Electronic Supplementary Material (ESI) for ChemComm.

SUPPORTING INFORMATION

Strong CPL of Achiral Liquid Crystal Fluorescent Polymer *via* Regulation of AIE-active Chiral Dopant

Kerui Liu,[a,b] Yihao Shen,[b] Xiaojing Li,[a] Yu Zhang,[b] Yiwu Quan*[b] and Yixiang Cheng*[a]

[a] Key Lab of Mesoscopic Chemistry of MOE and Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China. *E-mail: yxcheng@nju.edu.cn

[b] Key Laboratory of High-Performance Polymer Material and Technology of Ministry of Education, Department of Polymer Science and Engineering, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China. *E-mail: quanyiwu@nju.edu.cn

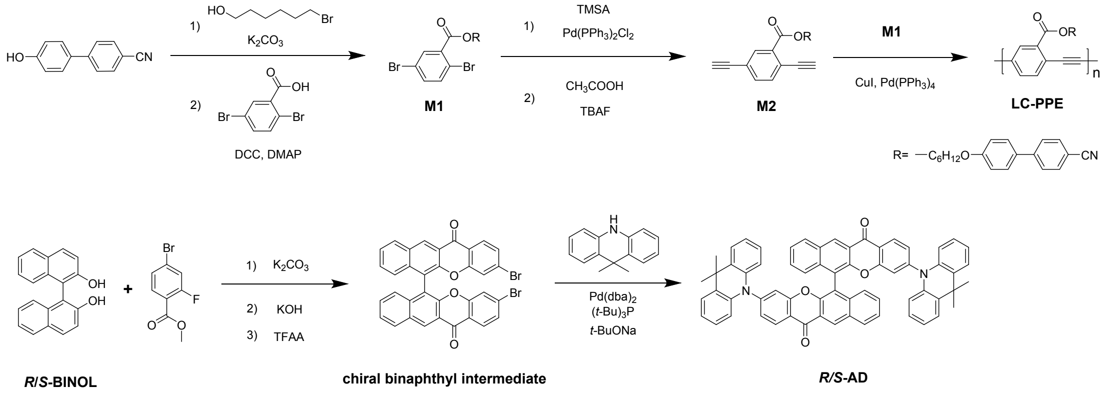
Table of Contents

1. **Instrumentation and Materials**
2. **Synthesis of LC-PPE and *R/S*-AD**
3. **Fluorescence spectra and UV-*vis* spectra of LC-PPE and *R/S*-AD**
4. **TGA and DSC Curves of LC-PPE**
5. **POM images of LC-PPE, CLCs and PD-CLCs**
6. **CD and CPL spectra of *R/S*-AD**
7. **CD spectra of CLCs**
8. **Fluorescence spectra of CLCs and PD-CLCs**
9. **CD spectra of PD-CLCs**
10. **^{1}H NMR and ^{13}C NMR spectra of compounds**

1. Instrumentation and Materials

NMR spectra were measured in $CDCl_3$ using Bruker AVANCE III-400 spectrometer with 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR. Chemical shifts are reported as parts per million (ppm) relative to tetramethylsilane (TMS; $\delta = 0$) as the internal reference. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were carried out by using a PerkinElmer Pyris-1 instrument under N_2 atmosphere. UV-visible (UV-*vis*) absorption spectra were obtained by using a Hitachi U-3900 spectrophotometer. Fluorescence (FL) spectra were recorded on a HORIBA Scientific Fluoromax-4 Spectrofluorometer. Circular dichroism (CD) spectra were measured by a JASCO *J*-810 Spectropolarimeter, and the length of the sample cell was 1 cm. Circularly polarized luminescence (CPL) spectra were measured by a JASCO CPL-300 Spectrofluoropolarimeter. The liquid crystalline textures were investigated and photographed using liquid crystal cells with a polarized optical microscope (POM) equipped with a Leitz-350 heating stage and an associated Nikon (D3100) digital camera. All starting materials were purchased from Energy, Acros, Bidepharm and used directly.

2. Synthesis of LC-PPE and *R/S*-AD



Scheme S1. The synthesis procedures of LC-PPE and *R/S*-AD.

