

Electronic Supplementary Information

Single Amino Acid Based Thixotropic Hydrogel Formation And pH-Dependent Morphological Change of Gel Nanofibers

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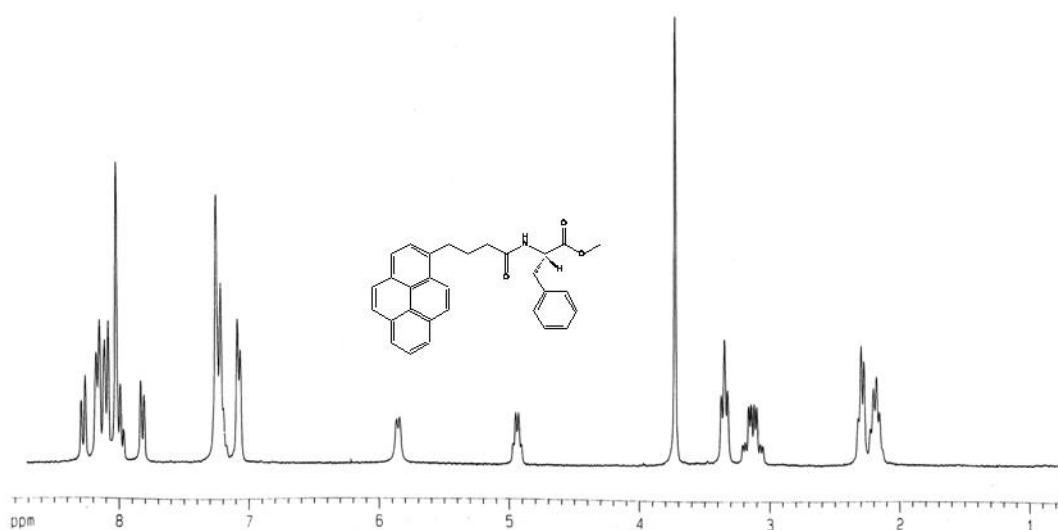


Figure S1. ¹H spectrum of Pyrene-Phe-OMe in CDCl₃ solvent in 300 MHz.

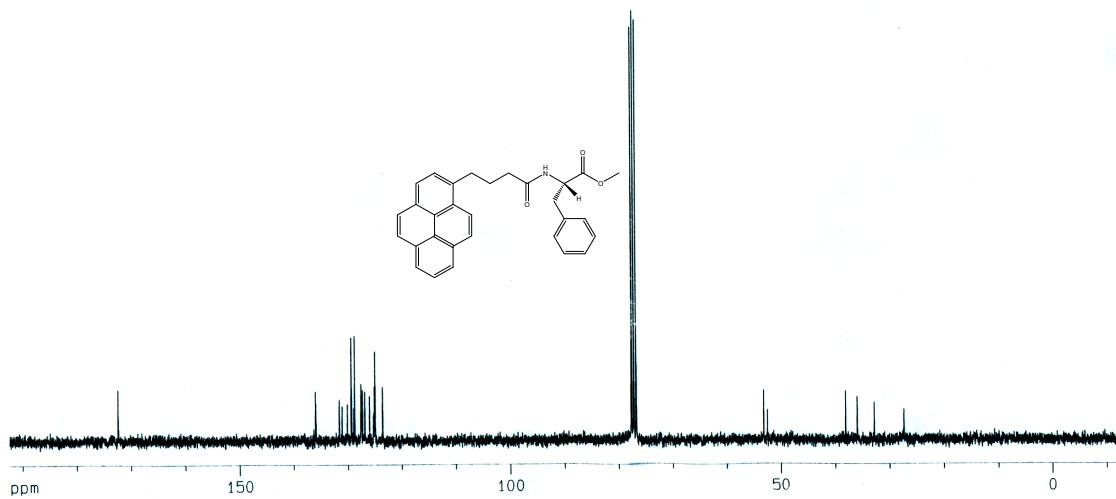


Figure S2. ¹³C spectrum of Pyrene-Phe-OMe in CDCl₃ solvent in 75 MHz.

