

Supporting Information,

Materials and general methods:

Chemicals: Naphthalene acetic acid and Taurine was obtained from Aladdin (Shanghai, China). Fmoc-amino acids were obtained from GL Biochem (Shanghai, China). 2-Cl-trityl chloride resin was obtained from Nankai University resin Co. Ltd. All the other starting materials were obtained from Alfa. Commercially available reagents were used without further purification, unless noted otherwise. All other chemicals were reagent grade or better.

characterization methods

The synthesized compounds were characterized by ^1H NMR (Bruker ARX 300) and ^{13}C NMR (100 MHz) using DMSO-d_6 as the solvent, the LC-MS spectrometric analyses were performed at the Thermo Finnigan LCQ AD System. HPLC was conducted at LUMTECH HPLC (Germany) system using a C_{18} RP column with MeOH (0.1% of TFA) and water (0.1% of TFA) as the eluents. Rheology was performed on an AR 2000ex (TA instrument) system using a parallel plates (40 mm) at the gap of 500 μm . TEM was done on a Tecnai G2 F20 system, operating at 200 kV. Circular dichroism (CD) data were collected on a Jasco J-715 CD spectrometer using demountable quartz cuvette with a path length of 0.1mm. Emission spectra were recorded on a Perkin-Elmer LC-55 luminance spectrometer at excitation wavelength of 265 nm.

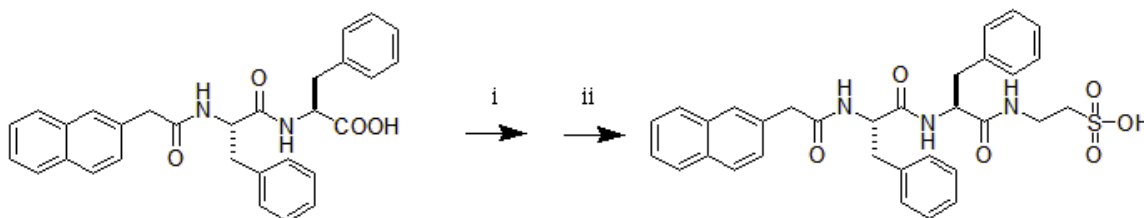
Syntheses of Nap-FF

Peptide synthesis: Peptide of Nap-FF was prepared by standard solid-phase peptide synthesis (SPPS) as previous described by Yang.¹ Briefly, the first Fmoc-Phe-OH was loaded on the resin at the C-terminal with the loading efficiency about 0.5 mmol/g. 20% piperidine in anhydrous $\text{N,N}'$ -dimethylformamide (DMF) was used during deprotection of Fmoc group. Then the second Fmoc-Phe-OH was coupled to the free amino group of first amino acid using O-(Benzotriazol-1-yl)- $\text{N,N,N}',\text{N}'$ -tetramethyluroniumhexafluorophosphate (HBTU) as the coupling reagent. At the final step, 2-Naphthalene acetic acid was used to cap the amine group of the peptide. After the

last coupling step, excessive reagents were removed by filter element. The resulting resin beared peptide was washed by DMF, followed by washing with DCM. The peptide was then cleaved from the resin using 95% of trifluoroacetic acid with 2.5% of TMS and 2.5% of H₂O for 30 minutes. After filtration, the resulting solution containing peptide was then added to ice-cold diethylether to precipitate the peptide (Nap-FF).

