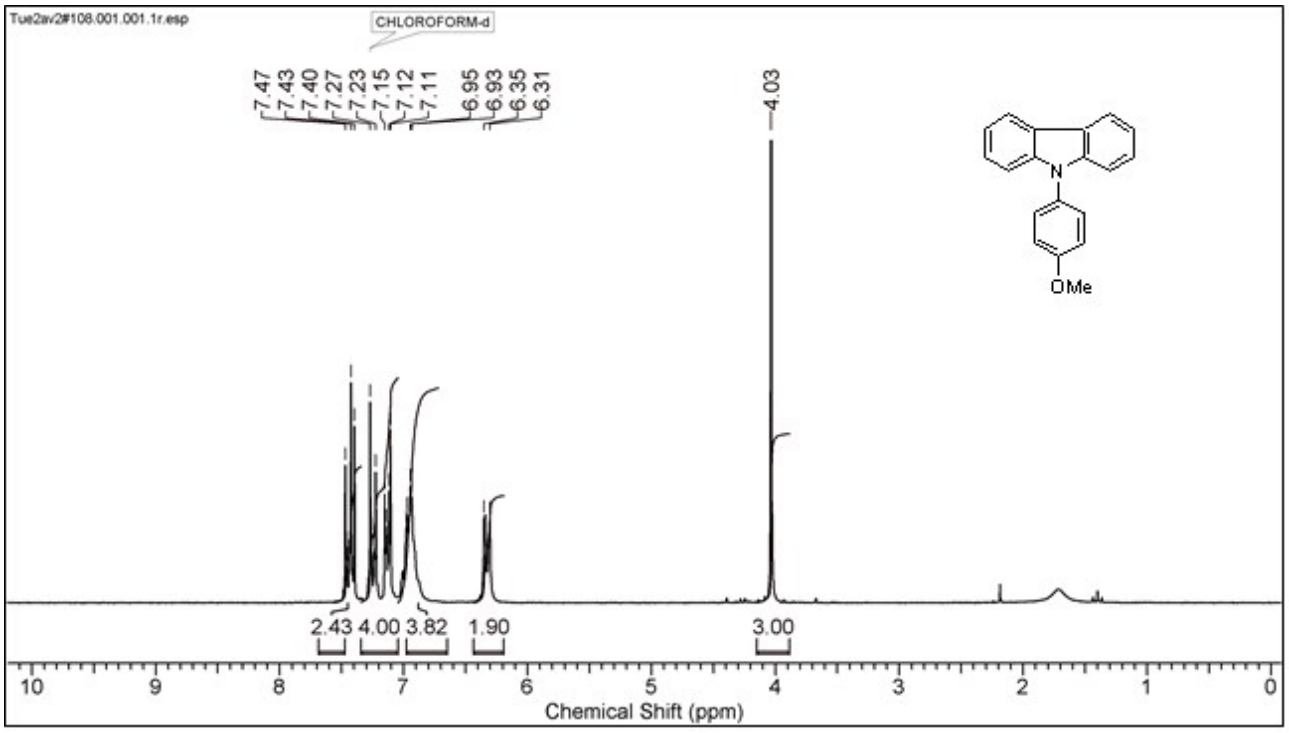
Supporting Information

Phenothiazine and Carbazole Substituted Pyrene Based Electroluminescent Organic Semiconductors for OLED Devices

Table of Contents:-



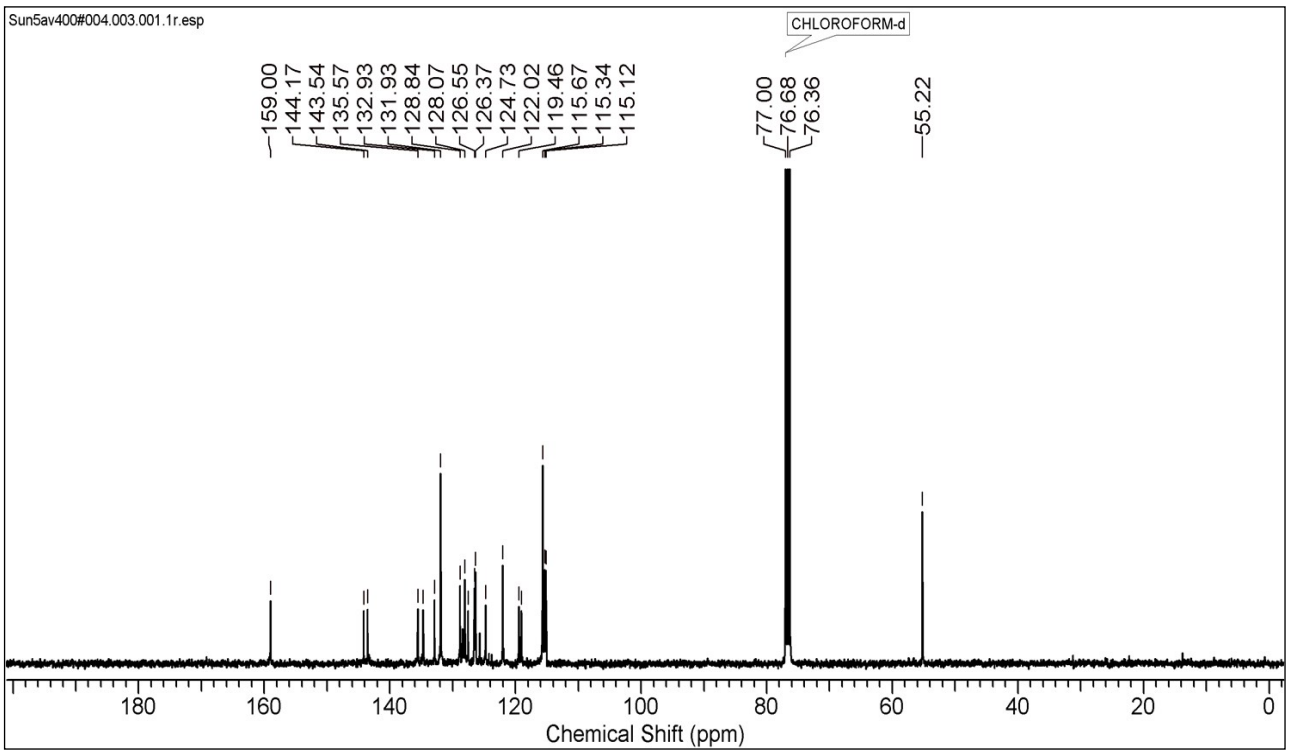
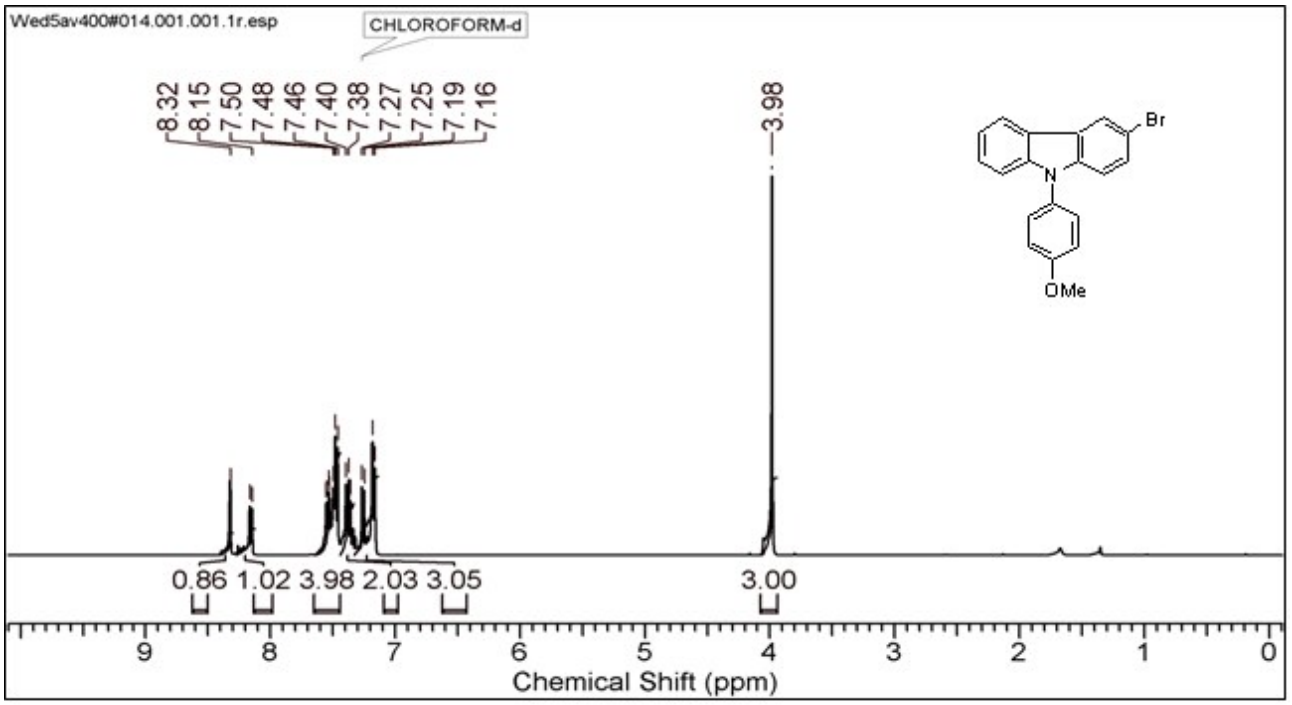


