

## SUPPORTING INFORMATION

# Strong CPL-active Liquid Crystal Materials Induced by Intermolecular Hydrogen-bonding Interaction and Chirality Induction Mechanism

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## 1. Instrumentation and Materials

### 1.1 Materials and Measurements

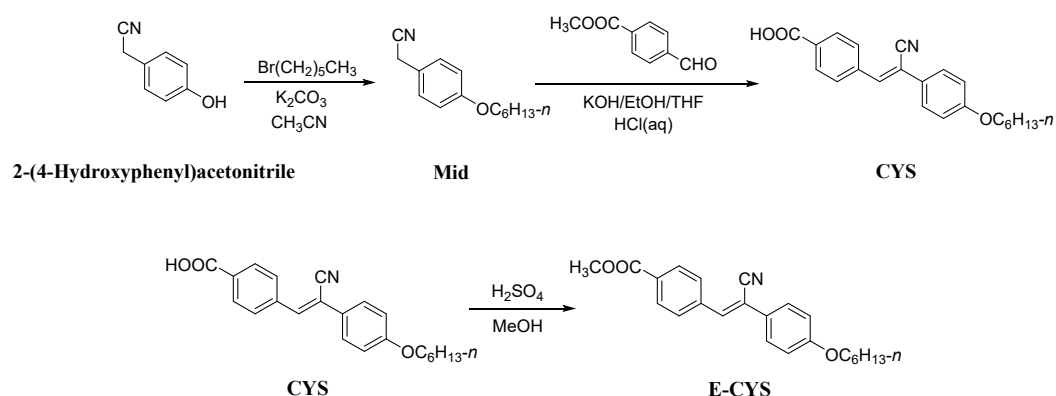
All NMR spectra were obtained by using Bruker AVANCE III-400 spectrometer with 400 MHz for  $^1\text{H}$  NMR and 100 MHz for  $^{13}\text{C}$  NMR. Chemical shifts are reported as parts per million (ppm) relative to tetramethylsilane (TMS;  $\delta = 0$ ). UV-visible (UV-*vis*) absorption spectra were measured by a Hitachi U-3900 spectrophotometer. Fluorescence (FL) spectra were tested from a HORIBA Scientific Fluoromax-4 Spectrofluorometer. DSC traces were measured by using Mettler DSC823e Differential Scanning Calorimetry. XRD patterns were obtained on a Bruker D8 ADVANCE X-Ray Powder Diffractometer. Circular dichroism (CD) spectra were collected on a JASCO J-810 spectropolarimeter, and the length of the sample cell was 1 cm. Circularly polarized luminescence (CPL) spectra were performed on a JASCO CPL-300 spectrofluoropolarimeter. In the CPL measurements, the excitation wavelength was 360 nm, scan speed was 200 nm/min, number of scans was 1, and slit width was 3000  $\mu\text{m}$ . The magnitude of CPL can be quantified by luminescence dissymmetry factor  $g_{\text{em}}$  ( $g_{\text{em}} = 2(I_{\text{L}} - I_{\text{R}}) / (I_{\text{L}} + I_{\text{R}})$ , where  $I_{\text{L}}$  and  $I_{\text{R}}$  represent the intensities of the left and right CPL, respectively). Experimentally, the value of dissymmetry factor  $g_{\text{em}}$  is defined as  $\Delta I/I = 2[\text{ellipticity} / (32980/\ln 10)] / (\text{total fluorescence intensity at the CPL extremum})$ .<sup>1</sup> All starting materials were purchased from Acros, Alfa Aesar, Energy and used directly.

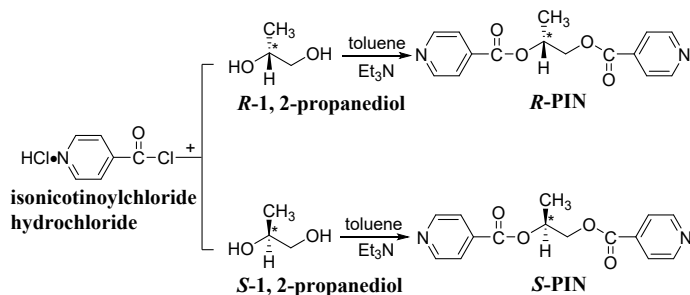
### 1.2 Measurements of liquid crystal textures

The liquid crystalline textures were investigated and photographed using a polarized optical microscope (POM) equipped with a Leitz-350 heating stage and an associated Nikon (D3100) digital camera.

## 2. Syntheses of CYS, E-CYS and R/S-PIN

**Scheme S1.** The synthesis procedures of R/S-PIN, CYS, E-CYS.





### Synthesis of Mid

To a 500 mL round-bottomed flask equipped with a magnetic stir bar were added (4-Hydroxyphenyl)acetonitrile (5.30 g, 0.040 mol),  $\text{K}_2\text{CO}_3$  (11.00 g, 0.080 mol) and  $\text{CH}_3\text{CN}$  (200 mL). After stirring for 15 min, 1-Bromohexane (7.88 g, 0.048 mol) was added to the mixture and the reaction was continued to stirring at room temperature for 24 h. After the reaction completed (detected by TLC), the reaction mixture was filtered and the solvent was removed under reduced pressure. The crude product was further purified by silica gel column chromatography, with a mixture solvent of *n*-hexane/AcOEt (20:1, v/v) as the eluent to obtain a yellow-green liquid. Yield: 68.2%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.12 (m, 2H), 6.79 (m, 2H), 3.85 (t,  $J = 6.4$  Hz, 2H), 3.57 (s, 2H), 1.69 (m, 2H), 1.36 (m, 2H), 1.25 (m, 4H), 0.82 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.92, 129.04, 121.58, 118.29, 115.08, 68.14, 31.59, 29.19, 25.71, 22.79, 22.62, 14.05.

