

Supplementary Information

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

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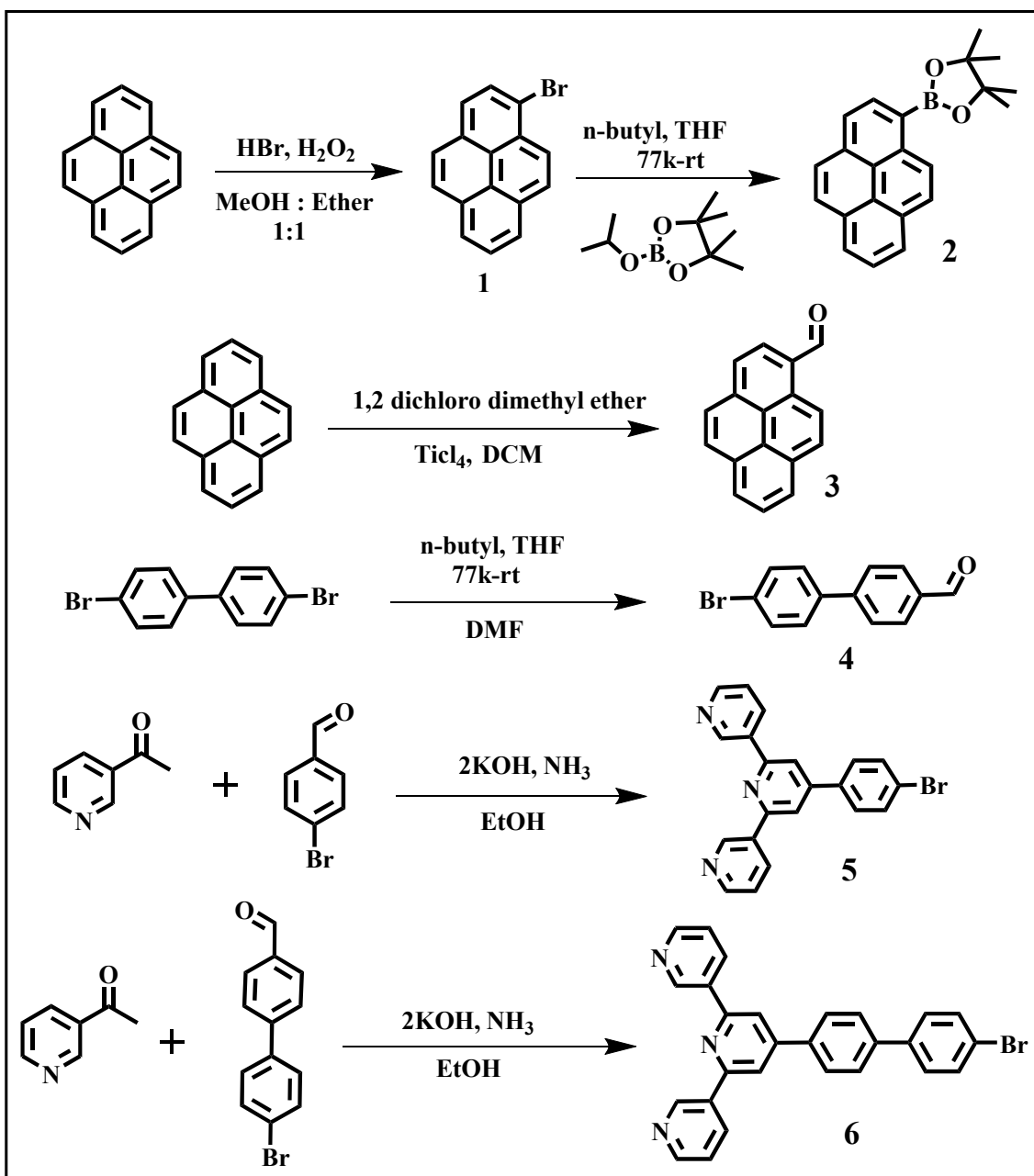
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Scheme S1. Synthetic route for intermediates

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 μ_e (D).

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

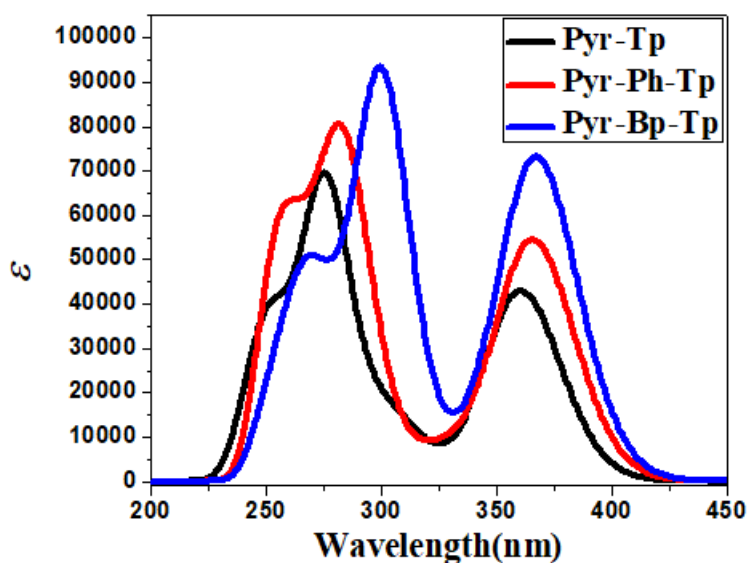


Figure S1. PBE0/6-311G (d,p) simulated absorption spectra of **Pyr-Tp**, **Pyr-Ph-Tp** and **Pyr-Bp-Tp** in chloroform solvent.

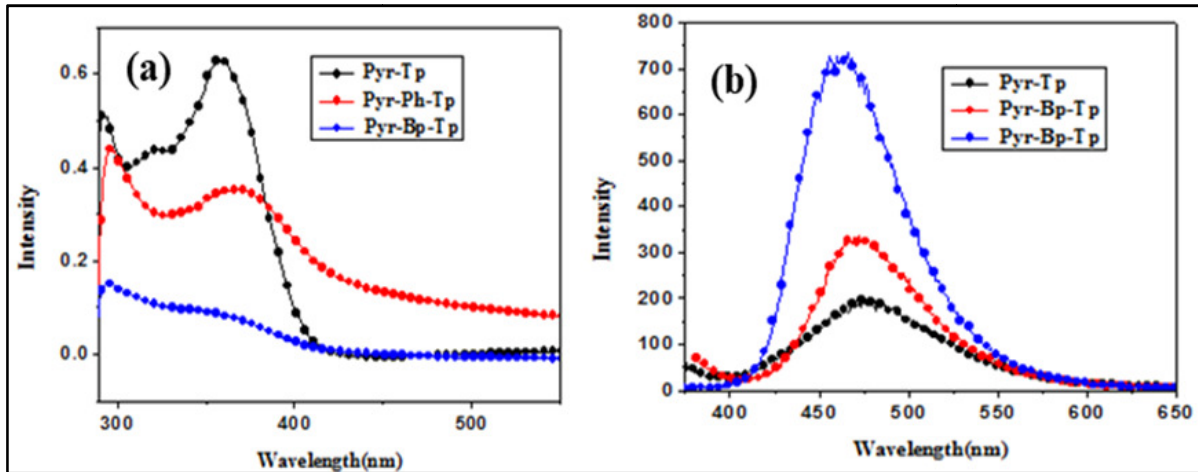


Figure S2.(a) Thin film UV-vis absorption spectra (b) Thin film Fluorescence spectra.