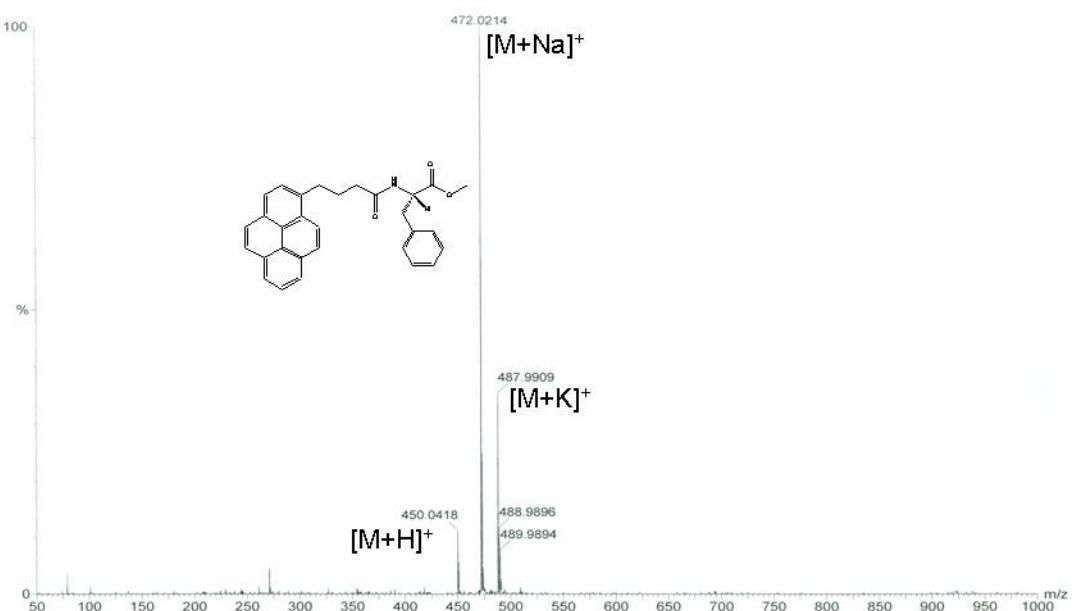


Figure S3. HRMS spectrum of Pyrene-Phe-OMe.

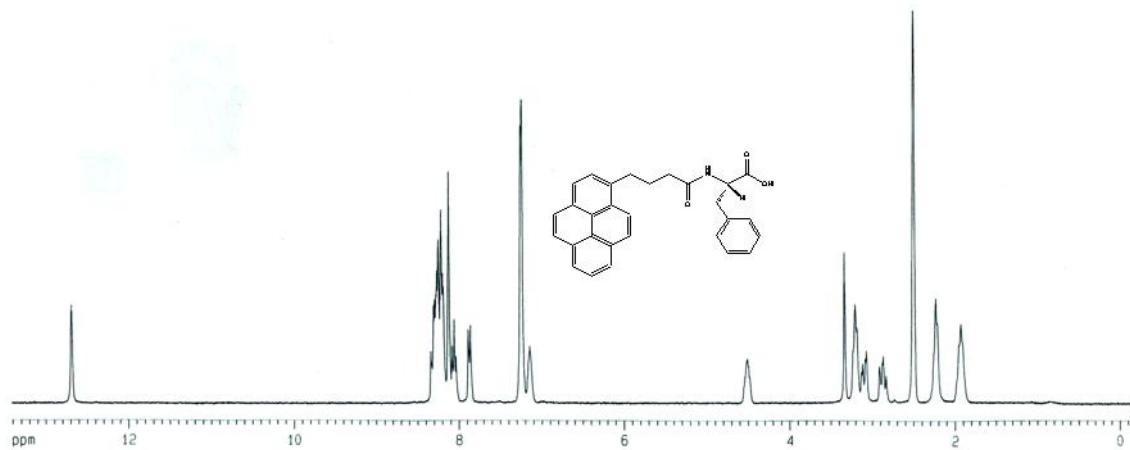


Figure S4. ^1H spectrum of Pyrene-Phe-OH in DMSO-d_6 solvent in 300 MHz.

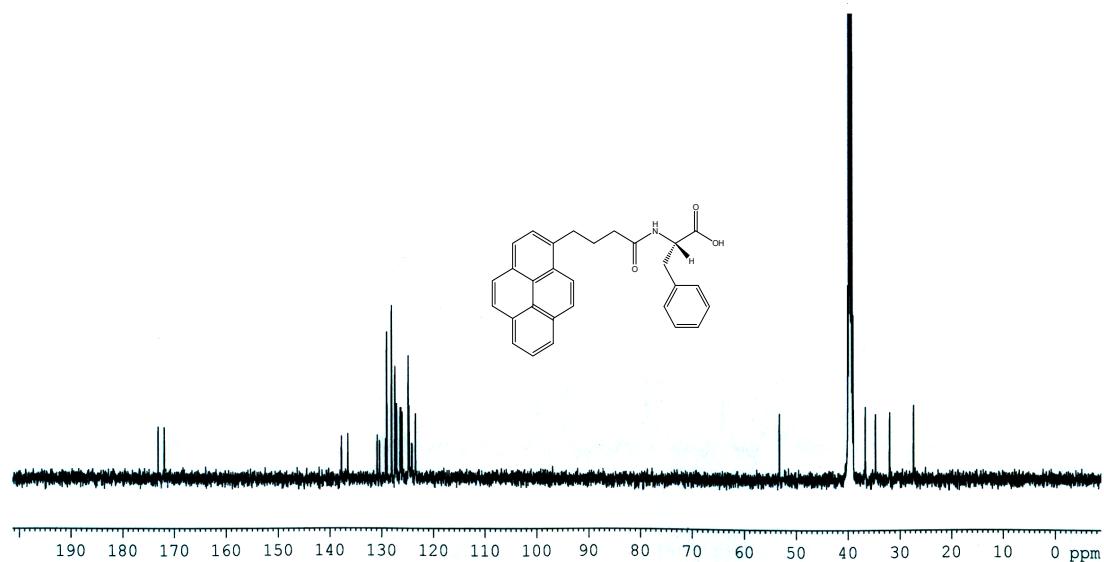


Figure S5. ¹³C spectrum of Pyrene-Phe-OH in DMSO-d₆ solvent in 75 MHz.

