# Electronic Supplementary Information

## Guest-activated Quaternary Ammonium Salt Hosts Emit Room Temperature Phosphorescence

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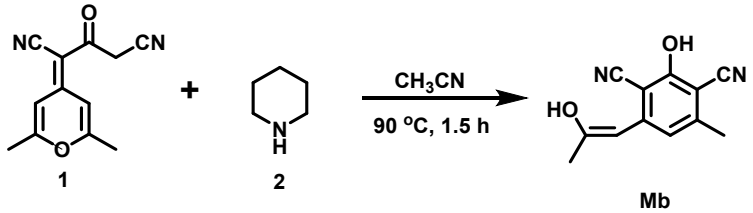
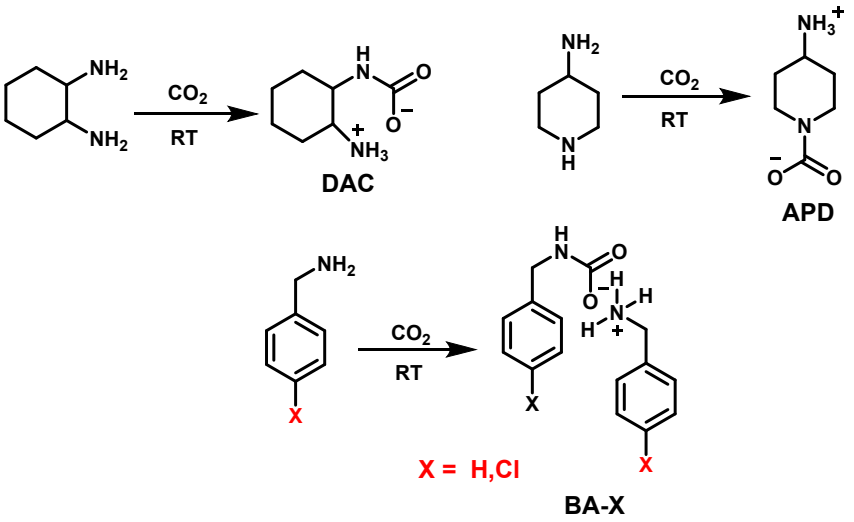
## 1. Materials and characterization

$^{1}H$ 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 and preparation of guest, hosts and doped materials.




**Scheme S1.** Synthesis of guest/**Mb**.




**Scheme S2.** Synthesis of hosts.

**General procedure for Mb.**

A mixture of compound **1** (0.64 g, 3 mmol), compound **2** (6 mmol) and $CH_3CN$ (15 mL) was stirred at 90 °C for 1.5 h.[1] After the reaction mixture was cooled to room temperature, it was filtered and concentrated under reduced pressure. Chromatography on a silica gel column using ethyl acetate/methanol (10/1, v/v) as eluent to afford the target product.

**2-hydroxy-4-(2-hydroxyprop-1-en-1-yl)-6-methylisophthalonitrile (Mb)**. Yellow solid (0.50 g, 78% yield). $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ 12.21 (s, 1H), 10.22 (s, 1H), 6.49 (s, 1H), 6.15 (s, 1H), 2.32 (s, 3H), 2.25 (s, 3H) ppm. $^{13}$C NMR (125 MHz, DMSO-$d_6$): $\delta$ 174.5, 165.9, 153.8, 153.1, 139.0, 118.0, 107.4, 106.5, 102.3, 100.4, 21.3, 18.4 ppm.

**General procedure for hosts.**

Put 10 ml of liquid raw materials (various amines) into the reaction flask, then pass carbon dioxide gas into the raw materials,[2] and white solids will be rapidly produced in the reaction flask. After ten minutes, the ventilation was stopped, the crude product was obtained by filtration, and washed three times with ethyl acetate to obtain the final pure product.

**DAC**. (2.75 g, 91%yield). $^1$H NMR (400 MHz, DMSO-*d*6): $\delta$ 2.67 (s, 1H), 2.34 (s, 4H), 2.06 (d, 1H), 1.71 (d, 1H), 1.59-1.57 (m, 1H), 1.48-1.45 (m, 2H), 1.34 (d, 1H), 1.20-1.13 (m, 2H), 0.98 (d, 1H) ppm. $^{13}$C NMR (100 MHz, DMSO-*d*6): $\delta$ 57.9, 52.1, 35.2, 30.9, 25.7, 22.2ppm.

**PAD**. (2.78g, 93% yield). $^1$H NMR (400 MHz, DMSO-*d*6): $\delta$ 2.85 (d, 2H), 2.56-2.53

(m, 1H), 2.41-2.35 (m, 2H), 1.63-1.60 (m, 2H), 1.10-1.00 (m, 2H) ppm. $^{13}$C NMR (100 MHz, DMSO-*d*6): *δ* 49.4, 45.5,37.2ppm.

**BA-H**. (2.90 g, 97%yield). $^{1}$H NMR (500 MHz, DMSO-*d*6): *δ* 7.30 (t, 8H), 7.22 (s, 2H), 5.78 (s, 3H), 4.14 (s, 2H), 3.77 (s, 2H) ppm. $^{13}$C NMR (125 MHz, DMSO-*d*6): *δ* 159.6, 142.6, 141.6, 128.6, 127.9, 127.4, 127.0, 126.9, 45.3, 44.5ppm.

**BA-Cl**. (2.90g, 97% yield). $^{1}$H NMR (500 MHz, DMSO-*d*6): *δ* 7.36-7.27 (m, 8H), 4.53 (s, 4H), 4.11 (s, 2H), 3.72 (s, 2H) ppm. $^{13}$C NMR (125 MHz, DMSO-*d*6): *δ*159.3, 142.8, 140.6, 131.3, 129.5, 129.3, 128.5, 45.0, 43.8ppm.

**References**


1. X. Y. Zhang, Y. B. Zhou, M. Z. Wang, Y. T. Chen, Y. B. Zhou, W. X. Gao, M. C. Liu, X. B. Huang, H. Y. Wu, *Chem. Asian J.* **2020**, *15*, 1692.
2. T. B. Yang, H. A. Lu, R. H. Qiu, L. Hong, S. F. Yin, Nobuaki Kambe, *Chem. Asian J.* **2019**, *14*, 1436.


**General procedure for doped materials.**

The doped materials are prepared by the solvent evaporation method: First, the corresponding amount of the guest was dissolved in 5 ml of dichloromethane, and the corresponding amount of the host was dissolved in 15 ml of methanol. After mixing the two, the solvent was distilled under reduced pressure with an oil pump to obtain the mixture. The doped materials with high guest-host molar ratio (1:20-1:200) are using direct weighing method, while for guest-host molar ratio (1:500-1:10000) doped materials, we use the indirect dilution method.

## 3. Experimental data

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

$E = 1240/\lambda_{em}$ (eV) (Where $\lambda_{em}$ is the fluorescence or phosphorescence emission peak).

