Electronic Supplementary Information

Host to Regulate the T_1-S_1 and T_1-S_0 Processes of Guest Excitons in Doped System to Control the TADF and RTP emissions

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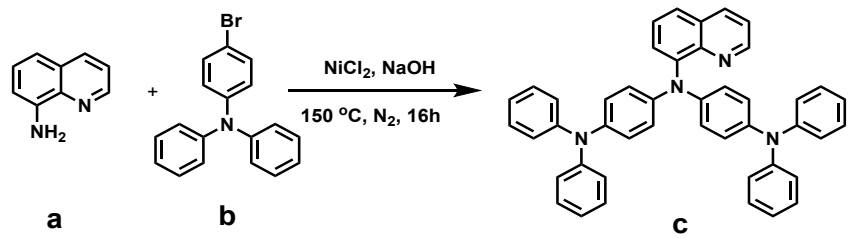
1. Materials and characterization

^1H and ^{13}C NMR spectra were carried out by a Bruker ARX500 spectrometer with $CDCl_3$ as the solvent. UV-vis absorption spectra were measured by a Persee TU-1901 spectroscopy. Fluorescence spectra were measured by a Hitachi F-7000 spectrophotometer. Phosphorescence spectra were measured by a FLS920 lifetime and steady state spectrometer. X-Ray crystal structure analyses were conducted on a Bruker-AXS SMART APEX2 CCD diffractometer. Solid-state emission quantum yields were collected on a FluoroMax-4 (Horiba Jobin Yvon) fluorimeter equipped with integrated sphere. The theoretical ground-state geometry and electronic structure were performed using the density functional theory (DFT) with B3LYP hybrid functional at the basis set level of 6-31+G (d, p). All the theoretical calculations were optimized using Gaussian 09 package. All the host and guest compounds were purified twice by column chromatography and then recrystallized using dichloromethane and methanol.

2. Synthesis of the guest



Scheme S1. Synthesis of **IQ-TPA**.

General procedure for IQ-TPA

A mixture of compound 8-aminoquinoline (1 mmol), 4-bromotriphenylamine (3 mmol), $NiCl_2$ (0.1 mmol), Sodium hydroxide (3 mmol), and DMF (10.0 mL) was stirred at 150 °C for 16 h under N_2 atmosphere. After being cooled to the room temperature, the reaction mixture was poured into CH_2Cl_2 (100 mL), and the organic layer was washed with water (50 mL) for three times, and then dried over Na_2SO_4. After the removal of solvent under reduced pressure, the residue was purified by flash chromatography on silica gel to afford the target product.

***N*^{1}-(4-(Diphenylamino)phenyl)-*N*^{4},*N*^{4}-diphenyl-*N*^{1}-(quinolin-8-yl)benzene-1,4-diamine (IQ-TPA).** Yellow solid (0.26 g, 41% yield). ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.83 (s, 1H), 8.17 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.60 (d, J = 5.0 Hz, 1H), 7.53 (d, J = 7.5 Hz, 1H), 7.40–7.36 (m, 1H), 7.21 (m, 8H), 7.07 (m, 8H), 6.94 (m, 12H) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 149.7, 148.0, 141.5, 136.4, 130.1, 129.1, 127.0, 125.8, 125.4, 123.4, 123.1, 122.1, 121.4. ppm.

Preparation of doped materials. Put the corresponding amount of host and guest salts together, and heat the mixture to 60-90℃ in air atmosphere. After the guests are completely dissolved in the molten hosts, the mixed systems are cooled to room temperature, and the mixed systems are crystallized to obtain the doped materials.

Calculated mothod of $\triangle E_{ST}$ ($\triangle E_{ST}$: The energy gap between the lowest singlet and triplet states):

$E = 1240/\lambda_{em}$ (eV) (Where λ_{em} of fluorescence is 440 nm, and λ_{em} of phosphorescence is 574 nm).

