

# Supplementary Material: Constructing ROS-Responsive Supramolecular Gel with Innate Antibacterial Properties

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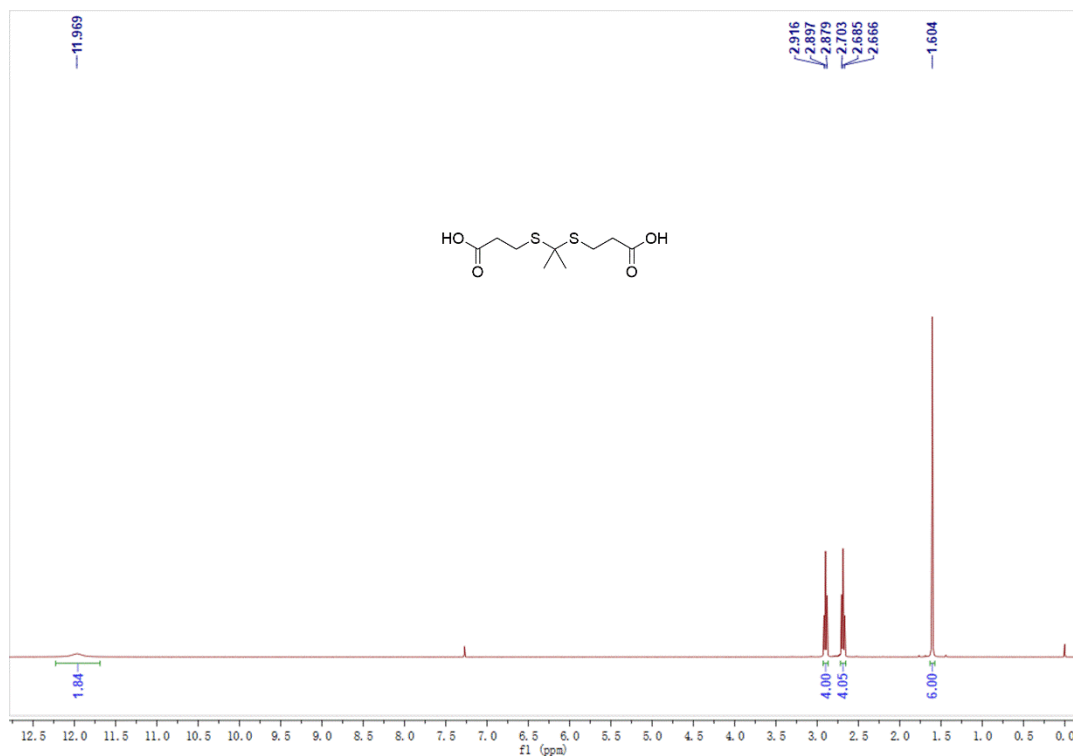


Figure S1. <sup>1</sup>H NMR spectra of TK1 (n=2).

