

Electronic Supplementary Information

A chiral single-component sol-gel platform with highly integrated optical properties

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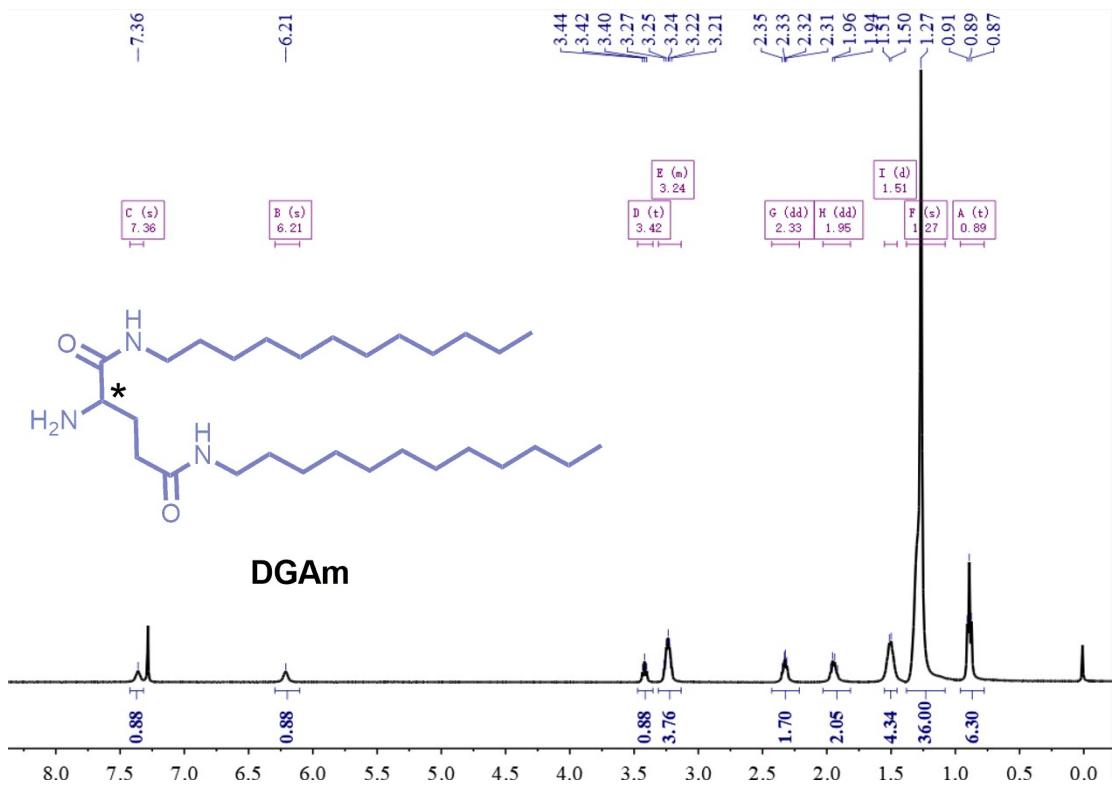


Fig. S1 ^1H NMR spectrum for compound **DGAm** (CDCl_3 , 298 K).

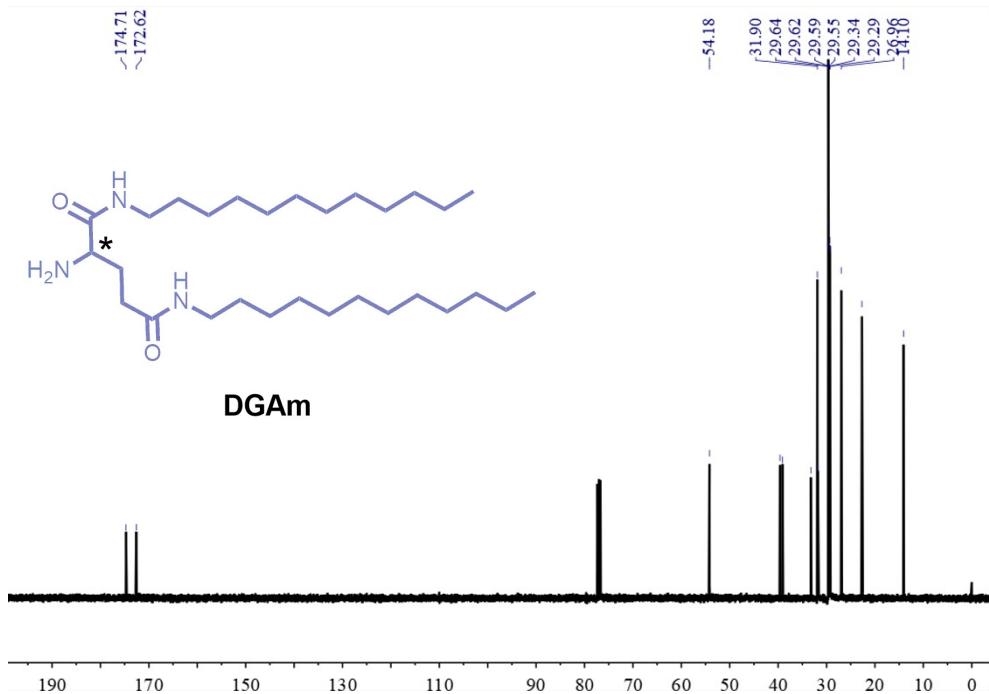


Fig. S2 ^{13}C NMR spectrum for compound **DGAm** (CDCl_3 , 298 K).

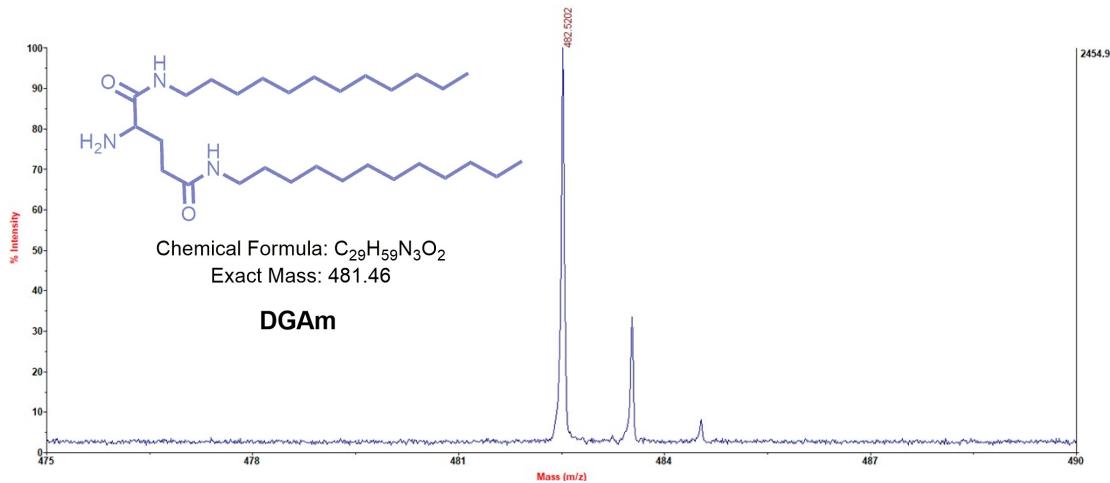


Fig. S3 MALDI-TOF MS Spectrum for compound **DGAm**.

