

*Supplementary Information*

# Pyrene appended terpyridine derivatives as electrochemiluminescence material for OLEDs: Characterization of photo-physical, thermal and electrochemical properties

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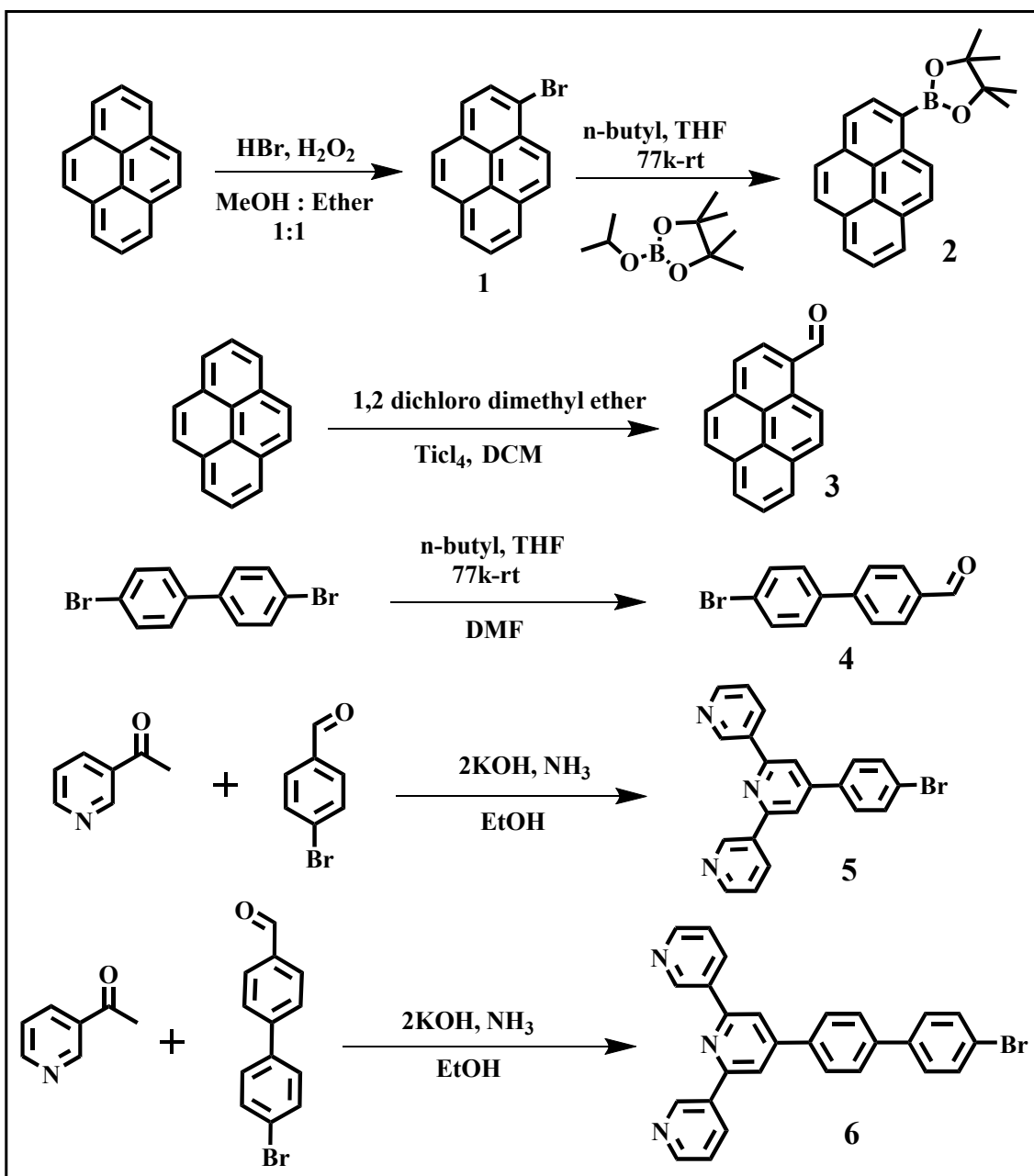
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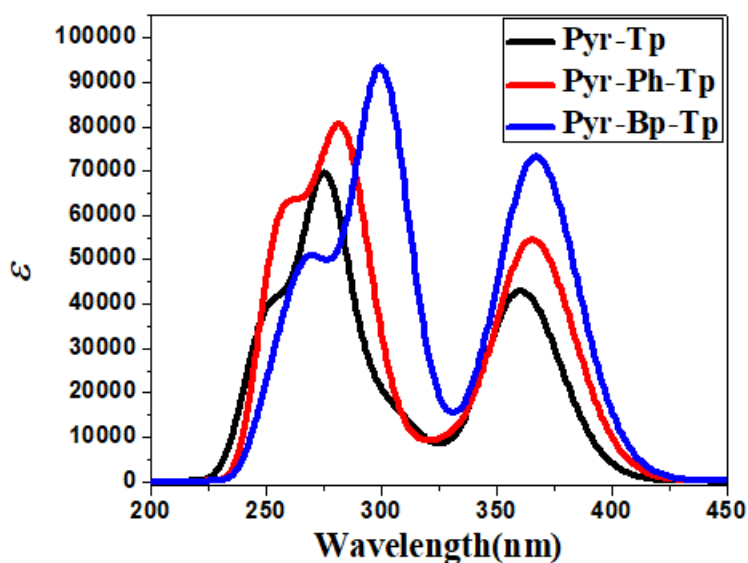
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Scheme S1. Synthetic route for intermediates

**Table S1.** Calculated properties of **Pyr-Tp**, **Pyr-Ph-Tp** and **Pyr-Bp-Tp** at PBE0/6-311G(d,p) level. HOMO and LUMO energies (eV), HOMO–LUMO gap HLG (eV), Oscillator strength  $f$ , the wavelength maxima, the major contribution (%) to the first excited state and the dipole moment  $\mu_e$  (D).

Molecule	HOMO (eV)	LUMO (eV)	HLG (eV)	$\lambda_{\max}$ (nm)	$f$	Major contribution (%)	$\mu_e$ (D)
<b>Pyr-Tp</b>	-6.01	-2.06	-3.95	360	0.5919	HOMO→LUMO (94%)	8.141
<b>Pyr-Ph-Tp</b>	-5.91	-2.01	-3.90	366	0.7472	HOMO→LUMO (96%)	7.916
<b>Pyr-Bp-Tp</b>	-5.85	-1.98	-3.87	367	1.0005	HOMO→LUMO (93%)	7.934



**Figure S1.** PBE0/6-311G (d,p) simulated absorption spectra of **Pyr-Tp**, **Pyr-Ph-Tp** and **Pyr-Bp-Tp** in chloroform solvent.

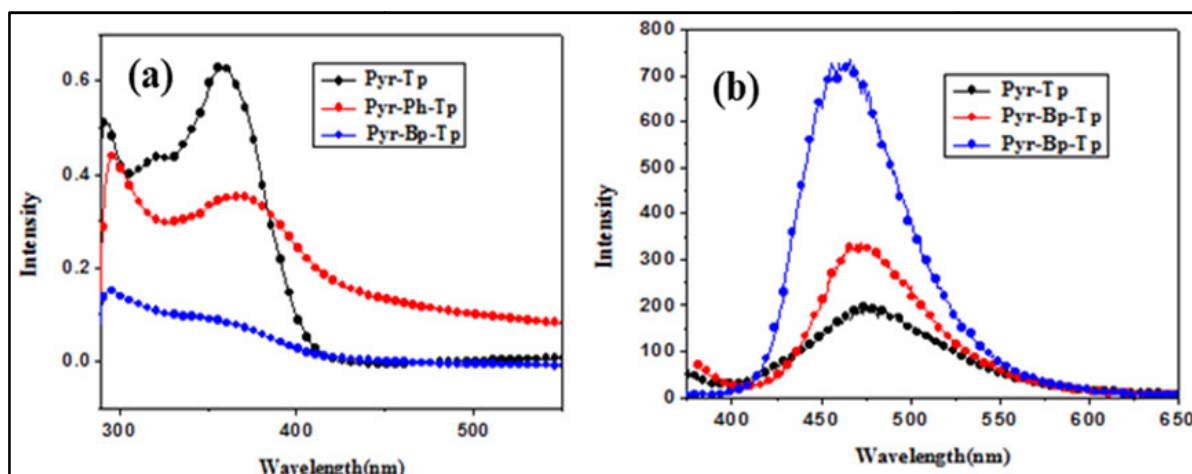


Figure S2.(a) Thin film UV-vis absorption spectra (b) Thin film Fluorescence spectra.

