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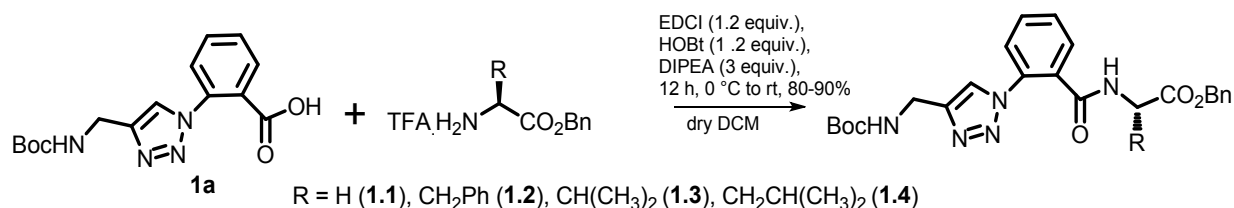
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General experimental information:

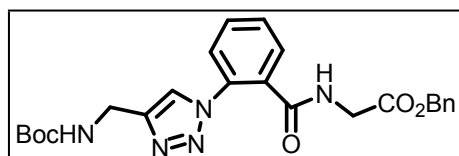
Experiments which required anhydrous conditions were carried out under nitrogen atmosphere in dry dichloromethane (DCM). Thin-layer chromatography (TLC) was performed on 0.25 mm silica gel plates (60 F254 grade) from Merck, and were analyzed using 254 nm UV light. Chromatographic separation was carried out on 100-200 mesh silica gel in gravity mode. ^1H NMR and ^{13}C NMR spectra were recorded on Bruker Avance 400 MHz and 500 MHz instruments, and the chemical shifts (δ) are reported in parts per million (ppm) relative to tetramethylsilane (TMS) with coupling constant (J) values in Hertz (Hz). The splitting patterns in ^1H NMR spectra are reported as follows: s = singlet; d = doublet; t = triplet; dd = doublet of doublet; m = multiplet, bs = broad singlet. ^{13}C NMR data are reported with the solvent peak (CDCl_3 , $\delta = 77.0$ ppm) as the internal standard. High resolution mass spectra (HRMS) were recorded on a Waters Q-ToF microTM spectrometer with lock spray source. Infrared spectra were recorded using a Nicolet 6700 FT-IR spectrophotometer. Powder X-Ray diffraction data was obtained on BRUKER D8-Advance diffractometer using $\text{CuK}\alpha$ radiation ($\lambda=1.5418$ Å) over the range of $0.5^\circ < 2\theta < 30^\circ$ at room temperature. Samples for SEM imaging were coated with Au-Pd (Gatan precision etching coating system (model No. 682) operating at 5 KeV) and analyzed by FEI Quanta FEG 200 High Resolution Scanning Electron Microscope operating at 10-30 kV. Rheological measurements were performed with a stress-controlled rheometer (MCR 301) equipped with steel-coated parallel-plate geometry (25 mm diameter). The gap distance was fixed at 1 mm and a solvent-trapping device was placed above the plate to prevent solvent evaporation. All measurements were done at 25 °C. UV experiments were carried out with a JASCO V660 spectrometer. Circular dichroism studies were performed with an Applied Photophysics Chirascan spectrometer. The synthetic strategy adopted to access various compounds reported here is presented in Schemes 1. Detailed experimental procedures are given subsequently. Compound **1.0** was synthesized based on protocols published earlier by us.¹

Synthesis of aryl-triazole peptides



Scheme S1. Synthetic scheme towards dipeptides **1.1** - **1.4**

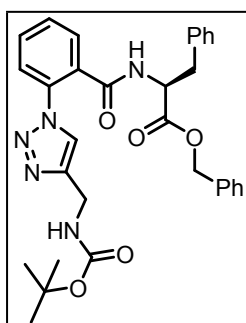
General reaction procedure for the synthesis, and spectral data of 1.1-1.4:



Dipeptide 1.1: To a stirred mixture of the acid **1a** (0.5 g, 1.57 mmol), HOBT (0.25 g, 1.88 mmol) and EDCI (0.36 g, 1.88 mmol) in dry dichloromethane (10 mL) at

0 °C was added DIPEA (3 mmol). After stirring for 1 h, the amine trifluoroacetate salt of Glycine benzylester (0.41 g, 1.57 mmol) in 5 mL of dry dichloromethane was added, and stirring continued for 12 h at room temperature. All the volatiles were then removed under reduced pressure, the residue dissolved in ethyl acetate and washed successively with 5% HCl (3 x 10 mL) and saturated NaHCO₃ (3 x 10 mL). After drying with sodium sulphate, the organic layer was evaporated under reduced pressure to get a residue which was purified by column chromatography using 50% ethyl acetate/hexane system to get the product as a white crystalline solid (0.63 g, 87 %). Analytical data: *R_f*, 0.23 (50 % Ethyl acetate- Hexane); mp 110-112 °C ¹H NMR (CDCl₃, 400 MHz): 7.85 (s, 1H), 7.73 (dd, 1H, *J* = 7.23, 1.8 Hz), 7.63-7.53 (m, 2H), 7.50 (dd, 1H, *J* = 7.5, 1.7 Hz), 7.40-7.30 (m, 5H), 6.46 (bs NH², 1H), 5.35 (bs, 1H, NH¹), 5.16 (s, 2H), 4.45 (d, 2H, *J* = 5.52 Hz), 4.07 (d, 2H, *J* = 5.5 Hz), 1.43 (s, 9H); ¹³C NMR (CDCl₃, 100 MHz): 169.2, 166.4, 155.8, 145.7, 134.9, 134.2, 131.8, 131.4, 130.03, 129.4, 128.64 (2C), 128.6, 128.4 (2C), 126.2, 124.3, 79.7, 67.4, 41.67, 36.23, 28.38 (3C) ; IR(neat): 3314, 3147, 2978, 1747, 1706, 1665, 1523, 1500, 1168 cm⁻¹; HRMS (ESI) exact mass calcd. for C₂₄H₂₇N₅O₅Na [M+Na]⁺ 488.1910, found [M+Na]⁺ 488.1928.

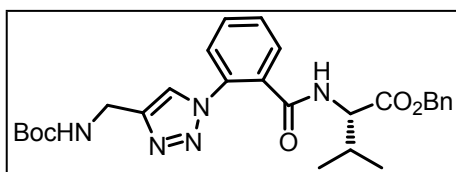
Dipeptide 1.2:



Use of the acid **1a** (0.5 g, 1.57 mmol) and Phenylalanine benzylester (0.56 g, 1.57 mmol) in the procedure discussed above (for **1.1**) resulted in 90% yield (0.78 g) of **1.2** as a white crystalline solid. Analytical data:

