Electronic Supplementary Information

Circularly Polarized Organic Room Temperature Phosphorescence Activated by Liquid Crystalline Polymer Network

Ao Huang [a], Jiang Huang [a], Hui-Yin Luo [a], Zhi-Wang Luo [a], Pu Wang [a], Ping Wang [a] *, Yan Guan [b], He-Lou Xie [a] *

[a] *Key Lab of Environment-friendly Chemistry and Application in Ministry of Education, and Key Laboratory of Advanced Functional Polymer Materials of Colleges, Universities of Hunan Province and College of Chemistry, Xiangtan University, Xiangtan Hunan, 411105, China.*

[b] *Beijing National Laboratory for Molecular Sciences, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Center for Soft Matter Science and Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

**To whom the correspondence should be addressed.*

E-mail: 90wangpu@xtu.edu.cn，395658023@qq.com (PW)，and and xhl20040731@163.com (HLX)

Materials. 2-Bromocarbazole (97%, Energy Chemical), 1, 4-Dibromobutane (97%, Energy Chemical), 1,8-Dibromooctane (97%, Energy Chemical), 1,12-Dibromododecane (97%, Energy Chemical), Tetrabutylammonium bromide (TBAB) (99%, Energy Chemical), Dibenzo[b,d]furan-4-yl boronic acid (98%, Bidepharm), Tetrakis(triphenylphosphine) palladium (99%, Energy Chemical), (R)-1,1'-Bi-2-naphthol (98%, Energy Chemical), (S)-1,1'-Bi-2-naphthol (98%, Energy Chemical), Sodium hydroxide(NaOH) (AR, Damao Chemical Reagent Factory), Sodium sulfate

($NaSO_4$) (AR, Tianjin Kemiou Chemical Reagent Co., Ltd.), Sodium carbonate ($NaCO_3$) (AR, Chron Chemical), Potassium carbonate(KCO_3) (AR, Tianjin Kemiou Chemical Reagent Co., Ltd.), Potassium iodide(KI) (AR, Tianjin Kemiou Chemical Reagent Co., Ltd.), Acetone (AR, Fuyu Chemical), E7 (AR, Hecheng Display), 2-Methyl-1,4-phenylene bis(4-(((4-(acryloyloxy)butoxy)carbonyl)oxy)benzoate) (LC-242) (97%, Energy Chemical), 2,2-Dimethoxy-2-phenylacetophenone (DMPA) (98%, Energy Chemical) were directly used without any treatment. Toluene was refluxed with metal sodium and distilled before used.

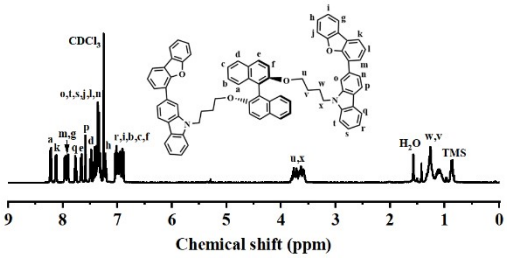
Instruments and Measurements.

The ^{1}H NMR and ^{13}C NMR experiments were carried out on a Bruker ARX400 spectrometer using deuterated chloroform ($CDCl_3$) as solvent and tetramethylsilane (TMS) as internal standard (frequency: 400 MHz). Matrix assisted laser desorption ionization tandem flight time mass spectrometry (MALDI-TOF) were determined on a Bruker Daltonics BIFLEX Ⅲ MALDI-TOF analyzer. Fourier transform infrared spectroscopy (FTIR) spectra were determined by a PE Spectrum on FTIR spectrometer under the powder state. Differential scanning calorimetry (DSC) experiments was performed on TA DSC Q100 calorimeter. UV-vis absorption spectra were measured by Cary 60 with the Flashing xenon lamp as the light source. Emission spectra were obtained using spectrofluorometer F-4600 with 1 cm quartz cuvettes. The UV irradiation light source is a hand-held ultraviolet lamp of 365 nm UV LED (FUWO, FUV-6BK 800 Wm^{-2}). Phosphorescence lifetime data were obtained on Horiba

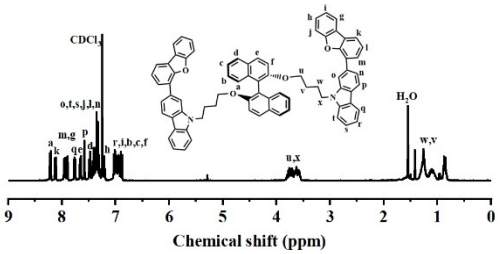
Deltaflex equipped with a microsecond flash-lamp and analyzed by DAS6 Analysis. The LC texture of the sample was investigated under polarized optical microscopy (Leica DMLM-P) with hot stage (Mettler FP82HT). 1D WAXD curves were recorded on a Bruker D8 Advance diffractometer. Circularly polarized luminescent spectra were measured with JASCO CPL-200, and circular dichroism (CD) spectra were obtained with JASCO J-1500. The thin films were prepared by spin coating the solution of 15 mg/mL in toluene with 2.5 kr/min.

Computational Details:

Density functional theory (DFT) and Time-dependent DFT methods were used to optimize the geometric structure of ground state and excited state. The B3LYP[1-2] hybrid functional and 6-31g* basis set[3] were used in all calculations. All the calculations were performed using the Gaussian 09 program.[4] All theoretical calculation diagrams were drawn by VMD 1.9.4[5] and Multiwfn 3.7 programs.[6]


CDCl3
H2O
w,v
TMS
u,x
Chemical shift (ppm)

(a)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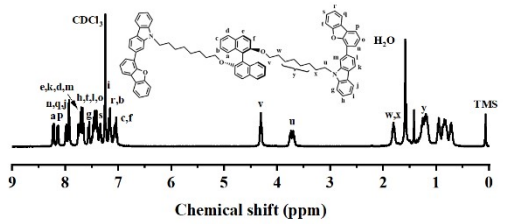
H2O
w,v
u,x
Chemical shift (ppm)

(b)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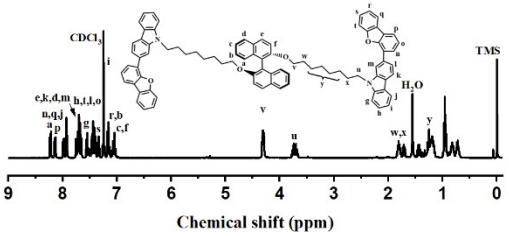
H2O
TMS
v
u
w,x
y
Chemical shift (ppm)