$\Delta E_{ST} = E_{singlet} - E_{triplet.}$

3. Experimental data

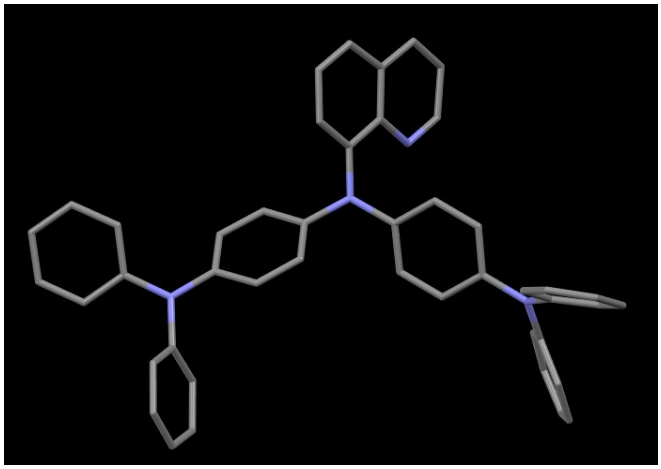


Figure S1. Single crystal structure of guest molecule (CCDC: 2159958).

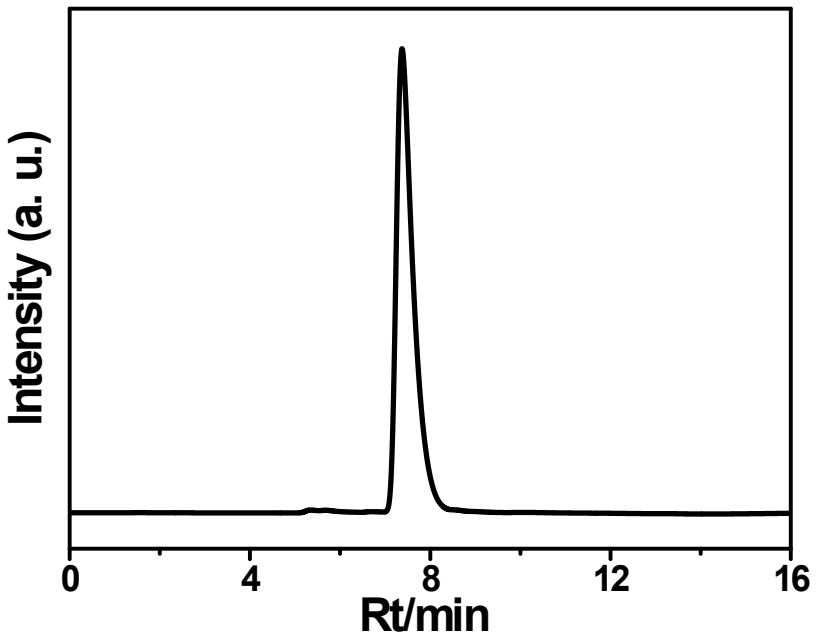


Figure S2. High performance liquid chromatography of **IQ-TPA**. (CH_3OH/H_2O= 80%: 20%)

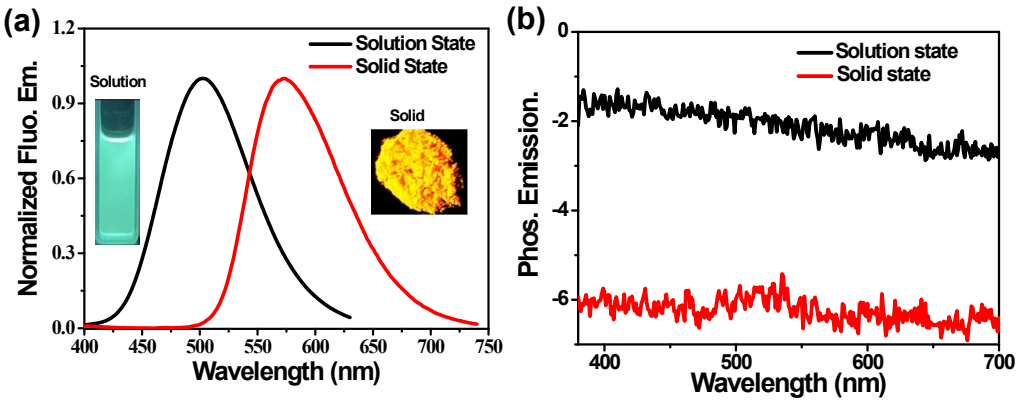


Figure S3. (a) Fluorescence emission spectra of guest in solution and solid state (Inset: Fluorescence images of guest in solution and solid state). (b) Phosphorescence spectra of guest in solution and solid states (Delayed time: 0.5 ms, Ex.: 380 nm). (Solvent: Acetone; Concentration: $1.0*10^{-5}$ mol/L)

