The first supramolecular peptidic hydrogelator consisting of taurine

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Supplementary Information

Materials

All the chemicals used in this work were purchased from Aldrich or Fluka, and used without further purification.

Instrumentation

NMR on 400 MHz Varian Unity Inova 400 using DMSO-d^6 as the solvent; sonication on Cole Parmer 8845-50. TEM images on Morgagni 268 transmission electron microscope; rheological studies on TA ARES G2 rheometer; MTT on DTX 880 plate reader.

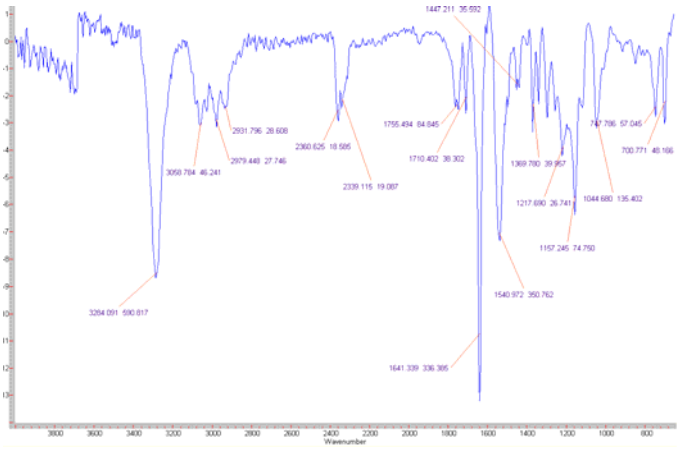
Characterization

^{1}H NMR (400 MHz, DMSO-*d6*) of **3**: δ 8.40 (d, *J*=8.4 Hz, 1H), 8. 25 (t, *J*=4.0 Hz, 1H), 8.17 (d, *J*=4.0 Hz 1H), 8.02 (m, 1H), 7.80 (m, *J*=4.0 Hz, 2H), 7. 62 (m, 1H), 7. 62 (m, 1H), 7.09 (m,10H), 6.98 (m, 2H), 4.53 (m, 1H), 4.39 (m, 1H), 3.56 (m, 4H), 3.01 (m, 2H), 2.72 (m, 2H), 2.54 (m, 2H).

^{13}C NMR (400 MHz, DMSO-d_6) of **3**: δ = 171.71, 170.26, 138.31, 138.11, 134.33, 132.16, 129.72, 129.67, 129.62, 128.44, 128.29, 128.07, 127.85, 127.80, 127.69, 126.37, 125.83, 54.26, 42.67, 39.32.

MS: calculated for $C_{32}H_{33}N_3O_6S$ is 587.20901, M^{-1} found 586.36666

IR spectrum:



Procedures

*Hydrogelation of **3***: 10 mg of compound **3** and 0.5 mL of DI water was added into glass vial. 1N NaOH was slowly added (1 μL each time) and mixed by stirring the solution using a needle to adjust the solution to desired pH. The solution was then heated by placing in a 70 ˚C water bath for 5 min. For the cooling process, the hot solution of **3** was immediately placed in a water bath at 20 ˚C for 1 min. For the

cooling plus sonication process, the hot solution of **3** was immediately placed in a turned-on sonicator with the temperature of the water at 20 ˚C. After 5 seconds of sonication, the sonicator was turned off and the vial continued to sit in the water for another 55 seconds.

Negative stained TEM: Carbon coated grids were glow discharged to increase their hydrophilicity before use. The sample solution (3 μL) was placed on the grid to cover the grid surface. After being rinsed for 10 s, the grid was tilted, allowing the sample-loaded surface to touch a drop of ddH_2O. The edge of the grid was immediately leaned to touch a filter paper for three times to remove water from the grid. The grid was stained by letting the grid touch a drop of 2.0 % (w/v) uranyl acetate with the sample-loaded surface. Excessive stain solution was removed by gently touching the edge of the grid on a filter paper for 3 times. The grid was air dried for a few minutes and was then examined immediately.