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

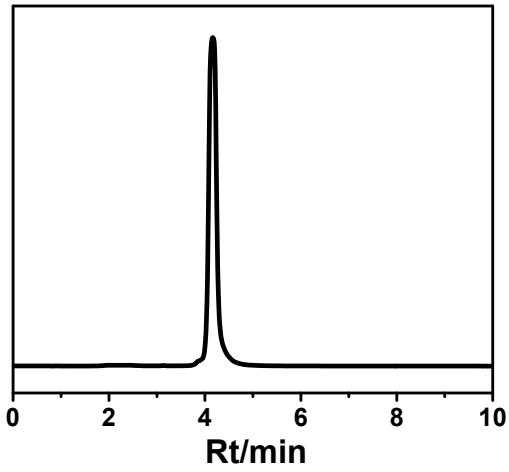



**Figure S1**. High performance liquid chromatography of **Mb**. ($CH_3OH/H_2O$= 80%: 20%)

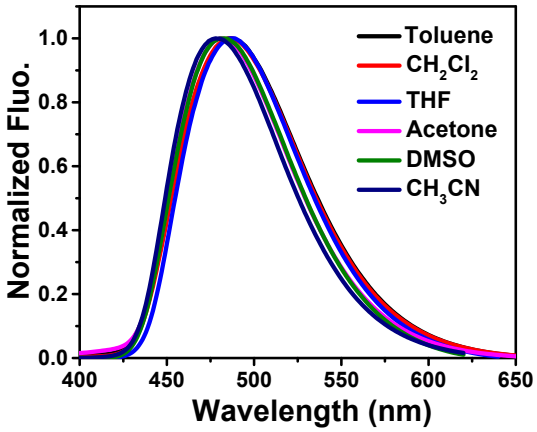



**Figure S2**. (a) Fluorescence wavelength of **Mb** in different solvents (Concentration: $1.0*10^{-4}$ mol/L, Ex.: 360 nm).

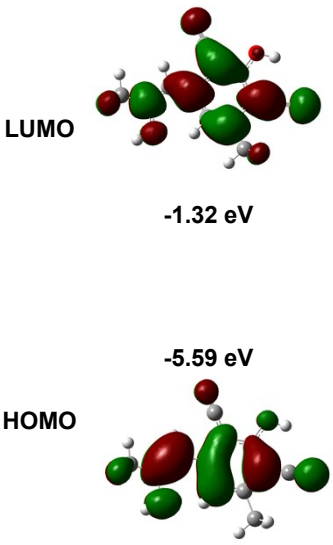



**Figure S3.** LUMO and HOMO distributions of **Mb**.

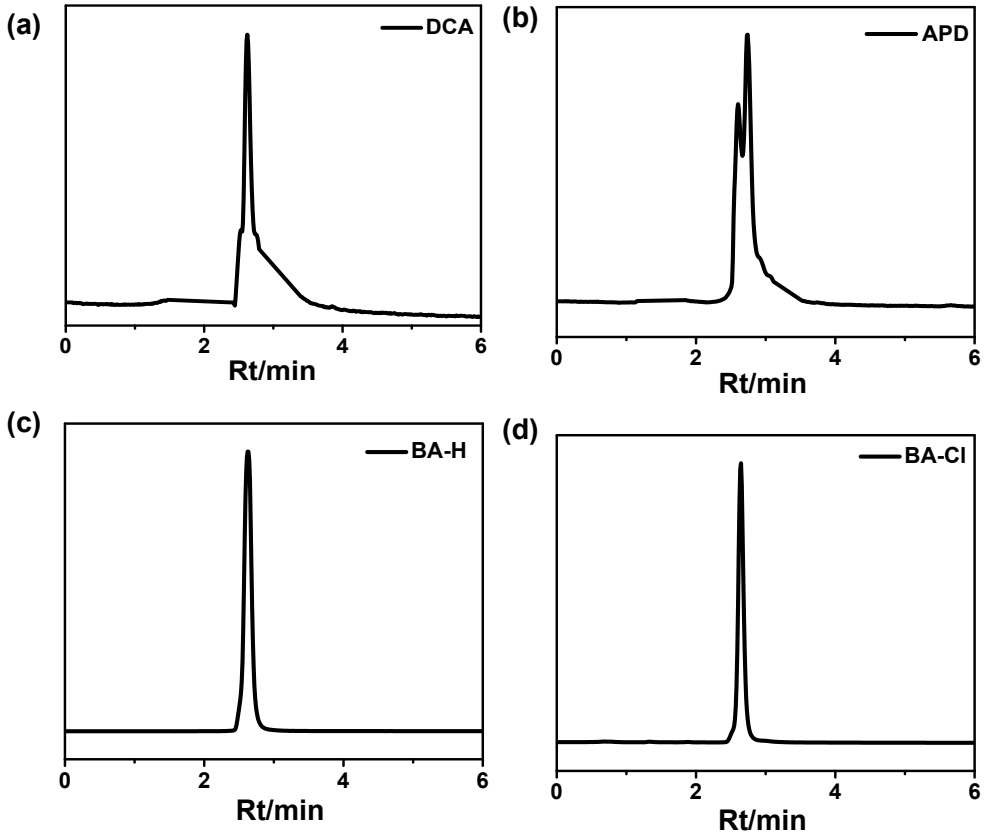



**Figure S4**. High performance liquid chromatography of hosts ($CH_3OH/H_2O$= 80%: 20%).

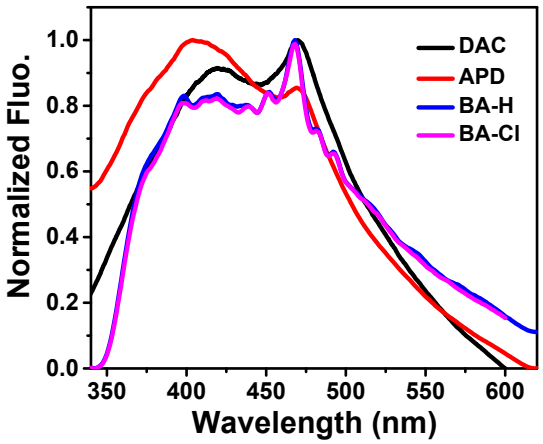



**Figure S5**. Fluorescence emission spectra of four hosts in solid state. (Ex.: 330 nm).

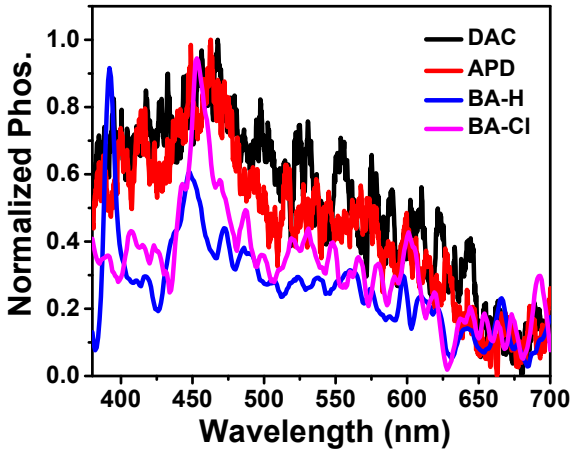



**Figure S6**. Delayed emission spectra of four hosts in solid state. (Delay time: 0.5 ms; Ex.: 380 nm).

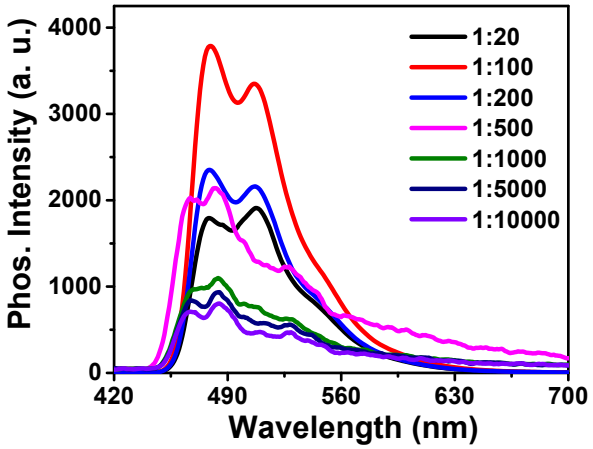



**Figure S7**. Delayed emission spectra of doped materials **Mb/BA-H** with different amounts of **Mb**. (Delayed time: 0.5 ms, Ex.: 380 nm).

