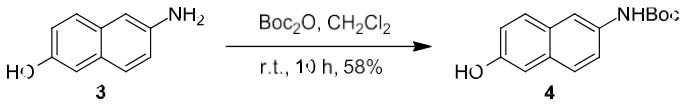
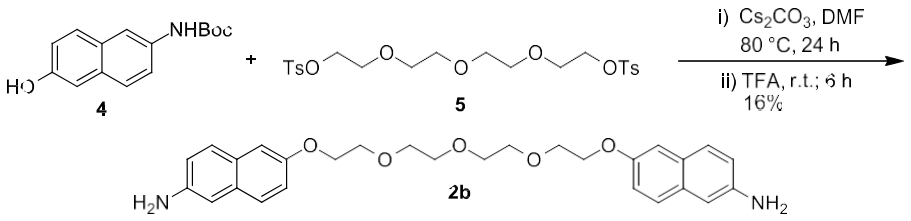
General methods: All solvents were dried following the standard procedures before use. Unless otherwise indicated, all starting materials were obtained from commercial suppliers and used without further purification. ^{1}H and ^{13}C NMR spectra were recorded on 400 or 500 MHz spectrometers in the indicated solvents by DMX 400 MHz (Bruker, Germany) or Varain Mercury 500 MHz (Varian, USA) NMR instruments. Chemical shifts were referenced to the residual solvent peaks. Mass spectra were obtained on Shimadzu LCMS-2010EV, IonSpec 4.7 Tesla FTMS and micro-TOF II spectrometers. UV-Vis absorption spectra were recorded with a Perlom Elmer Lambda 750S UV-Vis /NIR Spectrophotometer (PerkinElmer, USA). Fluorescence spectra were measured with F-4600 FL Spectrophotometer (Hitachi, Japan). DLS was performed on a Zetasizer Nano ZS90 light-scattering instrument (Malvern, UK). AFM images were recorded on a Nano scope IIIaMultiMode microscope. Transmission electron micrographs were recorded on a 2100F JEOL FETEM microscope at 120 kv aligned for low dose (10 $eÅ^{-2}$ s^{-1}) diffractive imaging. Synchrotron radiation SAXS and GISAXS experiments were performed on the BL16B beamline of Shanghai Synchrotron Radiation Facility, using a fixed wavelength of 0.124nm, a sample to detector distance of 1.87m an exposure time of 3600s and 4000 s, respectively.



3 4

Compound 4.[1] A solution of di-tert-butyl pyrocarbonate (0.19 g, 1.0 mmol) in CH_2Cl_2 (5 mL) was slowly added to a solution of compound **3** (0.16 g, 1.0 mmol) in CH_3OH (5 mL) within 1 hour under N_2 atmosphere. The mixture was stirred at room temperature for 10 hours and then concentrated with a rotavapor. After workup, the crude product was purified by flash column chromatography (ethyl acetate/petroleum ether, 1:4) to yield compound **4** as a white solid (0.16 g, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.92 (br, 1H), 7.65 (d, J = 8 Hz, 1H), 7.58 (d, J = 8 Hz, 1H), 7.29-7.26 (m, 2H), 7.08-7.05 (m, 2H), 6.56 (br, 1H), 1.55 (s, 9H); EI-MS m/z: 259.3 $[M]^{+}$.



4 5 2b

Compound 2b. To a stirred solution of compound **4** (0.26 g, 1.0 mmol) and Cs_2CO_3 (1.30 g 4.0 mmol) in anhydrous DMF (15 mL) was added a solution of compound **5**[2] (0.26 g, 0.5 mmol) in anhydrous DMF (5 mL) in 1 hour. The mixture was heated to 80 °C for 24 hours and then concentrated under reduced pressure. The resulting slurry was treated with water (5 mL) and the solid formed was filtrated off. The solid was dried and then suspended to trifluoroacetic acid (5 mL) at room temperature for 6 hours. The solution was then concentrated with a rotavapor and the resulting residue dissolved in dichloromethane (10 mL). The solution was washed with diluted sodium bicarbonate (0.5 M, 50 mL × 2), water (5 mL) and brine (5 mL), and dried over sodium sulfate. Upon removal of the solvent with a rotavapor, the resulting crude product was purified by flash column chromatography (ethyl acetate/petroleum ether, 2:1) to yield compound **2b** as a brown oil (0.096 g, 16%). ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.47 (d, J = 8 Hz, 2H), 7.42 (d, J = 4 Hz,