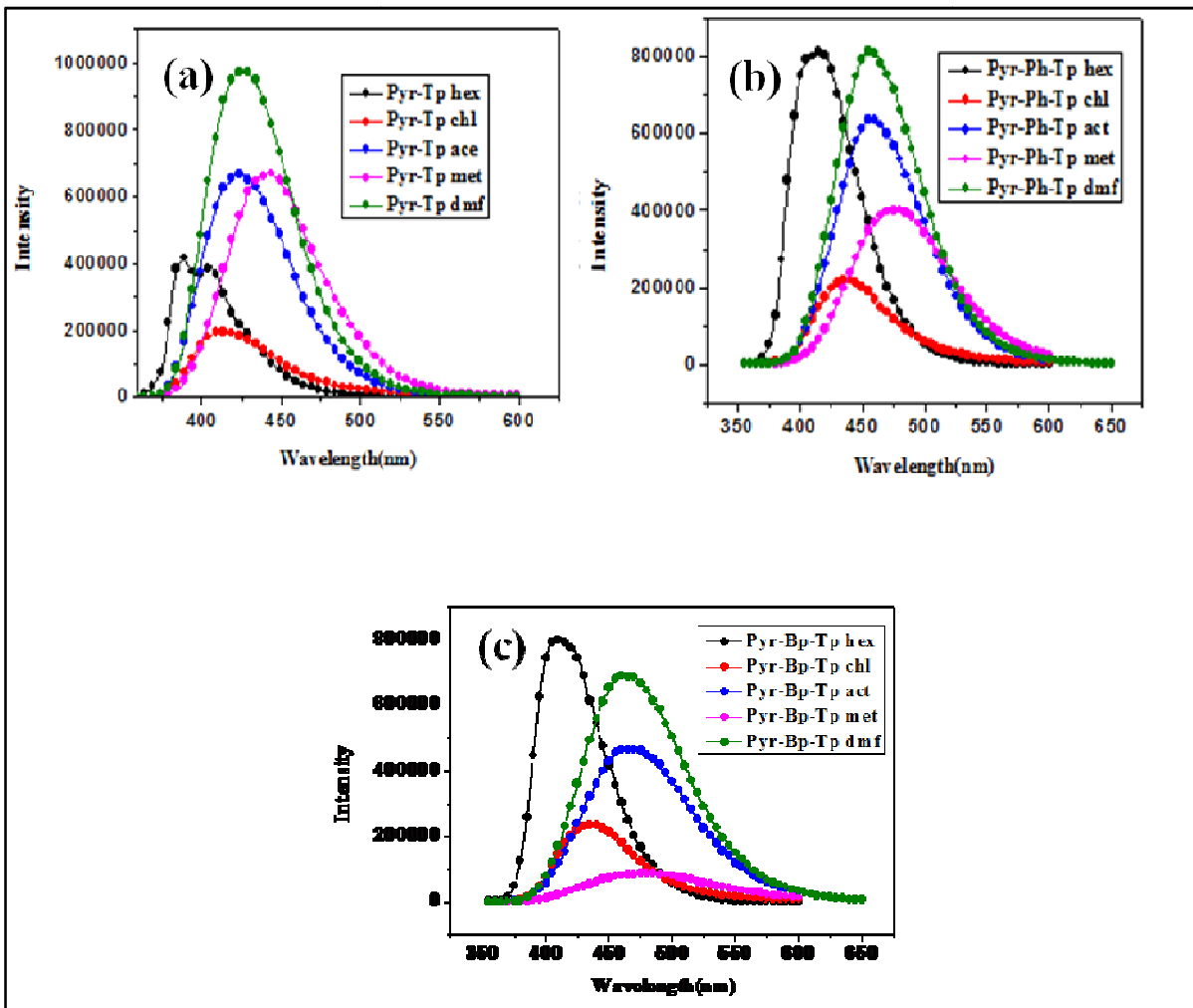


Figure S3.Solvatochromism spectra of Pyr-Tp, Pyr-Ph-Tp and Pyr-Bp-Tp

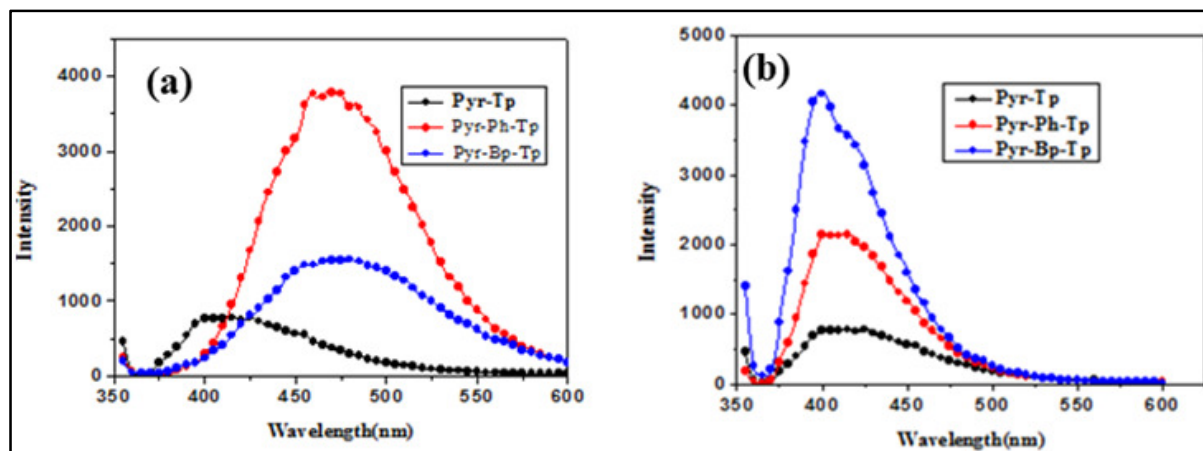


Figure S4. (a) Delayed fluorescence at RT (b) Delayed fluorescence at 77k

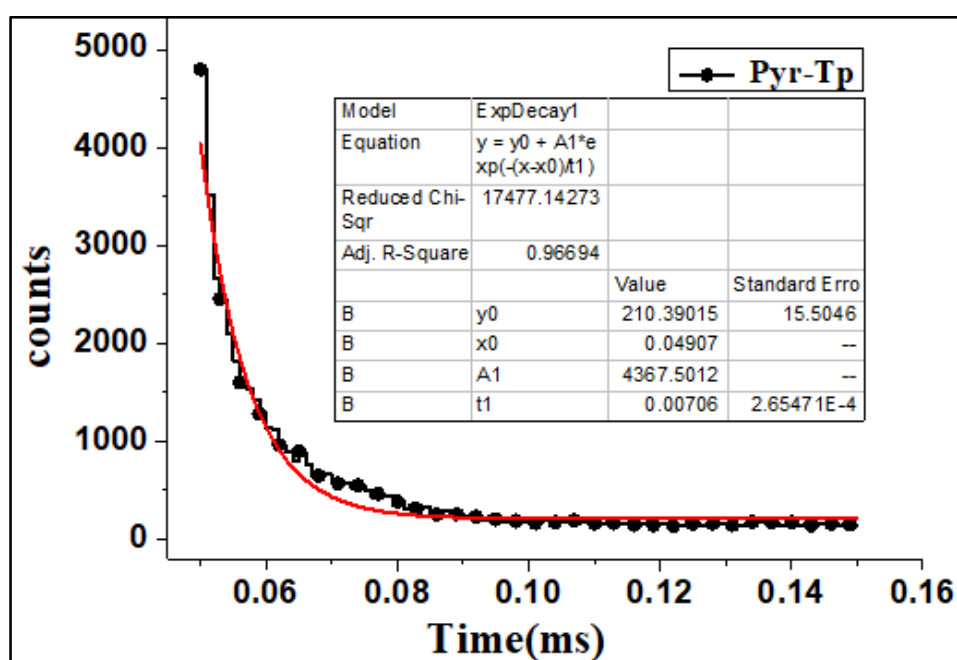