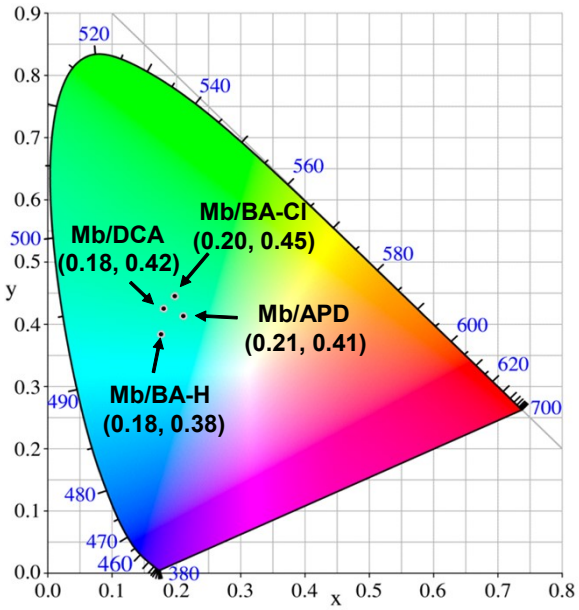



**Figure S8**. CIE coordinates of the doped materials.

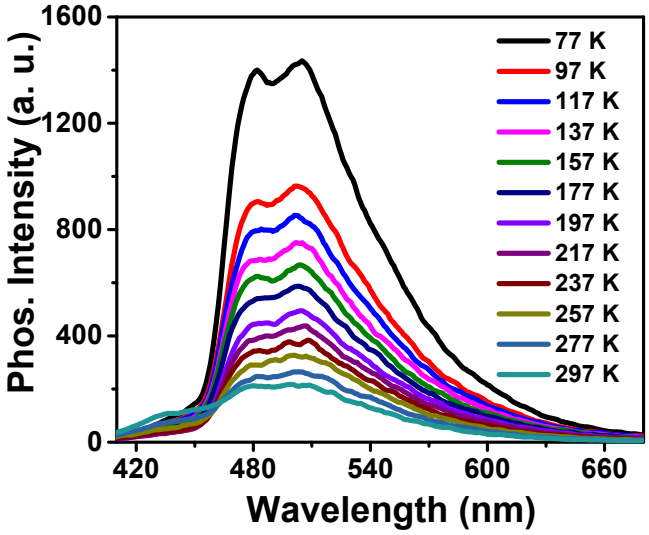



**Figure S9**. Delayed emission intensity of **Mb/BA-Cl** at different temperatures. (Delayed time: 0.5 ms, Ex.: 380 nm).