2H), 7.10 (d, J = 4 Hz, 2H), 6.98 (d,d, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 6.89 (d,d, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 2H), 6.78 (d, J = 4.0 Hz, 2H), 5.12 (s, 4H), 4.16-4.14 (m, 4H), 3.87-3.85 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 128.5, 127.5, 126.9, 121.3, 119.1, 118.9, 115.1, 107.6, 107.3, 107.0, 70.6, 70.5, 69.5, 67.5. HRMS (ESI): Calcd for $C_{28}H_{32}N_2O_5$ $[M + H]^+$: 477.2384. Found: 477.2381.

References:

1) L. Brockunier, E. R. Parmee and A. E. Weber, *Brit. UK Pat.*, 2001, 2356196.
2) R. A. Bartsch, Y. Liu, S. I. Kang, B. Son, G. S. Heo, P. G. Hipes and L. J. Bills, *J. Org. Chem.*, 1983, **48**, 4864-4869.

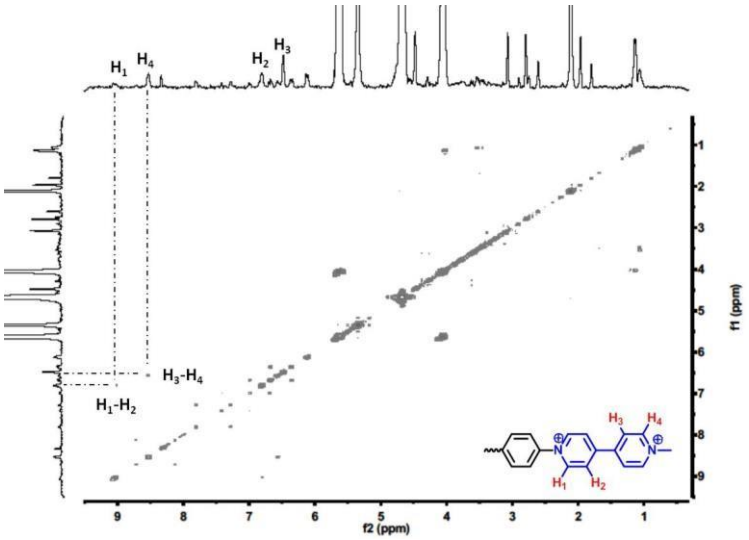


Fig. S1 2D COSY ^{1}H NMR spectrum (500 MHz) of the mixture of **1**, **2a** and CB[8] (1:1.5:3) in D_2O ([1] = 1.0 mM) at 25 °C.

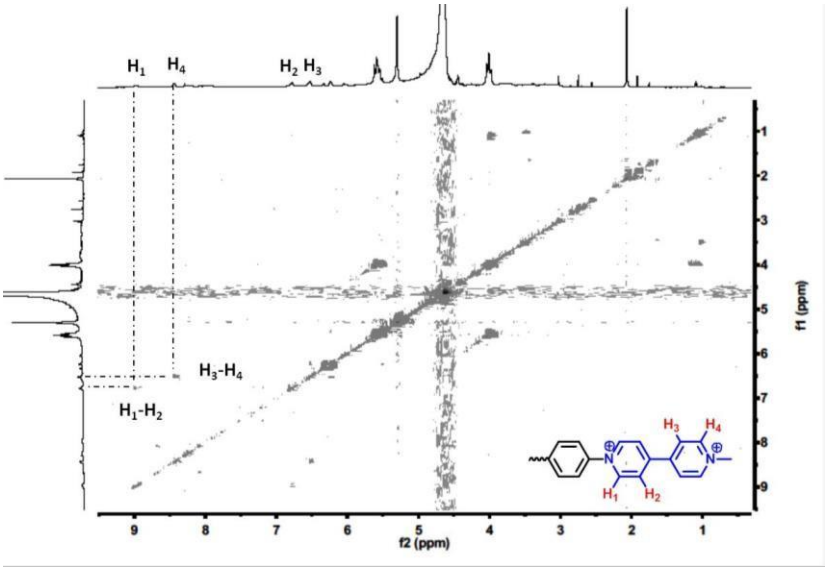


Fig. S2 2D COSY ^{1}H NMR spectrum (500 MHz) of the mixture of **1**, **2b** and CB[8] (1:1.5:3) in D_2O ([1] = 1.0 mM) at 25 °C.

