Supplementary information

Nanoarchitectonics of a covalent organic supramolecular cage (COSC) for fluorescent visual detection of macrolides

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Content

1. Supplemental Experimental Procedures

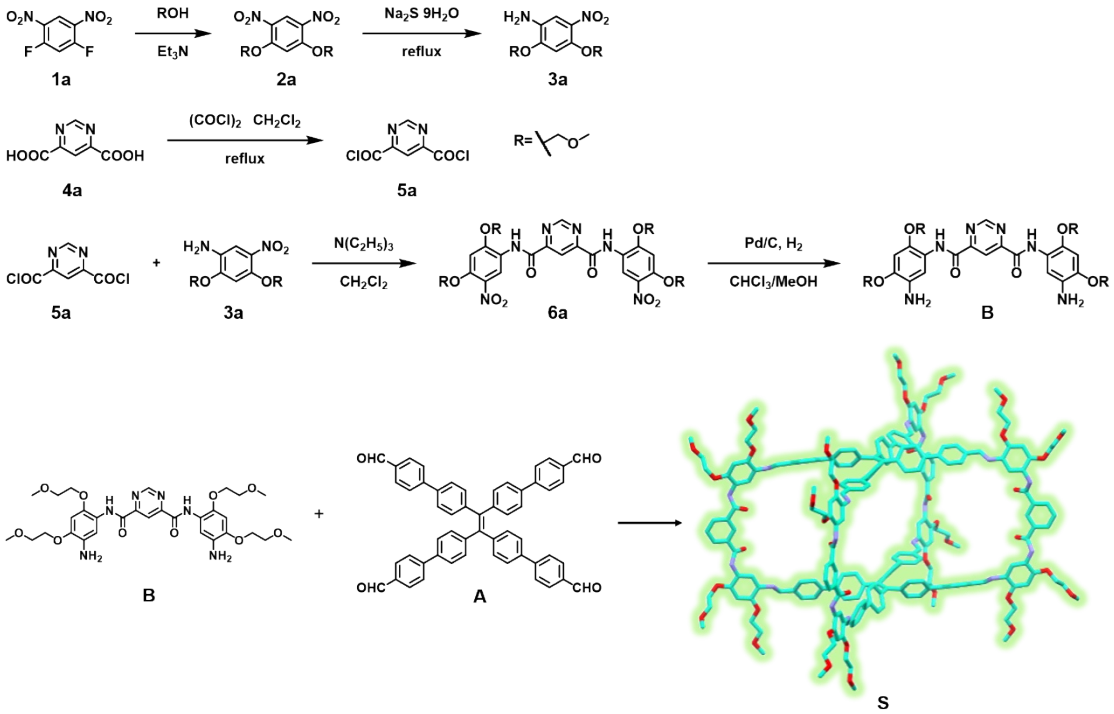
General Procedures. Reagents and solvents were purchased from Energy Chemical, Bidepharm, and used without purification. Thin-layer chromatography (TLC) was performed on flexible sheets (Greagent) precoated with Al_2O_3 (IB-F) and SiO_2 (IB2-F) and visualized by UV light. Column chromatography was conducted using neutral Al_2O_3 (200-300 mesh). ^1H, ^{13}C, 2D COSY and 2D ^1H-^1H NOESY NMR spectra were recorded on a Bruker NMR 500 MHz. Different NMR solvents were purchased from Bidepharm. ESI-MS was recorded with a Waters Synapt G2 Si tandem mass spectrometer, using solutions of 0.01 mg sample in 1 mL of $CHCl_3$/CH_3OH (1:3, v/v) for ligands or 0.5 mg sample in 1 mL of MeCN/MeOH (3:1, v/v) for **S**[1].

Molecular Modeling. Energy minimization of the macrocycles was conducted with the Materials Studio version 6.0 program, using the Anneal and Geometry Optimization tasks in the Forcite module (Accelrys Software, Inc.). The counterions were omitted. Geometry optimization used a universal forcefield with atom-based summation and cubic spline truncation for both the electrostatic and van der Waals parameters.

UV-vis absorption and fluorescence properties. UV-vis absorption spectra were recorded on a Thermo Fisher Scientific Evolution 201 spectrophotometer at room temperature and were corrected with the background spectrum of the solvent. Fluorescence properties were performed on Edinburgh-FS5 Fluorescence spectrometer at 298K.

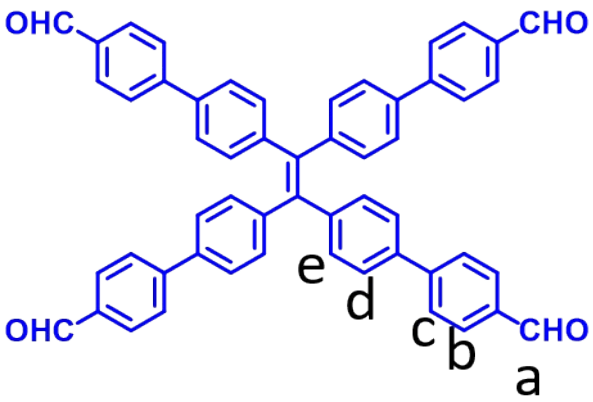
X. Computational details. Geometry optimization of the organic supramolecular cage and guest molecules was performed using the Forcite module with the Universal Force Field (UFF) in the Materials Studio 8.0 software package[2]. Subsequently, the host-guest conformational search was conducted using simulated annealing with the Monte Carlo method in the Adsorption Locator module with 20 cycles, 10000 steps per cycle, and the optimized guest molecule was selected as the adsorbate. Geometry optimization using Quasi-Newton algorithm was allowed during the calculation to obtain the most stable host-guest model. The electronic structure of the most stable

host-guest model was further studied using quantum mechanics/molecular mechanics (QM/MM) theory[3], implemented with the two-layer ONIOM approach[4] in the Gaussian 16 C.01 program[5]. Here, the guest molecule was treated as the QM part and set as the high layer, while the surrounding supramolecular cage was chosen as the MM part and defined as the low layer. The QM and MM parts were treated with the WB97XD[6]/Def2-SVP[7] functional and universal force field (UFF)[2], respectively.



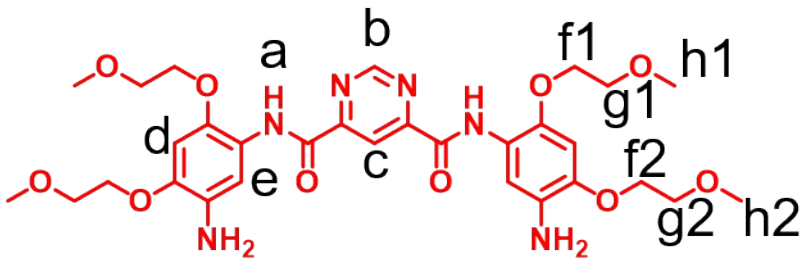
Scheme S1. Synthesis routes of **B** and **S**.

2. Synthesis of compounds and supramolecule

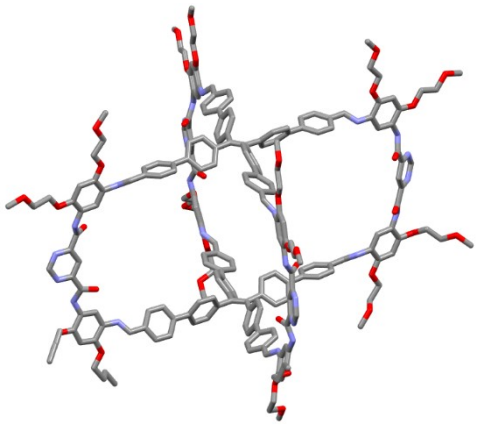


A was purchased from commercial supplier. In order to compare the ^{1}H NMR changes of **A+B** and **S**, the ^{1}H NMR of **A** and **B** were tested separately. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, ppm) δ 10.03 (s, 4H), 7.97 – 7.88 (m, 8H), 7.77 – 7.70 (m, 8H), 7.51 – 7.45 (m, 8H), 7.24 (d, *J* = 8.5 Hz, 8H). ^{13}C NMR (126 MHz, $CDCl_3$ 298 K, ppm) δ

191.87, 146.37, 143.64, 140.75, 137.95, 135.21, 132.13, 130.29, 127.41, 126.87.



B was synthesized as described in literature[8] with a little modification. Choose the glycol chain instead of alkyl chain. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, ppm) δ 10.42 (s, 2H), 9.33 (s, 1H), 9.00 (s, 1H), 8.08 (s, 2H), 6.63 (s, 2H), 4.15 (dt, *J* = 26.9, 4.7 Hz, 8H), 3.76 (dt, *J* = 10.1, 4.6 Hz, 8H), 3.46 (d, *J* = 8.4 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K, ppm) δ 159.62, 159.07, 156.48, 143.02, 140.82, 131.49, 122.31, 115.95, 107.80, 102.09, 71.12, 71.04, 70.53, 68.99, 59.26, 59.17. ESI-TOF (*m/z*): Calcd. for $[C_{30}H_{40}N_6O_{10}]^+$: 644.92. Found: 644.92.



Synthesis the cage S: A (75 mg, 1.0 eq, 0.1 mmol), **B** (130 mg, 2.0 eq, 0.2 mmol) and $CHCl_3$/MeOH (v/v= 3 mL: 1mL) were added to a 10 mL round-bottomed flask and stirred at 50 ℃ for 4 h. The reaction was continued for 2 h with the addition of 10 μL of trifluoroacetic acid, cooled to room temperature and then the solvent was removed under vacuum to give an orange-red solid (Yield: 98%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, ppm) δ 9.80 (s), 9.24 (s), 8.72 (s), 8.42 (d, *J* = 3.6 Hz), 7.74 (d, *J* = 8.1 Hz), 7.57 (d, *J* = 8.0 Hz), 7.06 (d, *J* = 8.3 Hz), 7.01 (d, *J* = 8.4 Hz), 6.68 (s), 4.16 (d, *J* = 4.9 Hz), 4.09 (d, *J* = 4.8 Hz), 3.71 (t, *J* = 4.4 Hz), 3.65 (d, *J* = 4.7 Hz), 3.34 (s), 3.32 (d, *J* = 4.9 Hz), 3.29 (d, *J* = 7.1 Hz). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K, ppm) δ 163.54, 163.23, 162.91, 162.59, 162.09, 161.75, 161.42, 134.22, 131.31, 130.58, 121.79, 120.06, 119.53, 117.79, 117.26, 115.00, 74.39, 73.31, 72.11, 62.98, 62.59, 57.76, 57.58, 57.40, 57.22, 57.04. ESI-TOF (*m/z*): 1933.7358 (S with a glycol chain lost), calculated: 1933.7358; 1611.6030 (S with L2 lost), calculated: 1611.6030; 1289.6642 (S with a glycol chain lost), calculated: 1289.6642; 967.2510 (S with a glycol chain lost), calculated: 967.2510.

