

Electronic Supplementary Information for

Selective shrinkage and separation of isomeric naphthoic acids via supramolecular gelation

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1: Experimental Section

Materials: All starting materials and solvents were purchased from TCI, or Beijing Chemicals and used as received unless otherwise stated. Solvents were purified and dried according to standard methods. Milli-Q water ($18.2 \text{ M}\Omega \text{ cm}^{-1}$) was used in all cases.

Instruments and methods: ^1H NMR spectra were recorded on a Bruker AV400 (400 MHz) spectrometer. Mass spectral data were measured by using a BIFLEIII matrix-assisted laser desorption/ionization time of flight mass spectrometry (MALDI-TOF MS) instrument. Elemental analysis was performed on a Carlo-Erba-1106

Thermo-Quest. Scanning electron microscopy (SEM) was carried out on a Hitachi S-4800 FE-SEM microscope. Xerogel on silica plate were prepared for the measurement of Fourier transform infrared (FT-IR) spectra on a JASCO FT/IR-660 plus spectrophotometer with a wave number resolution of 4 cm^{-1} at room temperature. X-ray diffraction (XRD) was carried out on a Rigaku D/Max-2500 X-ray diffractometer (Japan) with $\text{CuK}\alpha$ radiation ($\lambda=1.5406\text{ \AA}$), which was operated at 45 kV, 100 mA. High Performance Liquid Chromatography (HPLC, DIOMEX Pump Series 2489) equipped with a variable wavelength UV-200 detector and Diacel OB column ($4.6\text{ mm} \times 15\text{ cm}$), the mobile phase was a mixture of n-hexane/isopropyl alcohol/ acetic acid (99:2:0.002) at a flow rate of 0.5 mL/min. The epoxide product was identified by comparison to the HPLC retention time.

Procedures: For the SEM measurements, a small amount of gels was placed onto a single-crystal silicon plate (Pt-coated) after being vacuum dried for 12 h. In the case of preparing samples for XRD measurements, gels were cast onto glass plates and dried under vacuum. Pellets made from the mixture of vacuum-dried supramolecular polymers and KBr powders were used for FT-IR spectral measurements.

Gelation studies: All the supramolecular gels were prepared in septum-capped test tubes. The amphiphilic L-histidine (LHC18) and different naphthoic acids with equal molar ratio were dispersed in Milli-Q water and DMSO and then heated until transparent. The obtained clear solution was let cool to room temperature and the gels formation was confirmed by the tube-inversion method.

2: Supplementary table and figures

Table S1. The DMSO/water gelation volume ratios for forming LHC18/naphthoic acids two-component supramolecular gels.

