Supporting information

Imidazole-containing cyanostilbene-based molecules with aggregation-induced emission characteristics: photophysical and electroluminescent properties

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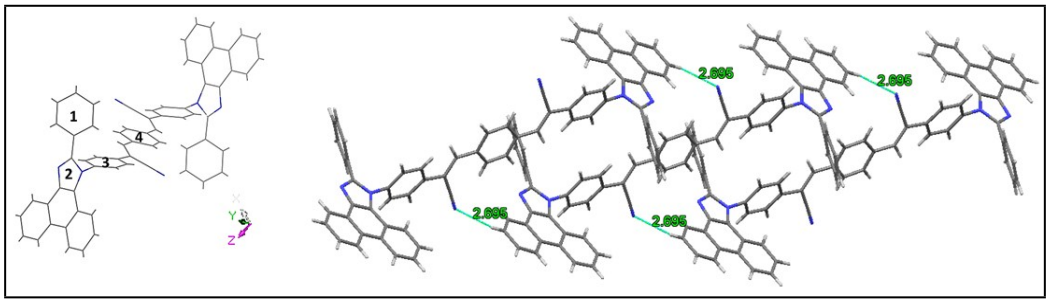

Fig. S1 Molecular structure and packing mode of **PPIA** in the crystal.

Table S1 Selected dihedral angle (deg) of the crystal structure of **PPIA**

Crystal	θ_{12} (°)	θ_{13} (°)	θ_{14} (°)	θ_{23} (°)	θ_{24} (°)	θ_{34} (°)
PPIA	52.0	78.9	77.5	84.7	73.8	12.6

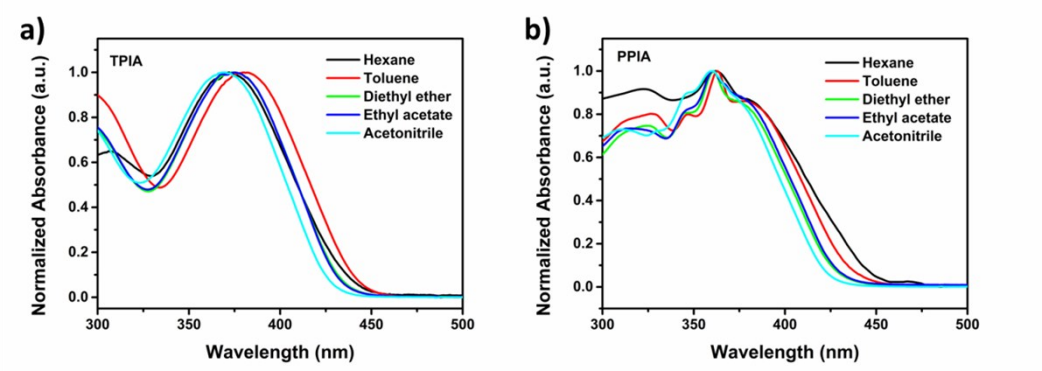

Fig. S2 Normalized absorption spectra of **TPIA** and **PPIA** in different solvents.

Table S2 Absorption and emission maxima of **TPIA** and **PPIA** in different solvents

Solvent		Hexane	Toluene	Diethyl ether	Ethyl acetate	Acetonitrile
TPIA	λ_{abs} (nm)	372	380	374	375	370
	λ_{em} (nm)	494	544	586	603	628
PPIA	λ_{abs} (nm)	362	363	361	360	360
	λ_{em} (nm)	528	556	580	601	624

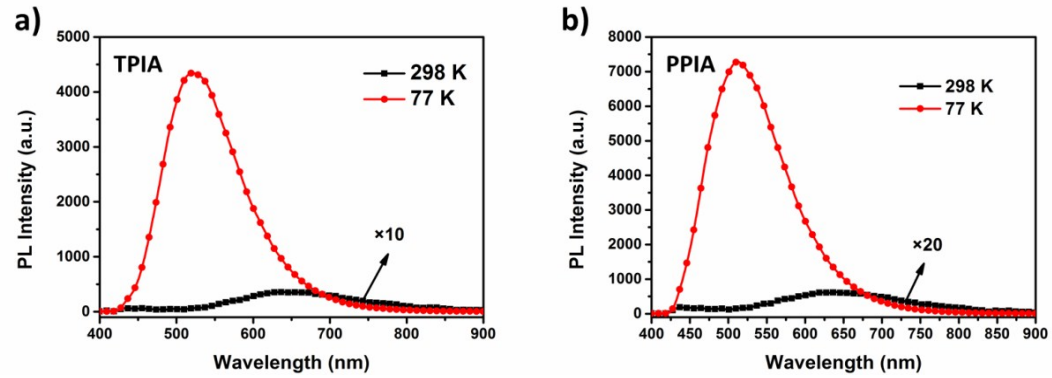

Fig. S3 PL spectra of **TPIA** and **PPIA** in THF at room temperature and 77 K.