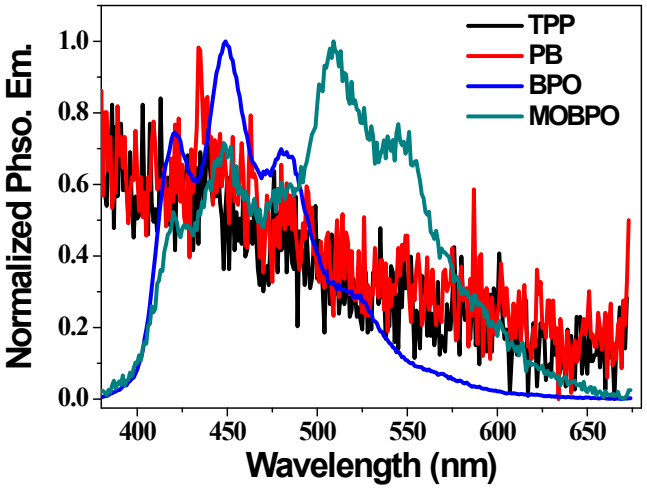


Figure S4. Phosphorescence spectra of four hosts in solid state. (Delayed time: 0.5 ms, Ex.: 380 nm).

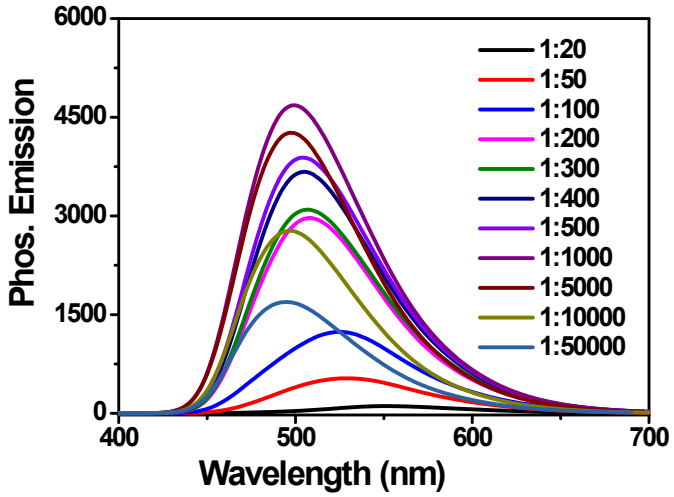


Figure S5. Delayed emission spectra of **IQ-TPA/TPP** doped materials with different amounts of **IQ-TPA**. (Delayed time: 0.5 ms, Ex.: 380 nm).

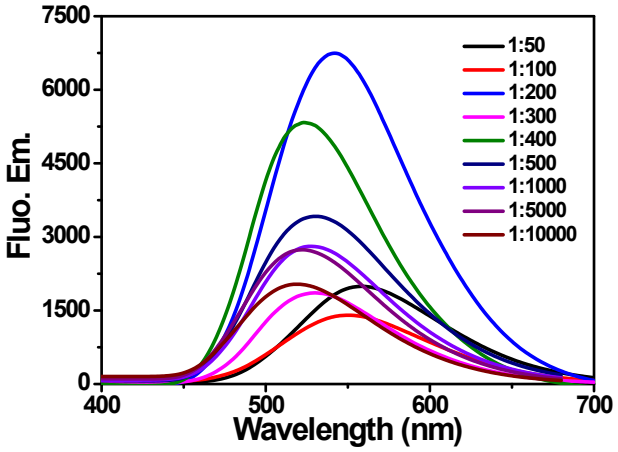


Figure S6. Prompt emission spectra of **IQ-TPA/TPP** doped materials with different amounts of **IQ-TPA**. (Ex.: 360 nm).