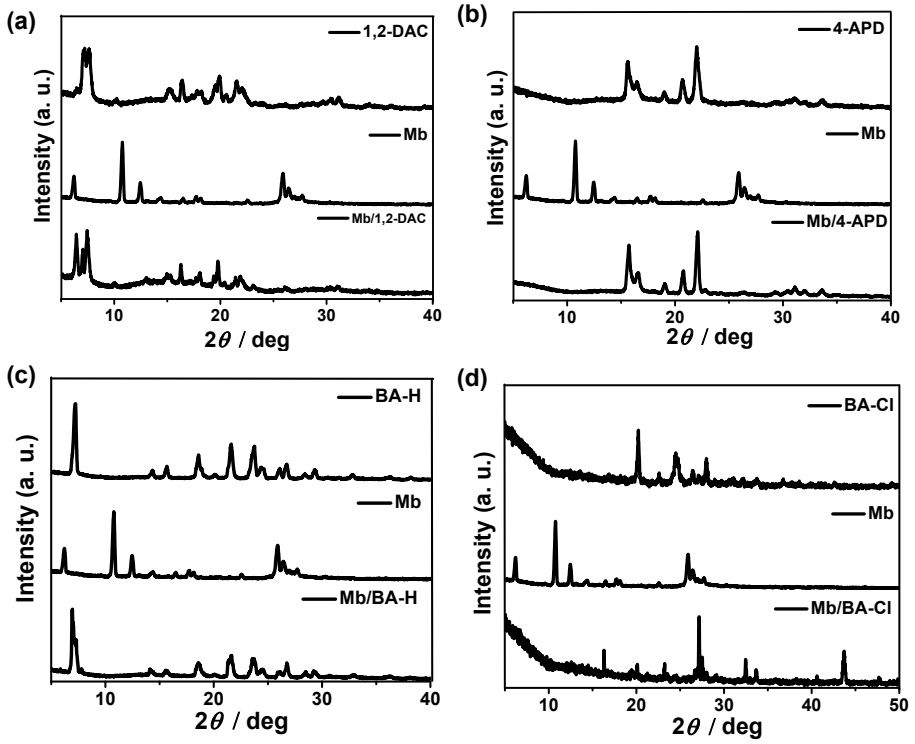



**Figure S10.** XRD curves of hosts, guest and doped materials.

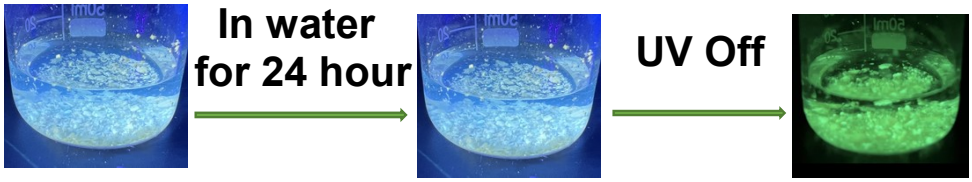



**Figure S11.** Phosphorescence photographs of **Mb/BA-Cl** in water.

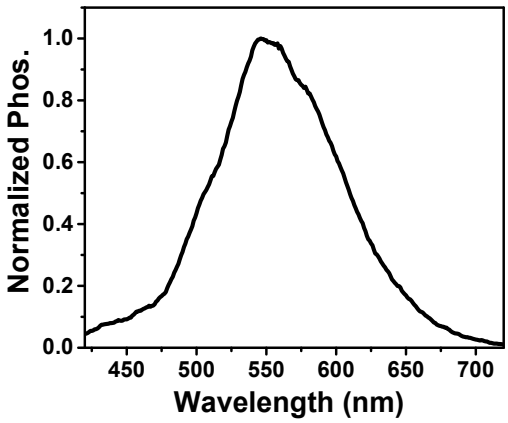



**Figure S12**. Delayed emission spectra of **Mb** in aggregate state in 77 K (Ex. = 380 nm, Delayed time: 0.5 ms).

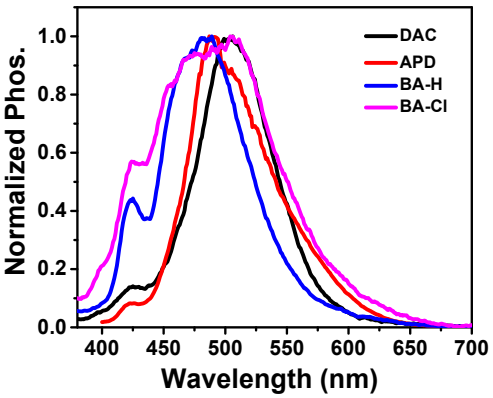



**Figure S13**. Delayed emission spectra of four hosts in solid state in 77 K (Ex. = 380 nm, Delayed time: 0.5 ms).

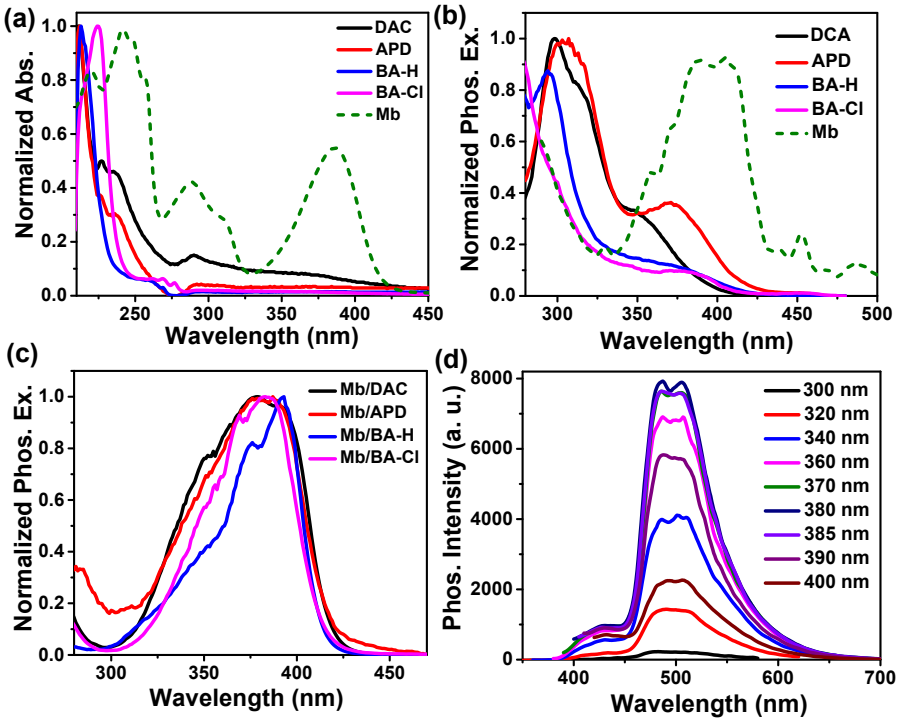



**Figure S14**. (a) Absorption spectra of guest and four salt hosts. (b) Excitation spectra of guest and four salt hosts. (c) Excitation spectra of four doped materials. (d) Delayed emission spectra of Mb/BA-Cl at different excitation wavelengths.

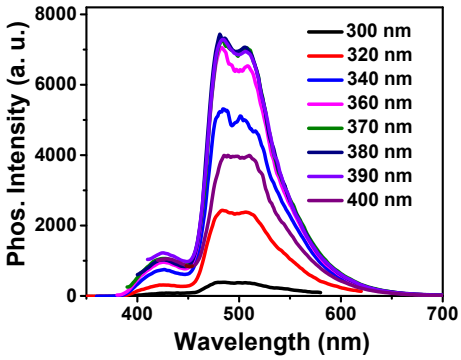



**Figure S15**. Delayed emission spectra of **Mb/DAC** at different excitation wavelengths.

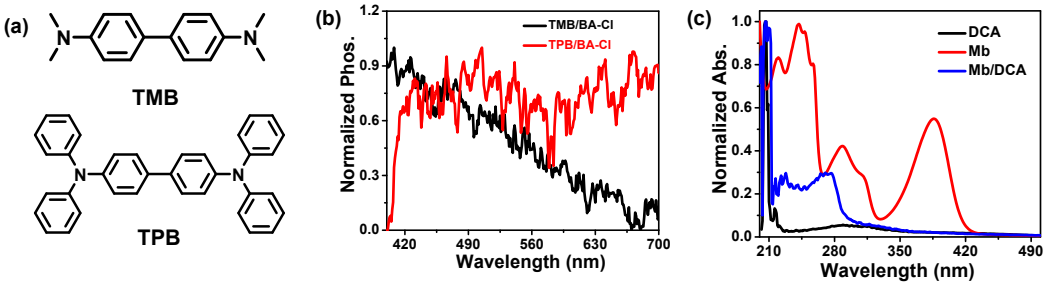



**Figure S16**. (a) Molecular structures of the control guests (**TMB** and **TPB**). (b) Delayed emission spectra of **TMB/BA-Cl** and **TPB/BA-Cl**. (c) Absorption spectra of guest (**Mb)**, host (**DCA)** and doped material (**Mb/DCA)**.

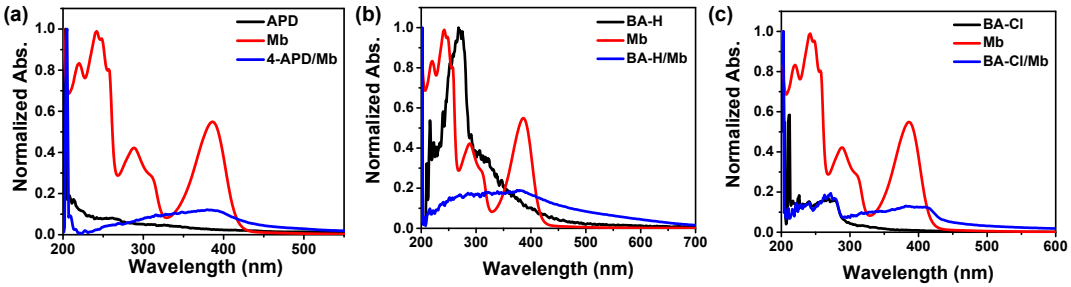



**Figure S17**. Absorption spectra of guest, hosts and doped materials.

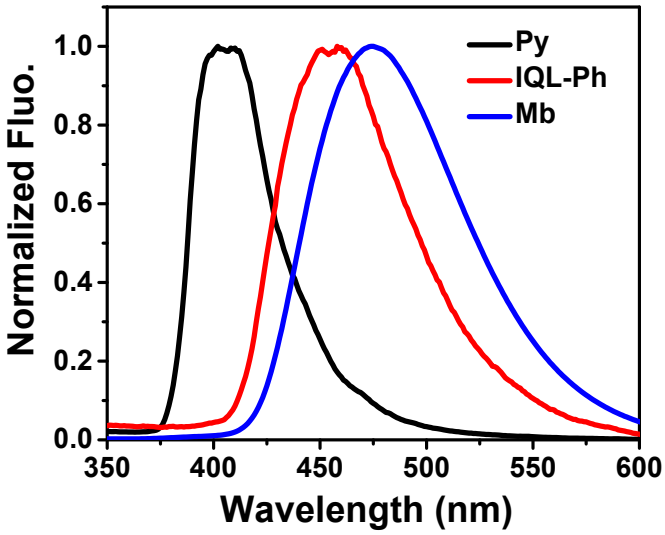



**Figure S18**. (a) Fluorescence wavelength of guests in toluene solvent (77 K). (Concentration: $1.0*10^{-4}$ mol/L, Ex.: 360 nm).