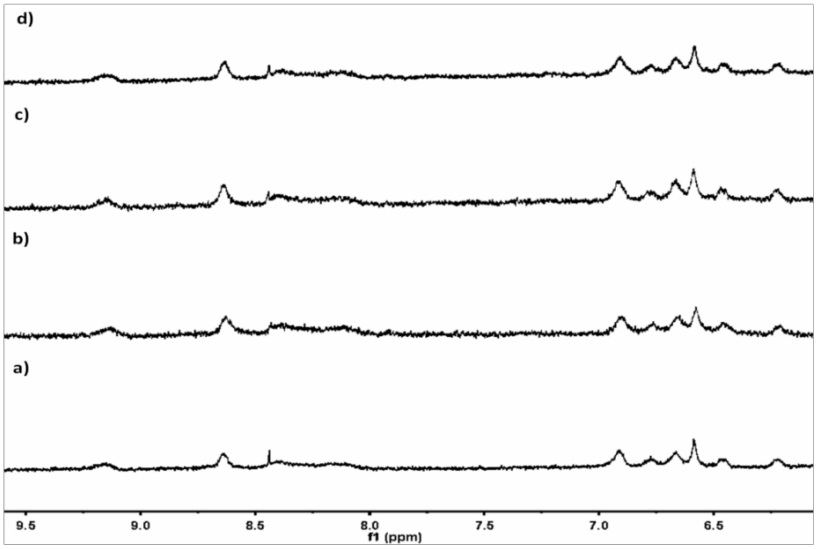


Fig. S3 Partial ^{1}H NMR spectra (400 MHz) of the mixture of **1**, **2a** and CB[8] (1:1.5:3) in D_2O at 25 °C. [**1**] = a) 1.0 mM, b) 0.5 mM, c) 0.25 mM and d) 0.125 mM.

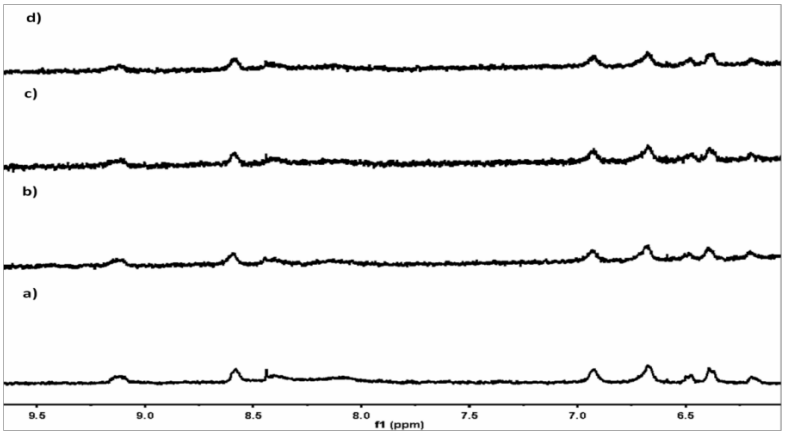


Fig. S4 Partial ^{1}H NMR spectra (400 MHz) of the mixture of **1**, **2b** and CB[8] (1:1.5:3) in D_2O at 25 °C: [**1**] = a) 1.0 mM, b) 0.5 mM, c) 0.25 mM and d) 0.125 mM.