R_f : 0.39 (50 % Ethyl acetate- Hexane); mp 116-118 °C ^1H NMR (CDCl_3 , 400 MHz): 7.80 (s, 1H), 7.61-7.45 (m, 4H), 7.40-7.33 (m, 3H), 7.33- 7.27 (m, 2H), 7.23-7.16 (m, 3H), 7.0-6.93 (m, 2H), 6.30 (d, 1H, $J = 7.5$ Hz), 5.26 (bs, 1H, NH^1), 5.20- 5.07 (m, 2H), 4.88 (td, 1H, $J = 7.5$, 6.0 Hz), 4.44 (d, 2H, $J = 5.6$ Hz), 3.1 (dd, 1H, $J = 13.6$, 5.9 Hz), 3.03 (dd, 1H, $J = 13.9$, 6.1 Hz), 1.43 (s, 9H); ^{13}C NMR (CDCl_3 , 100 MHz): 170.9, 165.8, 155.8, 145.6, 135.3, 134.9, 134.3, 131.8, 131.4, 129.9, 129.2 (2C), 129.06, 128.6 (6C), 128.57, 127.1, 126.2, 124.04, 79.6, 67.5, 53.7, 37.3, 36.2, 28.4 (3C); IR(neat): 3390, 3305, 3151, 3031, 2977, 1738, 1711, 1663, 1507, 1498, 1169 cm^{-1} ; HRMS (ESI) exact mass calcd. for $\text{C}_{31}\text{H}_{33}\text{N}_5\text{O}_5\text{Na}$ $[\text{M}+\text{Na}]^+$ 578.2379, found $[\text{M}+\text{Na}]^+$ 578.2380

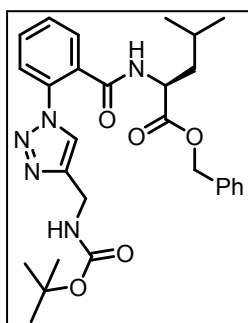
Dipeptide 1.3:



Use of the acid **1a** (0.5 g, 1.57 mmol) and Valine benzylester (0.48 g, 1.57 mmol) in the procedure discussed above (for **1.1**) resulted in 85% yield (0.68 g) of **1.3** as a white solid. Analytical data: R_f : 0.34 (50 %

Ethyl acetate- Hexane); mp 88-90 °C; ^1H NMR (CDCl_3 , 400 MHz): 7.82 (s, 1H), 7.72 (d, 1H, $J = 7.0$ Hz), 7.59 (m, 2H), 7.47 (d, 1H, $J = 7.1$ Hz), 7.59 (m, 5H), 6.31 (bs, 1H, NH^2), 5.31 (bs, 1H, NH^1), 5.20 (d, 1H, Bn CHH , $J = 12.1$ Hz), 5.11 (d, 1H, Bn CHH , $J = 12.0$ Hz), 4.56 (dd, 1H, $J = 8.5$, 4.5 Hz), 4.46 (d, 2H, $J = 4.96$ Hz), 2.22-2.04 (m, 1H), 1.43 (s, 9H), 0.83 (d, 3H, $J = 6.8$ Hz), 0.77 (d, 3H, $J = 6.84$ Hz); ^{13}C NMR (CDCl_3 , 100 MHz): 171.4, 166.2, 155.7, 145.7, 135.1, 134.0, 132.3, 131.3, 130.1, 129.4, 128.6 (2C), 128.5, 128.4 (2C), 126.4, 124.3, 79.66, 67.22, 57.7, 36.14, 30.9, 28.4 (3C), 18.8, 17.52; IR(neat): 3309, 3152, 2967, 1732, 1715, 1652, 1520, 1507, 1165 cm^{-1} ; HRMS (ESI) exact mass calcd. for $\text{C}_{27}\text{H}_{34}\text{N}_5\text{O}_5$ $[\text{M}+\text{H}]^+$ 508.2560, found $[\text{M}+\text{H}]^+$ 508.2584.

Dipeptide 1.4:



Use of the acid **1a** (0.5 g, 1.57 mmol) and amine trifluoroacetate salt of Leucine benzylester (0.5 g, 1.57 mmol) in the procedure discussed above (for **1.1**) resulted in 80% yield (0.65 g) of **1.4** as a white solid. Analytical data: R_f : 0.36 (50 % Ethyl acetate- Hexane); mp 72-74 °C; ^1H NMR (CDCl_3 , 400 MHz): 7.82 (s, 1H), 7.73-7.66 (m, 1H), 7.63-7.53 (m, 2H), 7.51-7.45 (m, 1H), 7.40- 7.28 (m, 5H), 6.26 (bs, 1H, NH^2), 5.32 (bs, 1H,

NH¹), 5.21- 5.08 (m, 2H), 4.68- 4.57 (m, 1H), 4.46 (d, 2H, $J = 4.8$ Hz), 1.64- 1.52 (m, 1H), 1.52- 1.45 (m, 2H), 1.43 (s, 9H), 0.87 (d, 6H, $J = 6.2$ Hz); ¹³C NMR (CDCl₃, 100 MHz): 172.2, 165.9, 155.7, 145.6, 135.2, 134.0, 132.2, 131.3, 130.1, 129.3, 128.6 (2C), 128.4, 128.3 (2C), 126.4, 124.4, 79.7, 67.2, 51.4, 40.8, 36.2, 28.4 (3C), 24.7, 22.7, 21.7; IR(neat): 3393, 2961, 1735, 1707, 1654, 1509, 1165 cm⁻¹; HRMS (ESI) exact mass calcd. for C₂₈H₃₅N₅O₅Na [M+Na]⁺ 544.2536, found [M+Na]⁺ 544.2520.

Gelation studies

Gelation study was carried out as discussed in our previous report.¹ In a typical experiment, 25 mg of the gelator was taken in a 5 mL glass vial and 500 μ L of the solvent was added to it. The mixture was gently heated to get a transparent solution, which on cooling to room temperature gave an immobilised gel, which was stable on vial inversion.

Table 1. Gelation behaviour for dipeptides **1.0** to **1.4**; G: gel, S: sol, I: insoluble, P: ppt.

Solvent	1.0 (wt%)	1.4 (wt%)	1.1 (wt%)	1.2 (wt%)	1.3 (wt%)
Toluene	G (0.6)	TG (5.6)	S	S	S
m-xylene	G (0.3)	TG (3.6)	S	S	S
Mesitylene	G (0.1)	TG (1.7)	S	S	S
Tetralin	G	TG (0.9)	S	S	S
Nitrobenzene	S	S	S	S	S
1,2-dichlorobenzene	S	S	S	S	S
Petrol oil	I	TG (0.5)	I	I	I
Diesel oil	I	TG (0.8)	I	I	I
Silicone oil	I	TG (1.2)	I	I	I
Dodecane	I	TG (2.0)	I	I	I
Carbontetrachloride	G (0.08)	TG (1.7)	I	I	S
Methanol	S	S	S	S	S
Ethanol	S	S	S	S	S
IPA	G	S	S	S	S
DMF	S	S	S	S	S
DMSO	S	S	S	S	S
n-Heptane	I	TG (0.1)	I	I	I