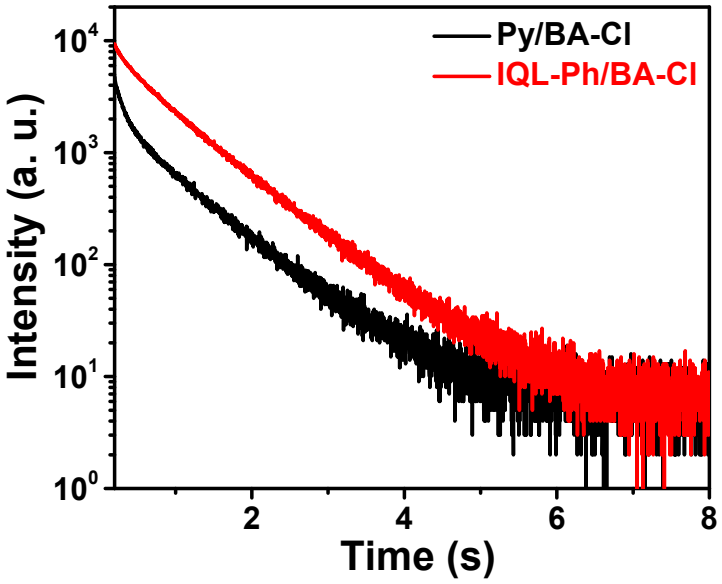



**Figure S19**. Phosphorescence decay curves of **Py/BA-Cl** and **IQL-Ph/BA-Cl**.

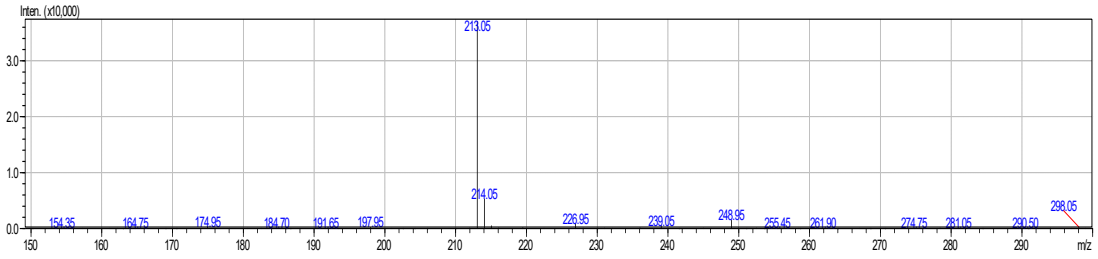



**Figure S20.** ESI-MS spectrum of compound **Mb**.

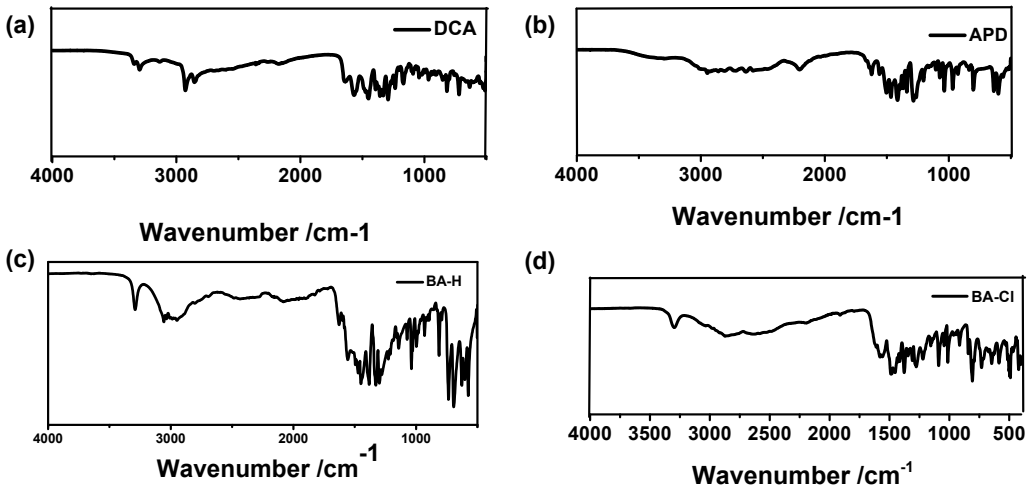



**Figure S21**. IR spectra of four hosts.

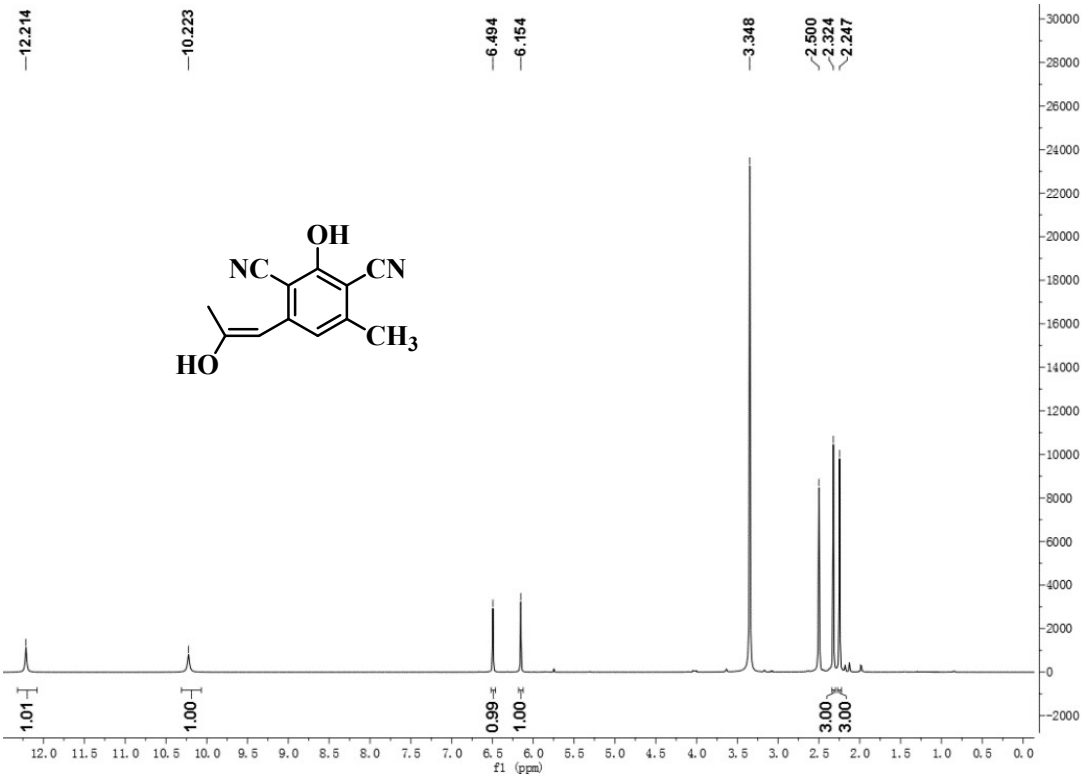