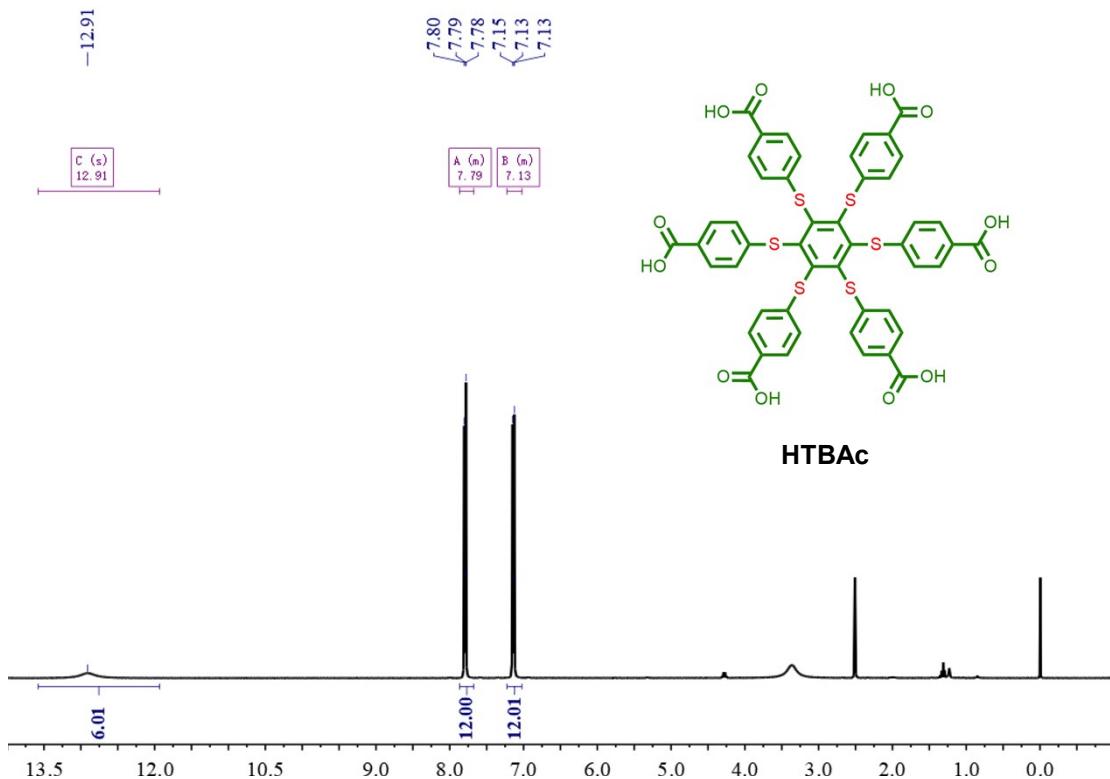


Fig. S4 1H NMR spectrum for compound **HTBAc** ($DMSO-d_6$, 298 K).

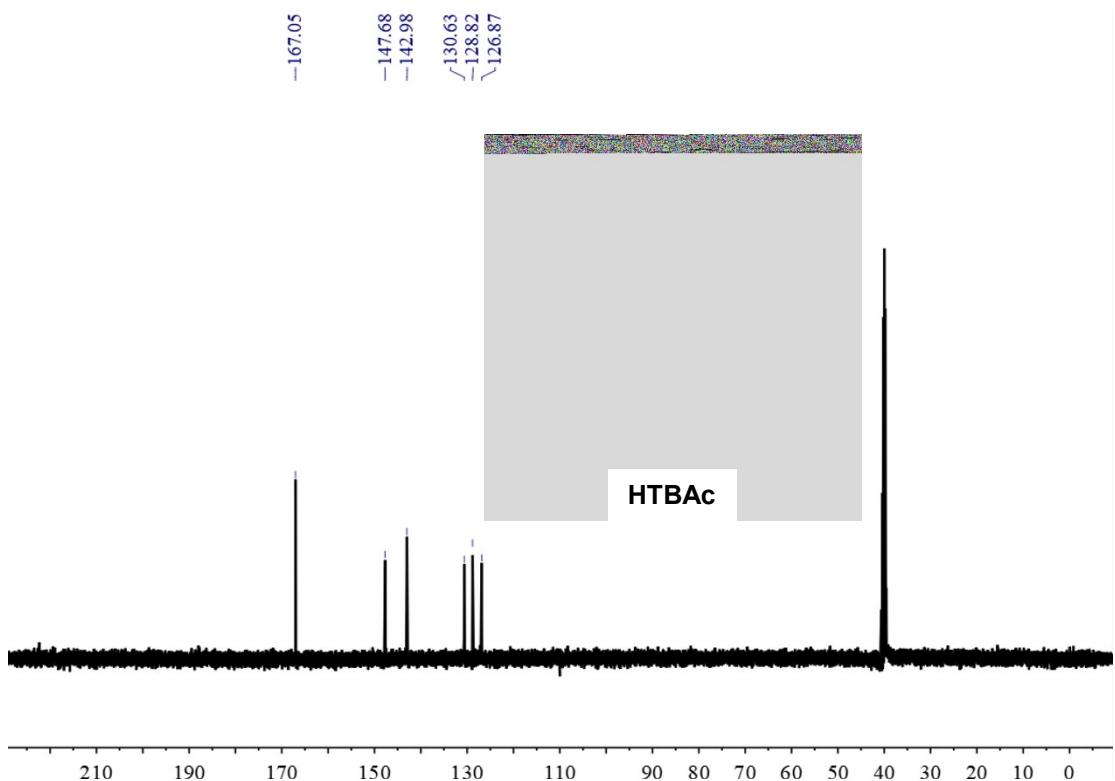


Fig. S5 ^{13}C NMR spectrum for compound **HTBAc** (DMSO- d_6 , 298 K).