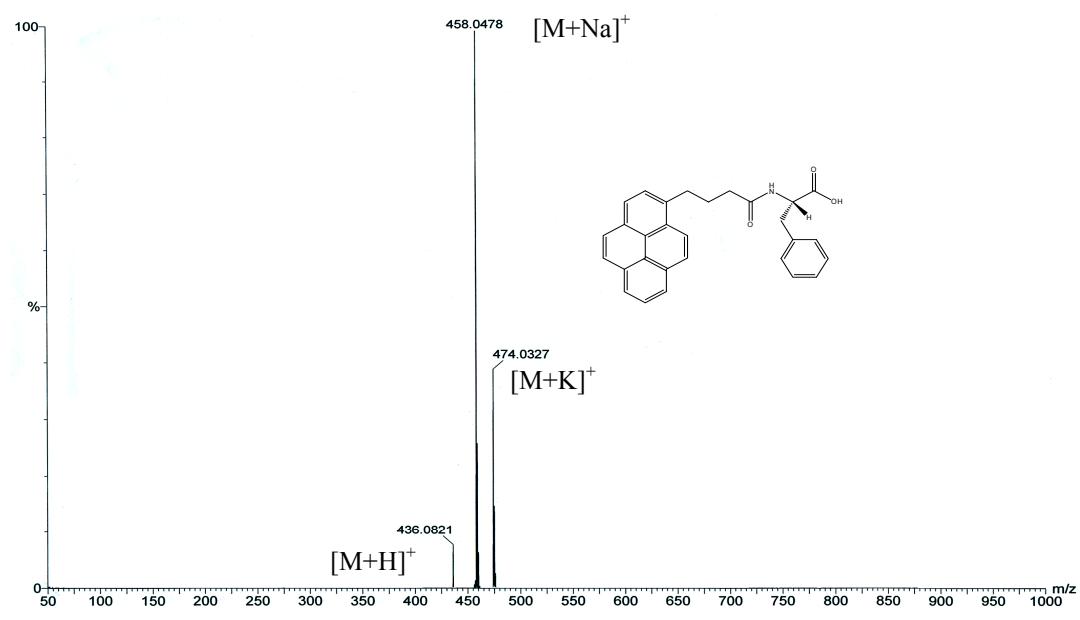


Figure S6. HRMS spectrum of Pyrene-Phe-OH.

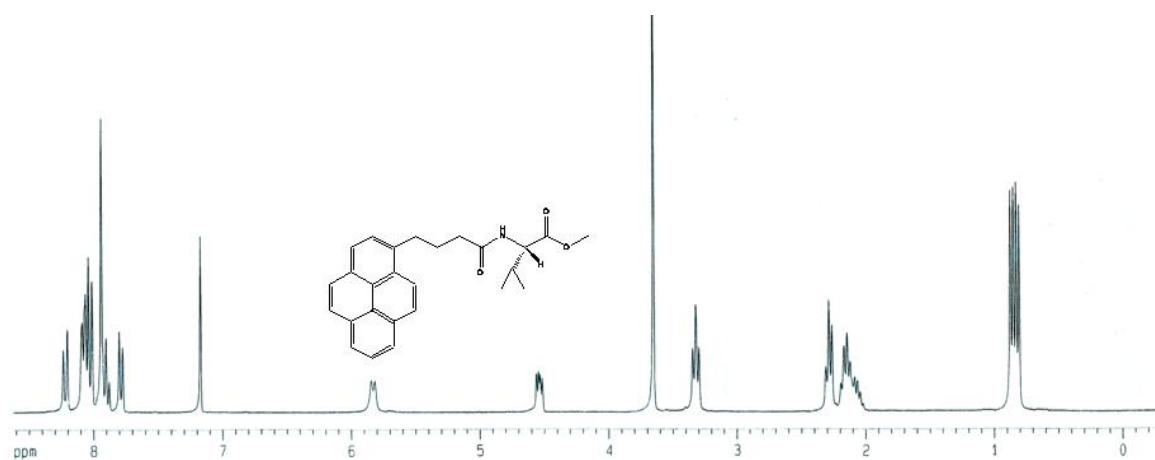


Figure S7. ¹H spectrum of Pyrene-Val-OMe in CDCl₃ solvent in 300 MHz.

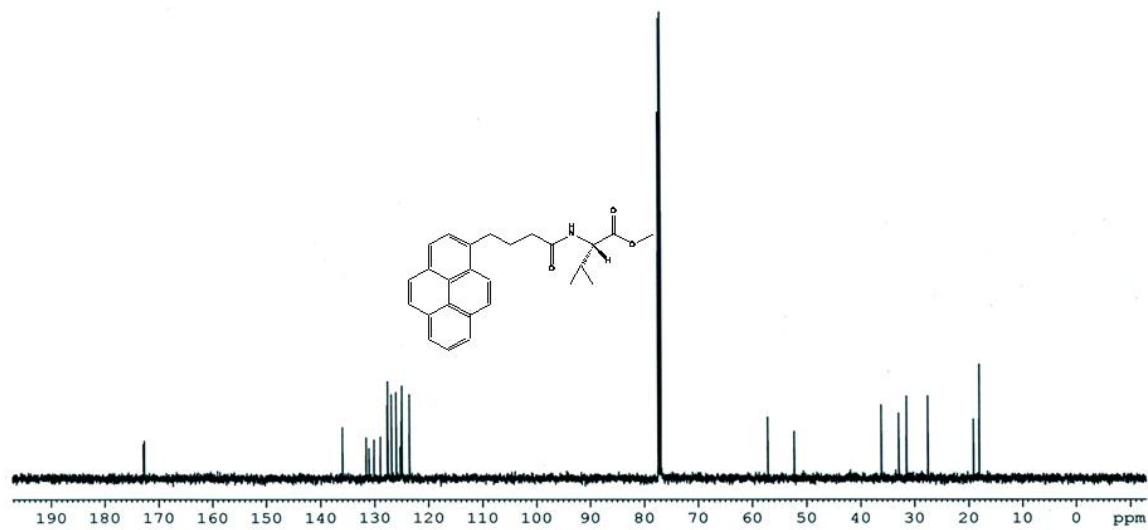


Figure S8. ¹³C spectrum of Pyrene-Val-OMe in CDCl₃ solvent in 75 MHz.