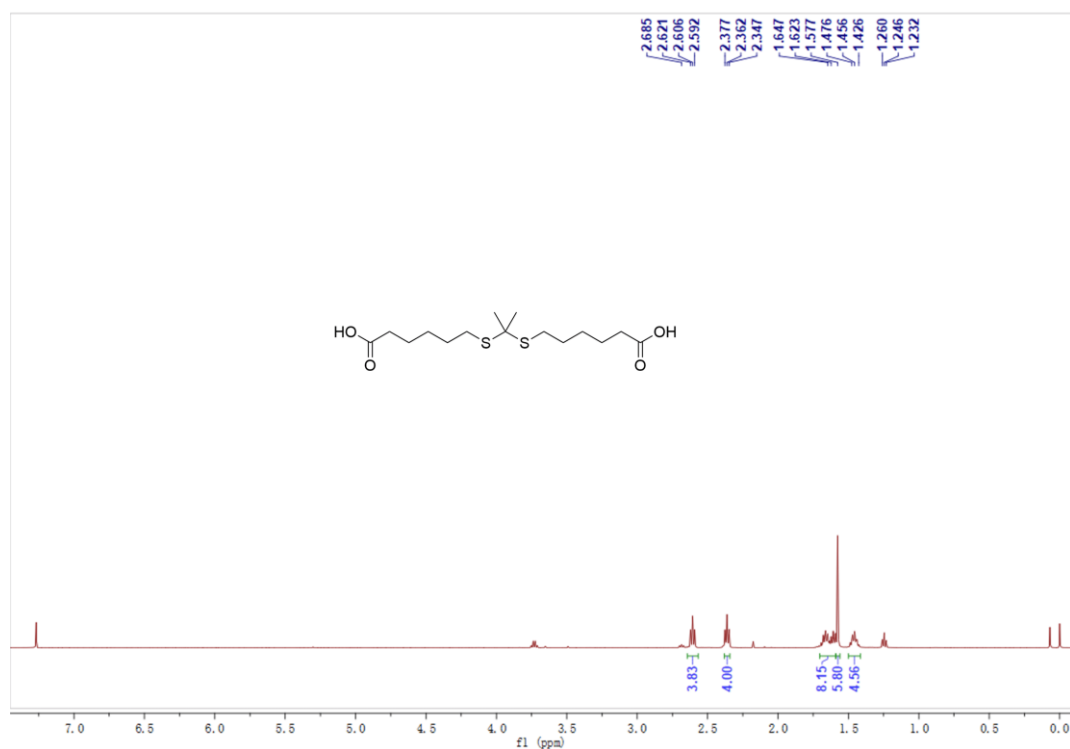


Figure S2. <sup>1</sup>H NMR spectra of TK2 (n=5).

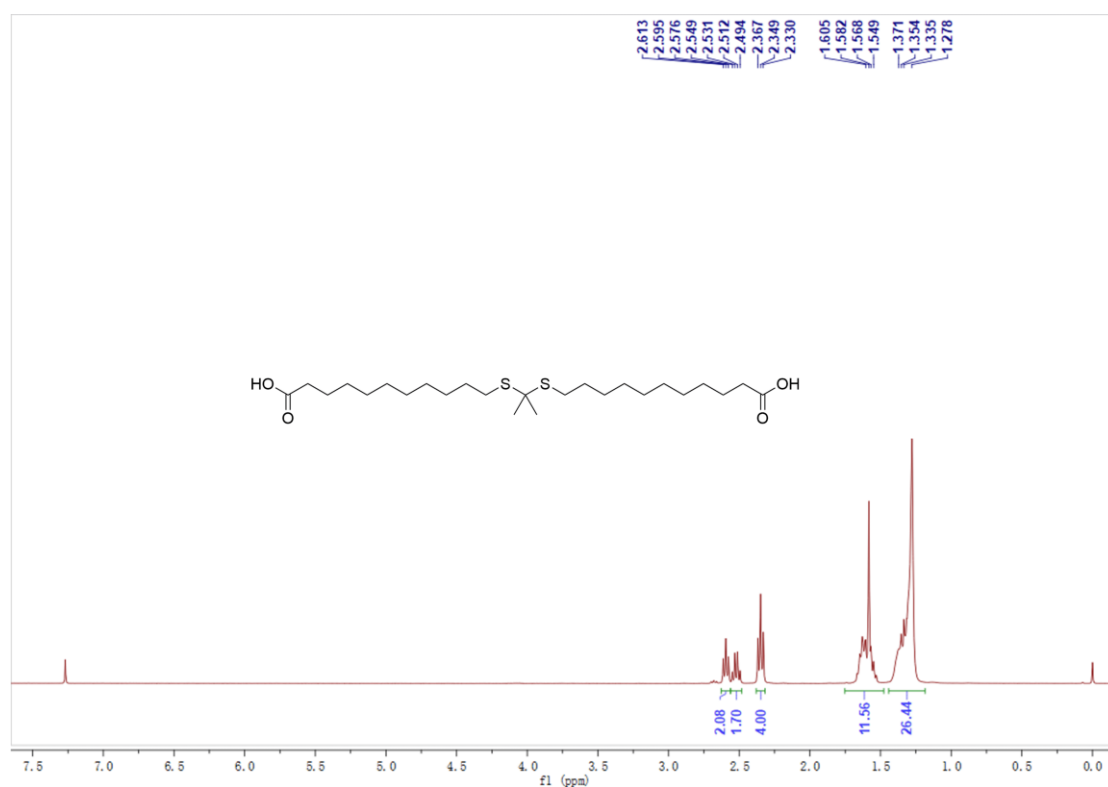


Figure S3. <sup>1</sup>H NMR spectra of TK3 (n=10).