(c)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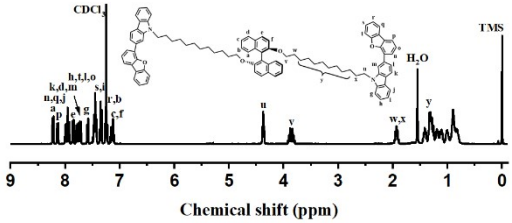
TMS
H2O
v
u
w,x
y
Chemical shift (ppm)

(d)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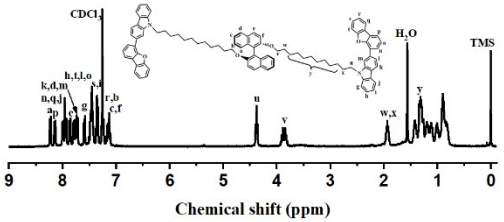
TMS
H2O
u
v
w,x
y
Chemical shift (ppm)

(e)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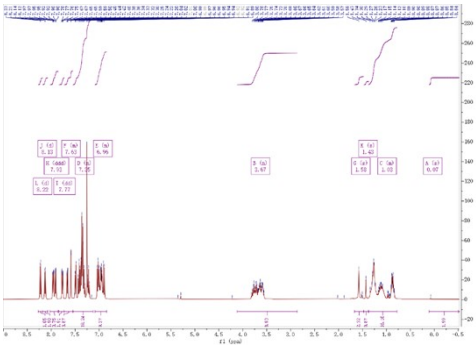
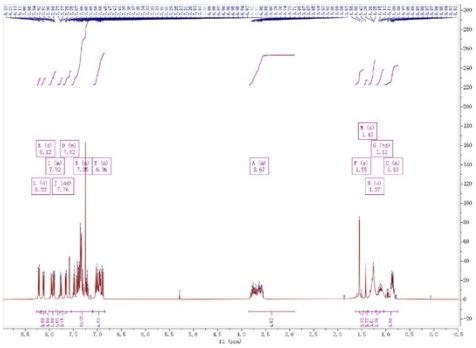
TMS
u
v
w,x
y
Chemical shift (ppm)

(f)



(g)



(h)

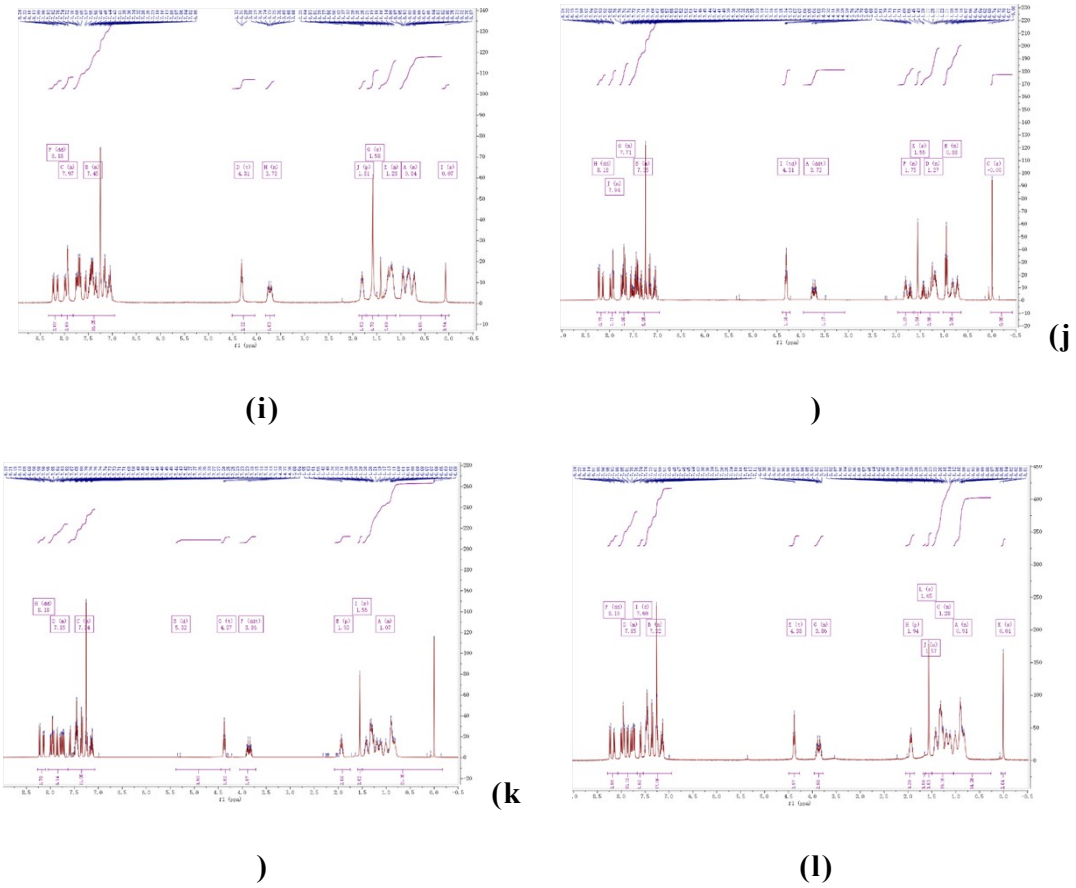
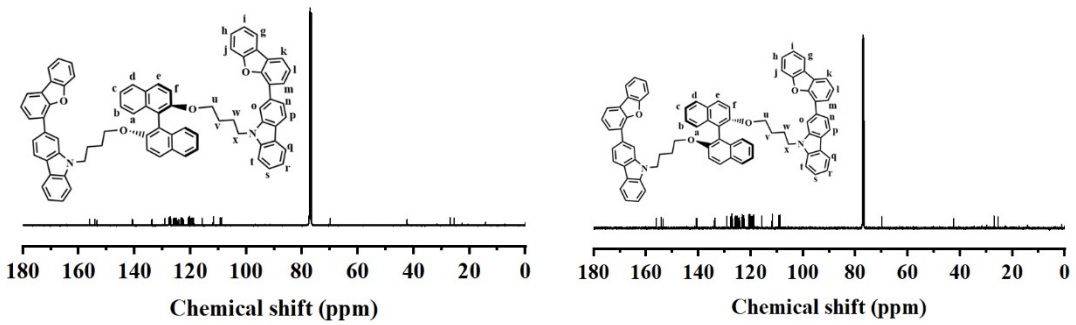
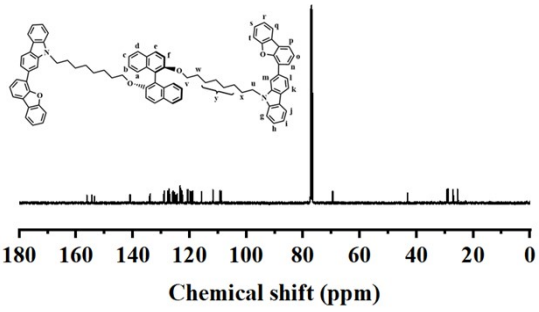