3. NMR Spectra

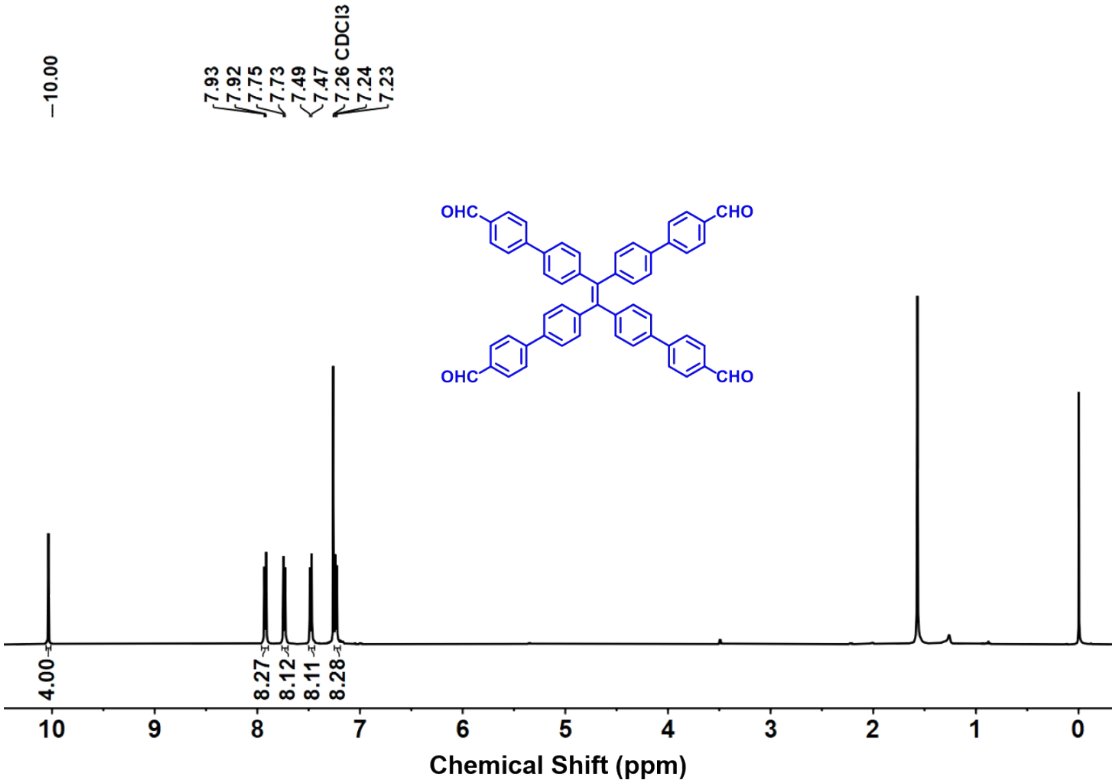


Figure S1. The ^{1}H NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **A**.

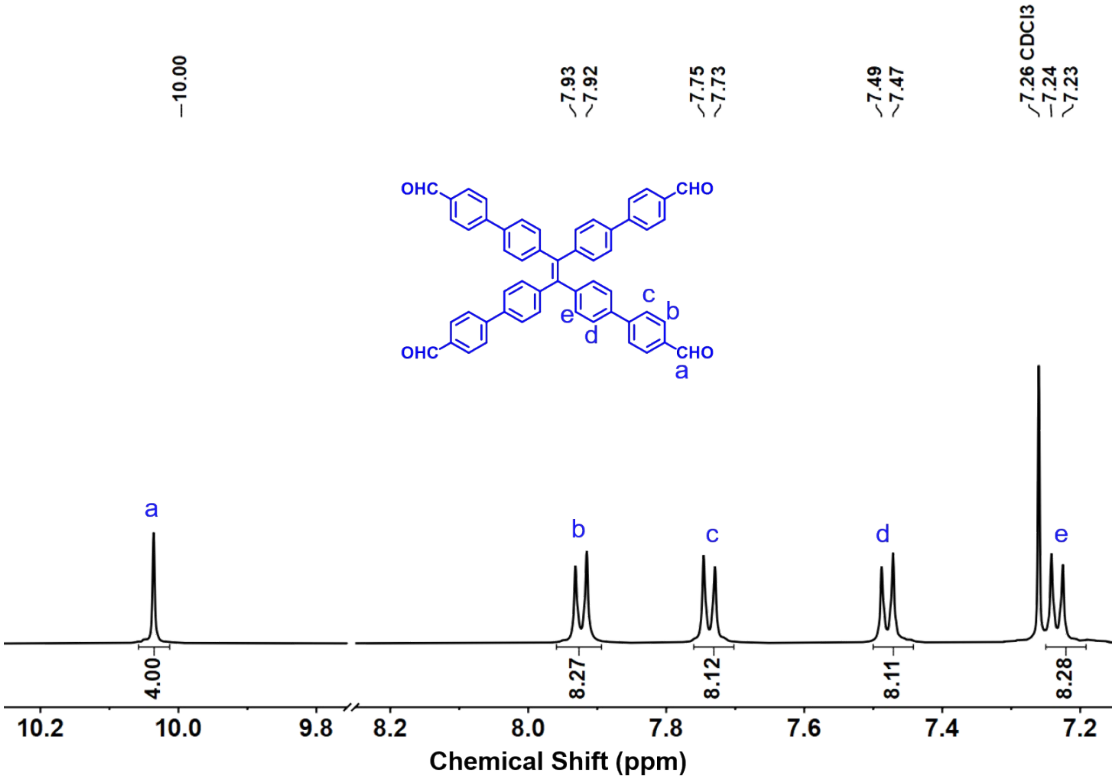


Figure S2. The aromatic region of ^{1}H NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **A**.

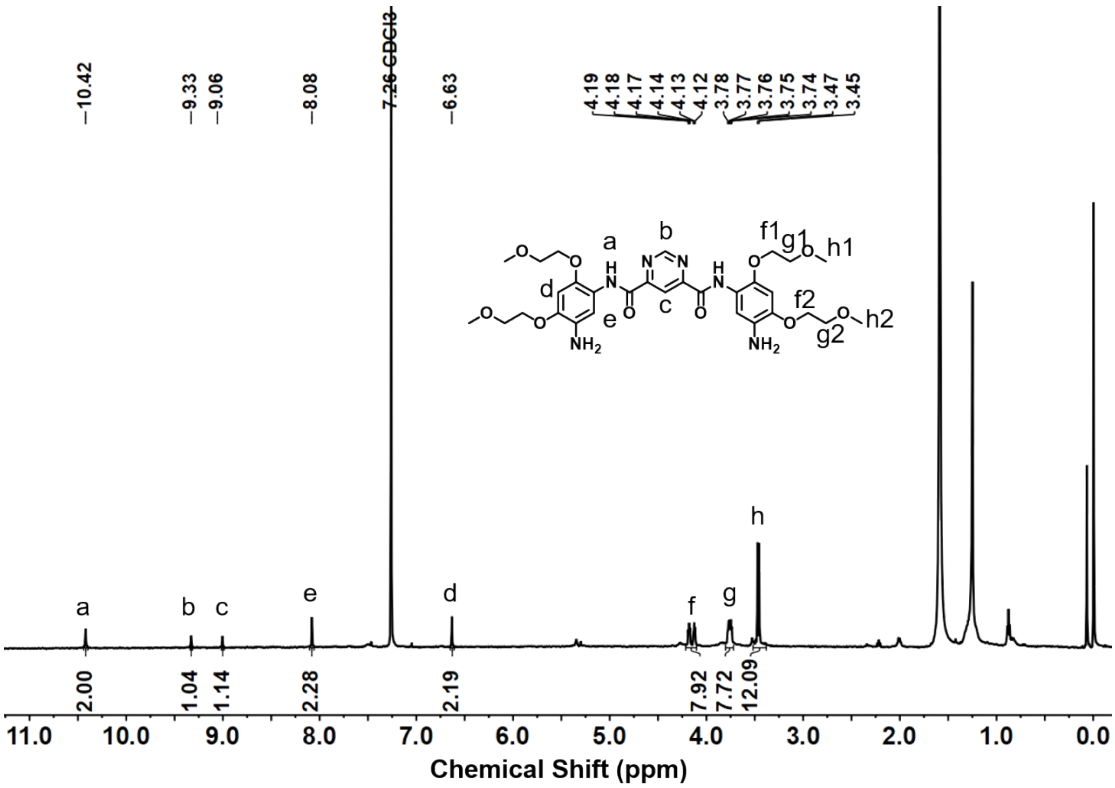


Figure S3. The ^{1}H NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **B**.