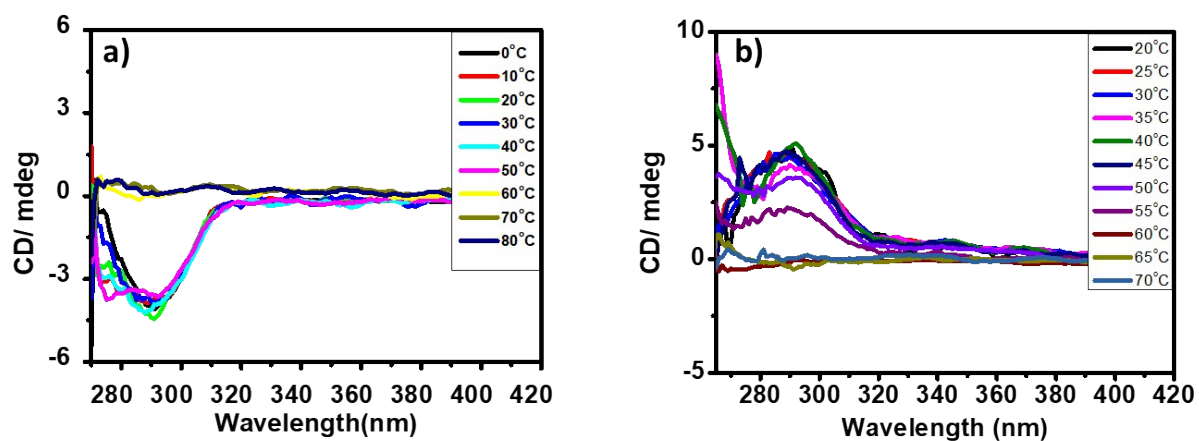


Fig. S1. Relevant region of the VT-CD spectra of **1.0** in CCl_4 : (a) sample with negative cotton effect and (b) sample with positive cotton effect

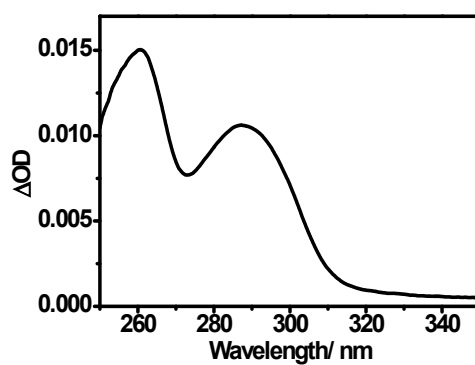


Fig. S2. a) LD spectrum of **1.0** in CCl_4 (0.2 wt%) at 20 °C

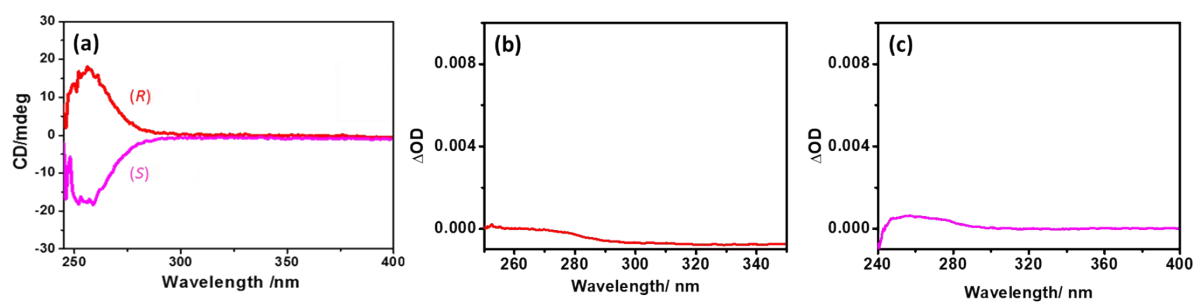


Fig. S3. a) CD spectra of enantiomers of **1.4** in CCl_4 (0.1 wt%); b) LD spectrum of ***R*-1.4** showing negligible orientational effects and c) LD spectrum of ***S*-1.4** showing negligible orientational effects

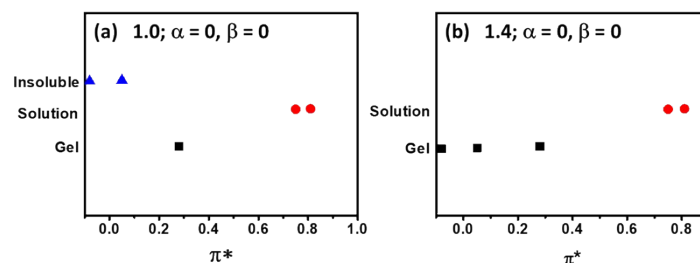


Fig. S4. Gelation behaviour of **1.0** and **1.4** assessed on the basis of kamlet-taft parameters of solvents: a) behaviour of **1.0** towards solvents with $\alpha = 0$; $\beta = 0$; the corresponding data from **1.4**.

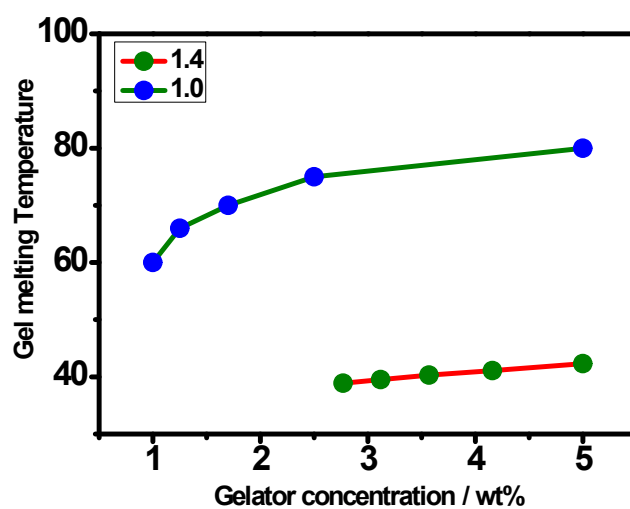


Fig. S5. Variation of gel-melting temperature (mesitylene gel) with increasing concentration of **1.0** and **1.4**.

Table 2. Comparison of gelation window of **1.0** and **1.4**; G: gel, S: sol, I: insoluble, P: ppt.

Solvents	1.0	1.4	Solvents	1.0	1.4	Solvents	1.0	1.4
Methanol	P	S	Acetone	S	S	DMSO	S	S
Ethanol	G	S	cyclohexanone	S	S	DMF	S	S
Isopropanol	G	S	Ethylacetate	S	S	Ethylacetate-hexane(1:1)	G	G
n-heptanol	G	S	n-butylacetate	S	S	Chloroform-hexane(1:1)	G	G
n-dodecanol	G	S	1,2 DME	S	S	Petrol oil	I	G
<i>t</i> -butanol	G	S	THF	S	S	Type 3 oil	I	G
Benzene	G	G	Chloroform	S	S	Coconut oil	I	G
Toluene	G	G	DCM	S	S	Groundnut oil	I	G
Mesitylene	G	G	CCl ₄	G	G	Mixture of oil	I	G
Bromobenzene	G	S	n- Heptane	I	G			
Chlorobenzene	G	S	n- Dodecane	I	G			
Iodobenzene	S	S	Diesel oil	I	G			

PXRD pattern of xerogel of **1.4**:

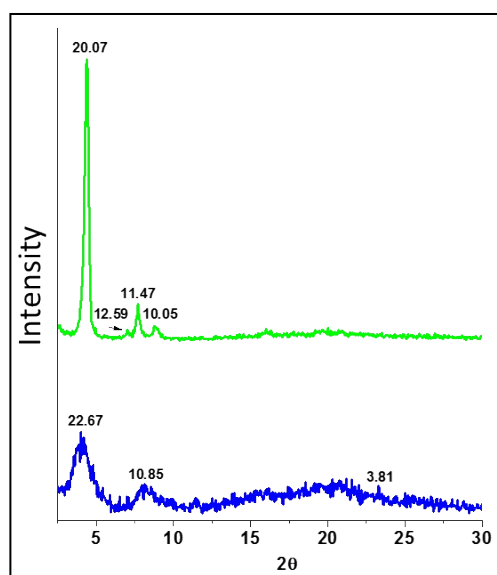


Fig. S6 Comparison of PXRD spectra of **1.4** of solid sample (green) and its xerogel from CCl_4 (blue) (2.5 wt%), The reflection at 2θ of 23.29 supports π - π interaction