Figure S1. [1]HNMR of (R/S)-B-n-CzO. (a) (R)-B-4-CzO, (b) (S)-B-4-CzO, (c) (R)-B-8-CzO, (d) (S)-B-8-CzO, (e) (R)-B-12-CzO and (f) (S)-B-12-CzO; the coupling constants, integration, chemical shift of [1]H NMR data of (R/S)-B-n-CzO. (g) (R)-B-4-CzO, (h) (S)-B-4-CzO, (i) (R)-B-8-CzO, (j) (S)-B-8-CzO, (k) (R)-B-12-CzO and (l) (S)-B-12-CzO.



(a) **(b)**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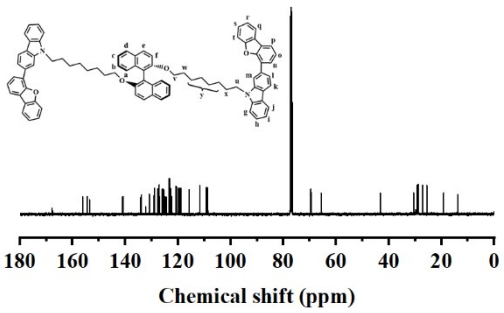
Chemical shift (ppm)

(c)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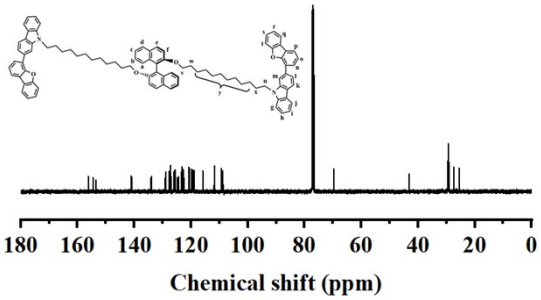
Chemical shift (ppm)

(d)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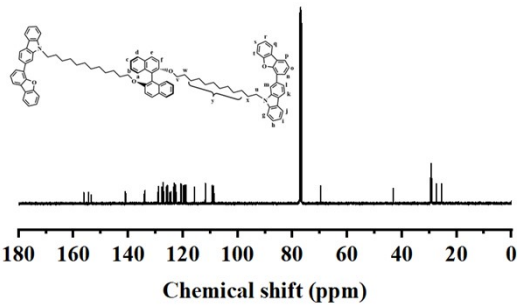
Chemical shift (ppm)

(e)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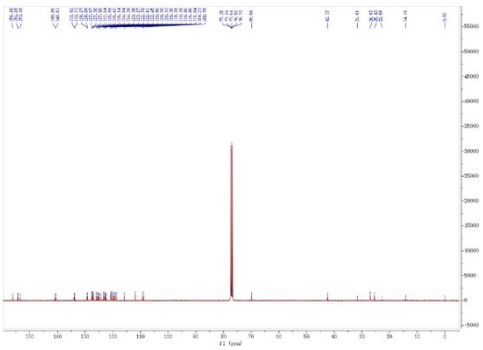
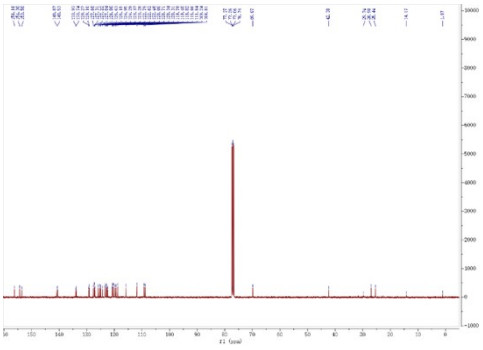
Chemical shift (ppm)

(f)



(g)



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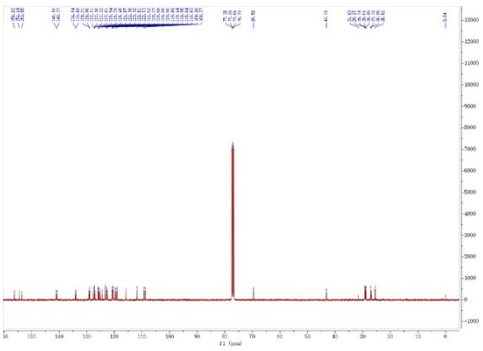
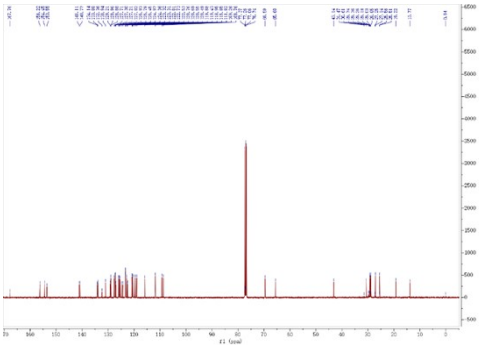
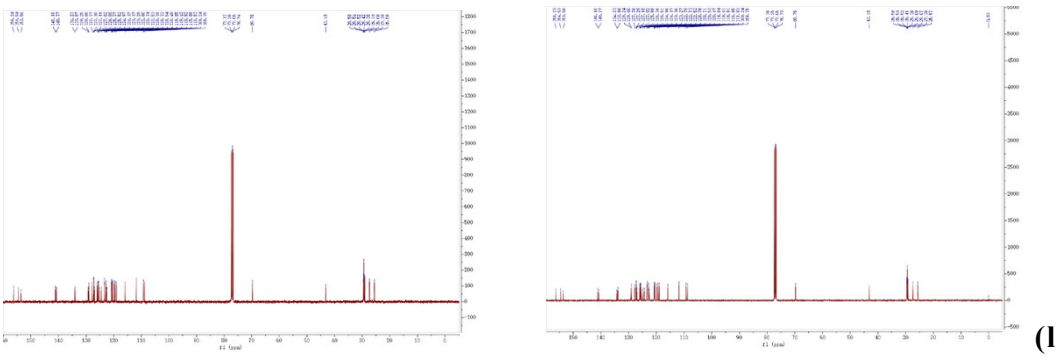


(i)



(j)



(k) (l)

Figure S2. ^{13}C NMR of (R/S)-B-n-CzO. (a) (R)-B-4-CzO, (b) (S)-B-4-CzO, (c) (R)-B-8-CzO, (d) (S)-B-8-CzO, (e) (R)-B-12-CzO and (f) (S)-B-12-CzO; the chemical shift of ^{13}C NMR of (R/S)-B-n-CzO. (g) (R)-B-4-CzO, (h) (S)-B-4-CzO, (i) (R)-B-8-CzO, (j) (S)-B-8-CzO, (k) (R)-B-12-CzO and (l) (S)-B-12-CzO.