### Synthesis of CYS

To a 250 mL round-bottomed flask equipped with a magnetic stir bar was added Mid (5.00 g, 0.023 mol), methyl 4-(cyanomethyl)benzoate (3.78 g, 0.023 mol) and THF (100 mL). After 5 min, KOH (3.87 g, 0.069 mol, dissolved in 50 mL EtOH) added into the above solution and the reaction was stirred at 50 °C for 24 h (detected by TLC). After that, the mixture was cooled to 0° C and hydrochloric acid was added dropwise until the pH of solution was 1. The crude product was further purified by silica gel column chromatography, with a mixture solvent of *n*-hexane/AcOEt (1:4, v/v) as the eluent to obtain a yellow-green solid. Yield: 53.1%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.18 (m, 2H), 7.95 (m, 2H), 7.64 (m, 2H), 7.47 (s, 1H), 6.97 (m, 2H), 4.01 (t,  $J = 6.4$  Hz, 2H), 1.81 (m, 2H), 1.47 (m, 2H), 1.35 (m, 4H), 0.92 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ),  $\delta$  (ppm): 170.62, 160.57, 139.02, 137.91, 130.71, 129.97, 128.98, 127.56, 126.14, 117.62, 115.09, 114.12, 68.31, 31.57, 29.14, 25.69, 22.60, 14.04.

### Synthesis of E-CYS

In a 150 mL round-bottomed flask equipped with a magnetic stir bar, 0.02 mL  $\text{H}_2\text{SO}_4$  added to a mixture of CYS (1.00 g, 0.003 mol) and methanol (50 mL). After stirring for 12 h, the solvent was removed under reduced pressure. The crude product was further purified by silica gel column chromatography, with a mixture solvent of *n*-hexane/AcOEt (20:1, v/v) as the eluent to obtain a

white solid. Yield: 86.2%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (m, 2H), 7.91 (m, 2H), 7.62 (m, 2H), 7.45 (s, 1H), 6.96 (m, 2H), 4.01 (t,  $J = 6.4$  Hz, 2H), 3.95 (s, 3H), 1.81 (m, 2H), 1.47 (m, 2H), 1.35 (m, 4H), 0.92 (m, 3H)  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ),  $\delta$  (ppm): 166.38, 160.48, 138.19, 138.16, 131.02, 130.07, 128.89, 127.51, 126.24, 117.70, 115.06, 113.66, 68.29, 52.32, 31.57, 29.13, 25.69, 22.60, 14.04.

### Synthesis of *R/S*-PIN

The isonicotinoylchloride hydrochloride (6.43 g, 0.036 mol) was dissolved in toluene (100 mL) to form a suspension. And then, triethylamine (20 mL, 0.145 mol) was added dropwise into the suspension under ice-water bath. After stirring for 0.5 h, to the above mixture was added *R/S*-1, 2-propanediol (1.10 g, 0.014 mol, dissolved in 50 mL THF) and the reaction was refluxed at  $110^\circ\text{C}$  for 24 h (detected by TLC). After the reaction completed, the precipitate was filtered off and the solvent was removed under reduced pressure. The crude product was further purified by silica gel column chromatography, with a mixture solvent of n-hexane/AcOEt (2:1, v/v) as the eluent to obtain a white solid with slightly yellow. Yield: 46.2%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.78 (m, 4H), 7.82 (m, 4H), 5.58 (m, 1H), 4.60 (m, 1H), 4.51 (m, 1H), 1.50 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.72, 164.45, 150.68, 150.65, 137.12, 136.75, 122.78, 122.76, 69.72, 67.04, 16.47.

### 3. Preparation of *R/S*-CYS-PIN, CYS-LC and *R/S*-CYS-PIN-LC

The proton donor CYS and the proton acceptor *R/S*-PIN were completely dissolved in  $\text{CH}_2\text{Cl}_2$  with a molar ratio of 2:1, *R/S*-CYS-PIN (yellowish rod solid) was obtained *via* natural evaporation at room temperature with stirring. The *R/S*-CYS-PIN films were obtained from the  $\text{CH}_2\text{Cl}_2$  solutions of *R/S*-CYS-PIN by spin coating on the quartz plates (1 cm  $\times$  3 cm) after  $\text{CH}_2\text{Cl}_2$  naturally evaporated. Covered the film with a clear quartz plate and formed a sandwich structure cell, heating the cell to the liquid crystal range, we froze the aggregation structures of *R/S*-CYS-PIN-LC by quick cooling with liquid nitrogen (rapid cooling quench treatment). The CYS and CYS-LC films were prepared in the same way.