Synthesis of M1

Into a 100 mL round-bottomed flask were added 1.50 g (7.68 mmol) of 4-(4-hydroxyphenyl)benzonitrile, 4.78 g (34.58 mmol) of K_2CO_3 and 30 mL acetonitrile. After all the reagents were dissolved, a solution of 6-bromo-1-hexanol (1.58 g, 8.45 mmol) was added to the flask. Then the solution was heated to 80 °C and refluxed under constant stirring. After the completion of the reaction, the solution was quenched by water and filtered. The white residue was dried under vacuum. Then, the white residue (2.20 g, 7.46 mmol), 2,5-dibromobenzoic acid (1.74 g, 6.22 mmol), DCC (5.77 g, 27.97 mmol) and DMAP (75.9 mg, 0.62 mmol) were added into a 100 mL round-bottomed flask, dissolved in CH_2Cl_2 (40 mL) and then stirred for 6 h. The solution was evaporated and purified by open column chromatography (silica gel, PE/EA = 40 : 1 as eluent). The collected liquid was evaporated and dried under vacuum to give **M1** (2.49 g, 6.22 mmol) as a white powder. Yield = 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (t, J = 4.5 Hz, 1H), 7.73 – 7.60 (m, 4H), 7.57 – 7.48 (m, 3H), 7.44 (dd, J = 8.5, 2.4 Hz, 1H), 7.04 – 6.93 (m, 2H), 4.36 (t, J = 6.6 Hz, 2H), 4.03 (t, J = 6.4 Hz, 2H), 1.90 – 1.75 (m, 4H), 1.62 – 1.50 (m, 4H).

Synthesis of M2

M1 (1.50 g, 2.69 mmol), $Pd(PPh)_2Cl_2$ (94.5 mg, 0.13 mmol) and CuI (51.3 mg, 0.27 mmol) were added in 10 mL Et_3N and 10 mL THF under Ar atmosphere. After continuous stirring, trimethylsilylacetylene (0.78 g, 8.07 mmol) and 5 mL THF was added to the solution. Then the solution was heated to 65 °C and left overnight. TLC indicated completion of the reaction. The solution was evaporated and purified by open column chromatography (silica gel, PE/EA = 40 : 1 as eluent). After removing the solvent, the white residue was added to a 100 mL round-bottom flask along with glacial acetic acid (0.21 g, 3.58 mmol), and 20 mL THF. After dissolving the reagents under constant stirring, the flask was placed in an ice bath, and TBAF (1.40 g, 5.37 mmol) was added dropwise to the above solution in the flask. After continuous stirring for 1 h, the solution was evaporated, and the residue was thoroughly washed with water and extracted with CH_2Cl_2 (30 mL) for three times. The organic layers were dried over anhydrous Na_2SO_4. The solution was evaporated and dried under vacuum to give **M2** (0.78 g, 1.74 mmol) as a yellow powder. Yield = 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.73 – 7.61 (m, 4H), 7.54 (dd, J = 17.5, 5.1 Hz, 4H), 7.04 – 6.92 (m, 2H), 4.37 (t, J = 6.6 Hz, 2H), 4.02 (t, J = 6.4 Hz, 2H), 3.48 (s, 1H), 3.21 (s, 1H), 1.90 – 1.78, 1.50 – 1.62 (m, 8H).

Synthesis of LC-PPE

Into a Schlenk flask were added **M1** (0.20 g, 0.36 mmol), CuI (6.83 mg, 35.89 μmol), $Pd(PPh_3)_4$ (20.74 mg, 17.94 μmol), and 3.0 mL THF under Ar atmosphere. After continuous stirring for 10 min, **M2** (0.16 g, 0.36 mmol) and 3.0 mL THF was added to the reaction solution. Then 2.0 mL Et_3N was added dropwise into the above solution. And the solution was heated to 70 °C and stirred for 24 h. The mixture was cooled to room temperature and was then filtered through a short silica gel column. After the solvent was removed, the mixture was dissolved in 2 mL CH_2Cl_2 and then added dropwise to 200 mL MeOH to precipitate the polymer. The polymer was filtered and washed with methanol several times and finally dried in vacuum to give 100.8 mg as a yellow solid with 64% yield. Mw: 21,420, Mw/Mn (PDI): 1.3 (GPC, PS calibration). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.03 (br, 1H), 7.73 – 7.35 (br, 8H), 7.06 – 6.77 (br, 2H), 4.48 – 4.28 (br, 2H), 4.07 – 3.81 (br, 2H), 1.89 – 1.39 (br, 8H).