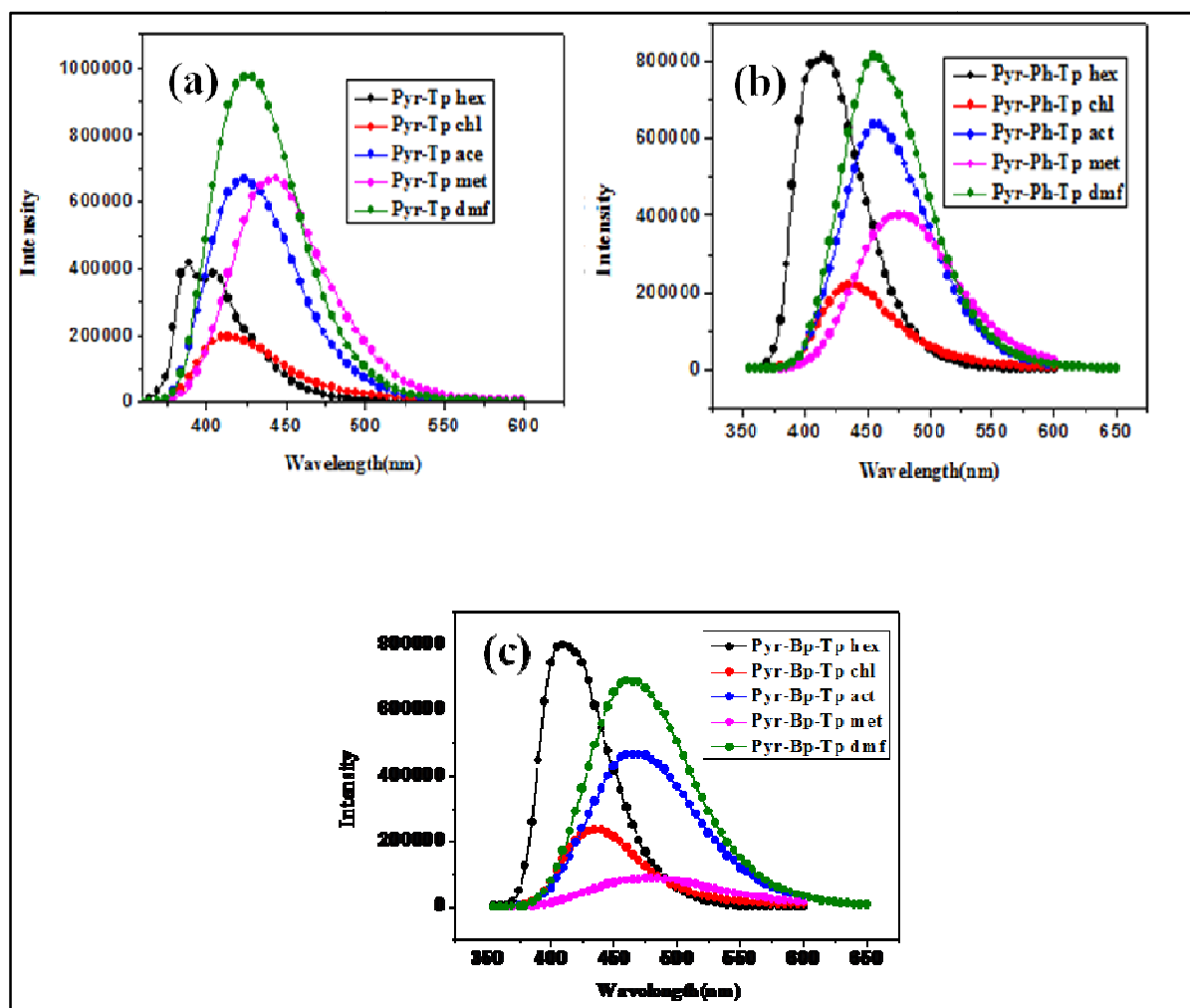


Figure S3.Solvatochromism spectra of Pyr-Tp, Pyr-Ph-Tp and Pyr-Bp-Tp

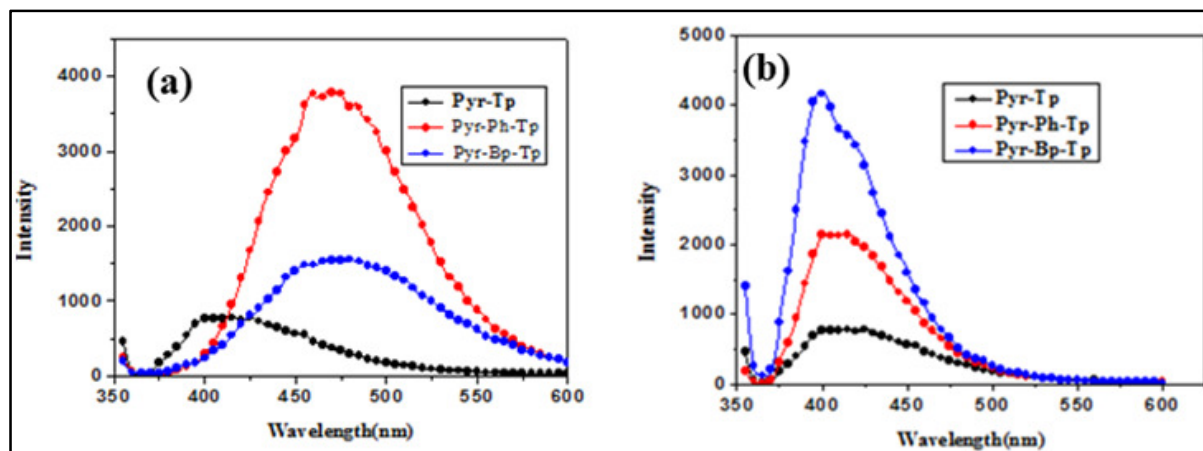


Figure S4. (a) Delayed fluorescence at RT (b) Delayed fluorescence at 77k

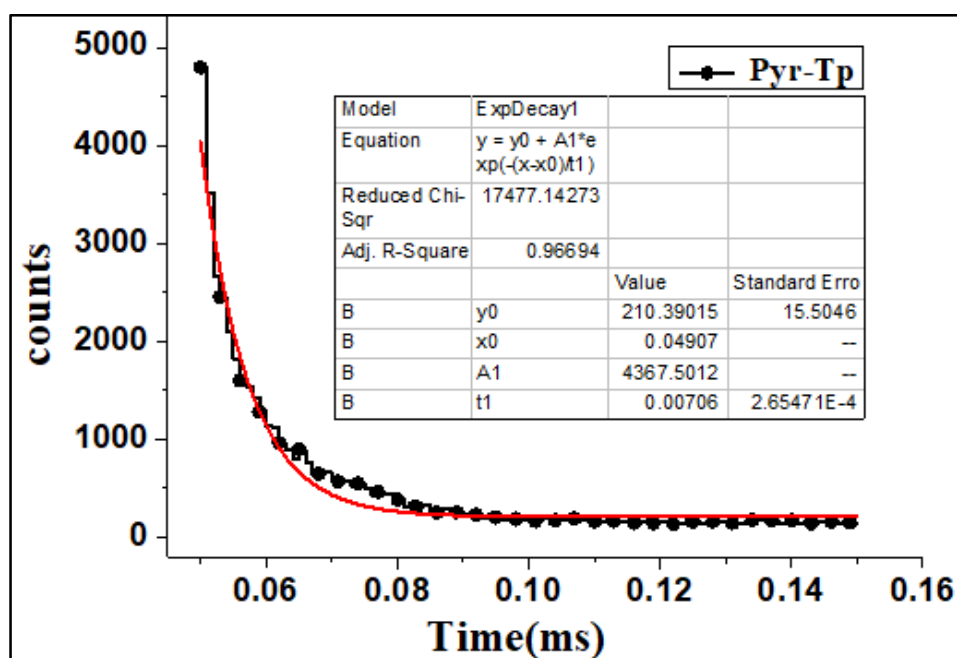