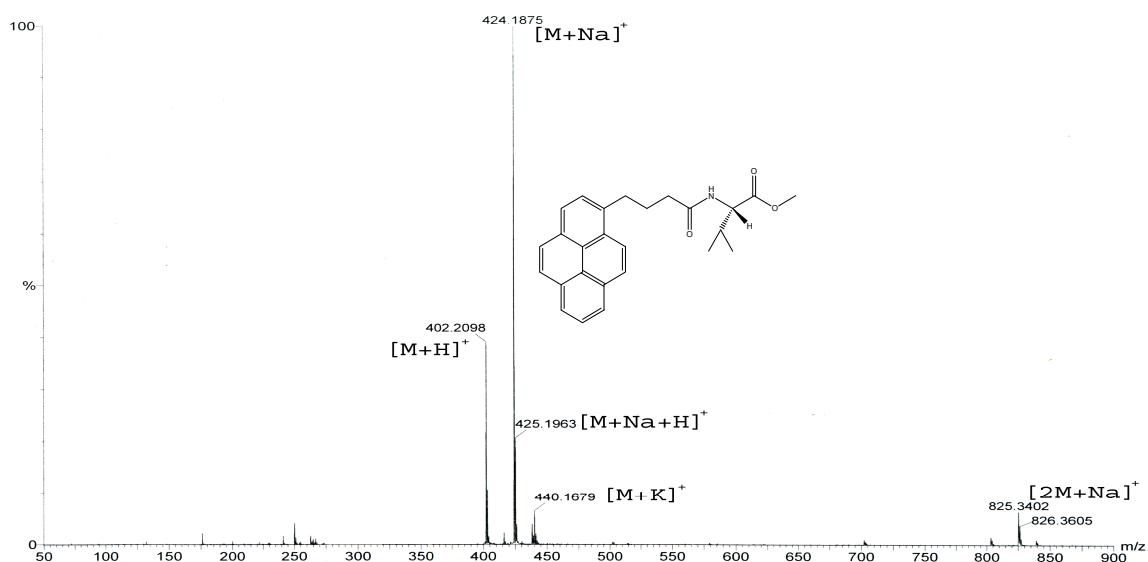


Figure S9. HRMS spectrum of Pyrene-Val-OMe.

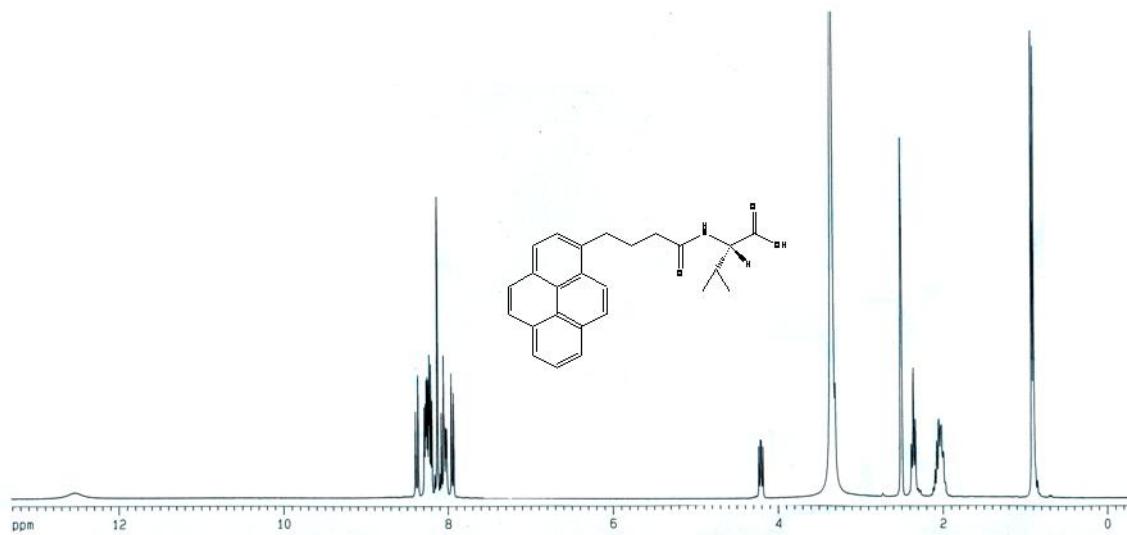


Figure S10. ^1H spectrum of Pyrene-Val-OH in DMSO-d_6 solvent in 300 MHz.