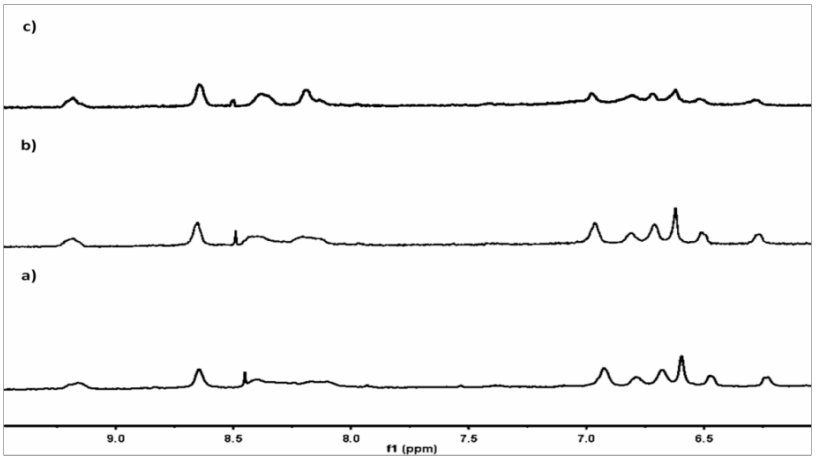


Fig. S5 Partial ^{1}H NMR spectra (400 MHz) of the mixture of **1**, **2a** and CB[8] (1:1.5:3) in D_2O ([**1**] = 1.0 mM) at a) 298 K, b) 313 K and c) 333 K.

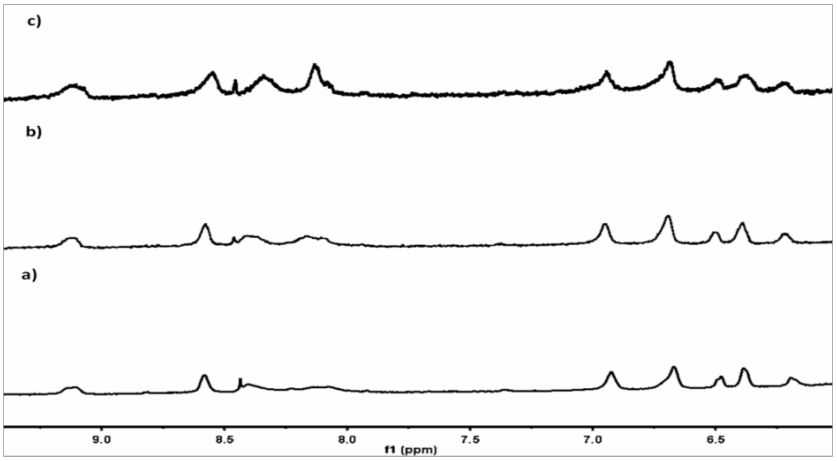


Fig. S6 Partial ^{1}H NMR spectra of mixture of **1**, **2b** and CB[8] (1:1.5:3) ([**1**] = 1.0 mM) in D_2O at a) 298 K, b) 313 K, and c) 333 K.

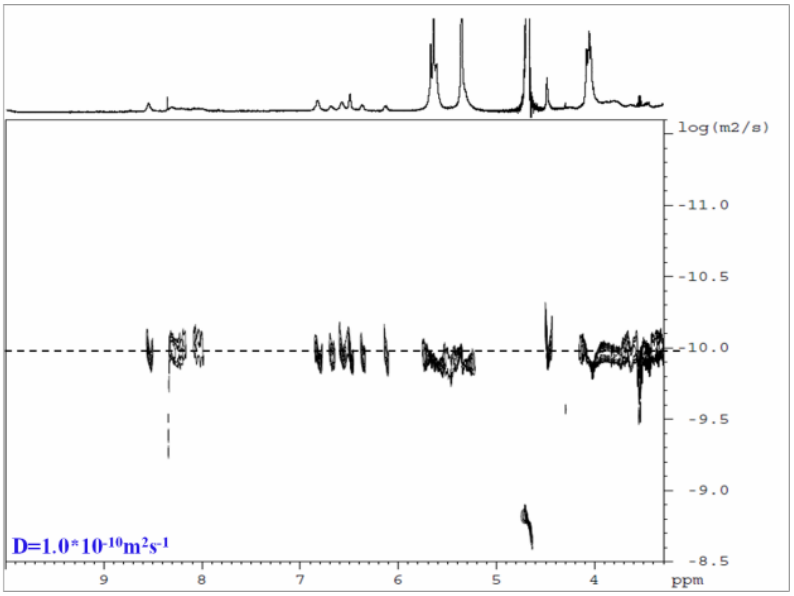


Fig. S7 DOSY-NMR spectra (500 MHz) of the mixture of **1**, **2a** and CB[8] (1:1.5:3) in D_2O at 25 °C ([**1**] = 0.8 mM).