Figure S5. Delayed fluorescence lifetime of Pyr-Tp

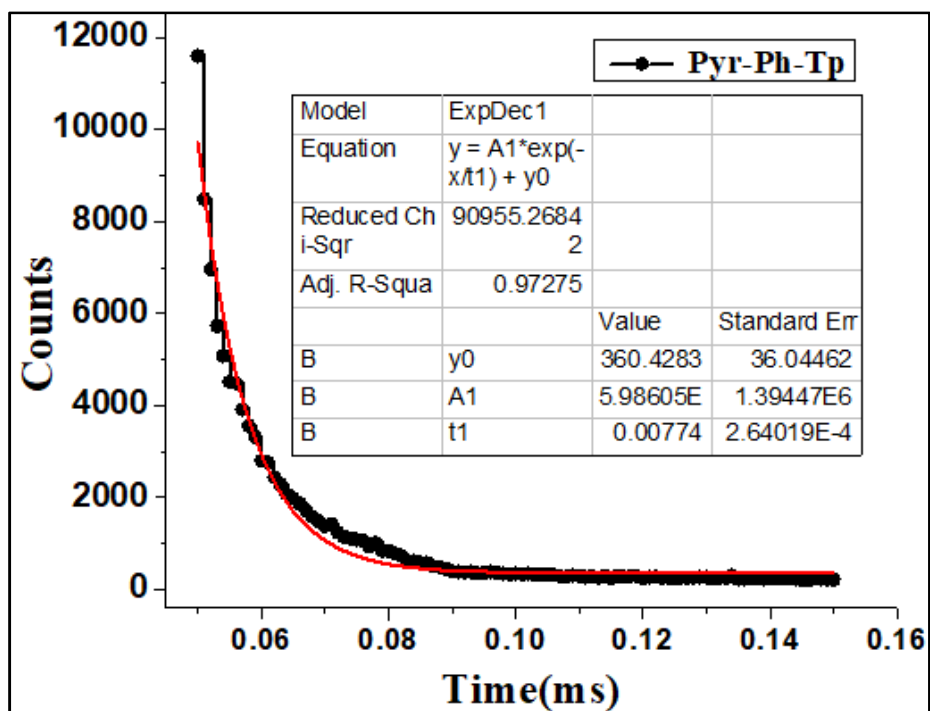


Figure S6. Delayed fluorescence lifetime of Pyr-Ph-Tp

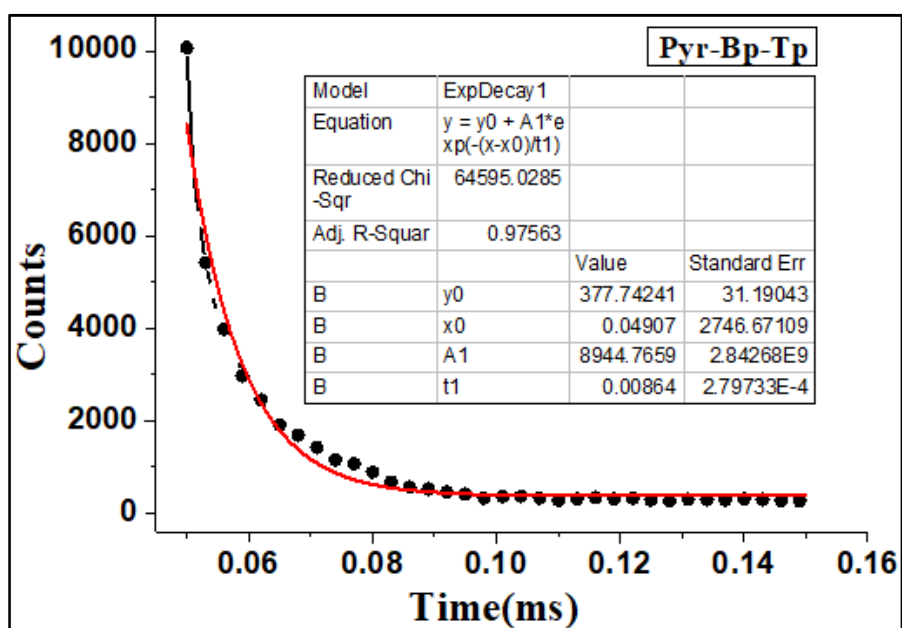
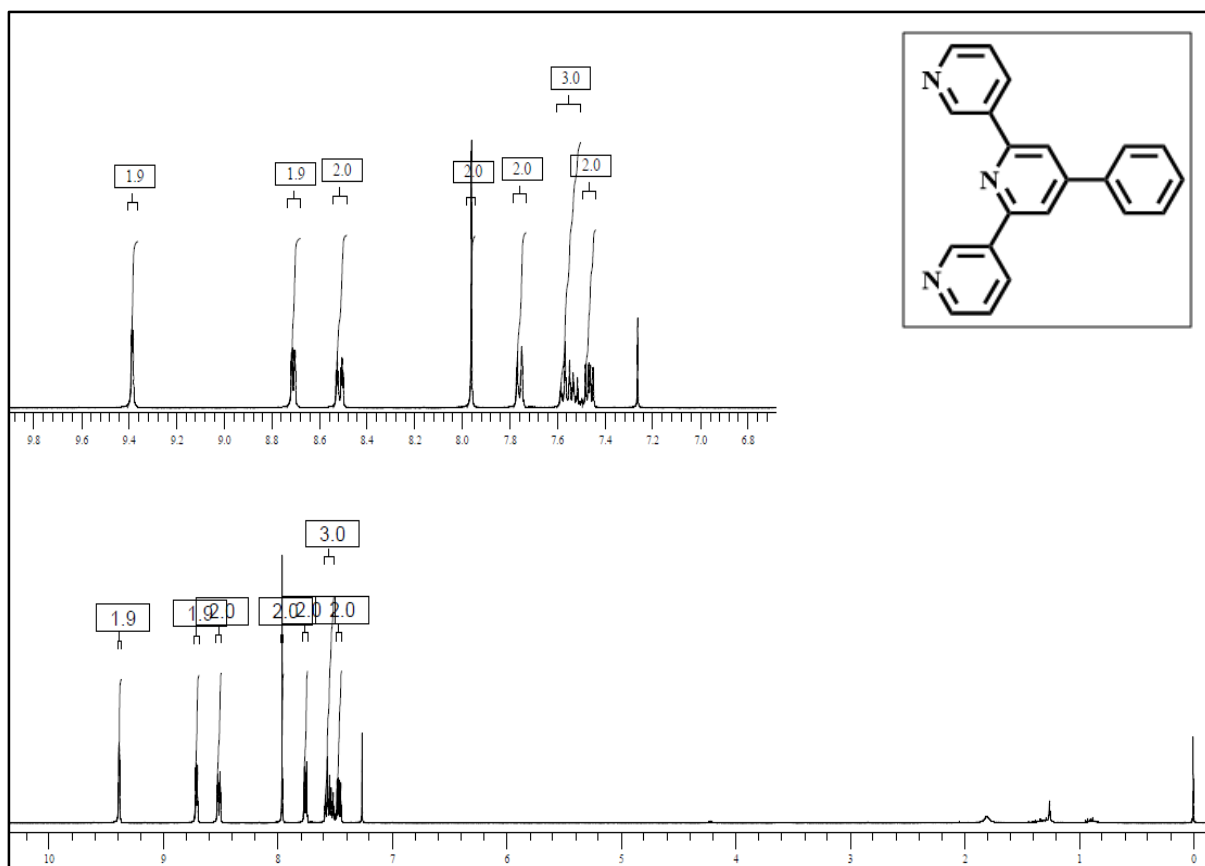
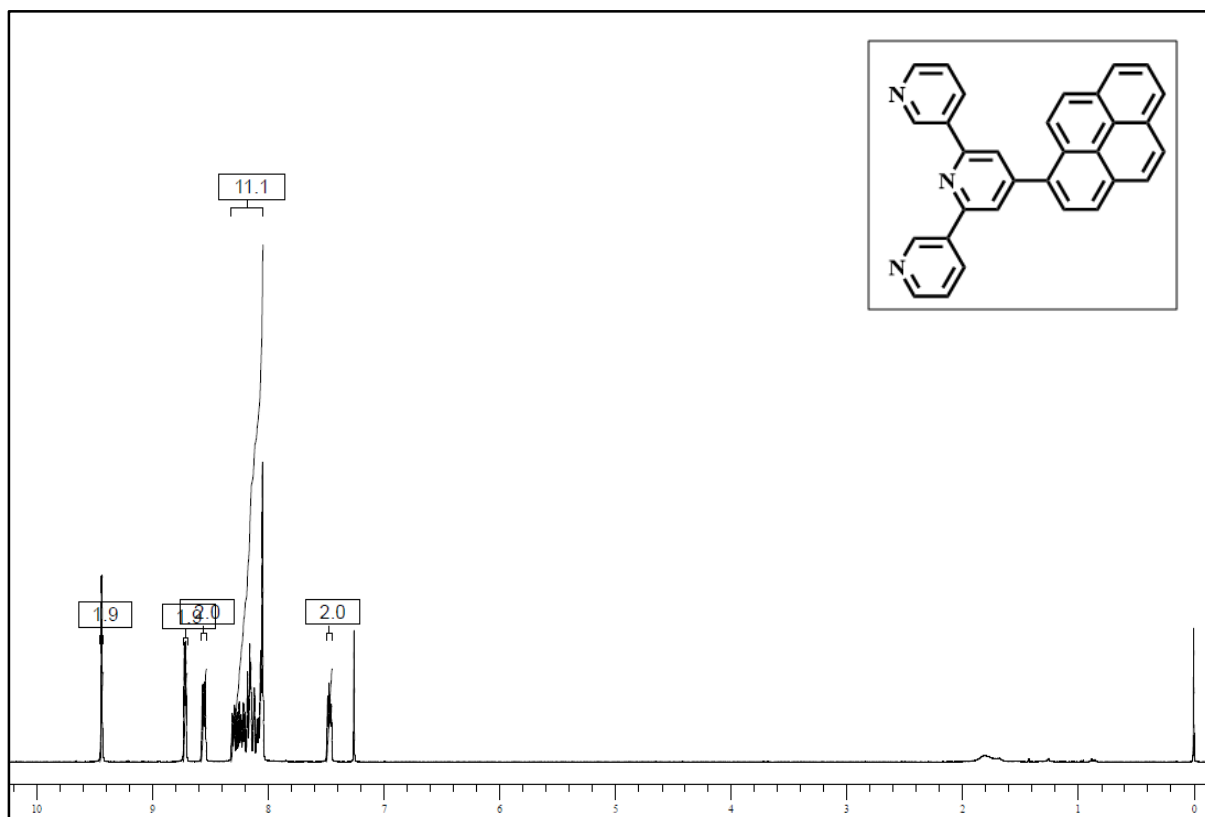