Fig. S1.[1]H NMR and [13]C NMR spectrum of 9H-carbazole-9-(4-methoxyphenyl).



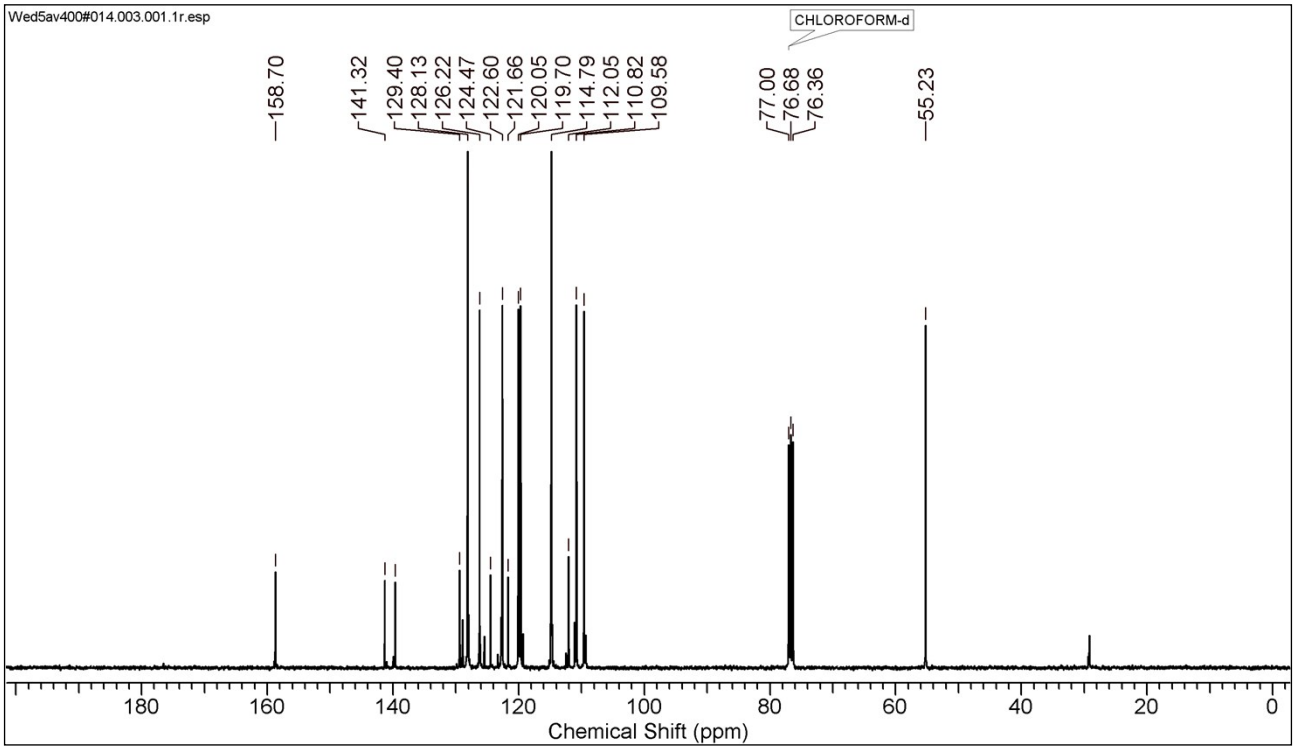
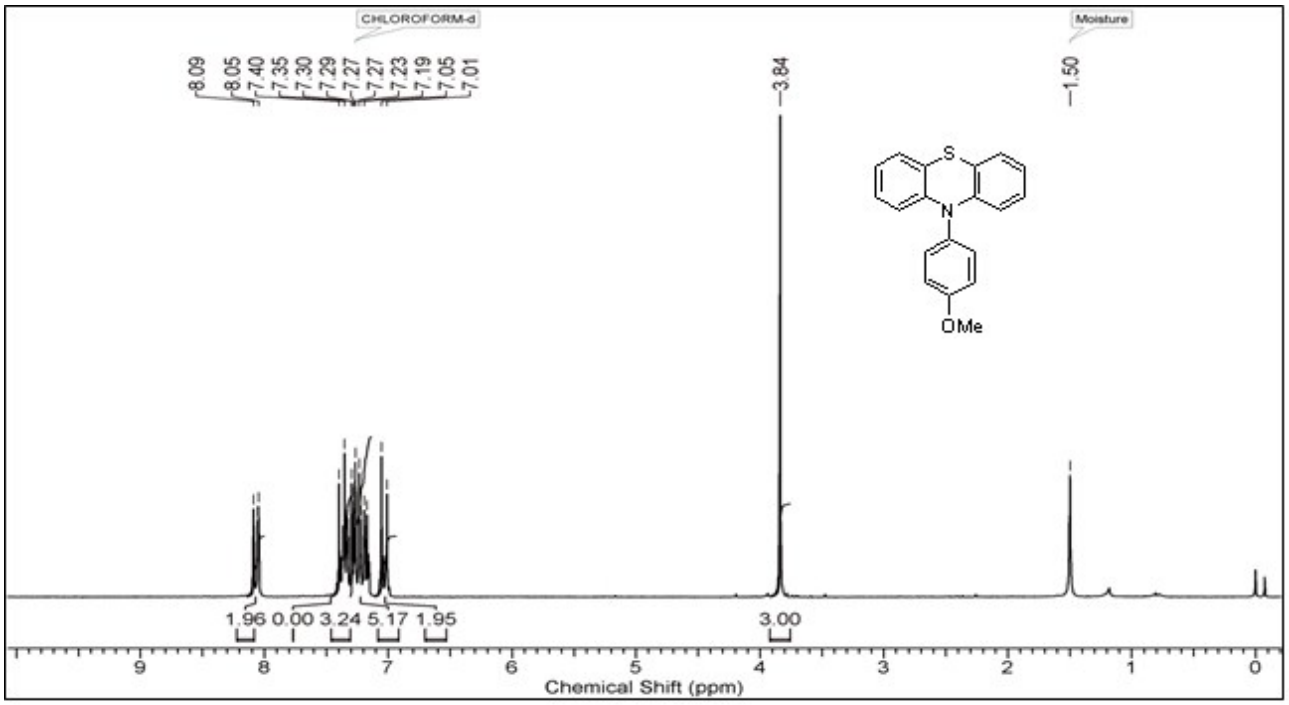


Fig. S2.[1]H NMR and [13]C NMR spectrum of 3-bromo-9-(4-methoxyphenyl)-9H-carbazole.