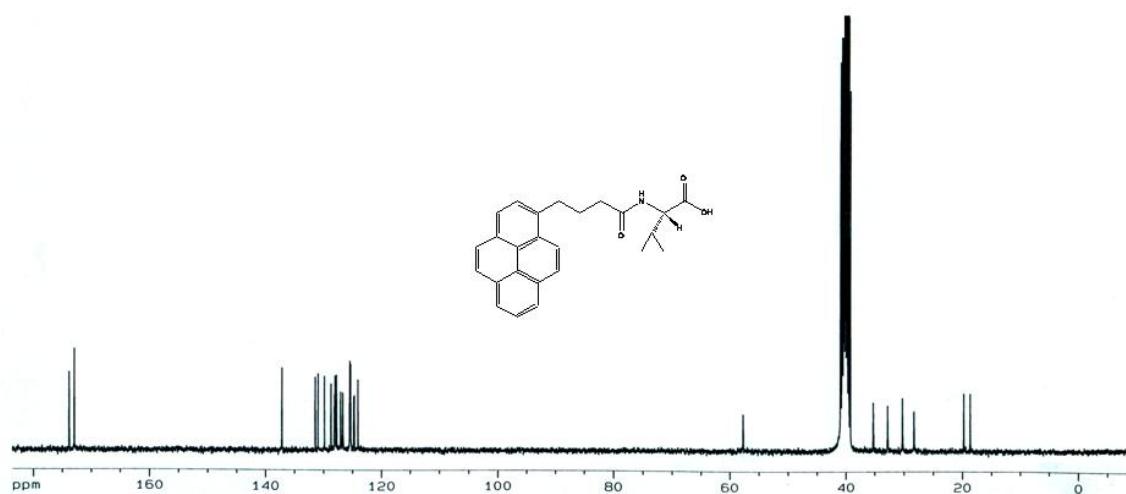


Figure S11. ¹³C spectrum of Pyrene-Val-OH in DMSO-d₆ solvent in 75 MHz.

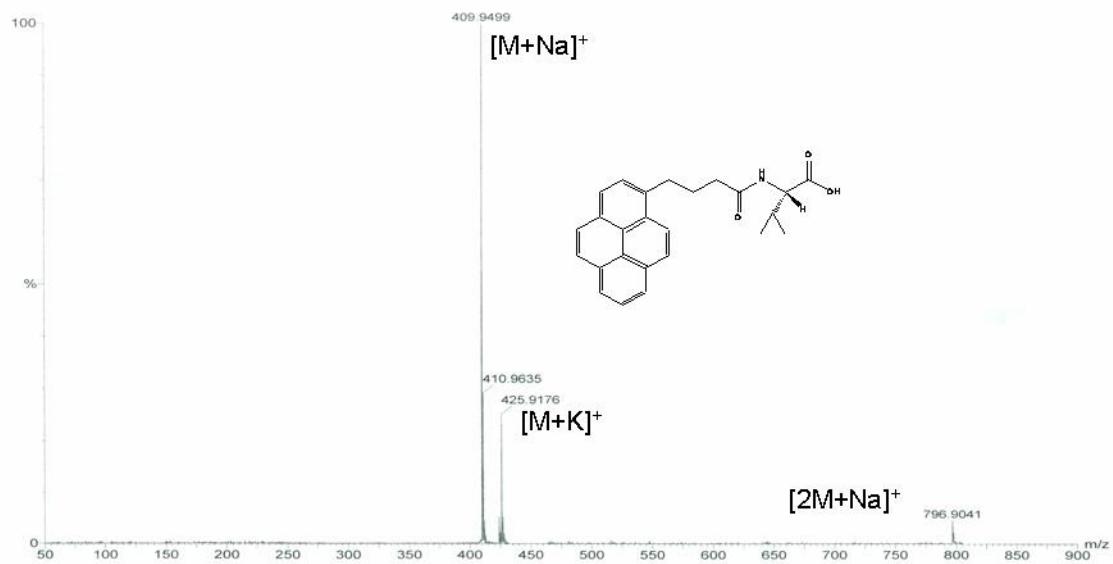


Figure S12. HRMS spectrum of Pyrene-Val-OH.

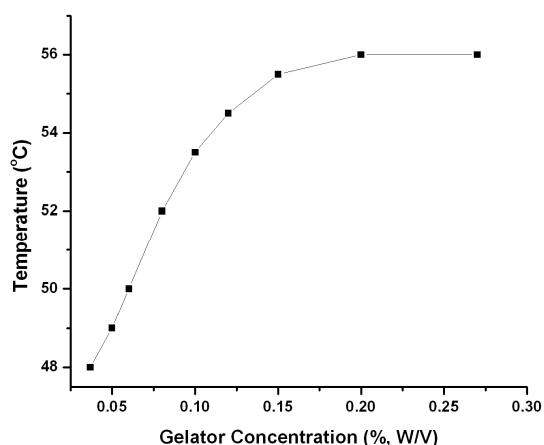


Figure S13. Changing of gel melting temperatures (T_m) with respect to gelator's concentration in phosphate buffer solution at pH 7.46.

Note. T_m values have been sharply increased, then slowed down and reached to a ‘platue region’ with the increase in the gelator’s concentration. The increase of gel melting temperature is due to the requirement of more energy to break the increased gelator-gelator interactions and the interactions among the gel nanofibers (Figure S14, ESI†) compare to that at lower gelator concentration. At minimum gelator concentration (MGC) 0.037 % (w/v), gel to sol transition has been taken place at 48 °C.