Figure S5. Delayed fluorescence lifetime of Pyr-Tp

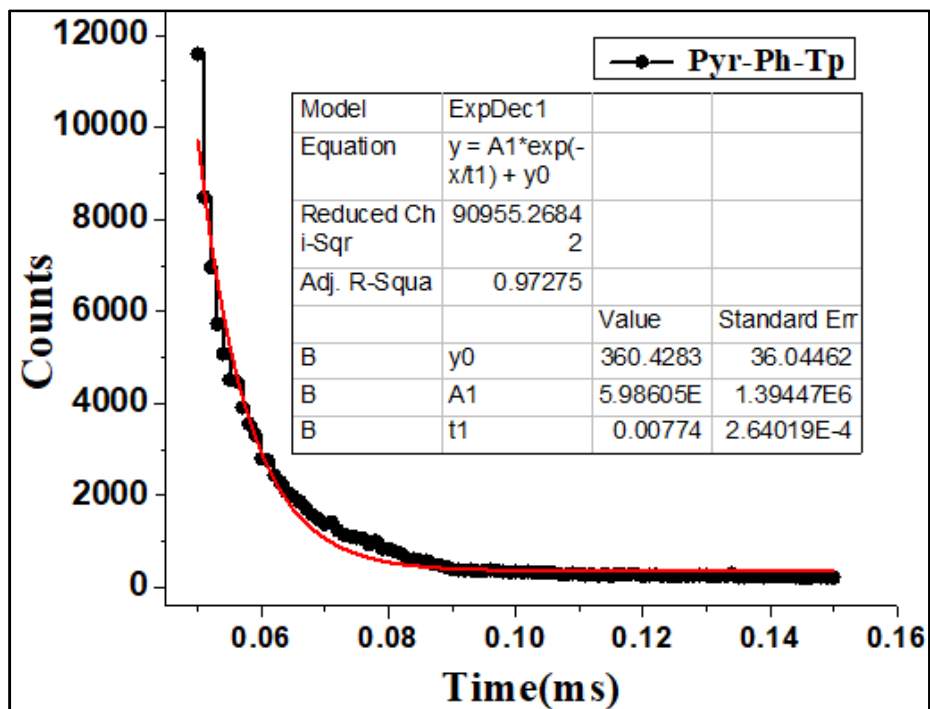


Figure S6. Delayed fluorescence lifetime of Pyr-Ph-Tp

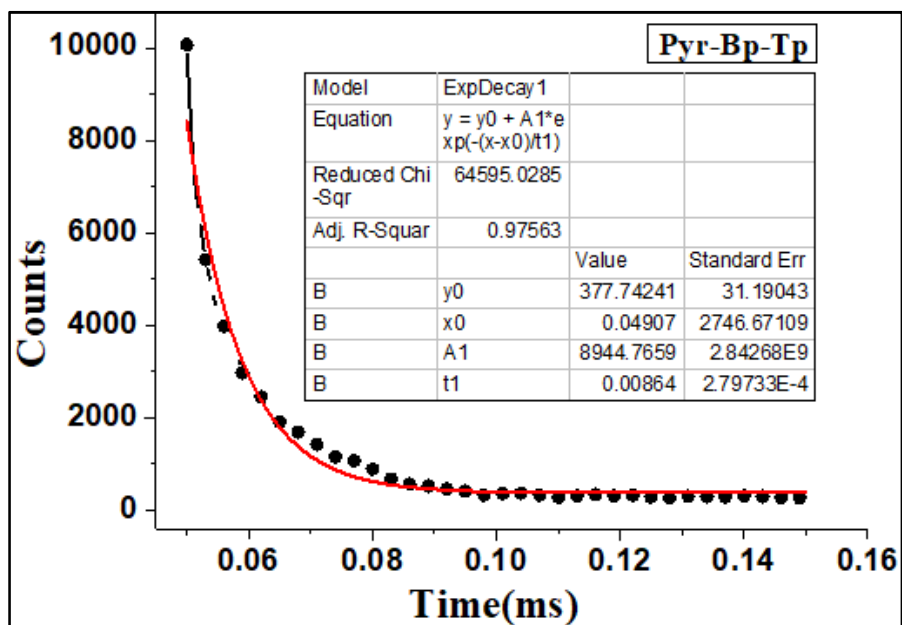


Figure S7. Delayed fluorescence lifetime of Pyr-Bp-Tp