MTT cell viability test: HeLa cells in exponential growth phase were seeded in a 96 well plate at a concentration of 2.0×10^4 cell/well in culture medium (MEM medium supplemented with 10% FBS and 1% penicillin-streptomycin). The cells were allowed to attach to the wells for 24 h at 37 ^oC, 5% CO_2, then the culture medium was removed, and 100 μL new culture medium dissolved with **3** at gradient concentrations was placed into each well. The as-prepared media containing **3** were prepared as follow: first slowly adding 5 μL of 1N of NaOH into **3** at 10 mM in water (200 μL) to dissolve **3**; as soon as the solutions turn transparent, it was quickly dilute into culture medium. Filtered media containing **3** were obtained by passing the as-prepared media gently through 0.22 μm nylon filter. After culturing at 37 ºC, 5% CO_2 for desired time, each well was added by 10 μL of 5 mg/mL MTT ((3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide), and then incubate in dark for 4 h. 100 μL 10% SDS with 0.01 M HCl was added to each well to stop the reduction reaction. After incubation of the cells at 37 ºC for overnight, the cell viability is measured. Data represented the mean ± standard deviation of three independent experiments.

Rheological tests: The U-gel and C-sol used for rheological tests were fresh prepared at the day of the experiments. The tests were performed on 25 mm parallel plate. The temperature of the experiments was set at 25 ^oC.

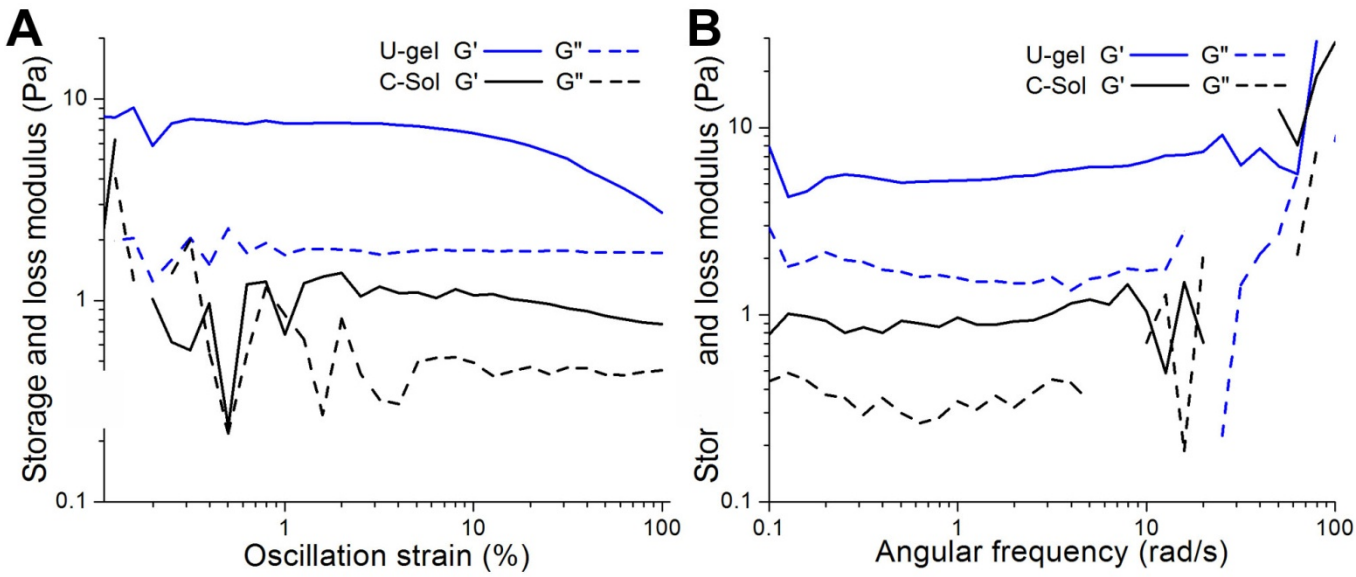


Fig. S1. Rheological property of U-gel and C-sol formed by 3 at 2 %, pH 3. (A) Strain sweep of U-gel and C-sol. (B) Frequency sweep of U-gel and C-sol.