Electronic Supplementary Information (ESI)

NMR Detection of chirality and enantiopurity for amines by using benzene tricarboxamide-based hydrogelators as chiral solvating agents

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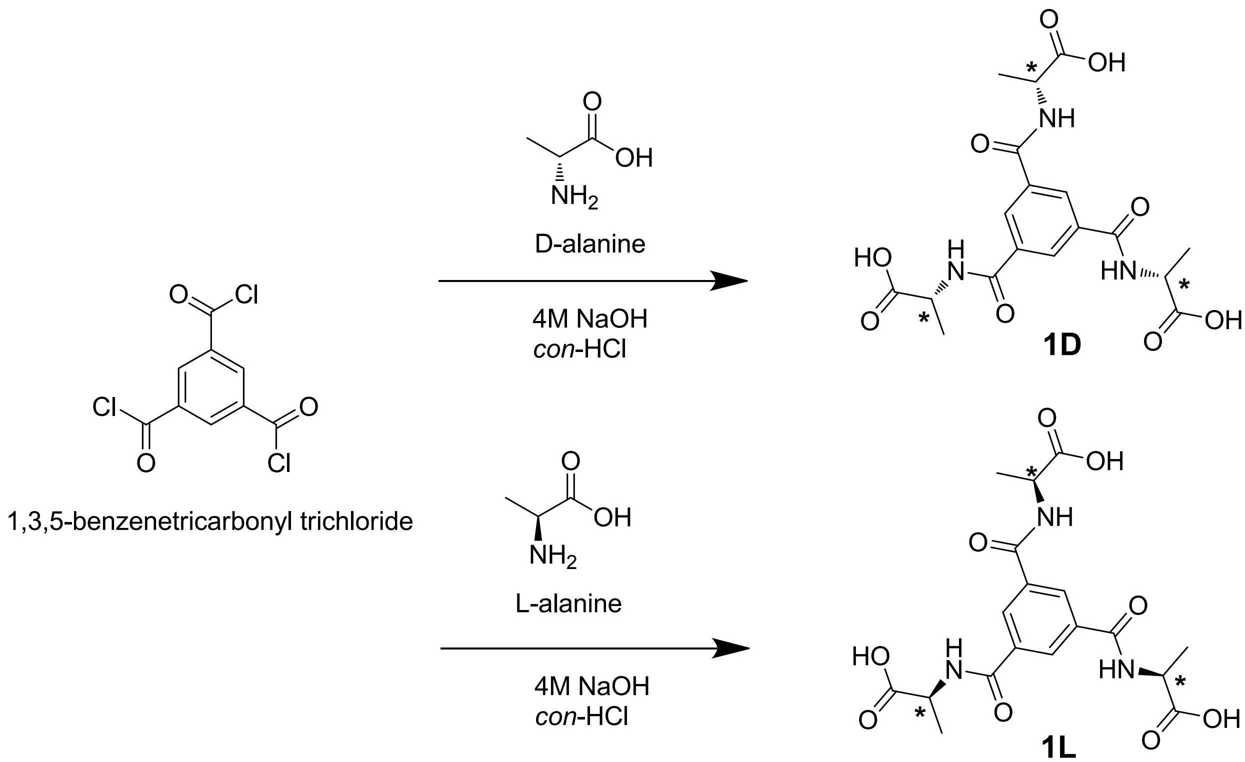


Scheme S1. Synthesis of **1D** and **1L**.

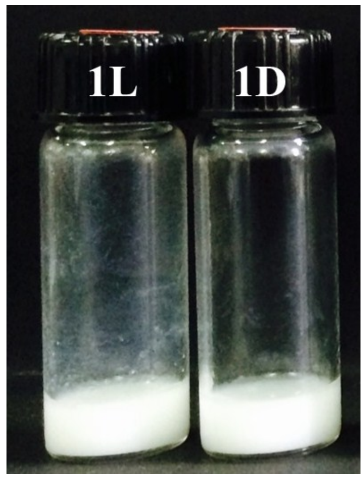


Fig. S1 Photograph of gelation test of gelator **1L** (left) and **1D** (right) in water (1.0 wt%).

