Supporting Information

Materials and methods:

Materials: Fmoc-amino acids were obtained from GL Biochem (Shanghai). Vancomycin was purchased from Aladdin Chemistry CO. Ltd. Commercially available reagents were used without further purification, unless noted otherwise. Nanopure water was used for all experiments. All other chemicals were reagent grade or better. The wastewater was taken from the liver outside of our research building. The urine sample was from the first author (Yongquan Hua).

General methods: The synthesized compounds were characterized by ^{1}H NMR (Bruker ARX 400) using DMSO-d_6 as the solvent and ESI-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 methanol (0.1% of TFA) and water (0.1% of TFA) as the eluents. LC-MS was conducted at the LCMS-2020 (Shimadzu) system, and rheology was performed on an AR 2000ex (TA instrument) system using a parallel plate (40 mm) at the gap of 500 μm. Fluorescence spectrum was recorded on a BioTek Synergy™ 4 Hybrid Microplate Reader. TEM was done on a Tecnai G2 F20 system.

Synthesis and characterization:

Peptide Synthesis: The peptide was prepared by solid-phase peptide synthesis (SPPS) using 2-chlorotrityl chloride resin and the corresponding *N*-Fmoc protected amino acids with side chains properly protected by a tert-butyl group or Pbf group or Boc group. After the first amino acid was loaded on the resin by its C-terminal, 20% piperidine in anhydrous *N, N'*-dimethylformamide (DMF) was used to deprotect Fmoc group. Then the next Fmoc protected amino acid was coupled to the free amino group using O-(benzotriazol-1-yl)-*N,N,N',N'*-tetramethyluranium-hexafluorophosphate (HBTU) as the coupling reagent and diisopropylethylamine (DIEA) as catalytic reagent. The growth of the peptide chain was according to the established Fmoc SPPS protocol. After the last amino acid was coupled, excessive

reagents were removed by a single DMF wash for 5 min (5 mL per gram of resin), followed by 5 times DCM wash for 2 min (5 mL per gram of resin). The peptide was cleaved using 95% of trifluoroacetic acid (TFA) with 2.5% of trimethylsilane (TMS) and 2.5% of H_2O for 30 min. TFA was removed by rotary evaporator, then 20 mL per gram of resin of ice-cold diethylether was added. The resulting precipitate was filtrated and washed by ice-cold diethylether. The resulting solid was further purified by HPLC and dried by lyophilizer.

Peptide Nap-GFFYEG^{D}A^{D}A : ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (t, *J* = 5.6 Hz, 1H), 8.17 (t, *J* = 8.2 Hz, 4H), 8.01 (dd, *J* = 7.6, 3.0 Hz, 3H), 7.84 (ddd, *J* = 11.1, 8.6, 5.6 Hz, 3H), 7.74 (s, 1H), 7.47 (pd, *J* = 6.9, 3.4 Hz, 2H), 7.41 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.27 – 7.17 (m, 4H), 7.18 – 7.09 (m, 6H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 4.50 (t, *J* = 9.3 Hz, 3H), 4.33 (dd, *J* = 14.0, 6.6 Hz, 1H), 4.28 (dd, *J* = 13.7, 7.9 Hz, 1H), 4.16 (dd, *J* = 14.6, 7.3 Hz, 1H), 3.75 – 3.71 (m, 1H), 3.68 (d, *J* = 5.4 Hz, 1H), 3.63 – 3.53 (m, 5H), 3.01 – 2.88 (m, 3H), 2.70 (ddd, *J* = 23.5, 18.8, 9.8 Hz, 3H), 2.27 (t, *J* = 8.1 Hz, 2H), 1.92 (dd, *J* = 14.1, 6.2 Hz, 1H), 1.83 – 1.72 (m, 1H), 1.26 (t, *J* = 8.1Hz, 3H), 1.21(d, *J* =7.1Hz, 3H).