Synthesis of *R/S*-AD

The chiral binaphthyl intermediate (300 mg, 0.46 mmol), 9,9-dimethyl-9,10-dihydroacridine (387.4 mg, 1.85 mmol), t-BuONa (266.8 mg, 2.77 mmol), Pd(dba)$_2$ (26.6 mg, 0.04 mmol) and (*t*-Bu)$_3$P (0.21 mL, 10 w% in toluene, 0.09 mmol) were dissolved in 15 mL anhydrous toluene, and the mixture was stirred at 110 °C under Ar atmosphere for 16 h. Then the mixture was added to 50 mL water and extracted with ethyl acetate. The combined organic layers were washed with saturated brine, dried over anhydrous Na_2SO_4, and then concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/DCM/ethyl acetate = 40: 10: 1) following with recrystallization in methanol to give *R/S*-AD (370 mg, 88 %) as yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 2H), 8.57 (d, J = 8.4 Hz, 2H), 8.23 (d, J = 8.3 Hz, 2H), 7.53 (dd, J = 11.1, 4.0 Hz, 2H), 7.41 (ddd, J = 16.0, 7.8, 1.4 Hz, 6H), 7.32 – 7.22 (m, 4H), 6.99 – 6.83 (m, 10H), 6.26 (dd, J = 7.7, 1.6 Hz, 4H), 1.58 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ=177.39, 158.57, 150.23, 148.16, 139.98, 136.35, 131.57, 130.47, 129.84, 129.81, 129.49, 129.36, 126.30, 125.91, 125.38, 125.26, 121.57, 121.45, 120.17, 118.65, 118.41, 115.05, 36.14, 30.93.

3. Fluorescence spectra and UV-*vis* spectra of LC-PPE and *R/S*-AD

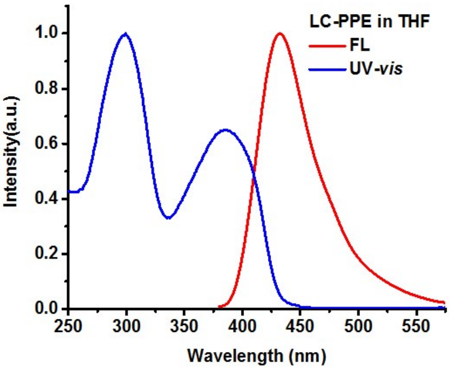


Fig. S1 The UV-*vis* absorption and fluorescence emission spectra of LC-PPE in the THF solution (1.0×10^{-5} mol L^{-1}, λ_{ex} = 300 nm).

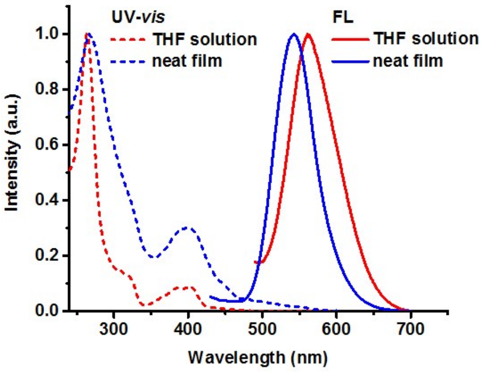


Fig. S2 The UV-*vis* absorption and fluorescence emission spectra of *R*-AD in the THF solution (1.0×10^{-5} mol L^{-1}, λ_{ex} = 373 nm) and neat film (λ_{ex} = 385 nm).

4. TGA and DSC Curves of LC-PPE

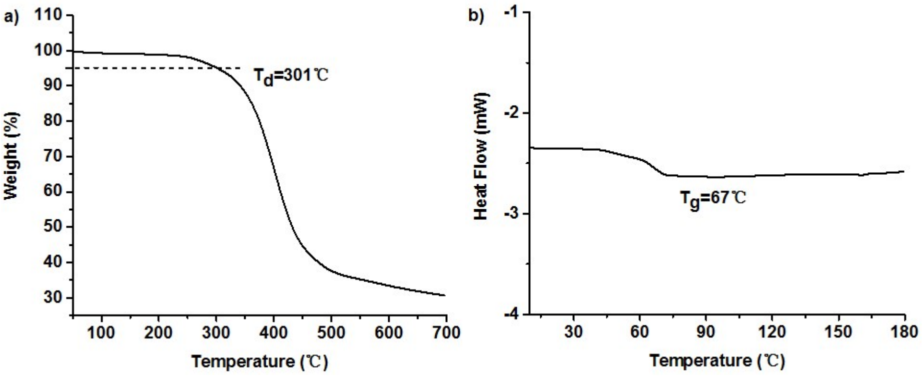


Fig. S3 a) TGA and b) DSC curves of LC-PPE.