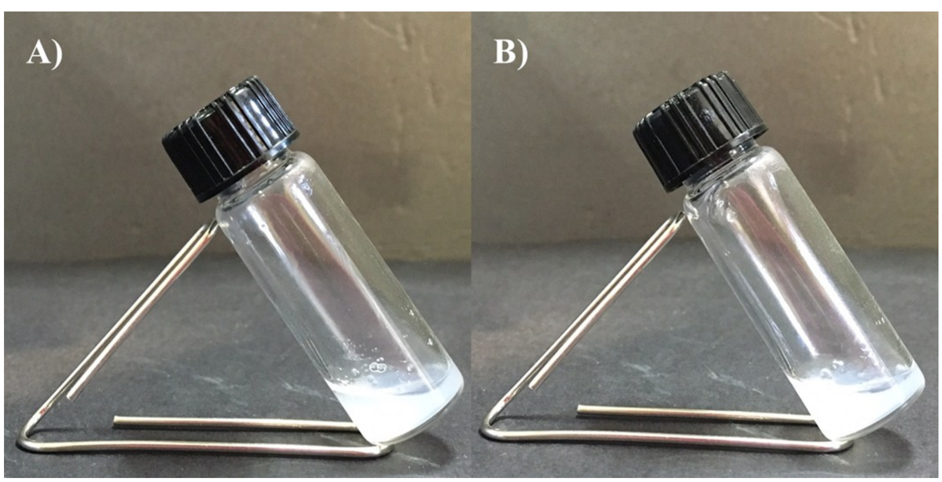


Fig. S2 Photograph of gelation test of gelator **1L+4R** (left) and **1D+4S** (right) D_2O and DMSO-d_6 mixtures (1.0 wt%).

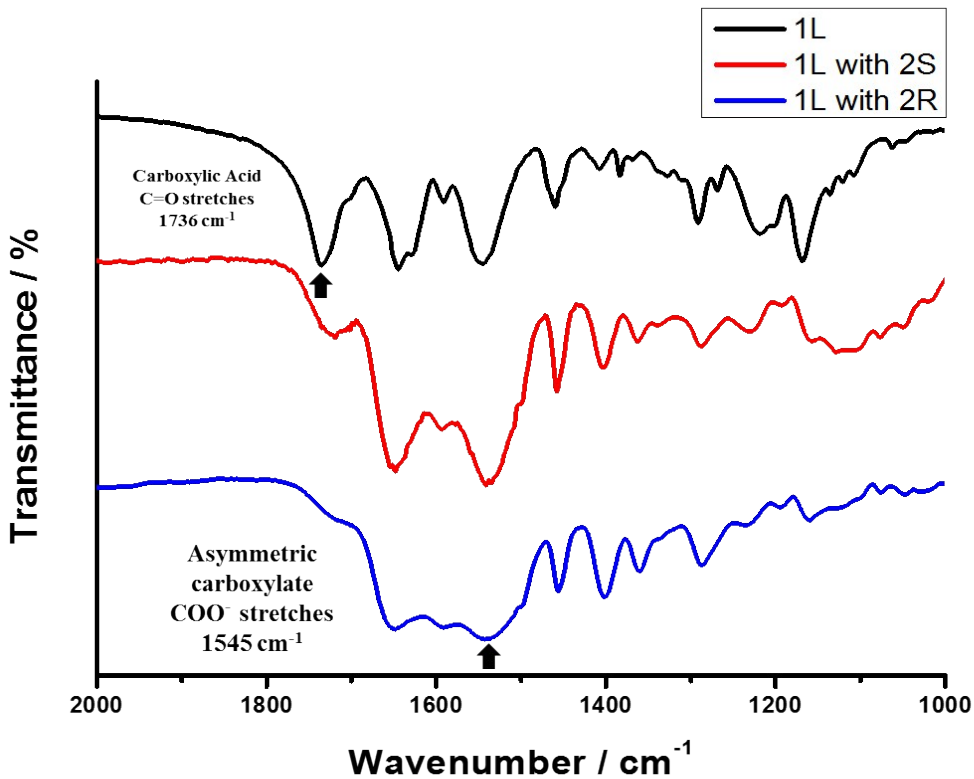


Fig. S3 IR spectra of **1L**, **1L** with **2S** and hydrogel of **1L** with **2R**.