Naphthoic acids	DMSO(μL)	H ₂ O(μL)
NA1	100	300
NA2	100	300

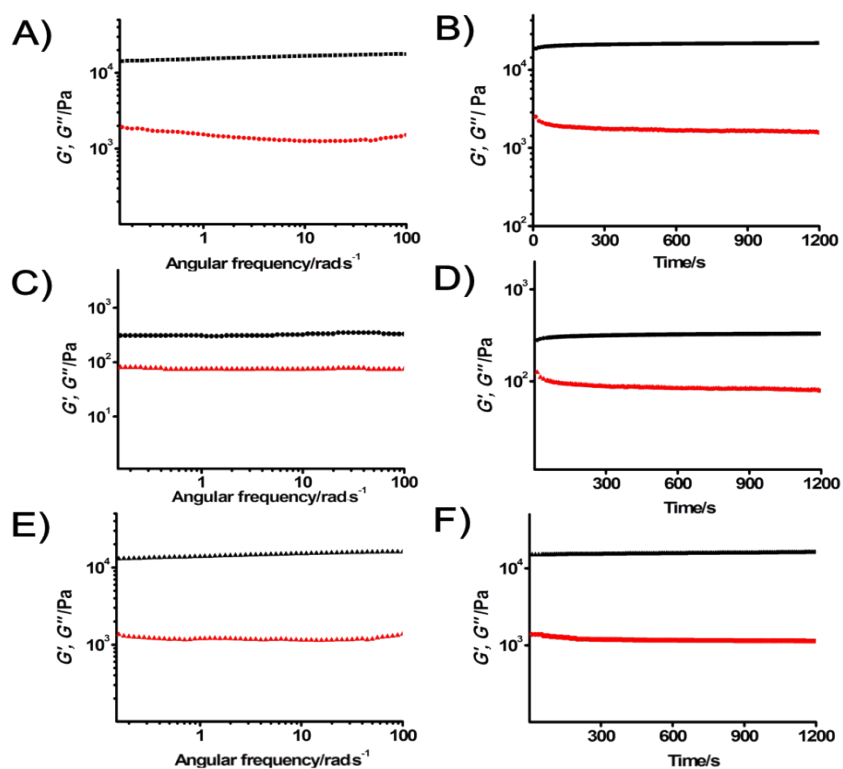


Figure. S1. Rheological studies of the as-prepared NA2/LHC18 (molar ratio=1:1) gels: (A) frequency sweeps and (B) time sweeps; Rheological studies of the shrunk NA2/LHC18 (molar ratio=1:1) gels: (C) frequency sweeps and (D) time sweeps; Rheological studies of the NA1/LHC18 (molar ratio=1:1) gels: (E) frequency sweeps and (F) time sweeps.

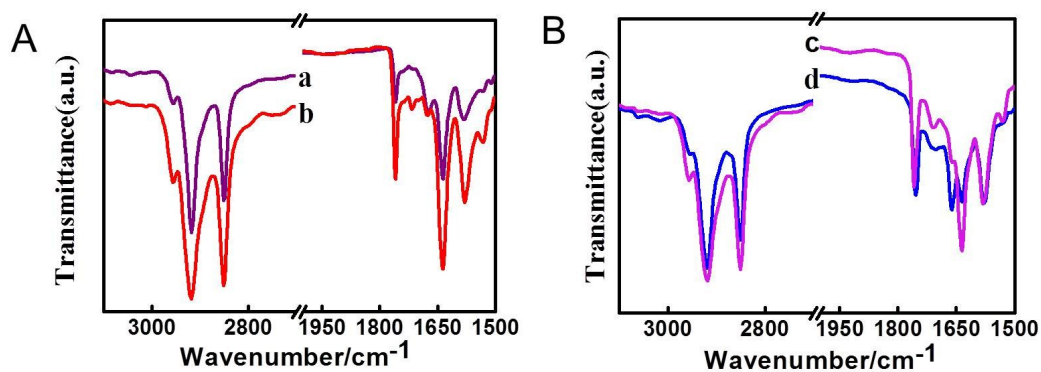


Figure. S2. A) FT-IR spectra of NA1/LHC18 gels before (a) and after (b) resting for 10 hours; B) FT-IR spectra of NA2/LHC18 gels before (a) and after (b) resting for 10 hours.

