

Supporting Information

Tunable aggregation-induced circularly polarized luminescence of chiral AIEgens *via* the regulation of mono-/di-substituents of molecules or nanostructures of self-assemblies

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1. General information

Materials and Instruments

Unless otherwise stated, all the solvents and reagents were analytical grade and directly used without further purification after gotten from the commercial suppliers. Tetrahydrofuran (THF) was distilled from sodium in the presence of benzophenone.. NMR spectra were measured on an Agilent 400-MR DD2 NMR spectrometer and reported as parts per million (ppm) from the internal standard TMS. HRMS data were taken on a Bruker Dalton maXis mass spectrometer. Mass spectra (MS) were obtained by using Bruker AutoFlex Matrix Assisted Laser Desorption/Ionisation (MALDI) Time of Flight (TOF)-Mass Spectrometer (MALDI-TOF-MS). UV-*vis* spectra were measured from UV-2550 ultraviolet spectrophotometer. Fluorescence spectra were obtained on an F-4500 spectrofluorometer. SEM images were collected on a Zeiss-Spura55 instrument with an accelerating voltage of 5 kV. Circular dichroism (CD) spectra were measured on a JASCO J-810 spectropolarimeter. Circularly polarized luminescence (CPL) spectra were performed on a JASCO CPL-300 spectrofluoropolarimeter.

Preparation of samples for optical measurement

Several stock solutions of the compounds were firstly prepared in THF (200 μ M). Then 10 μ L stock solutions were transferred to 2 mL THF/H₂O mixed solvents to afford sample solutions at the concentration of 10 μ M, which water fractions of the mixed solvents were from 0 to 99%. Then the optical measurements were taken after 2 hours later.

Sample Preparation of samples for SEM

Different THF/water mixtures of TPE-*L*-Glu, TPE-*D*-Glu, *cis*-TPE-*L*-DGlu and *trans*-TPE-*L*-DGlu with concentration of 10 μ M were first prepared, after 2 hours later, 10 μ L of the solution was then dropped onto the surface of silicon water, after vacuum drying for one hour, the samples were characterized by SEM.

2. Optical data

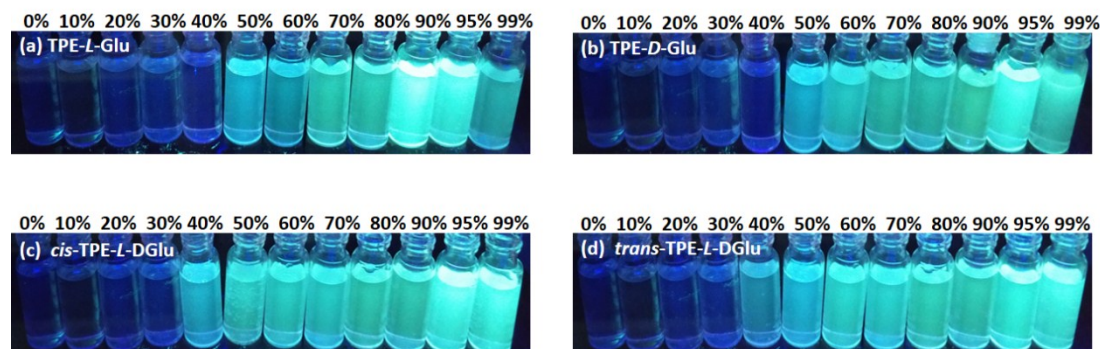


Figure S1. Photograph of A) TPE-*L*-Glu, B) TPE-*D*-Glu, C) *cis*-TPE-*L*-DGlu and D) *trans*-TPE-*L*-DGlu in THF/water mixed solvents with different f_w under 365 nm UV lamp. Concentration: 10 μ M.

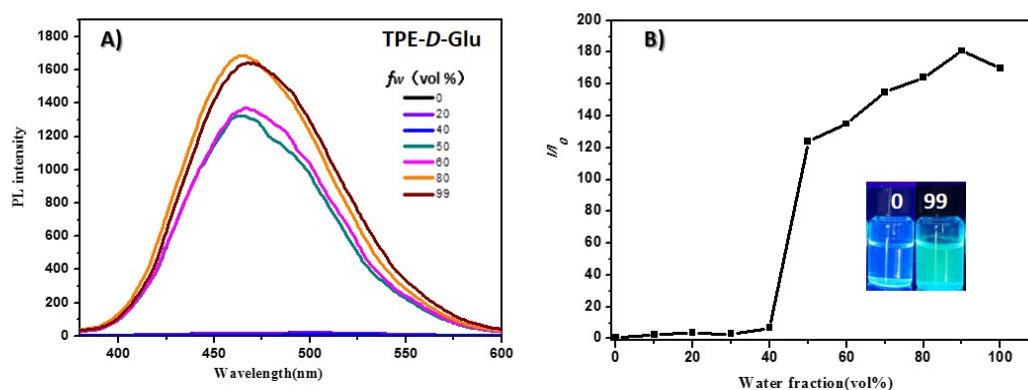


Figure S2. Fluorescent spectra of TPE-*D*-Glu and Plot of I/I_0 values versus f_w , where I_0 represents the emission intensity in pure THF. Inset: photographs of TPE-*D*-Glu in THF/water mixed solvents with 0 and 99% f_w under 365 nm UV lamp. Concentration: 10 μ M.