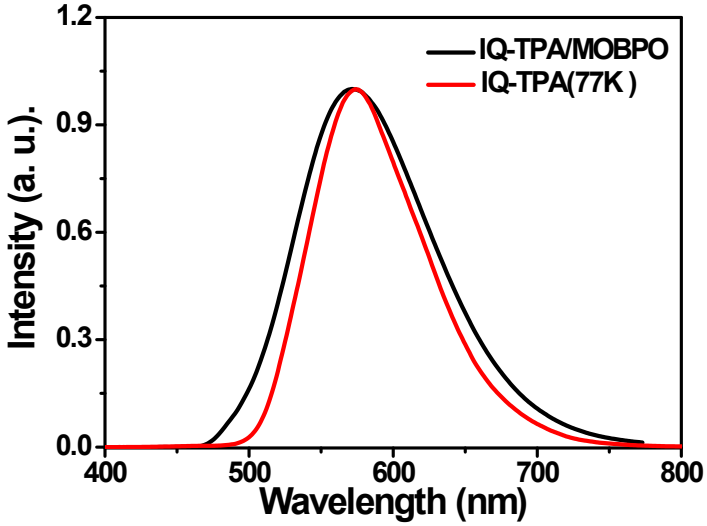


Figure S7. Phosphorescence spectra of **IQ-TPA/MOBPO** and **IQ-TPA** (Delayed time: 0.5 ms, Ex.: 380 nm).

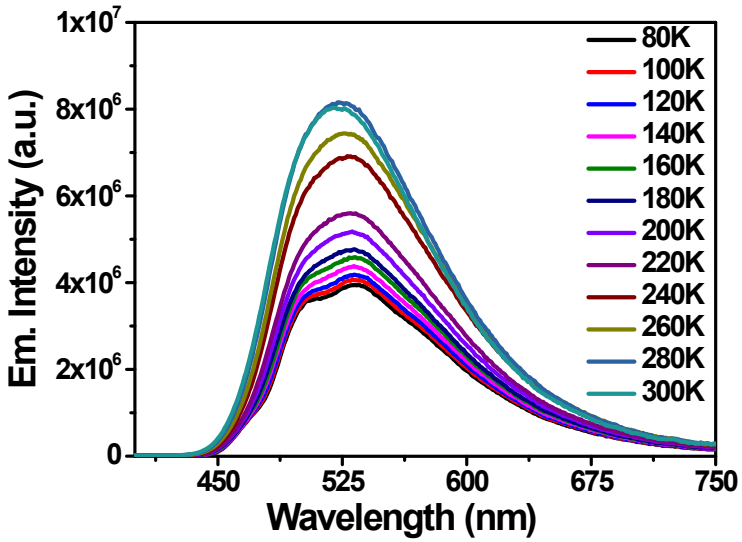


Figure S8. Prompt emission intensity of **IQ-TPA/TPP** at different temperatures. (Delayed time: 0.5 ms, Ex.: 380 nm).

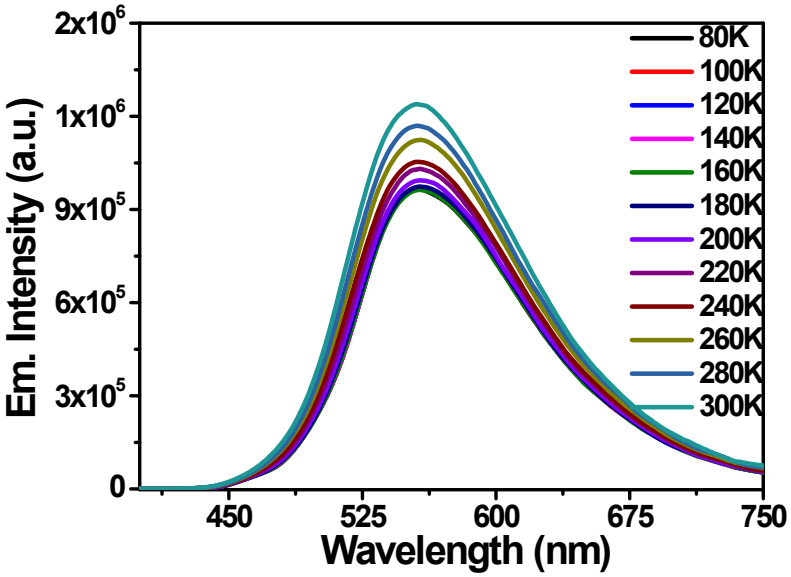


Figure S9. Prompt emission intensity of **IQ-TPA/PB** at different temperatures. (Delayed time: 0.5 ms, Ex.: 380 nm).