Synthesis and Characterization Nap-FF-Taurine

Fig.S1 shows synthetic pathway for Nap-FF-Taurine. Nap-FF (240.3 mg,0.5 mmol) and NHS (115.09 mg,1 mmol) was dissolved in 4 mL DMF, Taurine was dissolved in 0.8 mL water, then mixed them together in a flask. After being cooled to 0 °C in the ice bath, DIEPA was added to adjust the pH to about 8, then 95.85 mg EDC (0.5 mmol) was added three times per 20 min with the same amount. The reaction mixture was stirred overnight. The LC-MS spectrum of the resuting reaction solution showed that there were several peaks (Fig.S1A) which indicated that the reaction solution was not pure, so we used HPLC(with MeOH/ water (0.1%) as the eluents) to further purify reaction solution and collected target product. As shown in Fig.S1B, there was only narrow single peak indicating the target product was very pure. the MS data of target product ((MS: (M+1)⁺=588.69, HR-MS: (M+1)⁺ = 588.2165) (Fig.S2)was very consistence with that of Nap-FF-Taurine (calc: M⁺ = 587.69) proving pure Nap-FF-Taurine was obtained. The characteristic peaks of ¹H NMR (Fig.S3) were assigned as follows: ¹H NMR (400 MHz, DMSO-d₆) δ 8.25 (m,2H), δ 7.93 (m, 1H), δ7.86 (d, J=8.0 Hz ,1H), δ 7.79 (d,J=8.0 Hz, 1H), δ 7.76 (d,J=8.0 Hz, 1H),δ7.61 (s, 1H),δ7.18 (m,12H) , δ4.53 (m, 1H), δ4.38 (m, 1H), δ3.56 (m, 3H), δ3.31 (m, 3H), δ3.01 (m, 2H), δ2.78 (m,2H).



Scheme S-1. Synthetic pathway for Nap-FF-Taurine

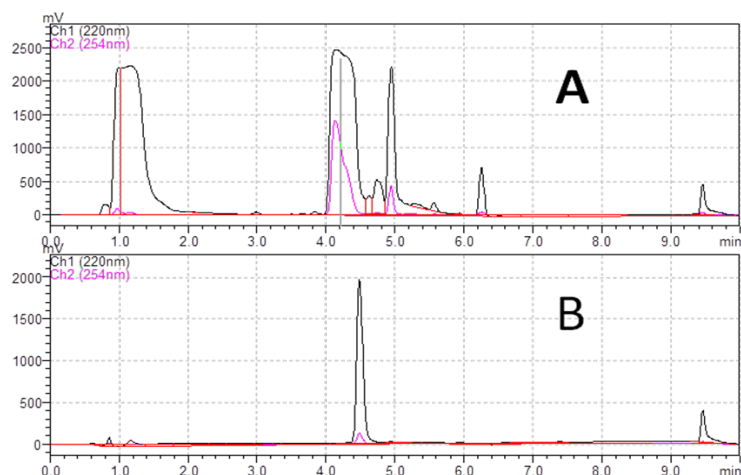


Fig.S1 The LC-MS spectrogram of Nap-FF-Taurine A) before HPLC separation B) after HPLC separation

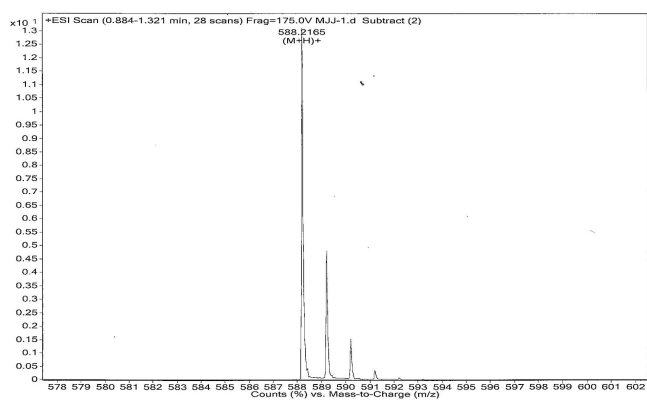


Figure S2. HR-MS of Nap-FF-Taurine

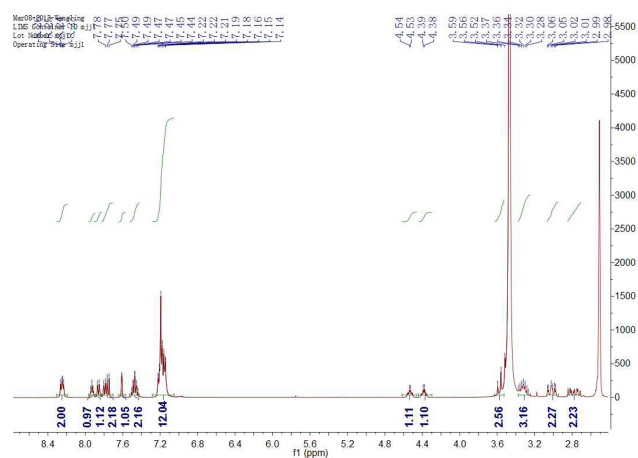


Figure S3. ¹H NMR of Nap-FF-Taurine

Formation of the hydrogels:

In order to investigate the hydrogel formation, The Nap-FF-Taurine was first dissolved in a small amount of PBS, then sodium carbonate solution was added to adjust the pH to about 7.4, afterward, a certain amount of PBS was supplemented to obtain Nap-FF-Taurine solution with desired concentration of Nap-FF-Taurine. As shown in Fig.S4, the hydrogels were formed after the additions of 0.5 or 0.7 equiv. of Ba^{2+} in PBS buffer solution. However, the hydrogels were not formed after the additions of Ca^{2+} , Cu^{2+} , Fe^{2+} , Pb^{2+} , Sr^{2+} , Mg^{2+} and Zn^{2+} in PBS buffer solution (Fig.S5)

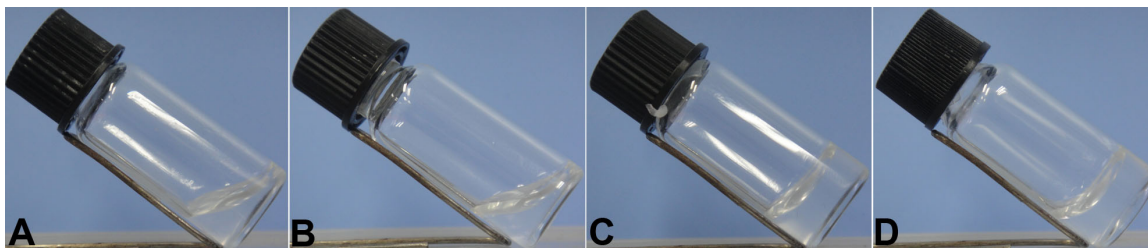


Figure S4. Optical images of the solution containing 0.2% of Nap-FF-Taurine with A) 0, B) 0.1, C) 0.5 and D) 0.7 equiv. of Ba^{2+} in PBS buffer solution

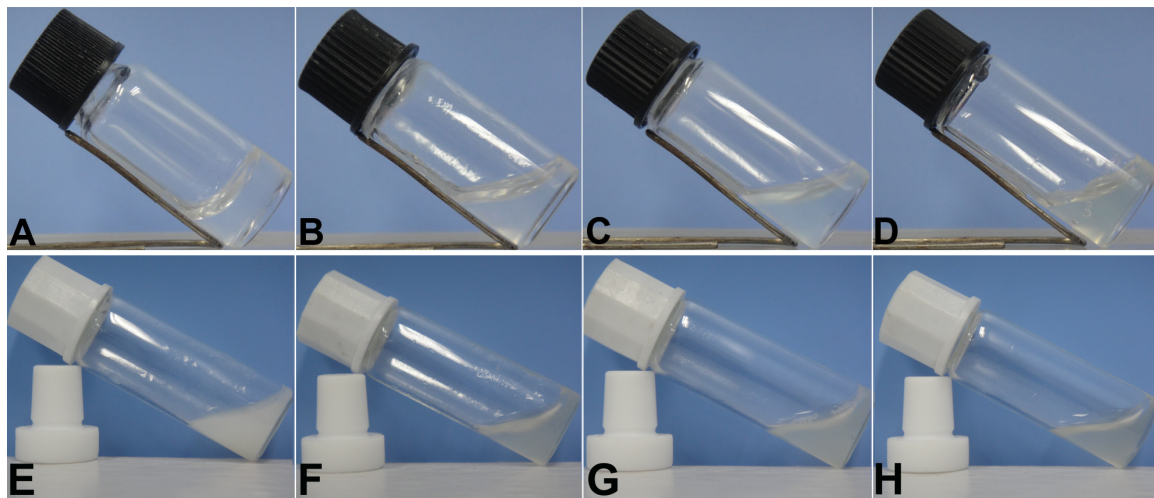


Figure S5. Optical images of the solution containing 0.2% of Nap-FF-Taurine with 1.0 equiv. of A) Ba^{2+} , B) Ca^{2+} , C) Cu^{2+} , D) Fe^{2+} , E) Pb^{2+} , F) Sr^{2+} , G) Mg^{2+} and H) Zn^{2+} in PBS buffer solution