3. CPL spectra and g_{lum} values of chiral AIEgens

3.1 CPL and PL spectra of chiral AIEgens

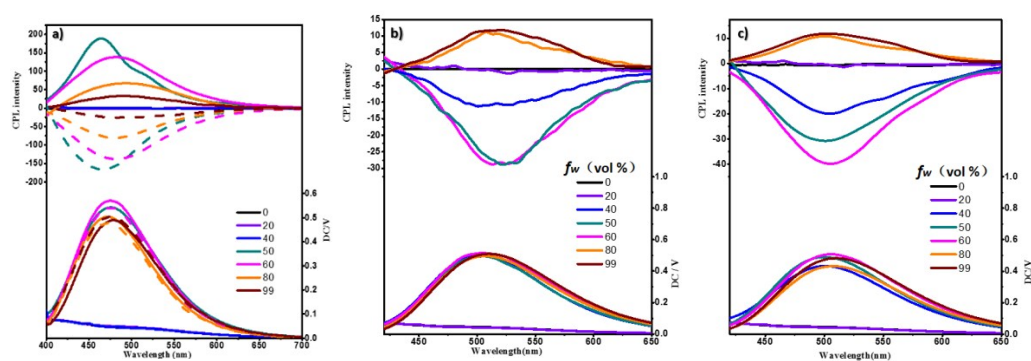


Figure S3. CPL and PL values for a) TPE-*L*-Glu and TPE-*D*-Glu, b) *cis*-TPE-*L*-DGlu and c) *trans*-TPE-*L*-DGlu in THF/water mixed solvents with different f_w . Concentration: 10 μ M; excitation wavelength: 340 nm.

3.2 g_{lum} values of chiral AIEgens

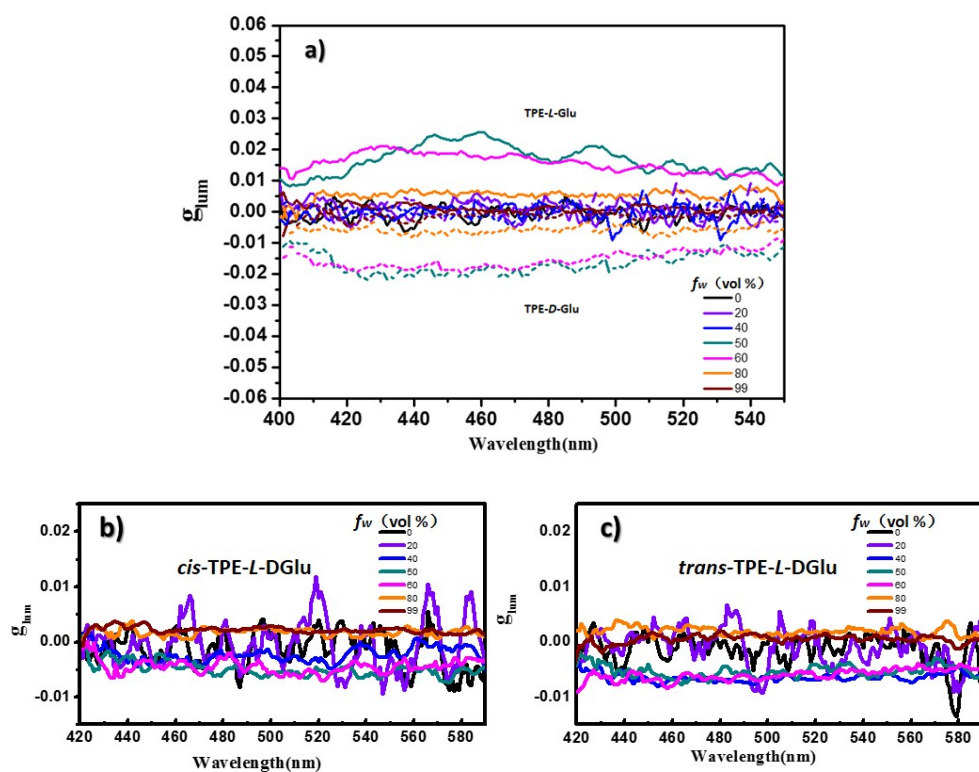


Figure S4. g_{lum} values versus wavelengths for a) TPE-L-Glu and TPE-D-Glu, b) *cis*-TPE-L-DGlu and *trans*-TPE-L-DGlu in THF/water mixed solvents with different f_w . Concentration: 10 μ M; excitation wavelength: 340 nm.