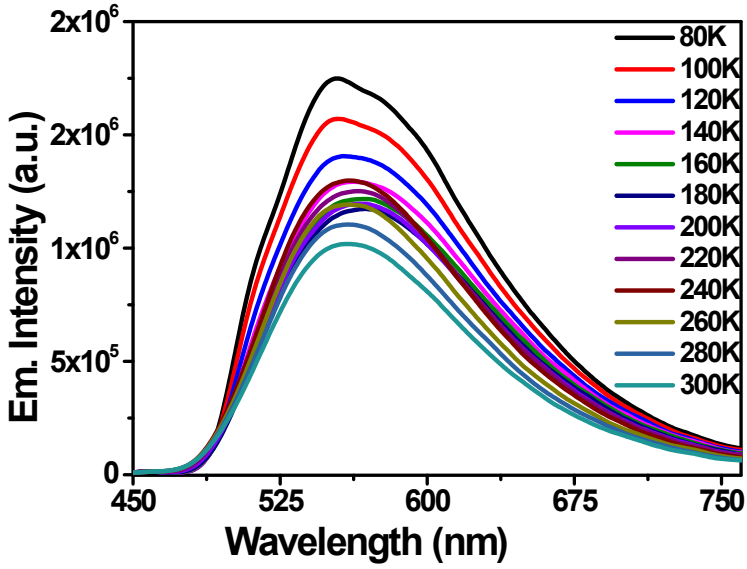


Figure S10. Prompt emission intensity of **IQ-TPA/BPO** at different temperatures. (Delayed time: 0.5 ms, Ex.: 380 nm).

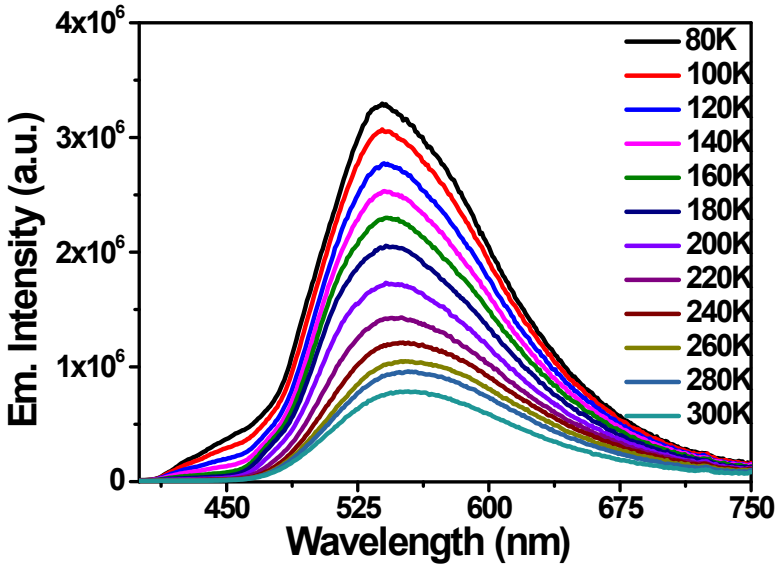


Figure S11. Prompt emission intensity of **IQ-TPA/MOBPO** at different temperatures. (Delayed time: 0.5 ms, Ex.: 380 nm).

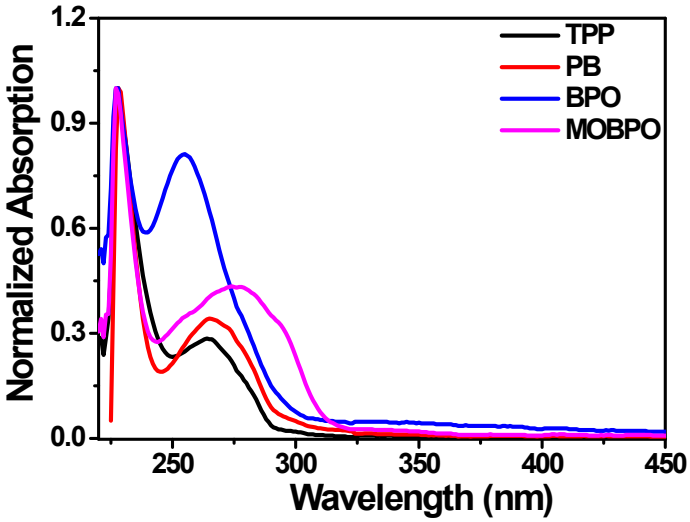


Figure S12. UV absorption spectra of four hosts in solution state (Solvent: Acetone; Concentration: $1.0*10^{-5}$ mol/L).