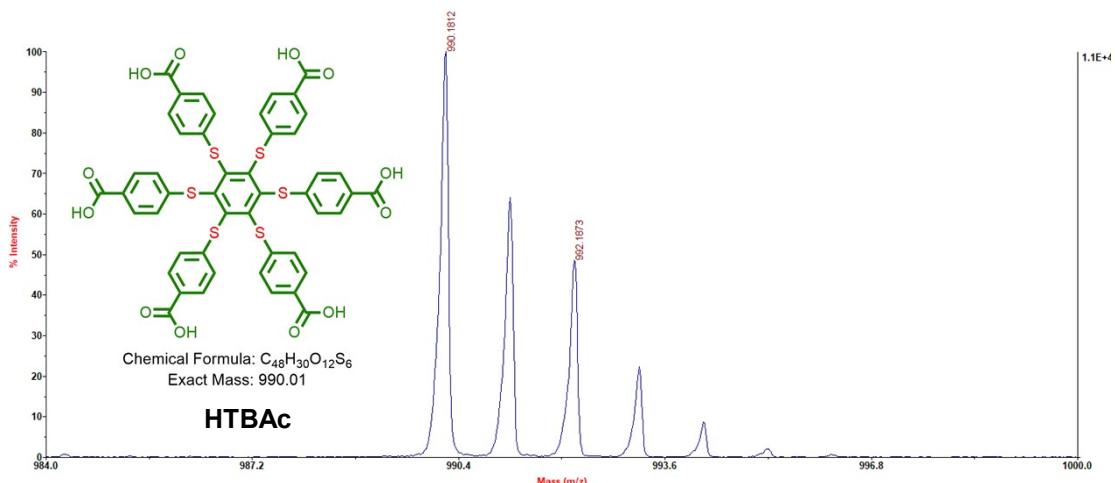


Fig. S6 MALDI-TOF MS Spectrum for compound **HTBAc**.

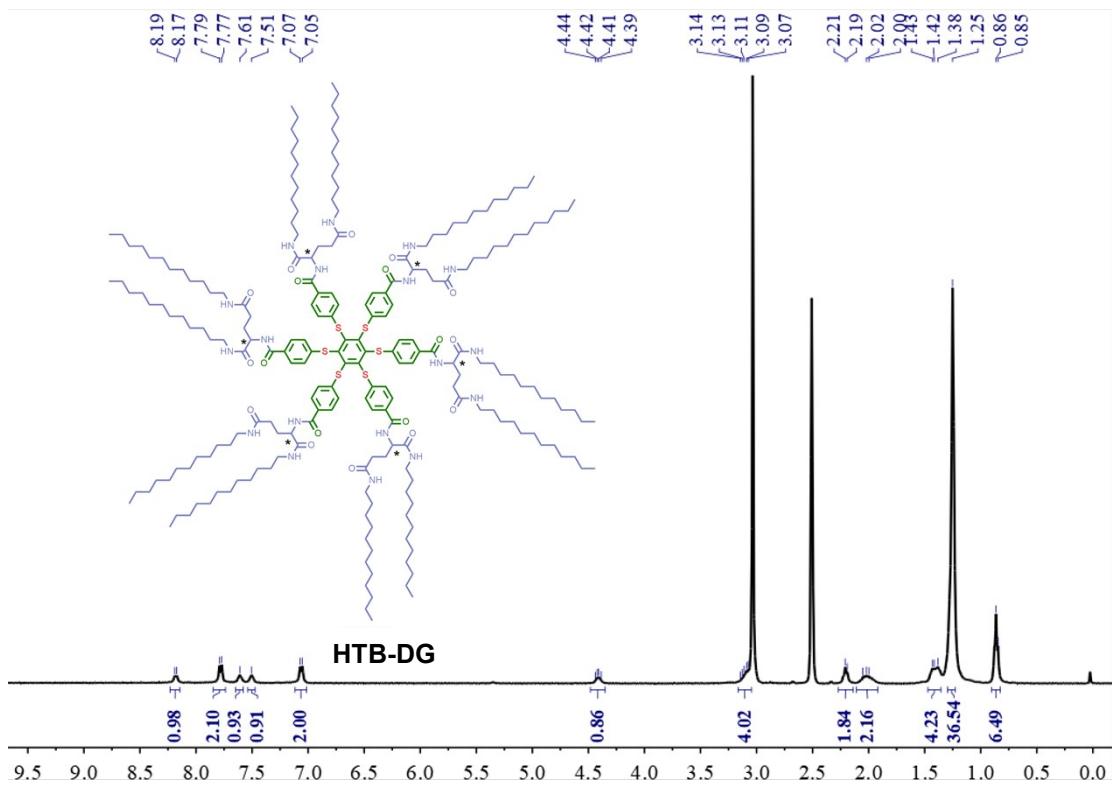


Fig. S7 ^1H NMR spectrum for compound **HTB-DG** ($\text{DMSO}-d_6$, 373 K).

MALDI-TOF MS Spectra for compound HTB-DG:

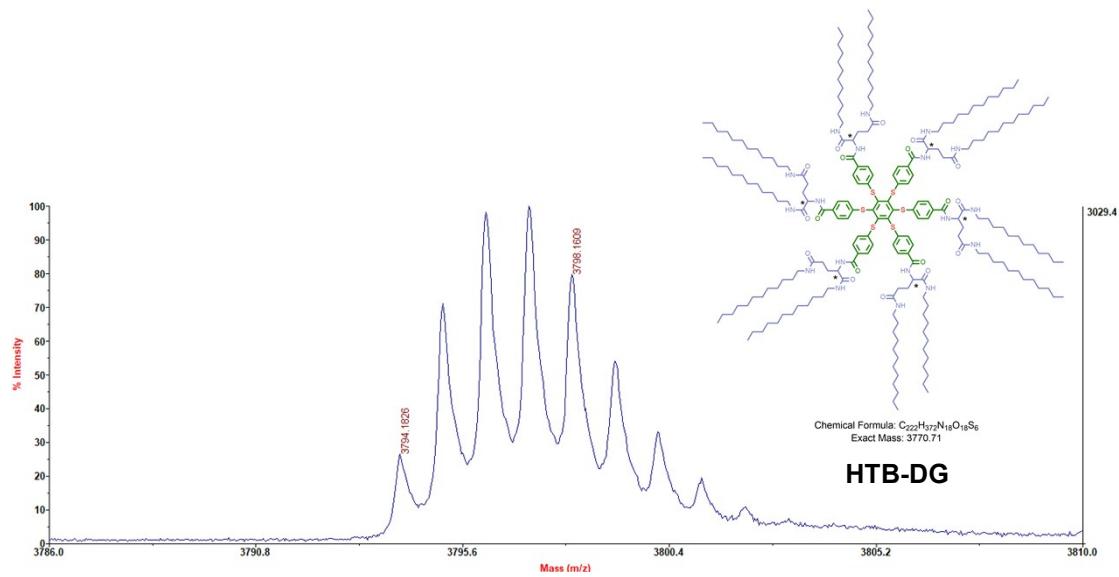


Fig. S8 MALDI-TOF MS Spectrum for compound **HTB-DG**.