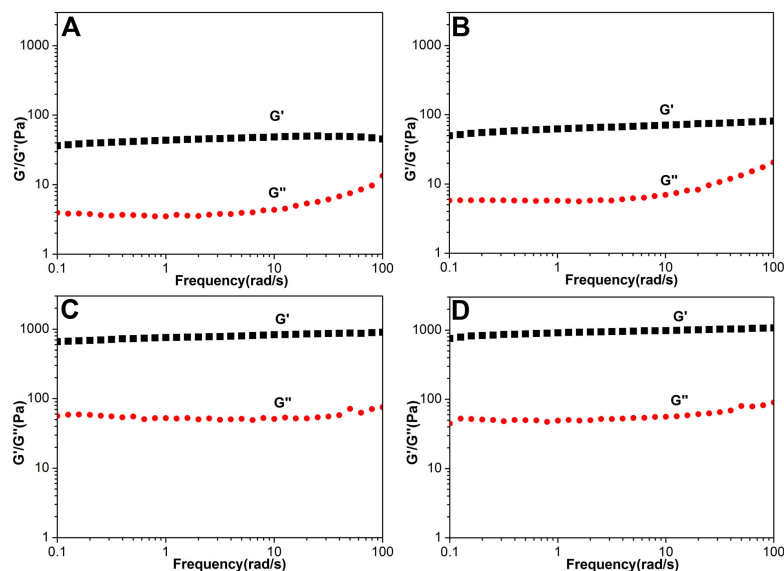


Figure S6. Rheological measurements with the mode of dynamic frequency sweep at the strain of 0.5% for the solution of Nap-FF-Taurine(0.2wt%) with A) 0, B) 0.1, C) 0.5 and D) 0.7 equiv.of Ba²⁺ in PBS buffer solution.

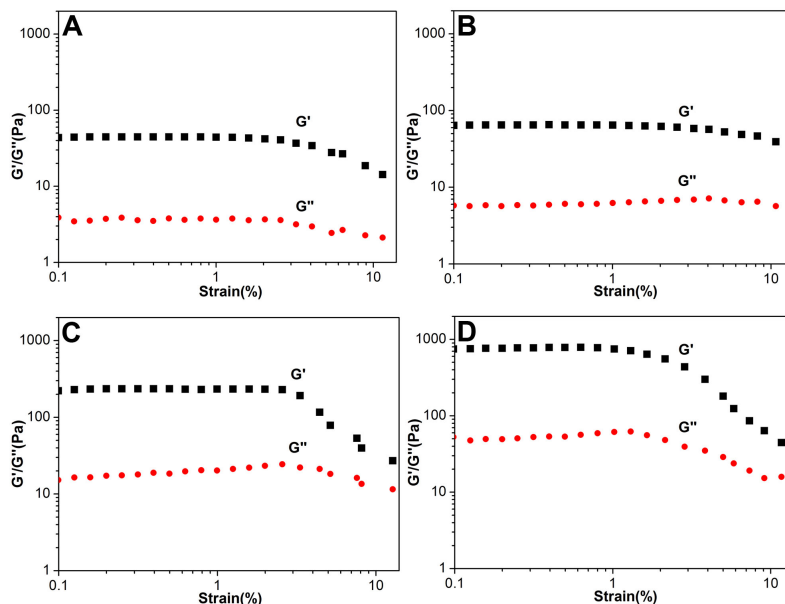


Figure S7. Rheological measurements with the mode of dynamic strain sweep at the frequency of 1.0 rad/s for the solution of Nap-FF-Taurine(0.2wt%) with A) 0, B) 0.1, C) 0.5 and D) 0.7 equiv.of Ba²⁺ in PBS buffer solution