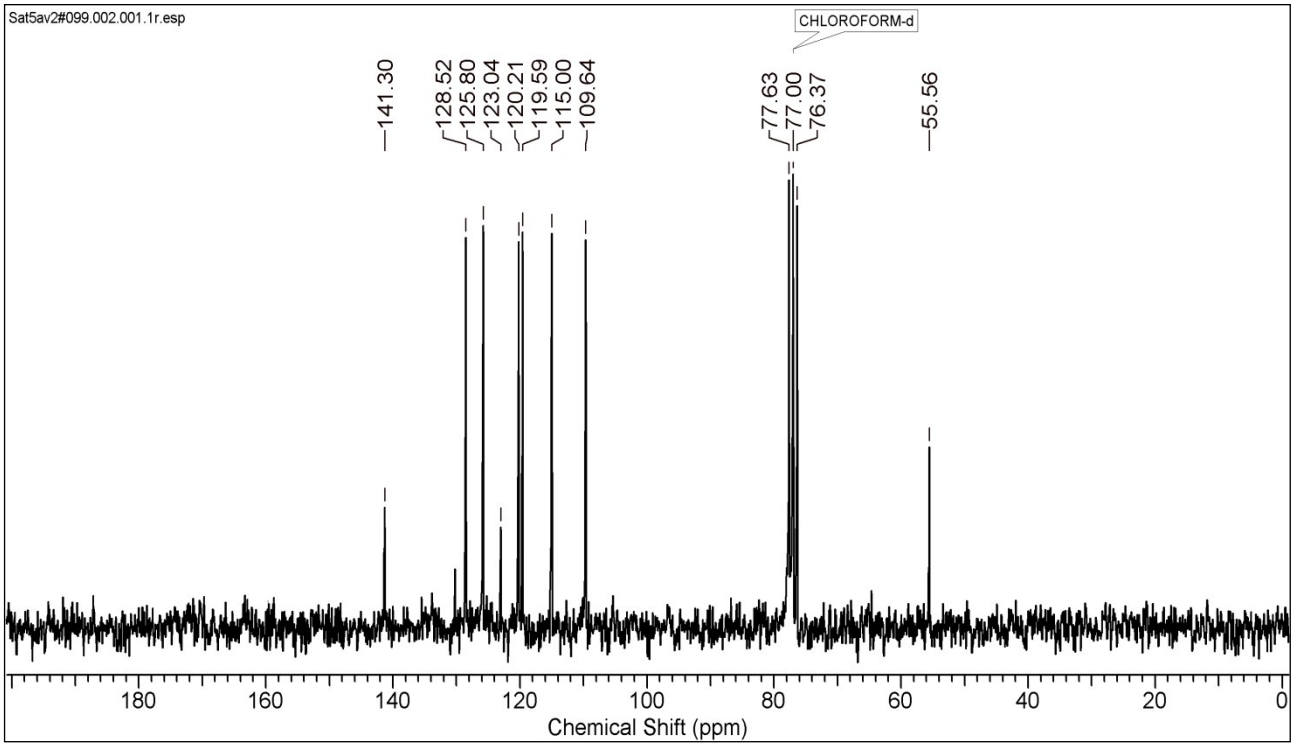


Fig.S3.[1]H NMR and [13]C NMR spectrum of 10-(4-methoxyphenyl)-10H-phenothiazine.

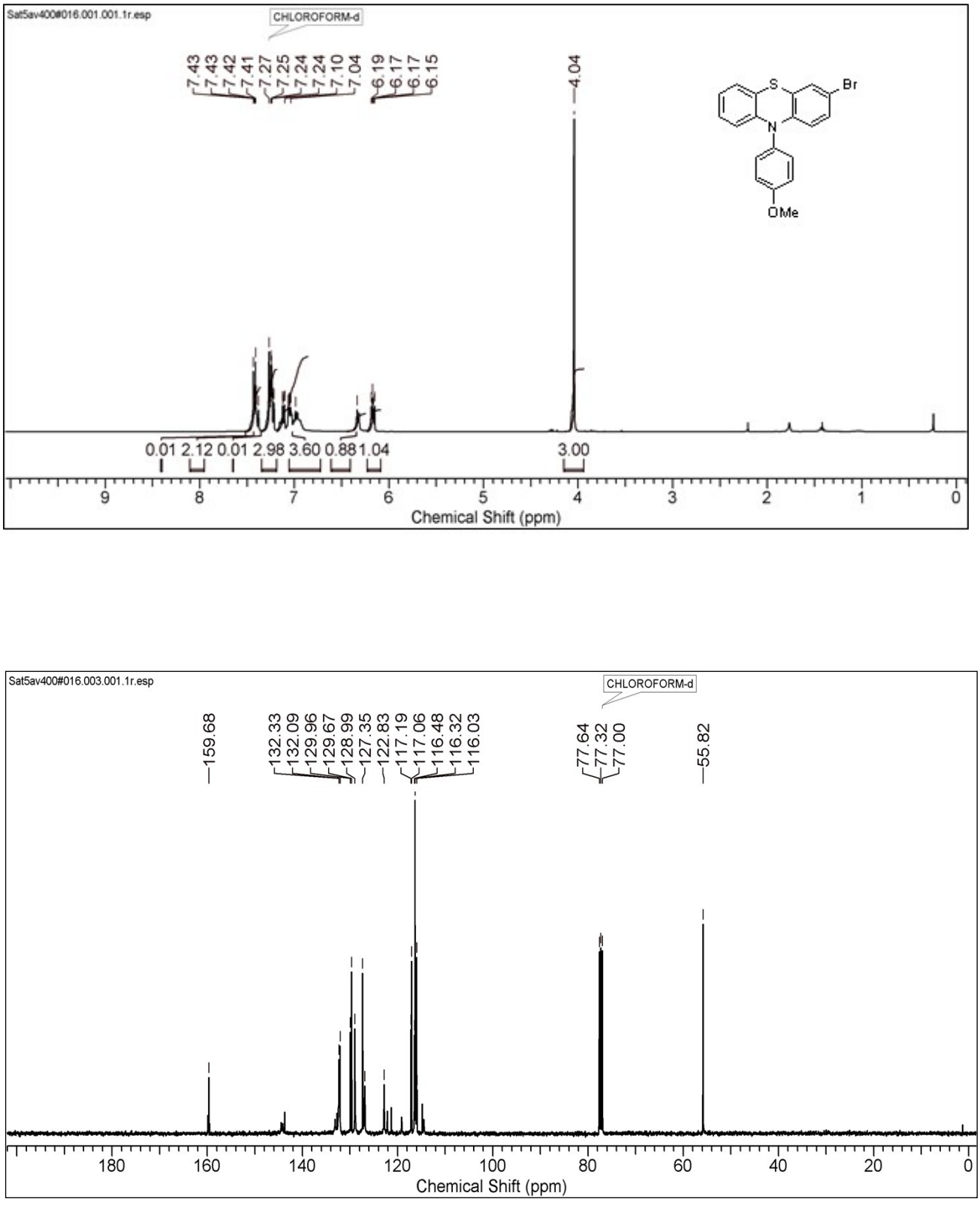


Fig. S4.[1]H NMR and [13]C NMR spectrum of 3-bromo-10-(4-methoxyphenyl)-10H-phenothiazine.