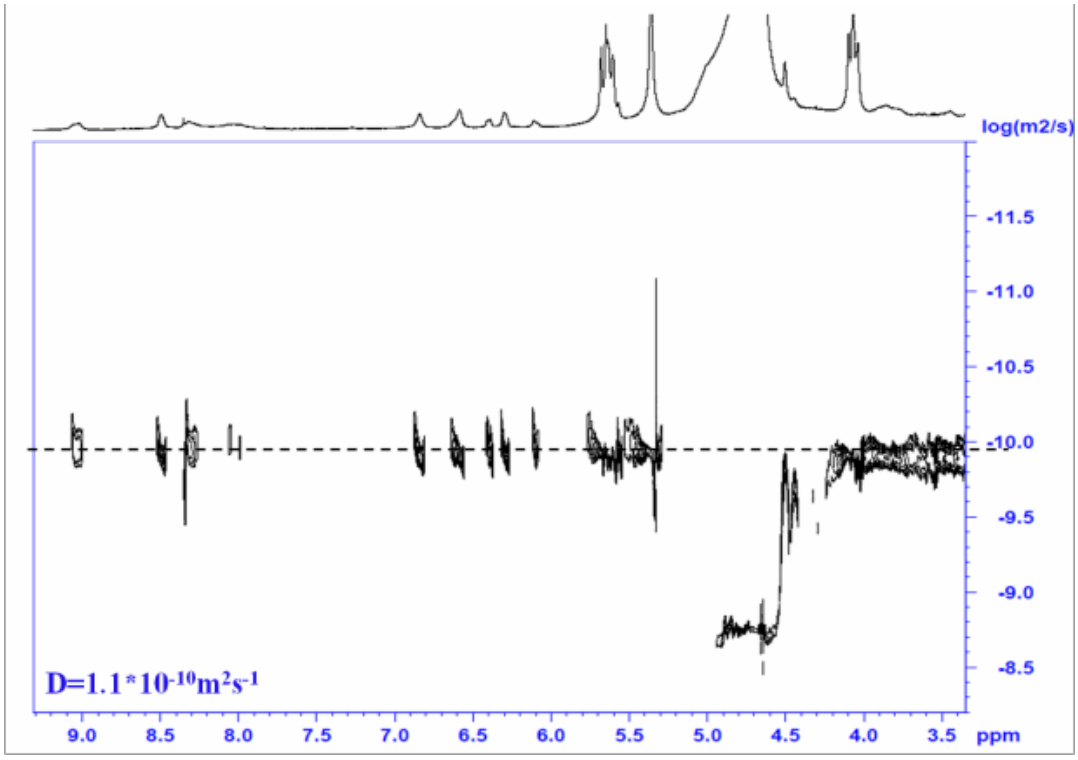


Fig. S8 DOSY-NMR spectra (500 MHz) of the mixture of **1**, **2b** and CB[8] (1:1.5:3) in D_2O at 25 °C ([**1**] = 0.8 mM).