4. Morphologies of the aggregates

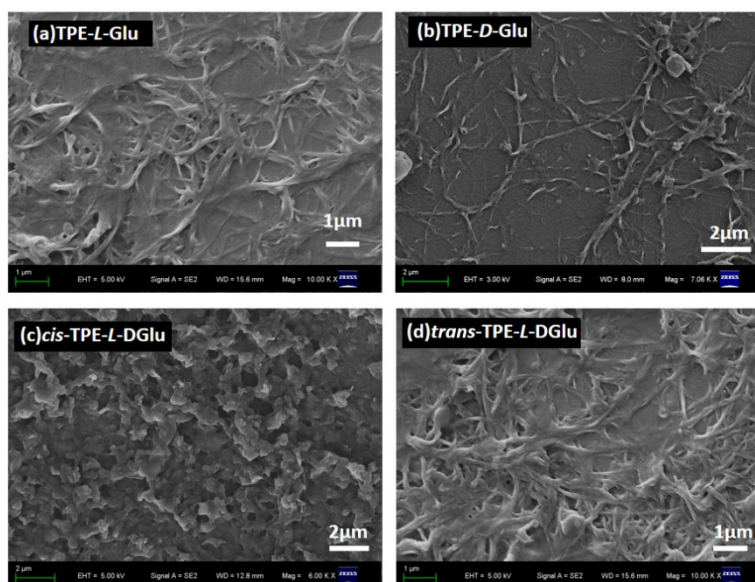


Figure S5. SEM images of aggregates of (a) TPE-L-Glu, (b) TPE-D-Glu, (c) *cis*-TPE-L-DGlu and (d) *trans*-TPE-L-DGlu formed in 20% f_w mixed THF/water mixed solvents. Concentration: 10 μ M.

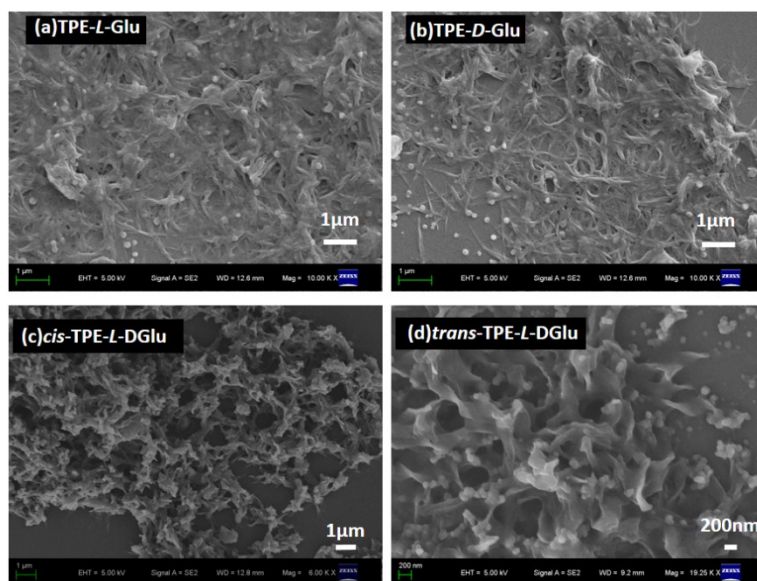


Figure S6. SEM images of aggregates of (a) **TPE-L-Glu**, (b) **TPE-D-Glu**, (c) **cis-TPE-L-DGlu** and (d) **trans-TPE-L-DGlu** formed in 60% f_w mixed THF/water mixed solvents. Concentration: 10 μ M.

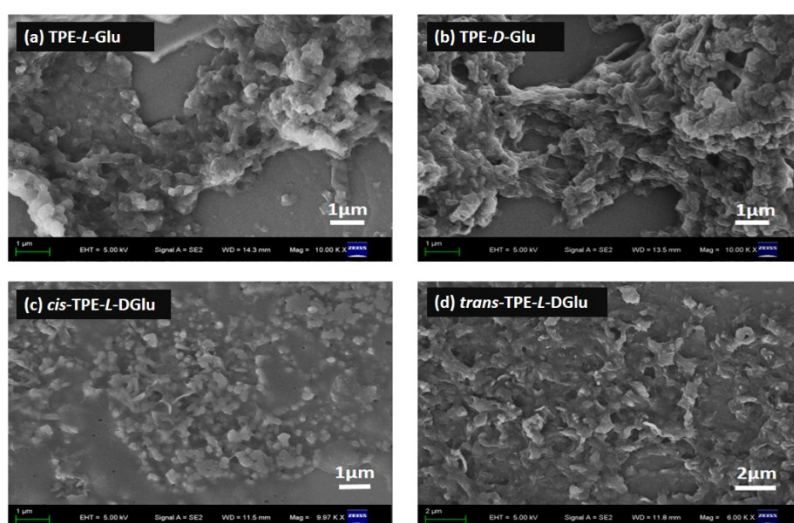
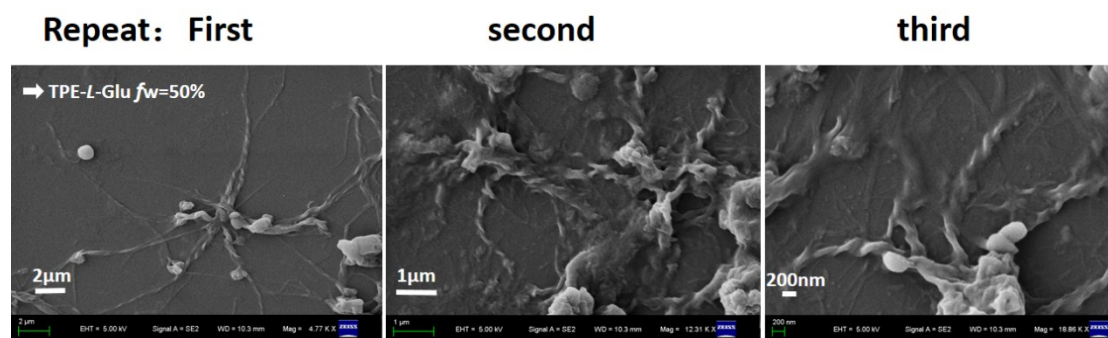