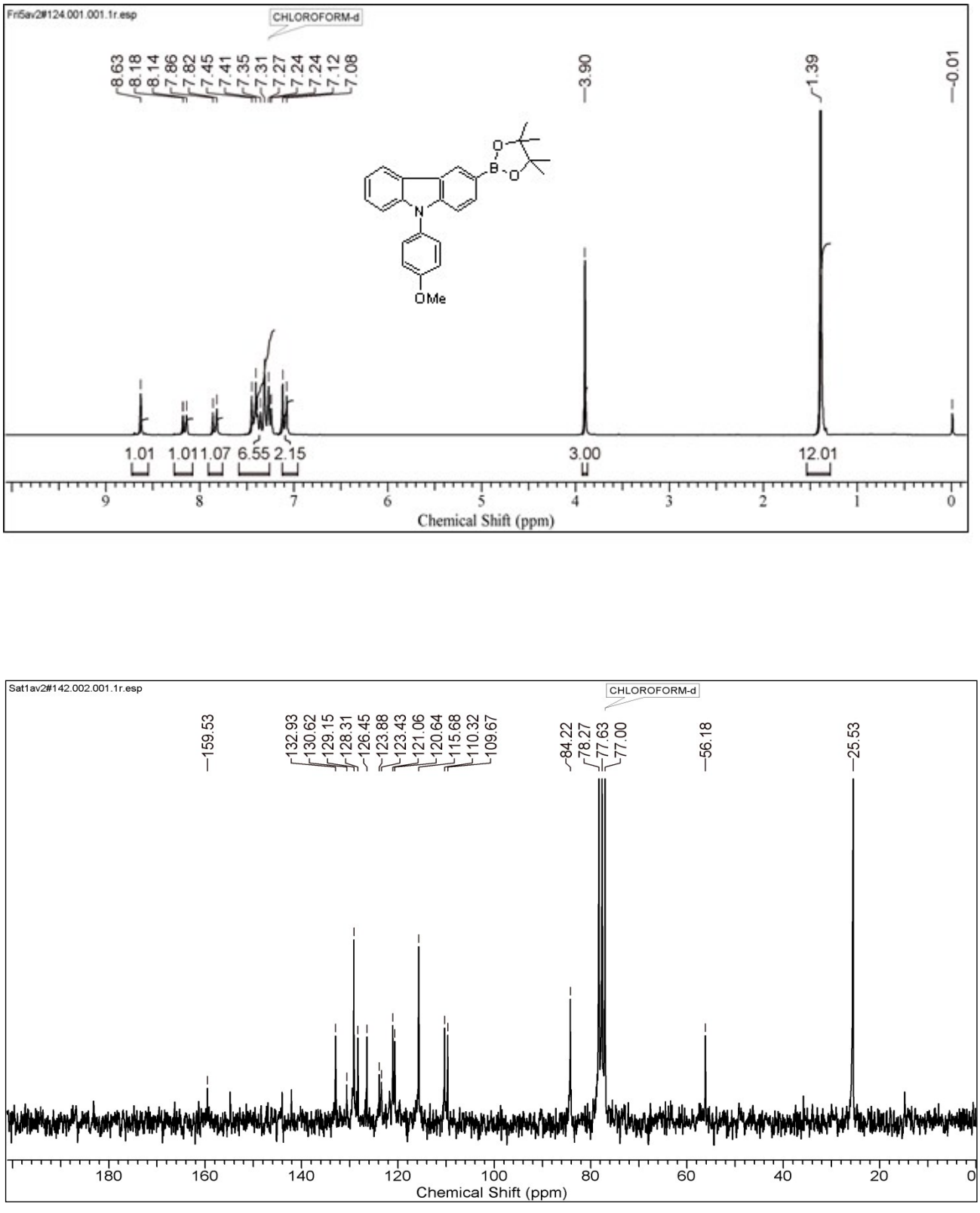
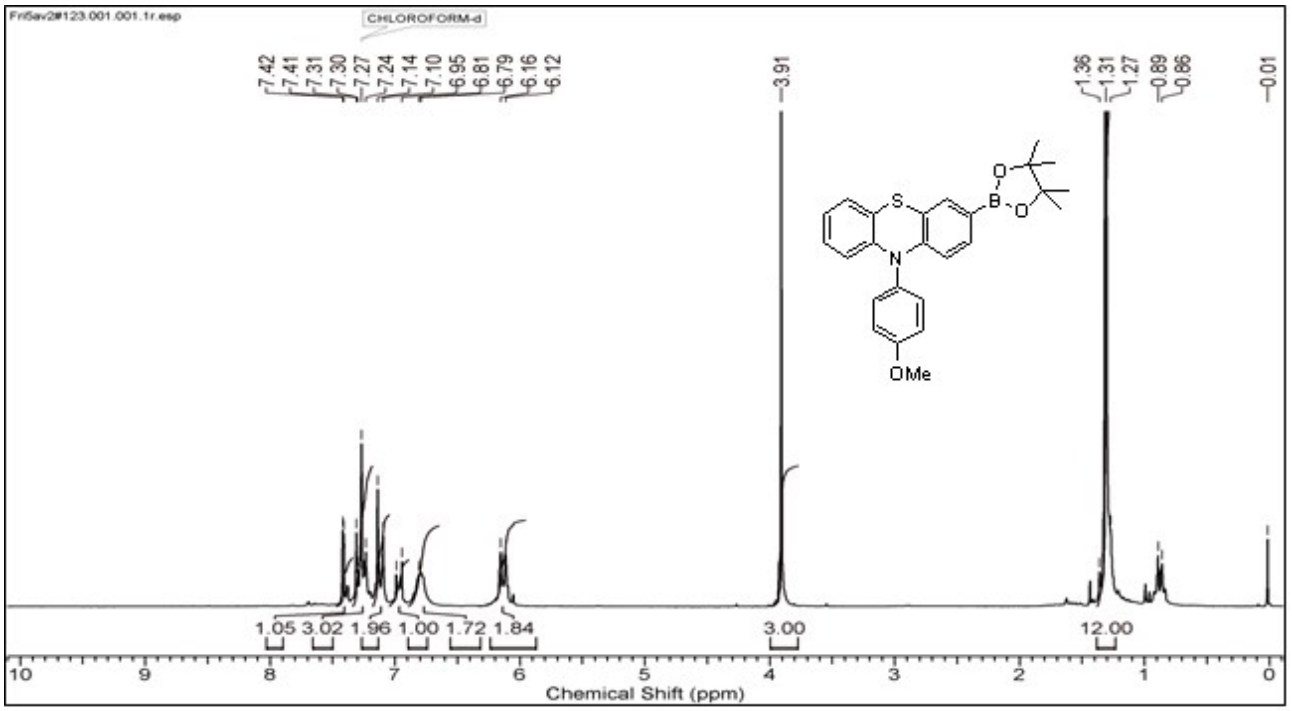


Fig. S5.[1]H NMR and [13]C NMR spectrum of 9-(4-methoxyphenyl)-3-(4,4, 5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (**4**).