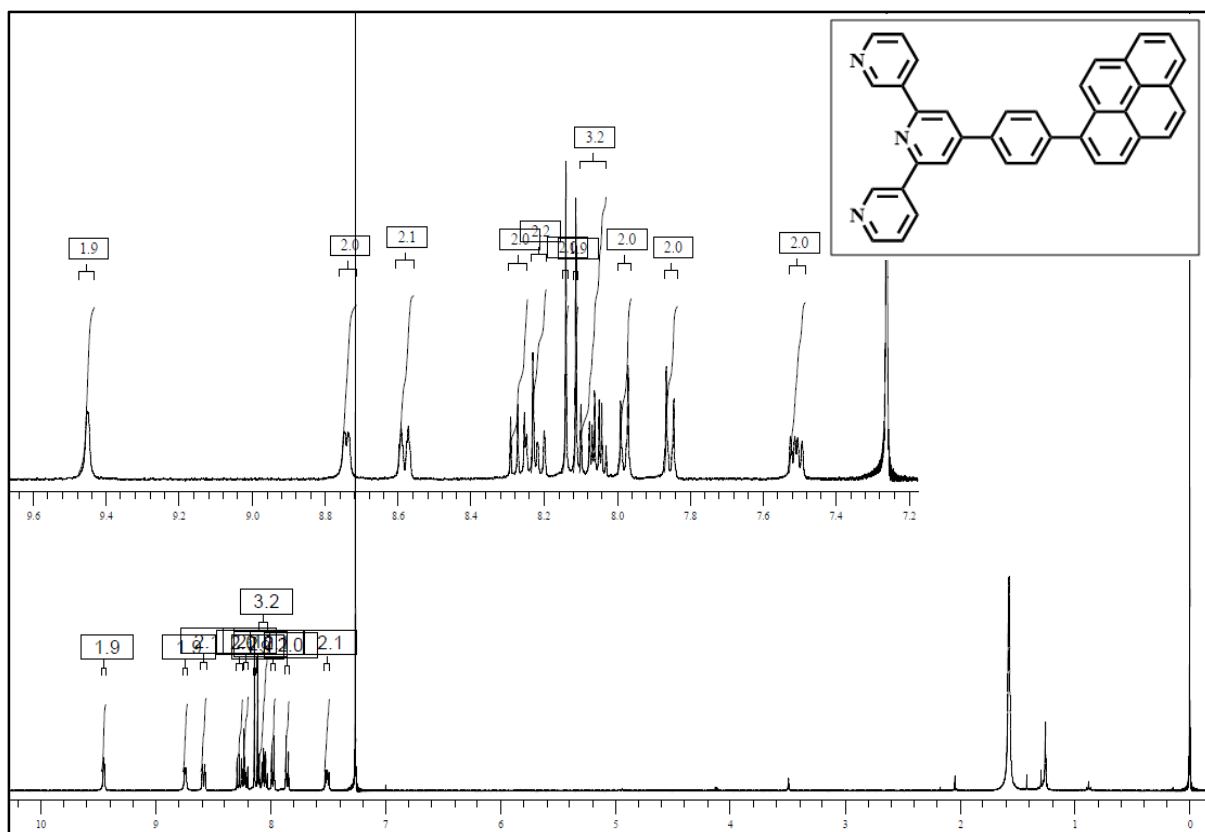
Figure S7. Delayed fluorescence lifetime of Pyr-Bp-Tp



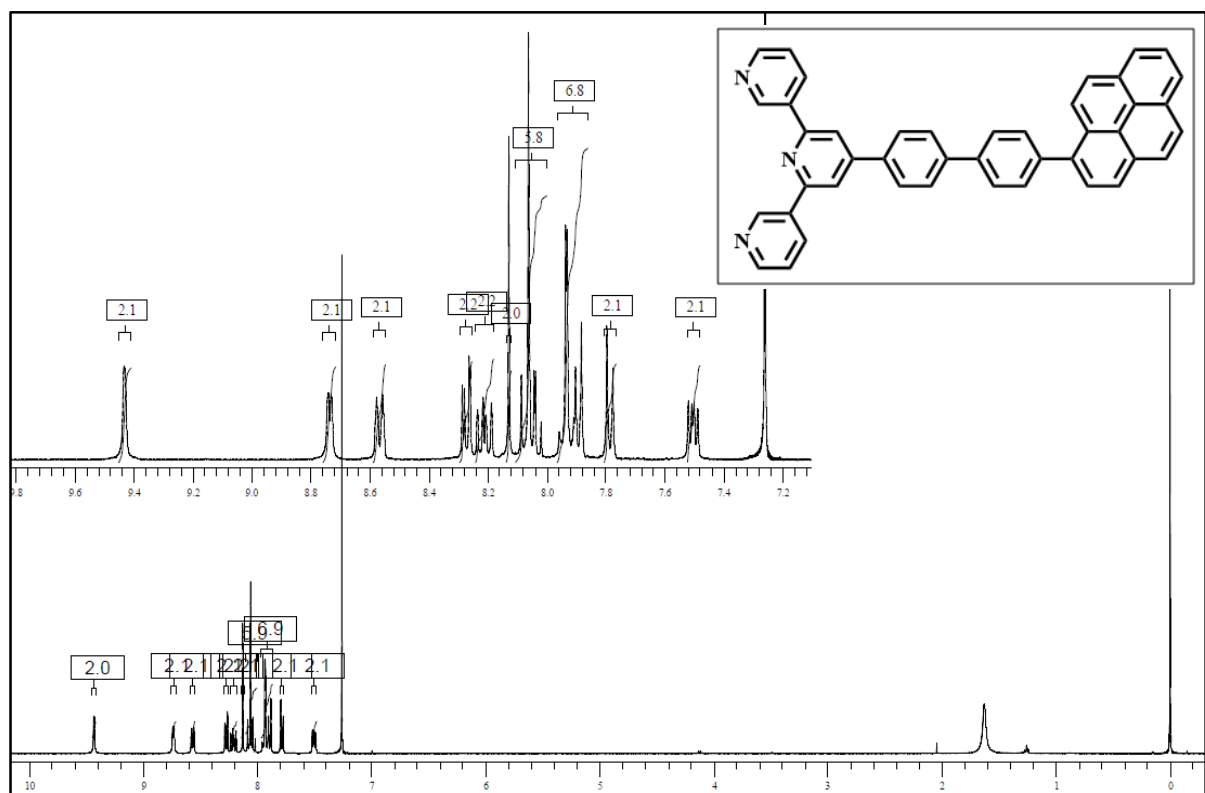
**Figure S8.** <sup>1</sup>H-NMR spectrum of **Ph-Tp**