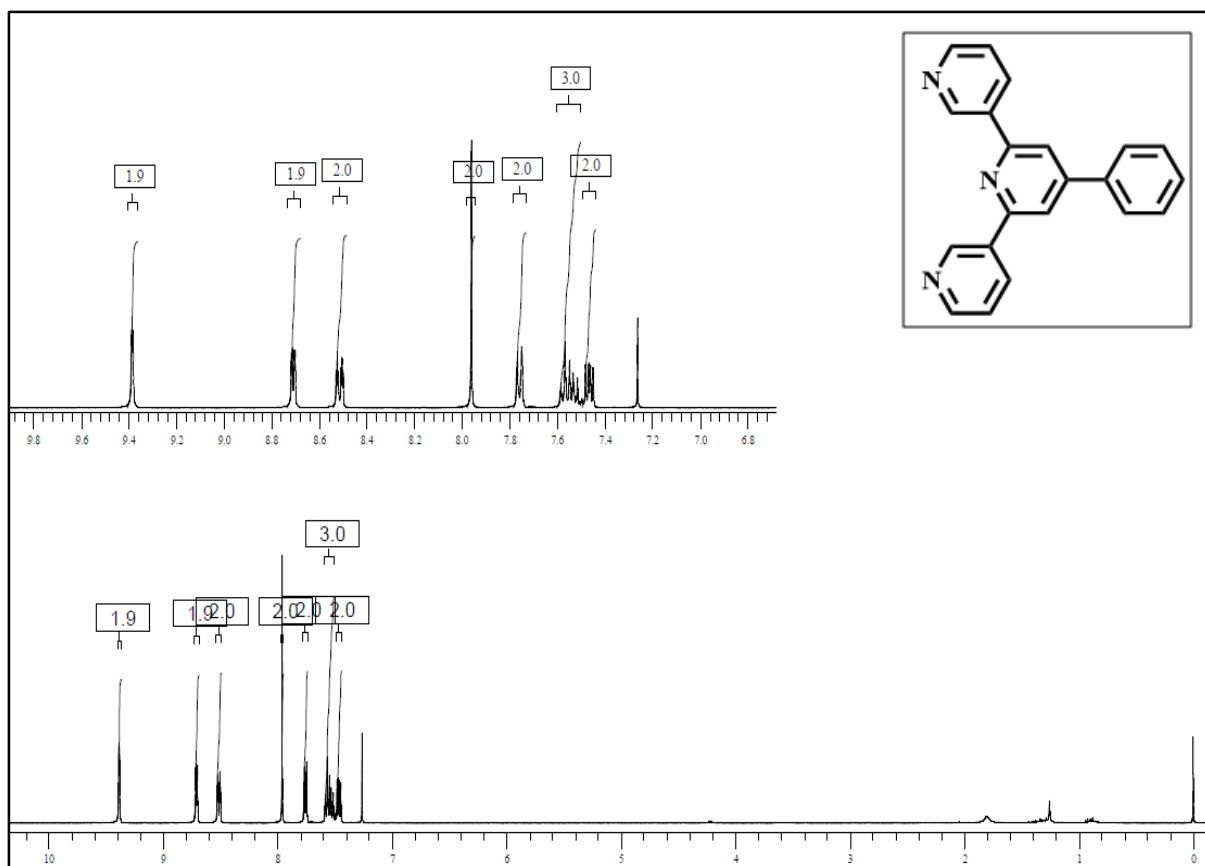


Figure S8. ¹H-NMR spectrum of **Ph-Tp**

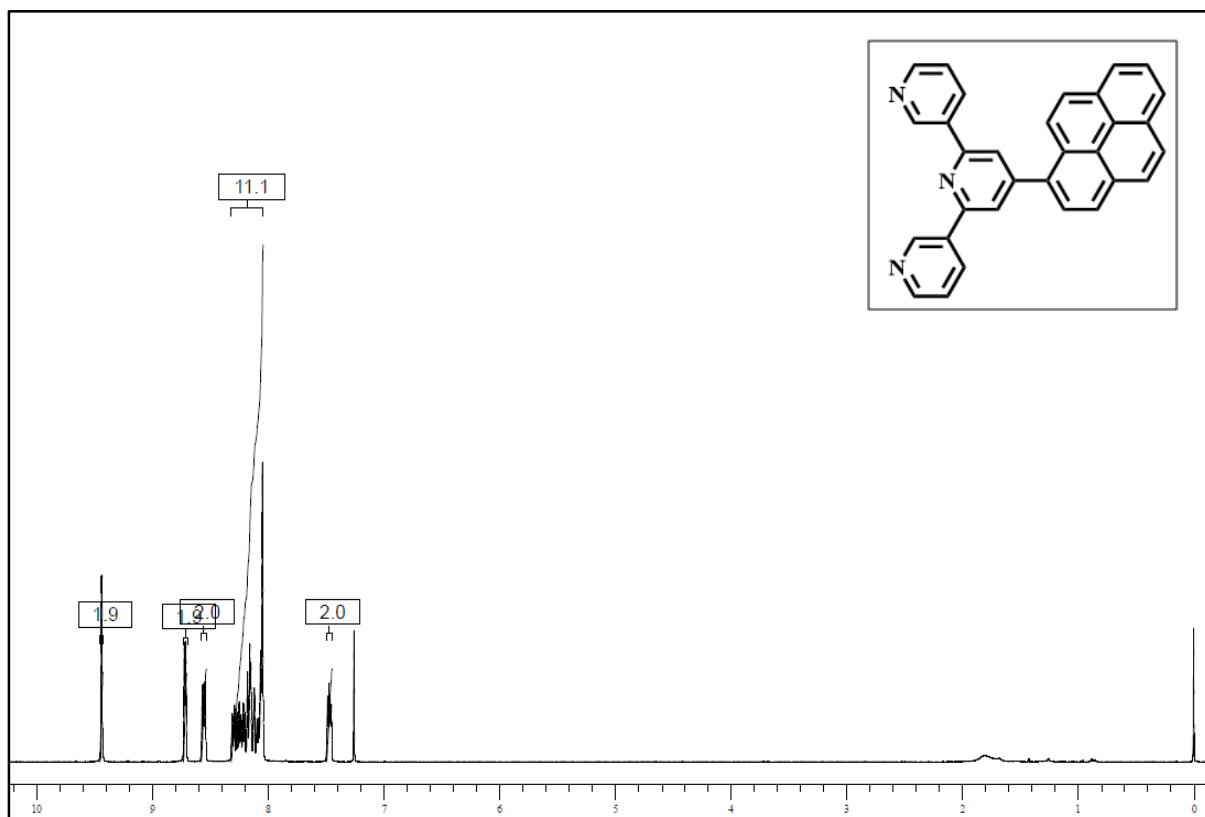


Figure S9. ¹H-NMR spectrum of **Pyr-Tp**

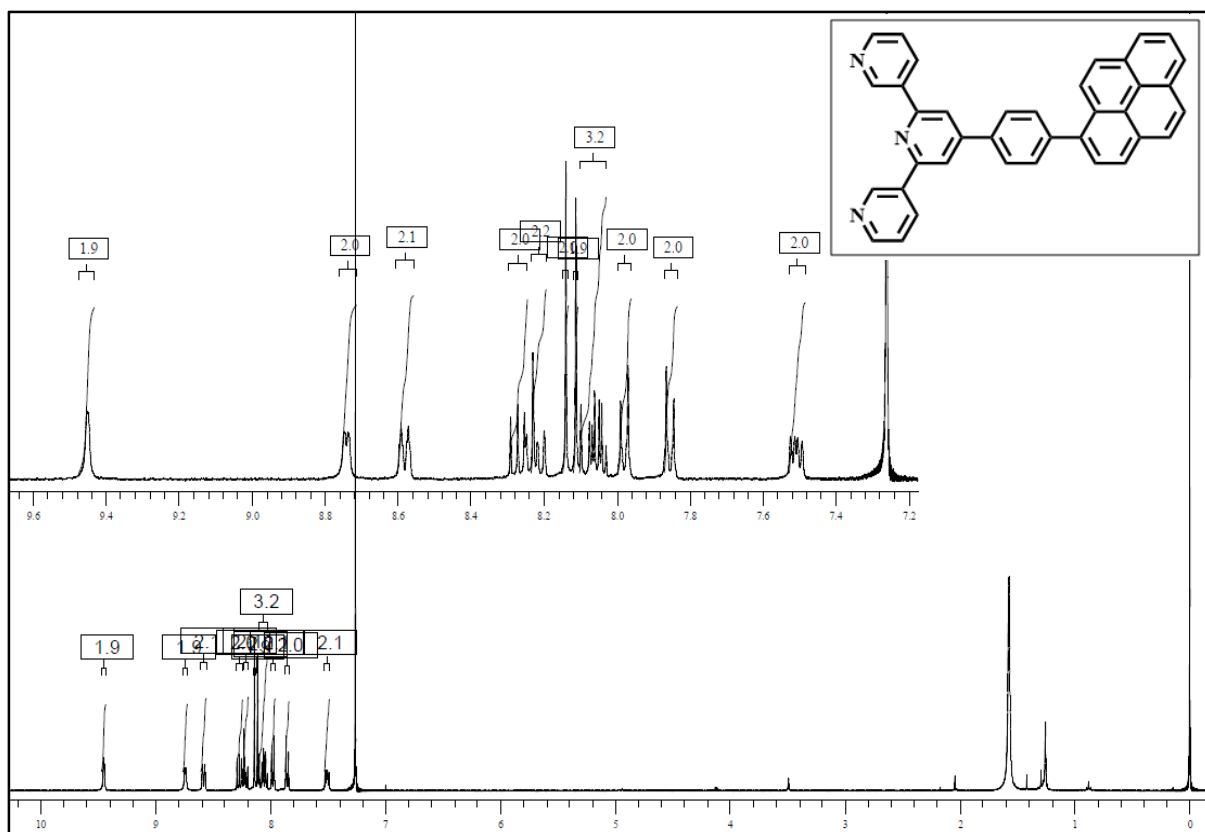


Figure S10. $^1\text{H-NMR}$ spectrum of **Pyr-Ph-Tp**

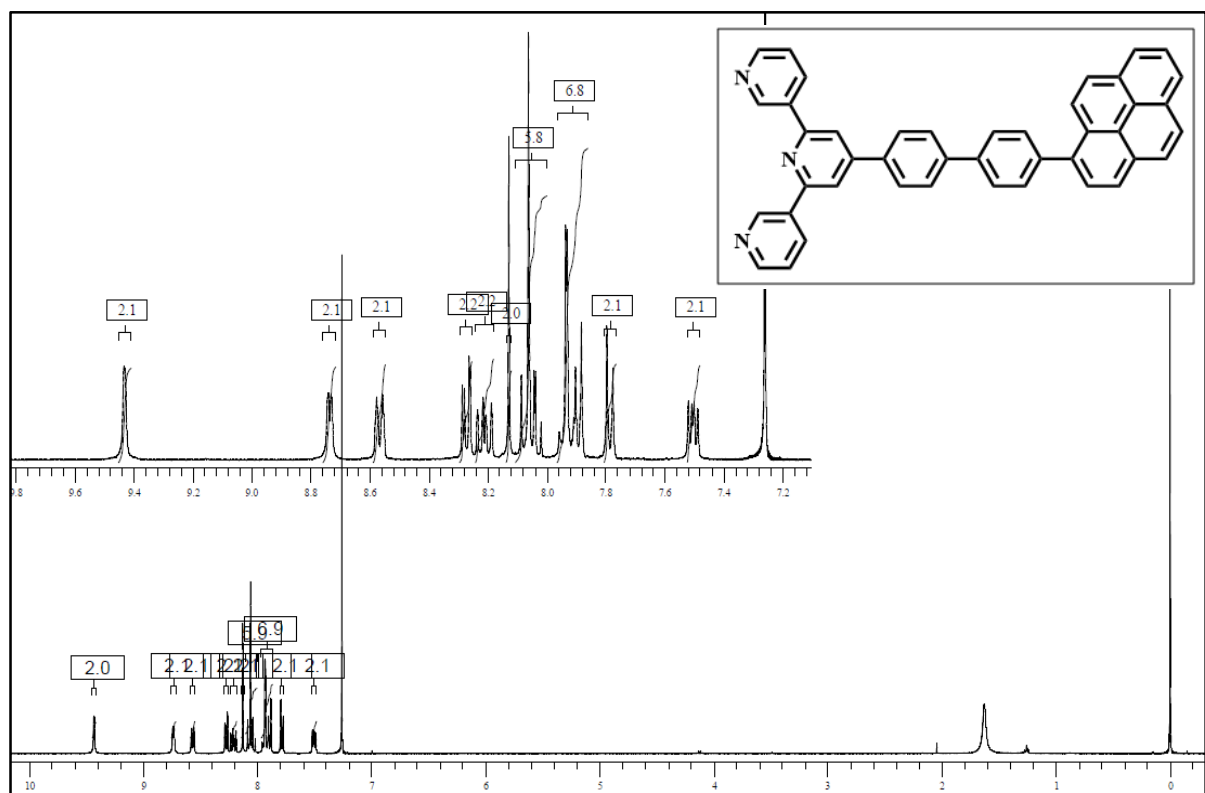