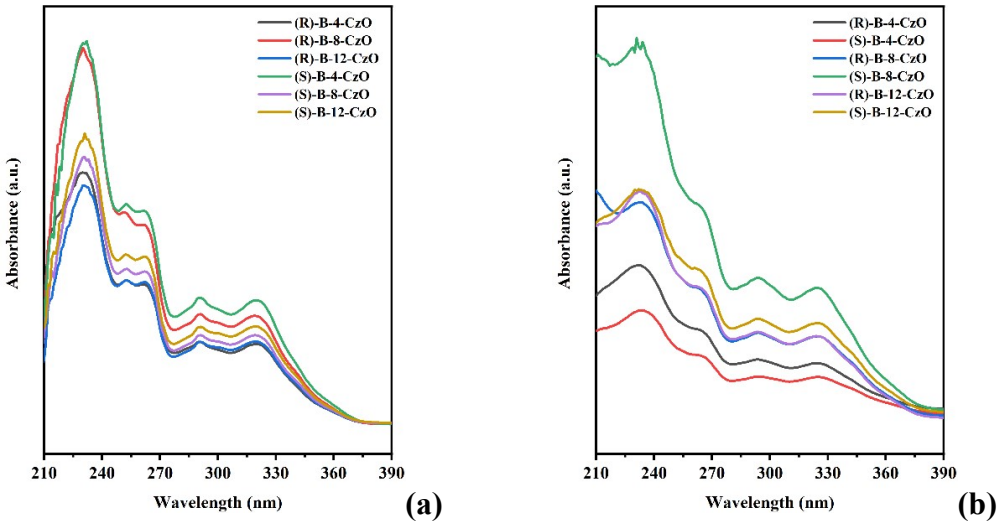


Figure S3. UV-Vis absorption of (R/S)-B-n-CzO in solution (a) and film (b).

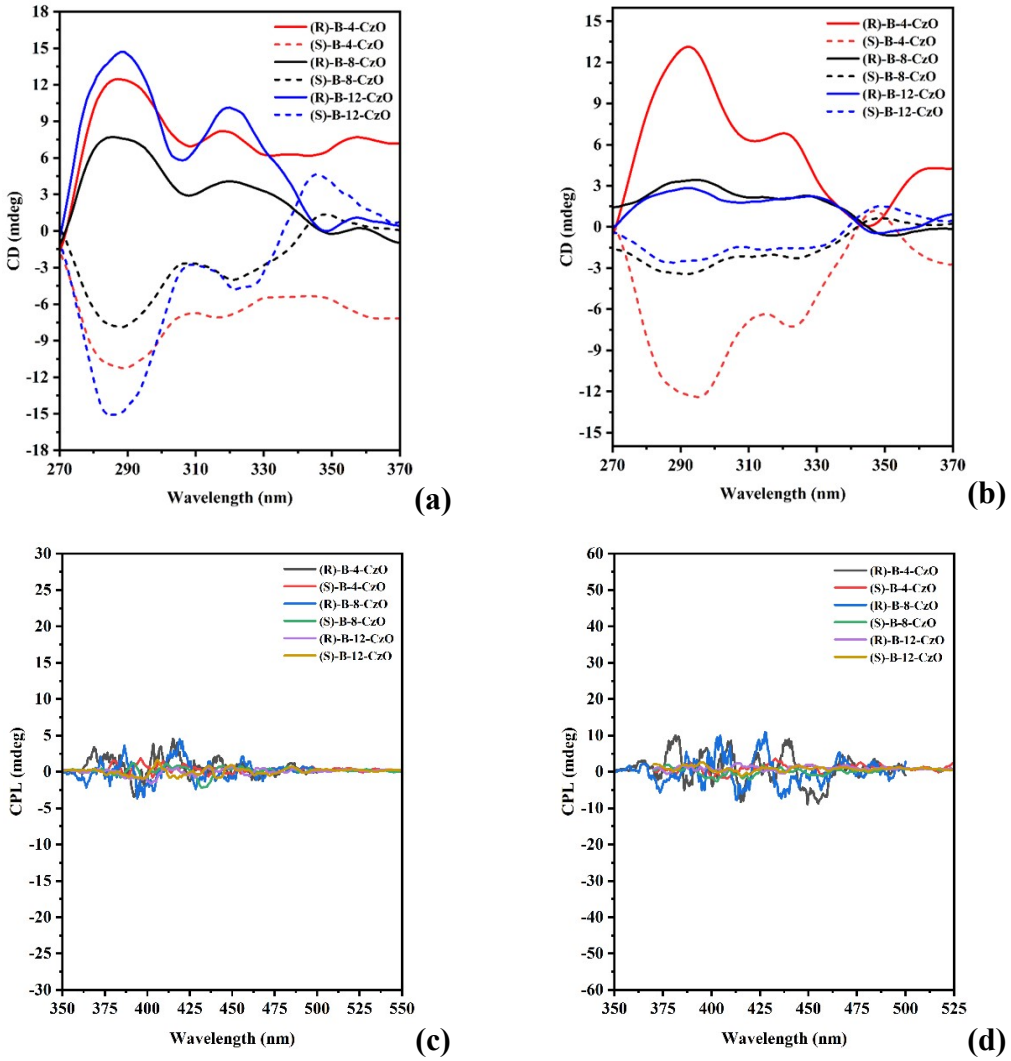


Figure S4. (a, b) CD spectra of (R/S)-B-n-CzO in solution (a) and film (b); (c, d) CPL spectra of (R/S)-B-n-CzO in solution (c) and film (d).