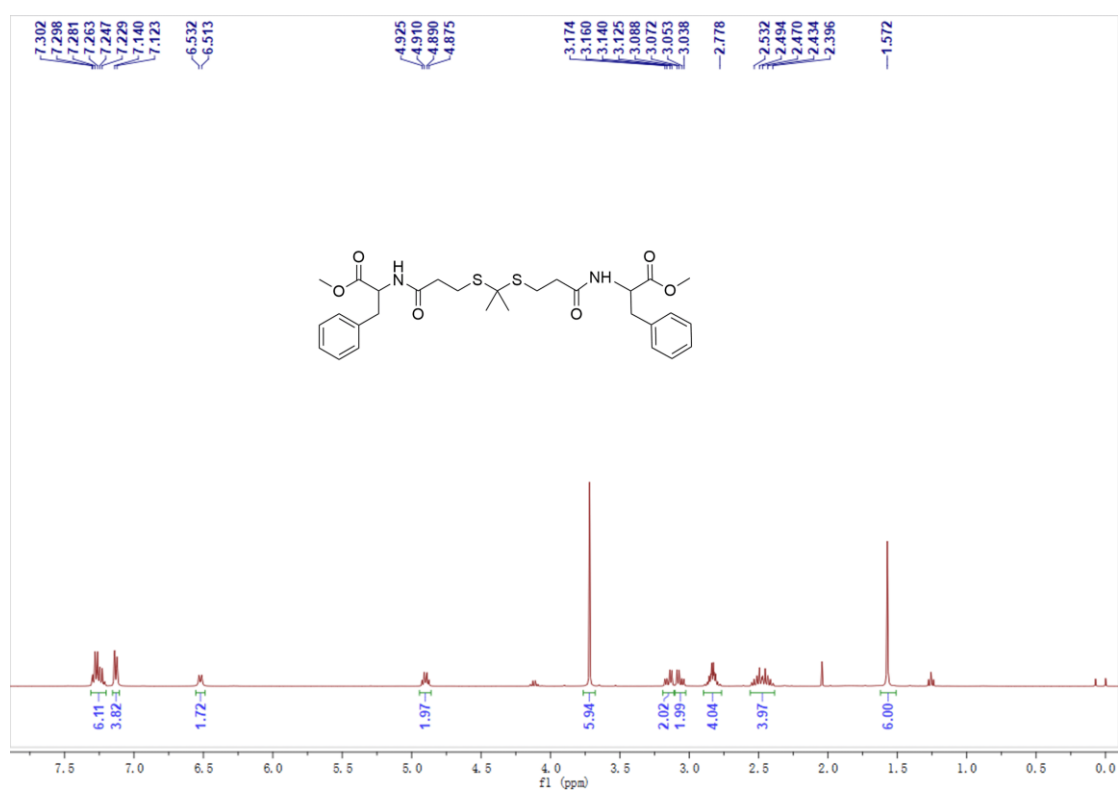


Figure S4. <sup>1</sup>H NMR spectra of Phe-TK1-Phe (n=2).