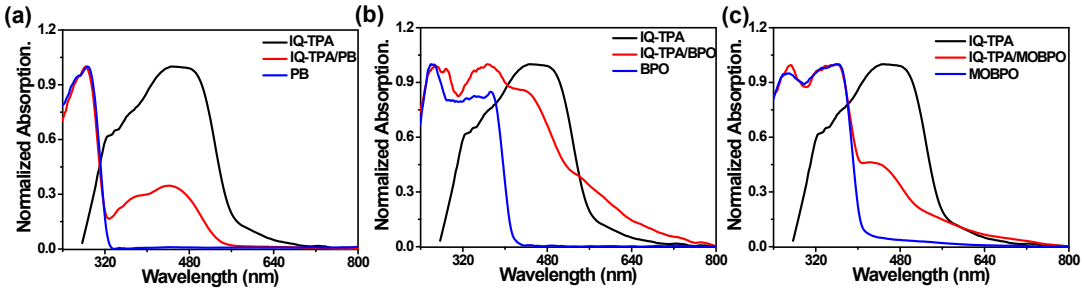


Figure S13. (b) Absorption spectra of individual guest/**IQ-TPA**, host/**PB** and doped material/I**Q-TPA/PB** in the solid state. (b) Absorption spectra of individual guest/**IQ-TPA**, host/**BPO** and doped material/I**Q-TPA/BPO** in the solid state. (c) Absorption spectra of individual guest/**IQ-TPA**, host/**MOBPO** and doped material/I**Q-TPA/MOBPO** in the solid state.

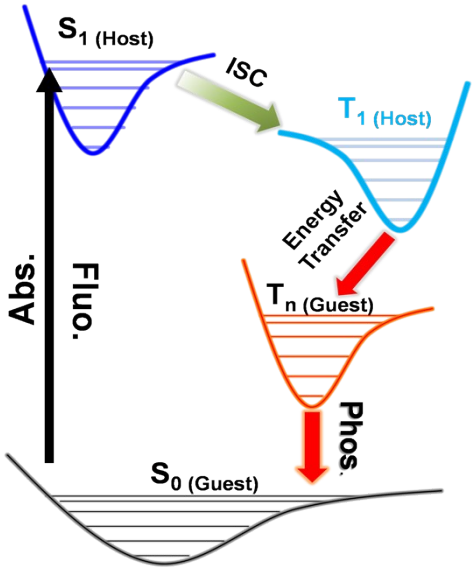


Figure S14. Proposed transfer path between guest and host.

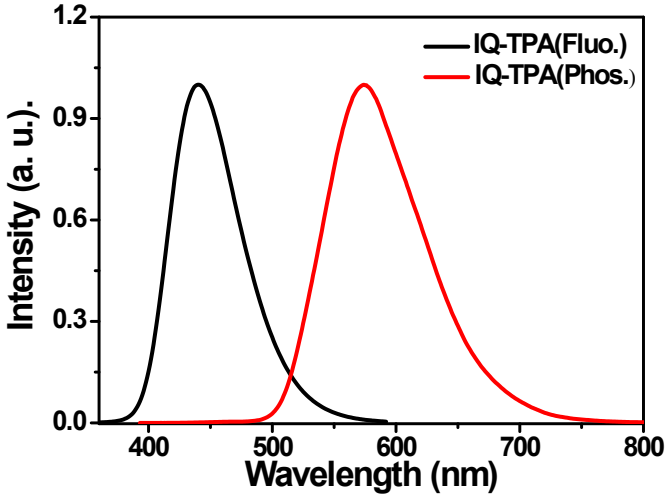


Figure S15. Fluorescence and phosphorescence spectra of IQ-TPA at low temperature (77 K). (Solvent: Toluene; Concentration: $1.0*10^{-5}$ mol/L)