**Figure S9.** <sup>1</sup>H-NMR spectrum of **Pyr-Tp**



**Figure S10.** <sup>1</sup>H-NMR spectrum of **Pyr-Ph-Tp**



**Figure S11.** <sup>1</sup>H-NMR spectrum of **Pyr-Bp-Tp**



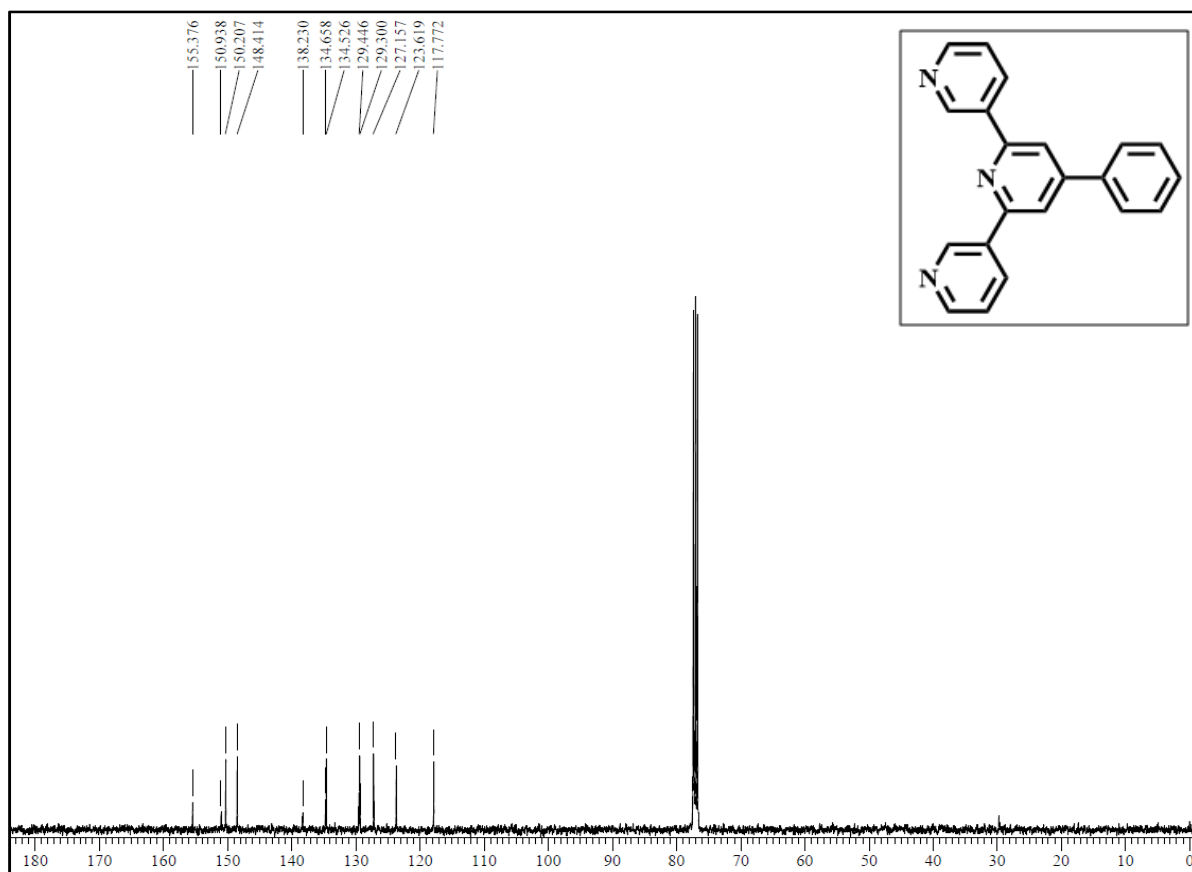


Figure S12.  $^{13}\text{C}$ -NMR spectrum of Ph-Tp