5. POM images of LC-PPE, CLCs and PD-CLCs

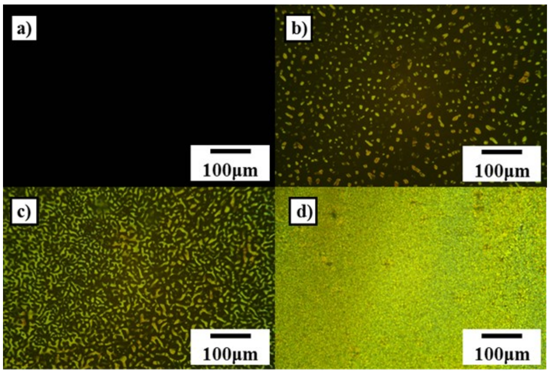


Fig. S4 POM images of LC-PPE upon cooling down from the isotropic melting at a rate of 20 °C/min, with temperatures respectively at a) 160 °C, b) 155 °C, c) 150 °C, and d) 145 °C.

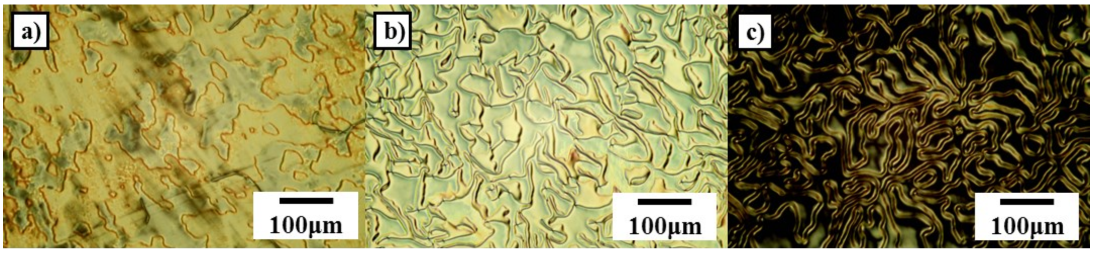


Fig. S5 POM images of CLCs doped with a) 0.5, b) 2.0, c) 3.0 wt% *R*-AD in flat cells at 25 °C.

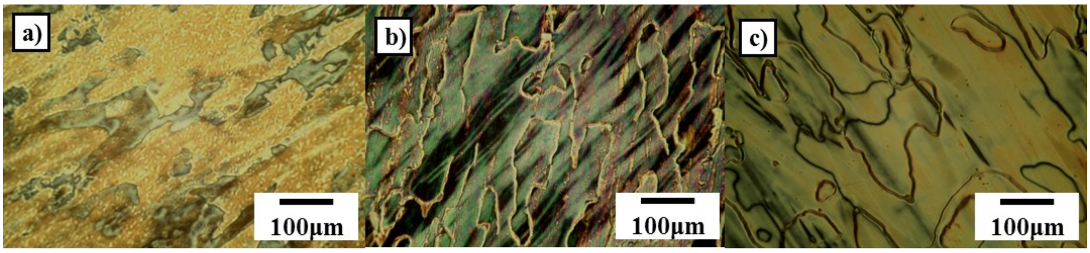


Fig. S6 POM images of PD-CLCs doped with 1.0 wt% *R*-AD and LC-PPE of a) 2.0, b) 4.0, c) 6.0 molar ratio in flat cells at 25 °C.

6. CD and CPL spectra of *R/S*-AD

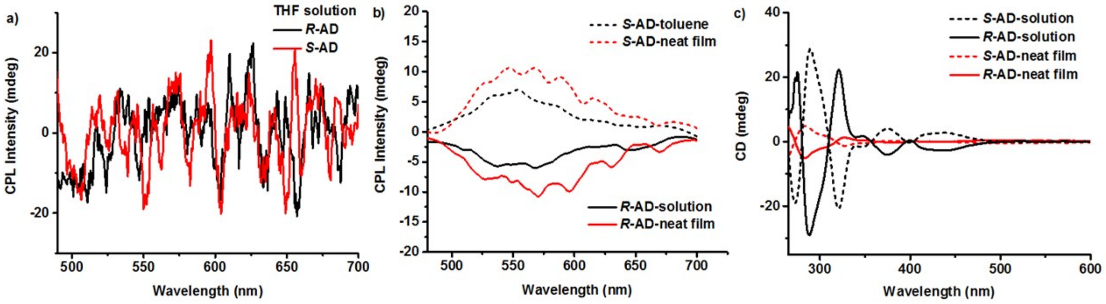


Fig. S7 a) CPL spectra of *R*/*S*-AD in THF (λ_{ex} = 373 nm, 1.0×10^{-4} mol L^{-1}); b) CPL spectra of *R*/*S*-AD in toluene (λ_{ex} = 373 nm, 1.0×10^{-4} mol L^{-1}) and neat films (λ_{ex} = 385 nm); c) CD spectra of *R*/*S*-AD in toluene and neat films.