Rheological experiments (Flow behaviour of Organogels):

The characterisation of visco-elastic behaviour of gels was done using rheology. In this study we performed two types of experiments, namely strain sweep experiment and frequency sweep experiment. Firstly, for having an idea of the linear visco-elastic region, we performed the strain sweep experiment at the angular frequency of 10 rad/sec (Figure S7a). As can be seen, the storage modulus or elastic modulus G' followed a straight line path and then crossed the loss modulus at a critical strain of 0.09%. The critical strain point (value) can be defined as a point below which gel behaviour is predominant and above which sol behaviour is predominant. Next, we performed the frequency sweep experiment at 0.01% strain (range 0.4 rad/s to 300 rad/s) and found that storage and loss modulus are independent of increase in frequency in this range. The results clearly showed that gels formed from compound **1.4** are real and strong gels ($G' \sim 10^5$) which remain in the gel state over a wide range of frequency (Figure S7b).

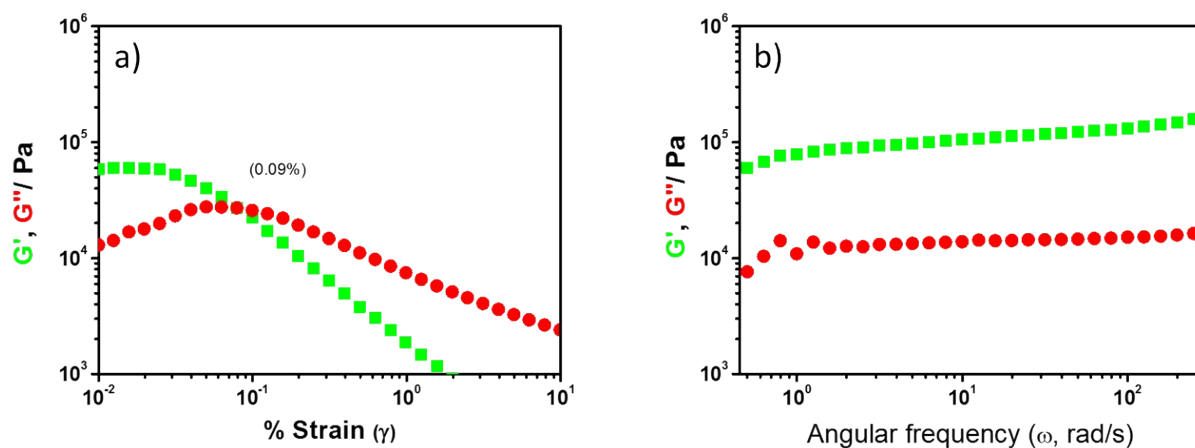


Fig. S7. (a) Amplitude sweep experiment showing gel behavior upto 0.09% strain and then collapse of the gel; (b) Frequency sweep experiment recorded at 0.01% strain, showing independence of storage and loss moduli on applied angular frequency in the range of 0.4 to 110 rad/sec.

Scanning Electron Microscopic images:

Morphological analysis of different xerogels was done using SEM. The SEM images of xerogels of **1.4** from DCM-Hexane (1:1), Mesitylene and Heptane are shown in Figure S8. The fibrillar assembly was observed in all the cases as shown.

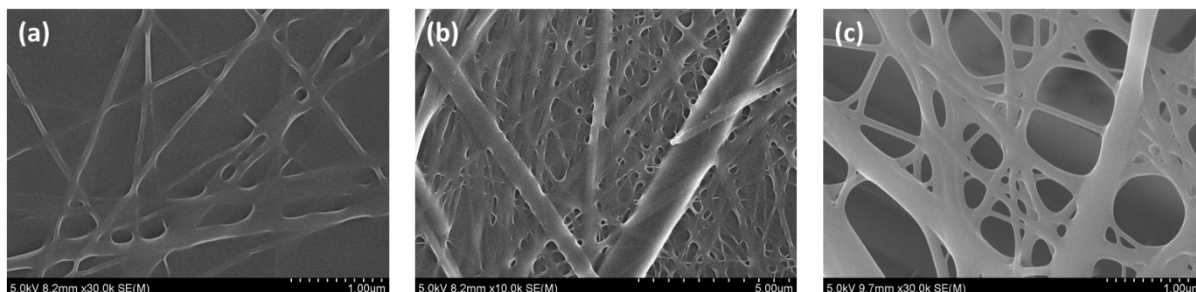


Fig. S8. SEM images of the xerogels of **1.4** from (a) DCM-hexane, (b) Mesitylene, (c) n-Heptane

Self-standing ability mesitylene gel of **1.4** at different concentration:

To find out the minimum gelation concentration required to get the self-standing gel blocks of mesitylene using **1.4**, a series of experiments were conducted by varying the gelator concentration as shown in Figure S9 (50 mg of **1.4** in 1 mL Mesitylene was initially tested and then diluted to get other concentrations). As can be seen, the gel block was self-standing until 2.0 wt% and collapsed on further dilution.

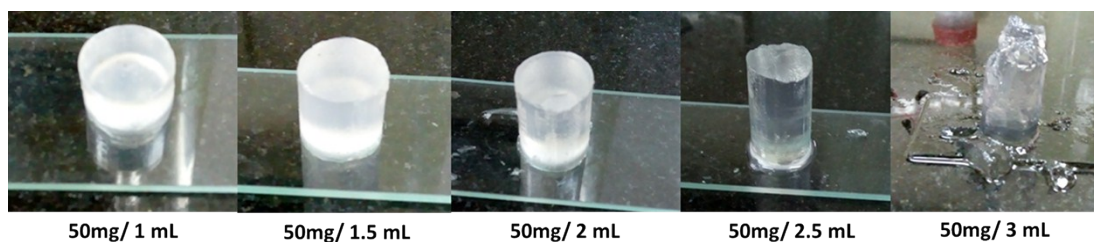


Fig. S9 Demonstration of self-standing property in the Mesitylene gel of **1.4** at different concentrations.