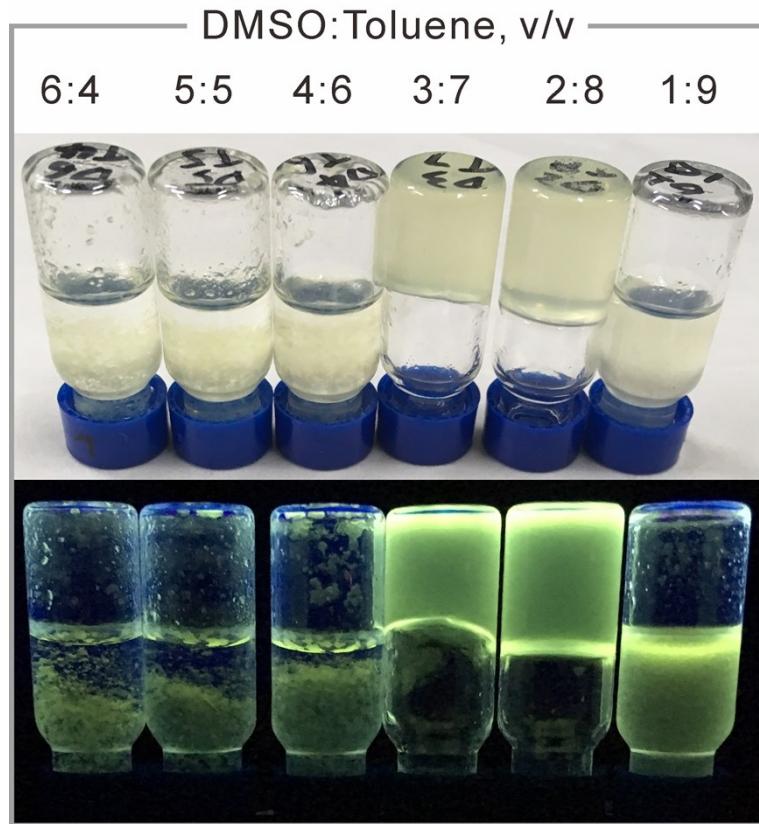


Fig. S9 Solvent ratio test between DMSO and toluene for gel formation. The concentration of **HTB-DG** was 3 mg/mL.

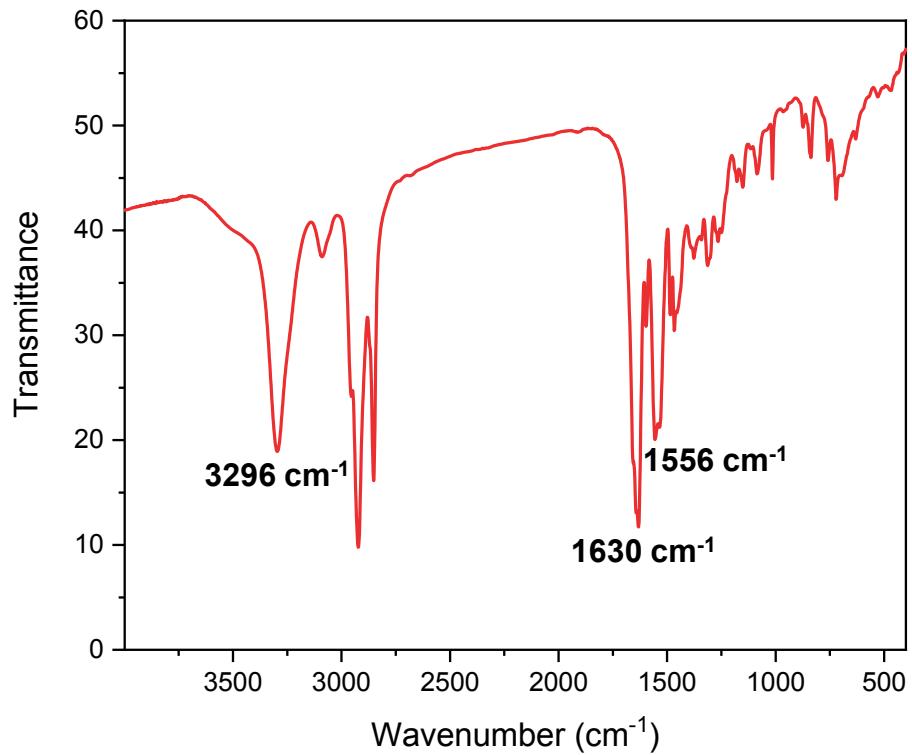


Fig. S10 FTIR spectra of HTB-DG xerogel.

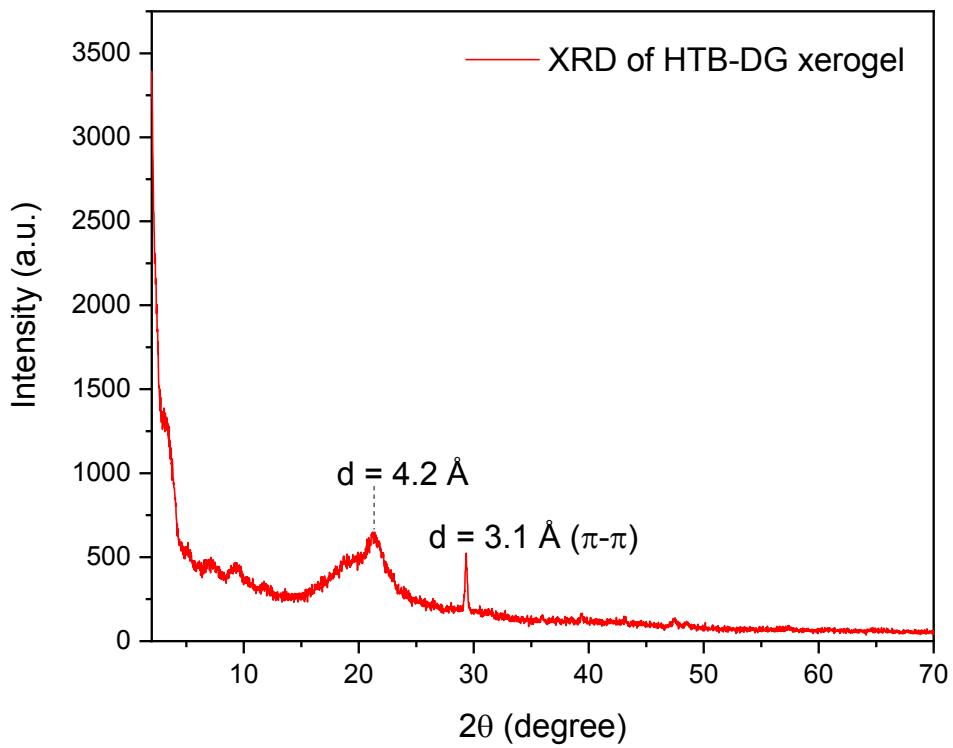


Fig. S11 XRD pattern of HTB-DG xerogel.