Figure S11. $^1\text{H-NMR}$ spectrum of **Pyr-Bp-Tp**

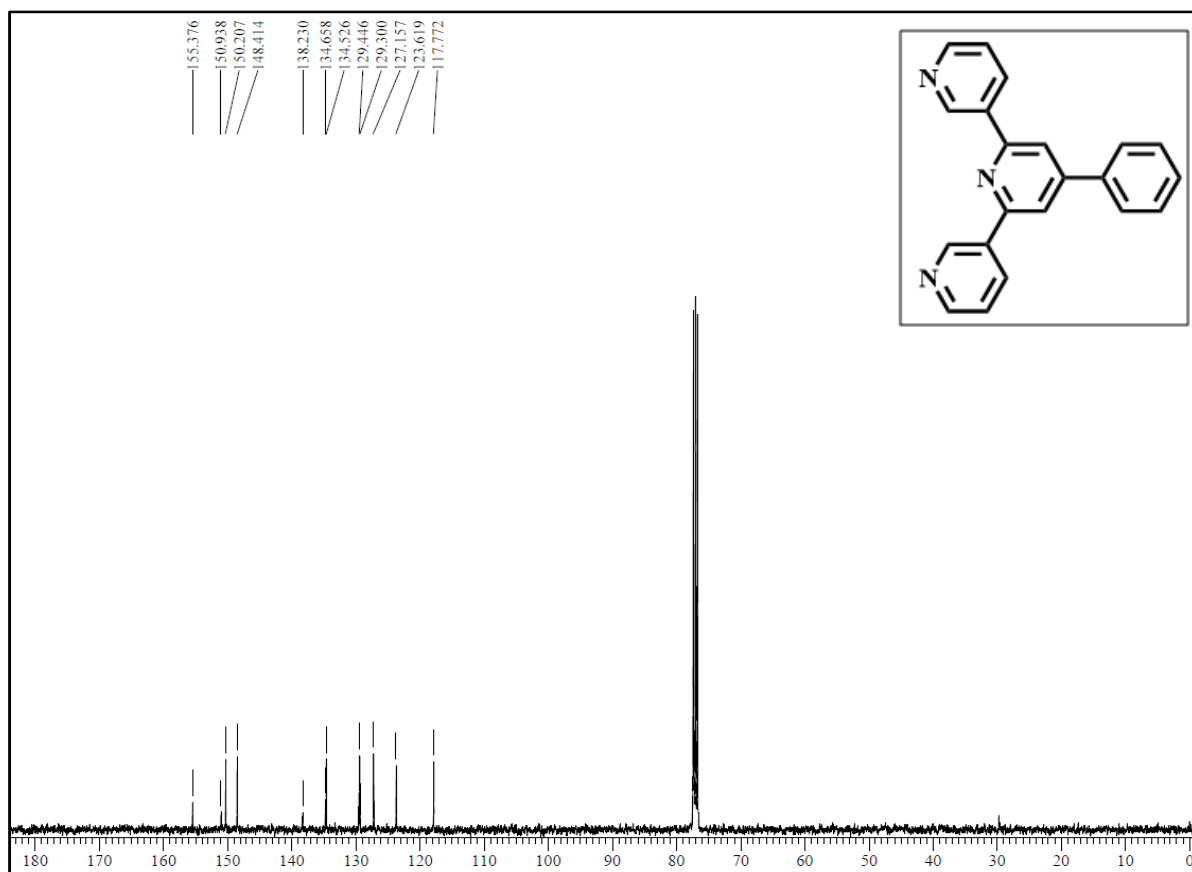


Figure S12. ^{13}C -NMR spectrum of Ph-Tp

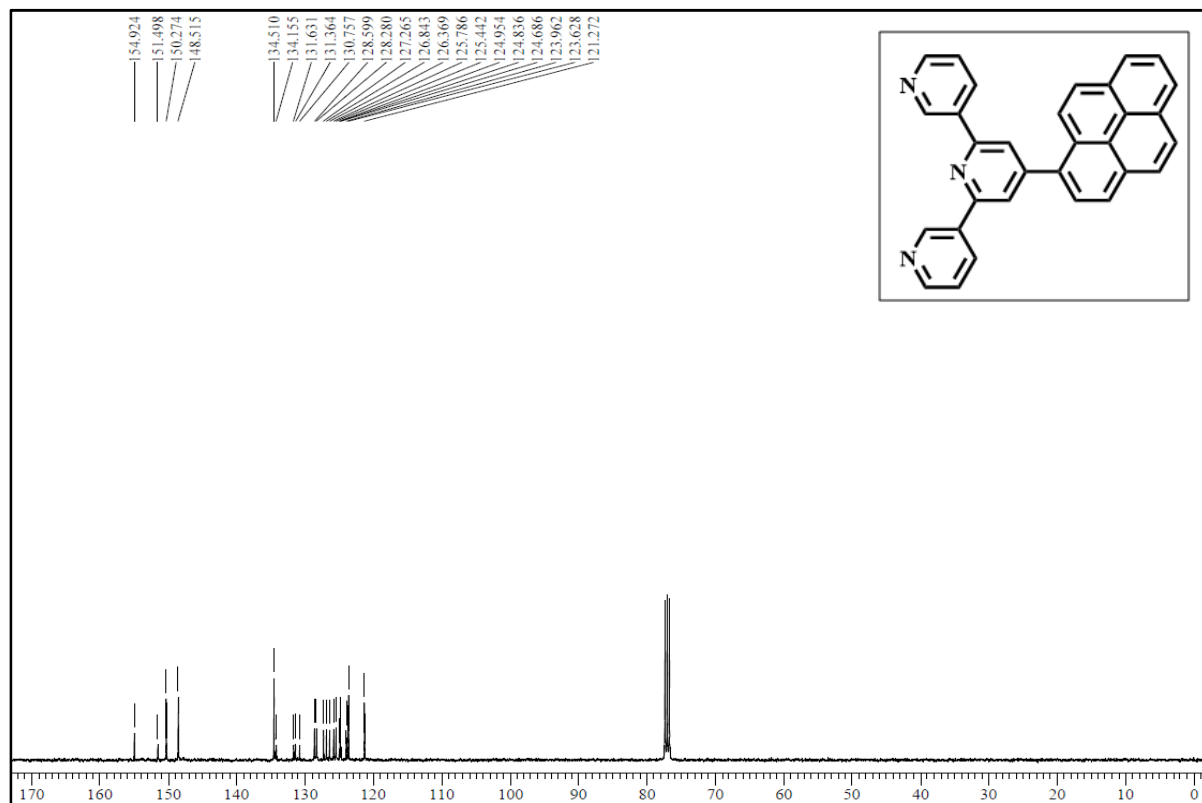


Figure S13. ^{13}C -NMR spectrum of Pyr-Tp

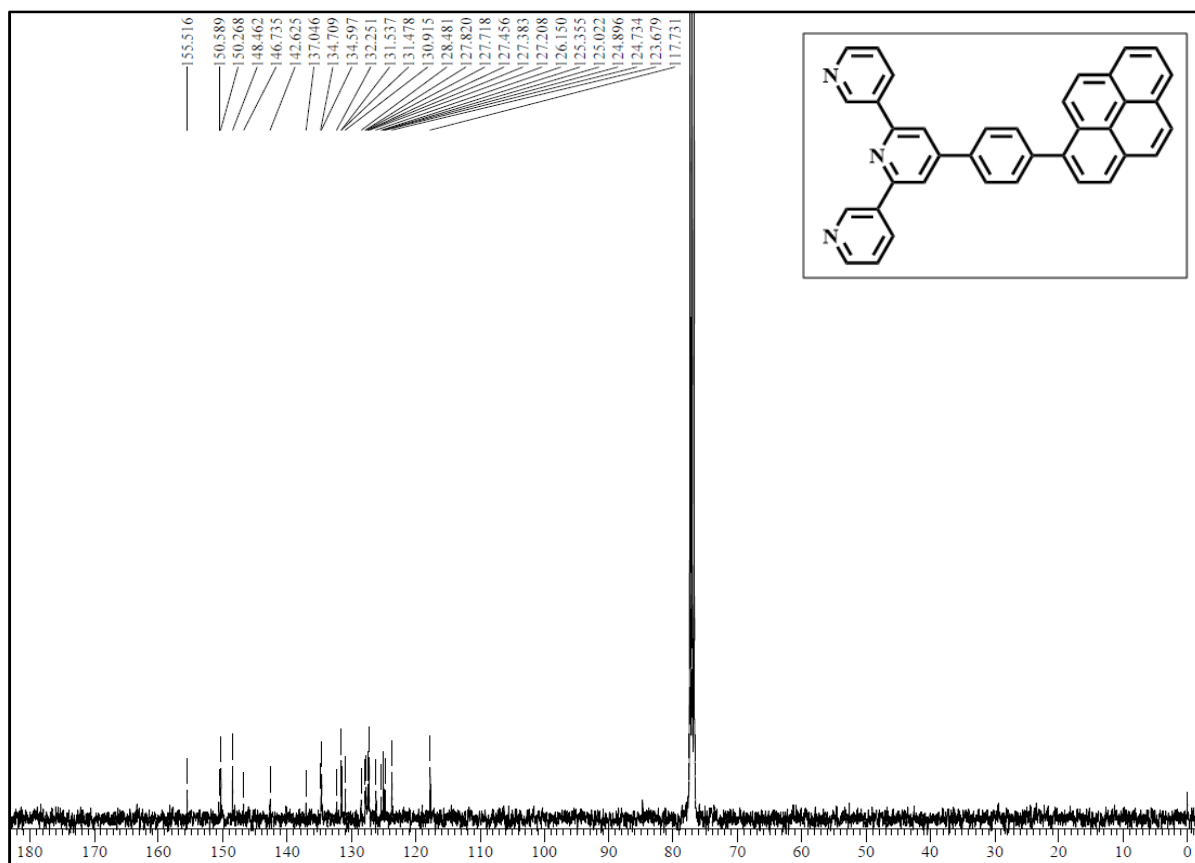