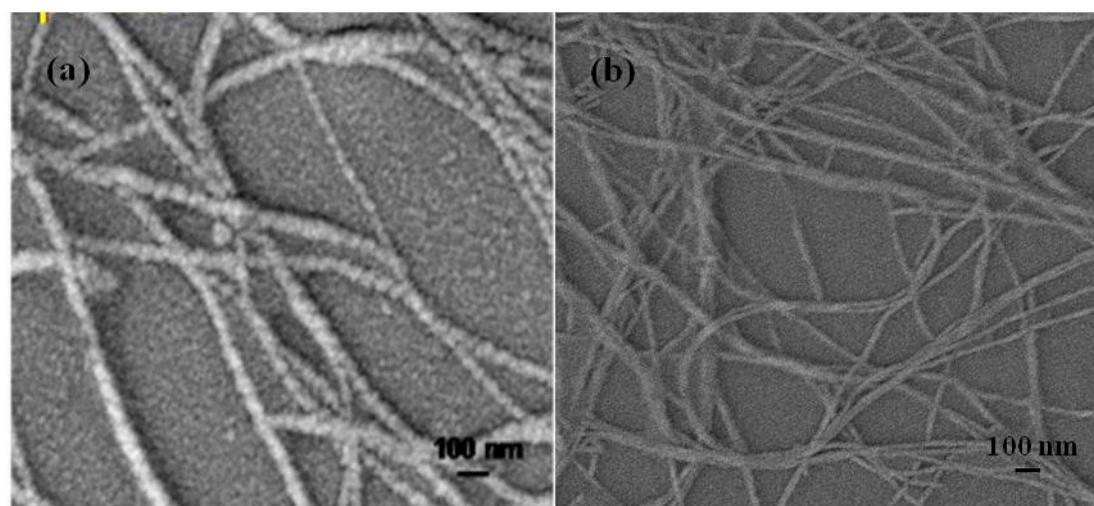


Figure S14. Comparative study morphological studies of the hydrogel materials having different concentration of gelator (a) 0.037 % (w/v) and (b) 0.31 % (w/v). FE-SEM study indicates that increase of gel fibers network density with the increase of the gelator concentration in gel state.

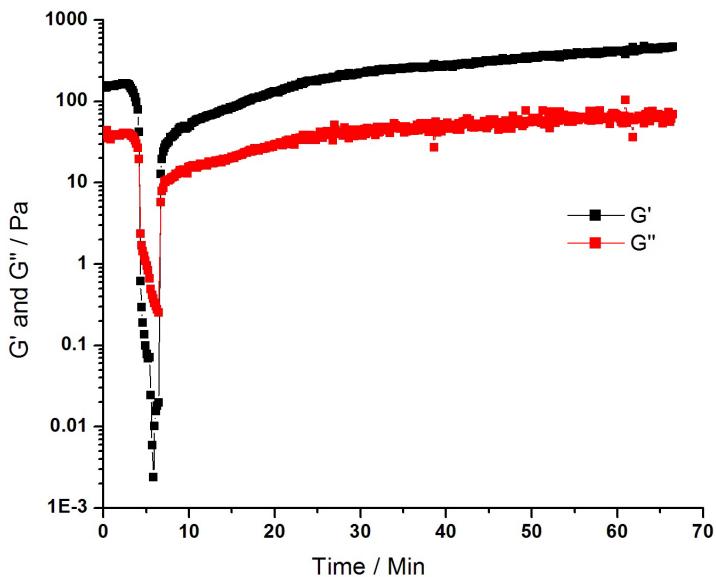


Figure S15. The recovered gel is strengthened with an increase of the recovery time.

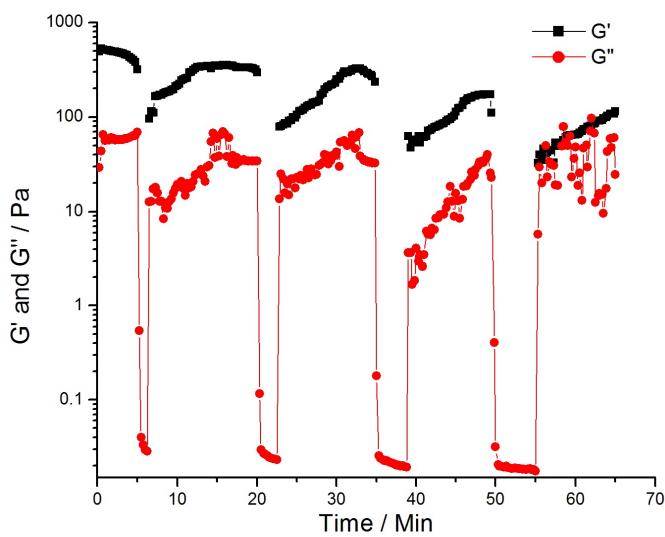


Figure S16. Demonstration of thixotropic property of the hydrogel material (0.42 % w/v) prepared at pH 8.5. Variation of storage modulus and loss modulus has been studied under application and release of shear stress in cyclic way. Though sol to gel recovery taking place, gel strength is not fully recovered.

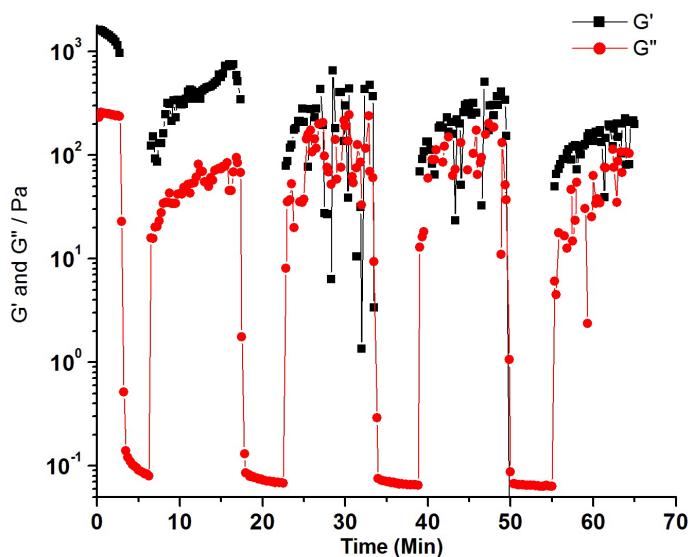


Figure S17. Demonstration of thixotropic property of the hydrogel material (0.42 % w/v) prepared at pH 10.5. Variation of storage modulus and loss modulus has been studied under application and release of shear stress in cyclic way. Strength of the hydrogel is not fully recovered and after first cycle, recovery of gel strength is not recovered properly.