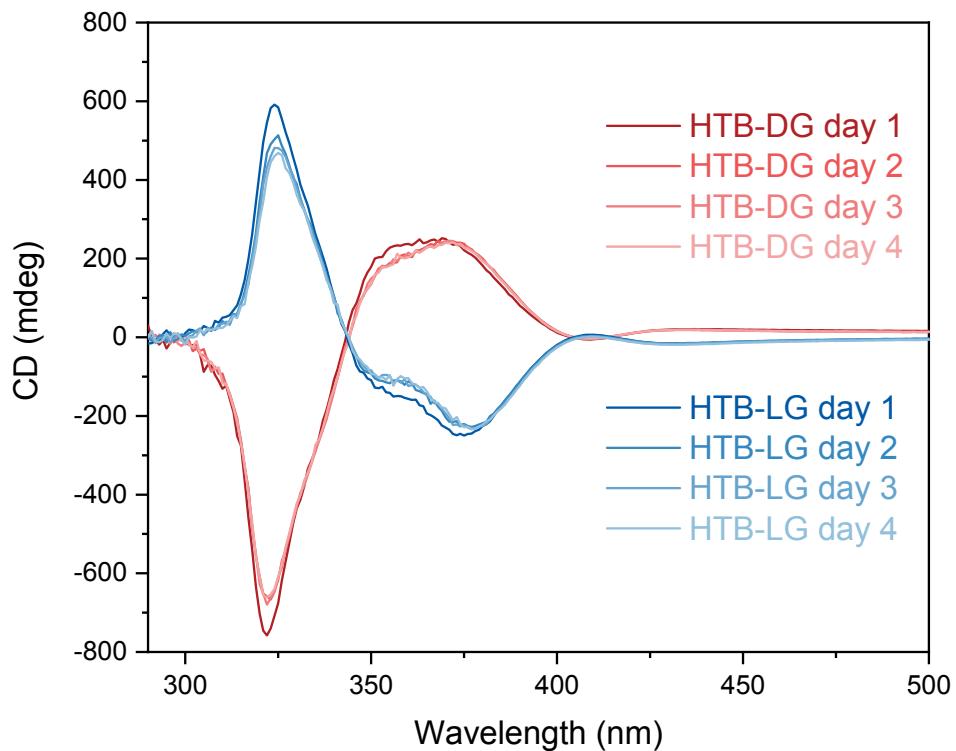


Fig. S12 Time-dependent CD spectra of **HTB-DG** (red lines) and **HTB-LG** (blue lines), concentration: 3 mg/mL, 2 mm cuvette.

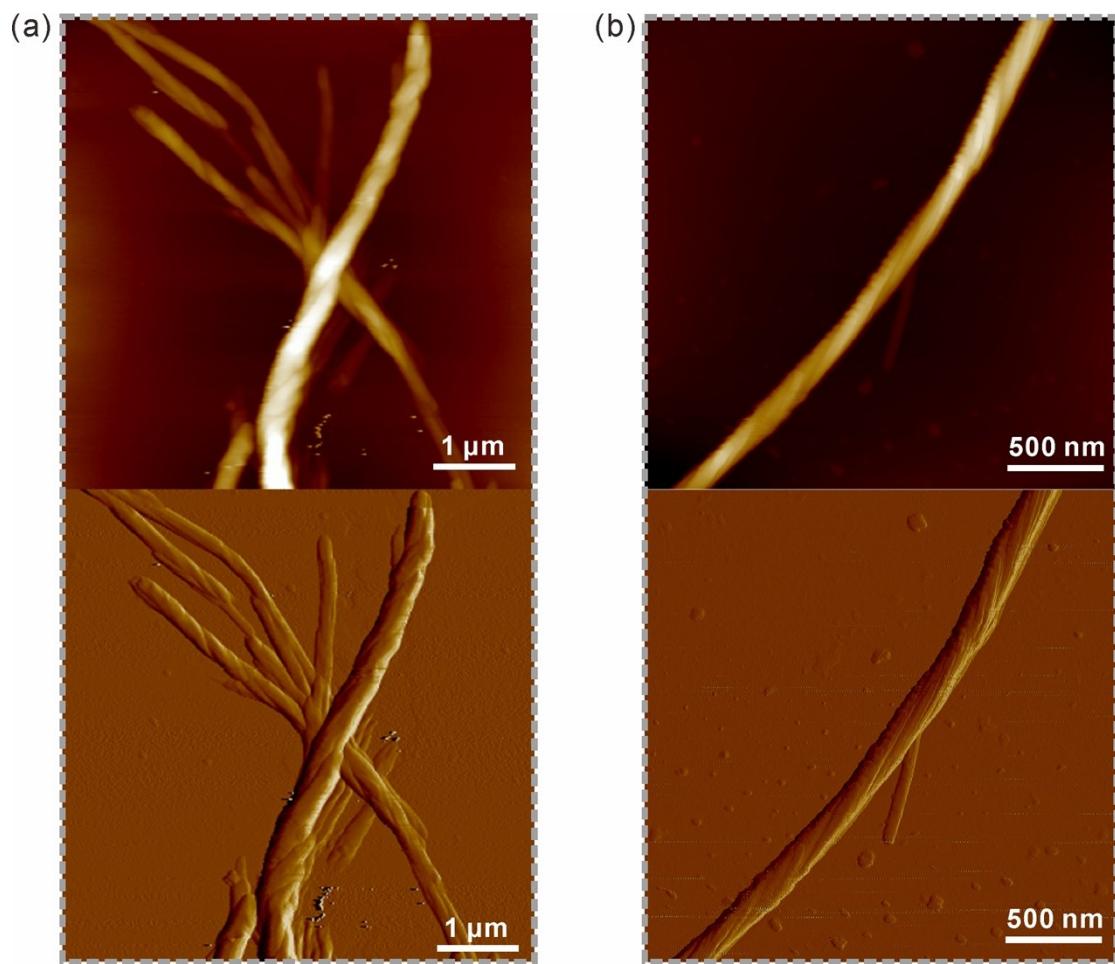


Fig. S13 AFM images of **HTB-DG** (a) and **HTB-LG** (b) xerogels showing helical self-assembly of **HTB-D/LG**.

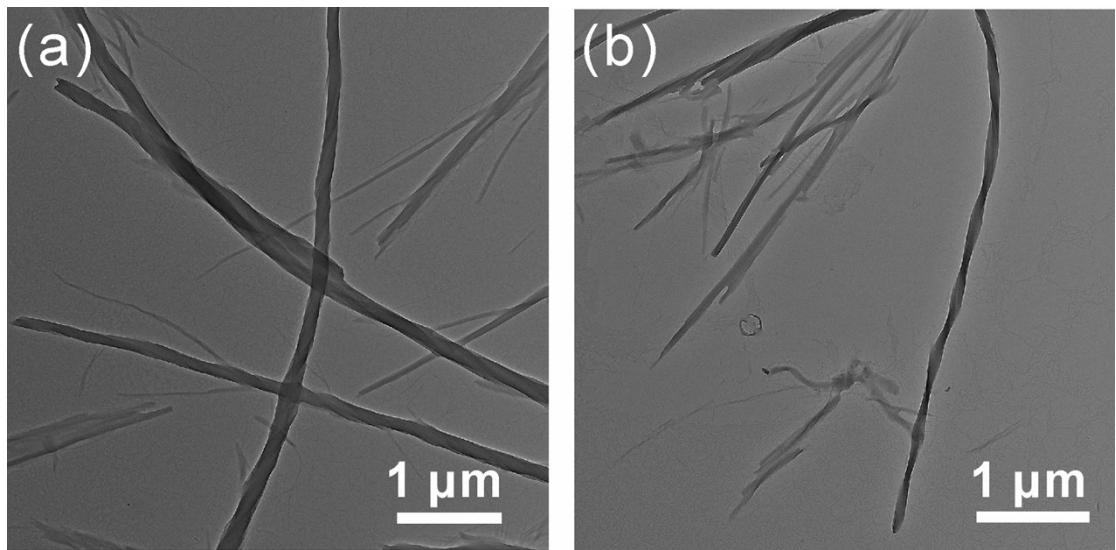


Fig. S14 TEM images of **HTB-DG** (a) and **HTB-LG** (b) xerogels showing helical self-assembly of **HTB-D/LG**.