7. CD spectra of CLCs

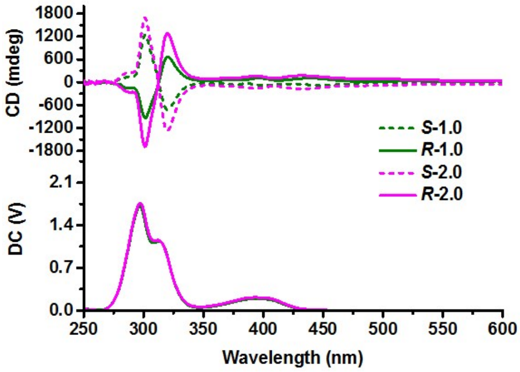


Fig. S8 CD spectra of CLCs (5CB doped with 1.0 and 2.0 wt% *R/S*-AD).

8. Fluorescence spectra of CLCs and PD-CLCs

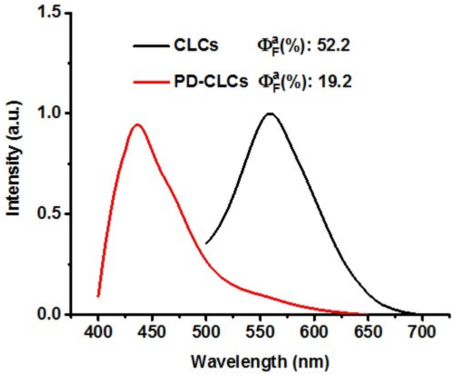


Fig. S9 Fluorescence emission spectra of CLCs (λ_{ex} = 380 nm) and PD-CLCs (λ_{ex} = 370 nm). CLCs of 5CB doped with 1.0 wt% *R*-AD; PD-CLCs of 5CB doped with 1.0 wt% *R*-AD and 2.0 molar ratio of LC-PPE in flat LC cells at 25 °C; ^{a} absolute quantum yields.

9. CD spectra of PD-CLCs

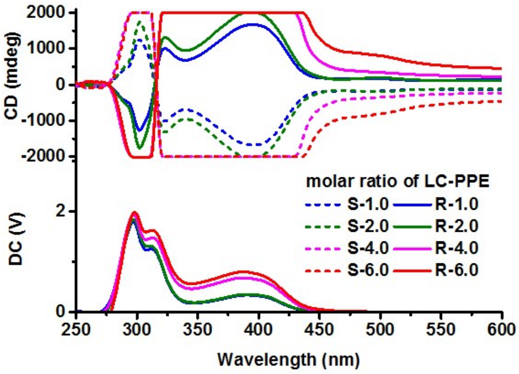


Fig. S10 CD spectra of PD-CLCs of 5CB doped with 1.0 wt% *R/S*-AD and 1.0, 2.0, 4.0, 6.0 molar ratio of LC-PPE in flat LC cells at 25 °C.