### 4. FT-IR spectra of the CYS, *R*-PIN, *R*-CYS-PIN and *R*-CYS-PIN-LC

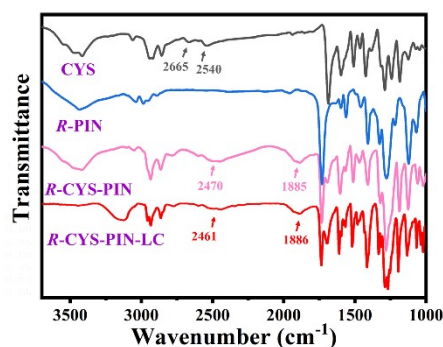
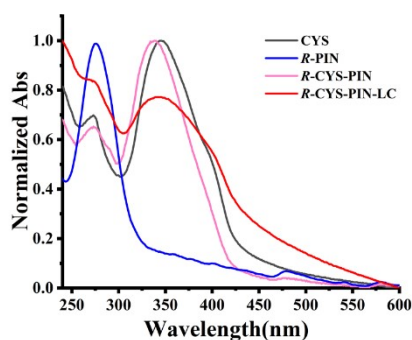


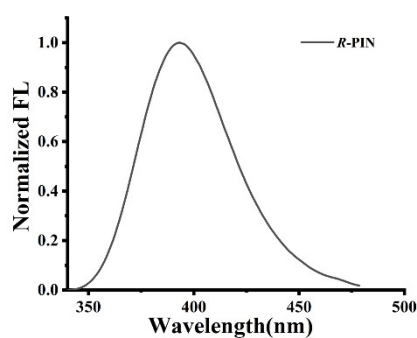
Fig. S1 FT-IR spectra of the CYS, *R*-PIN, *R*-CYS-PIN and *R*-CYS-PIN-LC.

## 5. UV-vis spectra of CYS, *R*-PIN, *R*-CYS-PIN and *R*-CYS-PIN-LC



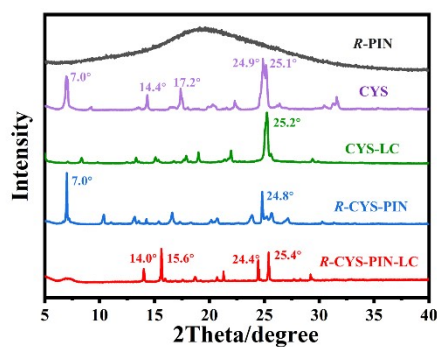
**Fig. S2** UV-vis absorption and fluorescence emission spectra of CYS, *R*-PIN, *R*-CYS-PIN and *R*-CYS-PIN-LC in film state. The maximum absorption of CYS, *R*-PIN, *R*-CYS-PIN and *R*-CYS-PIN-LC occurred at 345, 275 and 339 and 343 nm.

## 6. Fluorescence spectra of *R*-PIN



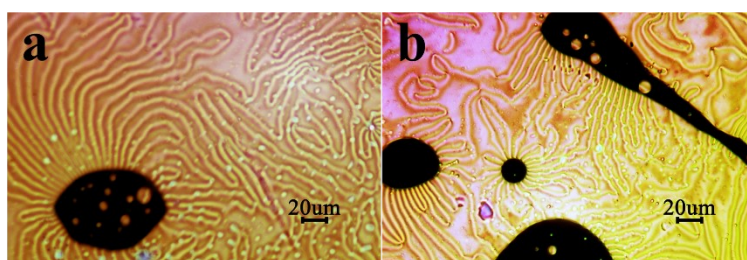
**Fig. S3** Fluorescence spectra of *R*-PIN in film state ( $\lambda_{\text{ex}} = 250$  nm,  $\lambda_{\text{em}} = 393$  nm)

## 7. XRD patterns for *R*-PIN, CYS, CYS-LC, *R*-CYS-PIN and *R*-CYS-PIN-LC



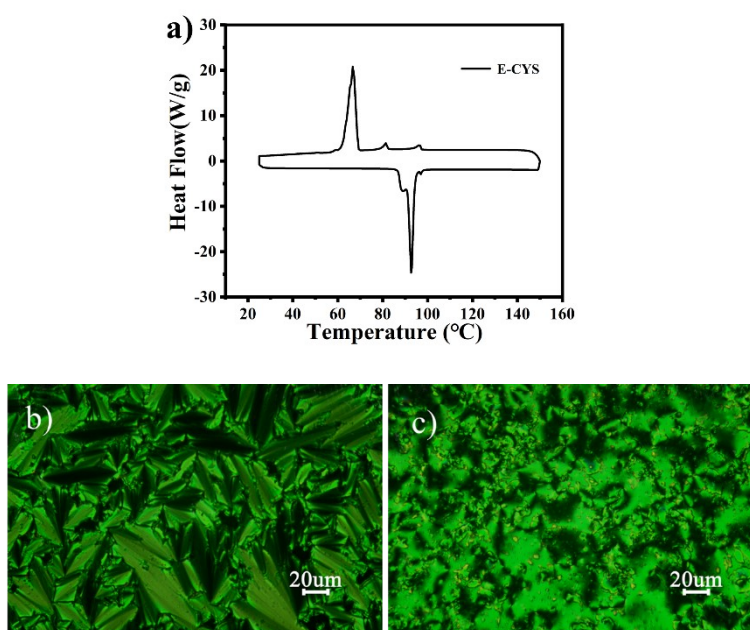
**Fig. S4** Powder XRD patterns for *R*-PIN, CYS, CYS-LC, *R*-CYS-PIN and *R*-CYS-PIN-LC.