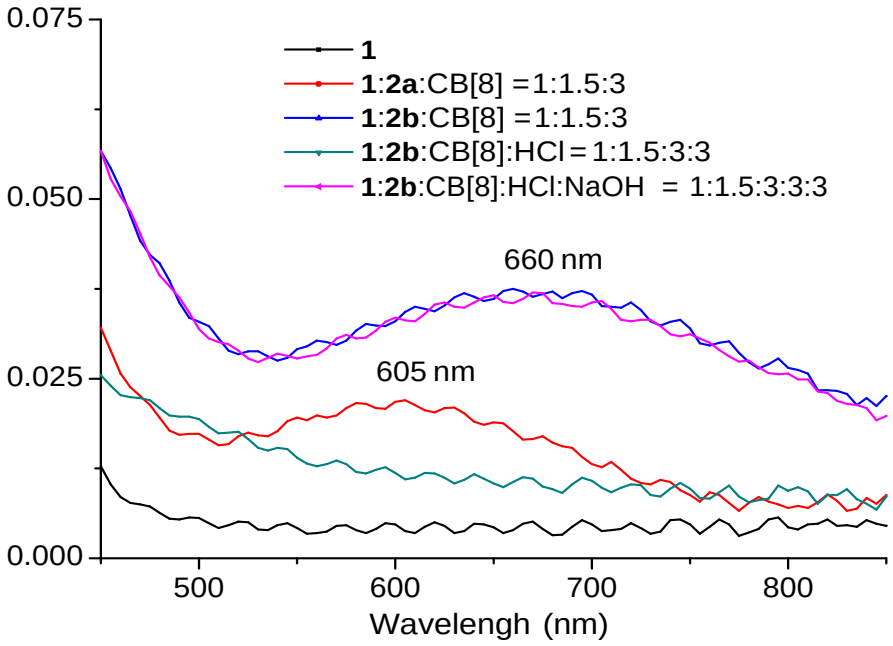


Fig. S9 The absorption spectra of **1** (50 μM) and the mixtures of **1**, CB[8] with **2a** and **2b** in water, without and with the addition of HCl and further addition of NaOH at 25 °C.

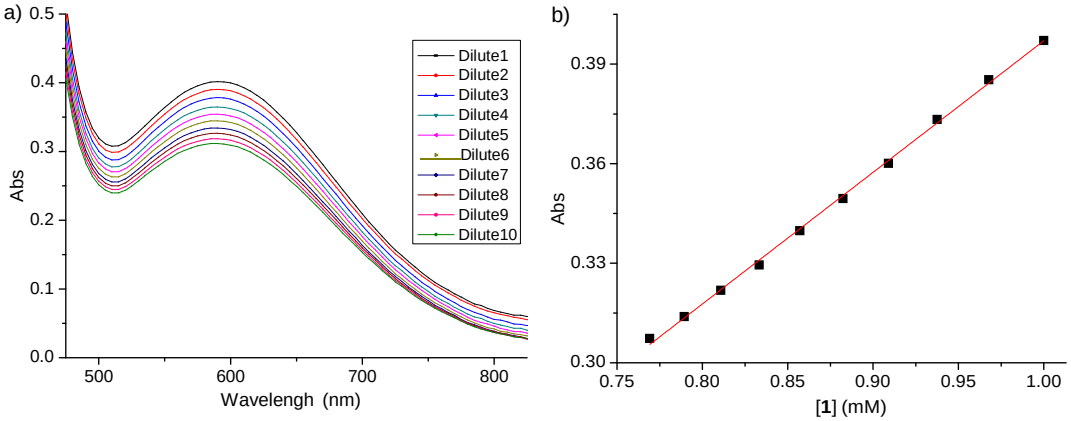


Fig. S10 a) The absorption spectra of the mixture of **1**, **2a** and CB[8] (1:1.5:3) in water at different concentrations at 25 °C. b) The plot of absorption vs [**1**].