Figure S7. SEM images of aggregates of (a) **TPE-L-Glu**, (b) **TPE-D-Glu**, (c) **cis-TPE-L-DGlu** and (d) **trans-TPE-L-DGlu** formed in 99% f_w mixed THF/water mixed solvents. Concentration: 10 μ M.



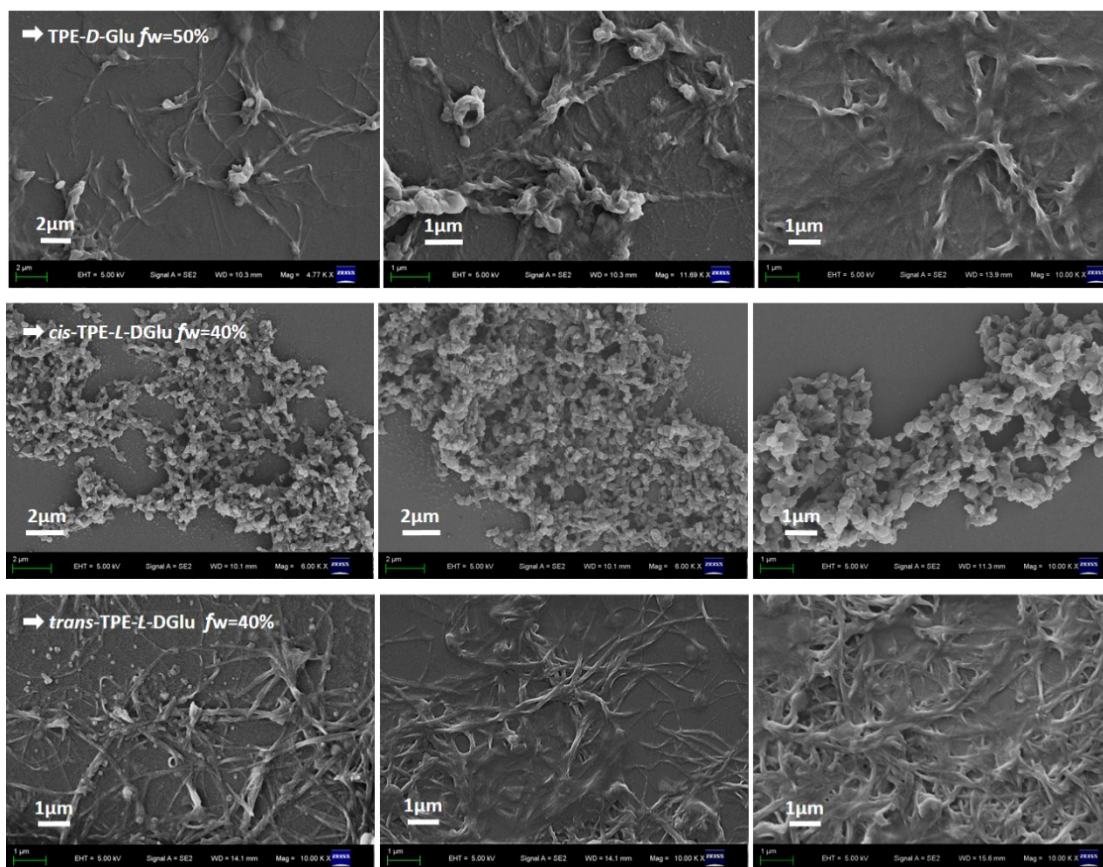


Figure S8. SEM images of aggregates of **TPE-L-Glu** and **TPE-D-Glu** formed in THF/water mixed solvents (5/5, v/v), **cis-TPE-L-DGlu** and **trans-TPE-L-DGlu** formed in THF/water mixed solvents (6/4, v/v). Concentration: 10 μM. The above experiments were repeated three times under the same conditions.