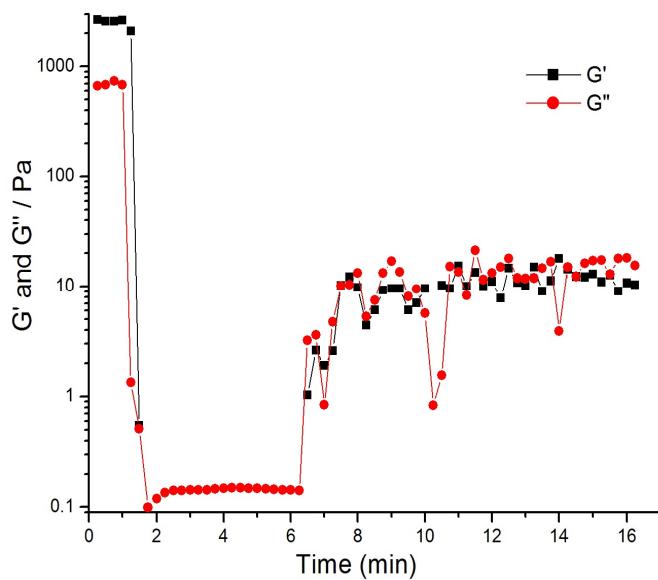


Figure S18. Rheological study of hydrogel (0.42 % w/v) prepared using aqueous solution of pH 14. Hydrogel materials are unable to recover into the gel state after removal of stress.

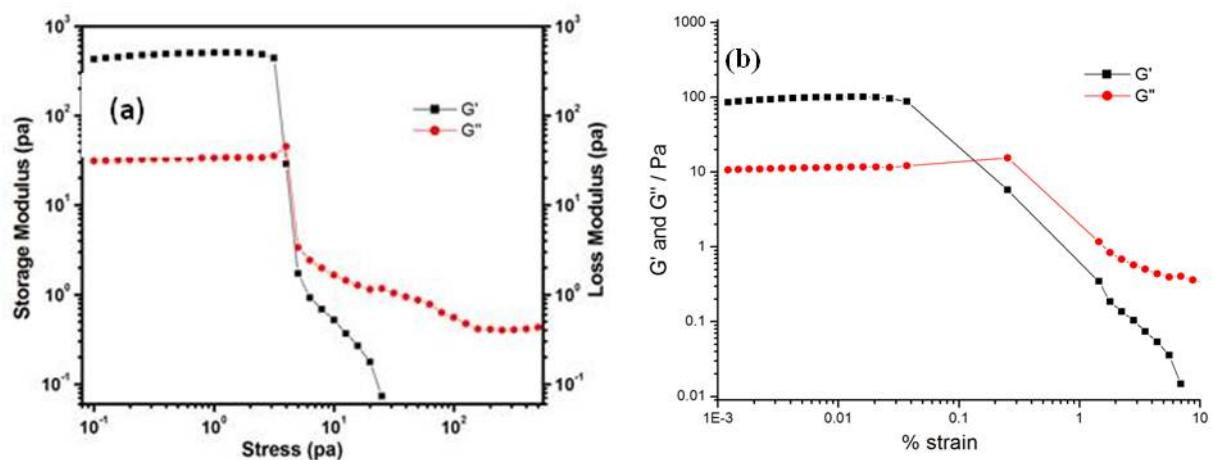


Figure S19. (a) Stress sweep and (b) strain sweep experiments of the hydrogel (0.3 % w/v)

prepared using phosphate buffer solution of pH 7.46.

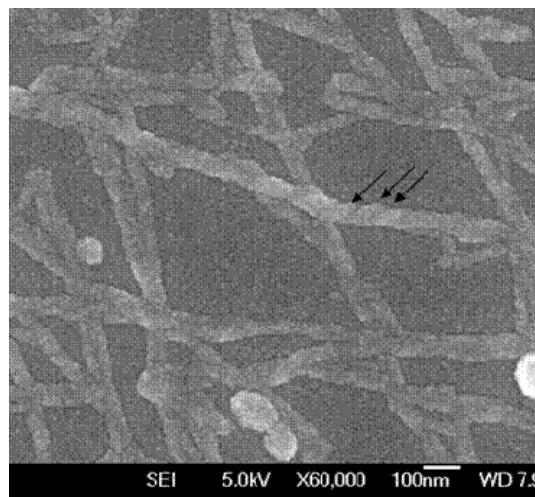


Figure S20. FE-SEM image of the hydrogel (0.037 %, w/v) at pH 7.46 after recovery process.
The black arrows indicates the left-handed helicity of the gel nanofiber.