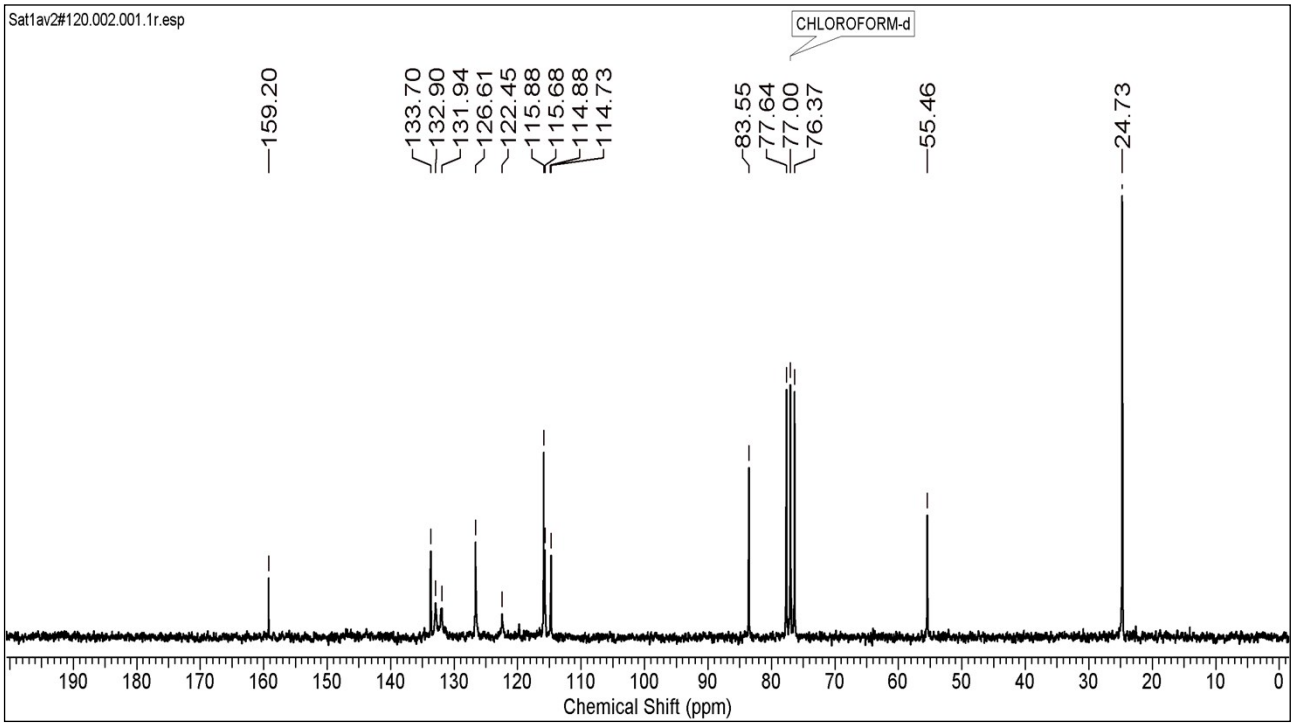
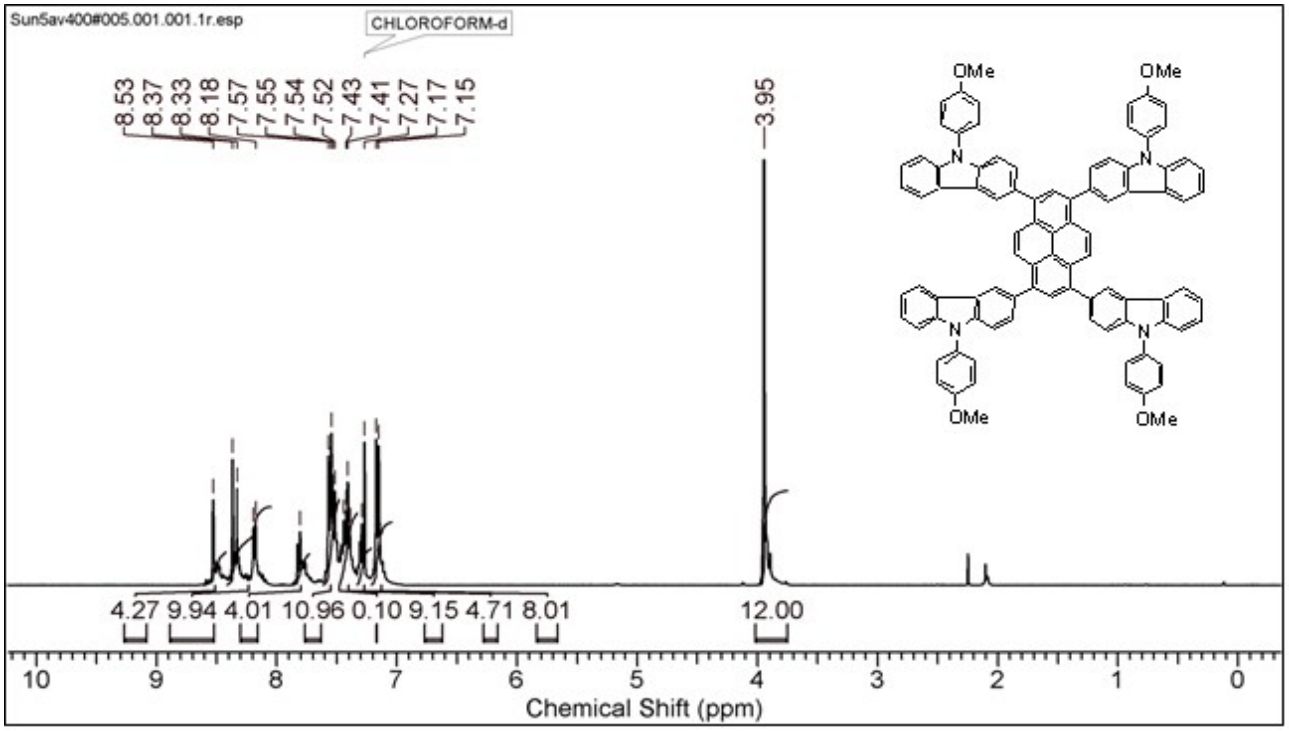


Fig. S6.[1]H NMR and [13]C NMR spectrum of10-(4-methoxyphenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-10H-phenothiazine (**8**).



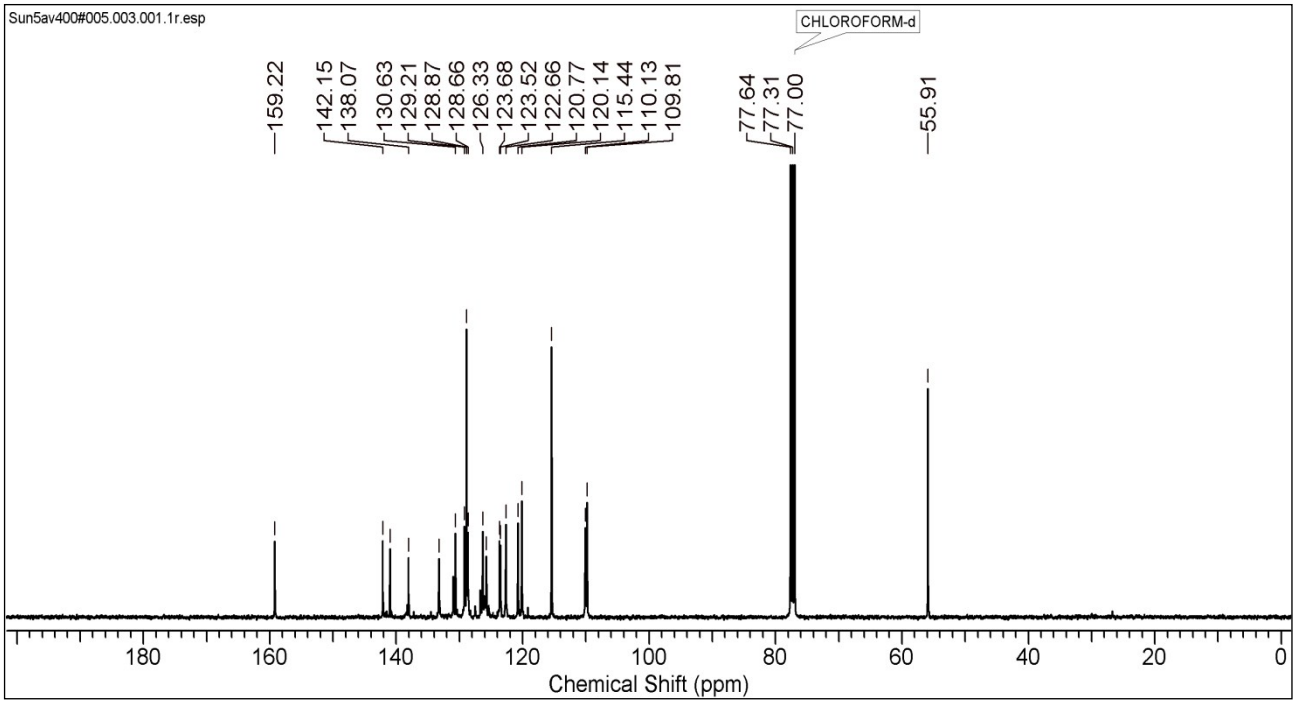


Fig. S7.[1]H NMR and [13]C NMR spectrum of 1, 3, 6, 8-tetrakis (9-(4-methoxyphenyl)-9H-carbazol-3-yl)pyrene (**PY-CA**).