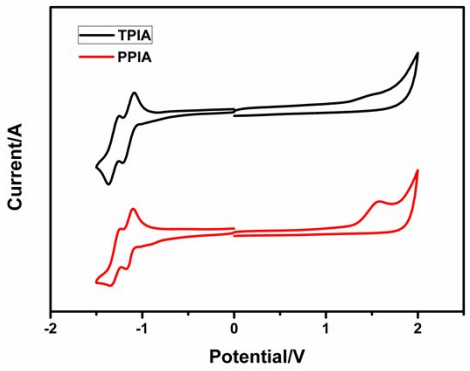

Fig. S4 Cyclic voltammograms of **TPIA** and **PPIA** in CH_2Cl_2, measured with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte at a scan rate of 100 mV s^{-1}.

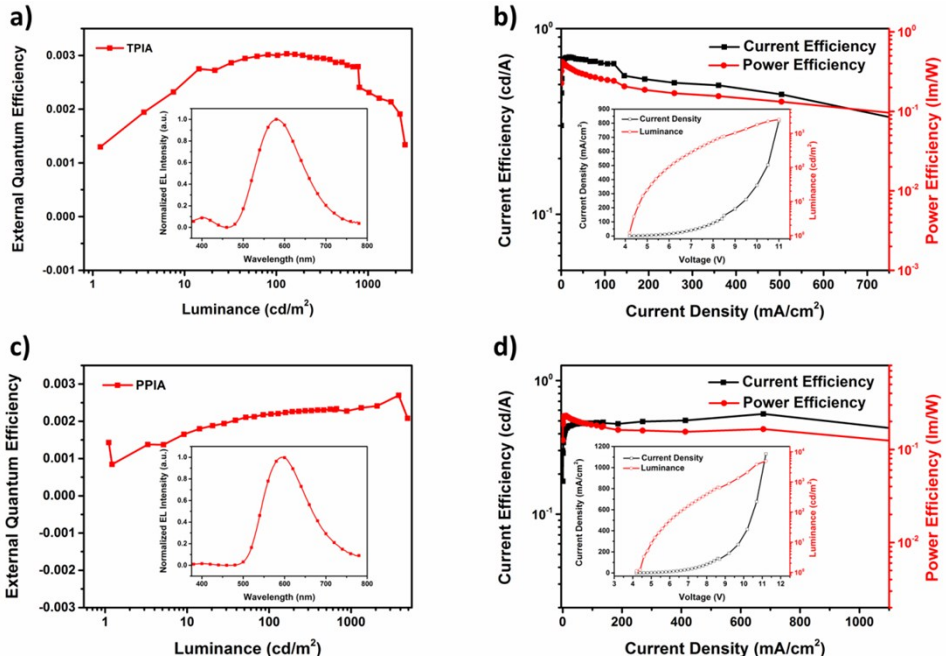

Fig. S5 (a: **TPIA**, c: **PPIA**) External quantum efficiency with the luminance and EL spectrum (Inset) of the fabricated OLED device I. (b: **TPIA**, d: **PPIA**) Current efficiency-current density-power efficiency curves and current-voltage-luminance characteristic curves (Inset) of the fabricated OLED device I. Device I configuration: ITO/HATCN (5 nm)/NPB (40 nm)/emitting layer (20 nm)/TPBi (40 nm)/LiF/Al.

Table S3: Crystal data and structure refinement results of **PPIA**

	PPIA
CCDC	1862218
empirical formula	$C_{72}H_{54}N_8O_2$
formula wt	1063.23
T, K	173(2)
crystal system	Triclinic
space group	*P*-1
a, Å	10.123(2)
b, Å	11.857(2)
c, Å	12.208(2)
α, degree	107.99(2)
β, degree	99.32(2)
γ, degree	97.49(2)
V,Å3	1349.7(5)
Z	1
density, Mg/m^3	1.308
M (Mo K α), mm^{-1}	0.080
θ range, degree	2.50-28.32
no. of reflcns collected	9082
no. of unique reflcns	6357
R(int)	0.0153
GOF	0.931
R1 [$I > 2\sigma(I)$]	0.0469
wR2 [$I > 2\sigma(I)$]	0.1281
R1 (all data)	0.0581
wR2 (all data)	0.1400