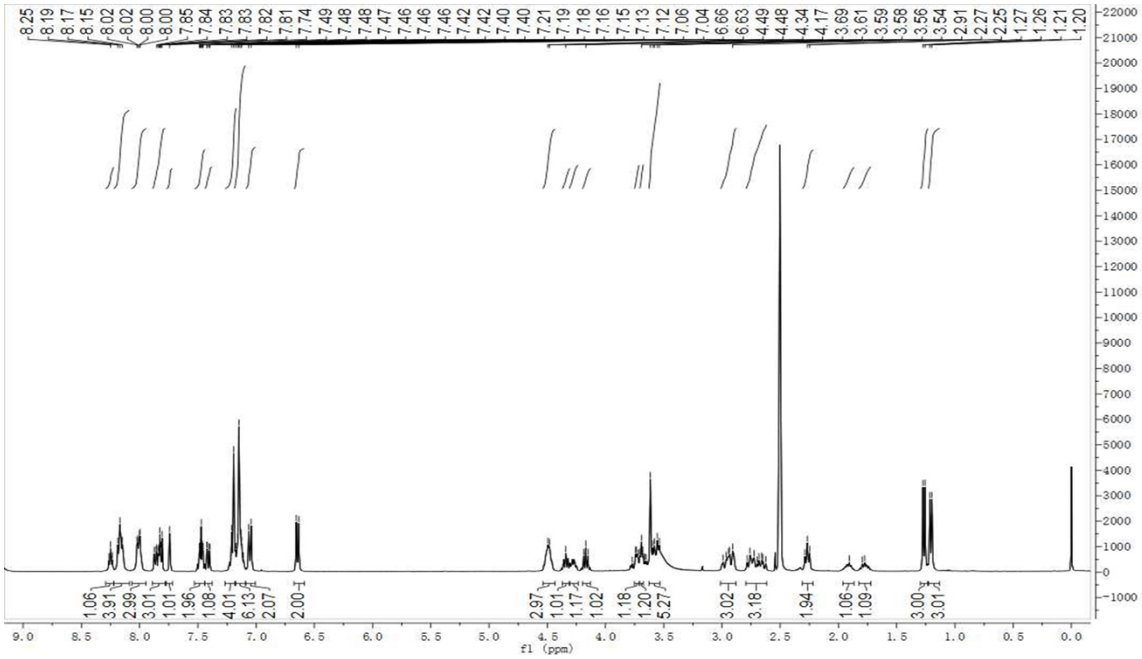

Fig. S-1. ^{1}H NMR of Nap-GFFYEG^{D}A^{D}A

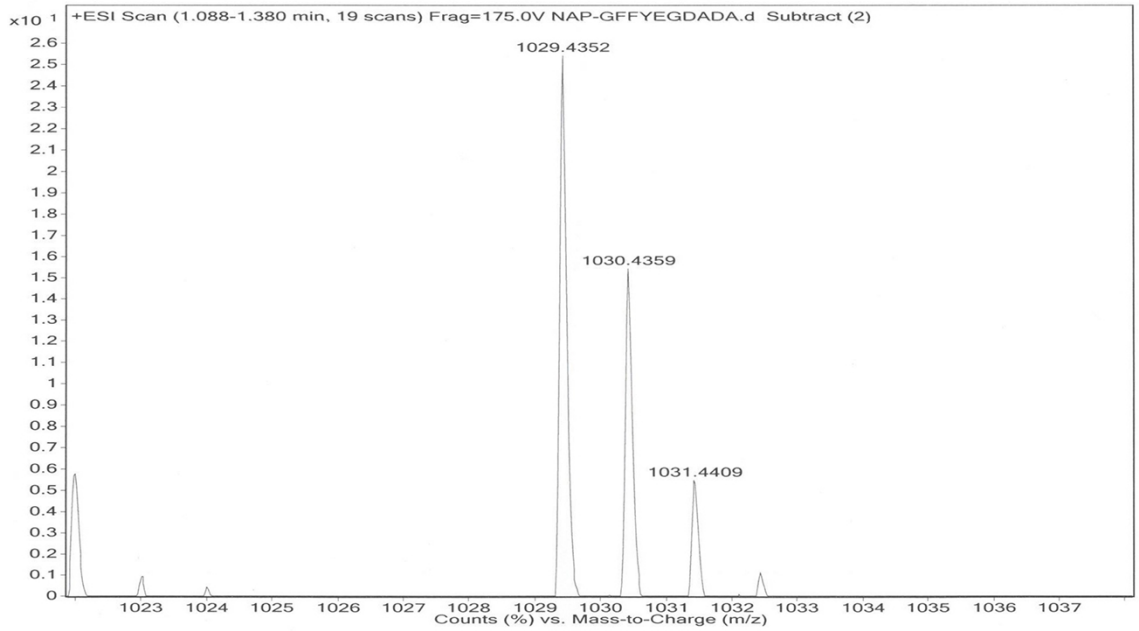

Fig. S-2. HR-MS of Nap-GFFYEG^{D}A^{D}A

Peptide Nap-GFFYEG^{L}A^{L}A : ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 – 8.19 (m, 2H), 8.15 (d, *J* = 7.6 Hz, 3H), 8.00 (d, *J* = 7.1 Hz, 3H), 7.84 (ddd, *J* = 11.1, 8.6, 5.7 Hz, 3H), 7.74 (s, 1H), 7.52 – 7.45 (m, 2H), 7.41 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.20 (d, *J* = 6.3 Hz, 4H), 7.14 (d, *J* = 6.5 Hz, 6H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 4.54 – 4.45 (m, 3H), 4.30 (dt, *J* = 13.9, 7.6 Hz, 2H), 4.20 – 4.14 (m, 1H), 3.80 – 3.72 (m, 2H), 3.68 (s, 2H), 3.61 (d, *J* = 5.8 Hz, 3H), 3.01 – 2.89 (m, 3H), 2.81 – 2.71 (m, 2H), 2.65 (dd, *J* = 13.8, 9.6 Hz, 1H), 2.54 (s, 1H), 2.28 (t, *J* = 8.0 Hz, 2H), 1.96 – 1.87 (m, 1H), 1.76 (dd, *J* = 13.9, 8.0 Hz, 1H), 1.26 (d, *J* = 7.3 Hz, 3H), 1.20 (d, *J* = 7.0 Hz, 3H).