5. NMR spectra

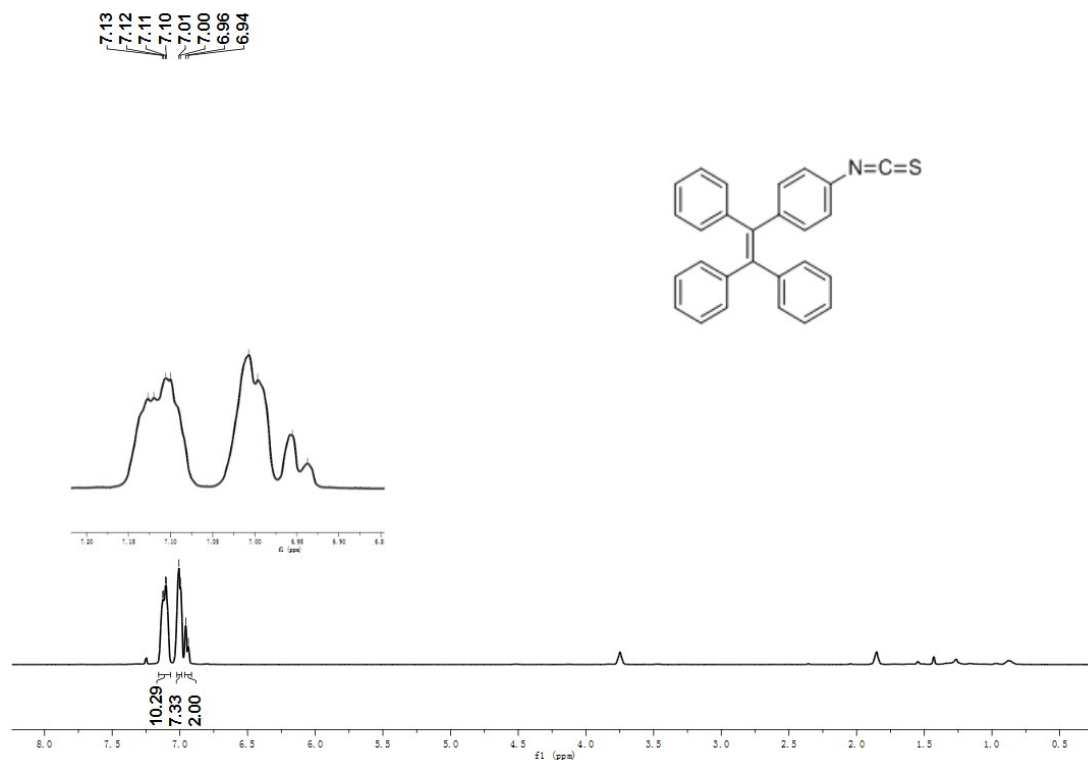


Figure S9. ¹H NMR of compound **3** in CDCl₃

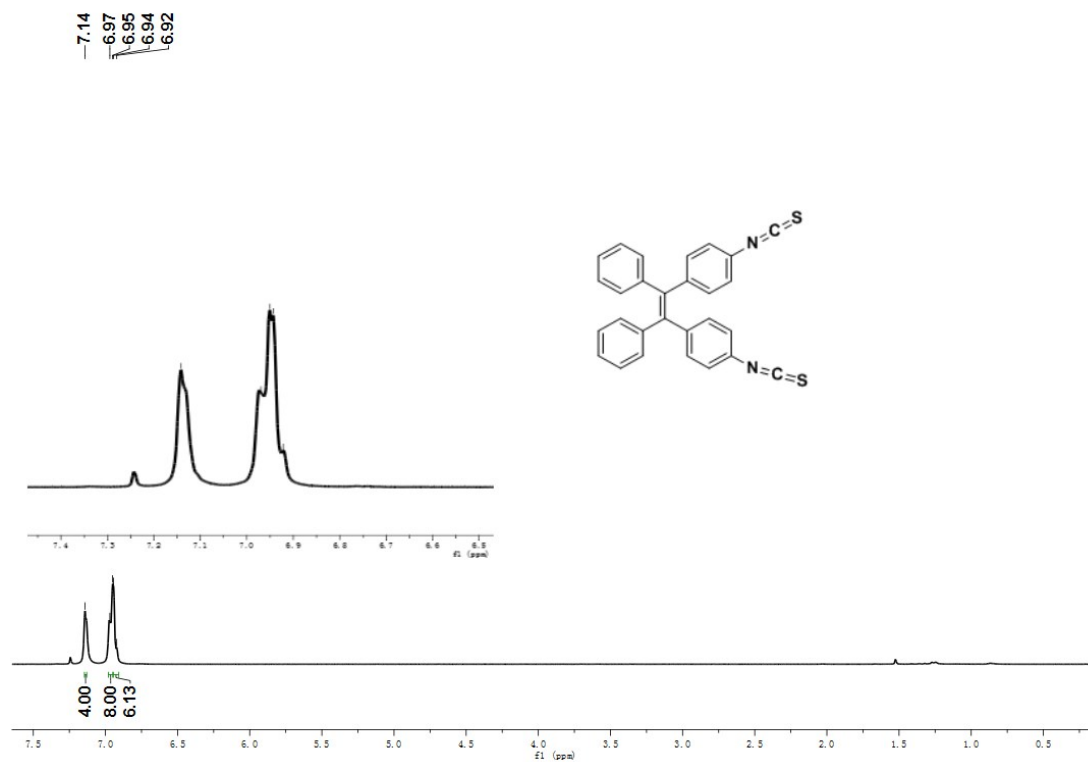