## 8. POM images of chiral emissive liquid crystals at a 1:1 ratio (CYS: *R/S*-PIN)



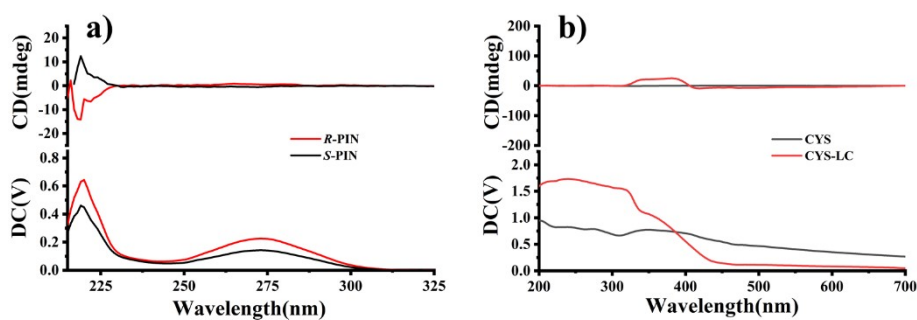
**Fig. S5** POM images of (a) CYS: *R*-PIN = 1:1 in film state at 125 °C; (b) CYS:*S*-PIN = 1:1 in film state at 125 °C.

## 9. DSC traces and POM images of E-CYS



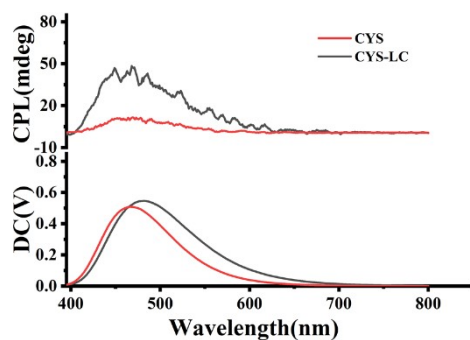
**Fig. S6** (a) DSC traces of E-CYS recorded during the first heating/cooling at the rate of 10 °C/min under nitrogen atmosphere; POM images of (b) E-CYS in liquid crystal (LC) state at 70 °C and (c) E-CYS in liquid crystal (LC) state at 88 °C.

## 10. CD spectra of *R/S*-PIN, CYS , CYS-LC



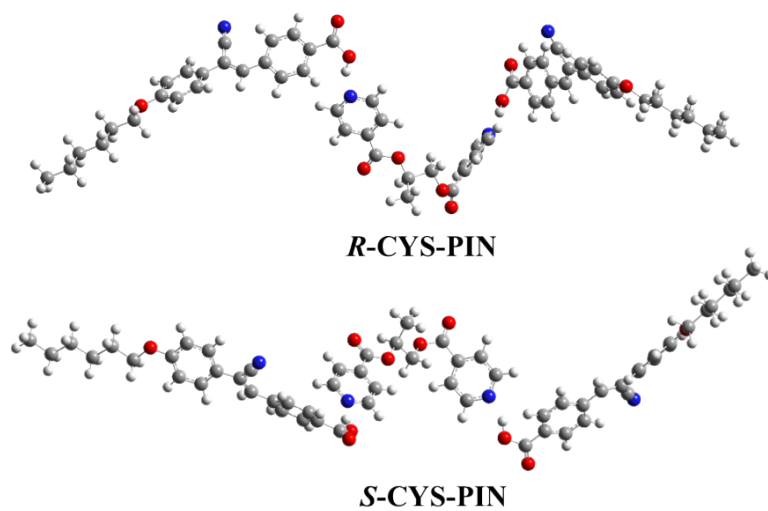
**Fig. S7** CD spectra of (a) *R/S*-PIN in film state and (b) CYS and CYS-LC in film state.

## 11. CPL spectra of CYS and CYS-LC



**Fig. S8** CPL spectra of CYS and CYS-LC in film state ( $\lambda_{\text{ex}} = 330$  nm).

## 12. Stereoscopic structure of *R/S*-CYS-PIN



**Fig. S9** Stereoscopic structure of *R/S*-CYS-PIN; the blue, grey, red, and white balls indicate nitrogen, carbon, oxygen, and hydrogen atoms.