Figure S14. ^{13}C -NMR spectrum of Pyr-Ph-Tp

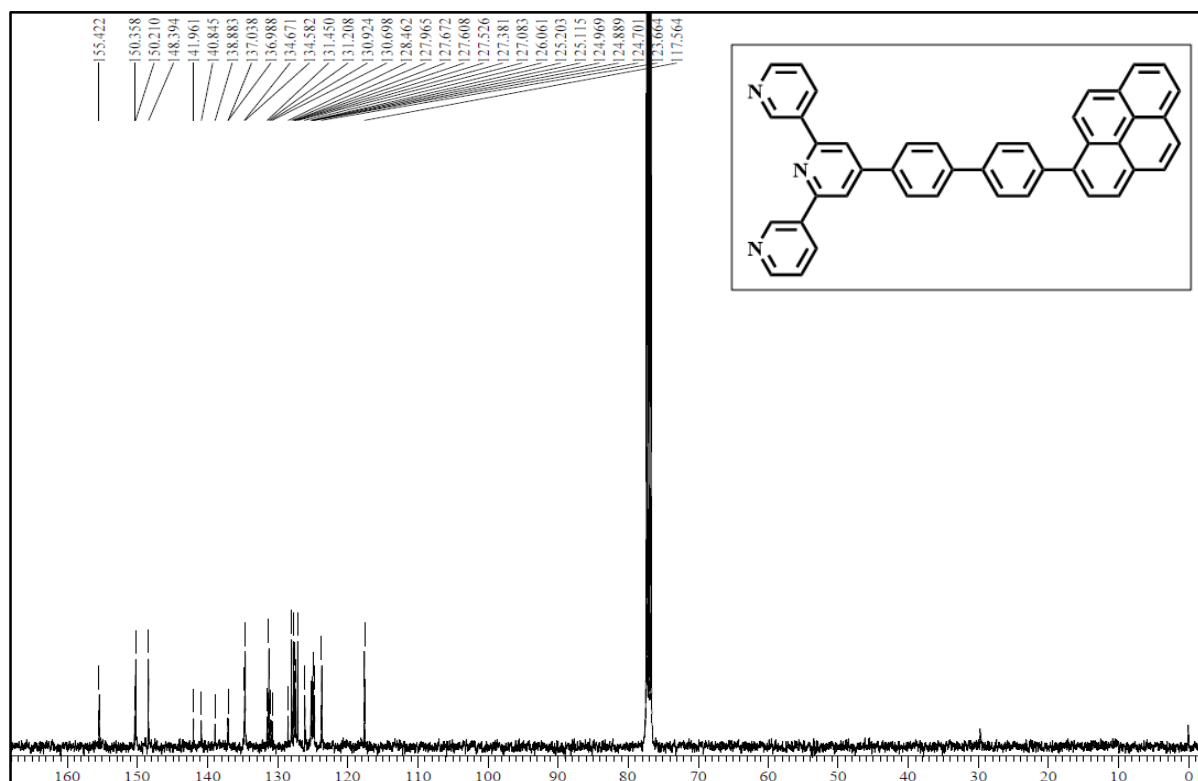


Figure S15. ^{13}C -NMR spectrum of Pyr-Bp-Tp

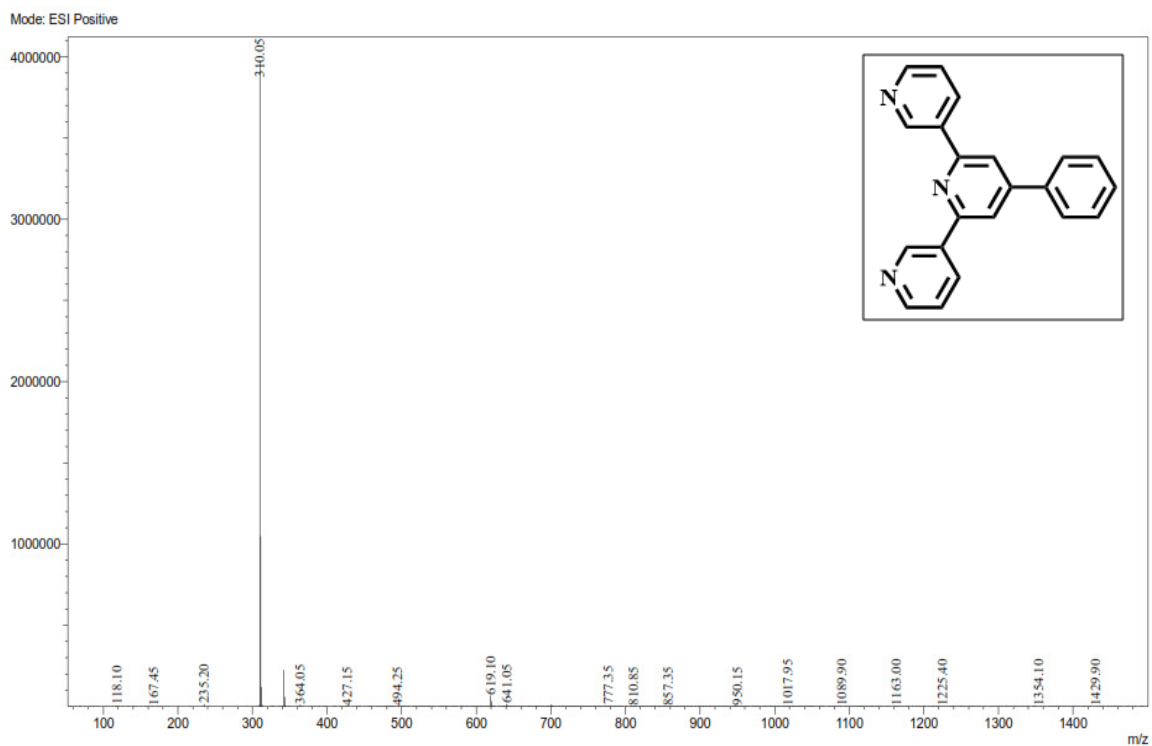


Figure S16. LC-MS spectrum of Ph-Tp

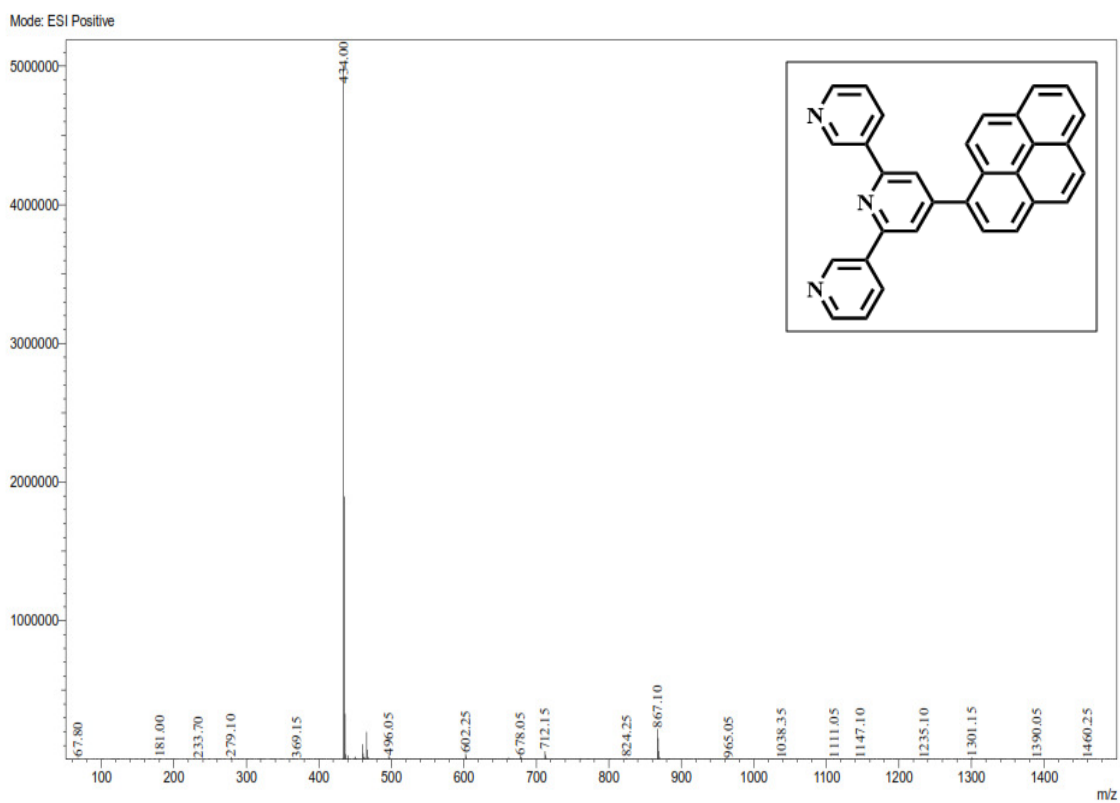