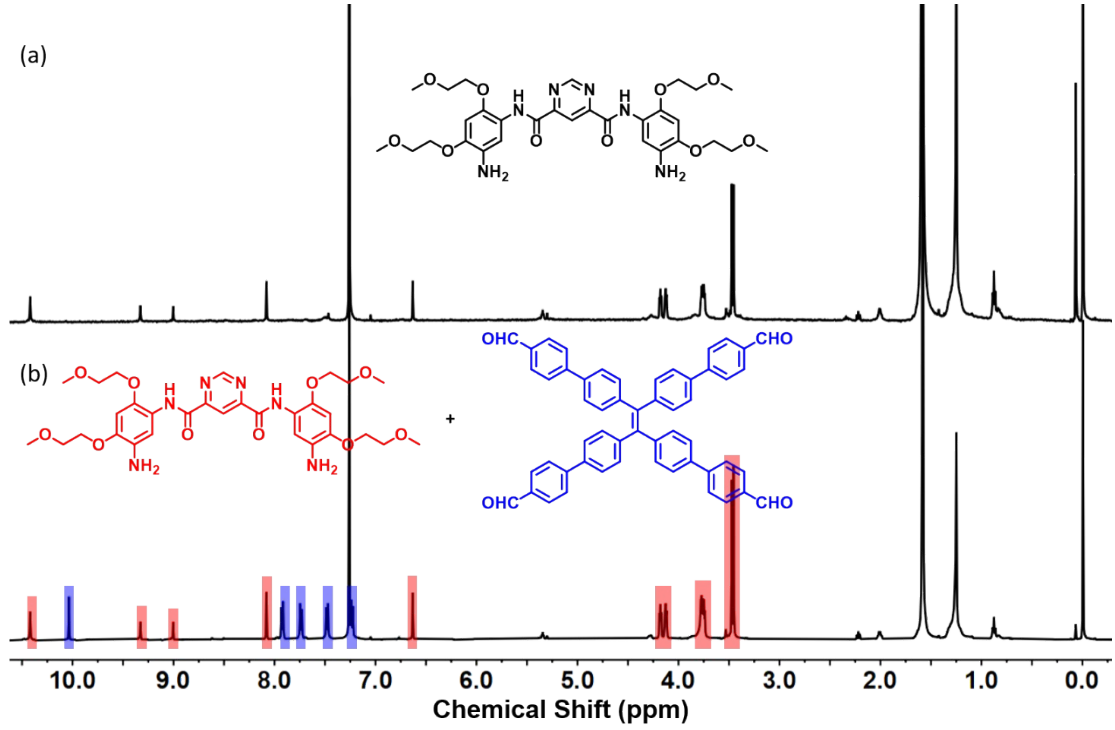


Figure S4. The comparison of the ^{1}H NMR (500 MHz, 298 K, $CDCl_3$) spectra of (a) **B** and (b) **A+B**.

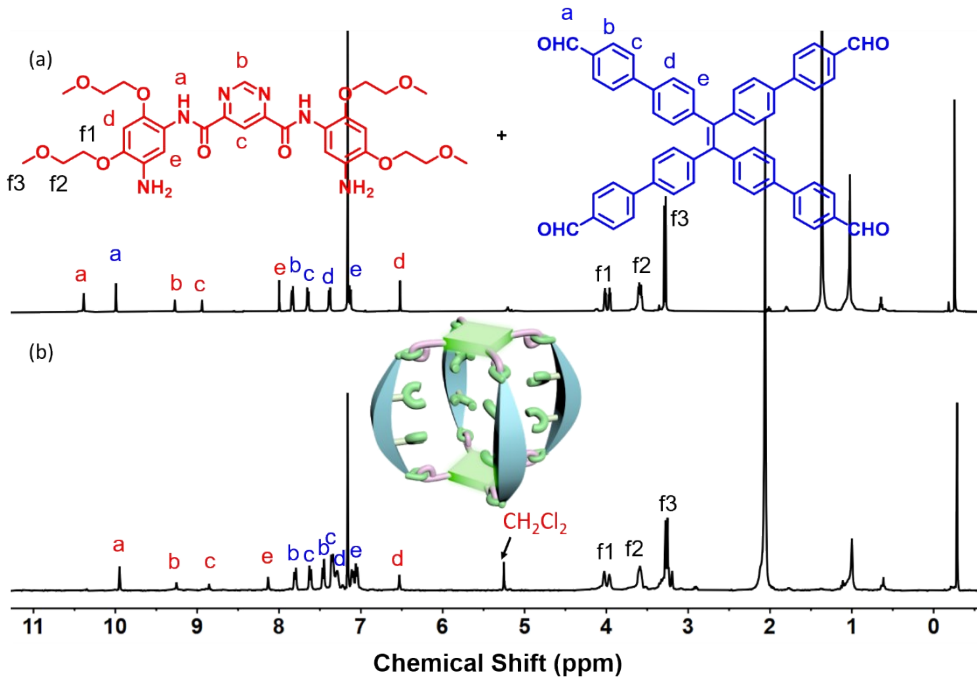


Figure S5. The comparison of the ^{1}H NMR (500 MHz, 298 K, $CDCl_3$: CD_3OD= 5:1) spectra of (a) **A+B** and (b) **S**.

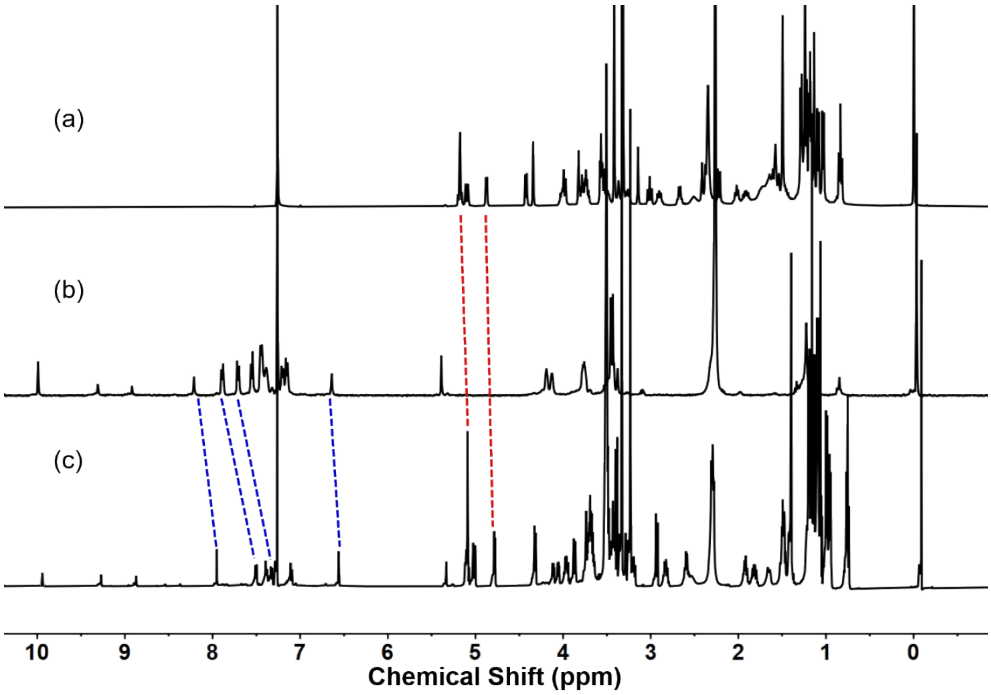


Figure S6. The comparison of the ^{1}H NMR (500 MHz, 298 K, $CDCl_3$) spectra of (a) **G**,(b) **S** and (c) **G⊂S**.

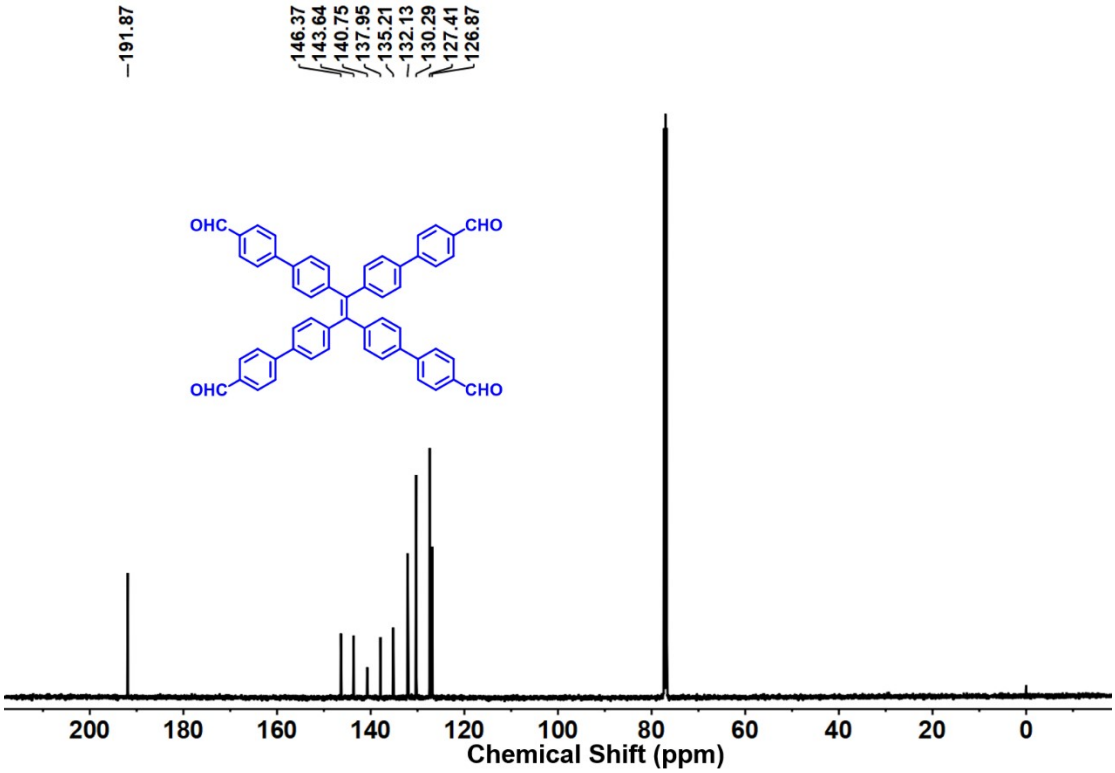


Figure S7. The ^{13}C NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **A**.