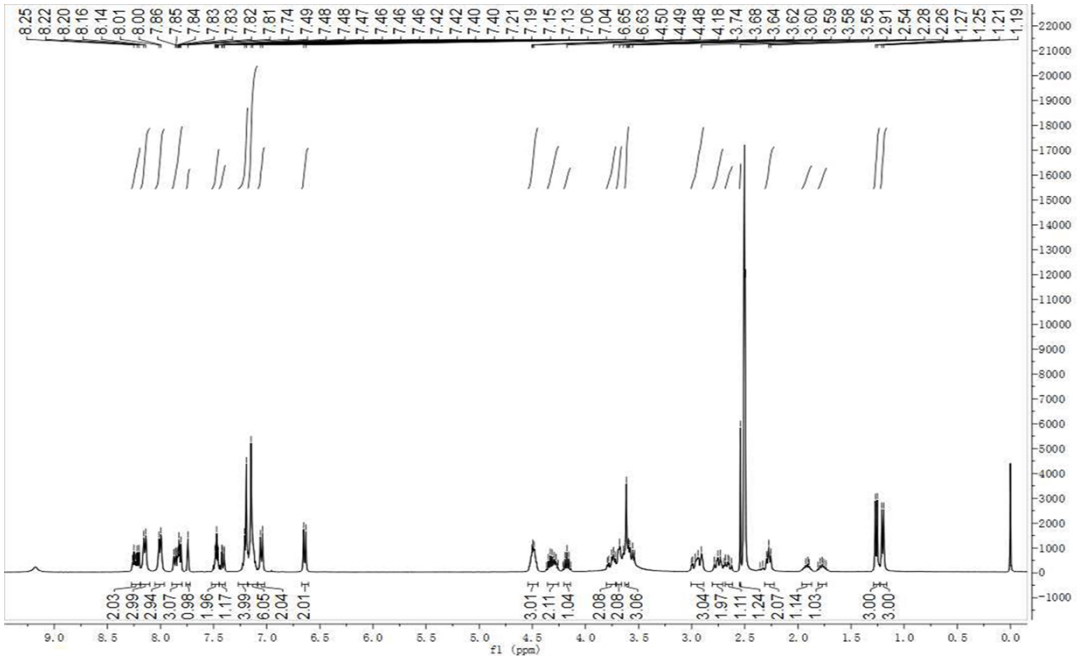

Fig. S-3. ^{1}H NMR of Nap-GFFYEG^{L}A^{L}A

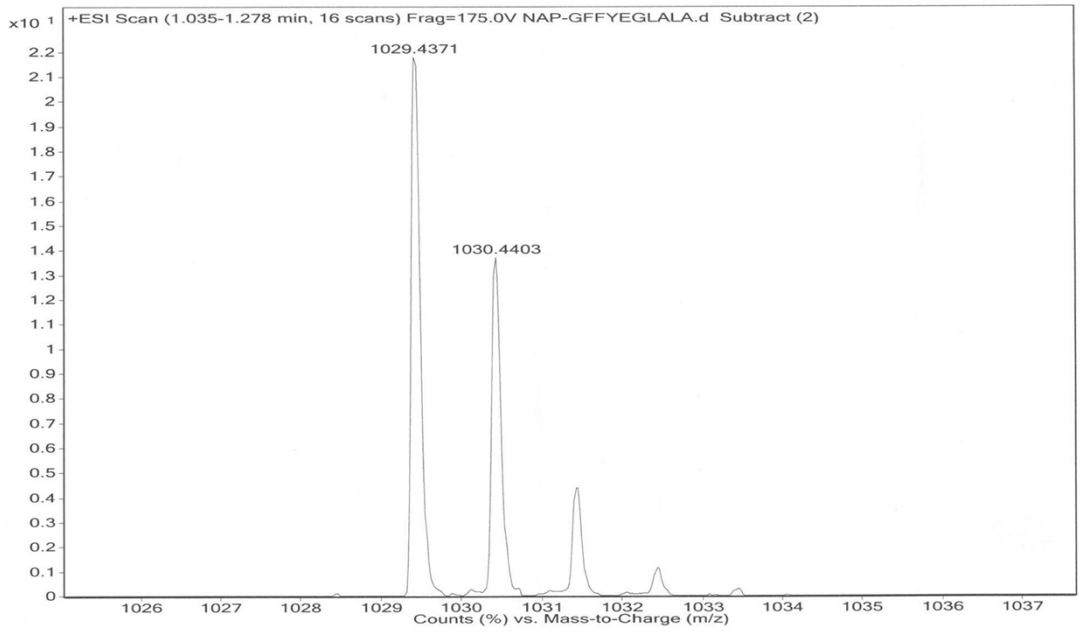

Fig. S-4. HR-MS of Nap-GFFYEG^{L}A^{L}A

Rheology: Rheology test was carried out on an AR 2000ex (TA instrument) system, 40 mm parallel plate was used during the experiment at the gap of 500 μm. For the dynamic time sweep, the sample after heating was directly transferred to the rheometer and it was performed at the frequency of 1 rad/s and the strain of

0.5%. The gel was characterized for the dynamic frequency sweep in the frequency region of 0.1-100 rad/s at the strain of 0.5%. For dynamic strain sweep, it was characterized in the strain region of 0.1-10 % at the frequency of 1 rad/s.