Figure S17. LC-MS spectrum of Pyr-Tp

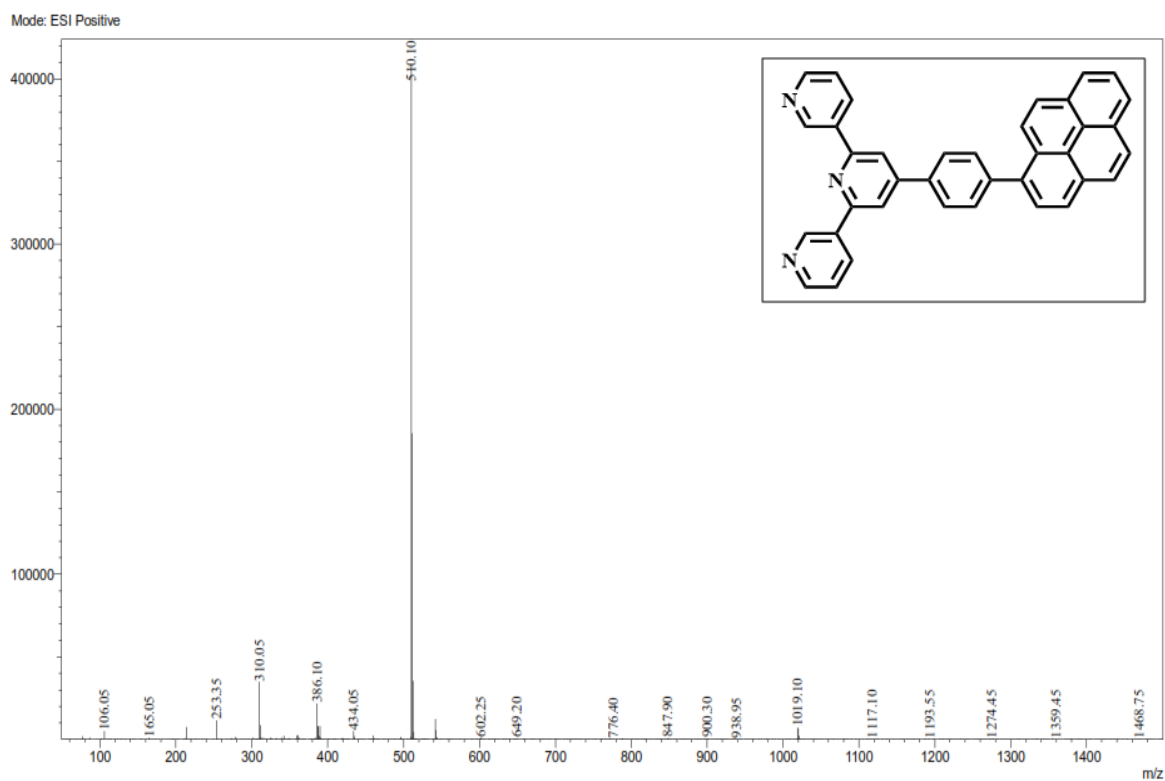


Figure S18. LC-MS spectrum of **Pyr-Ph-Tp**

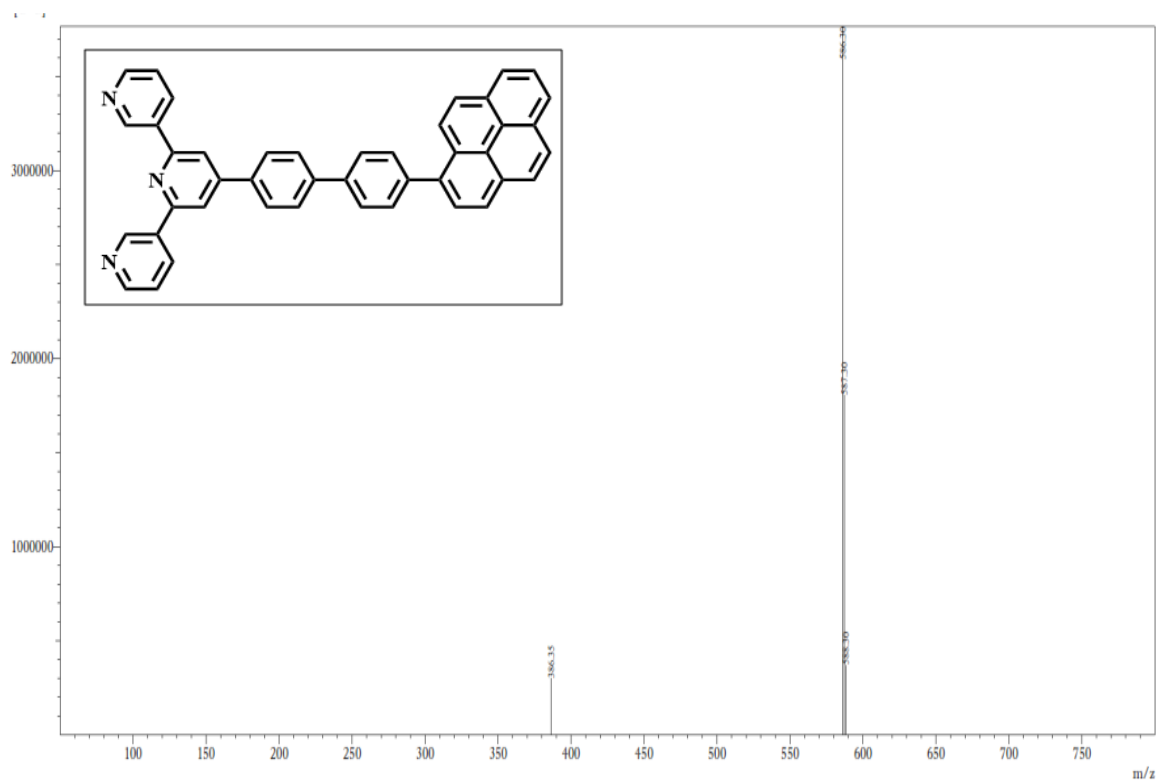


Figure S19. LC-MS spectrum of **Pyr-Bp-Tp**

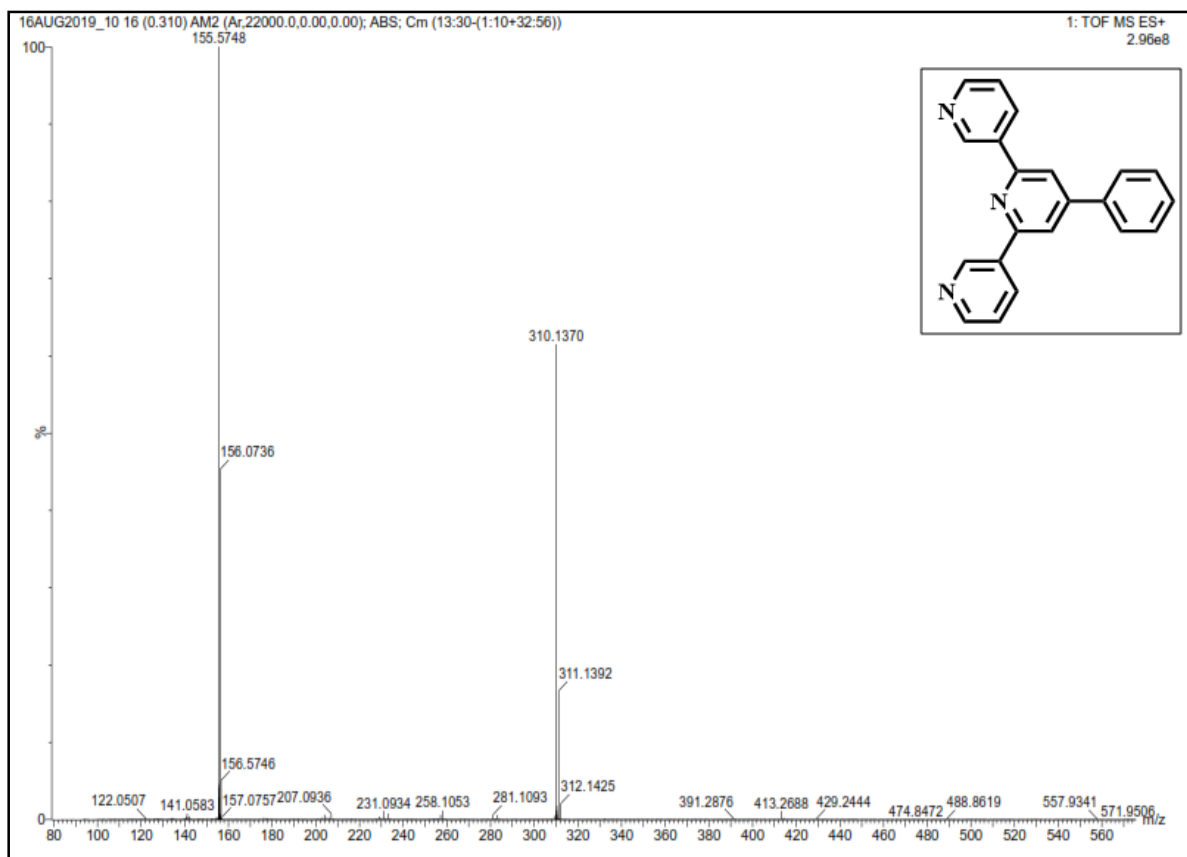