Figure S10. ¹H NMR of *cis*-**4** in CDCl₃

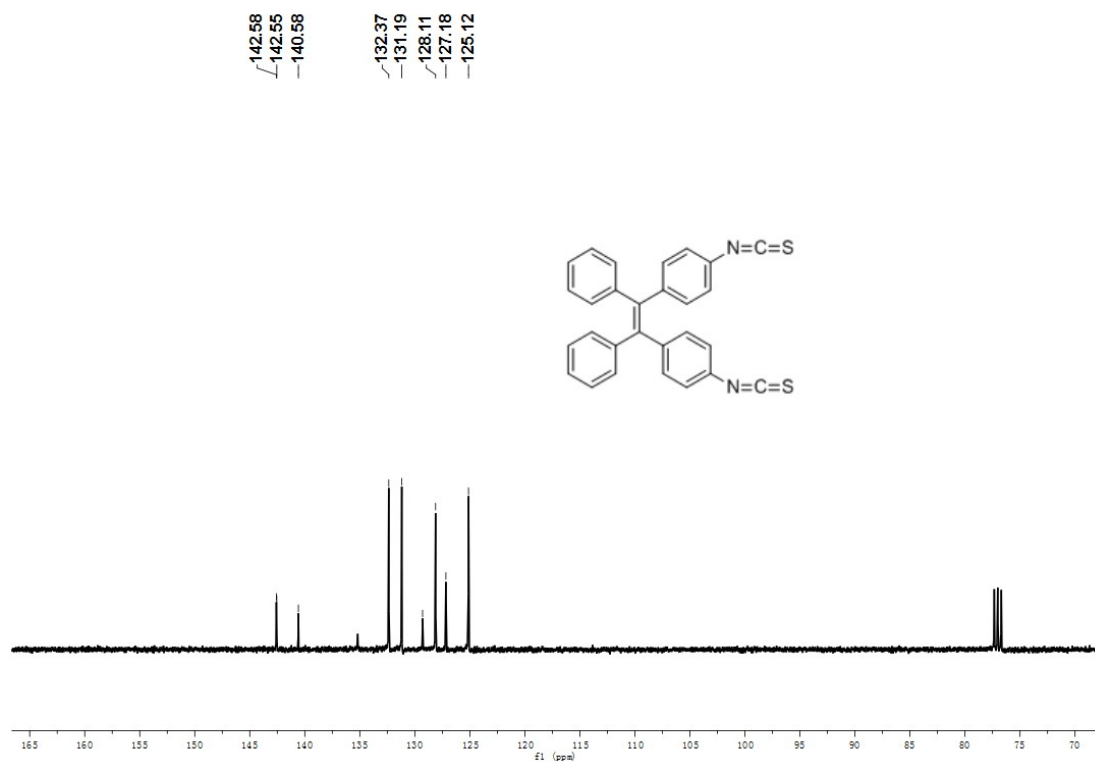


Figure S11. ^{13}C NMR of *cis*-4 in CDCl₃

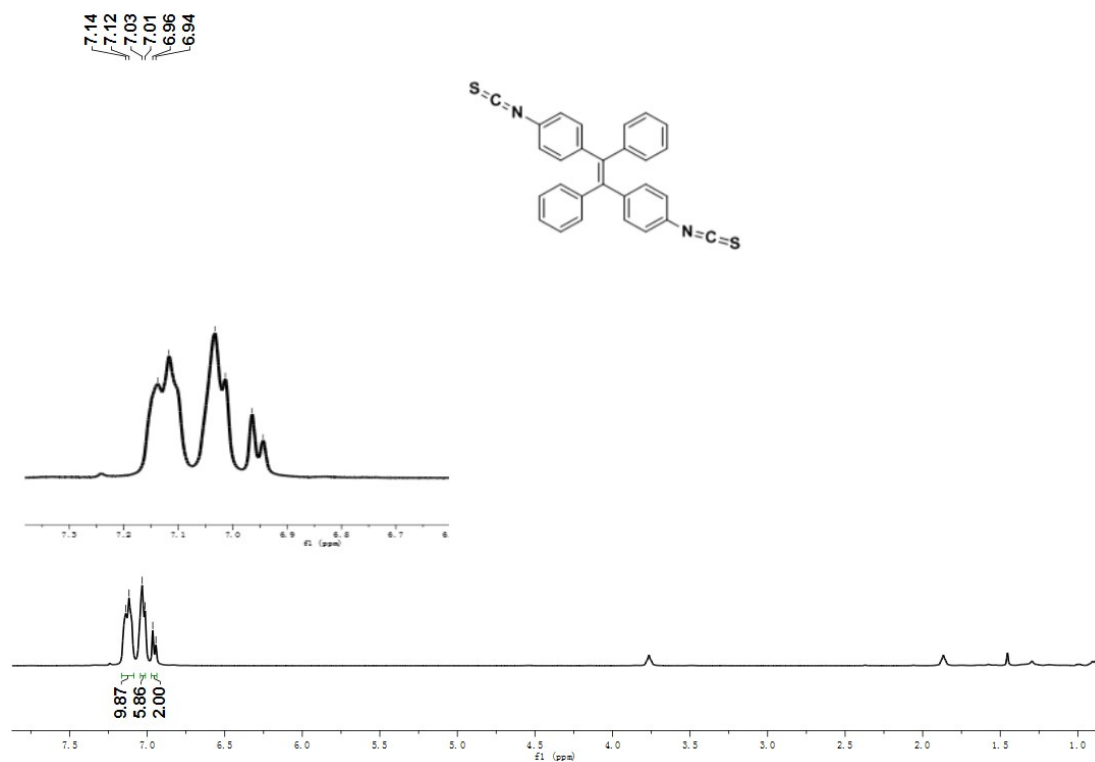