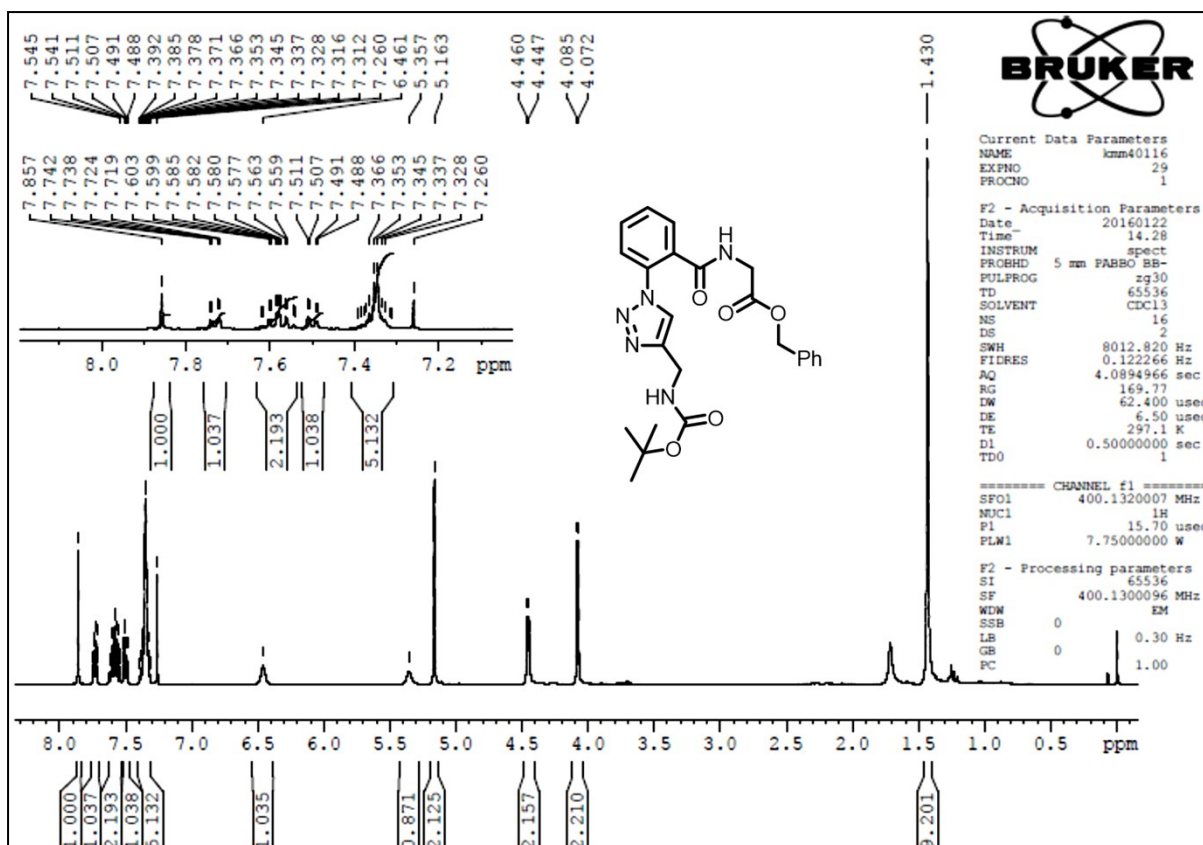


Fig. S10 ^1H NMR (400 MHz) spectrum of **1.1** in CDCl_3

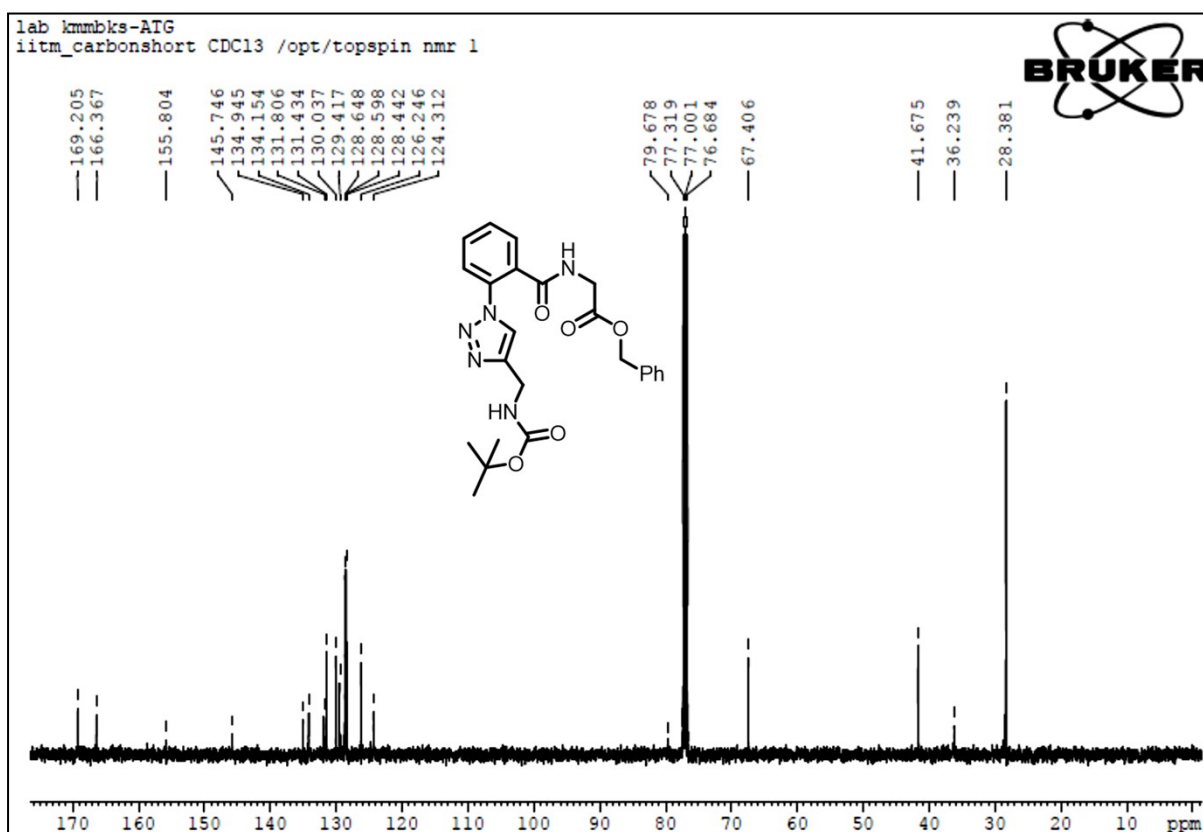


Fig. S11 ^{13}C NMR (100 MHz) spectrum of **1.1** in CDCl_3

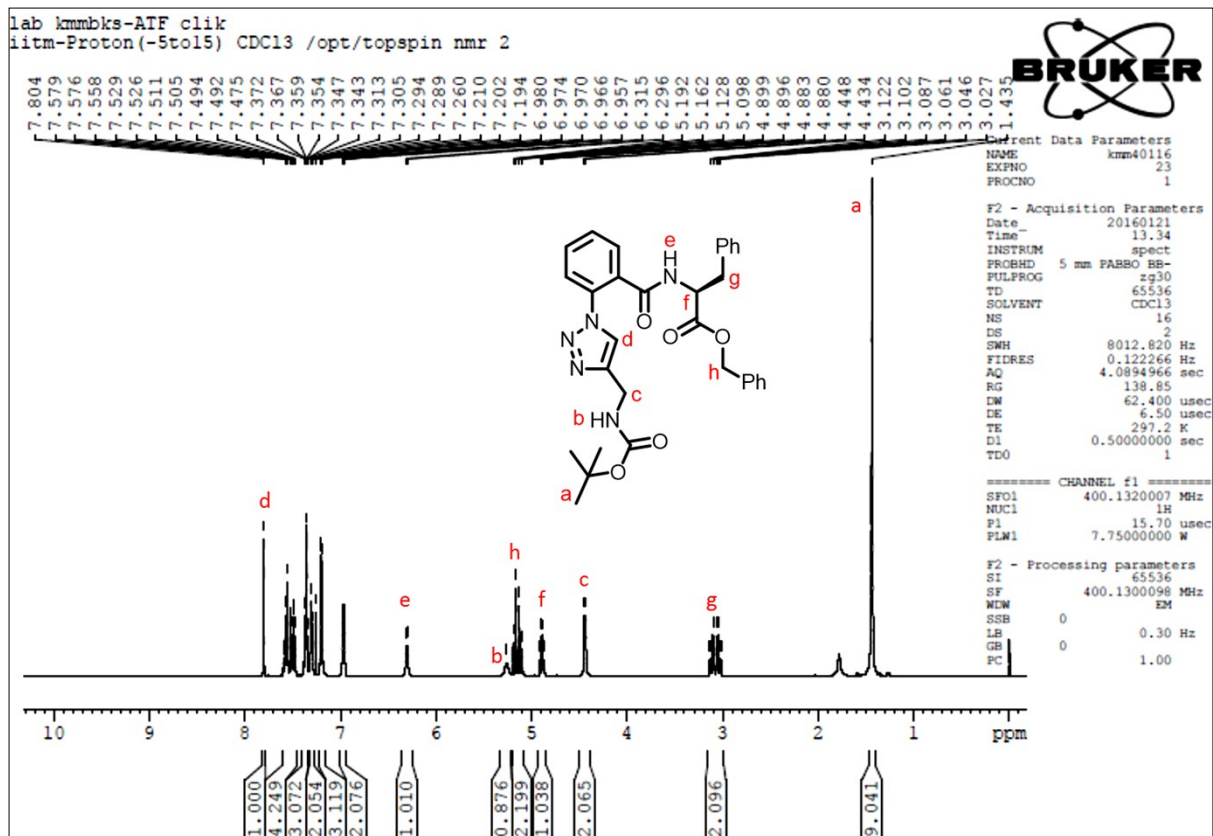


Fig. S12 ^1H NMR (400 MHz) spectrum of **1.2** in CDCl_3