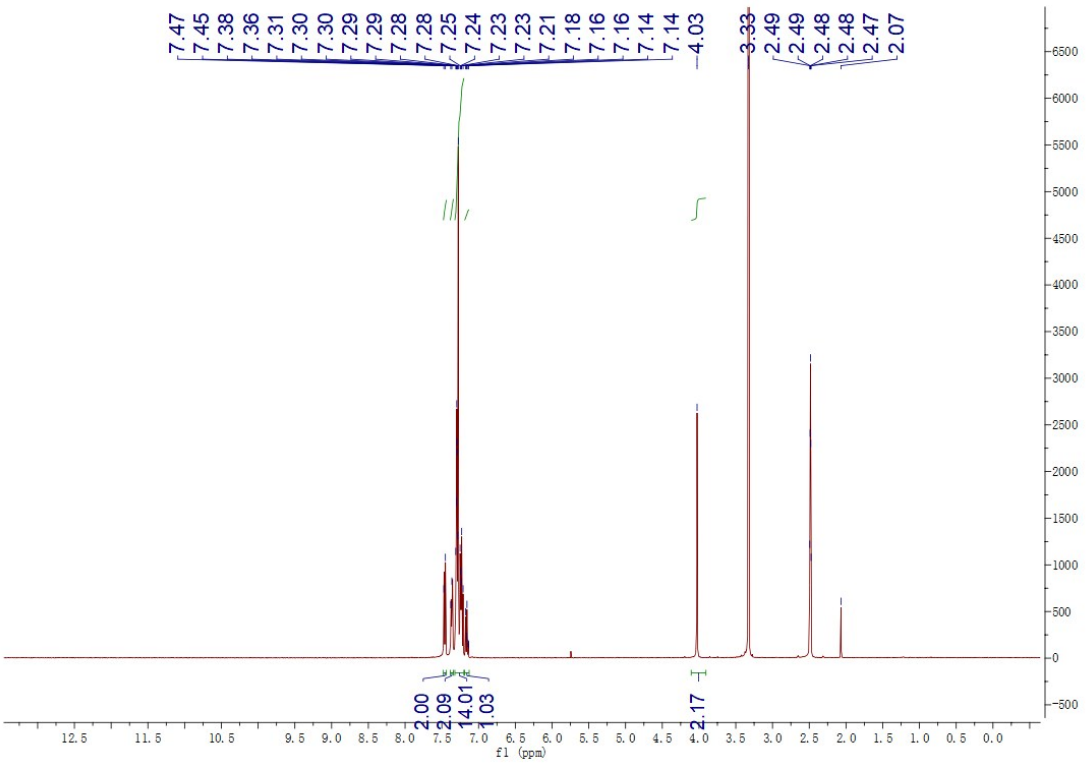

Fig. **S6**. ^{1}H NMR spectrum of compound **CN-1**.

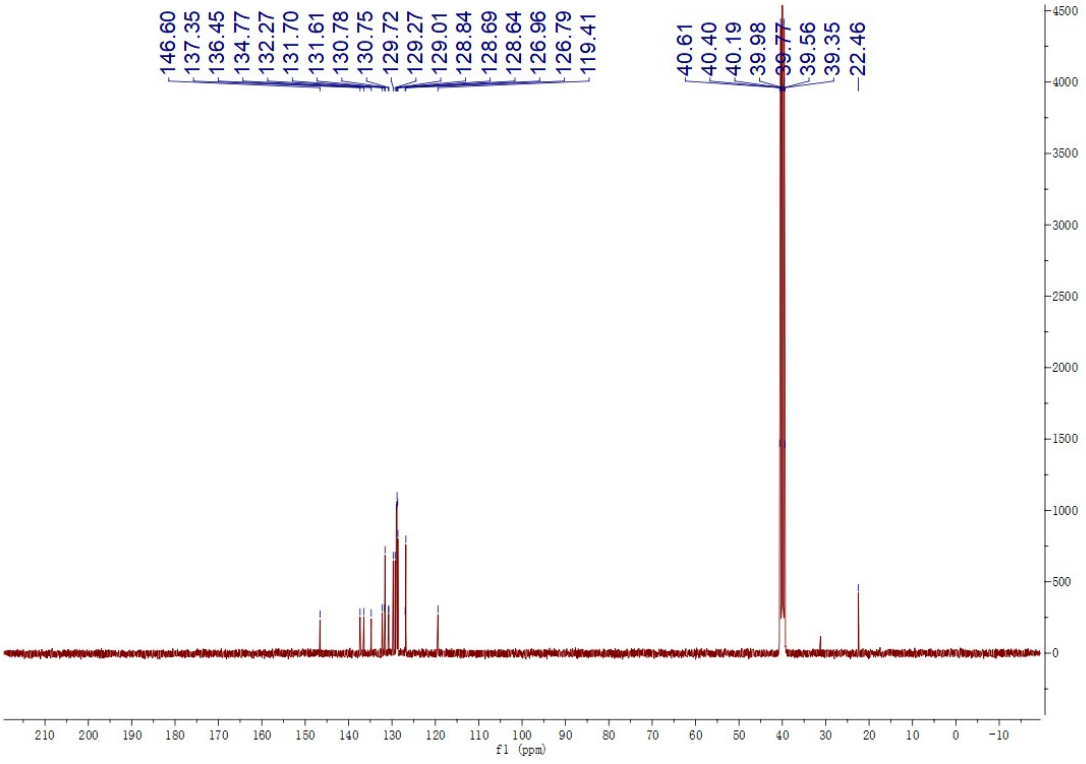

Fig. **S7**. ^{13}C NMR spectrum of compound **CN-1**.