4. NMR spectra

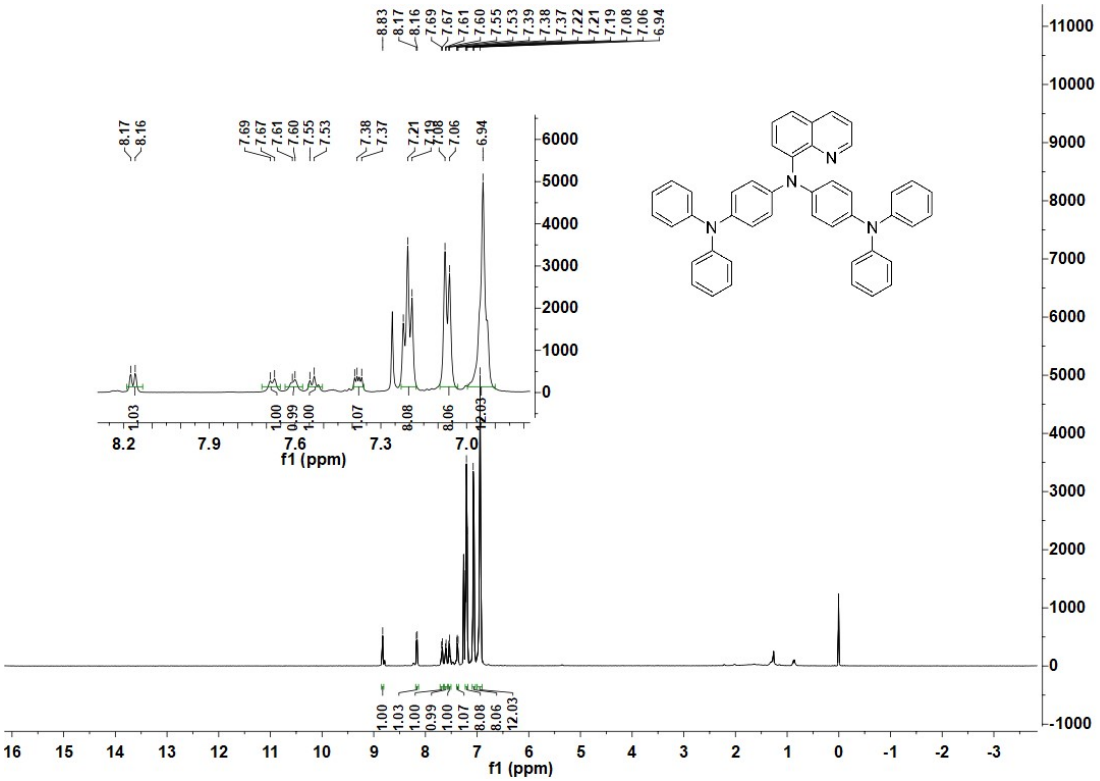


Figure S16. ^{1}H NMR of **IQ-TPA** ($CDCl_3$, 500 MHz).