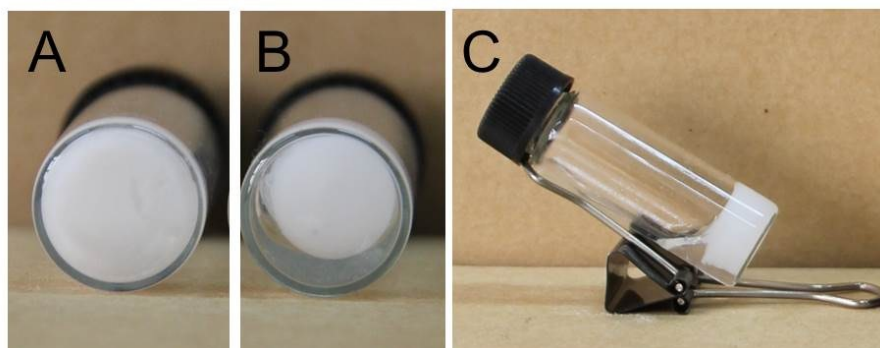
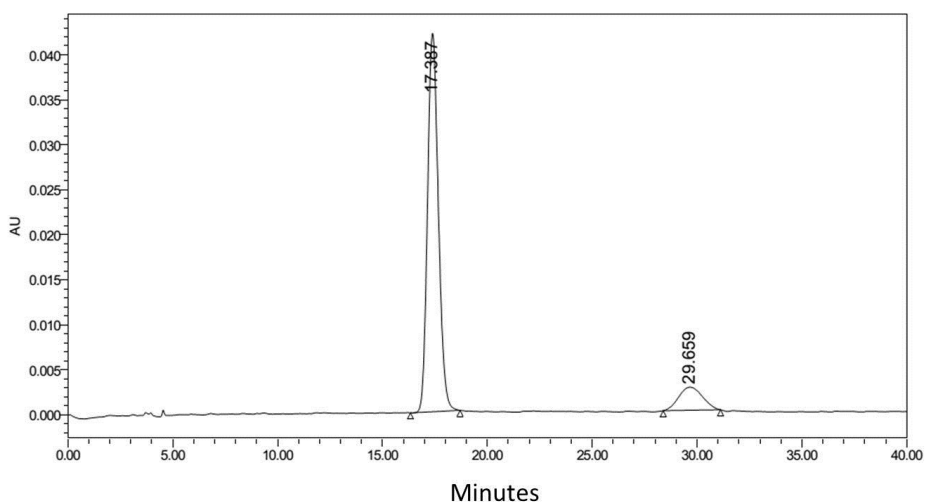
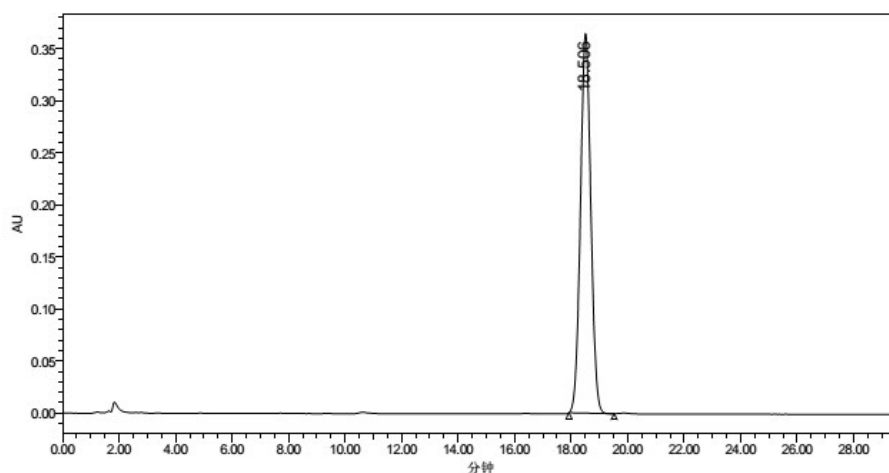


Figure. S3. The photographs of the two-component and three-component gels. A) NA1/LHC18 gel after resting for 10 hours; B) NA2/LHC18 gel after resting for 10 hours; C) NA1/NA2/LHC18 gel after resting for 10 hours.



	RT	Area	% Area	Height
1	17.387	1529493	89.47	94.22
2	29.659	180030	10.53	5.78

Fig. S4. High-performance liquid chromatography (HPLC) graph of the corresponding squeezed solution from NA1/NA2/LHC18=1/1/2 gel after 10 hours. The peaks at 1 and 2 correspond to NA2 and NA1, respectively,



	RT (min)	Area (峰*sec)	% Area	Height (峰)	% Height
1	18.506	9268815	100.00	364968	100.00

Fig. S5. High-performance liquid chromatography (HPLC) graph of the corresponding squeezed solution from NA2/LHC18=1/1 gel after 10 hours.

High Performance Liquid Chromatography was equipped with a Diacel OB column, and the mobile phase was a mixture of n-hexane/isopropyl alcohol/ acetic acid (99:2:0.002) at a flow rate of 0.5 mL/min. The compounds in the corresponding squeezed solution were identified according to the HPLC retention time. The peak at $t_R=18$ min indicates the 2-naphthoic acid, whereas the peak at $t_R=29$ min indicates 1-naphthoic acid.