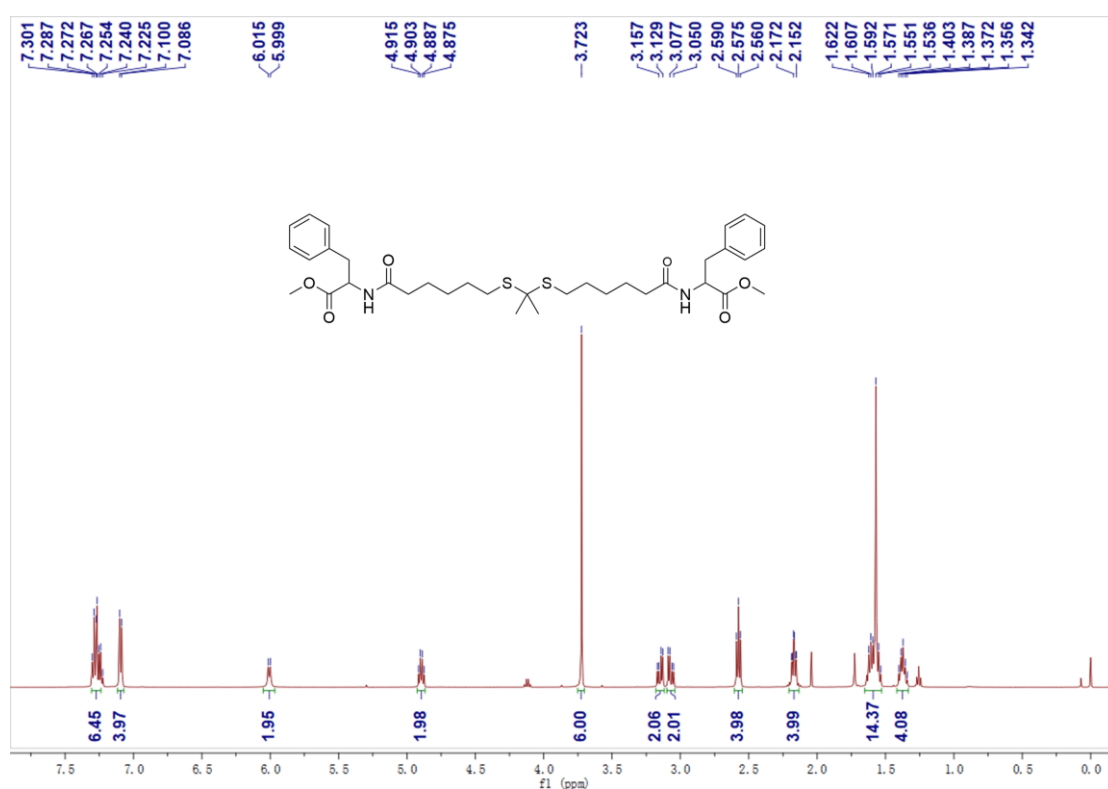


Figure S5.  $^1\text{H}$  NMR spectra of Phe-TK2-Phe (n=5).