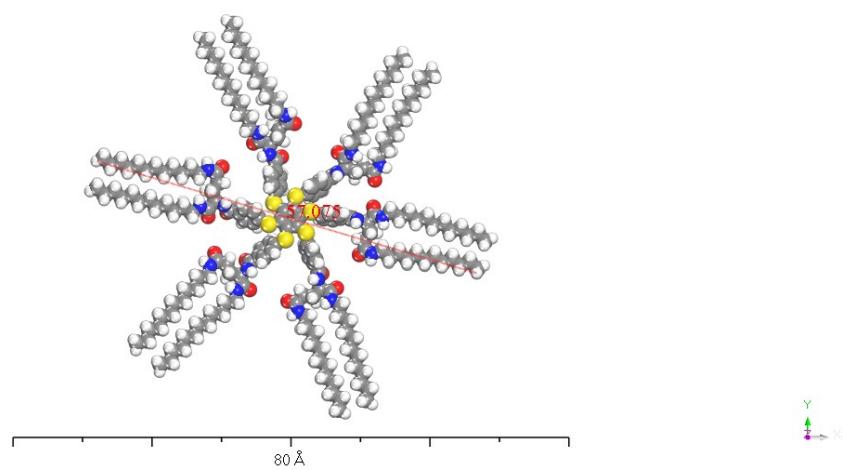


Fig. S15 Estimation of the length of an extended **HTB-D/LG** molecule calculated with Materials Studio package.

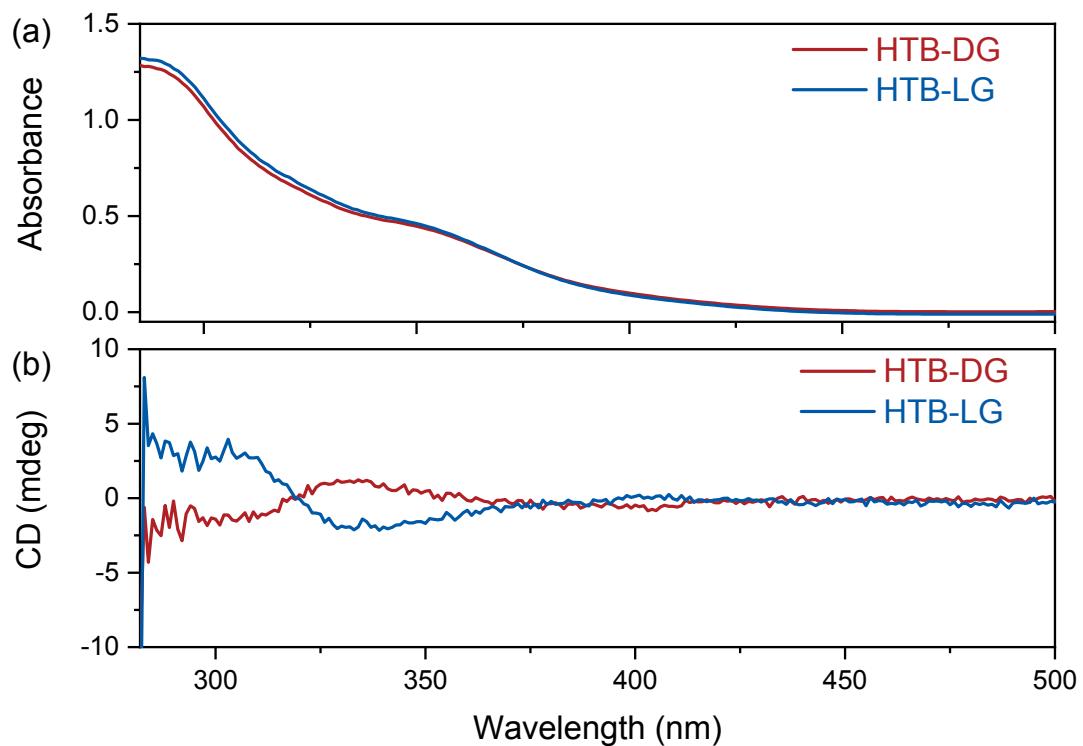


Fig. S16 UV-Vis (a) and corresponding CD (b) spectra of dilute solution of **HTB-DG** (red line) and **HTB-LG** (blue line) in DMSO/toluene (2/8, v/v) mixed solvent, concentration at 15 μ M, 1 cm cuvette.

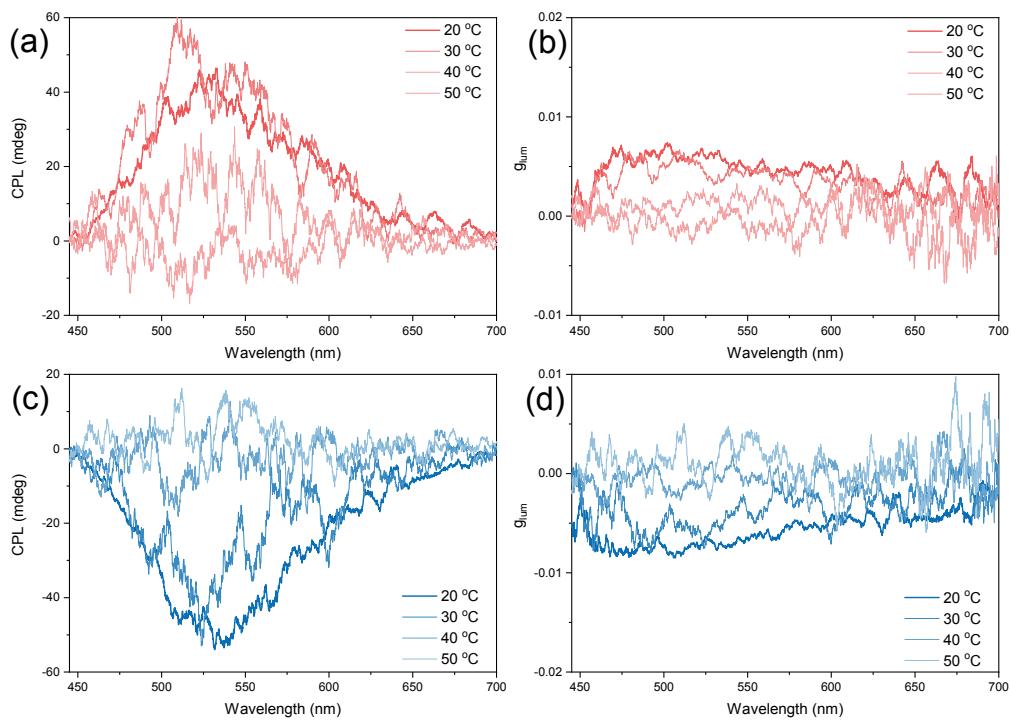


Fig. S17 CPL spectra (a, c) and corresponding g_{lum} (b, d) curves of **HTB-DG** (red lines) and **HTB-LG** (blue lines) organogel depended on temperature ($\lambda_{\text{ex}} = 365$ nm).