Figure S12. ^1H NMR of *trans*-4 in CDCl₃

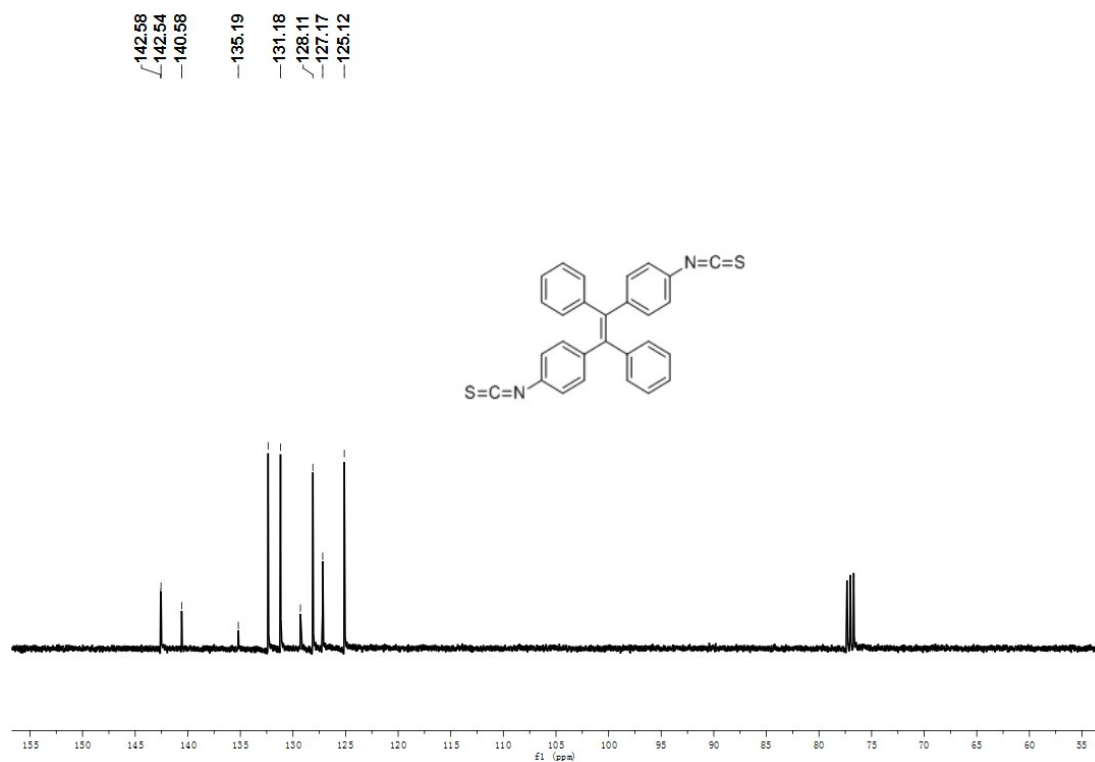


Figure S13. ¹H NMR of *trans*-4 in CDCl₃

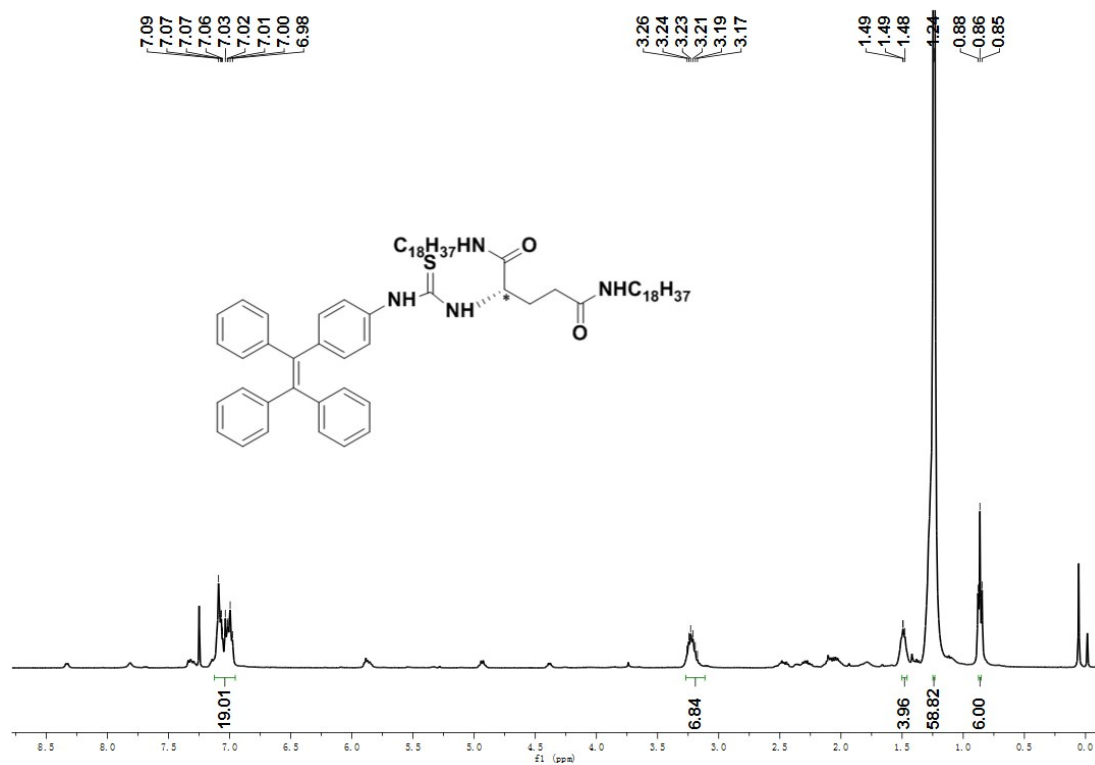