### 13. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compounds

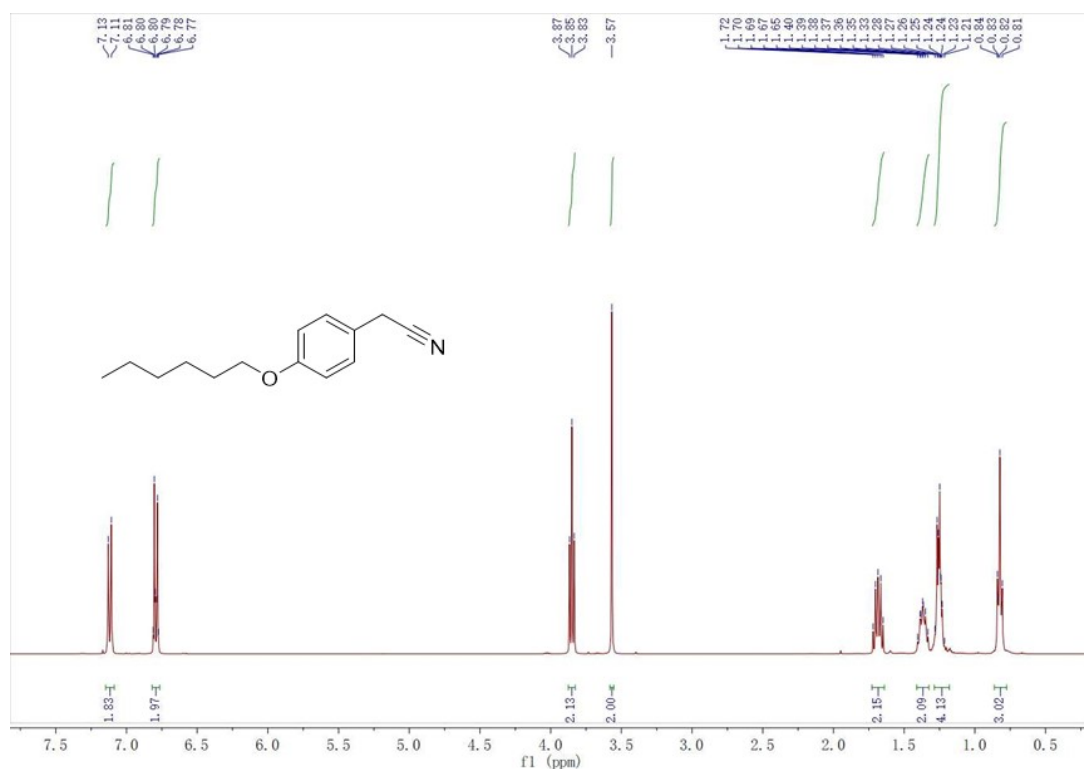


Fig. S10 <sup>1</sup>H NMR of Mid (400 MHz, CDCl<sub>3</sub>).