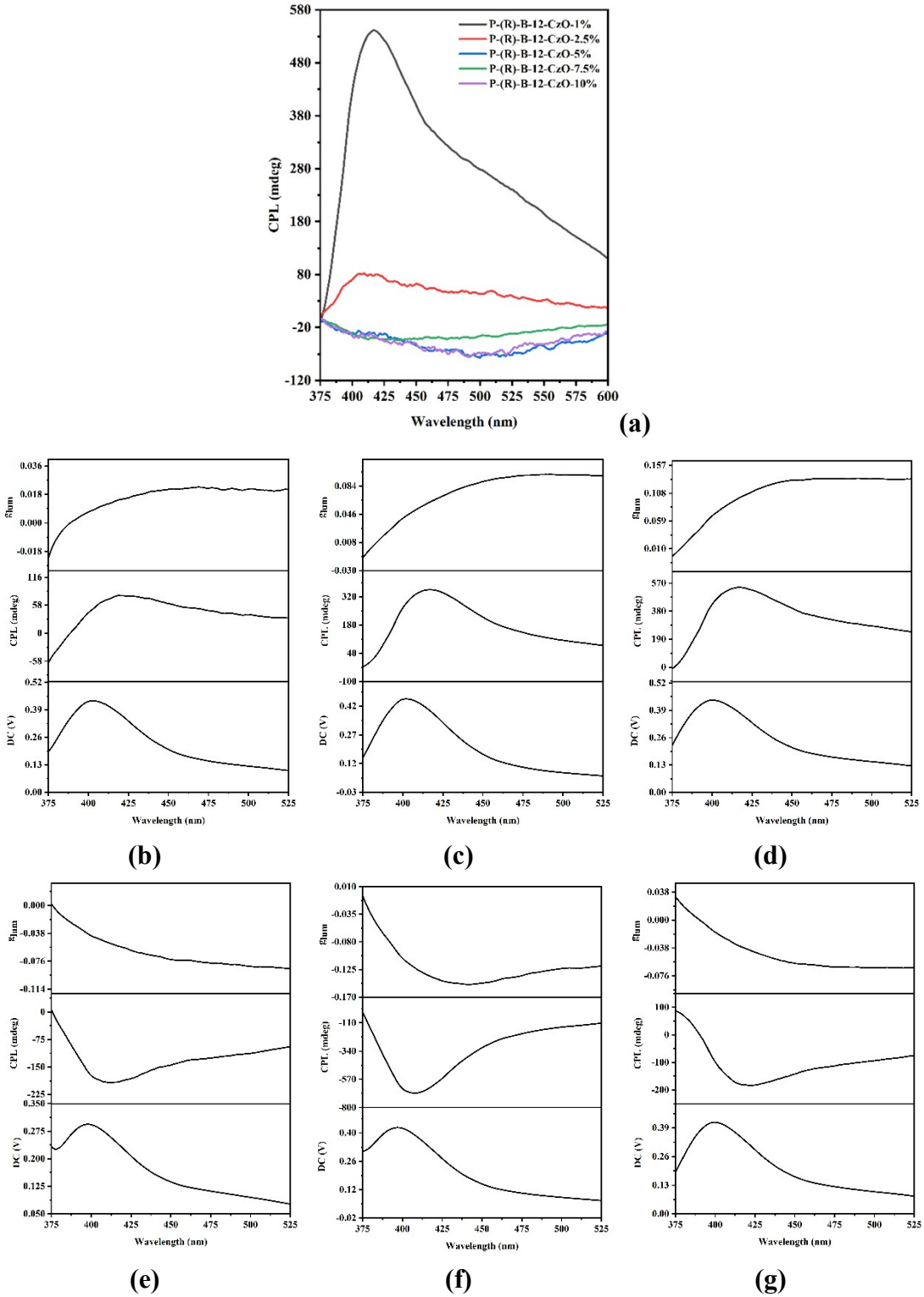


Figure S5. (a) CPL spectra of different concentrations of doped LC-242; (b-g) CPL spectra and g_{lum} of (b) P-(R)-B-4-CzO, (c) P-(R)-B-8-CzO, (d) P-(R)-B-12-CzO, (e) P-(S)-B-4-CzO, (f) P-(S)-B-8-CzO, (g) P-(S)-B-12-CzO.