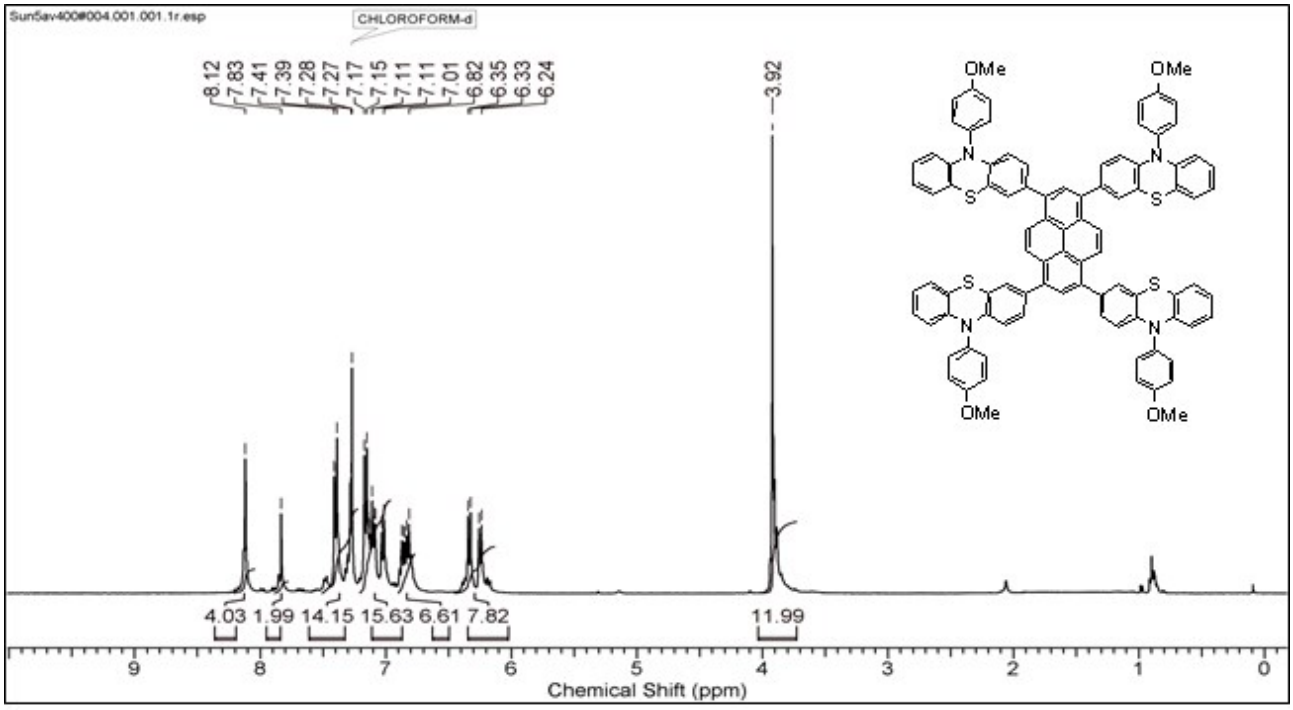


Fig. S8.[1]H NMR and [13]C NMR spectrum of 1,3,6,8-tetrakis(10-(4-methoxyphenyl)-10H-phenothiazin-3-yl)pyrene (**PY-PH**).