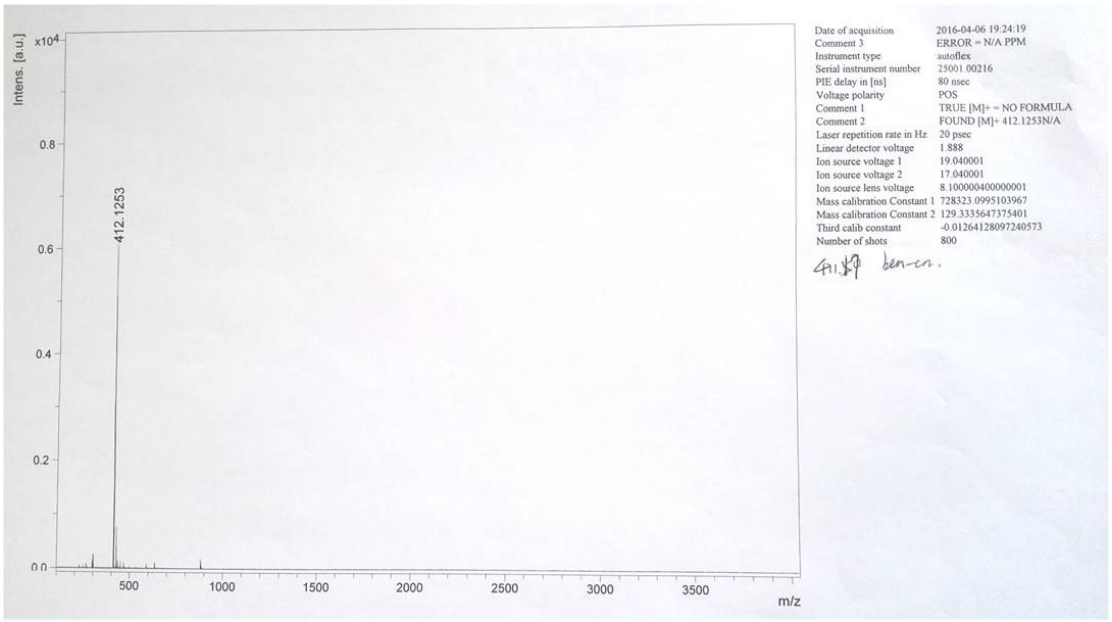

Fig. S8. Mass spectrum of compound **CN-1**.

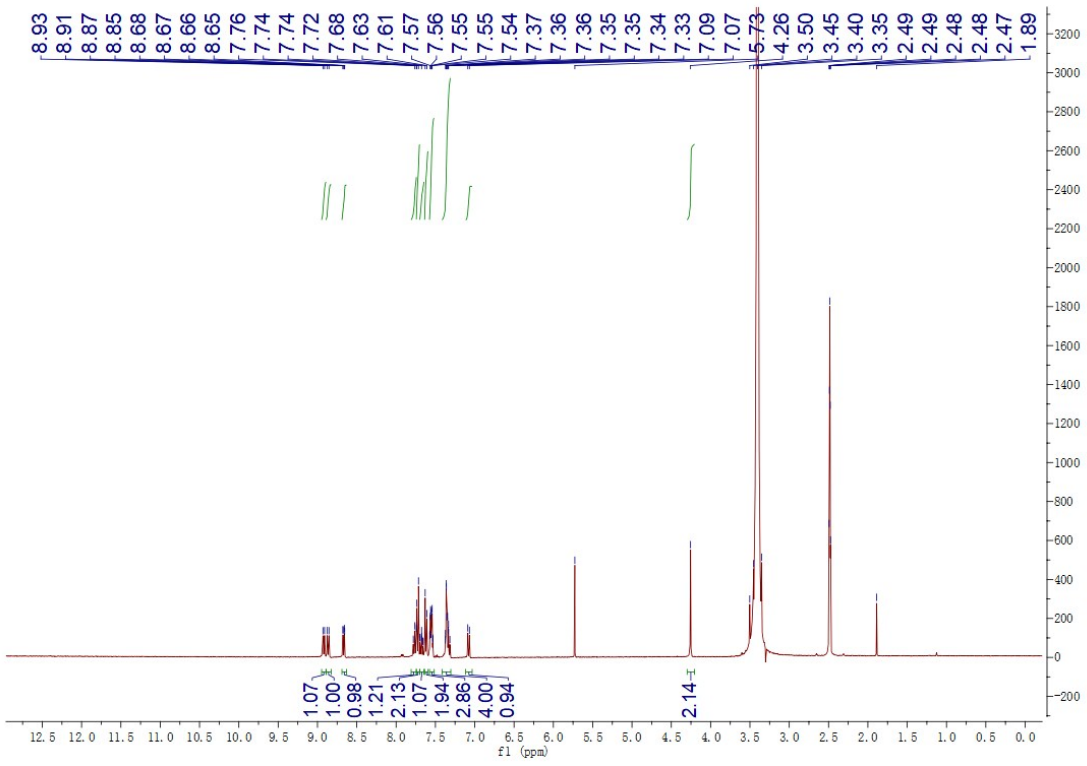

Fig. **S9**. ^{1}H NMR spectrum of compound **CN-2**.