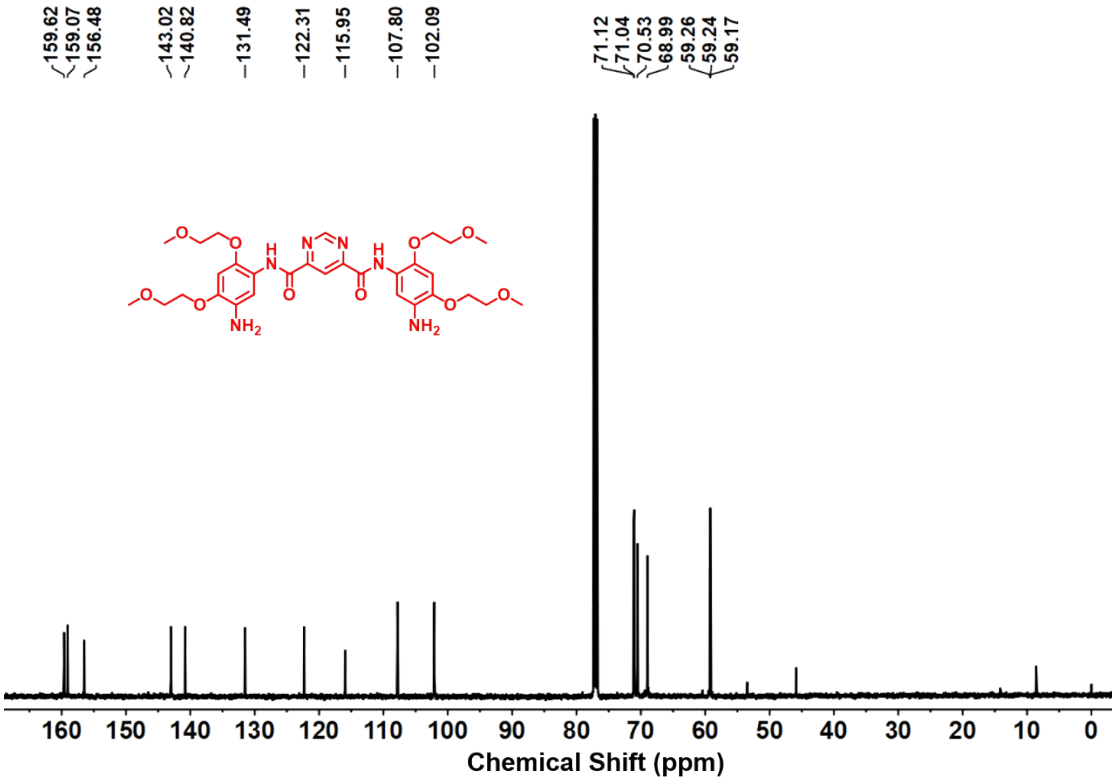


Figure S8. The ^{13}C NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **B**.

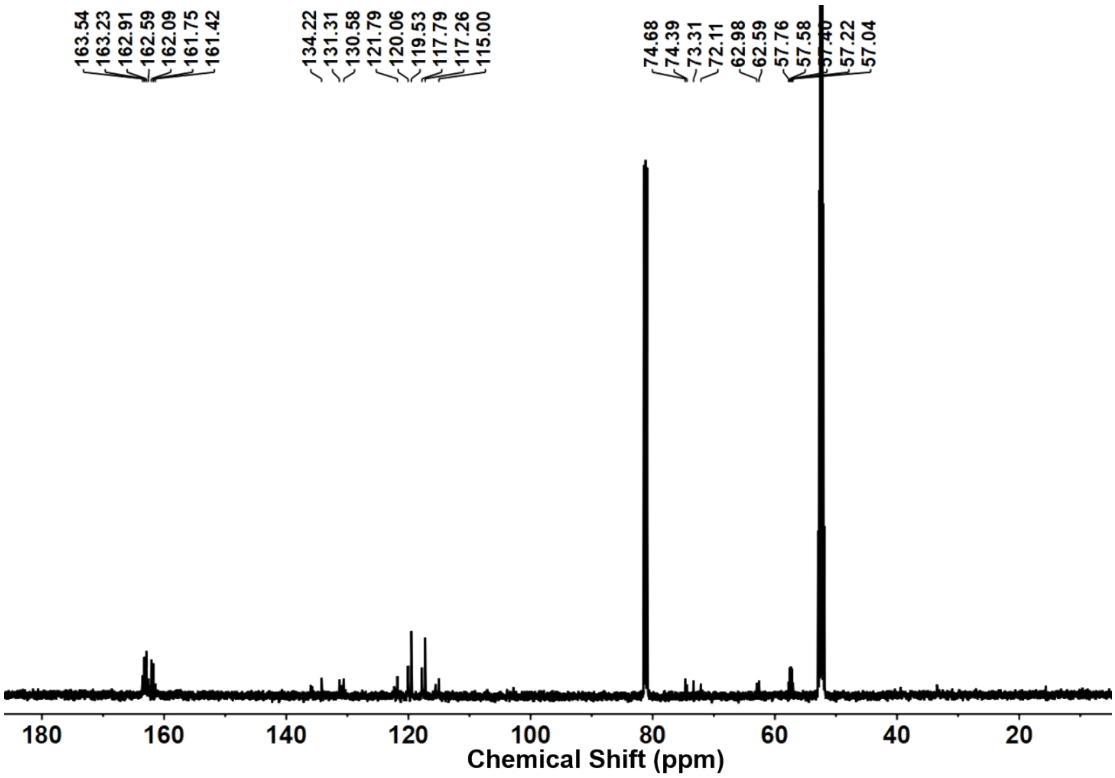


Figure S9. The ^{13}C NMR (500 MHz, 298 K, $CDCl_3$) spectrum of **S**.

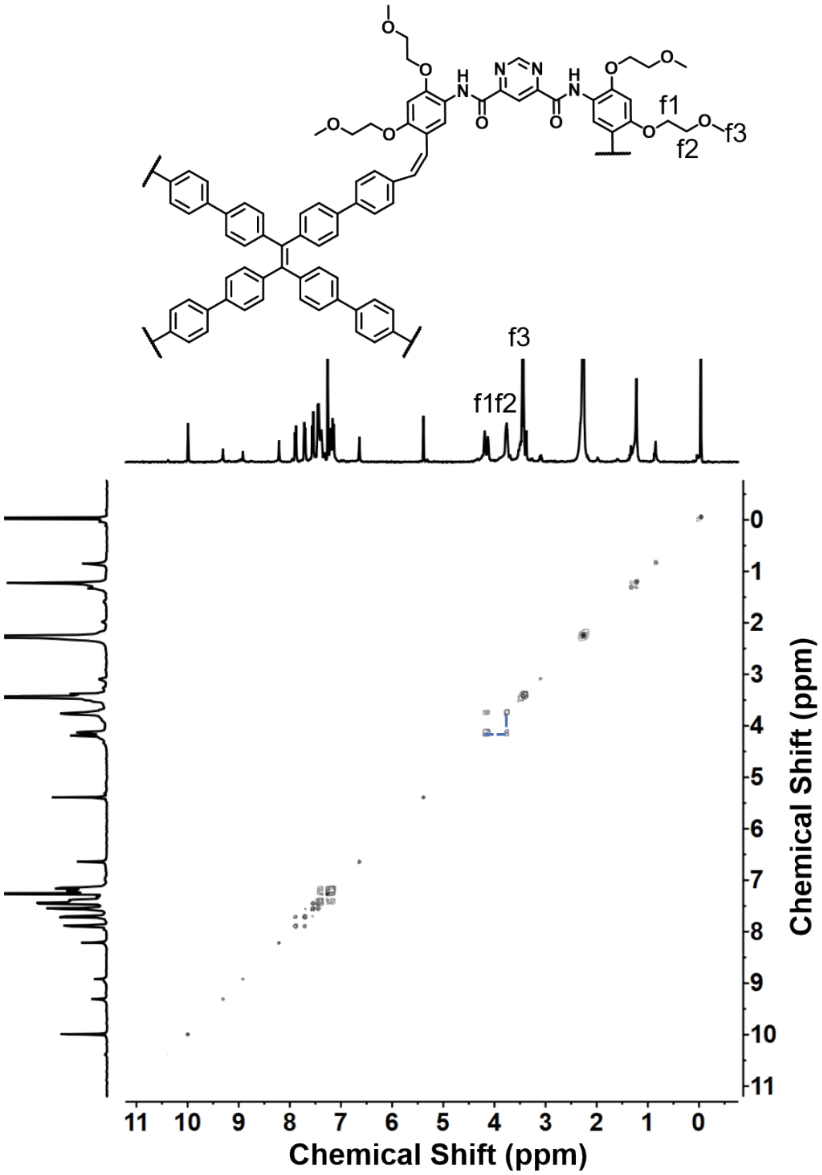


Figure S10. 2D ^{1}H-^{1}H COSY NMR (500 MHz, 298 K) spectrum of **S** in $CDCl_3$

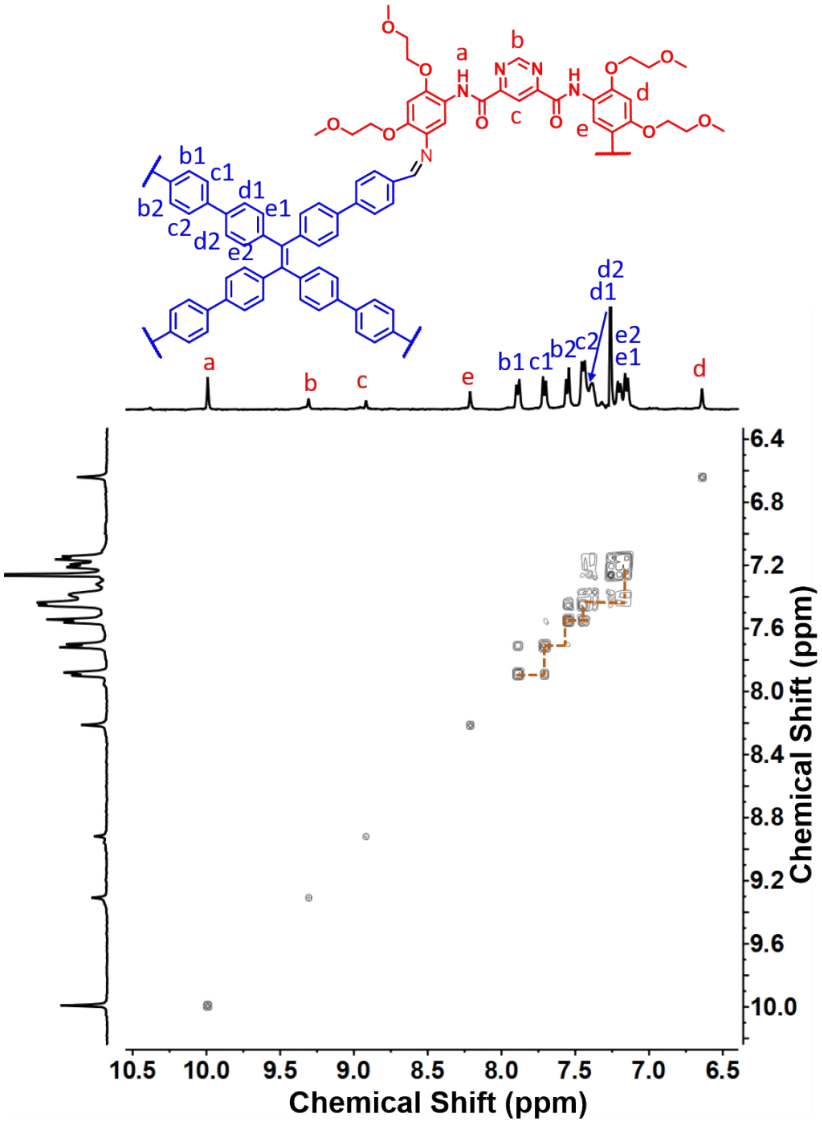


Figure S11. 2D ^{1}H-^{1}H COSY NMR (500 MHz, 298 K) spectrum of **S** in $CDCl_3$ (aromatic region)