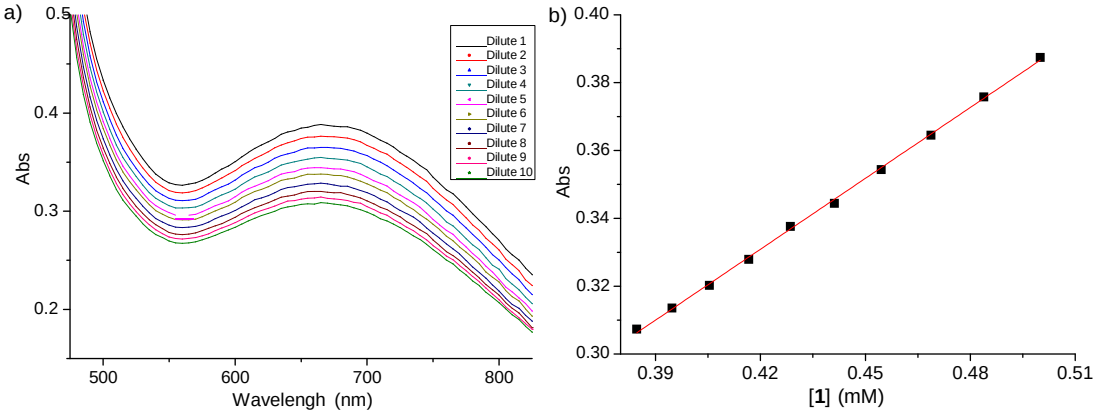


Fig. S11 a) The absorption spectra of the mixture of **1**, **2b** and CB[8] (1:1.5:3) in water at different concentrations at 25 °C. b) The plot of absorption vs [**1**].

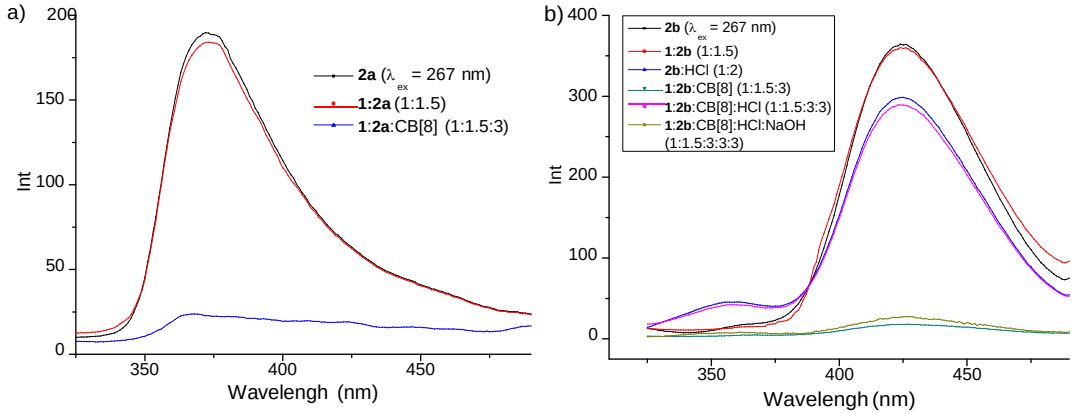


Fig. S12 Fluorescence spectra (λ_{ex} = 267 nm) of a) **2a** (7.5 μM) and its mixture with **1** (5.0 μM) in the presence and absence of CB[8] (15 μM) in water. b) Fluorescence spectra (λ_{ex} = 267 nm) of **2b** (15 μM) and its mixture with **1** (10 μM) in the presence and absence of CB[8] (30 μM) in water, without and with the addition of HCl (30 μM) and further addition of NaOH (30 μM).

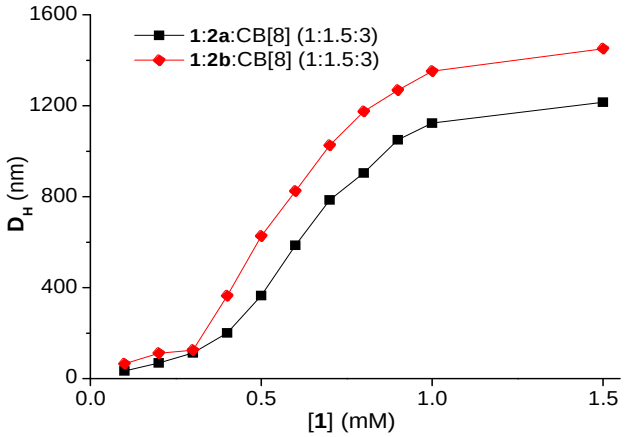


Fig. S13 DLS results of the mixtures of **1**, CB[8] with **2a** and **2b** at different concentration.