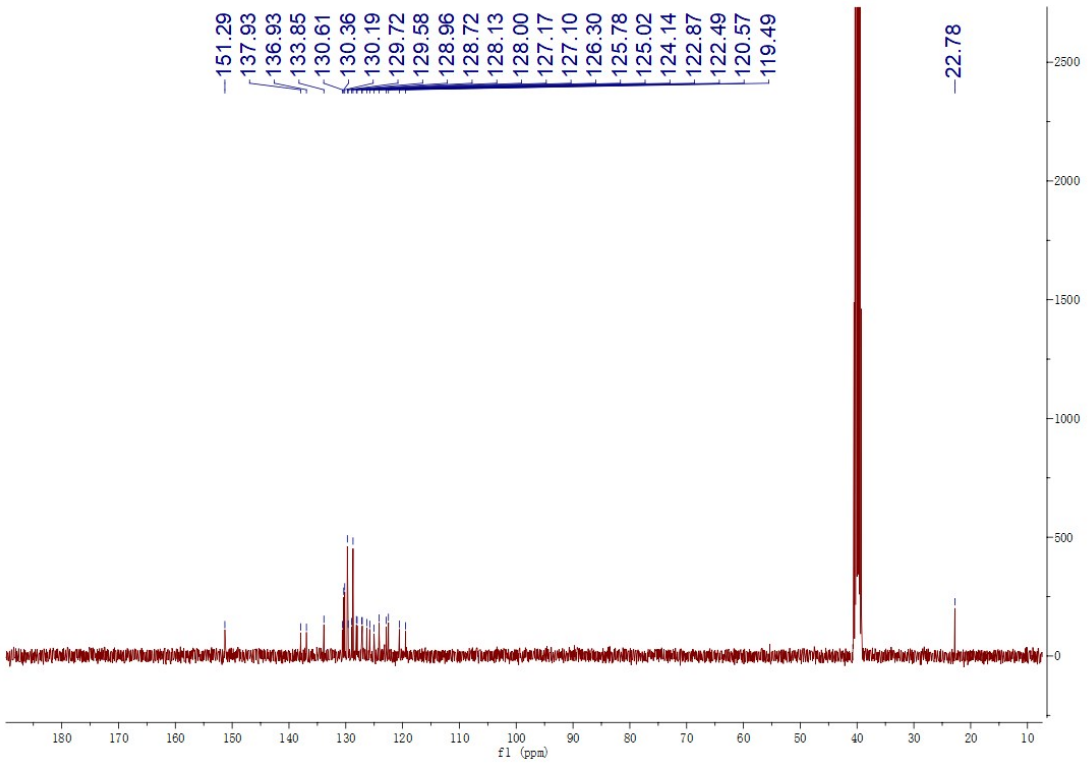

Fig. **S10**. ^{13}C NMR spectrum of compound **CN-2**.

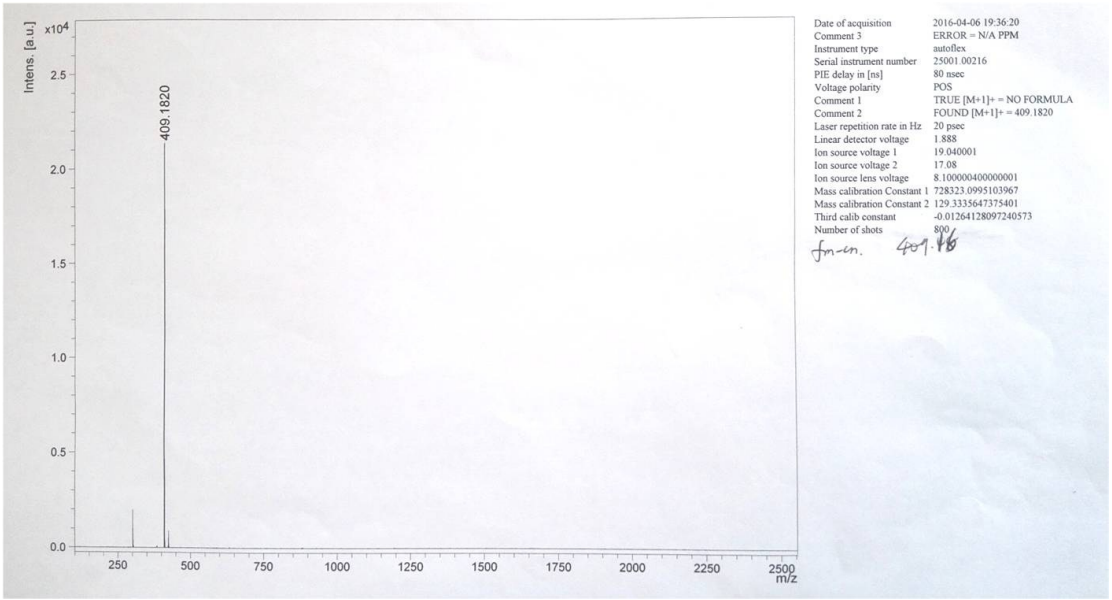

Fig. S11. Mass spectrum of compound **CN-2**.