Figure S14. ¹H NMR of TPE-*L*-Glu in CDCl₃

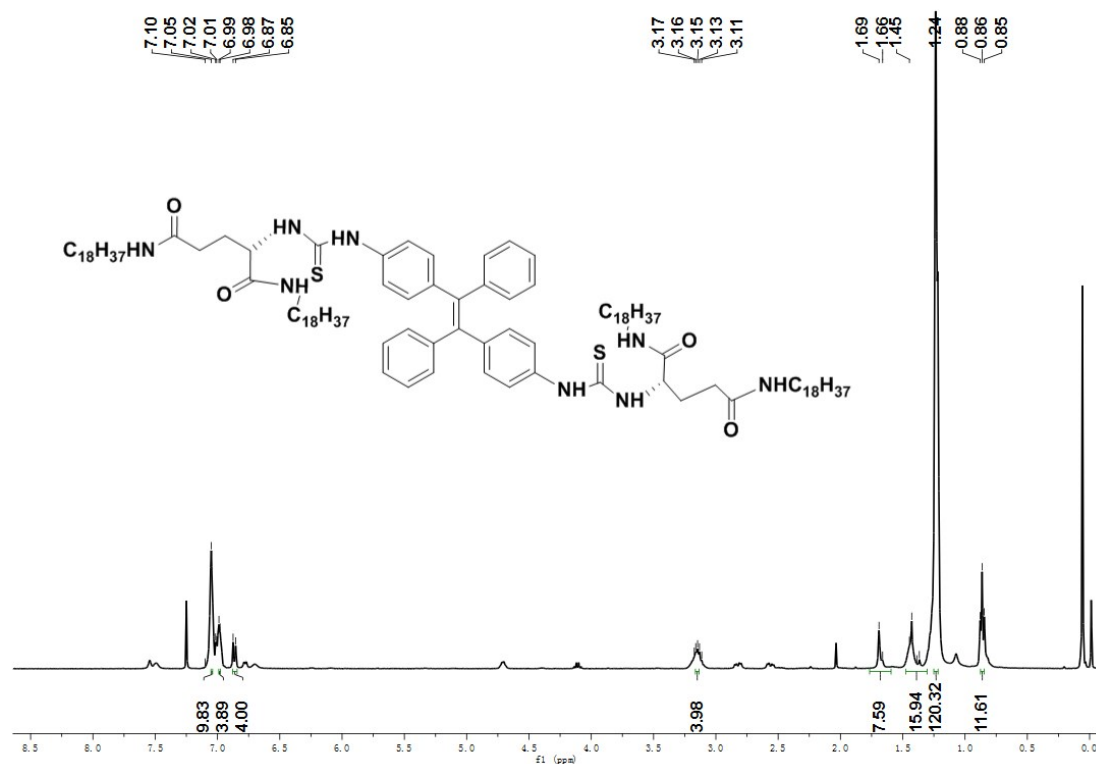


Figure S17. ¹H NMR spectrum of *trans*-TPE-*L*-DGlu in CDCl₃