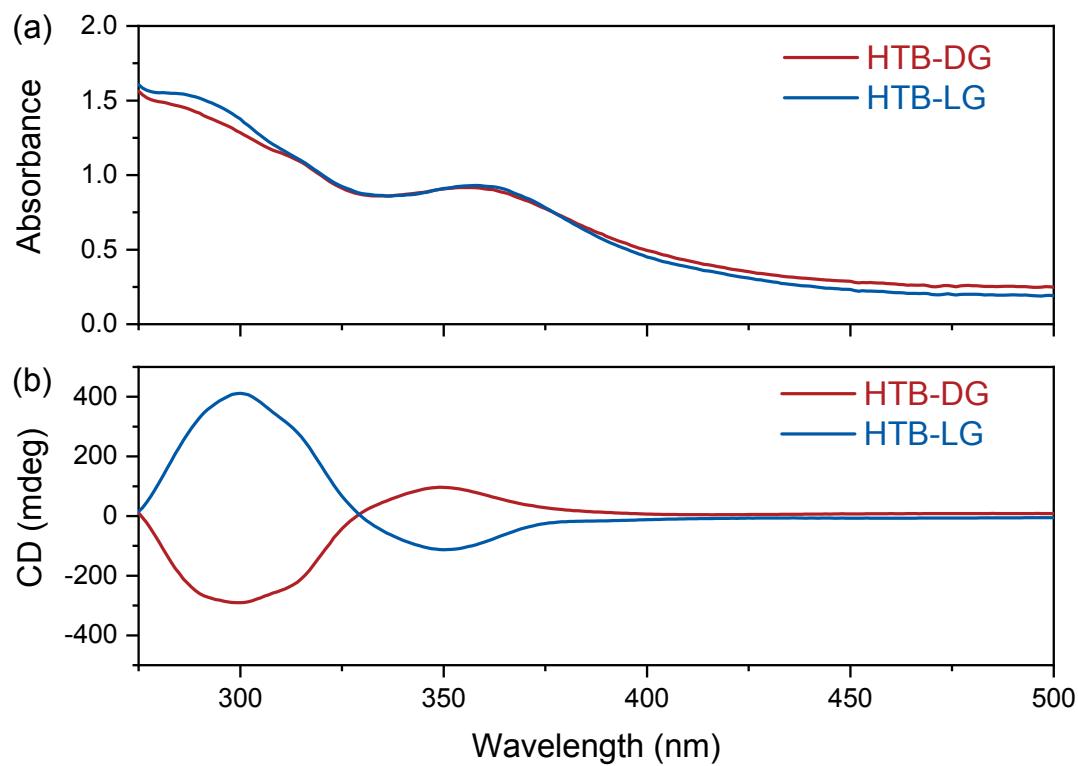


Fig. S18 UV-Vis (a) and corresponding CD (b) spectra of **HTB-DG** (red line) and **HTB-LG** (blue line) organogels, concentration at 10 mg/mL, 0.1 mm cuvette.

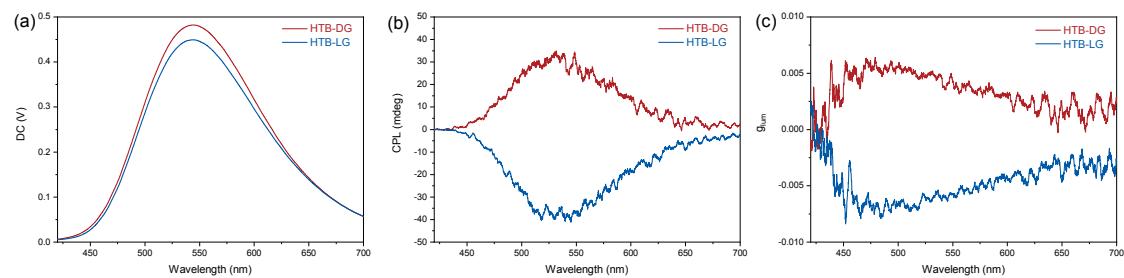


Fig. S19 Photoluminescence (a), CPL spectra (b) and corresponding g_{lum} curves (c) for **HTB-DG** (red line) and **HTB-LG** (blue line) organogels ($\lambda_{ex} = 365$ nm), concentration: 10 mg/mL.

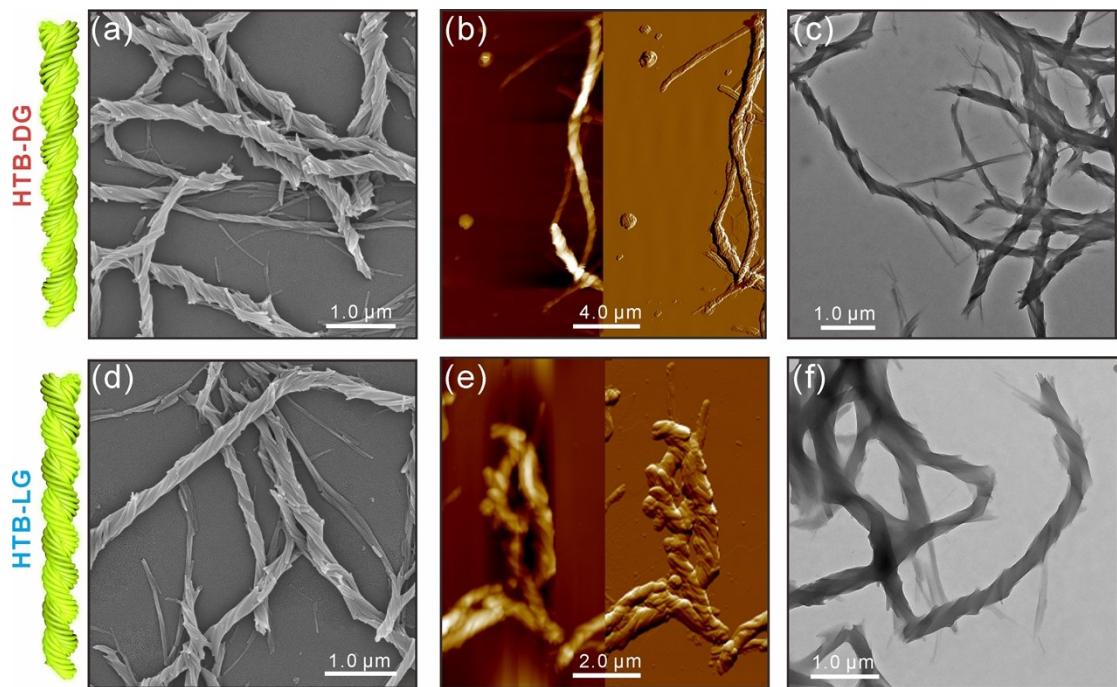


Fig. S20 SEM (a and c), AFM (b and e) TEM (c and f) images for **HTB-DG** (top) and **HTB-LG** (bottom) xerogels, concentration at 10 mg/mL.