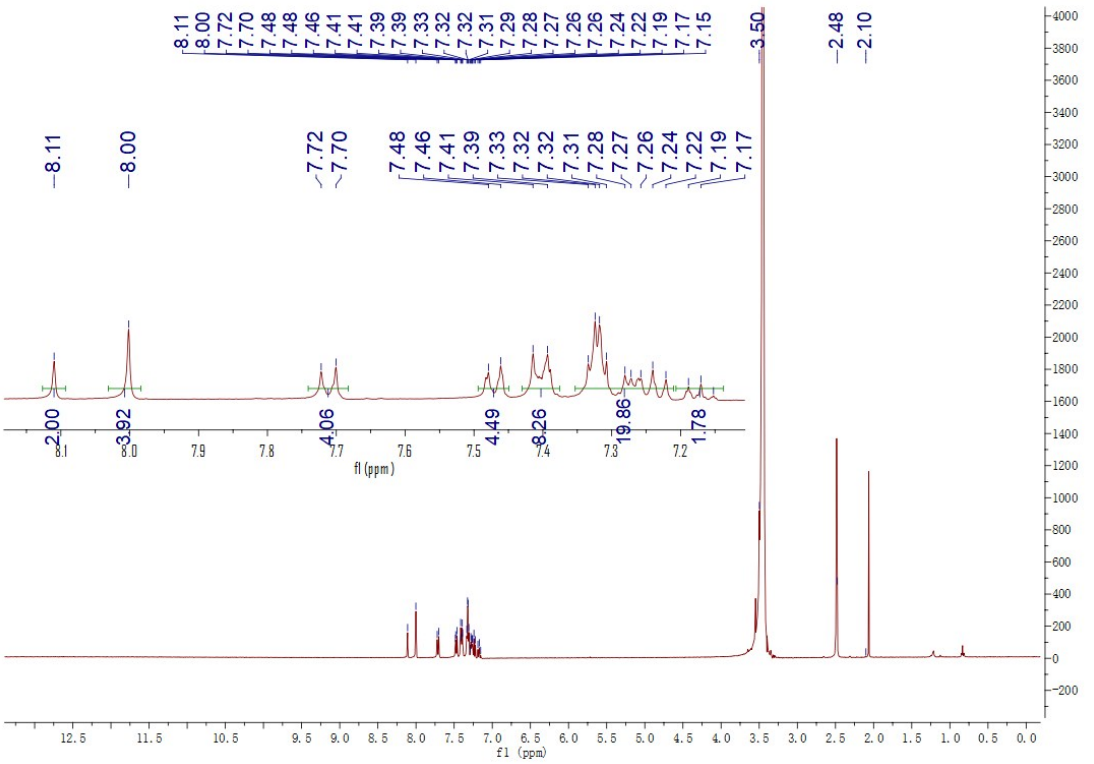

Fig. **S12**. ^{1}H NMR spectrum of compound **TPIA**.

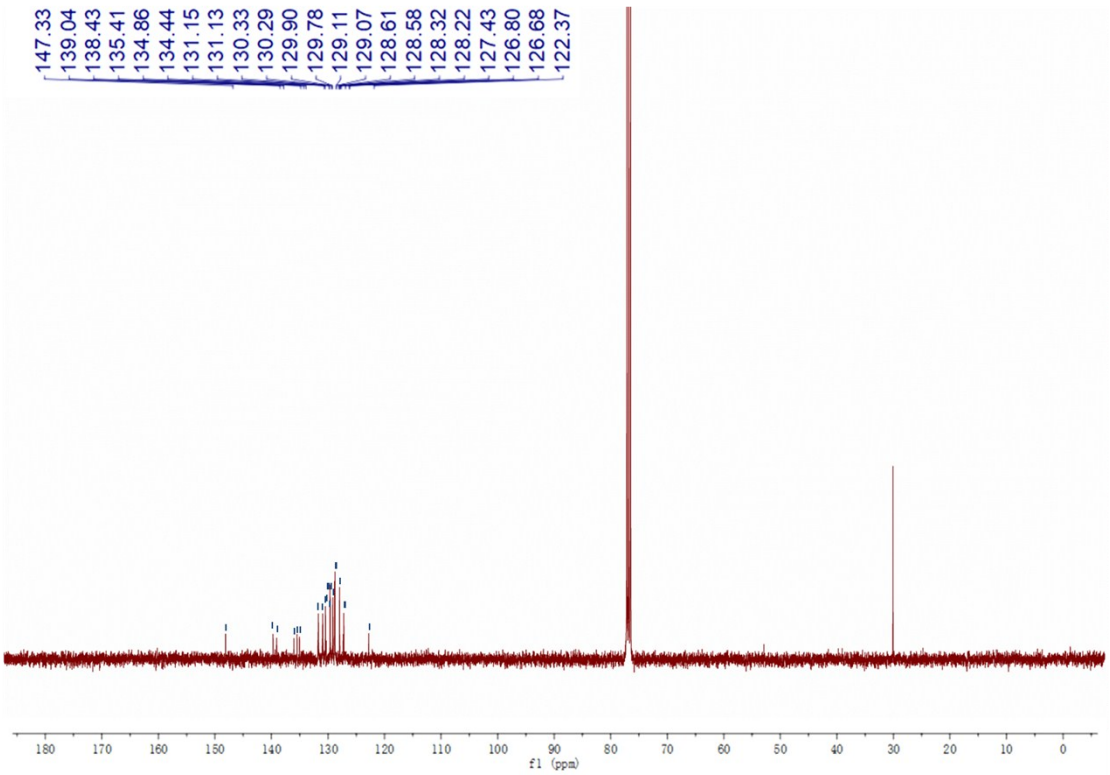

Fig. **S13**. ^{13}C NMR spectrum of compound **TPIA**.