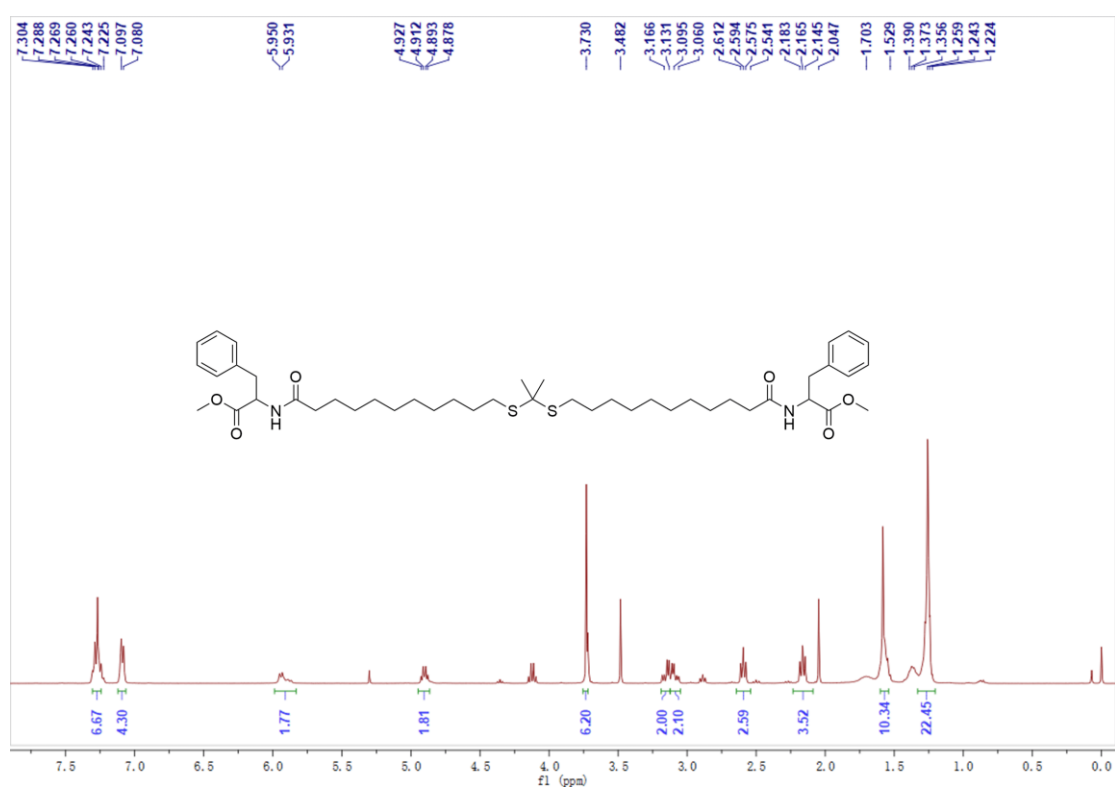


Figure S6.  $^1\text{H}$  NMR spectra of Phe-TK3-Phe (n=10).

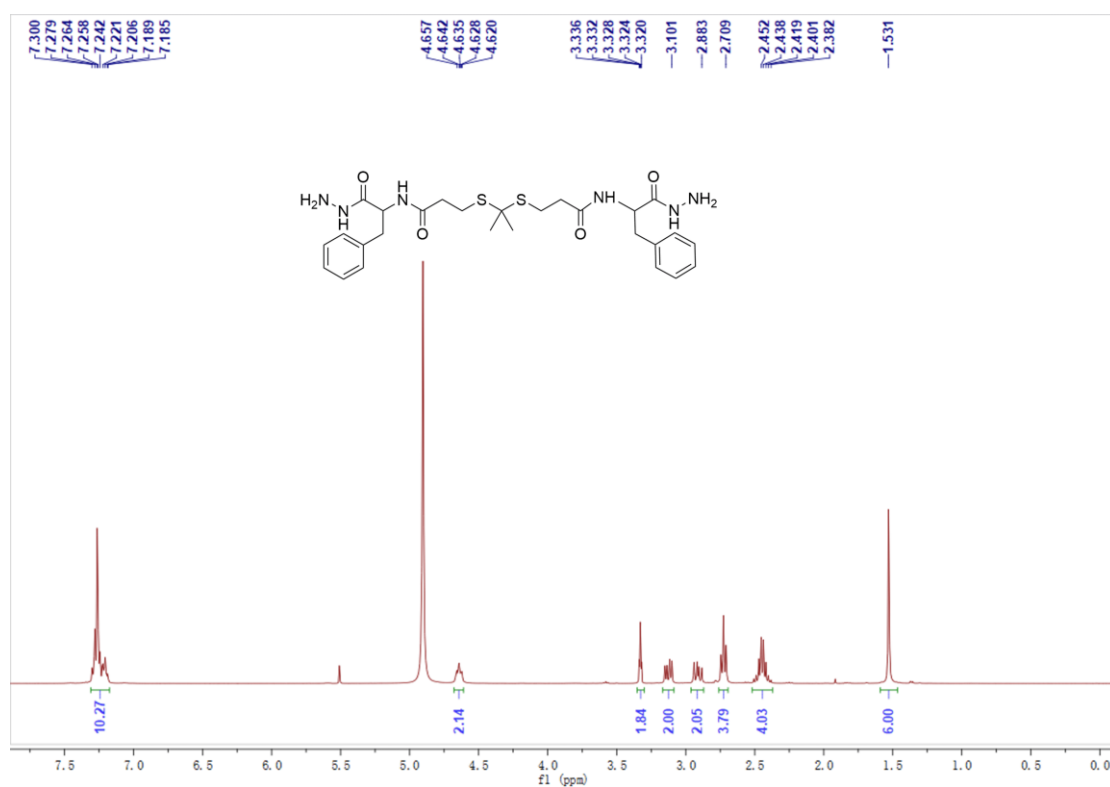


Figure S7. <sup>1</sup>H NMR spectra of gelator 1 (n=2).