**Figure S22.** $^{1}$H NMR of **Mb** (DMSO-*d*6, 500 MHz).

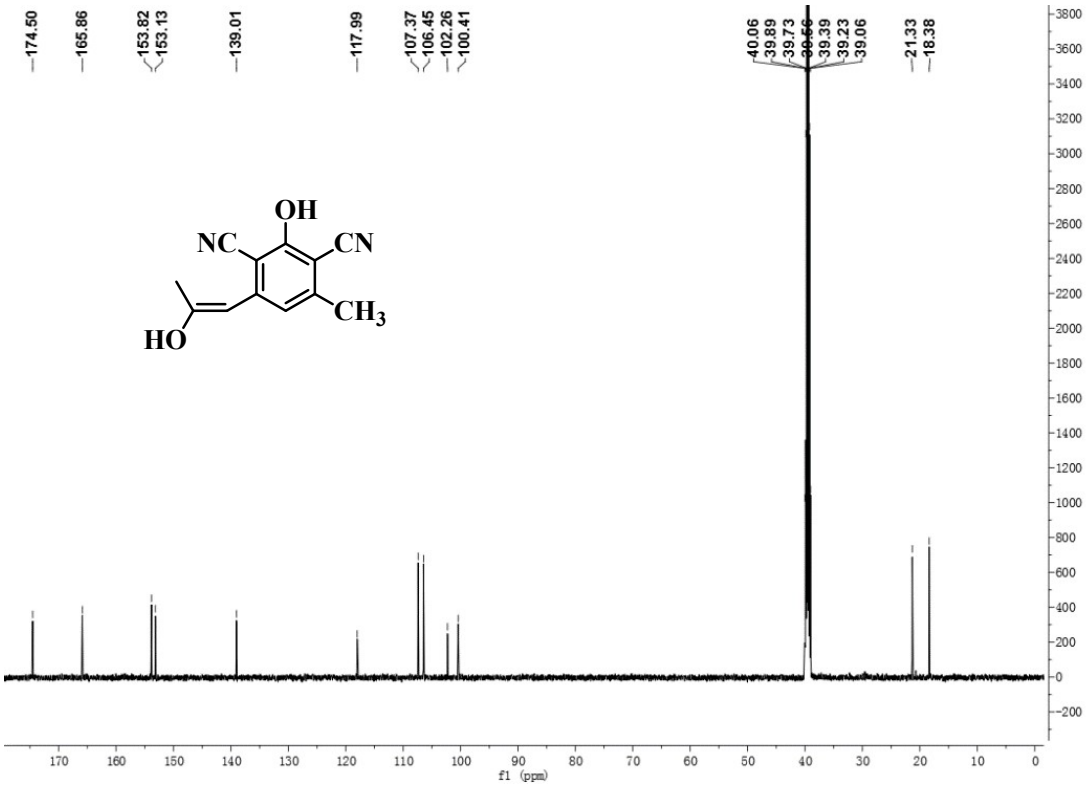



**Figure S23.** $^{13}$C NMR of **Mb** (DMSO-*d*6, 125 MHz).

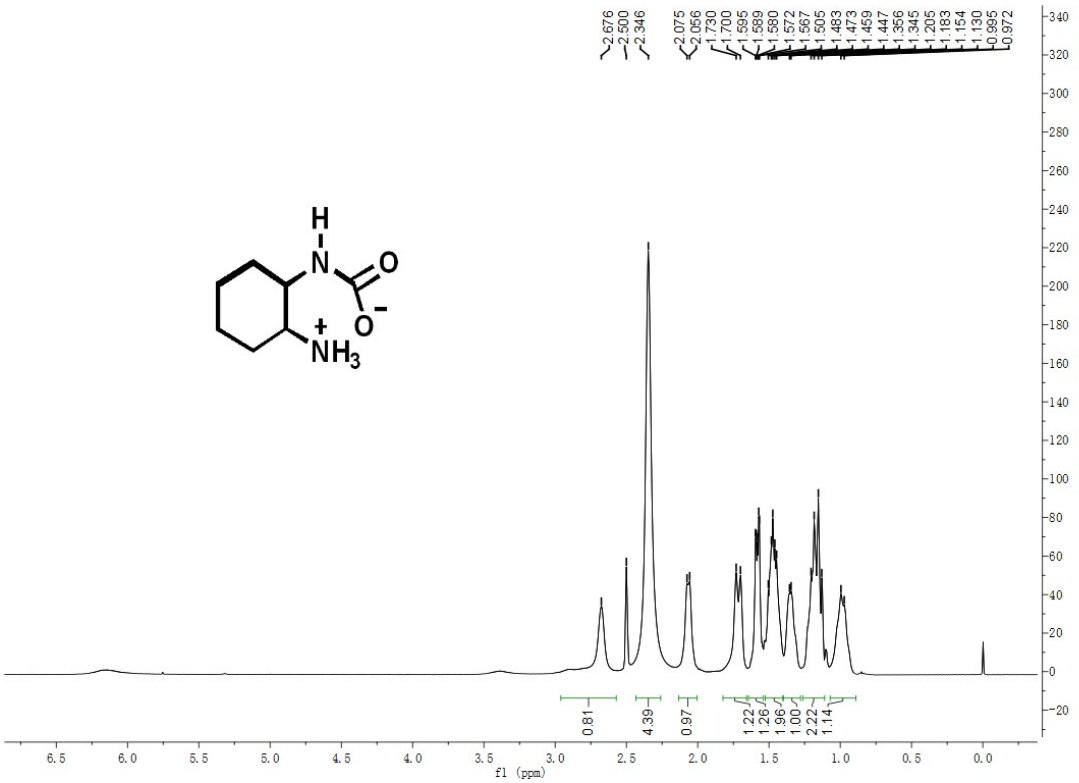



**Figure S24.** $^{1}$H NMR of **DCA** (DMSO-*d*6, 400 MHz).

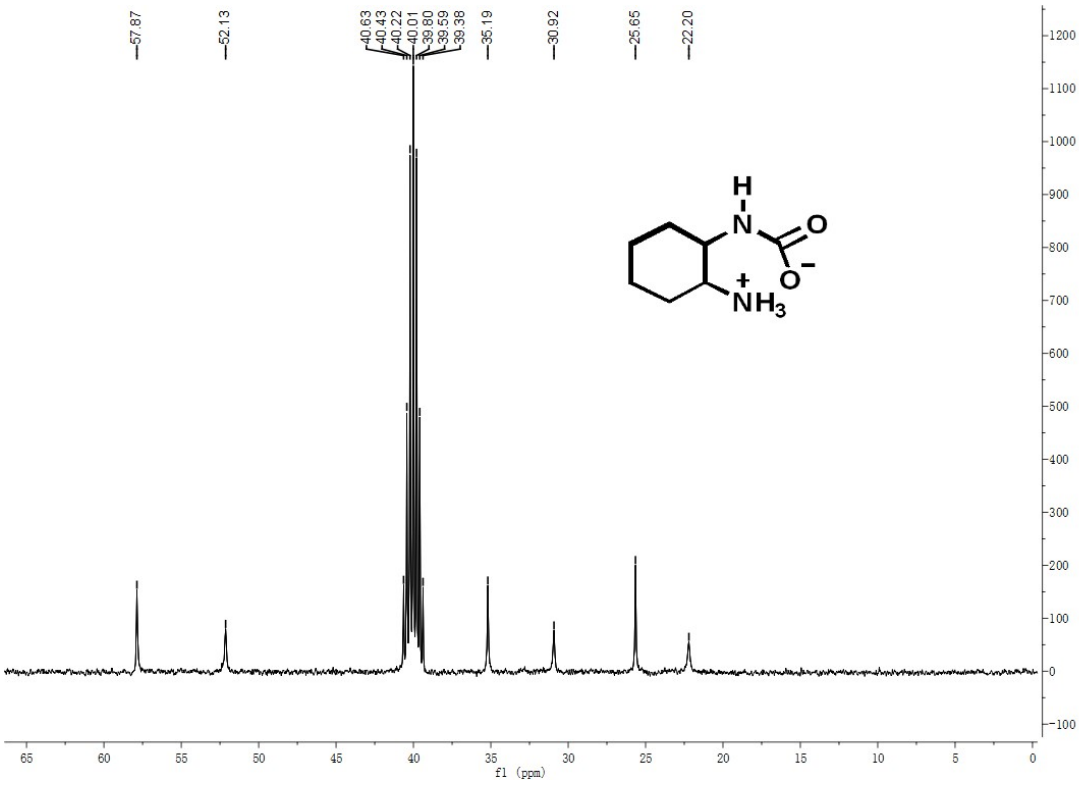