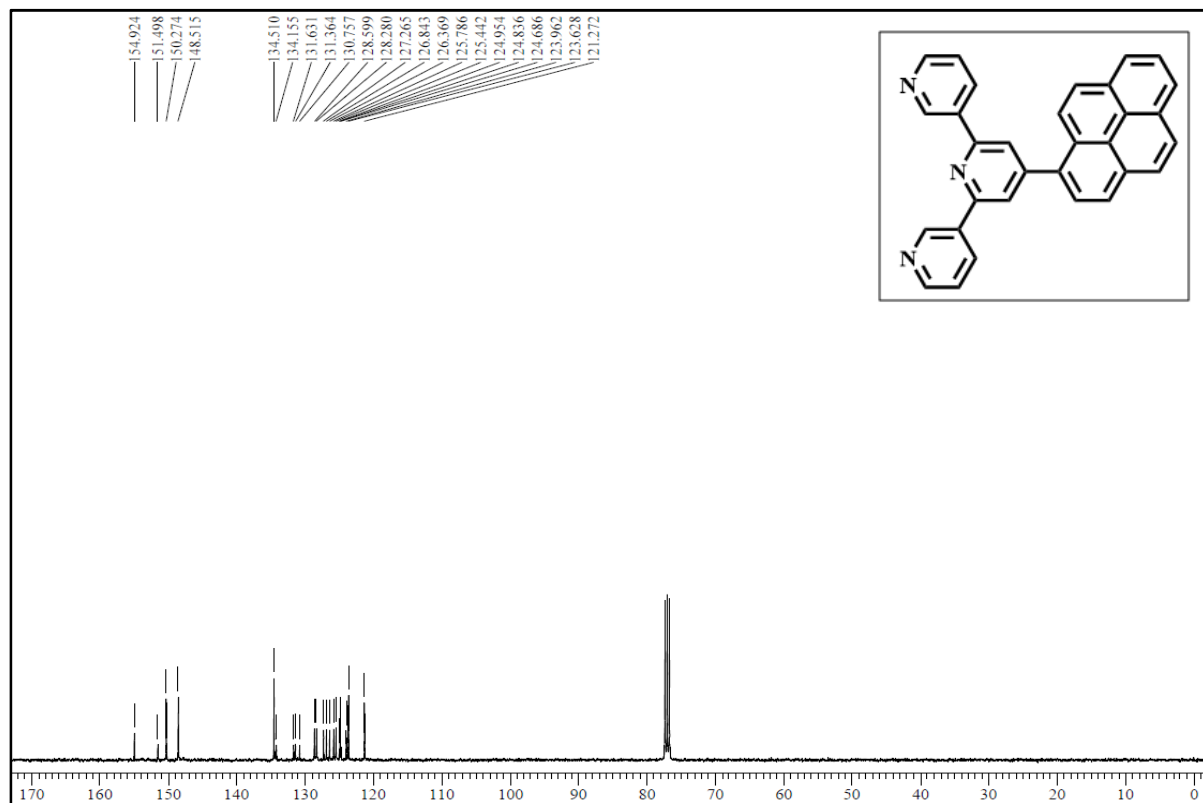


Figure S13.  $^{13}\text{C}$ -NMR spectrum of Pyr-Tp

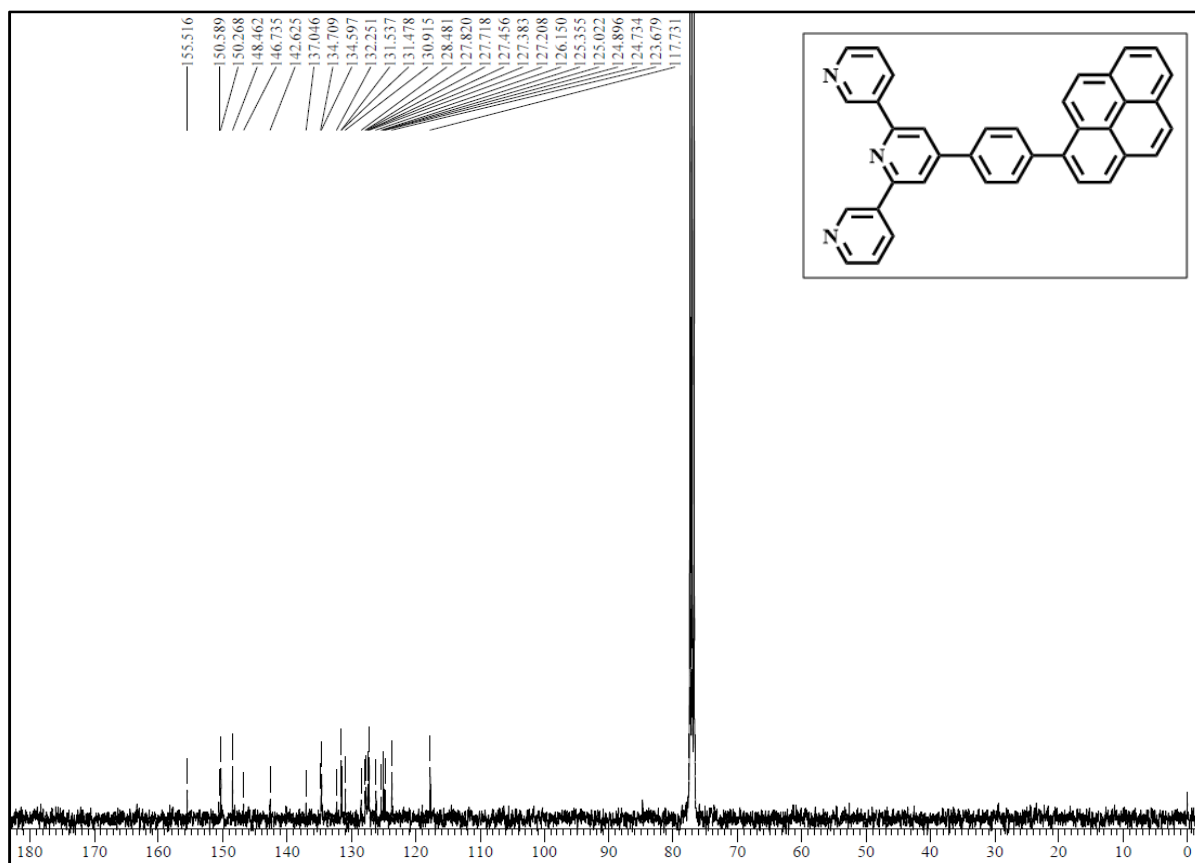


Figure S14.  $^{13}\text{C}$ -NMR spectrum of Pyr-Ph-Tp

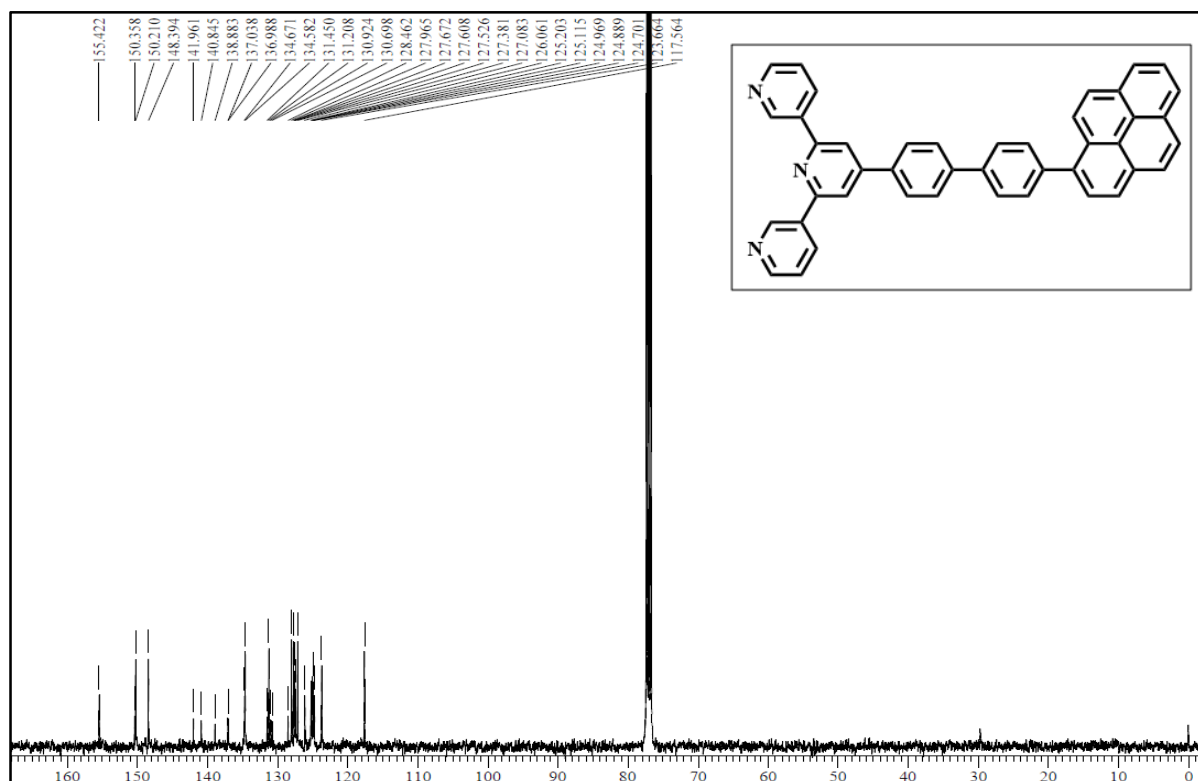
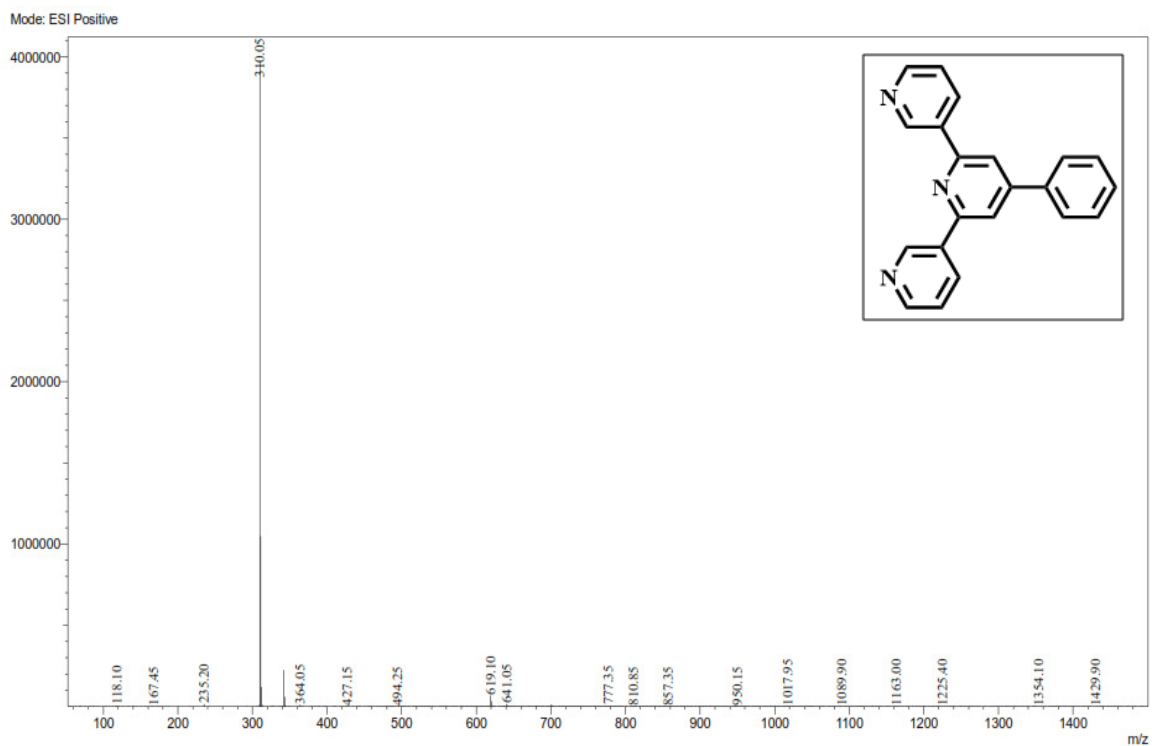
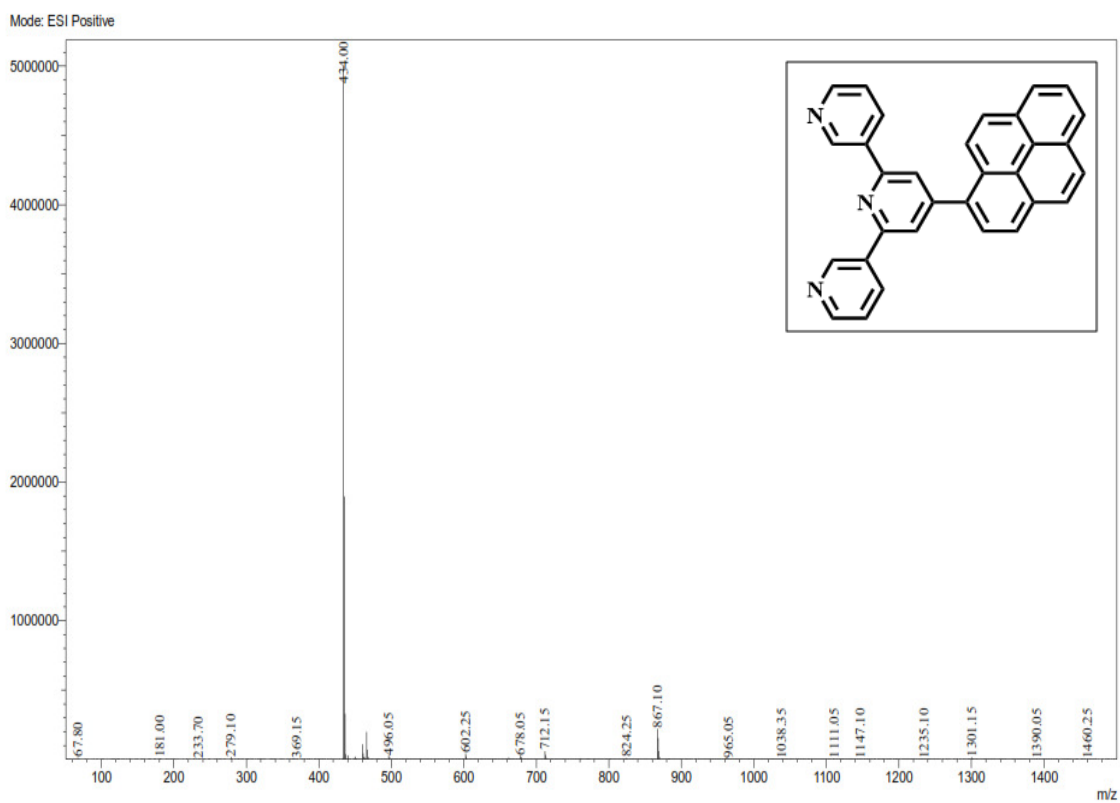