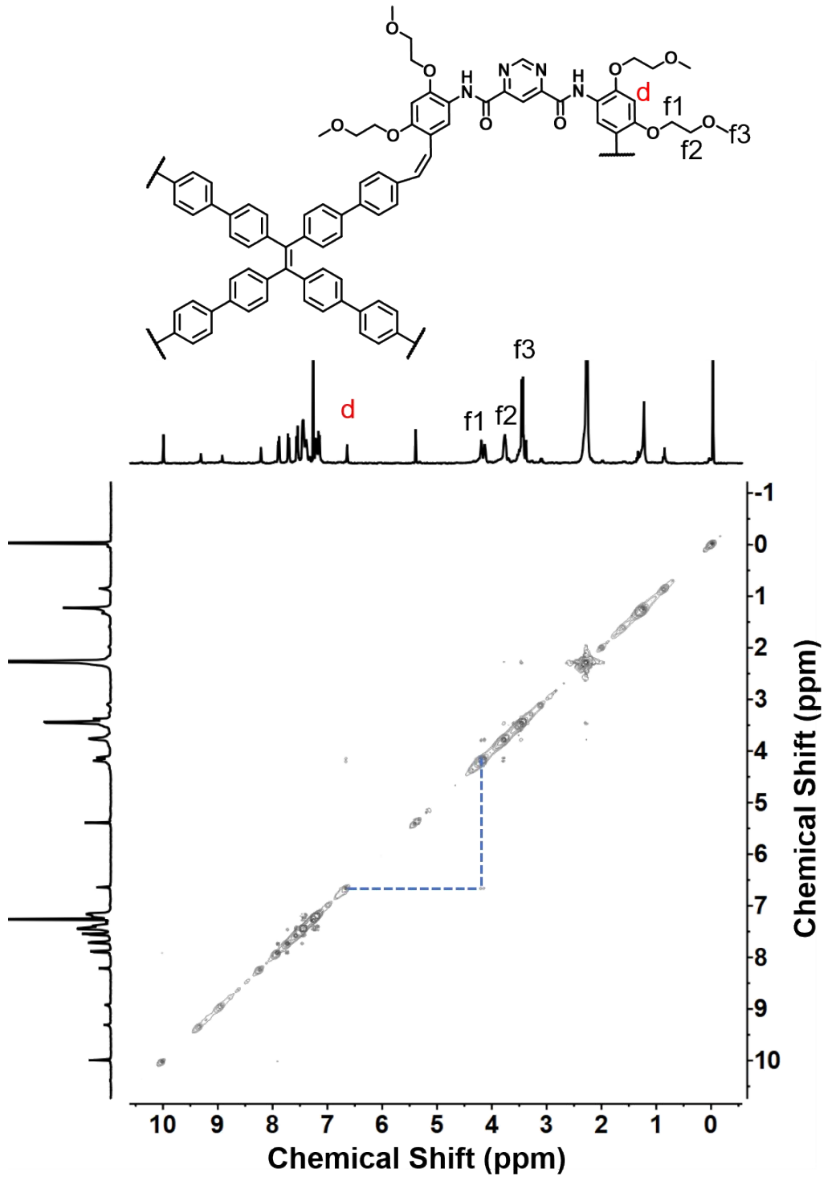


Figure S12. 2D ^{1}H-^{1}H NOESY NMR (500 MHz, 298 K) spectrum of **S** in $CDCl_3$

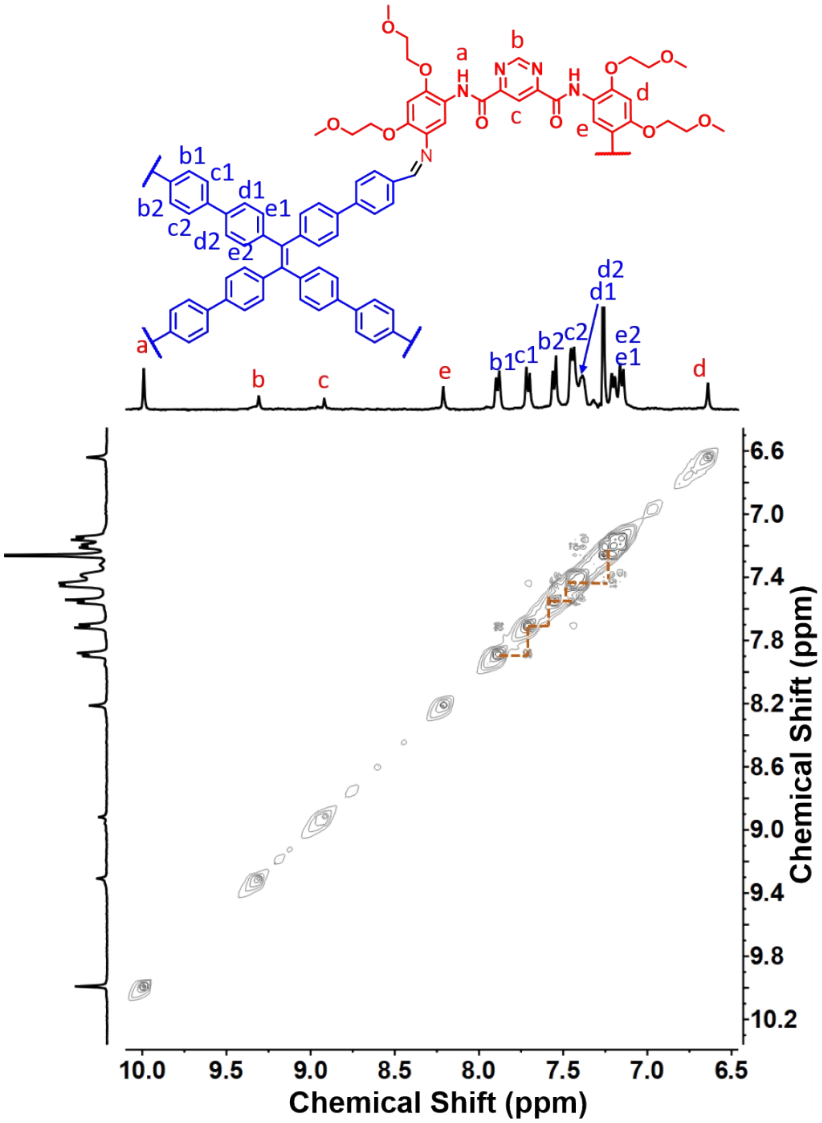


Figure S13. 2D ^{1}H-^{1}H NOESY NMR (500 MHz, 298 K) spectrum of **S** in $CDCl_3$ (aromatic region)

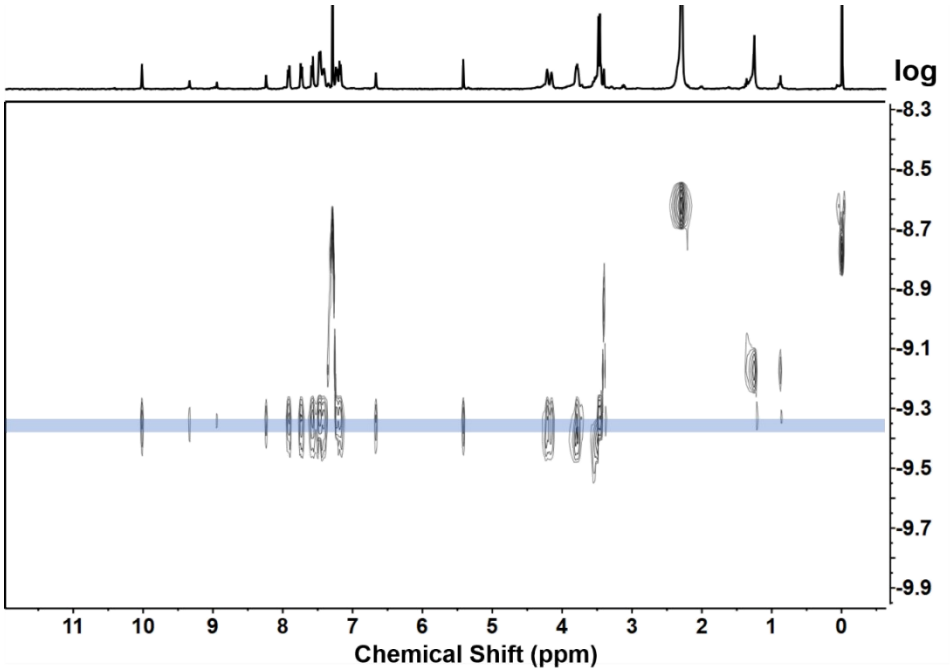


Figure S14 The DOSY (500 MHz, 298 K, $CDCl_3$) spectra of **S** in $CDCl_3$

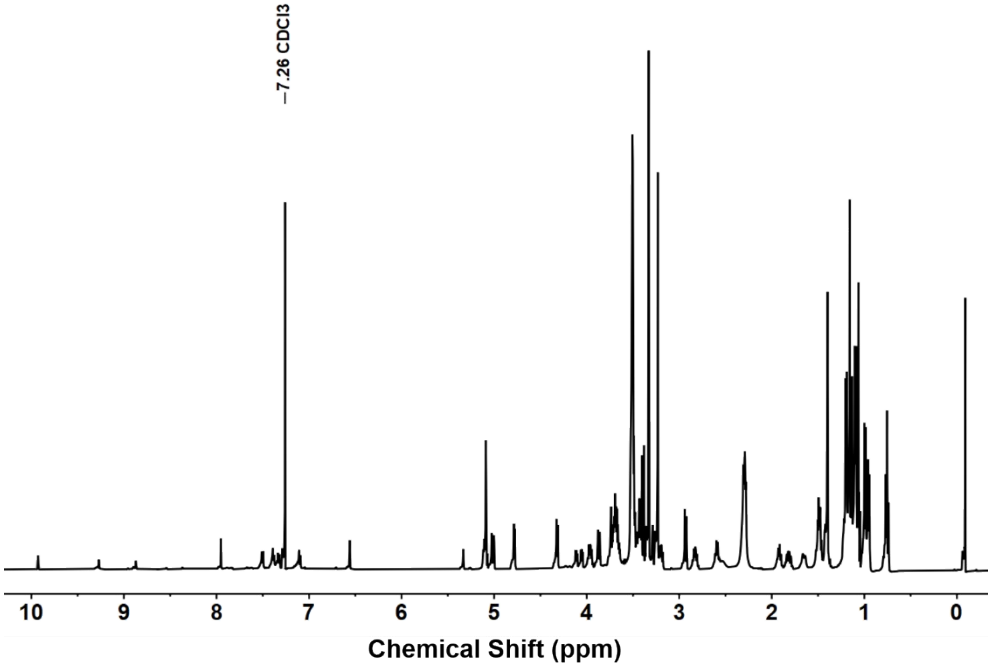


Figure S15. The ^{1}H NMR (500 MHz, 298 K) spectrum of **G**$\subset$**S** in $CDCl_3$: CD_3OD (1:1).