10. ^{1}H NMR and ^{13}C NMR spectra of compounds

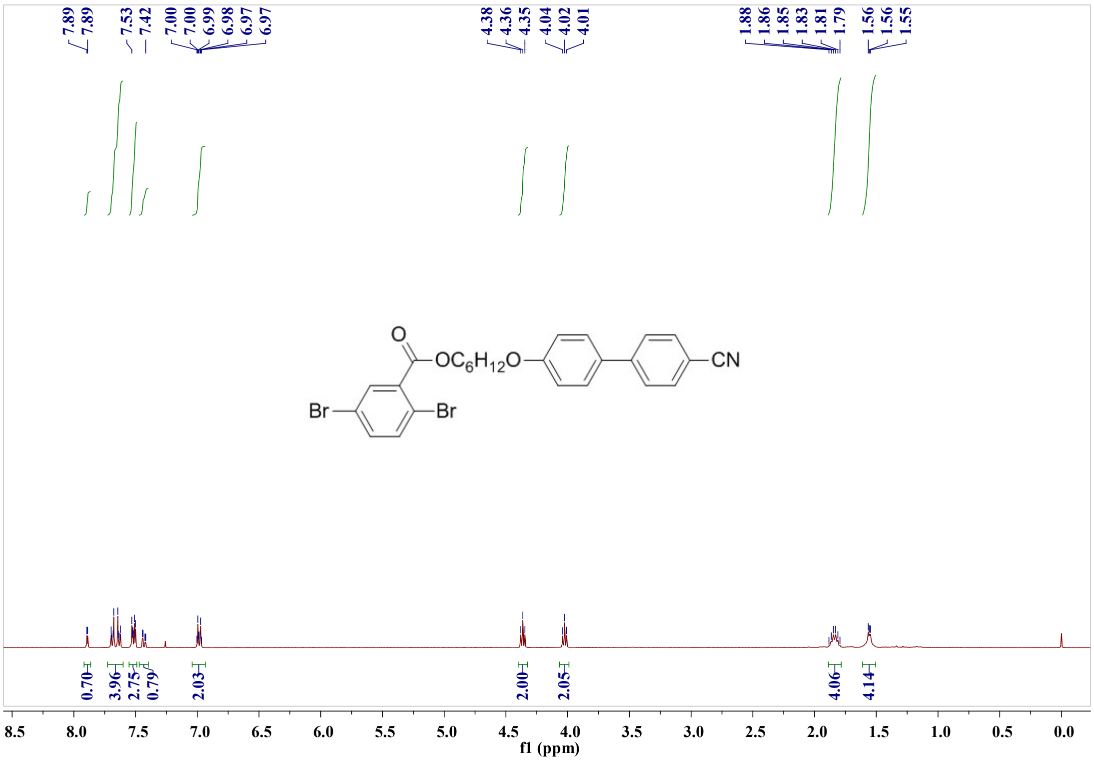


Fig. S11 ^{1}H NMR of M1 (400 MHz, $CDCl_3$).

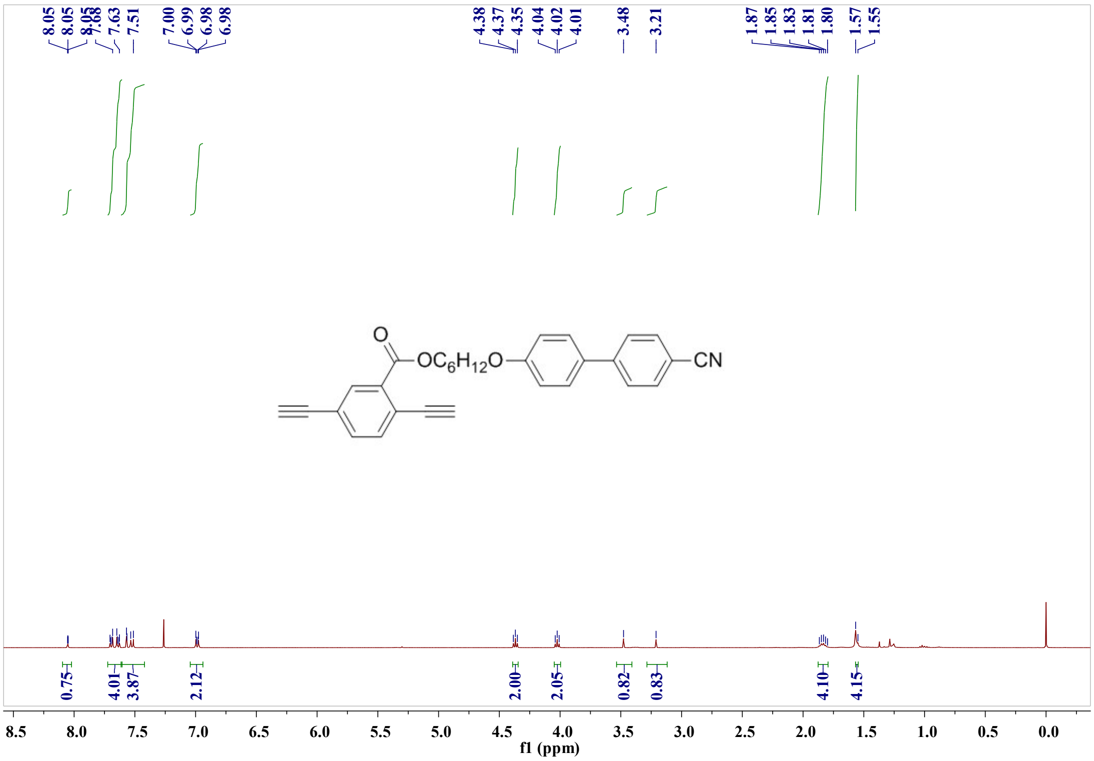


Fig. S12 ^{1}H NMR of M2 (400 MHz, $CDCl_3$).