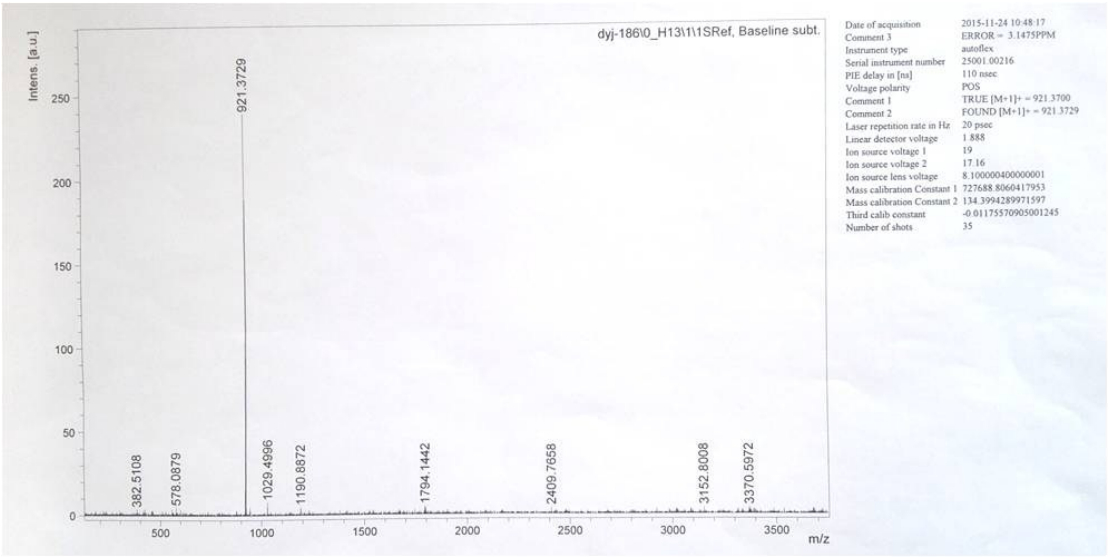

Fig. S14. Mass spectrum of compound **TPIA**.

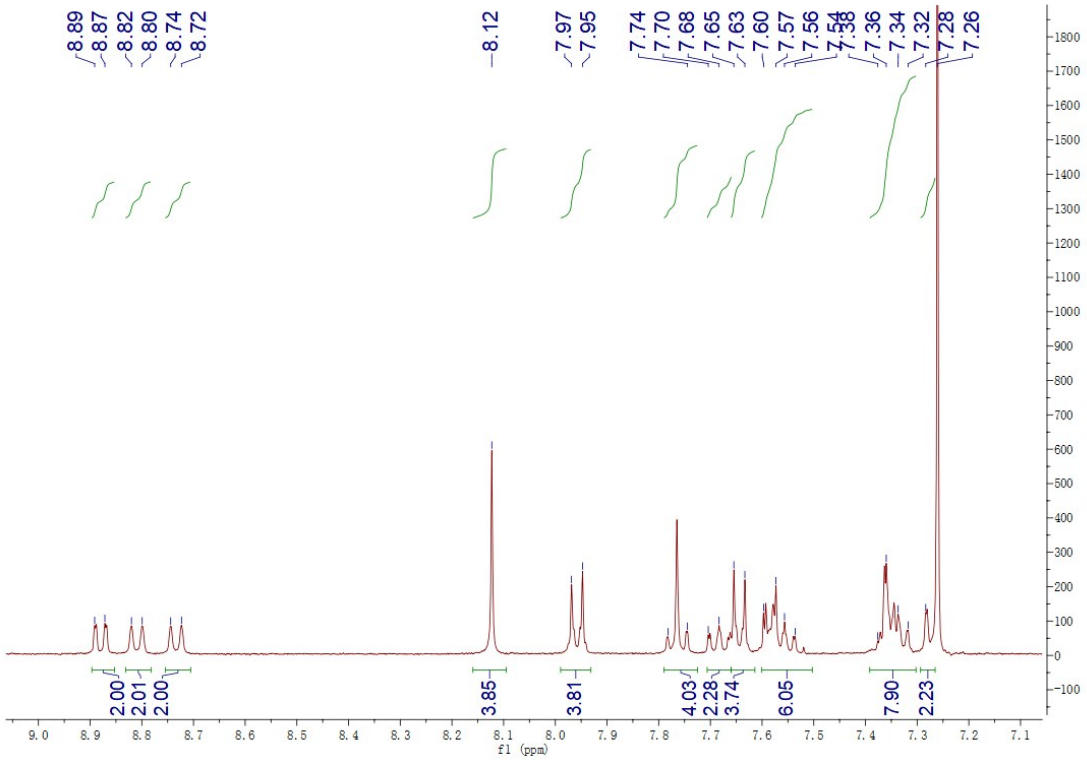

Fig. **S15**. ^{1}H NMR spectrum of compound **PPIA**.