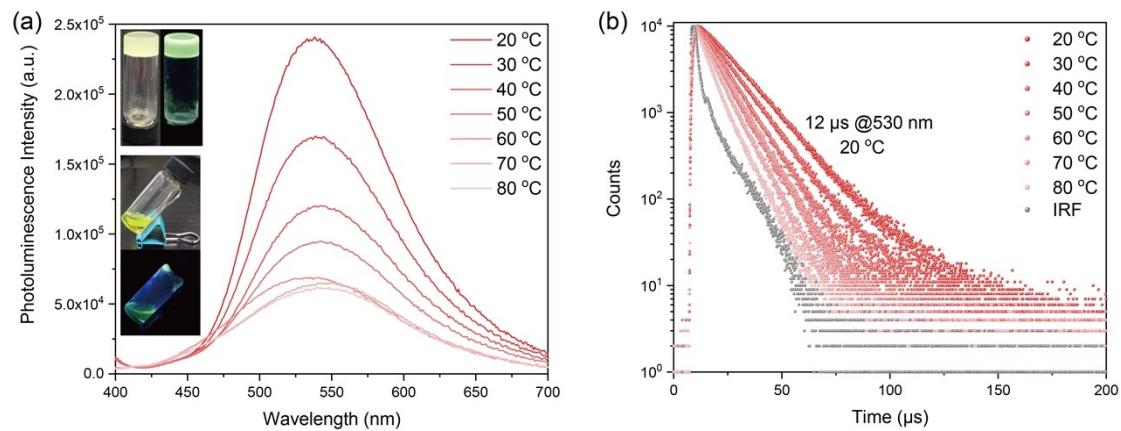


Fig. S21 Temperature-dependent photoluminescence (a) and lifetime (b) spectra of **HTB-DG** organogel ($\lambda_{\text{ex}} = 365 \text{ nm}$), concentration at 10 mg/mL. Insets: photographs of **HTB-DG** in gel state (top) and partial sol state (bottom) under ambient light and UV light.

Table S1. Comparison of the chiral response of **THB-D/LG** with reported literatures.

Material	Chiral Response	Other Features	Ref
HTB-D/LG	thermo ON-OFF CD and CPL response	gel, AIE, RTP	this work
S-TPE-Ph- PEA	solvent polarity driven CD and CPL inversion	AIE	Ref S1
DGG/PTPE	stoichiometry-controlled CD and CPL inversion	gel, AIE	Ref S2
cis/trans-TPE- L/D-DGlu	water fraction-controlled CD and CPL inversion in THF/water mixture	AIE	Ref S3
PPA-ACe	thermo-induced helical inversion	Ba ²⁺ response	Ref S4
Molecule-2a	thermo-induced helical inversion	encapsulation of C ₆₀	Ref S5
PF8	chiral solvent induced CD and CPL; thermo ON-OFF chiropticity	gel	Ref S6
Poly(quinoxali- ne-2,3-diyl)	solvent-dependent helix inversion	sergeants- and-soldiers effect	Ref S7
Poly-1-H	chiral amine induced macromolecular helicity and chiropticity	helicity memory	Ref S8
(2'S)-(P/M)-3- PHIC	light-controlled chiroptical switch (UV and visible light)	liquid crystalline phase	Ref S9
TPA-SDA	CPL-irradiation-induced helicity	photopolyme- rization	Ref S10
Poly-R-MPA	helical sense tuning by mono- and divalent metals	dynamic helical polymers	Ref S11
BTACA	vortex mixing-induced CD and CPL	gel	Ref S12

References

- S1. Q. Ye, F. Zheng, E. Q. Zhang, H. K. Bisoyi, S. Y. Zheng, D. D. Zhu, Q. H. Lu, H. L. Zhang and Q. Li, *Chem. Sci.*, 2020, **11**, 9989-9993.
- S2. P. Li, B. Lu, D. Han, P. Duan, M. Liu and M. Yin, *Chem. Commun.*, 2019, **55**, 2194-2197.
- S3. S. Zhang, J. Fan, Y. Wang, D. Li, X. Jia, Y. Yuan and Y. Cheng, *Mater. Chem. Front.*, 2019, **3**, 2066-2071.
- S4. F. Wang, C. Zhou, K. Liu, J. Yan, W. Li, T. Masuda and A. Zhang, *Macromolecules*, 2019, **52**, 8631-8642.
- S5. Z. Huang, S. K. Kang, M. Banno, T. Yamaguchi, D. Lee, C. Seok, E. Yashima and M. Lee, *Science*, 2012, **337**, 1521-1526.
- S6. Y. Zhao, N. A. Abdul Rahim, Y. Xia, M. Fujiki, B. Song, Z. Zhang, W. Zhang and X. Zhu, *Macromolecules*, 2016, **49**, 3214-3221.
- S7. Y. Nagata, T. Yamada, T. Adachi, Y. Akai, T. Yamamoto and M. Sugino, *J. Am. Chem. Soc.*, 2013, **135**, 10104-10113.
- S8. K. Maeda, M. Nozaki, K. Hashimoto, K. Shimomura, D. Hirose, T. Nishimura, G. Watanabe and E. Yashima, *J. Am. Chem. Soc.*, 2020, **142**, 7668-7682.
- S9. D. Pijper, M. G. M. Jongejan, A. Meetsma and B. L. Feringa, *J. Am. Chem. Soc.*, 2008, **130**, 4541-4552.
- S10. J. Kim, J. Lee, W. Y. Kim, H. Kim, S. Lee, H. C. Lee, Y. S. Lee, M. Seo and S. Y. Kim, *Nat. Commun.*, 2015, **6**, 6959.
- S11. F. Freire, J. M. Seco, E. Quinoa and R. Riguera, *Angew. Chem. Int. Ed.*, 2011, **50**, 11692-11696.
- S12. Y. Sang, D. Yang, P. Duan and M. Liu, *Chem. Sci.*, 2019, **10**, 2718-2724.