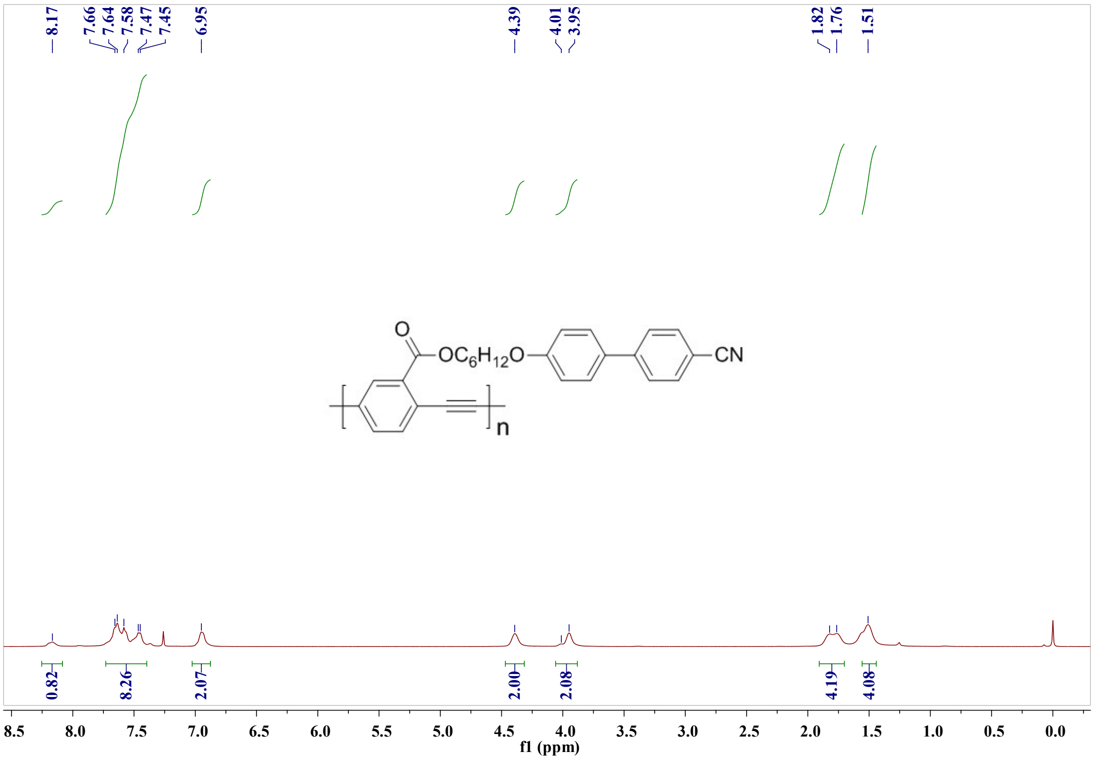


Fig. S13 ^{1}H NMR of LC-PPE (400 MHz, $CDCl_3$).