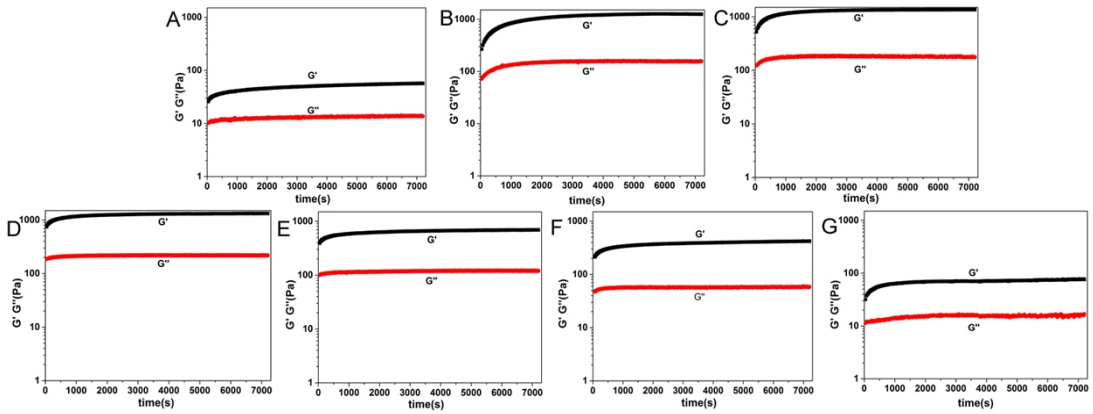

Fig. S-5. Rheological measurement with the mode of dynamic time sweep at the frequency of 1 rad/s and strain of 0.5% for the gels of Nap-GFFYEG^{D}A^{D}A with different equivalent of vancomycin: A (0.005 equiv.), B (0.01 equiv.), C (0.02 equiv.), D (0.05 equiv.), E (0.1 equiv.), F (0.2equiv.), and G (0.3 equiv.).

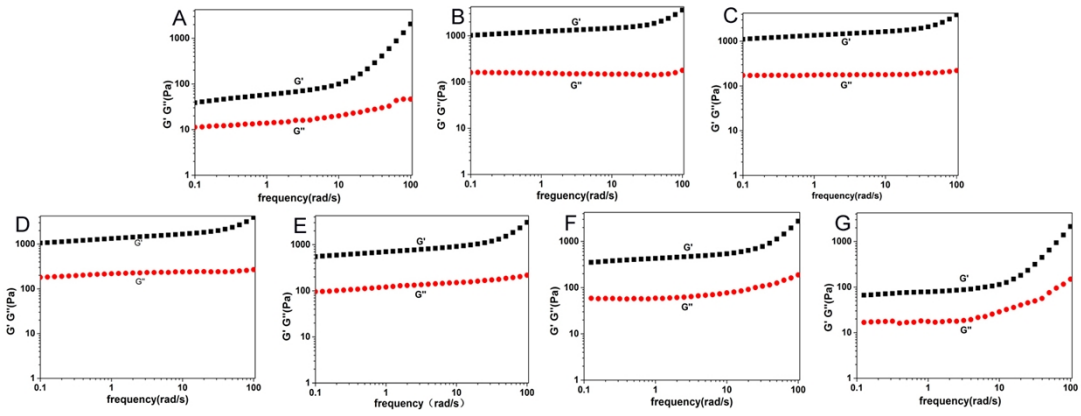

Fig. S-6. Rheological measurement with the mode of dynamic frequency sweep at the frequency of 1 rad/s and strain of 0.5% for the gel of Nap-FFYGK-CA with different equivalent of vancomycin: A (0.005 equiv.), B (0.01 equiv.), C (0.02 equiv.), D (0.05 equiv.), E (0.1 equiv.), F (0.2 equiv.), and G (0.3 equiv.)

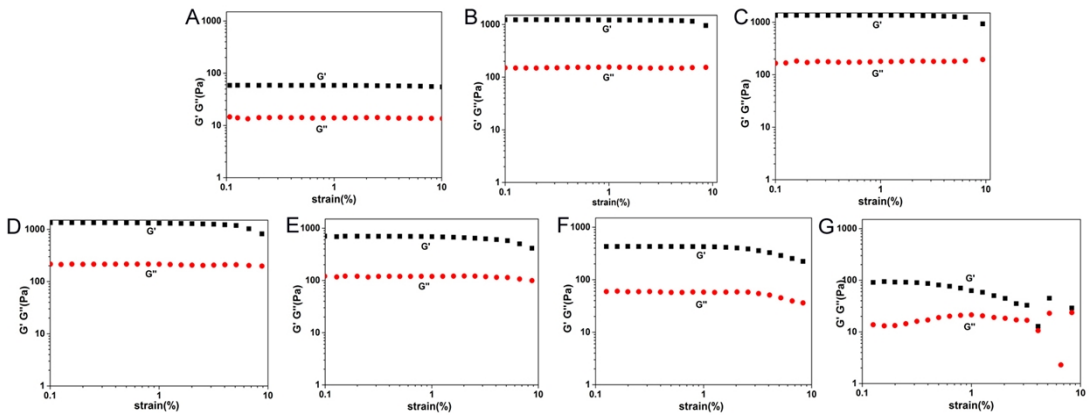

Fig. S-7. Rheological measurement with the mode of dynamic strain sweep at the frequency of 1 rad/s and strain of 0.1% for the gel of Nap-FFYGK-CA with different equivalent of vancomucin: A (0.005 equiv.), B (0.01 equiv.), C (0.02 equiv.), D (0.05 equiv.), E (0.1 equiv.), F (0.2equiv.), and G (0.3 equiv.)