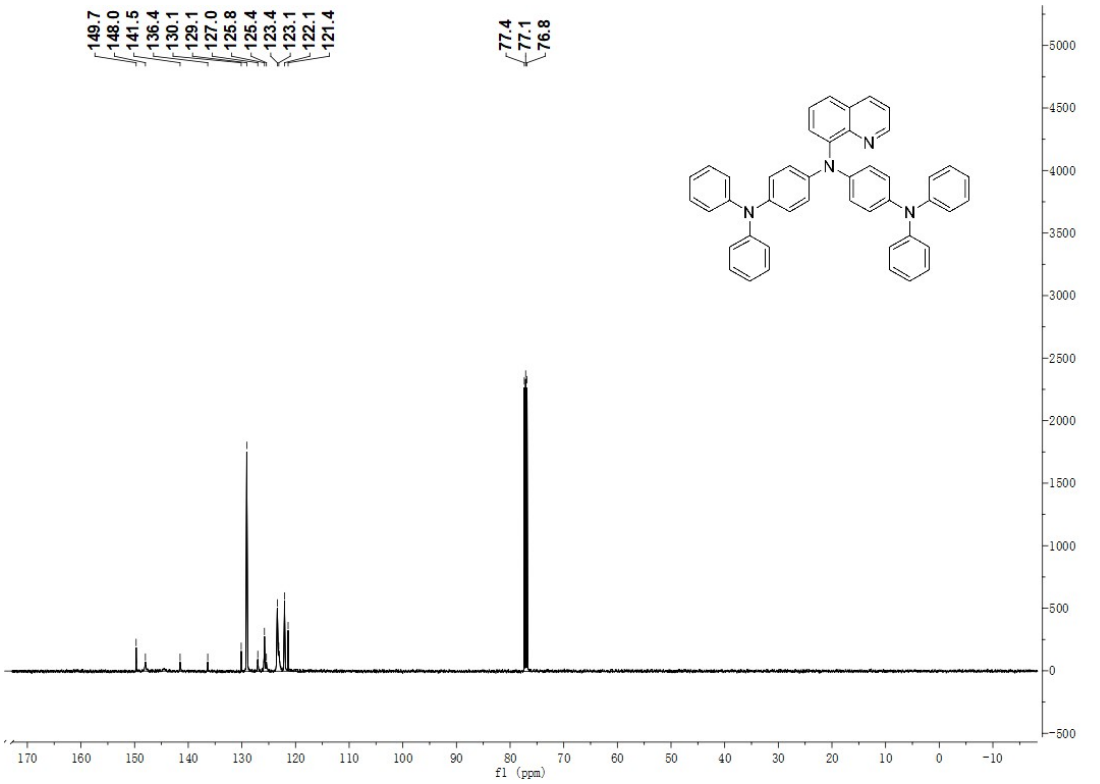


Figure S17. ^{13}C NMR of **IQ-TPA** ($CDCl_3$, 125 MHz).

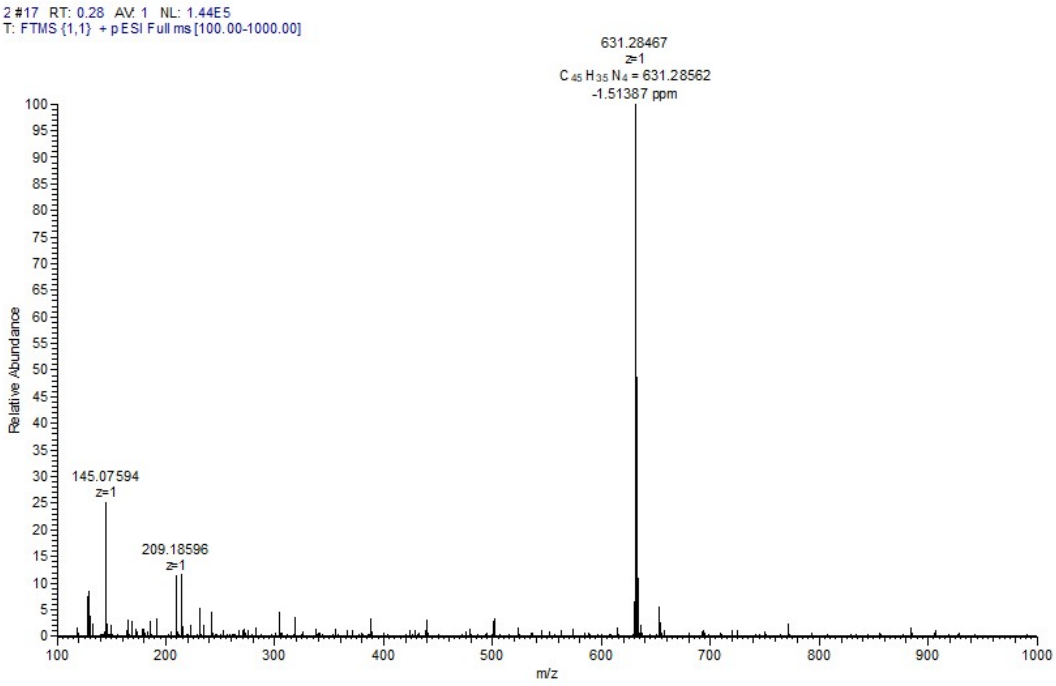


Figure S18. High-resolution mass spectrometry of **IQ-TPA**.