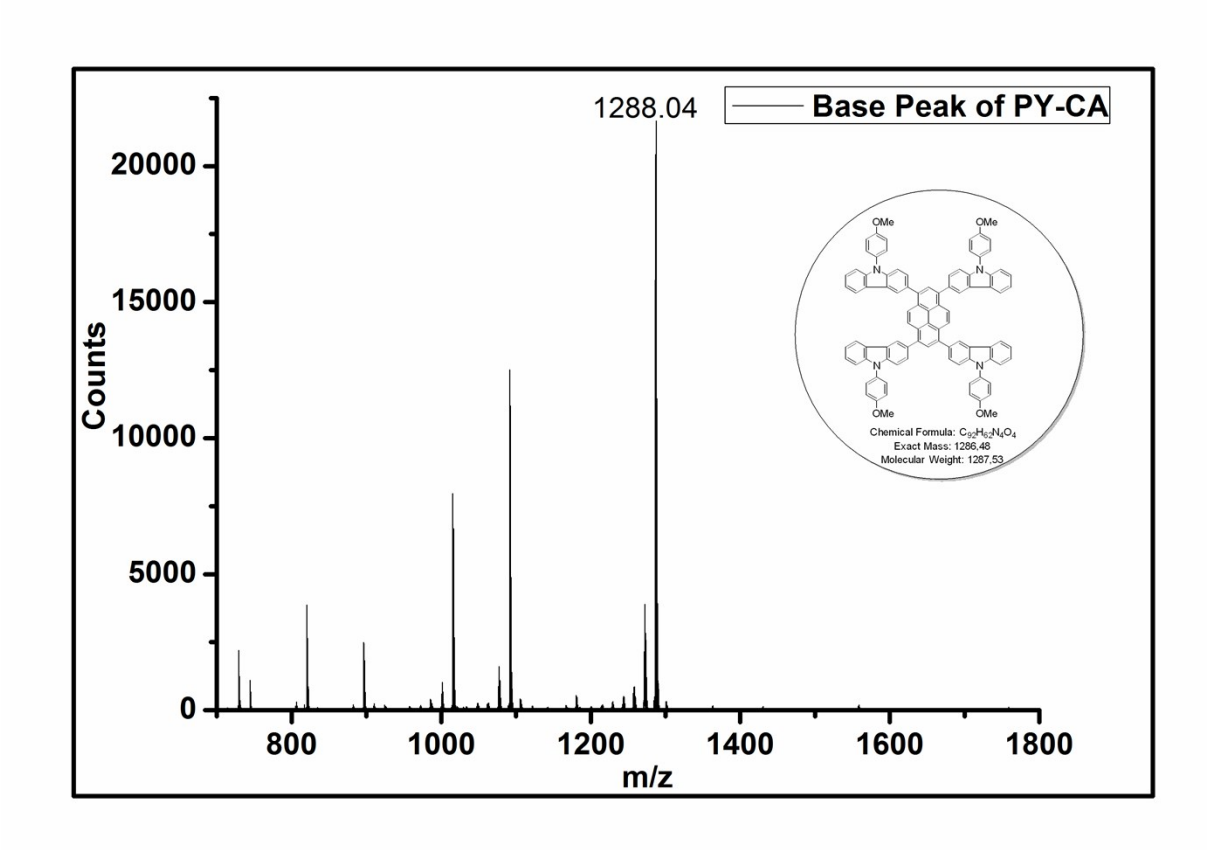


Fig. S9. MALDI-TOF spectrum of **PY-CA**

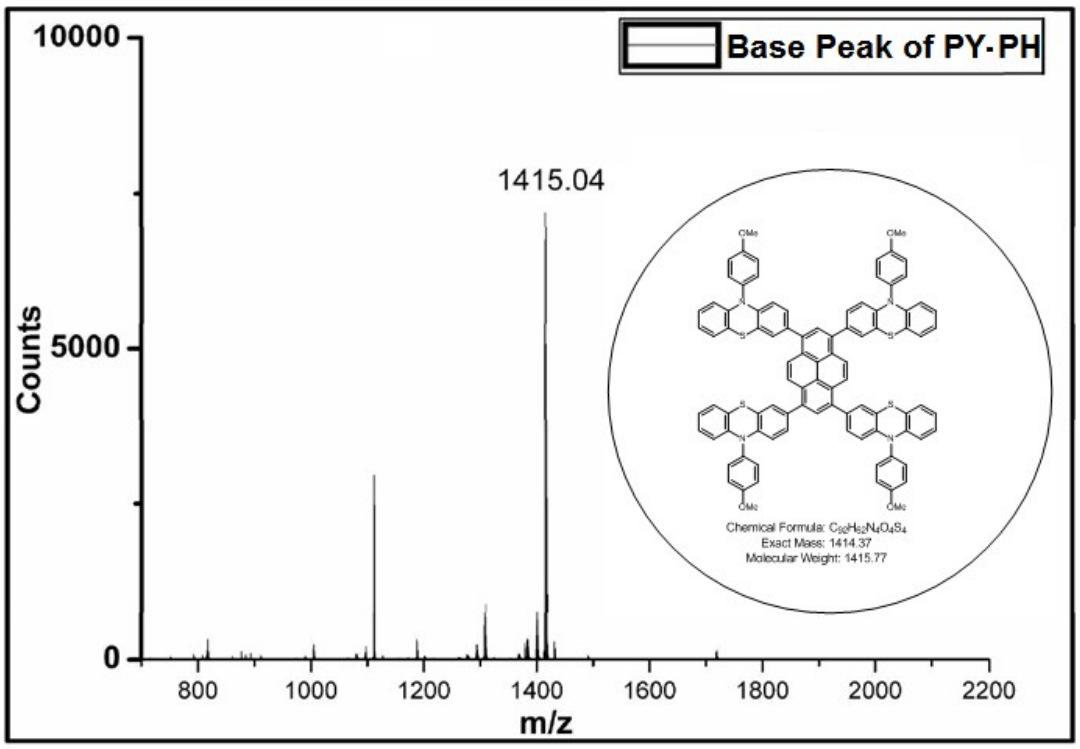
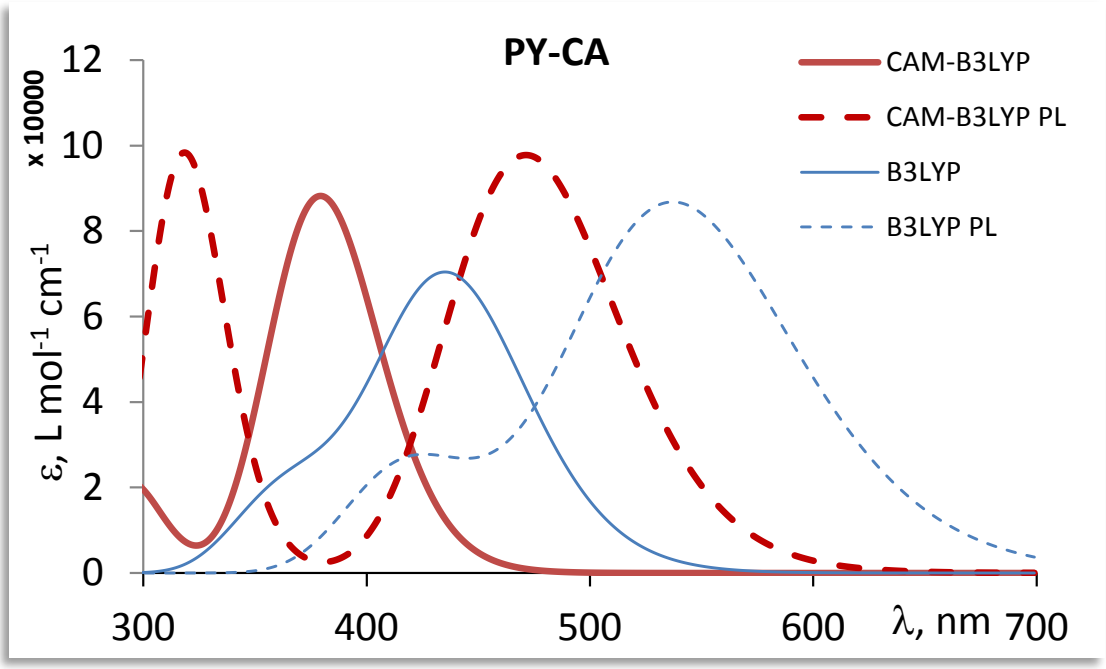


Fig. S10. MALDI-TOF spectrum of **PY-PH.**



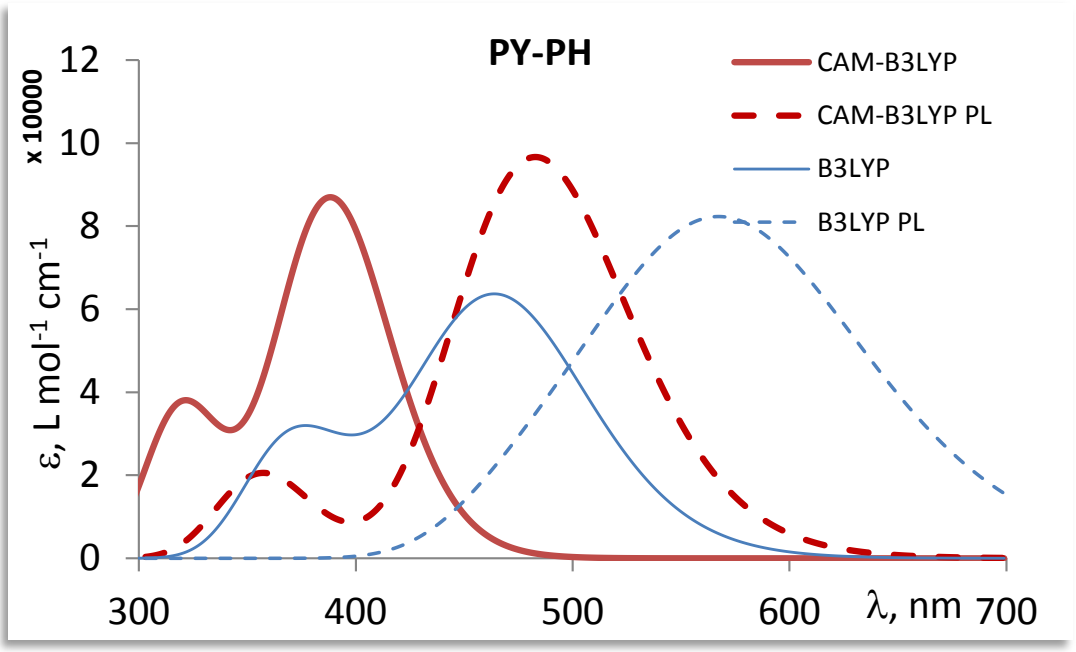


Fig. S11. Theoretical UV-vis absorption spectra of **PY-CA** and **PY-PH** in chloroform computed with B3LYP and CAM-B3LYP functionals. Here and elsewhere, the extinction coefficient ε in L mol^{-1} cm^{-1} is calculated from the oscillator strengths f computed with DFT at excitation energies E_{exc}as $\epsilon = \frac{1.35 \times 10^4}{\sigma} f exp\left[-2.7472 \left(\frac{E - E_{exc}}{2\sigma} \right) \right]$ where σ=0.25 eV is the HWHM broadening.