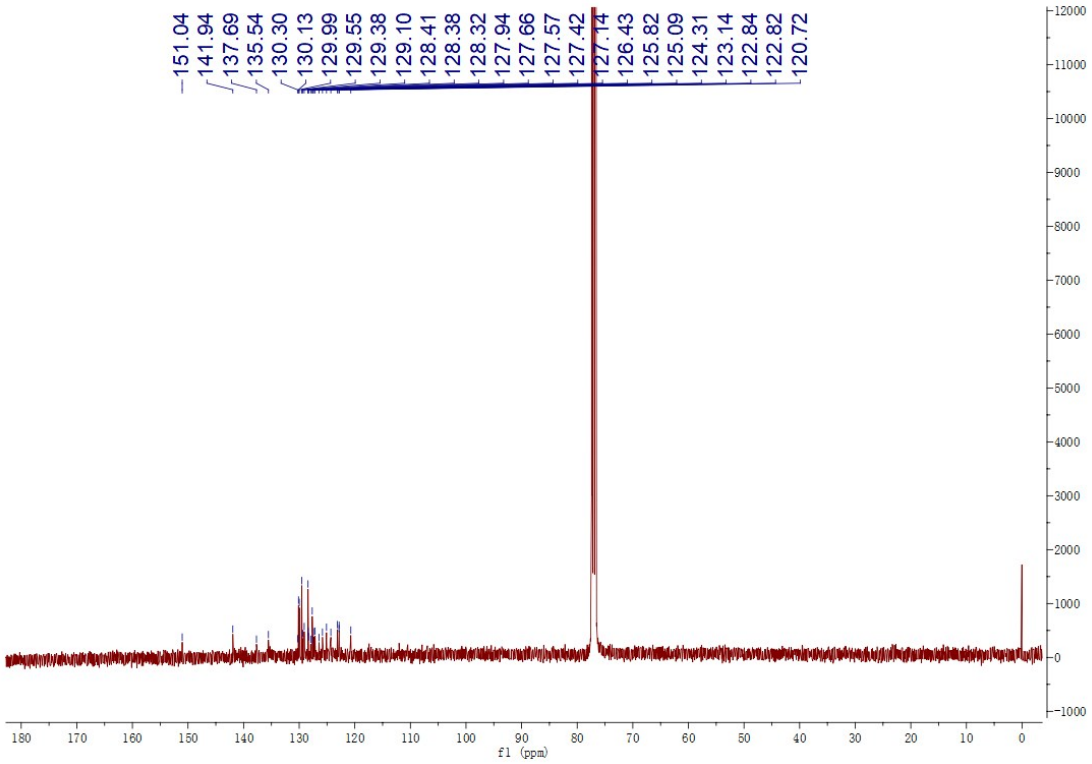

Fig. **S16**. ^{13}C NMR spectrum of compound **PPIA**.

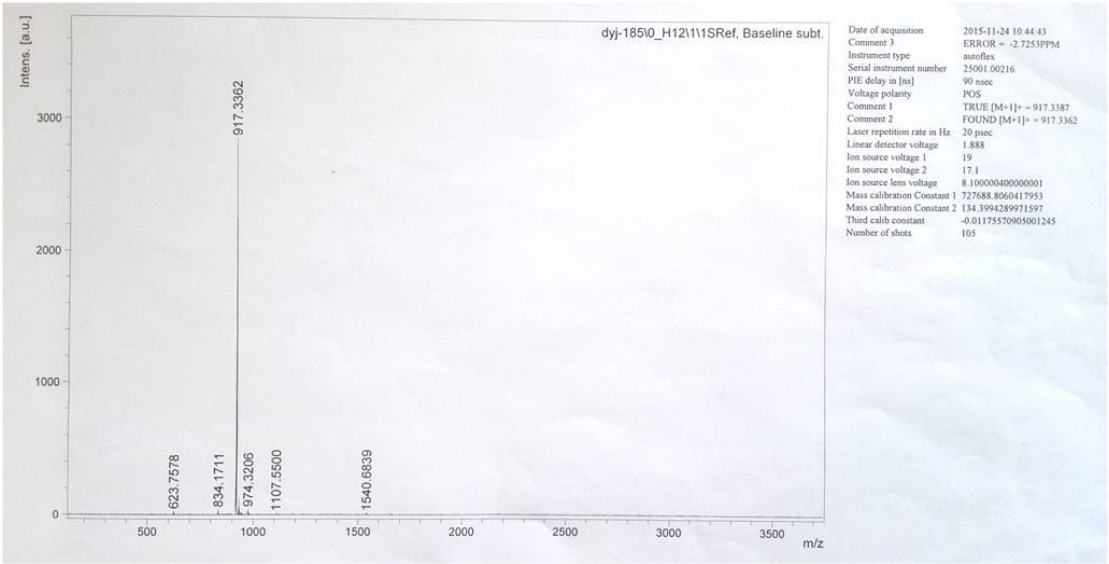

Fig. S17. Mass spectrum of compound **PPIA**.