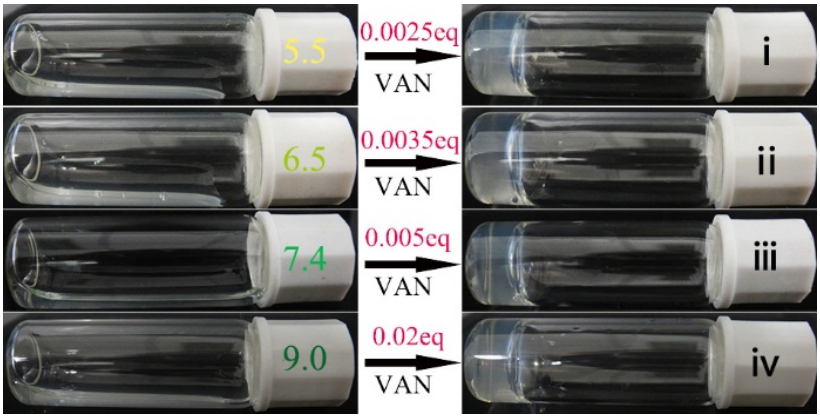

Fig. S-8. The effect of pH value on the minimum equiv. of VAN required for gelation in 0.01 M of PBS solution (the peptide concentration was 1.5 wt%, the temperature was 25 ^{o}C).

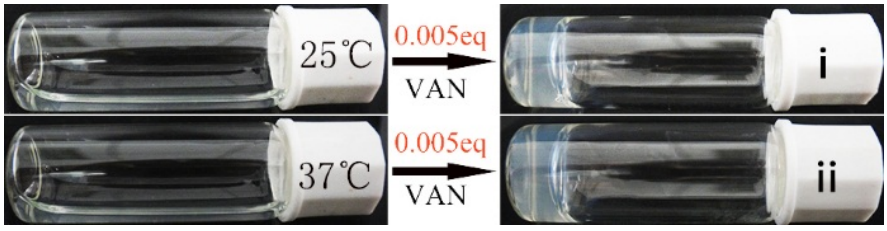

Fig. S-9. The effect of temperature on the minimum equiv. of VAN required for gelation in 0.01 M of PBS solution (the peptide concentration was 1.5 wt%, pH=7.4).

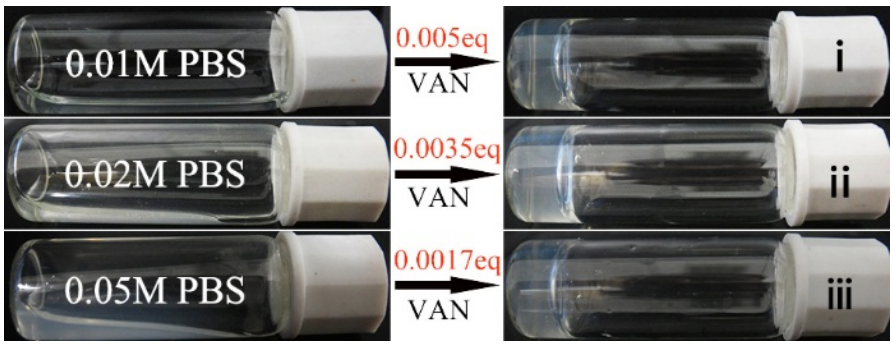

Fig. S-10. The effect of ionic strength on the minimum equiv. of VAN required for gelation in PBS solution (the peptide concentration was 1.5 wt%, the temperature was 25 °C, pH=7.4).

Fig. S-11. The minimum equiv. of VAN needed to gelate the PBS solution of the peptide (1.5 wt%, 0.05 M PBS, pH=5.5) is about 0.001 (20 μg/mL) at 25 °C.