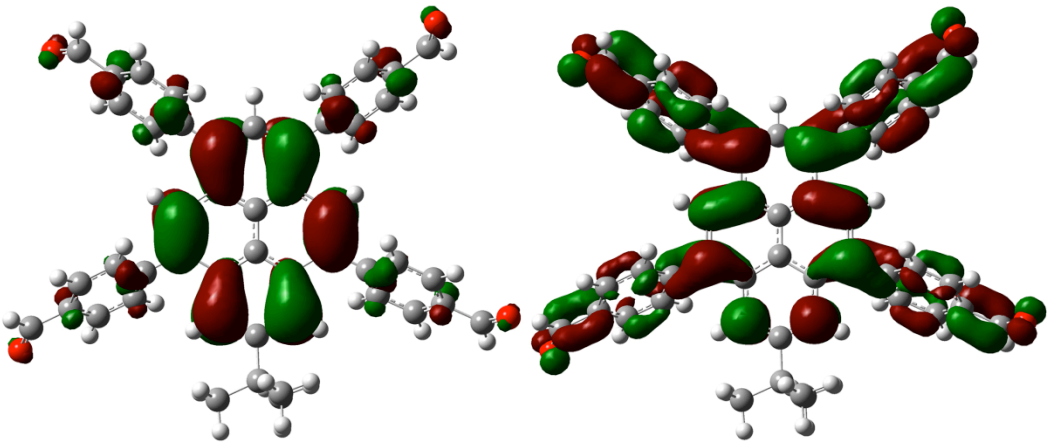

Figure S**4-3**. Computed molecular orbital plots (B3LYP/6–31G*) of the compound **4f**. The left plots represent the HOMOs, and the right plots represent the LUMOs.

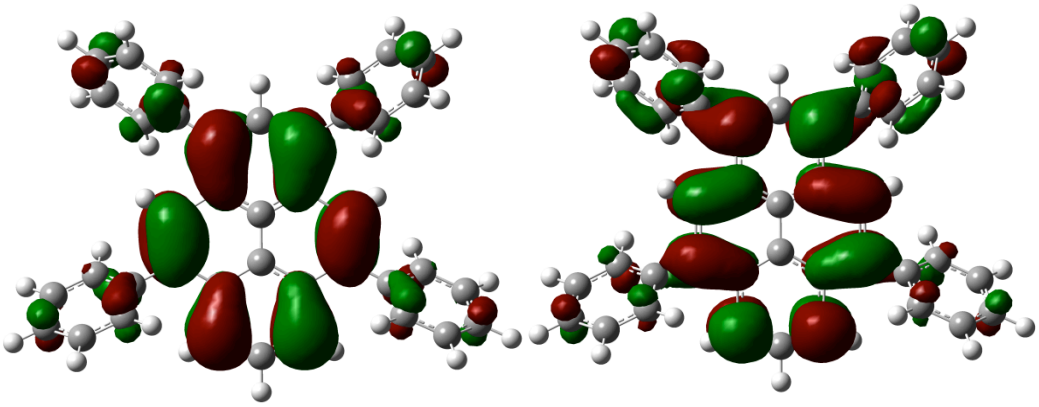

Figure S**4-4**. Computed molecular orbital plots (B3LYP/6–31G*) of the compound **6**. The left plots represent the HOMOs, and the right plots represent the LUMOs.