Figure S20.HRMS spectrum of Ph-Tp

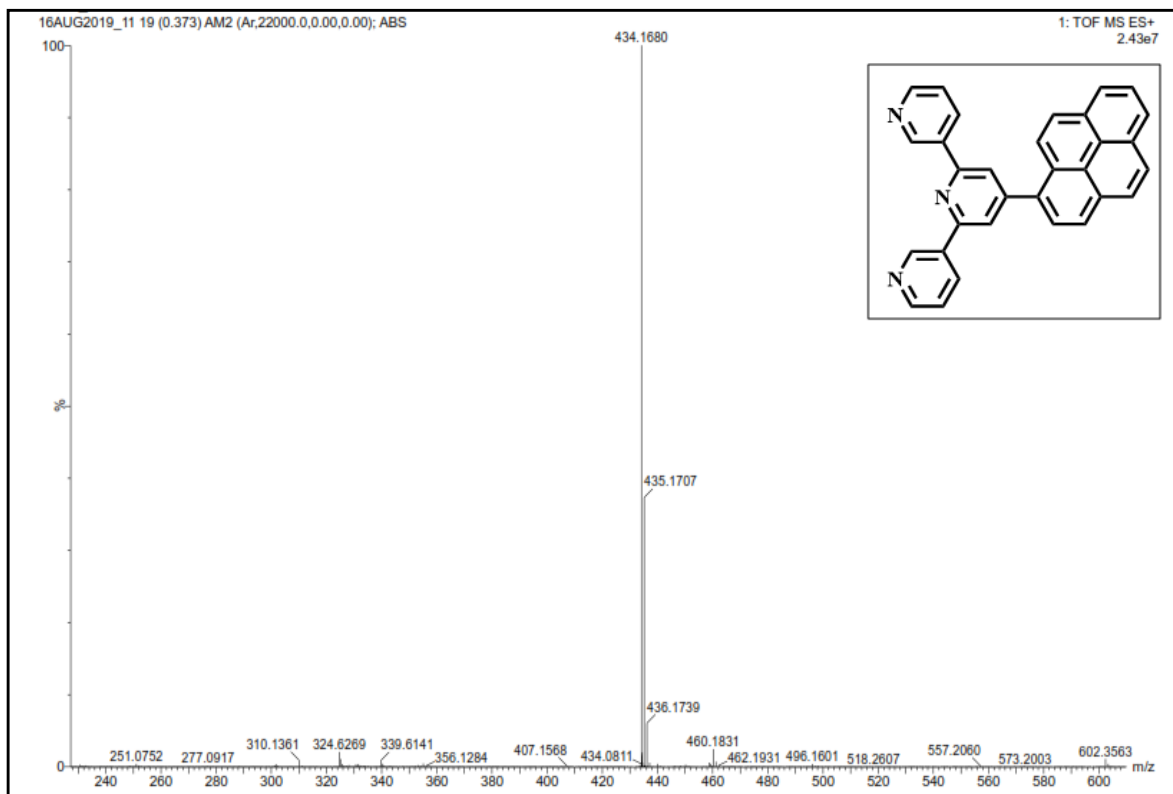


Figure S21.HRMS spectrum of Pyr-Tp

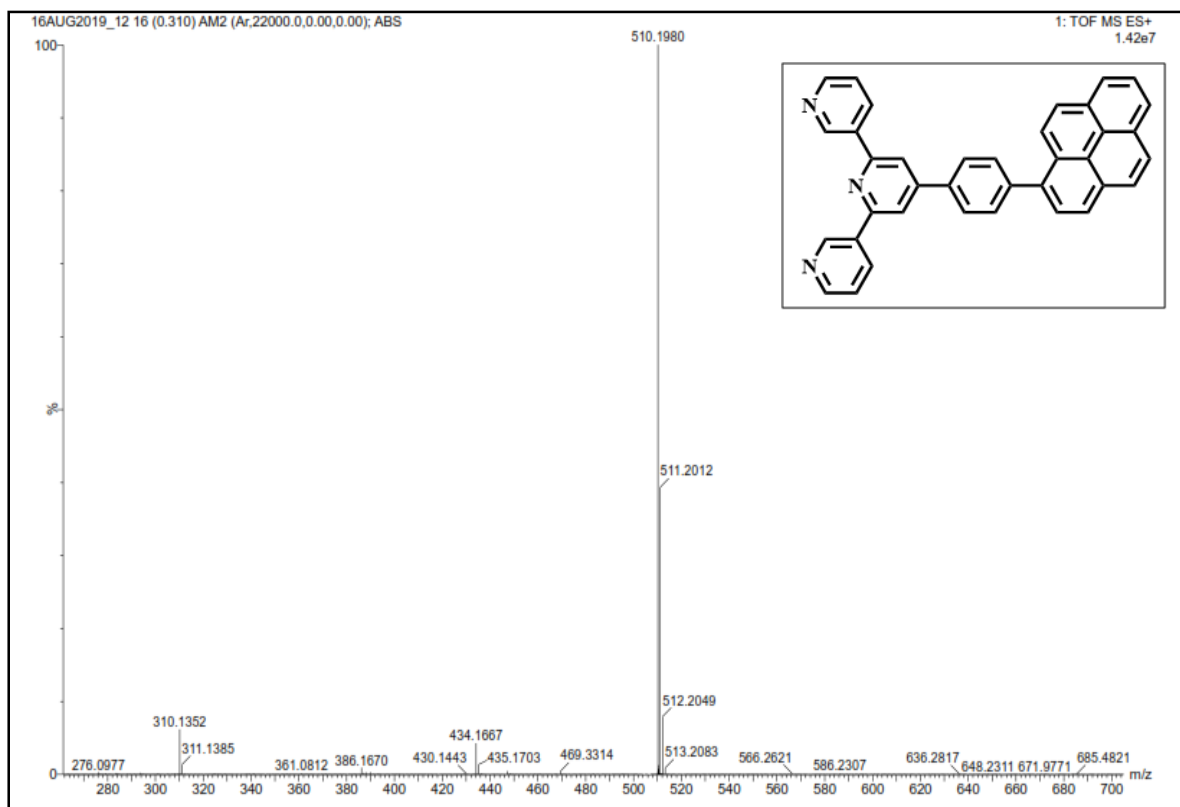


Figure S22. HRMS spectrum of Pyr-Ph-Tp

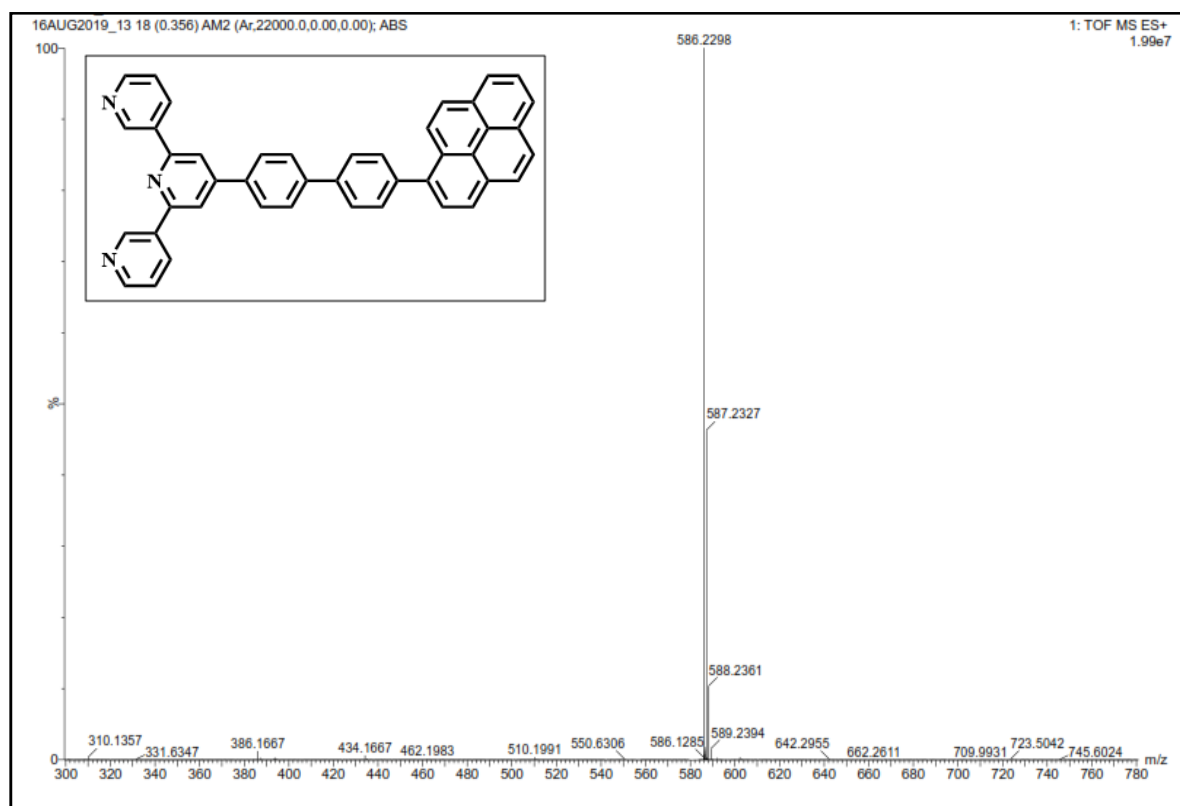


Figure S23. HRMS spectrum of Pyr-Bp-Tp