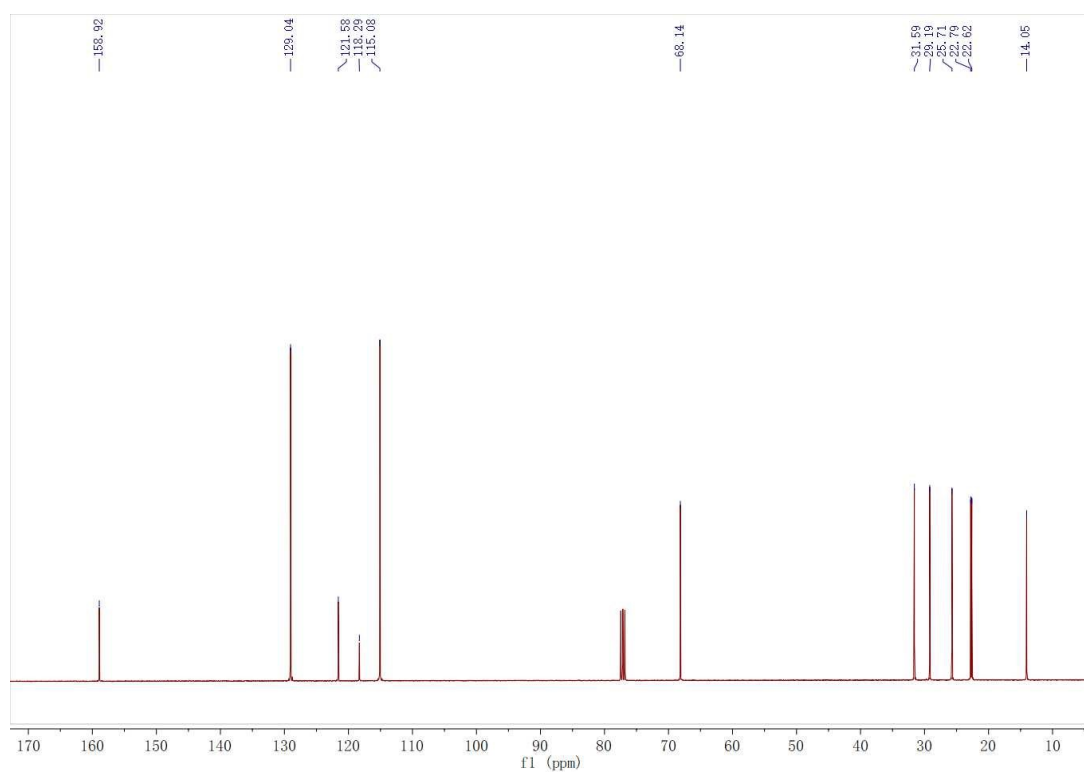
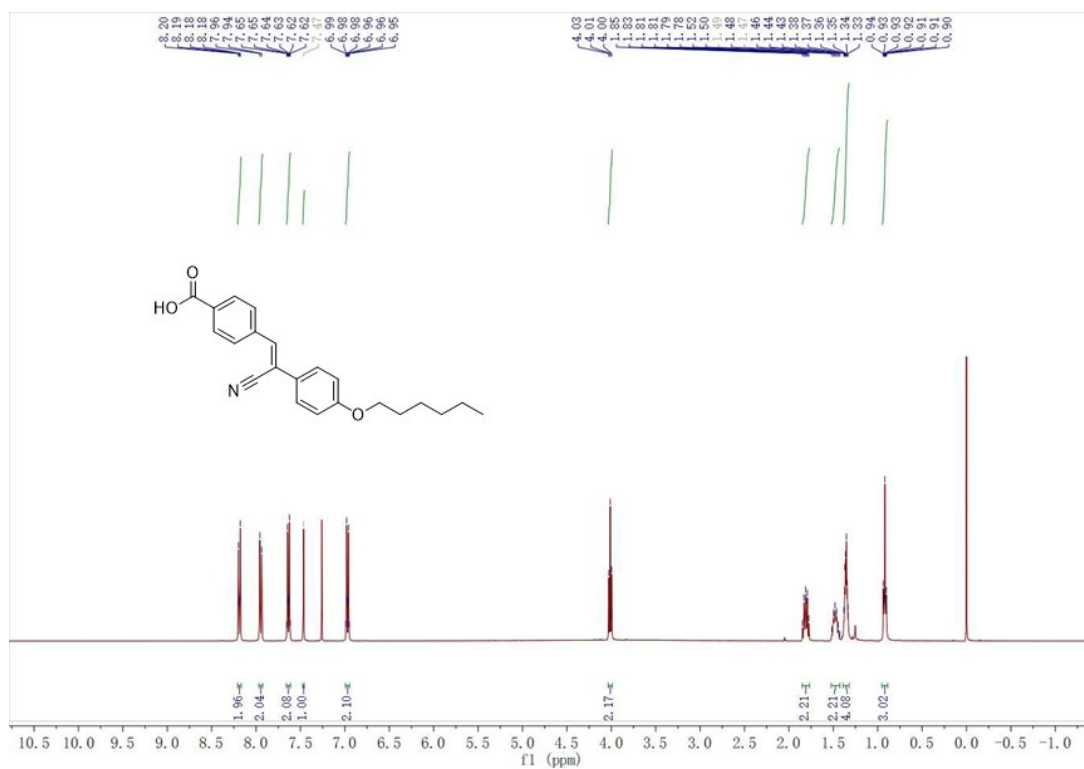
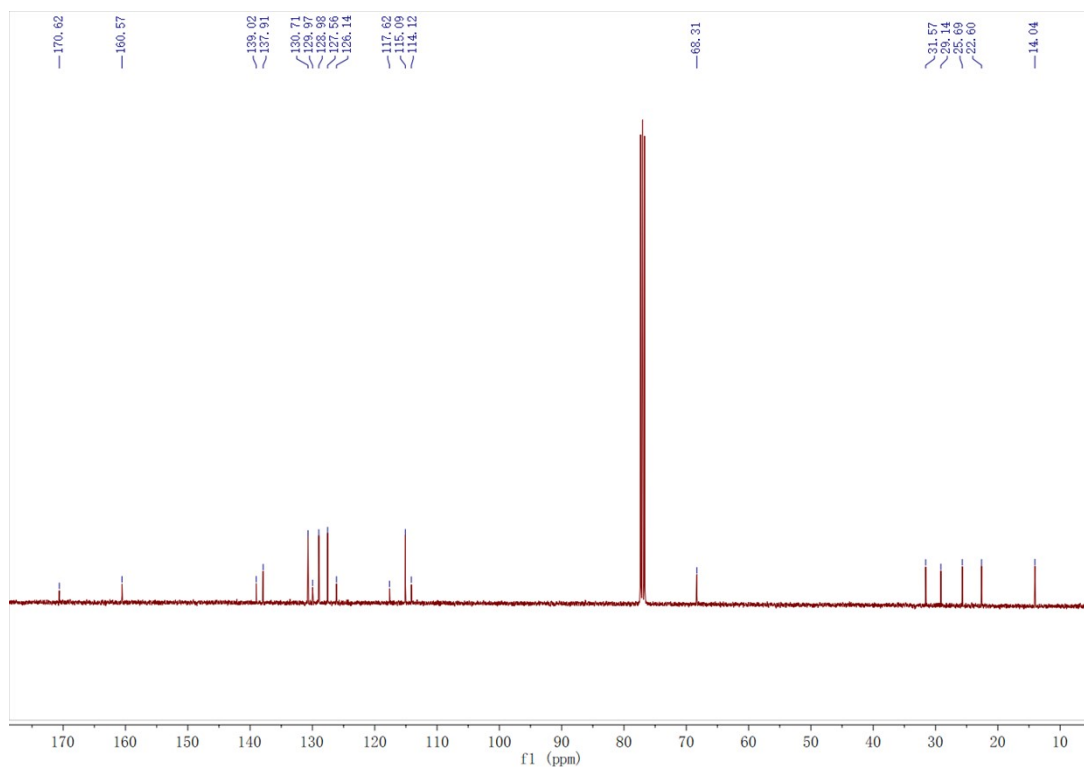


Fig. S11 <sup>13</sup>C NMR of Mid (100 MHz, CDCl<sub>3</sub>).