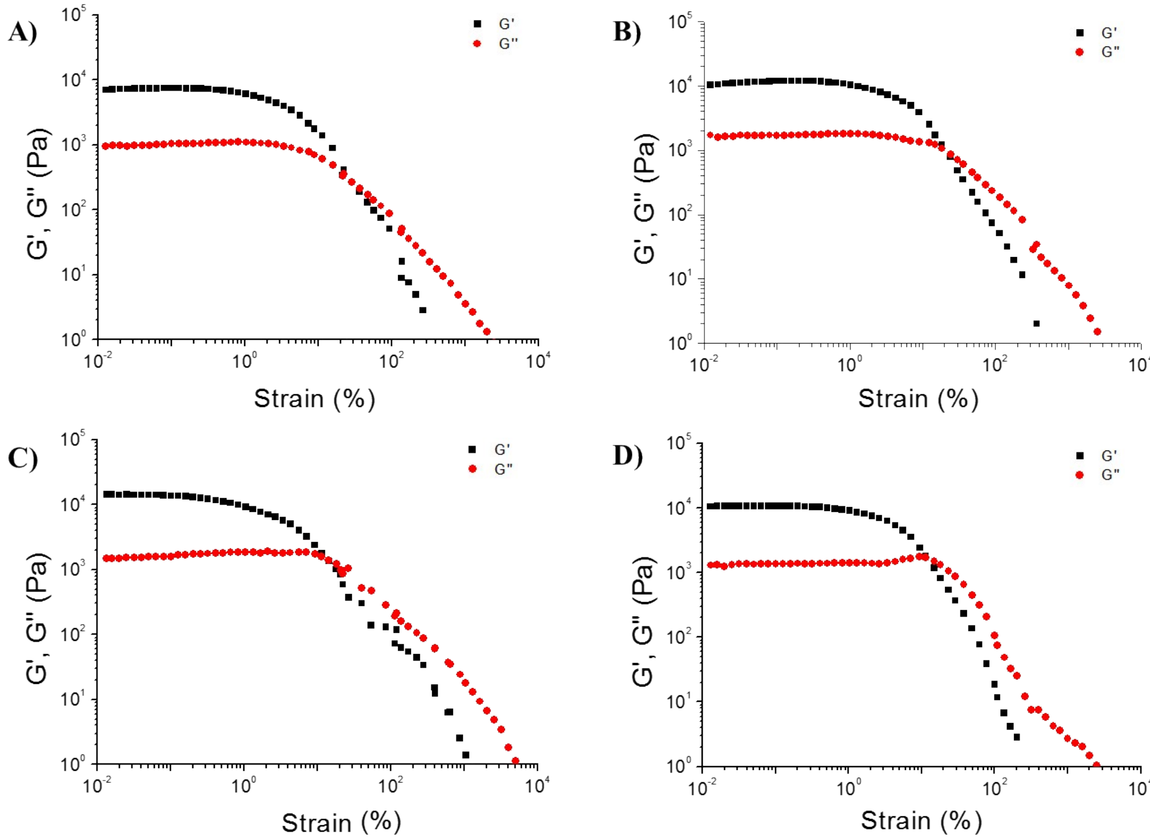


Fig. S4 Measurements of strain sweep tests at a strain of 0.1 to 1.0% for (A) **1L+2R** (1.5 equiv.) hydrogel, (B) **1D+2S** (1.5 equiv.) hydrogel, (C) **1L+2R** (3.0 equiv.) hydrogel and (D) **1D+2S** (3.0 equiv.) hydrogel.