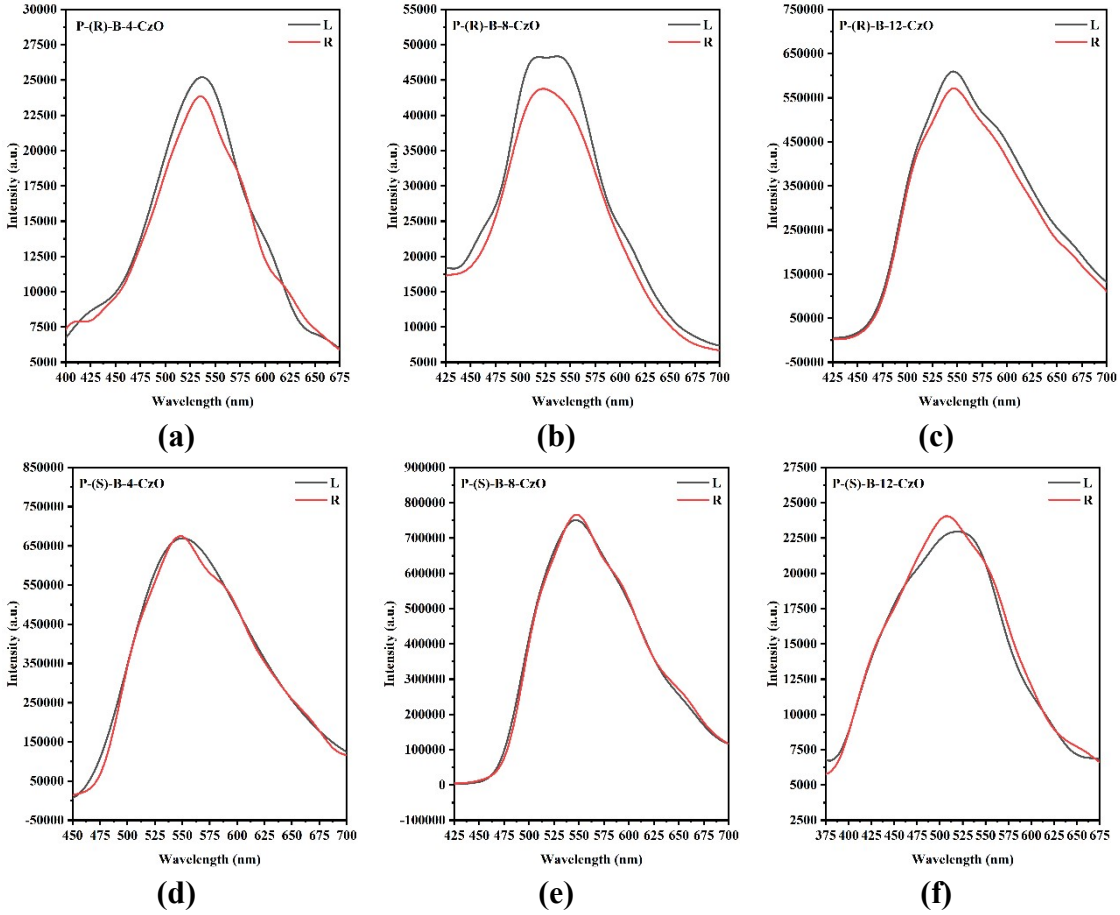


Figure S6. Phosphorescence emission spectra of P-(R/S)-B-n-CzO recorded with an L-CPF or R-CPF.

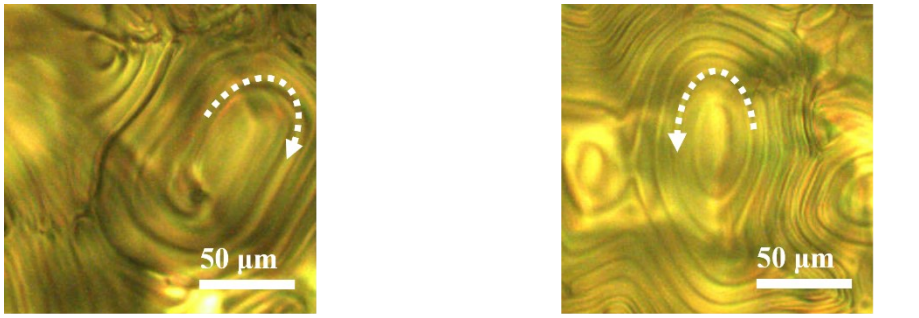


Figure S7. POM images of N*-LC films including (a) 5wt% (R)-B-4-CzO and (b) 5wt% (S)-B-4-CzO at room temperature.

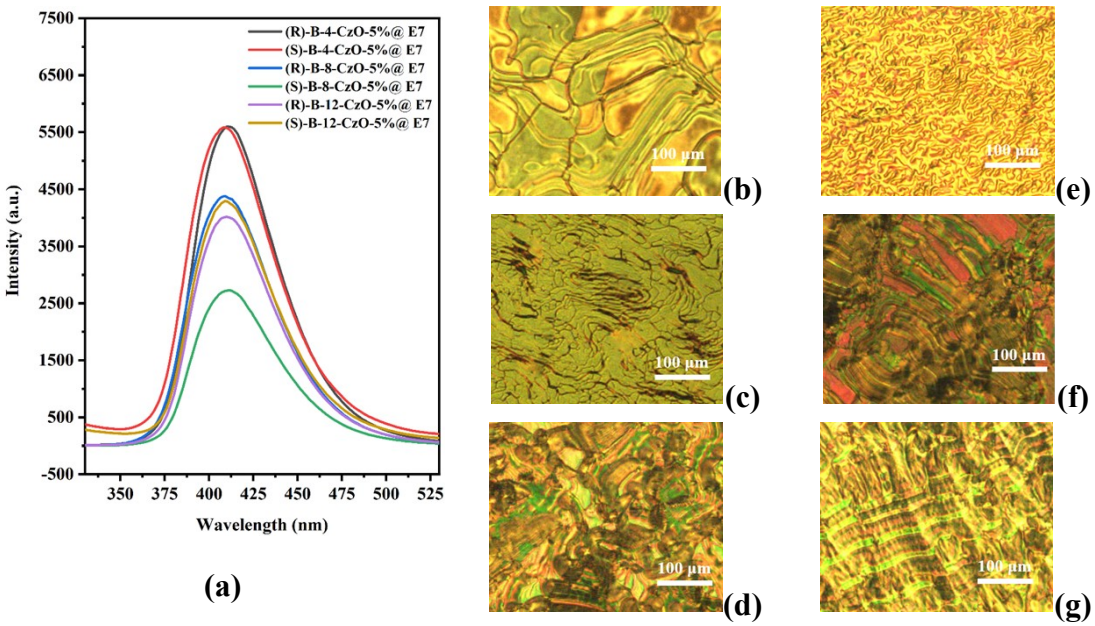


Figure S8. (a) Emission spectra of (R/S)-B-n-CzO-5%@E7; (b-g) the POM images of the mixture containing (b) (R)-B-4-CzO-5%@E7, (c) (R)-B-8-CzO-5%@E7, (d) (R)-B-12-CzO-5%@E7, (e) (S)-B-4-CzO-5%@E7, (f) (S)-B-8-CzO-5%@E7, (g) (S)-B-12-CzO-5%@E7.