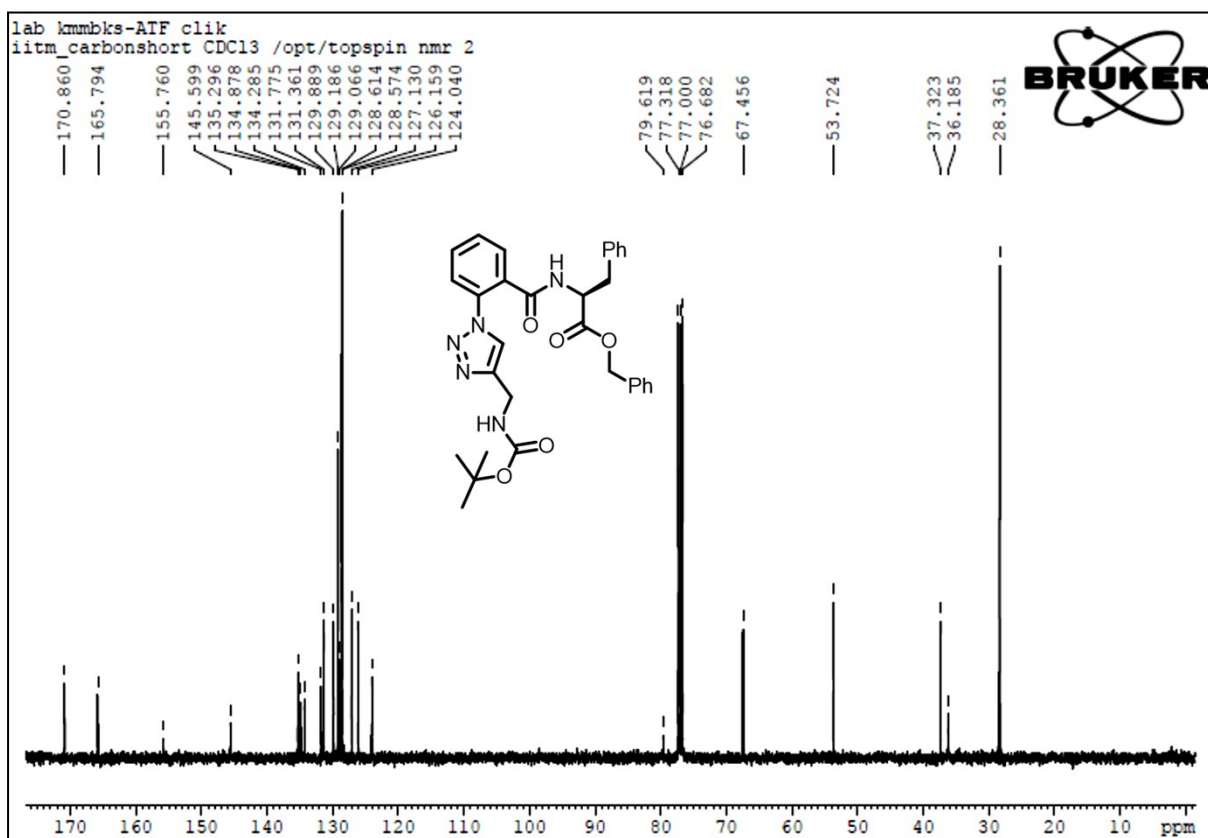


Fig. S13 ^{13}C NMR (100 MHz) spectrum of **1.2** in CDCl_3

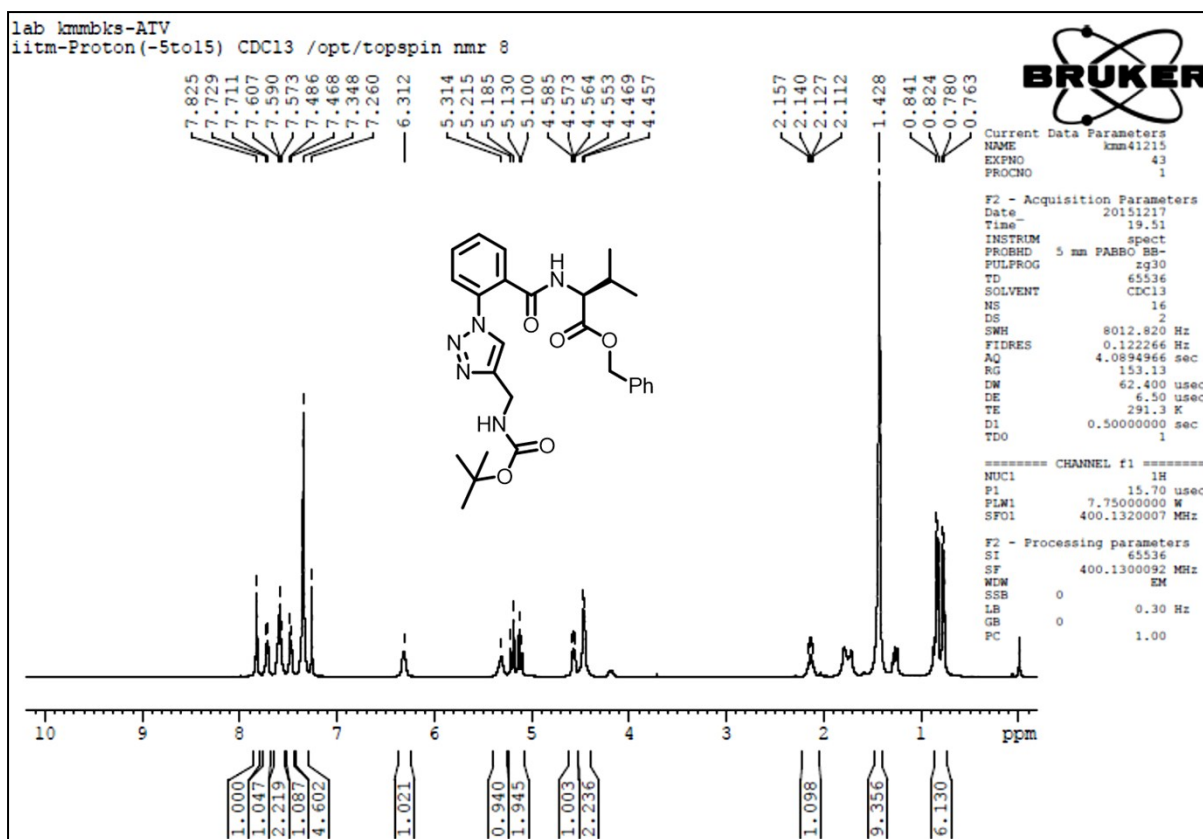


Fig. S14 ^1H NMR (400 MHz) spectrum of **1.3** in CDCl_3

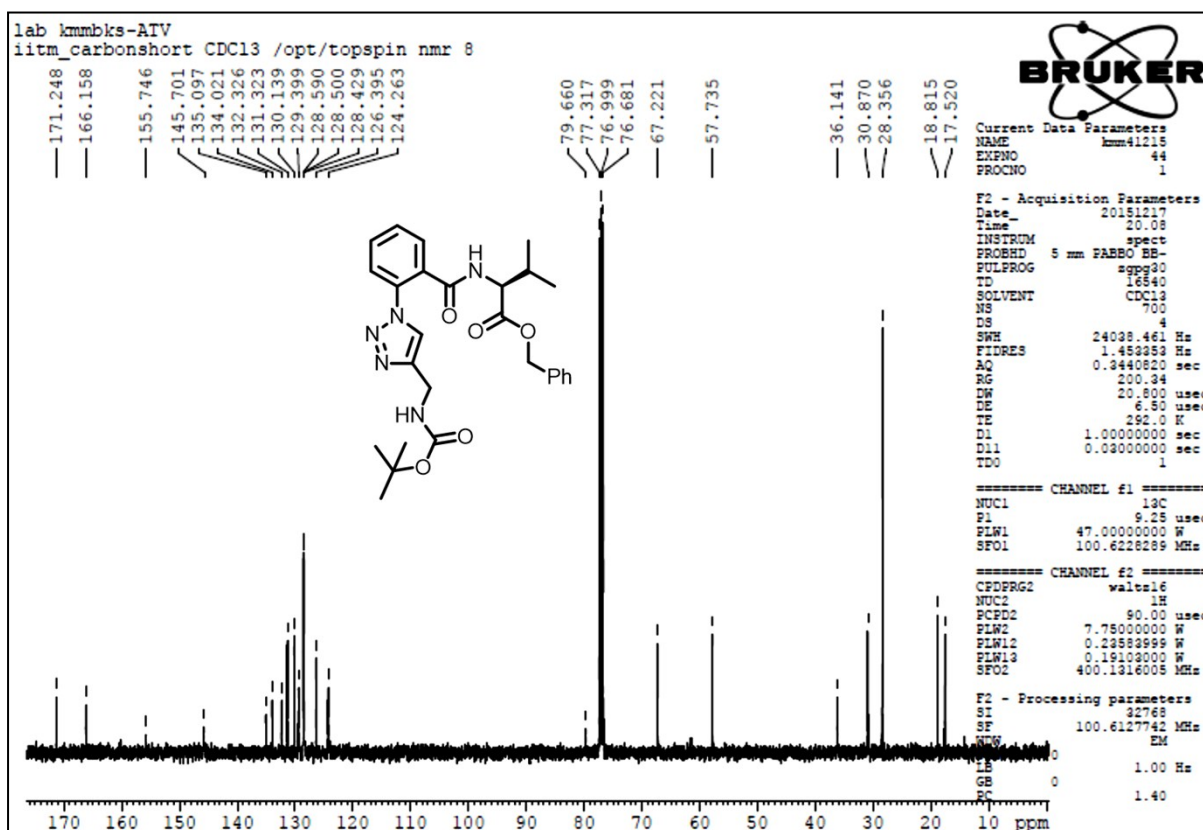


Fig. S15 ^{13}C NMR (100 MHz) spectrum of **1.3** in CDCl_3

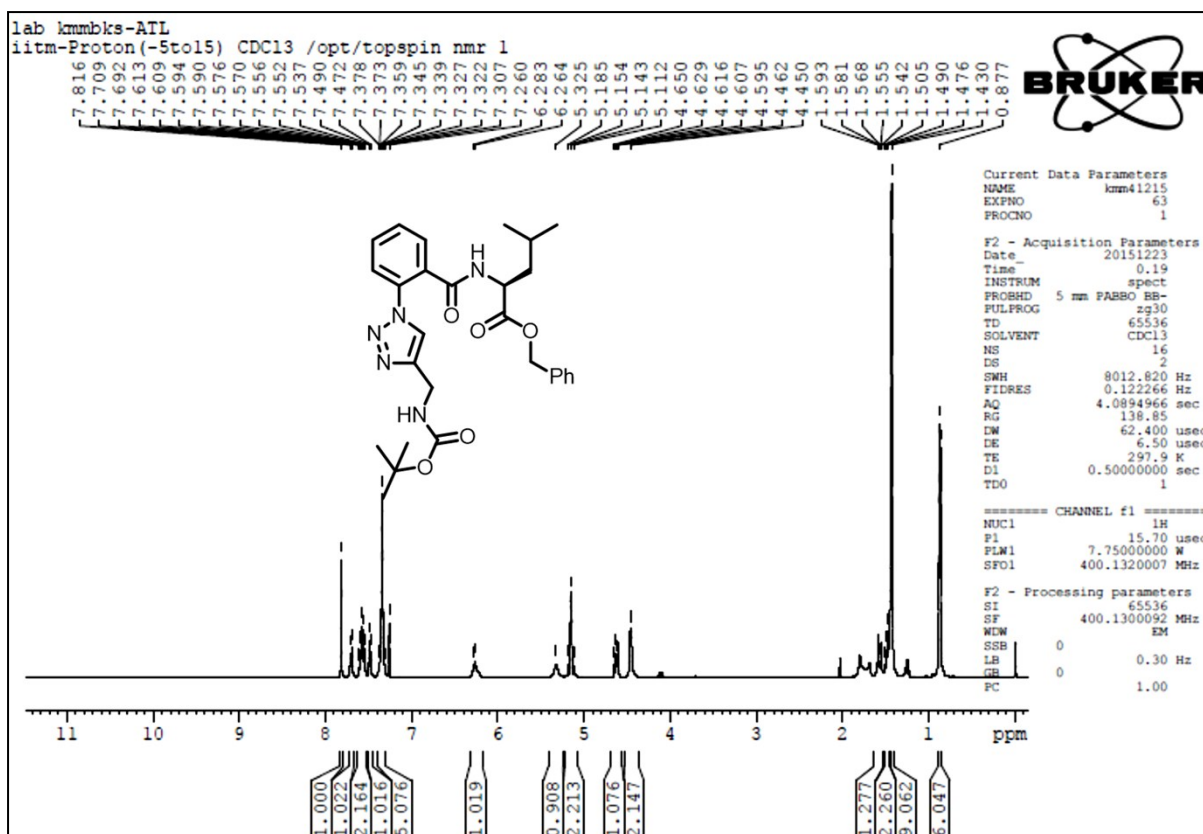