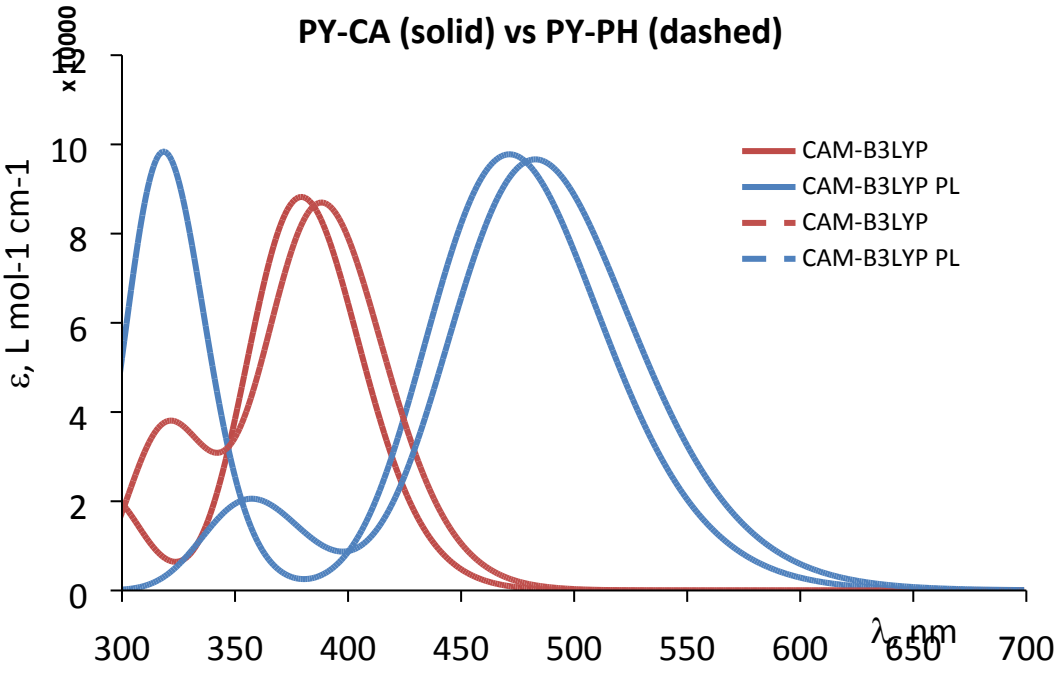


Fig.S12. Comparative theoretical UV-vis absorption and photoluminescence spectra of **PY-CA** and **PY-PH** in chloroform computed with the CAM-B3LYP functional.

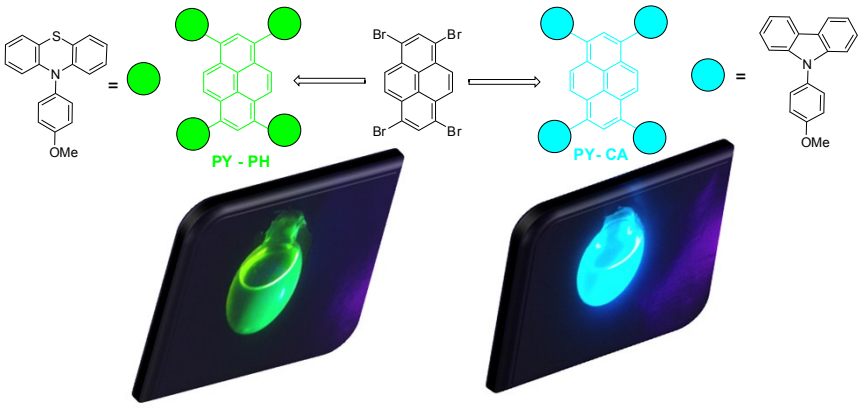


Figure S13. **PY-PH** and **PY-CA** and their emission under UV-vis lamp.

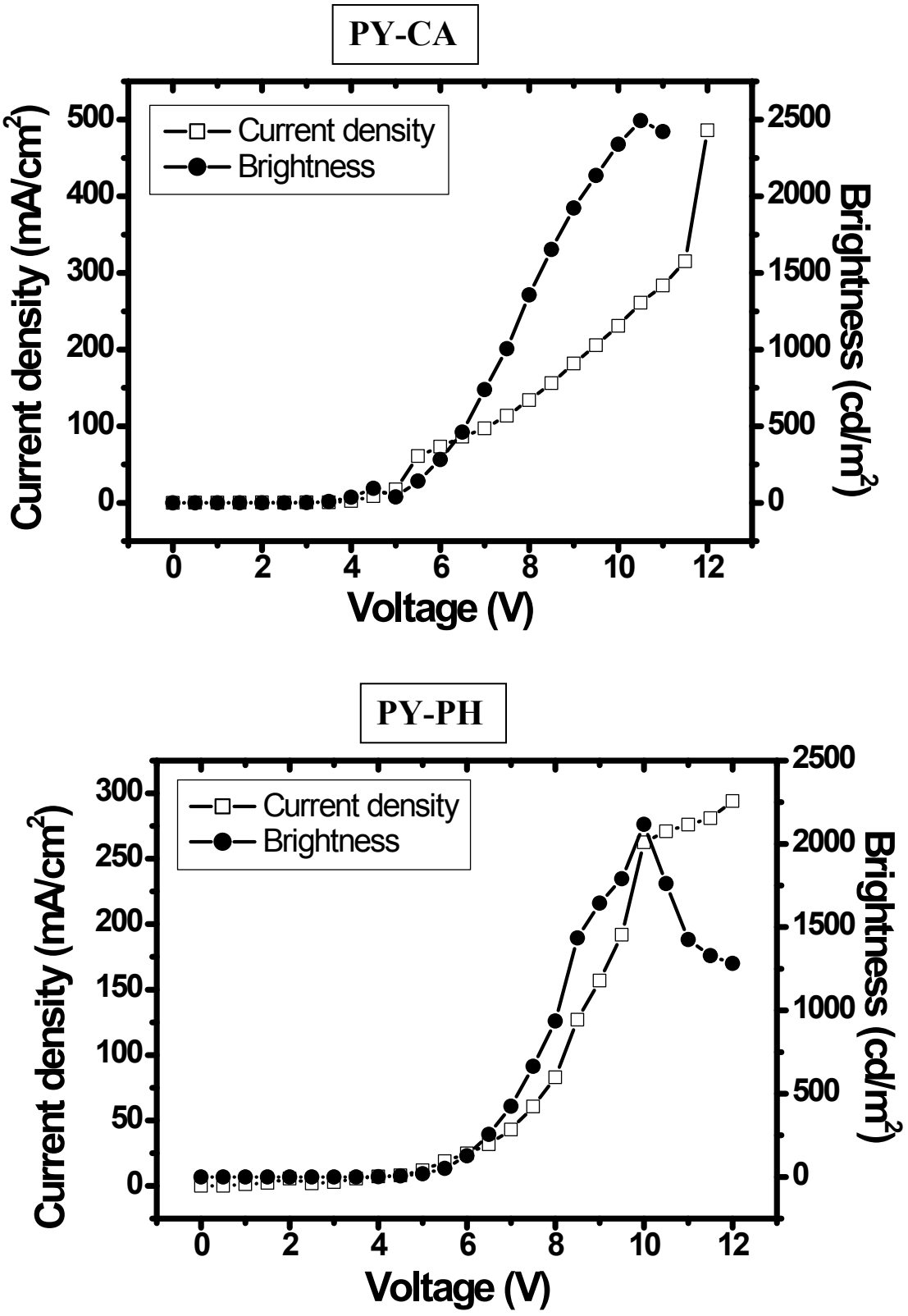


Fig. S14. Current density-Voltage-Brightness characteristics of the **PY-CA** device and the **PY-PH** device.