**Figure S25.** $^{13}$C NMR of **DCA** (DMSO-*d*6, 100 MHz).

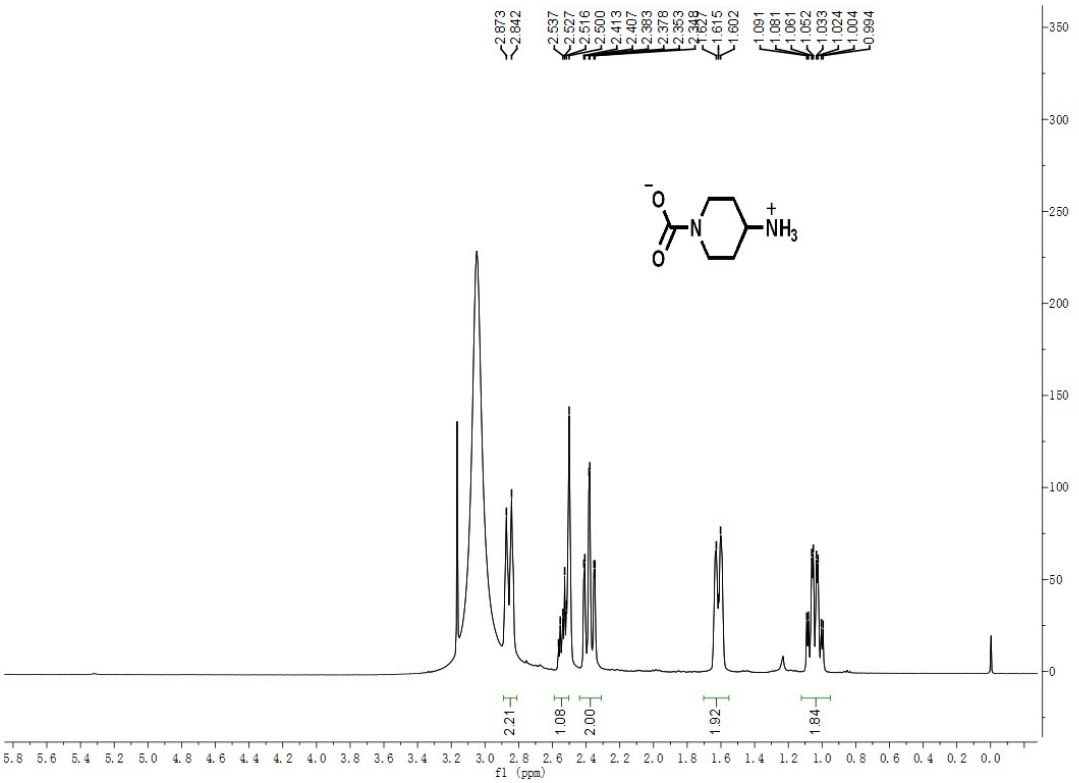



**Figure S26.** $^{1}$H NMR of **APD** (DMSO-*d*6, 400 MHz).

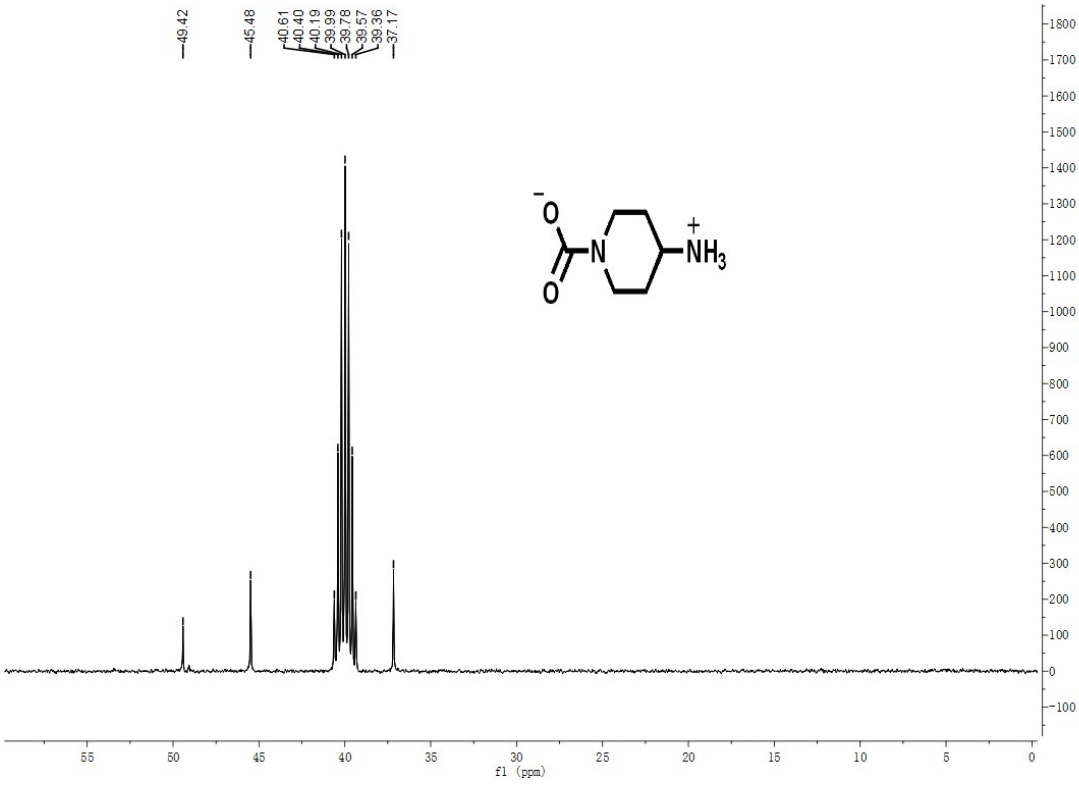



**Figure S27.** $^{13}$C NMR of **APD** (DMSO-*d*6, 100 MHz).

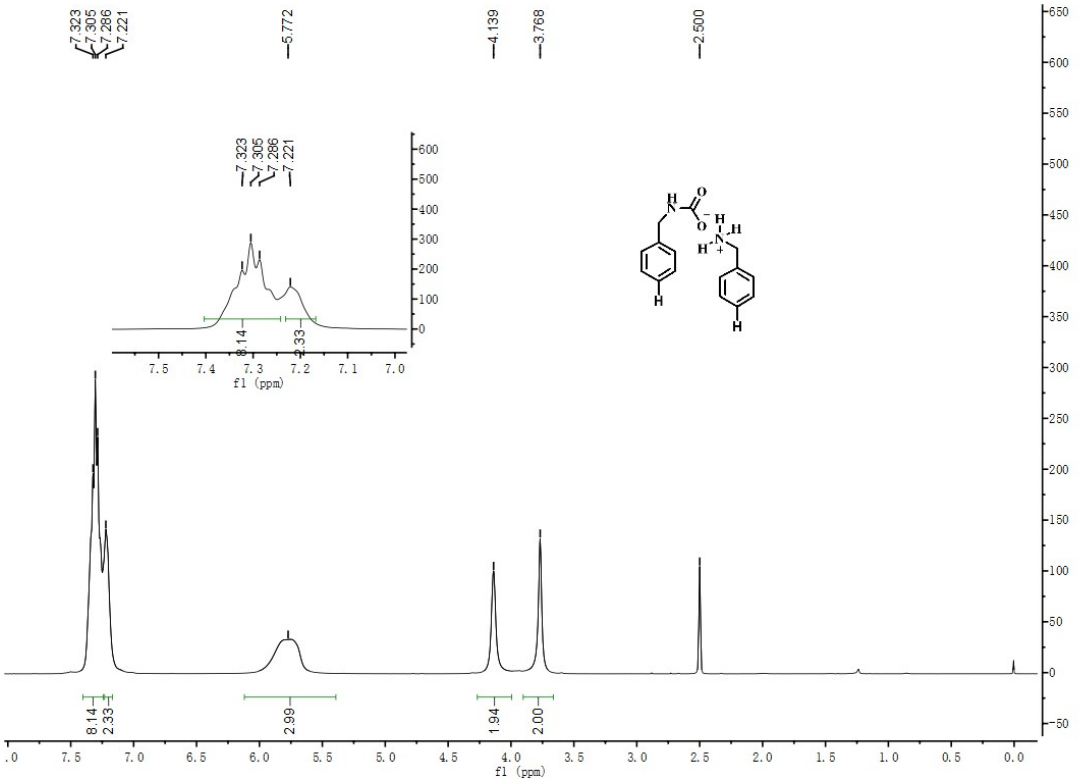