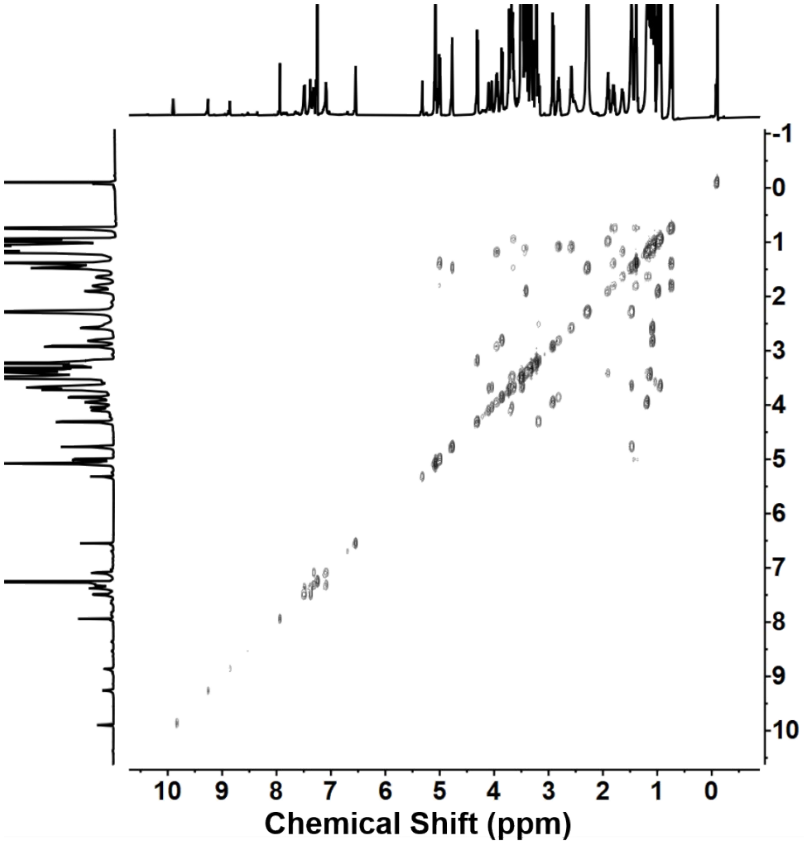


Figure S16. 2D ^{1}H-^{1}H COSY NMR (500 MHz, 298 K) spectrum of **G⊂S** in $CDCl_3$: CD_3OD (1:1).

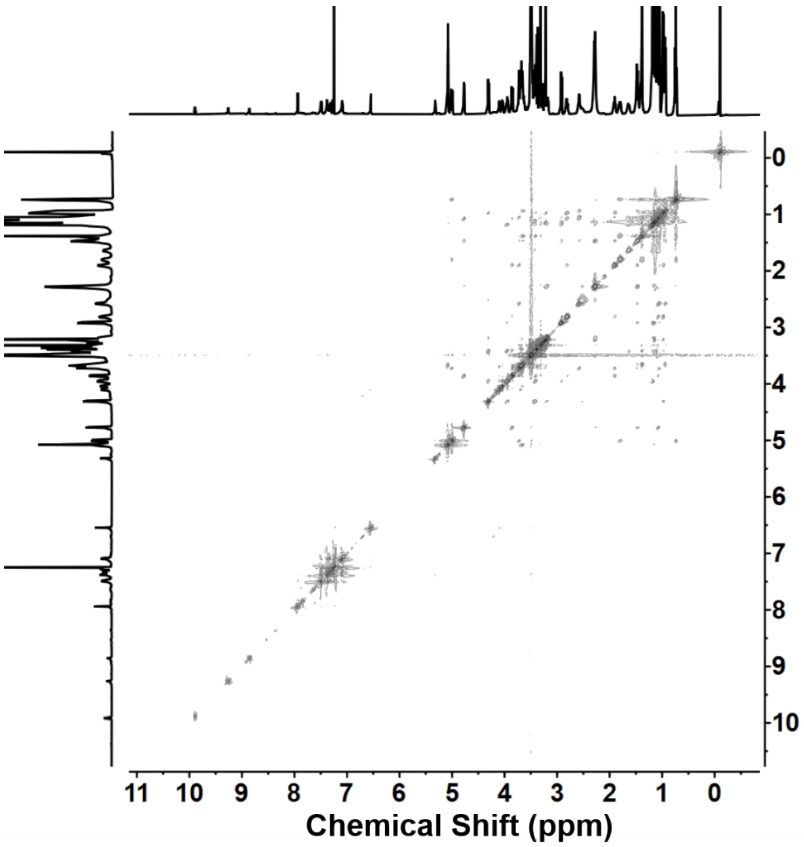


Figure S17. 2D ^{1}H-^{1}H NOESY NMR (500 MHz, 298 K) spectrum of **G⊂S** in $CDCl_3$: CD_3OD (1:1).

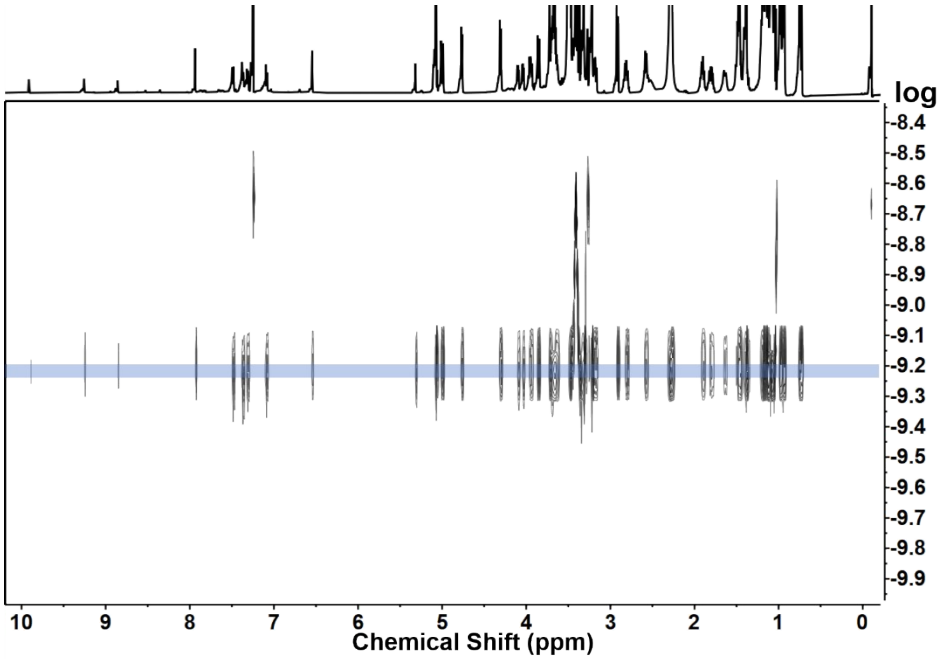


Figure S18. The DOSY (500 MHz, 298 K, $CDCl_3$) spectra of **G⊂S** in $CDCl_3$: CD_3OD = 1: 1.

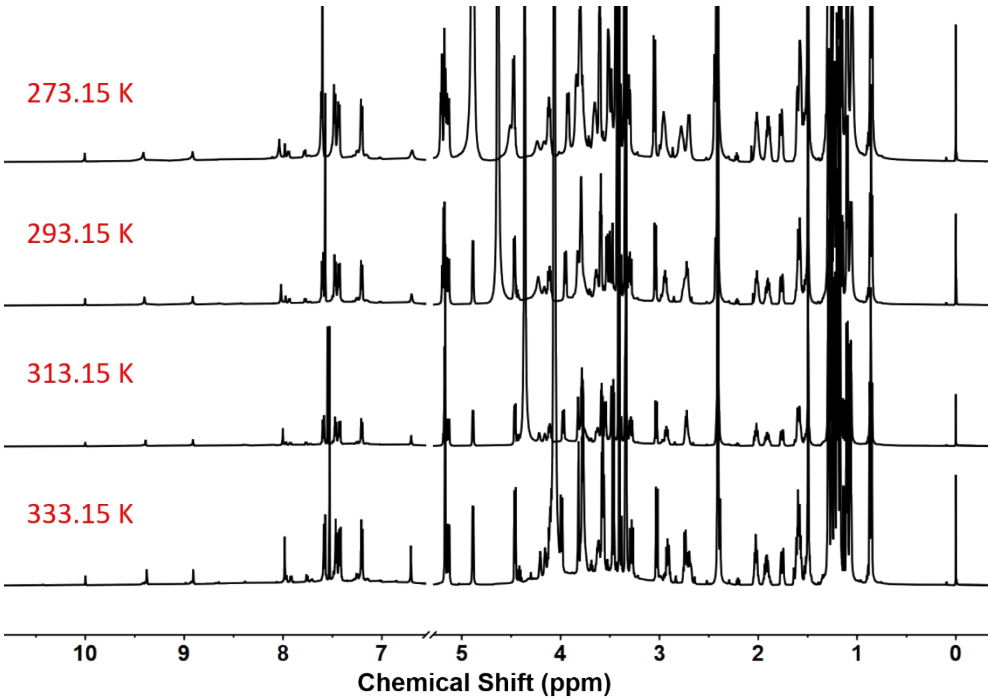


Figure S19. The VT ^{1}H NMR (500 MHz, 273.15 K -333.15 K) spectrum of **G⊂S** in $CDCl_3$: CD_3OD (1:1).