**Fig. S12** <sup>1</sup>H NMR of CYS (400 MHz, CDCl<sub>3</sub>).



**Fig. S13** <sup>13</sup>C NMR of CYS (100 MHz, CDCl<sub>3</sub>).

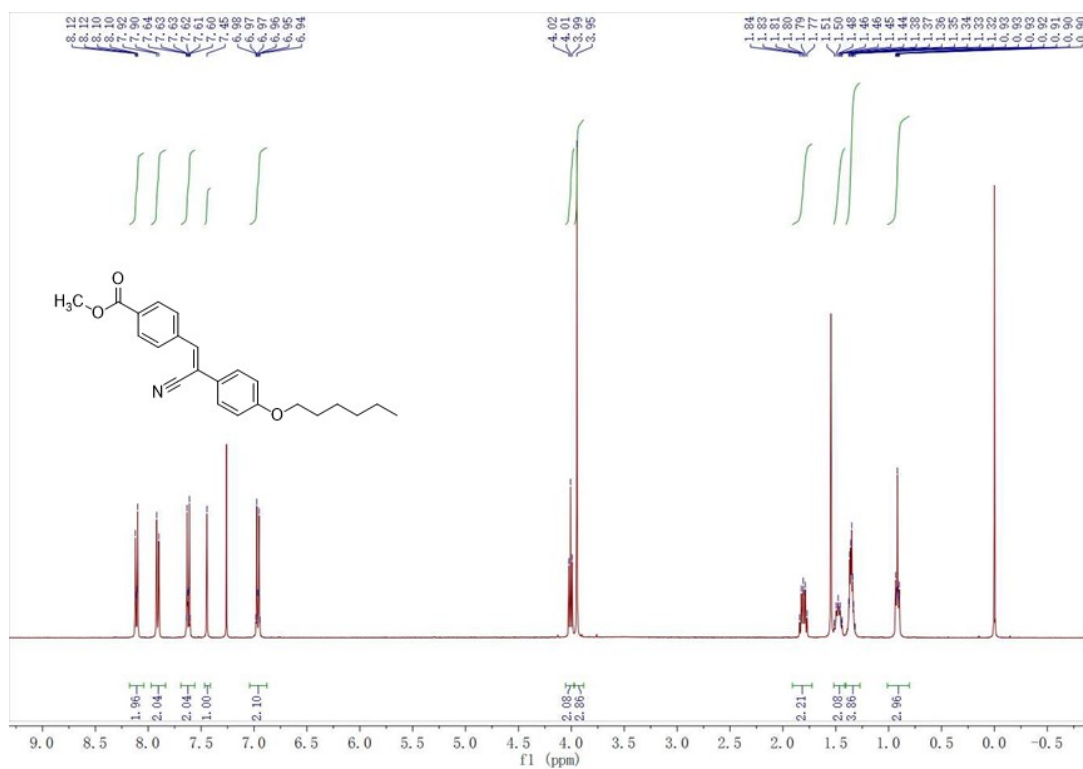


Fig. S14 <sup>1</sup>H NMR of E-CYS (400 MHz, CDCl<sub>3</sub>).