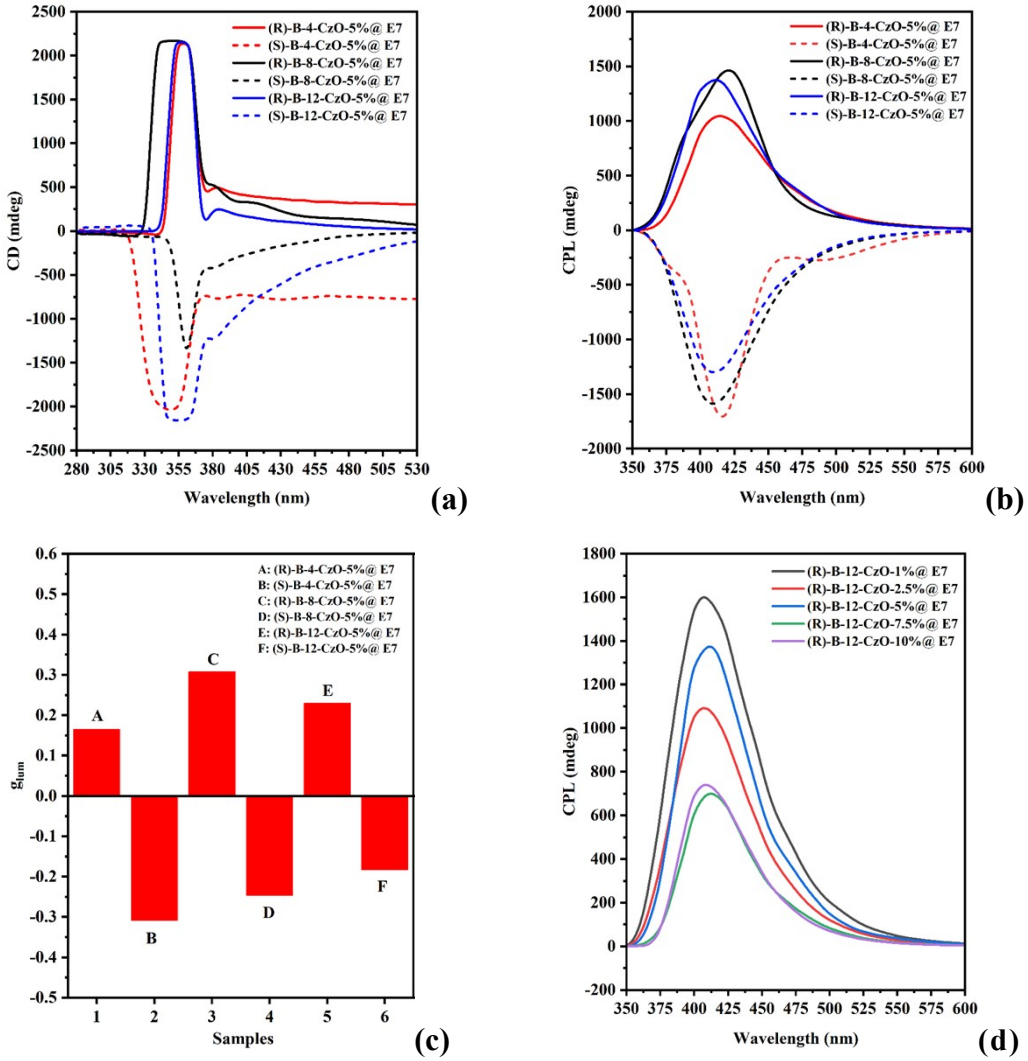


Figure S9. (a) CD spectra, (b) CPL spectra, (c) g_{lum} values of the (R/S)-B-n-CzO-5%@E7, (d) CPL spectra of different concentrations of doped E7.

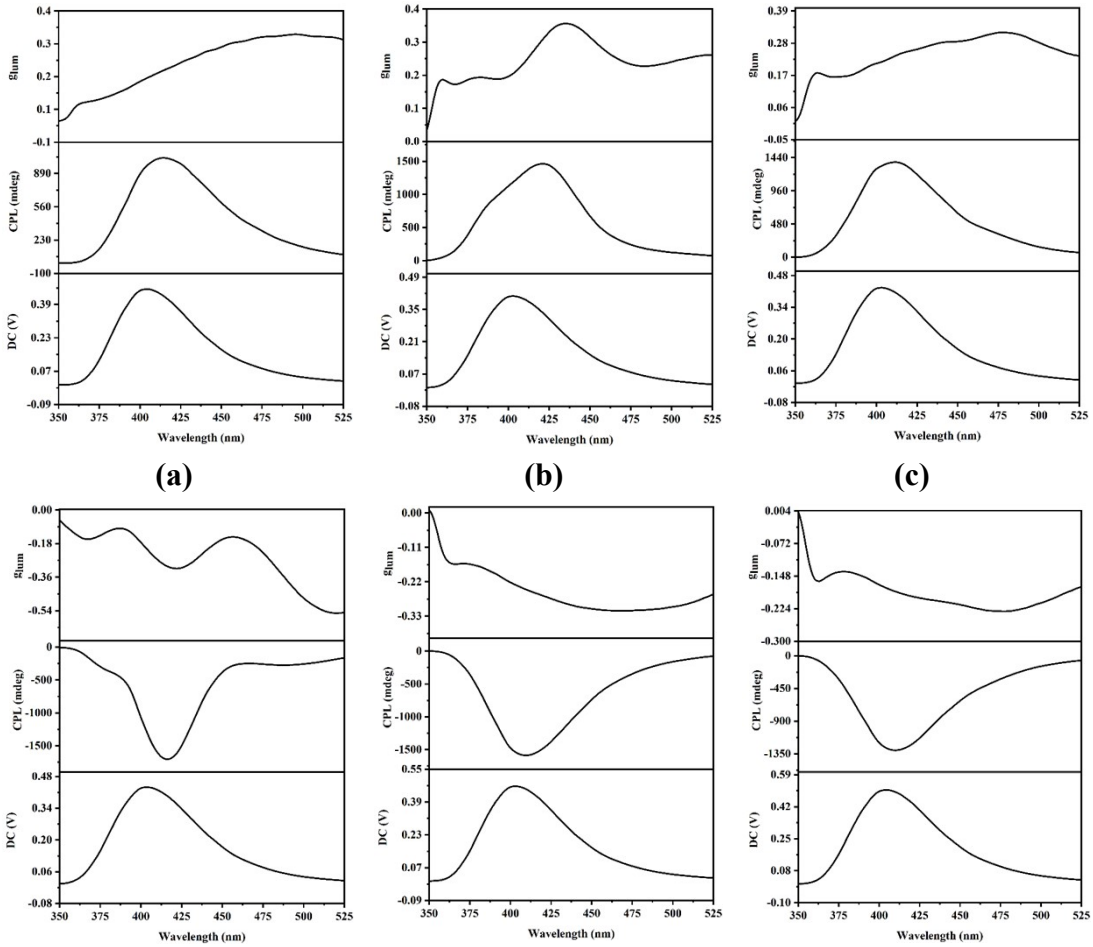


Figure S10. (a-f) CPL spectra and g_{lum} of (a) (R)-B-4-CzO-5%@E7, (b) (R)-B-8-CzO-5%@E7, (c) (R)-B-12-CzO-5%@E7, (d) (S)-B-4-CzO-5%@E7, (e) (S)-B-8-CzO-5%@E7, (f) (S)-B-12-CzO-5%@E7.