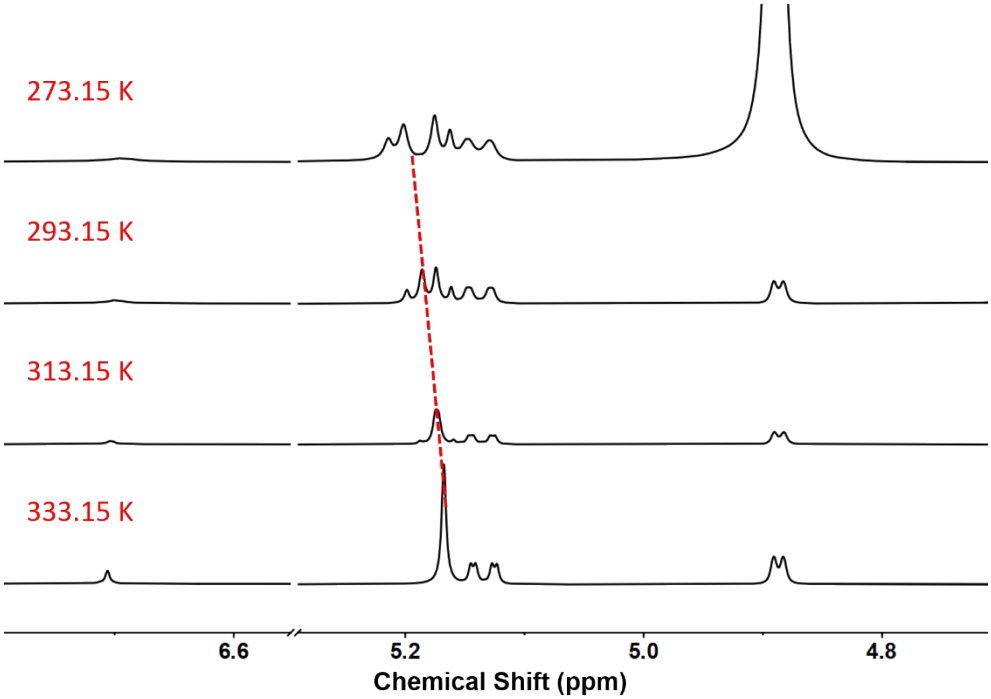


Figure S20. The VT ^{1}H NMR (500 MHz, 273.15 K -333.15 K) spectrum of **S** in $CDCl_3$: CD_3OD (1:1) at 6.6 ppm-4.8 ppm.

4. ESI and fluorescence Spectra

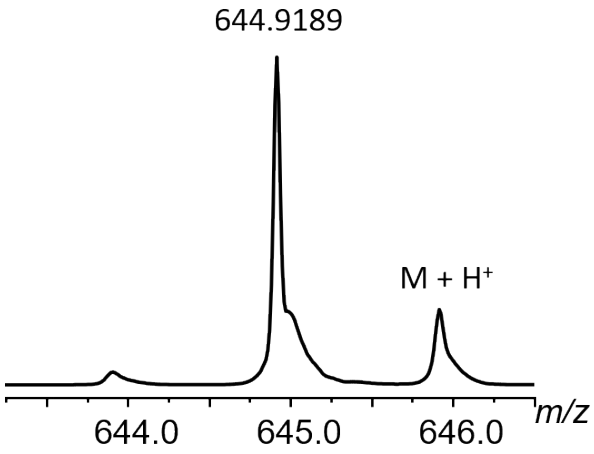


Figure S21. The ESI spectrum of **B**.

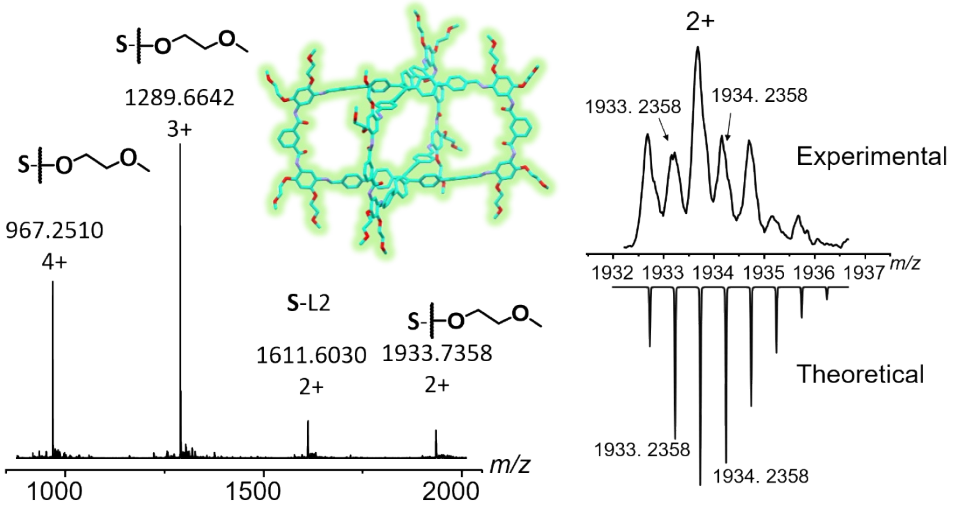


Figure S22. The ESI spectrum of **S**.

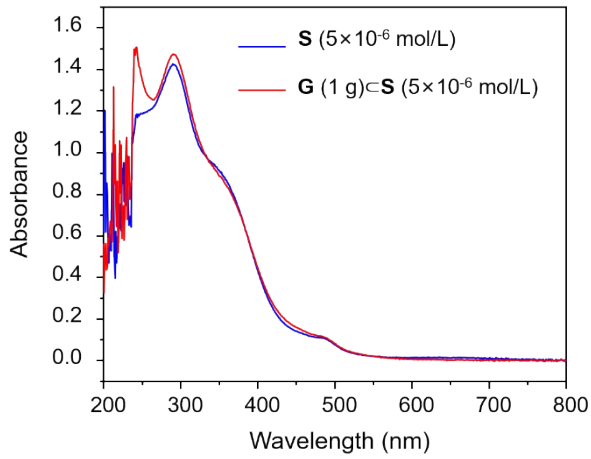


Figure S23. The UV-vis spectra of **G** and **G⊂S**

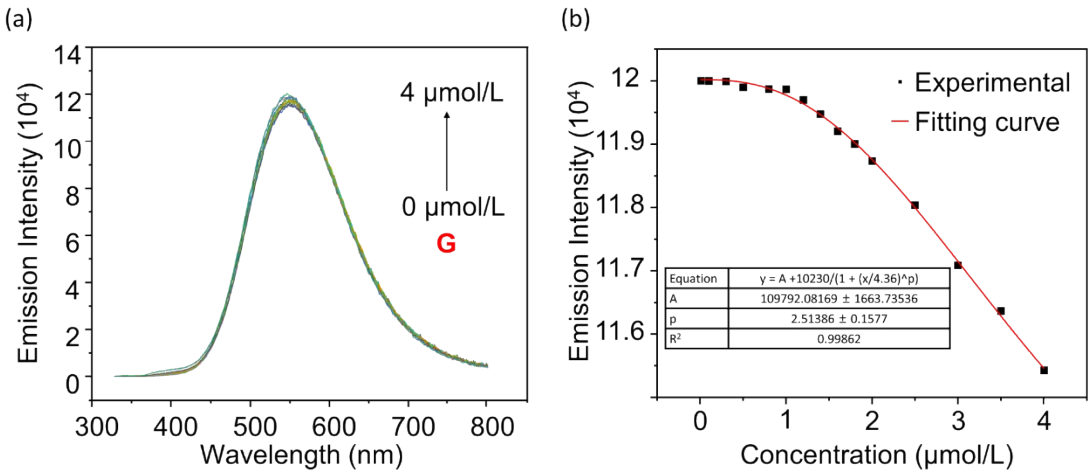


Figure S24. (a)The fluorescence spectrum of **G⊂S** which concentration was 0–4 μmol/L. (b)The measured (dot) emission peak intensities and their corresponding linear test (solid lines).