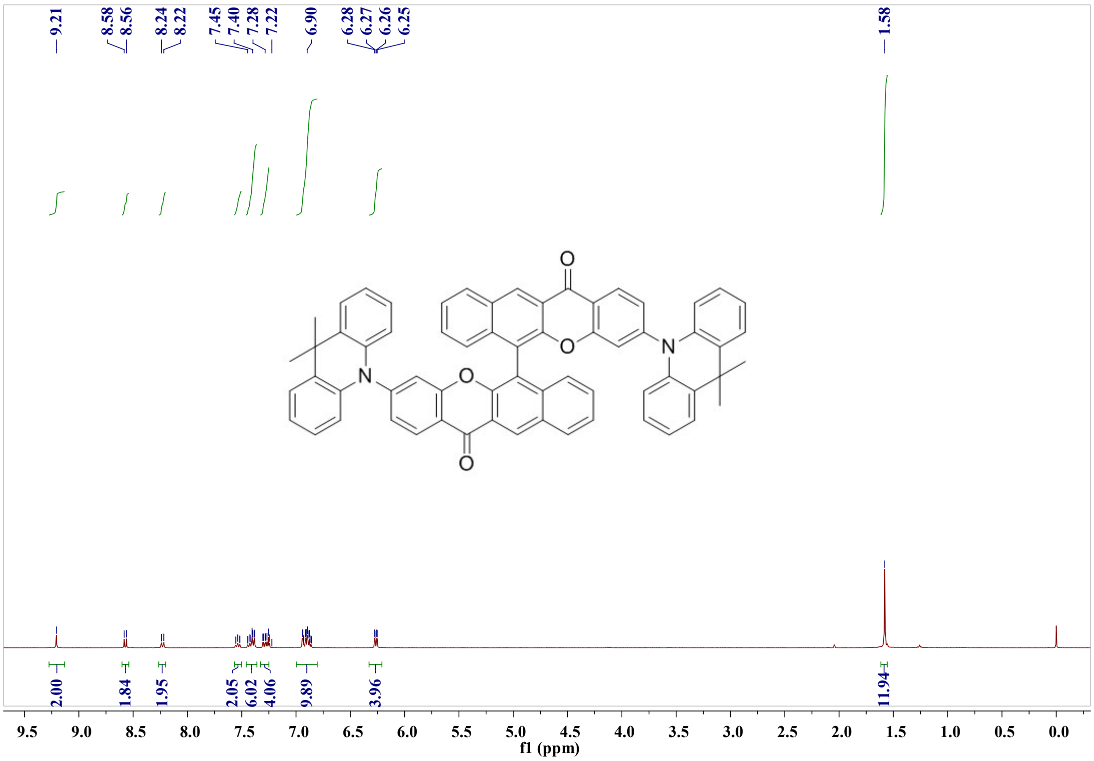


Fig. S14 ^{1}H NMR of *R/S*-AD (400 MHz, CDCl$_3$).

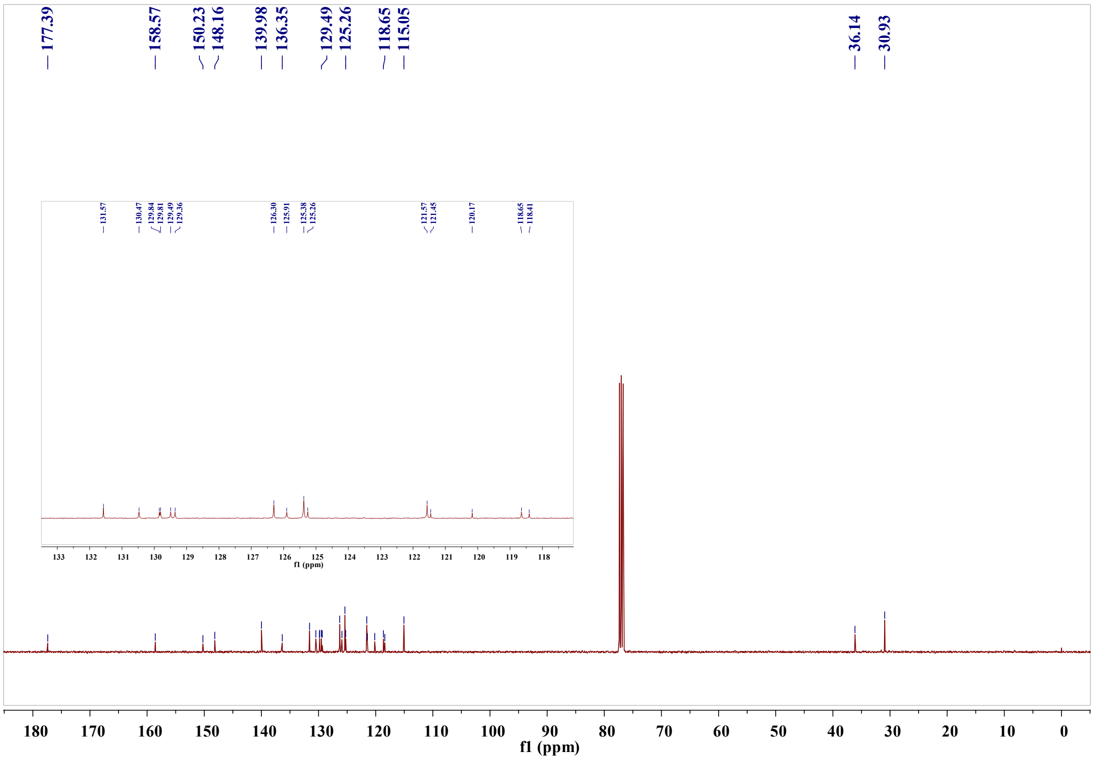


Fig. S15 ^{13}C NMR of *R/S*-AD (100 MHz, CDCl$_3$).