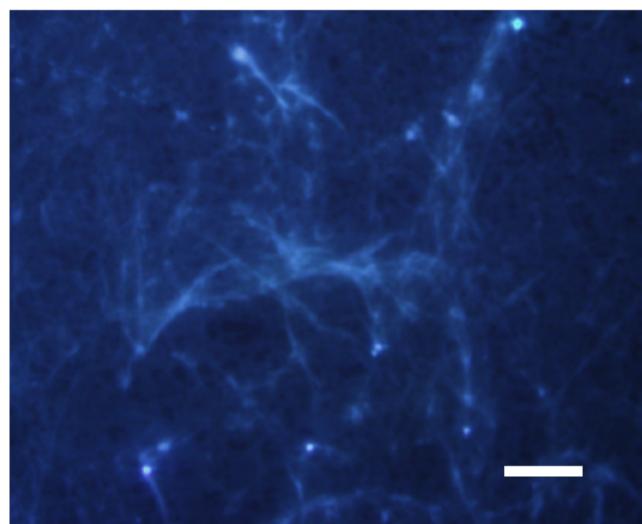


Figure S21. Fluorescence microscopic image of the native wet hydrogel at 0.05 % (w/v) prepared using phosphate buffer solution at pH 7.46 (scale bar 50 μm).

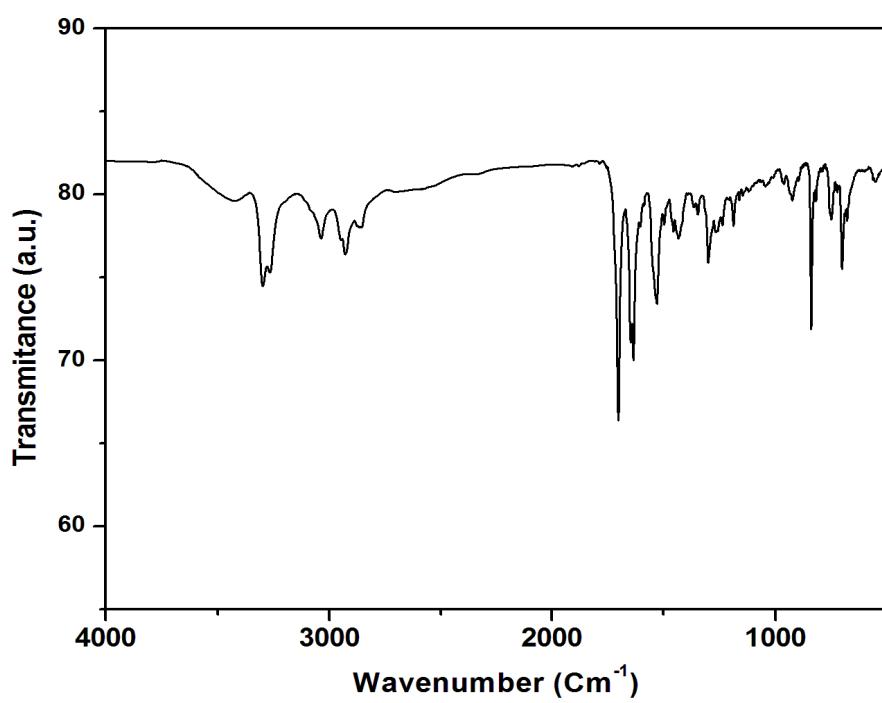


Figure S22. FTIR spectrum of the gelator in the solid state.

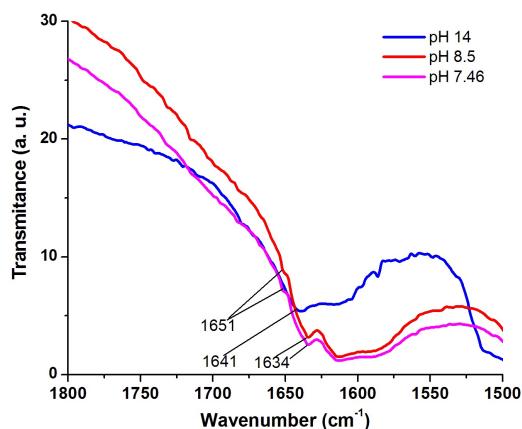


Figure S23. FTIR spectra of the gelator in wet gel state.

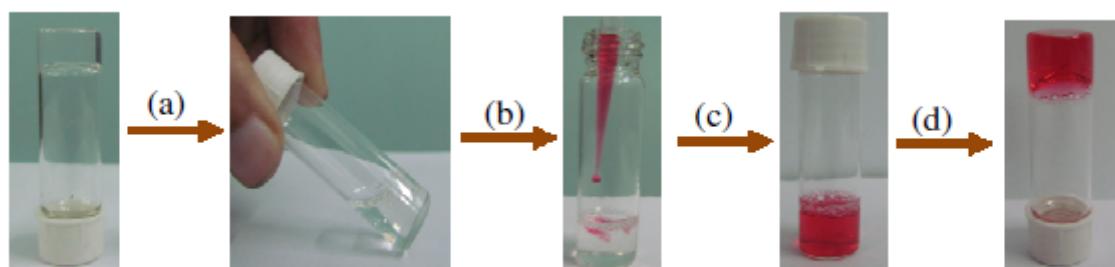


Figure S24. Demonstration of encapsulation of vitamin B₁₂ within the hydrogel matrix using the thixotropic of this hydrogel (Pyr 1) at pH 7.46: (a) breaking of hydrogel upon mechanical shaking, (b) addition of aqueous solution of vitamin B₁₂, (c) homogenized using a vortex and (d) further gel formation upon resting for about an hour.