$$LOD_{response} = \bar{X}_{blank} + 3\sigma_{blank}$$

$\bar{X}_{blank}$: Mean response value for blank samples

$3\sigma_{blank}$: Standard deviation of blank samples

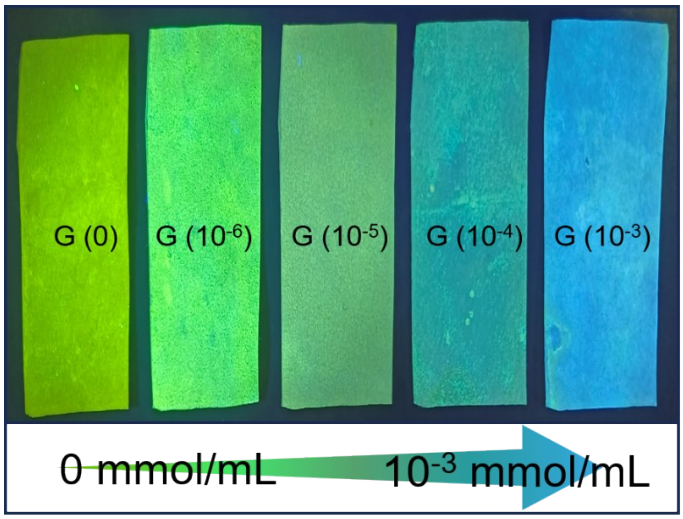


Figure S25. The image of **G** and different centration of **G⊂S**

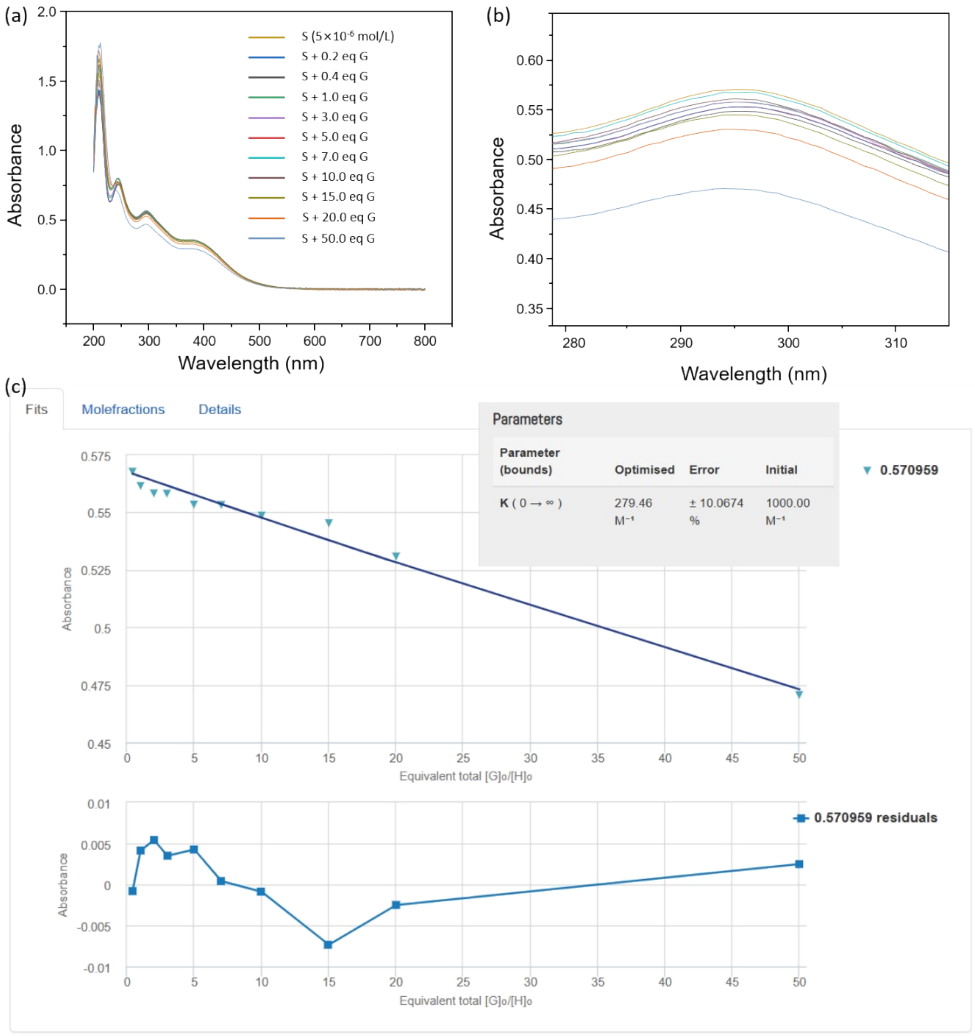


Figure S26. (a) The UV-vis spectra of **G⊂S** titration experiment. (b) The zoom in UV-Vis spectra of G⊂S titration experiments at 280 nm-310 nm. (c) The calculation of quantitative binding constants for **G⊂S**.

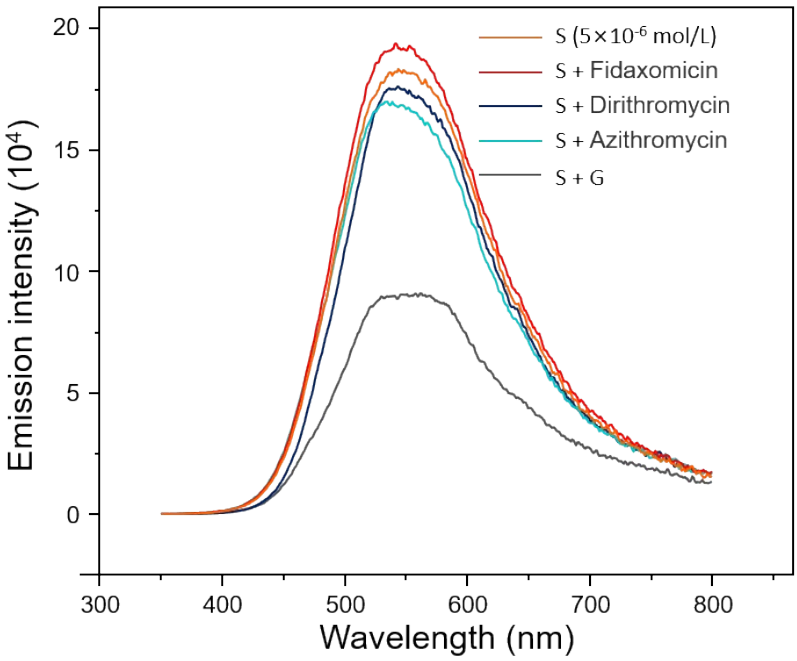


Figure S27. The fluorescence spectra of S (10^{-5} mol/L) in water with different macrolides (20.0 eq)

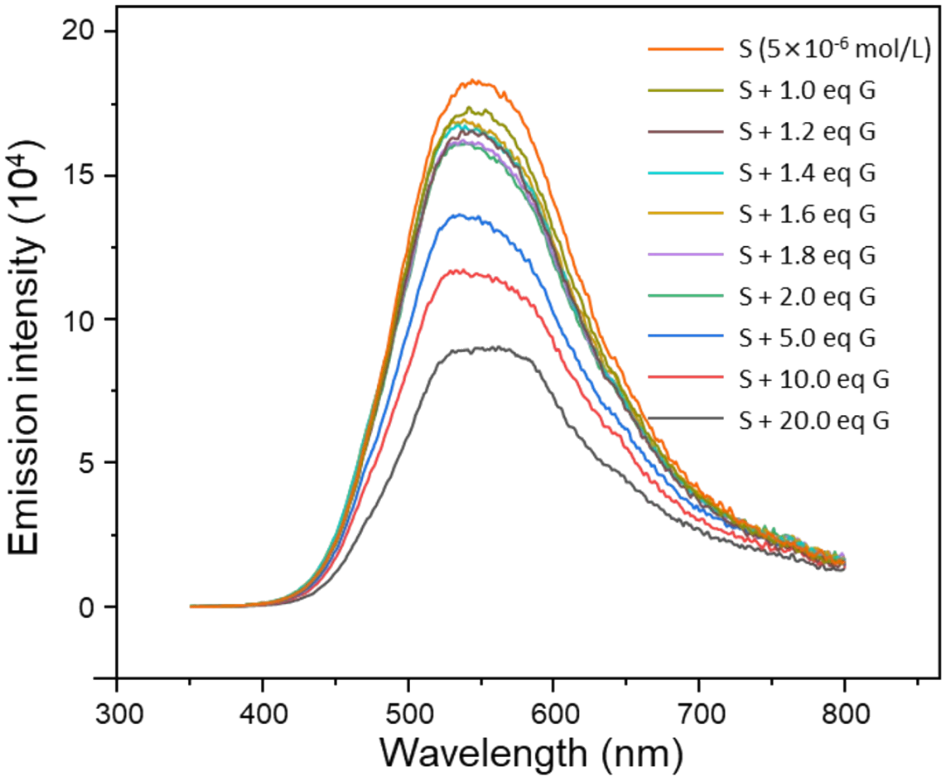


Figure S28. The fluorescence spectra of S (10^{-5} mol/L) in water with different equivalents of G

5. Density Functional Theory (DFT) Calculations

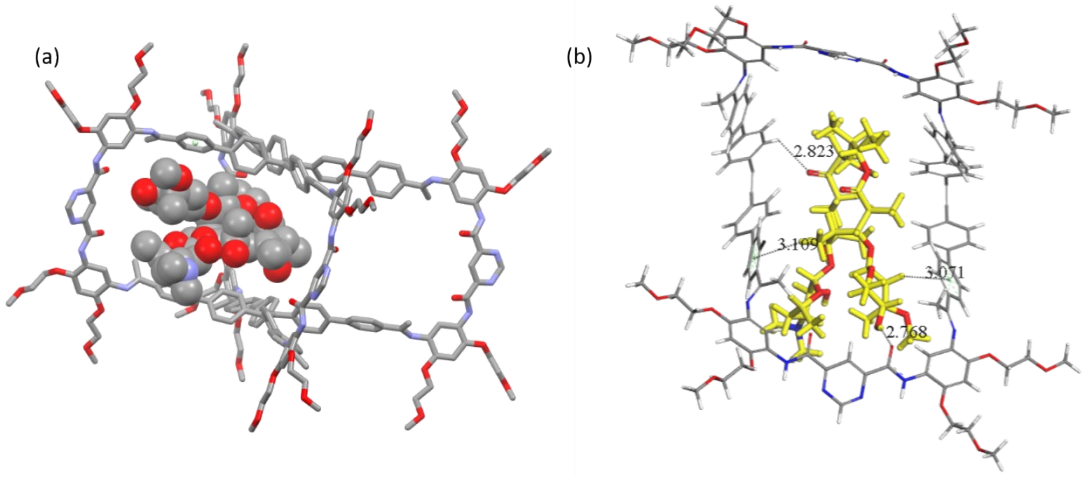


Figure S29. (a) The Material Studio image of the **G⊂S**. (b) the view showing C-H…O and C-H…π interactions between **G** and **S**. Color coding: N = blue; O = red; C = gray.

The cartesian coordinates (xyz) for the host-guest complex.

C	-0.40647480	0.82014387	0.00000000
C	-0.79237280	1.73693987	-0.90958400
C	-2.06027780	2.47662387	-0.74206600
C	-2.84707680	2.24147587	0.32113900
C	-2.43923580	1.22199087	1.31462300
C	-1.28598380	0.56091987	1.17101500
C	-4.11650780	2.98000887	0.50654500
C	-4.16824580	4.33400887	0.61601500
C	-5.35693080	2.17933387	0.52282800
C	-2.94933580	5.18367487	0.70862200
C	-5.47777680	5.01600787	0.70141700
C	-6.03856380	1.96551987	-0.61325800
C	-7.31072080	1.21966687	-0.58269300
C	-7.79656680	0.74961187	0.58097400
C	-7.03268080	0.97247887	1.83123800
C	-5.88386680	1.65780987	1.80512300
C	-6.09054180	5.46279787	-0.40642800
C	-7.41406680	6.10971587	-0.31337700
C	-8.03582080	6.21842787	0.87564100
C	-7.36935480	5.69190587	2.09273200
C	-6.15420480	5.13802787	2.01188500
C	-1.95924380	4.89374887	1.57315400
C	-0.75710180	5.74818687	1.65503500
C	-0.65348280	6.86299187	0.90406300
C	-1.77248880	7.20923287	-0.01084800
C	-2.84448180	6.41635187	-0.10936200
C	0.87484220	0.08092687	-0.15582500
C	-9.06451580	-0.00375213	0.62071400
C	-9.36589880	6.85612587	0.98541700
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