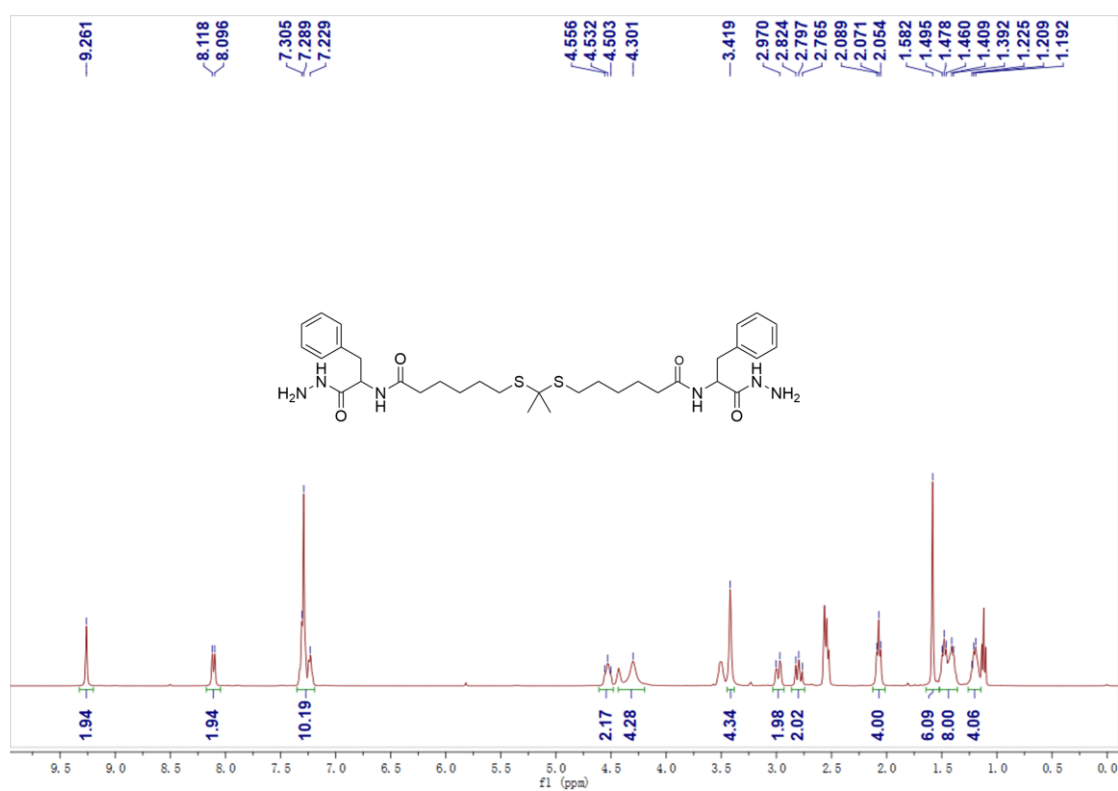
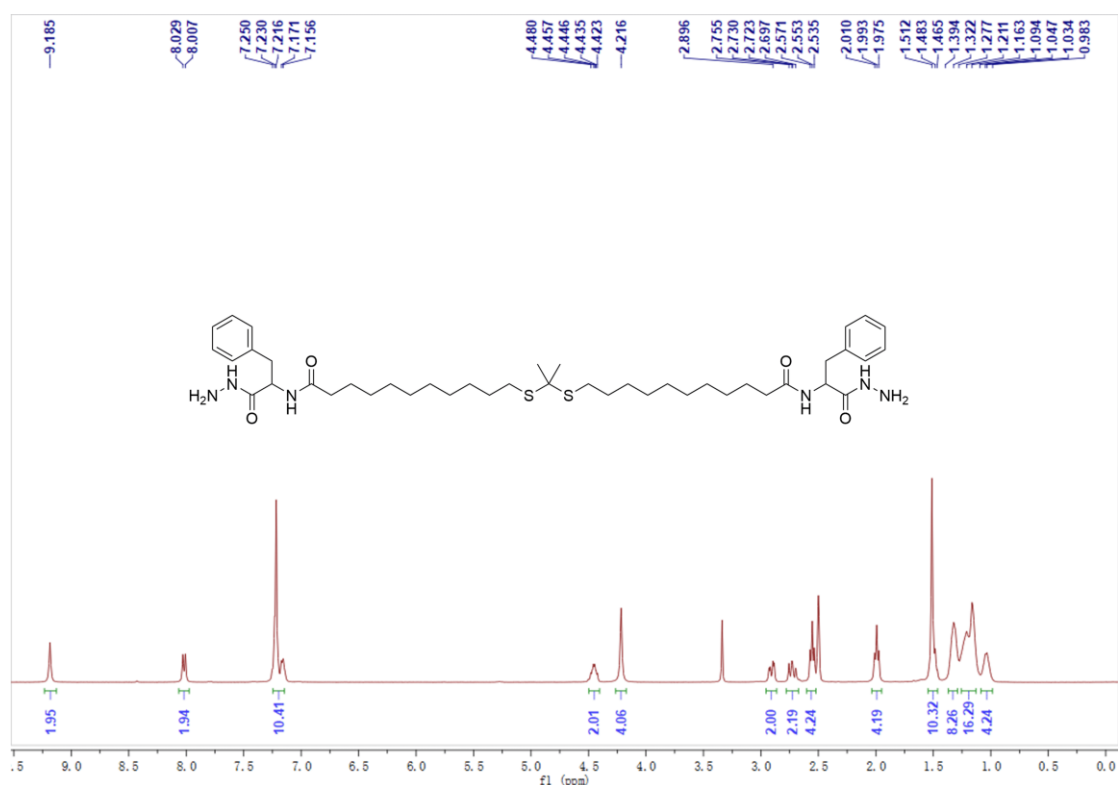