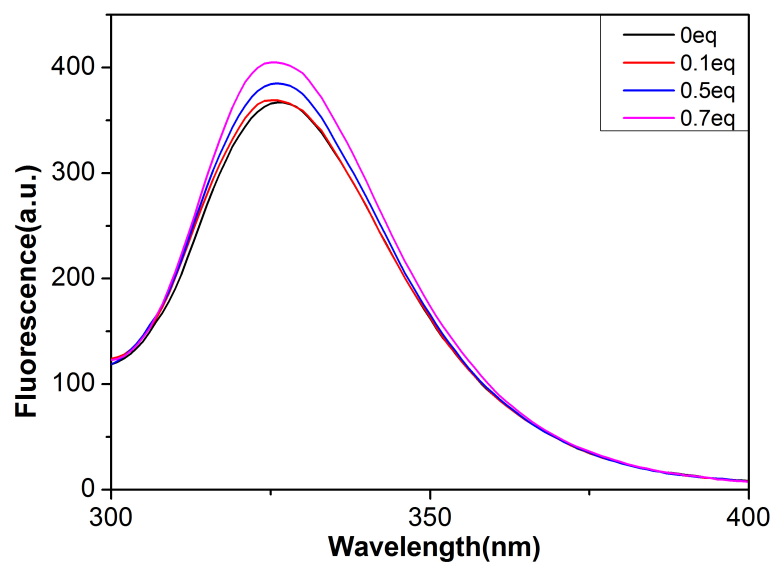


Figure S8. Emission spectra of the the solution of Nap-FF-Taurine(0.02wt%) with 0 , 0.1, 0.5 and 0.7 equiv.of Ba^{2+} in PBS buffer solution.

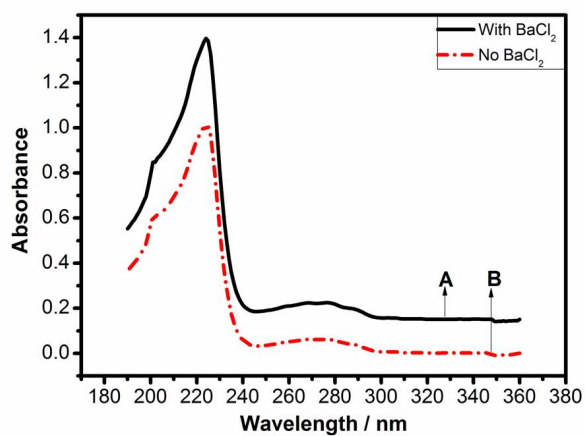


Figure S-9. UV-vis spectrum of Nap-FF-Taurine (0.05wt%) with A) 1.0 equiv.of BaCl_2 , B) no BaCl_2

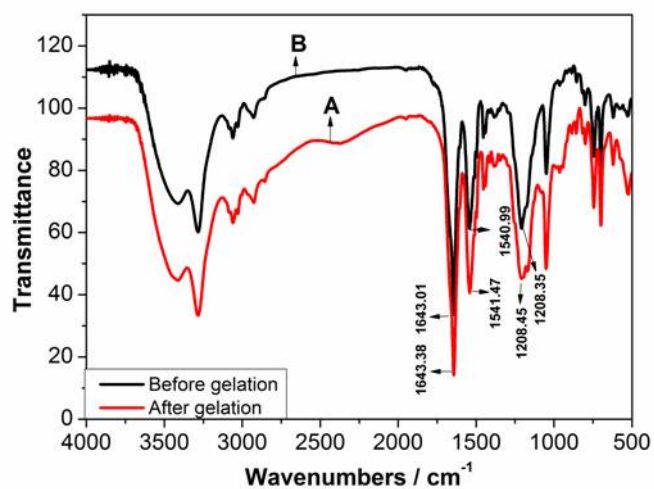


Figure S-10. FTIR of Nap-FF-Taurine (0.5wt%) with A) 1.0 equiv.of BaCl₂ , B) no BaCl₂

REFERENCE

1. Zhimou Yang, Gaolin Liang, Bing Xu, *Chem. Commun.*, 2006, 47, 738.