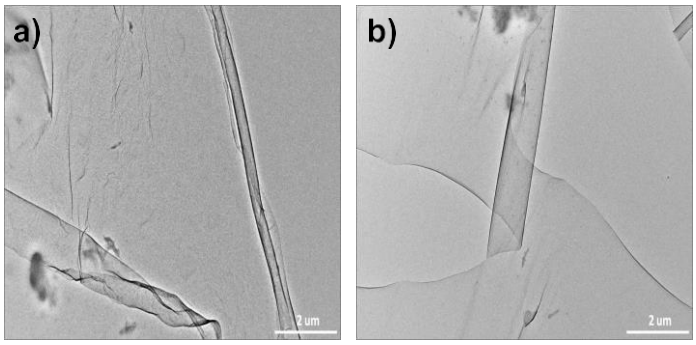


Fig. S14 TEM images of a) the mixture of **1**, **2a** and CB[8] (1:1.5:3) and b) the mixture of **1**, **2b** and CB[8] (1:1.5:3) ([**1**] = 50 μM).

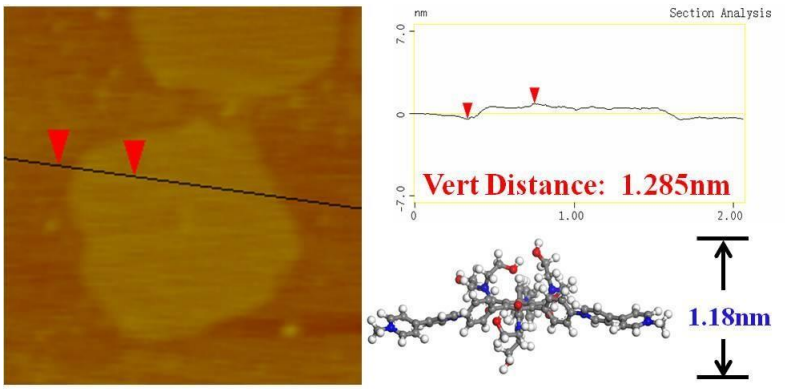


Fig. S15 Tapping-mode AFM image and cross-section analysis of the sample prepared by evaporating the solution of **1**, **2b** and CB[8] (1:1.5:3) in water ([**1**] = 10 μM).

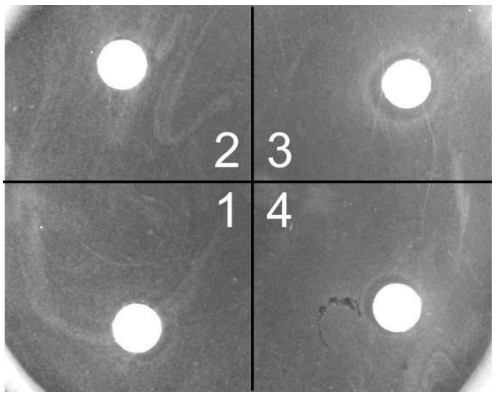


Fig. S16 Antimicrobial assays against *Staphylococcus aureus* SIPI-JD1002. (1) 6 nM **1**; (2) 6 nM **1** and 18 nM CB[8]; (3) a mixture containing 6 nM **1**, 18 nM CB[8], and 7.5 nM **2b**; (4) a mixture containing 6 nM **1**, 18 nM CB[8], and 7.5 nM **2a**.

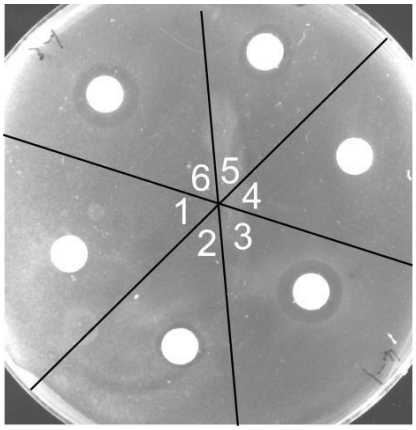


Fig. S17 Dose-dependent antimicrobial activity of SOFs. 1-3) 2 ul, 4 ul, and 8 ul of the mixture containing 3 mM **1**, 4.5 mM **2b** and 9 mM CB[8]; 4-6) 2 ul, 4 ul, and 8 ul of the mixture containing 3 mM **1**, 4.5 mM **2a** and 9 mM CB[8].