**Figure S28.** $^{1}$H NMR of **BA-H** (DMSO-*d*6, 500 MHz).

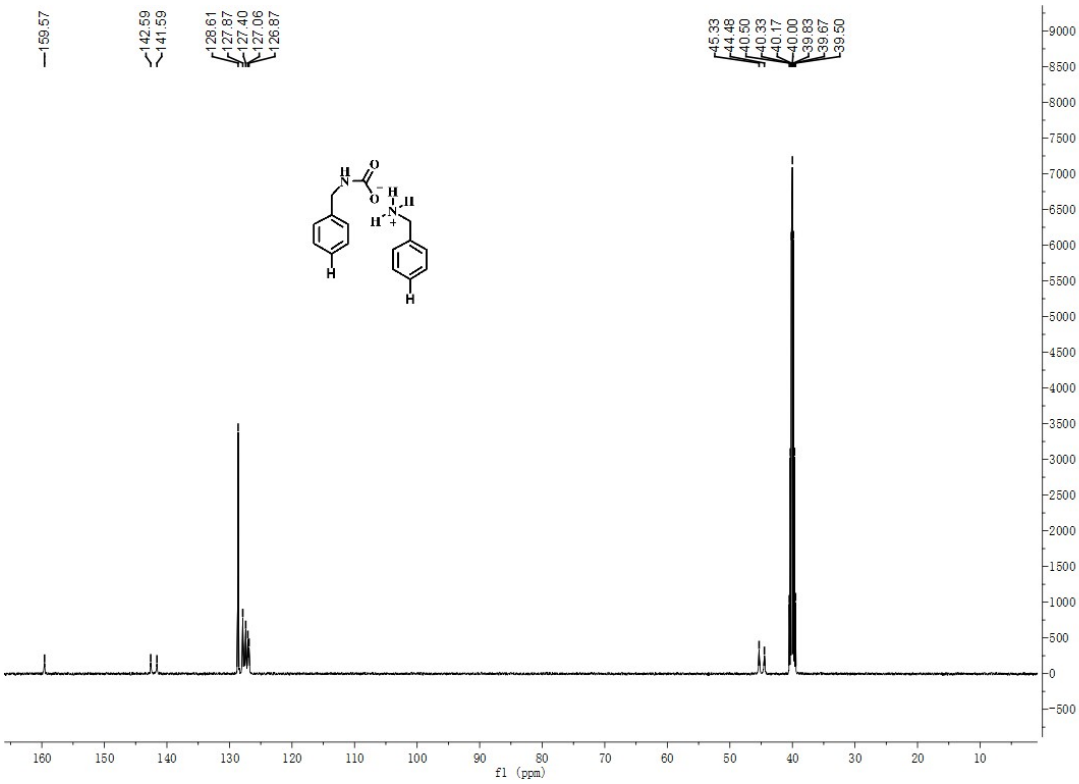



**Figure S29.** $^{13}$C NMR of **BA-H** (DMSO-*d*6, 125 MHz).

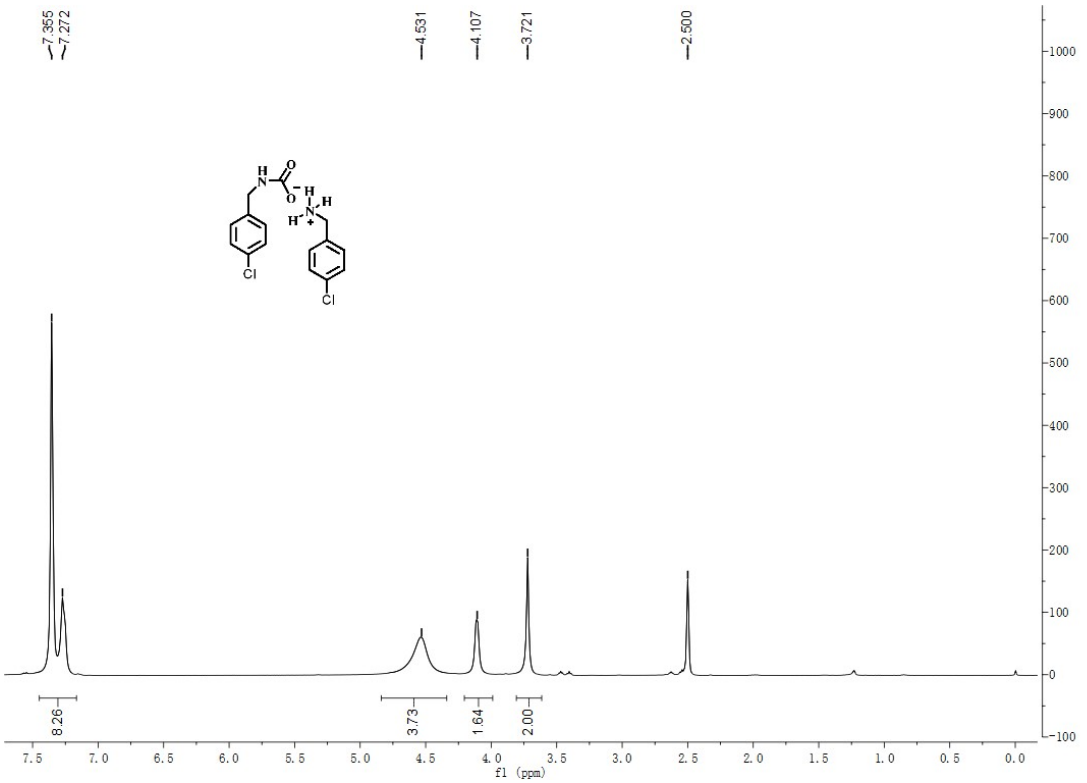



**Figure S30.** $^{1}$H NMR of **BA-Cl** (DMSO-*d*6, 500 MHz).

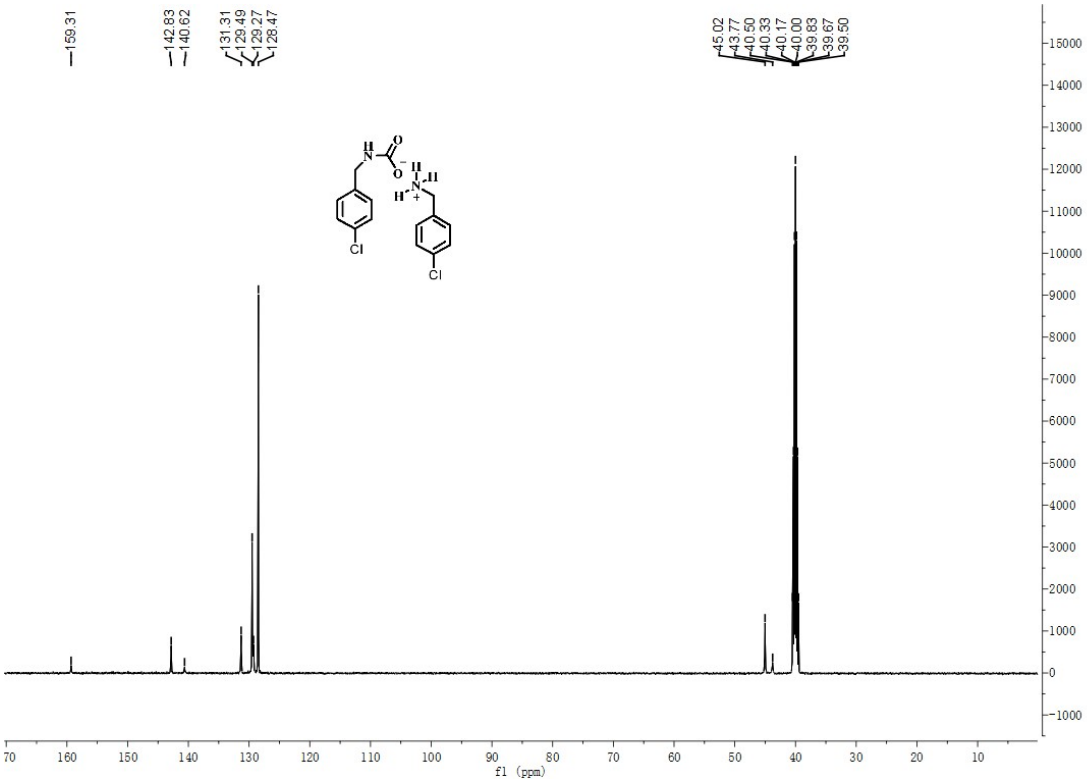



**Figure S31.** $^{13}$C NMR of **BA-Cl** (DMSO-*d*6, 125 MHz).