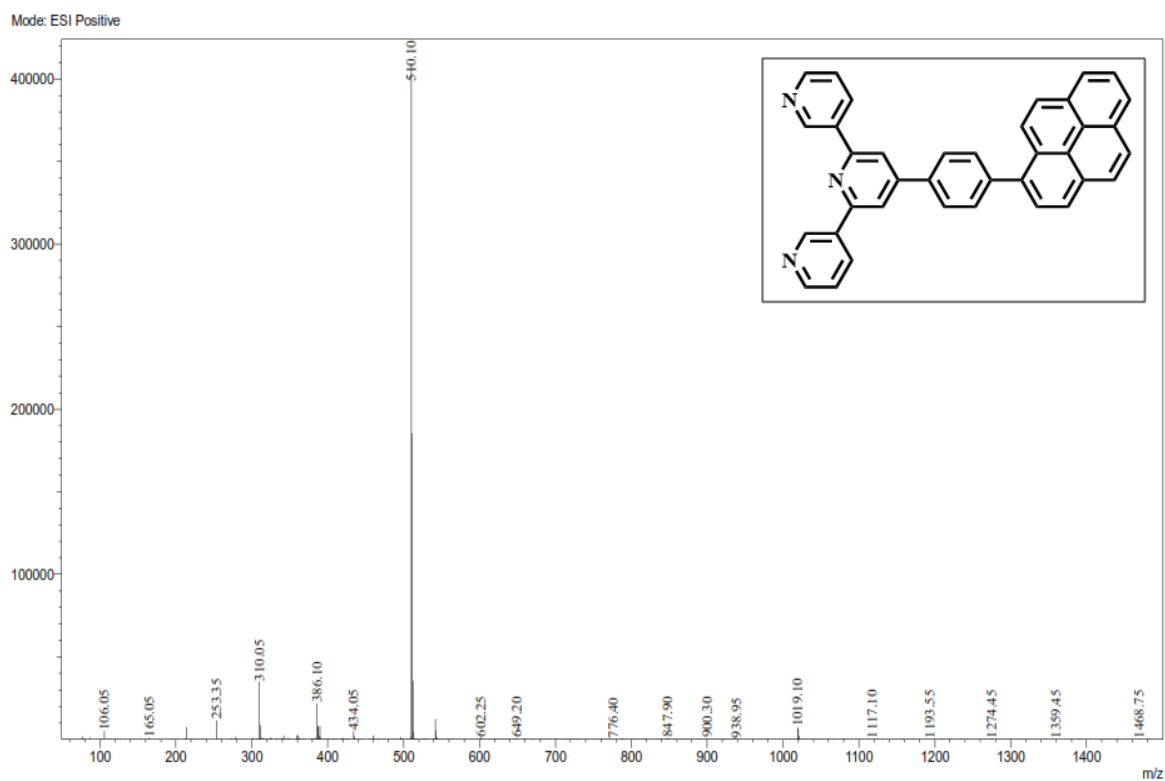
Figure S15.  $^{13}\text{C}$ -NMR spectrum of Pyr-Bp-Tp