Figure S8. <sup>1</sup>H NMR spectra of gelator 2 (n=5).



**Figure S9.**  $^1\text{H}$  NMR spectra of gelator 3 ( $n=10$ ).

**Table S1.** Critical gelation concentration and gelation behavior of three gelators in different solvents.

| Entry | Organic solvent                  | Gelator 1 CGC at 25°C<br>(mg/mL) | Gelator 2 CGC at 25°C<br>(mg/mL) | Gelator 3 CGC at 25°C<br>(mg/mL) |
|-------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| 1     | Petroleum ether                  | I                                | I                                | I                                |
| 2     | Cyclohexane                      | I                                | I                                | I                                |
| 3     | Diethyl ether                    | I                                | I                                | I                                |
| 4     | Ethyl acetate                    | G (10 mg/mL)                     | G (6 mg/mL)                      | G (5 mg/mL)                      |
| 5     | Dichloromethane                  | G (10 mg/mL)                     | G (7 mg/mL)                      | G (3 mg/mL)                      |
| 6     | Chloroform                       | G (9 mg/mL)                      | G (10 mg/mL)                     | G (10 mg/mL)                     |
| 7     | Acetone                          | S                                | S                                | S                                |
| 8     | Acetonitrile                     | G (15 mg/mL)                     | G (5 mg/mL)                      | G (2 mg/mL)                      |
| 9     | Methanol                         | S                                | S                                | G (7 mg/mL)                      |
| 10    | Ethanol                          | S                                | G (18 mg/mL)                     | G (6 mg/mL)                      |
| 11    | Ethylene glycol                  | S                                | G (5 mg/mL)                      | G (12 mg/mL)                     |
| 12    | Dimethyl sulfoxide               | S                                | S                                | S                                |
| 13    | PEG200                           | S                                | S                                | G (15 mg/mL)                     |
| 14    | PEG400                           | S                                | P                                | P                                |
| 15    | H <sub>2</sub> O                 | P                                | P                                | P                                |
| 16    | Ethanol : H <sub>2</sub> O (1:1) | I                                | G (10 mg/mL)                     | G (2 mg/mL)                      |
| 17    | PEG200 : H <sub>2</sub> O (1:1)  | P                                | G (22 mg/mL)                     | G (18 mg/mL)                     |
| 18    | PEG200 : H <sub>2</sub> O (3:2)  | P                                | G (28 mg/mL)                     | G (13 mg/mL)                     |

a) I: insoluble, if the gelator is completely insoluble in the solvent;

b) G: gel, if the gelator is able to gelation the solvent;

c) S: solution, if the gelator is completely soluble in the solvent;

d) P: precipitate, if the gelator dissolves after heating, and precipitates after cooling to room temperature.