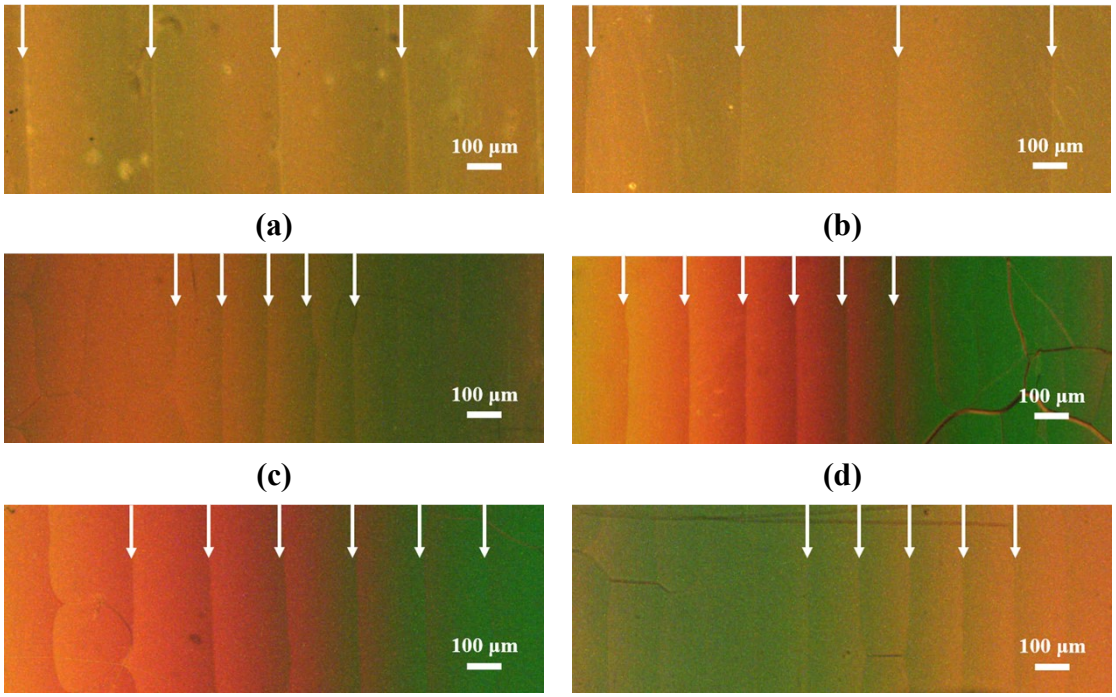


Figure S11. Images of Grandjean-Cano wedge cells (crossed polarizers) showing Grandjean steps (lines) of (a) (R)-B-4-CzO-5%@E7, (b) (S)-B-4-CzO-5%@E7, (c) (R)-B-8-CzO-5%@E7, (d) (S)-B-8-CzO-5%@E7, (e) (R)-B-12-CzO-5%@E7, (f) (S)-B-12-CzO-5%@E7.

Table 1. Helical Pitch (p) Values (μm) and HTP (β) values (μm^{-1}) of (R/S)-B-n-CzO-5%@E7.

	s/μm	p/μm	β/μm^{-1}
(R)-B-4-CzO-5%@E7	400.00	4.00	19.10
(S)-B-4-CzO-5%@E7	361.54	6.40	11.92
(R)-B-8-CzO-5%@E7	150.00	1.95	43.27
(S)-B-8-CzO-5%@E7	126.46	1.89	44.48
(R)-B-12-CzO-5%@E7	165.23	2.30	40.13
(S)-B-12-CzO-5%@E7	123.08	2.40	38.48

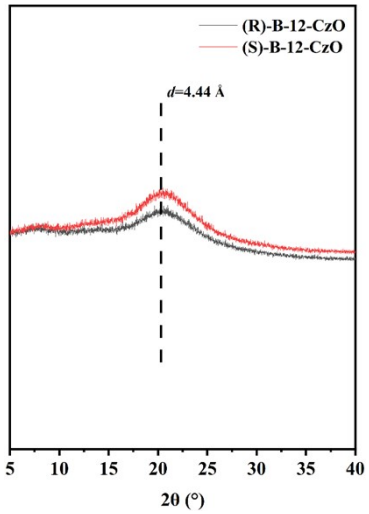


Figure S12. Powder XRD pattern of solid powder (R/S)-B-12-CzO.

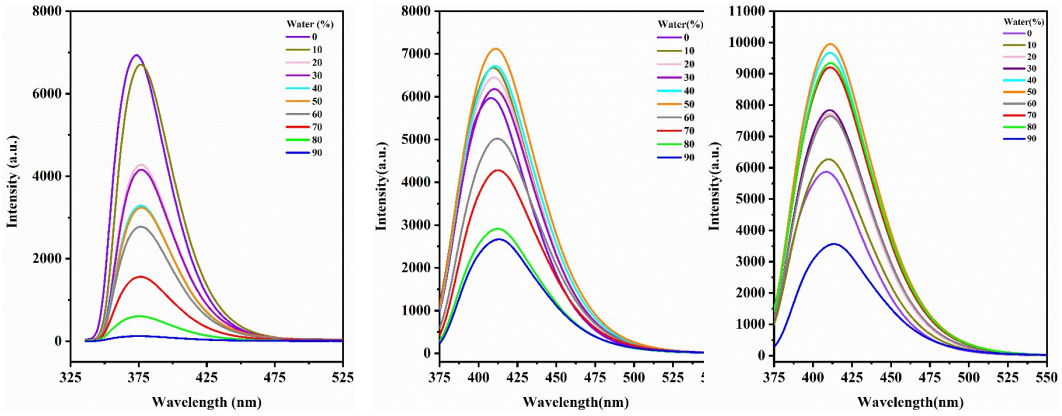


Figure S13. Emission spectra of binaphthol (a), (R)-B-12-CzO (b) and (S)-B-12-CzO (c) in THF and THF/water mixtures with varied volume fraction of water (%).

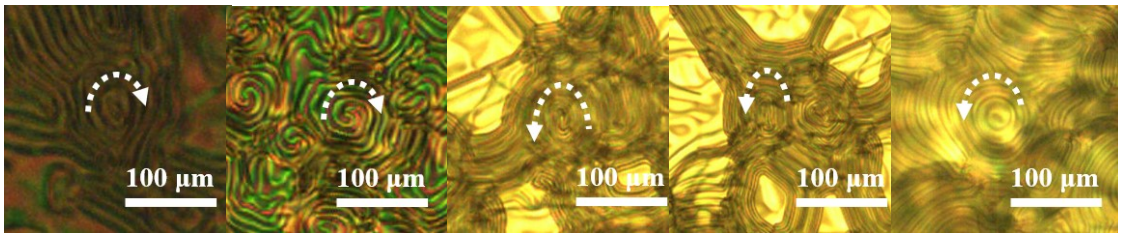


Figure S14. POM images of N*-LC films including (a) 1wt%, (b) 2.5wt%, (c) 5wt%, (d) 7.5wt%, (e) 10wt% P-(R)-B-4-CzO.

References

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