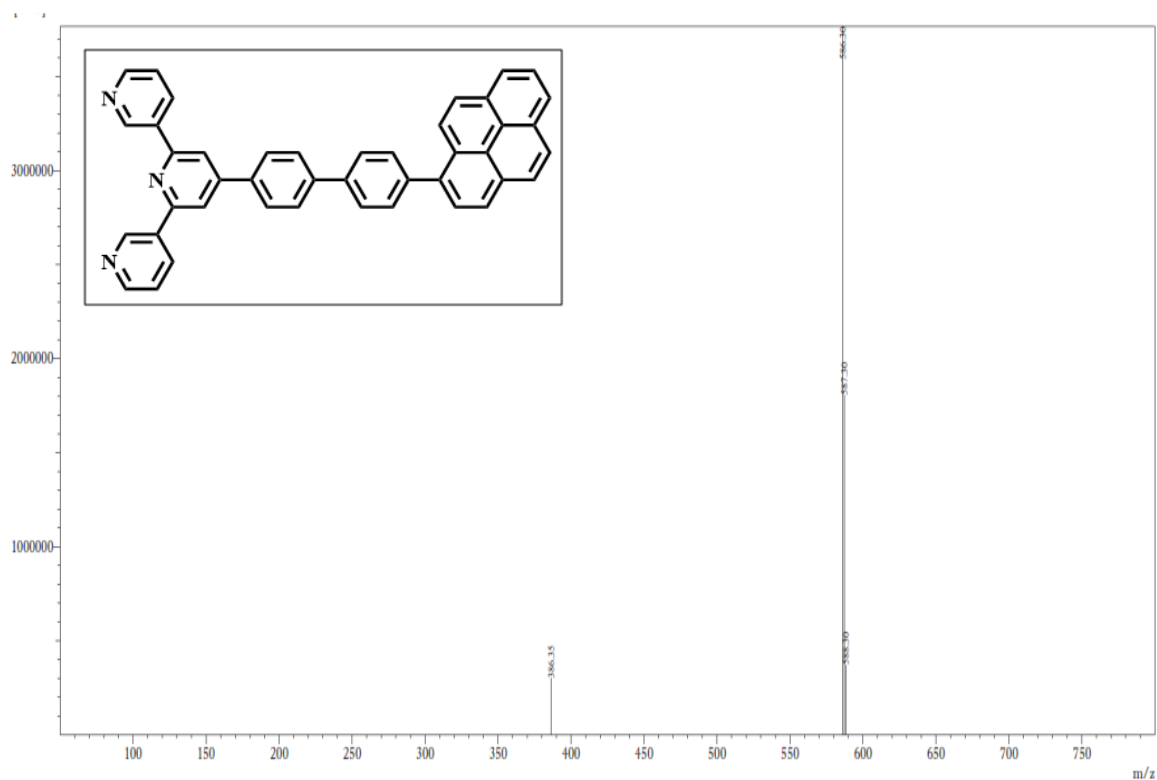
**Figure S16.** LC-MS spectrum of Ph-Tp



**Figure S17.** LC-MS spectrum of Pyr-Tp



**Figure S18.** LC-MS spectrum of **Pyr-Ph-Tp**



**Figure S19.** LC-MS spectrum of **Pyr-Bp-Tp**

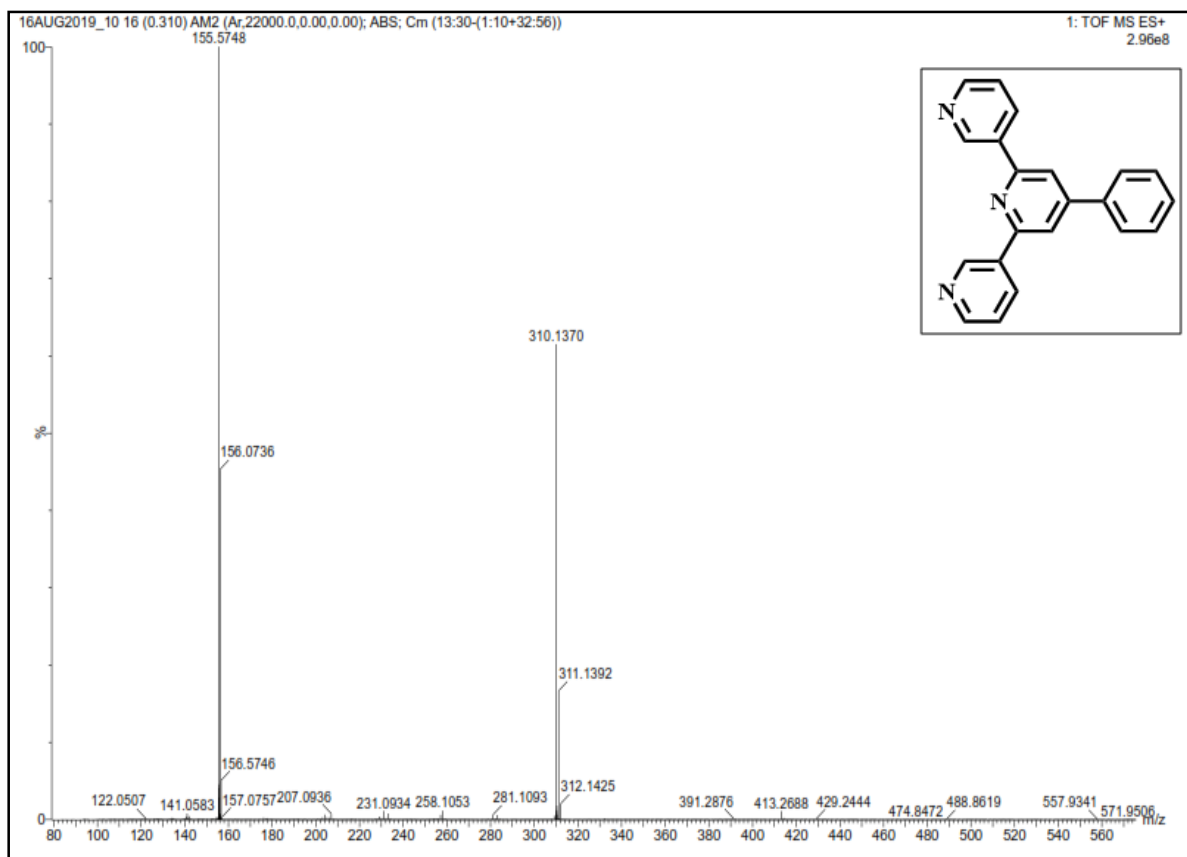


Figure S20.HRMS spectrum of Ph-Tp

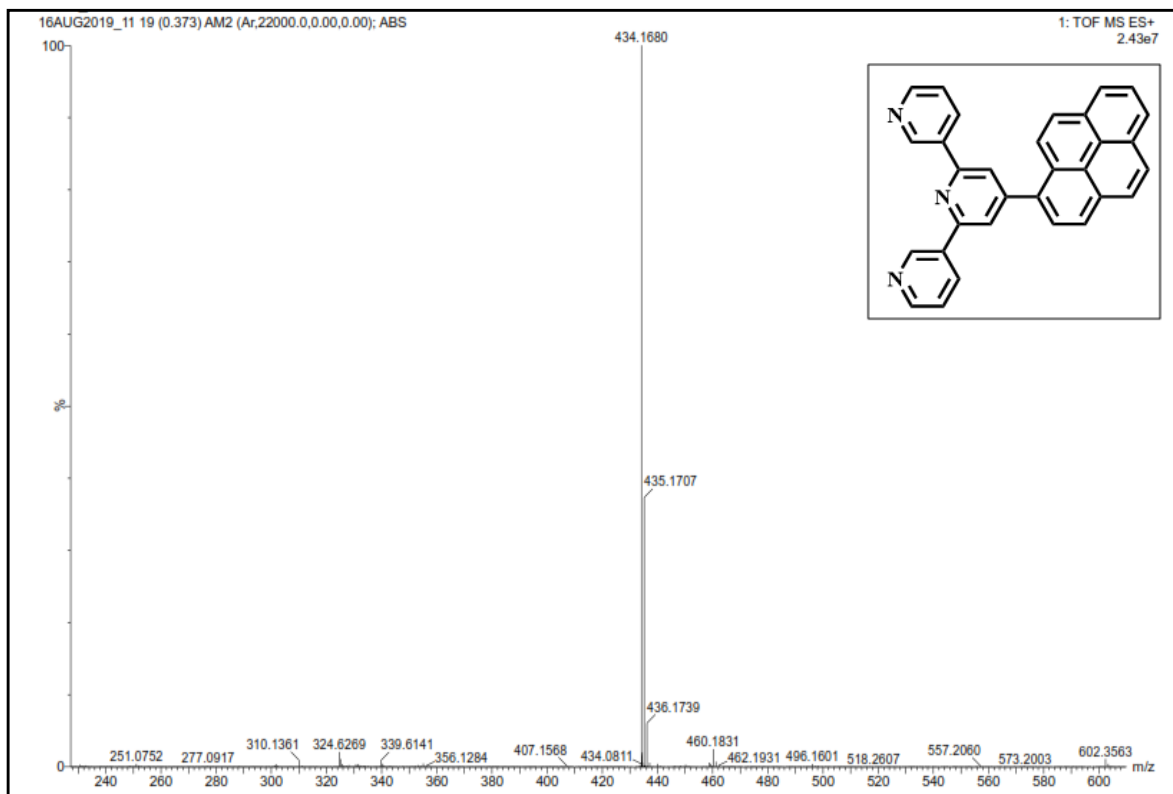
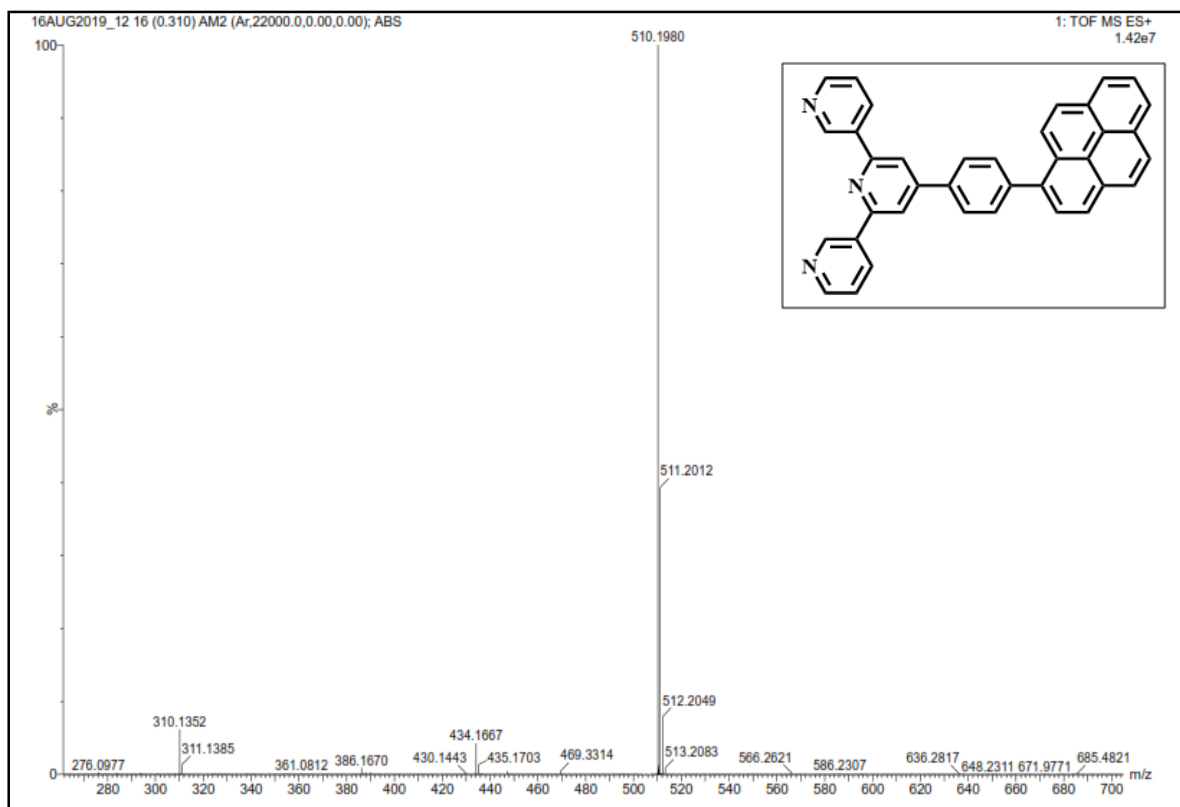
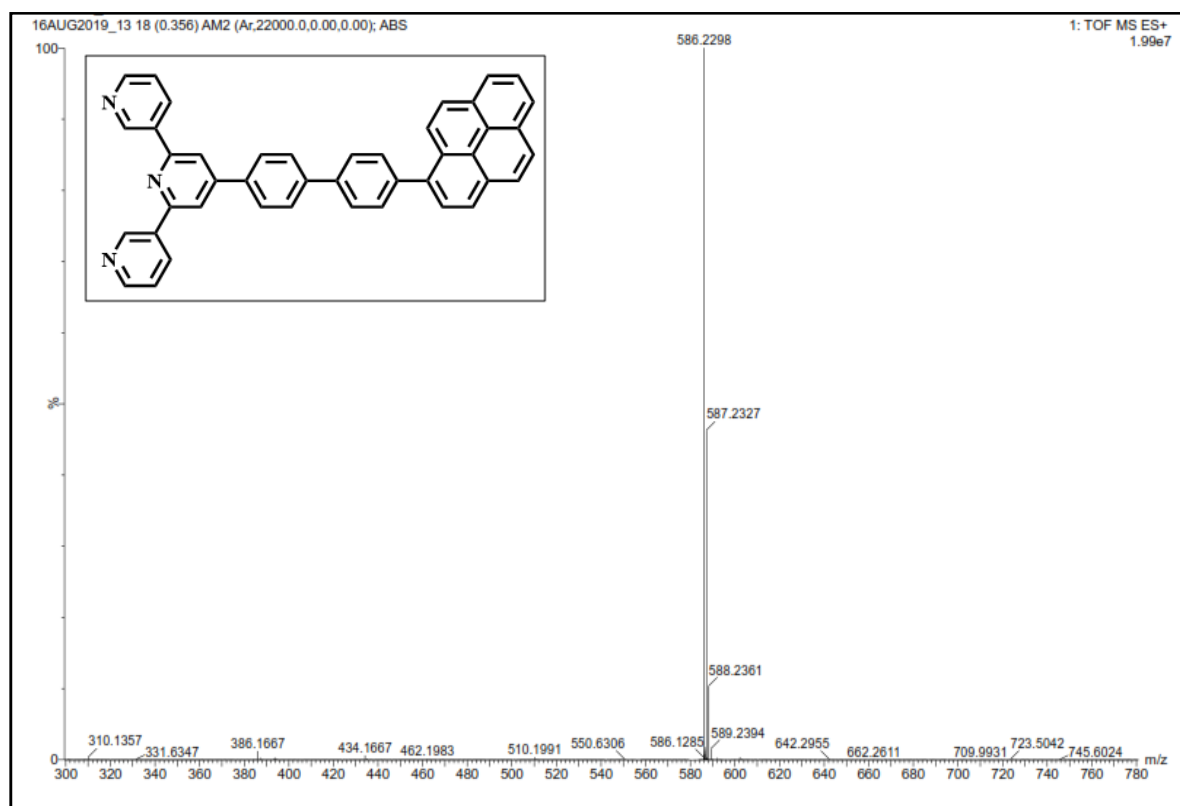


Figure S21.HRMS spectrum of Pyr-Tp



**Figure S22.** HRMS spectrum of Pyr-Ph-Tp



**Figure S23.** HRMS spectrum of Pyr-Bp-Tp