Fig. S16 ^1H NMR (400 MHz) spectrum of **1.4** in CDCl_3

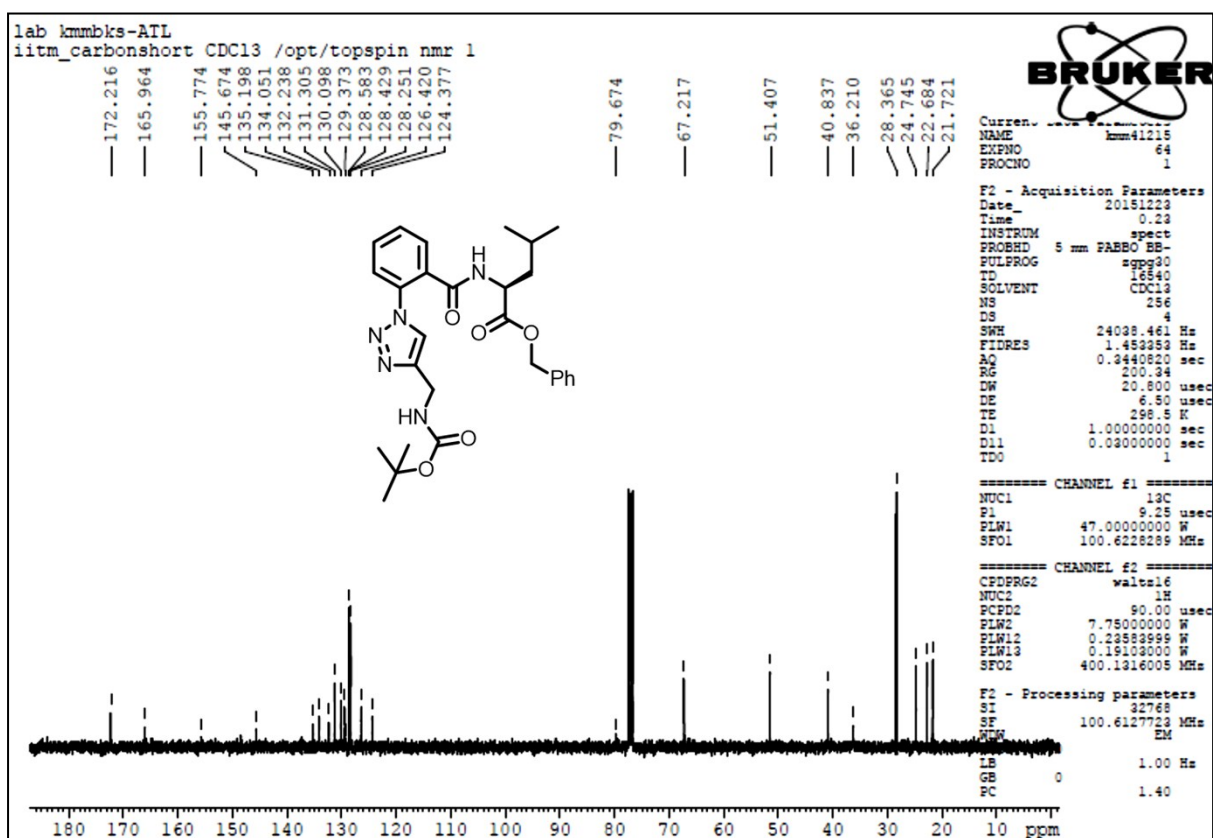


Fig. S17 ^{13}C NMR (100 MHz) spectrum of **1.4** in CDCl_3

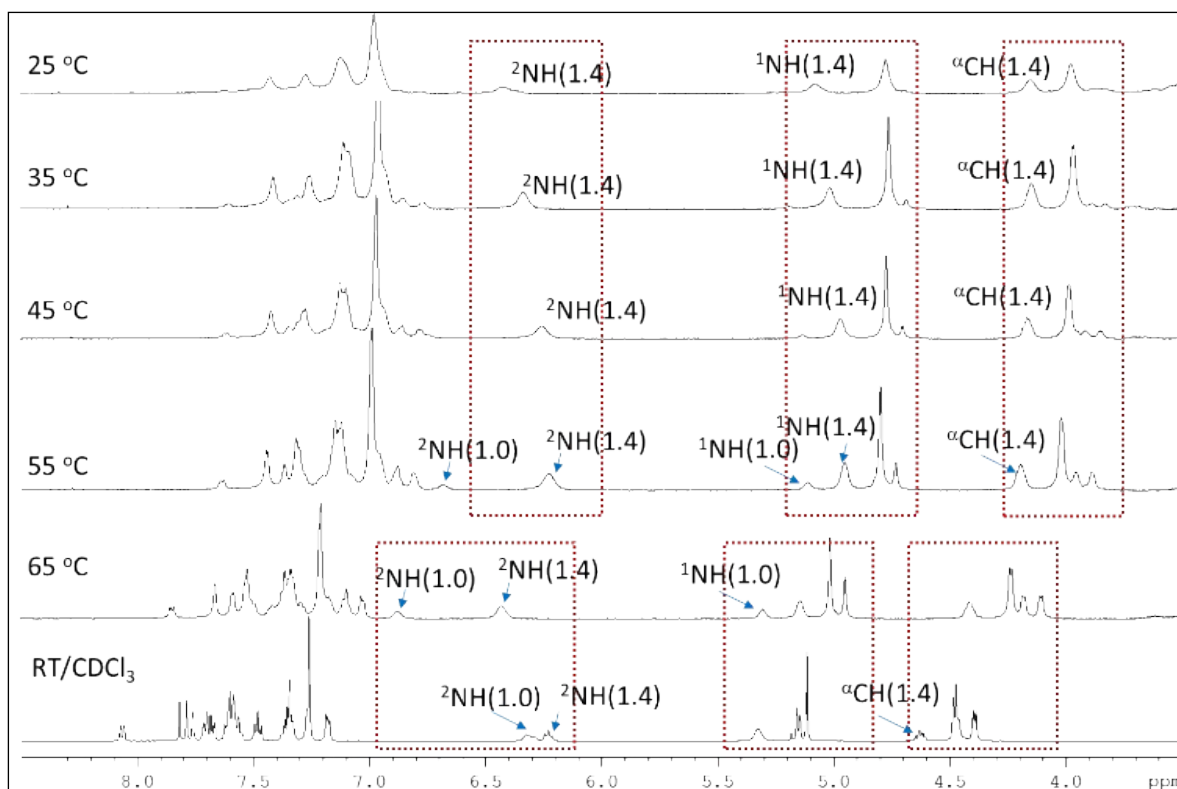


Fig. S18. Temperature dependent ^1H NMR of a 1:1 mixture of 1.0 and 1.4 showing gelator network formation predominantly from 1.0 at lower temperature.

Supporting video:

- 1) Supporting video 1 is included which shows the effect of mechanical disturbance on shape persistence of a self-healed material made from Tetralin gel of **1.4**.

References:

- 1) B. K. Srivastava and M. K. Manheri, *RSC. Adv.*, 2016, **6**, 29197-29201.