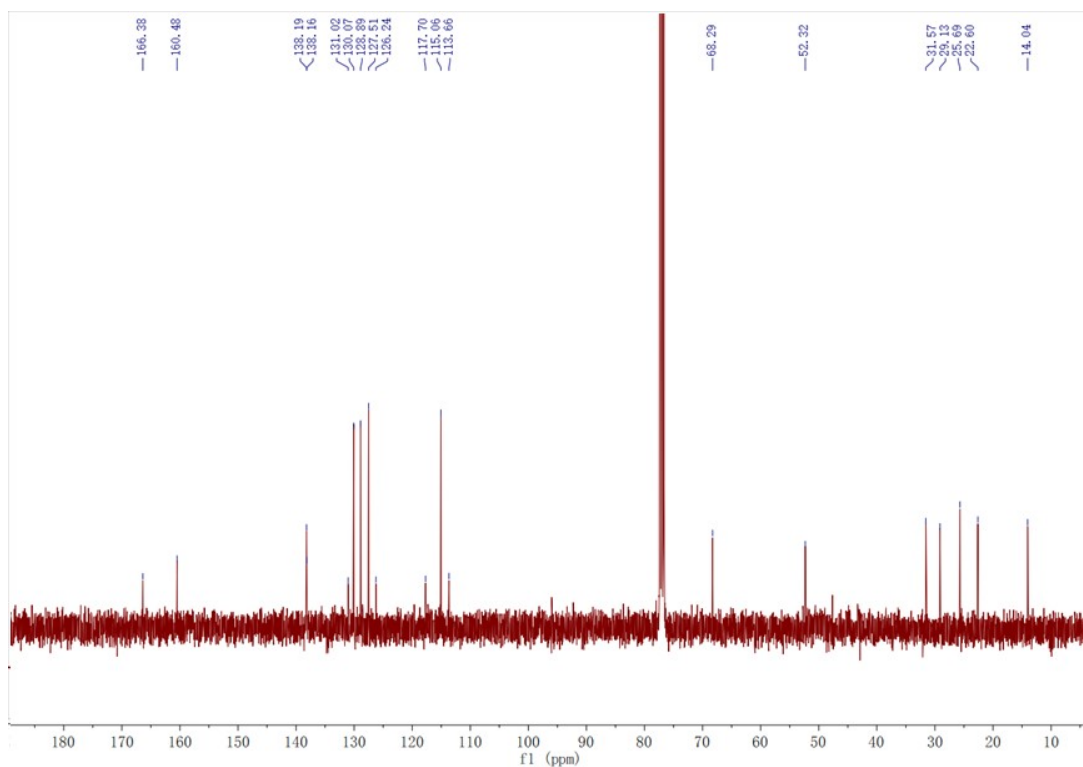
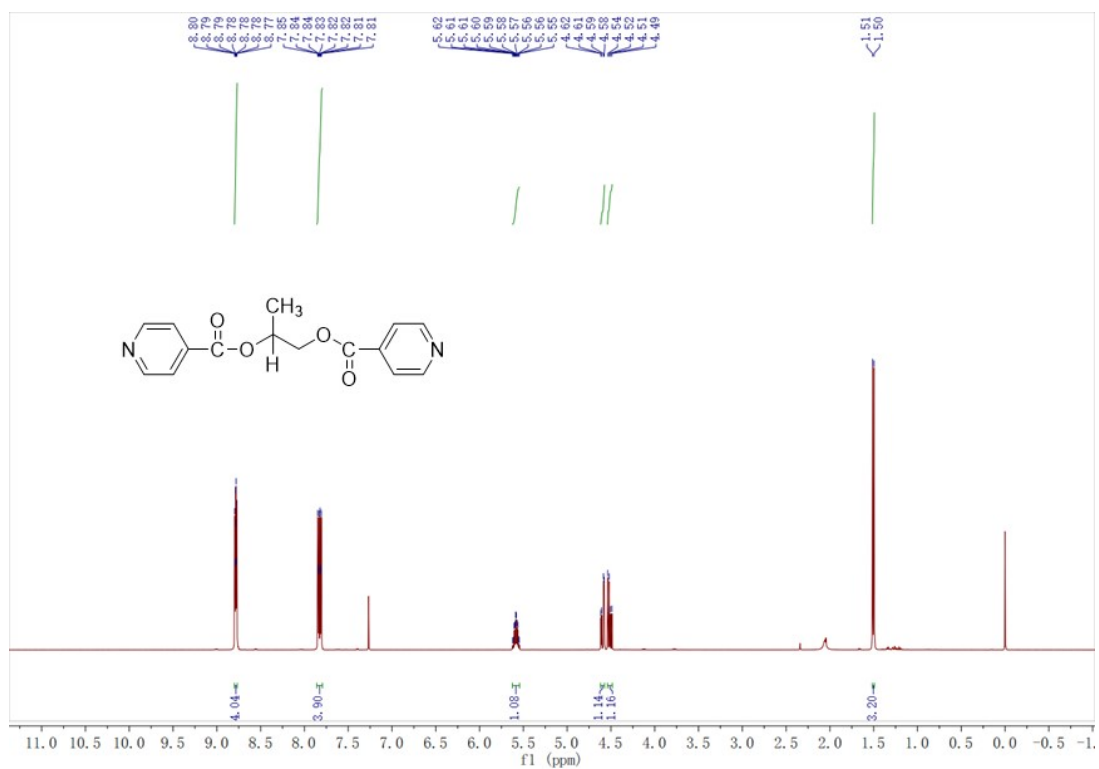
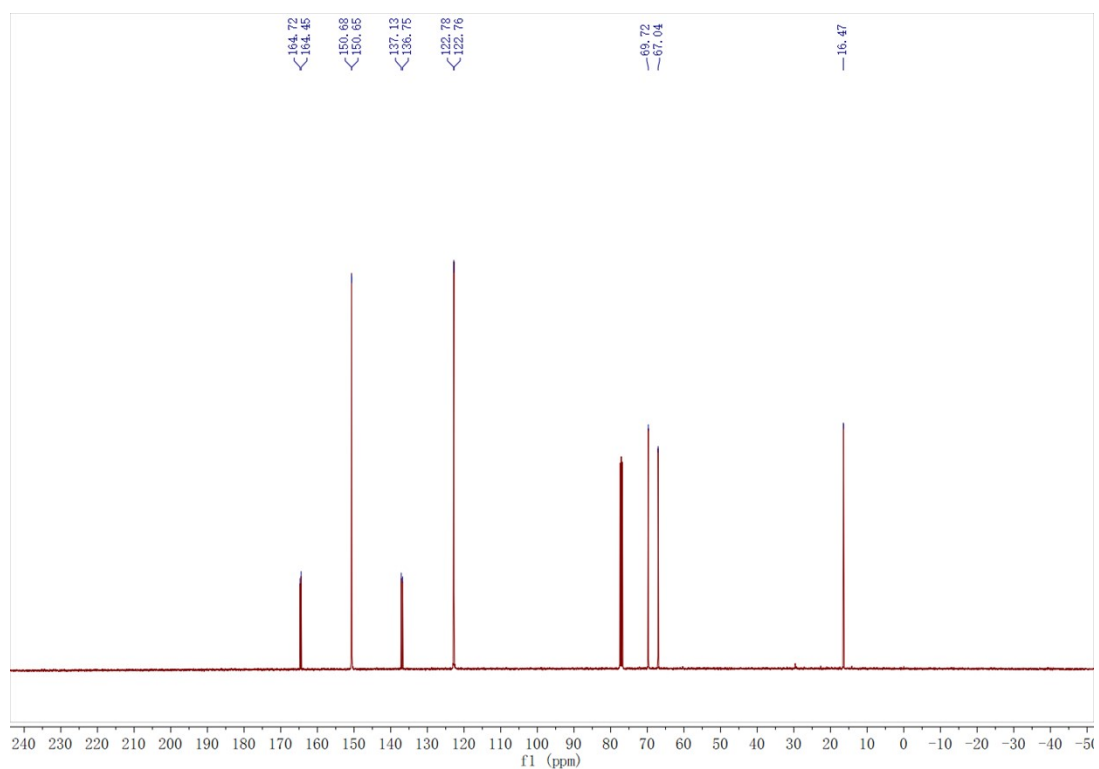


Fig. S15 <sup>13</sup>C NMR of E-CYS (100 MHz, CDCl<sub>3</sub>).



**Fig. S16**  $^1\text{H}$  NMR of *R*-PIN (400 MHz,  $\text{CDCl}_3$ ).



**Fig. S17**  $^{13}\text{C}$  NMR of *R*-PIN (100 MHz,  $\text{CDCl}_3$ ).

## 14. References

S1 D. Yang, P. F. Duan, L. Zhang and M. H. Liu, *Nat. Commun.*, 2017, **8**, 15727.