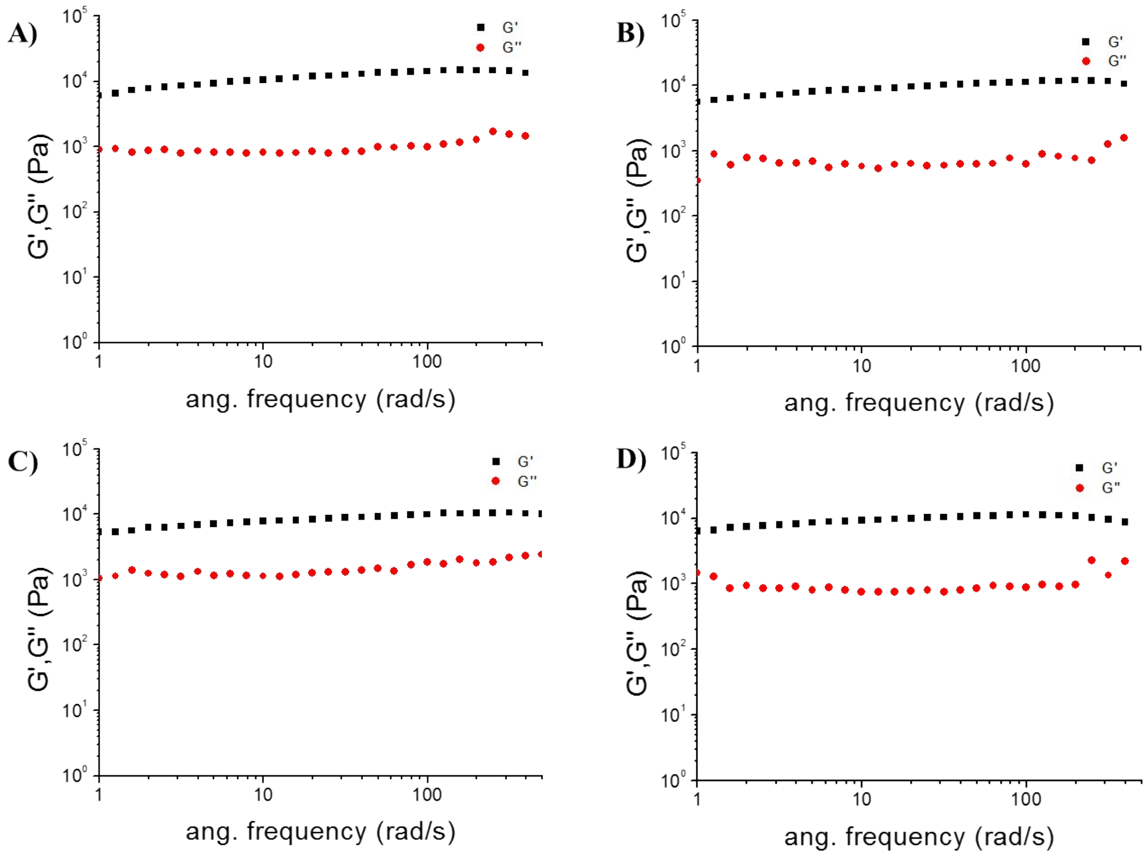


Fig. S5 Frequency sweep tests (from 0.1 to 100 rad/s) for (A) **1L+2R** (1.5 equiv.) hydrogel, (B) **1D+2S** (1.5 equiv.) hydrogel, (C) **1L+2R** (3.0 equiv.) hydrogel and (D) **1D+2S** (3.0 equiv.) hydrogel.

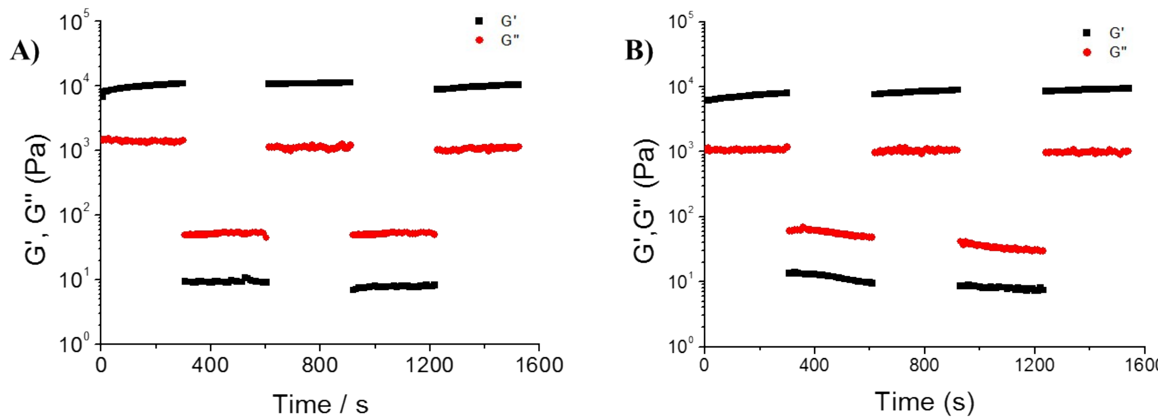
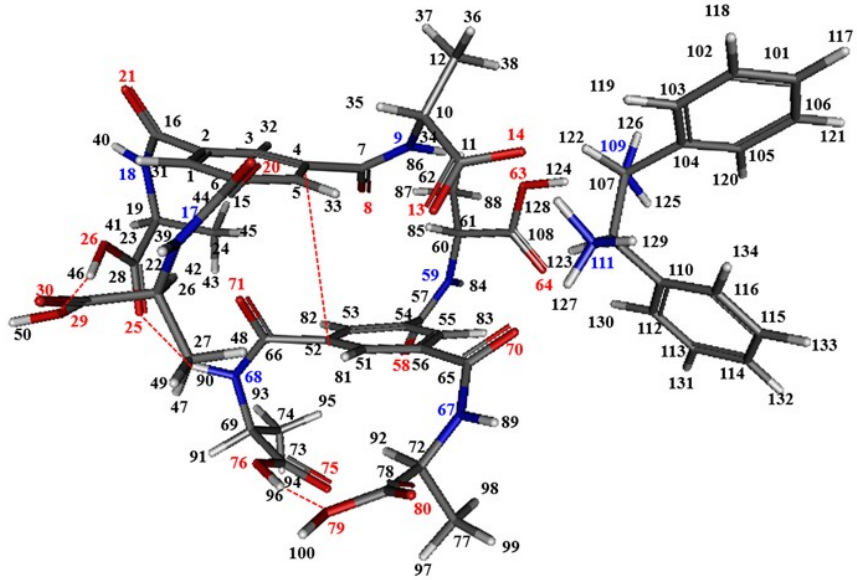


Fig. S6 Continuous step strain measurements for (A) **1L+2R** (1.5 equiv.) hydrogel and (B) **1D+2S** (1.5 equiv.) hydrogel.

A)



B)

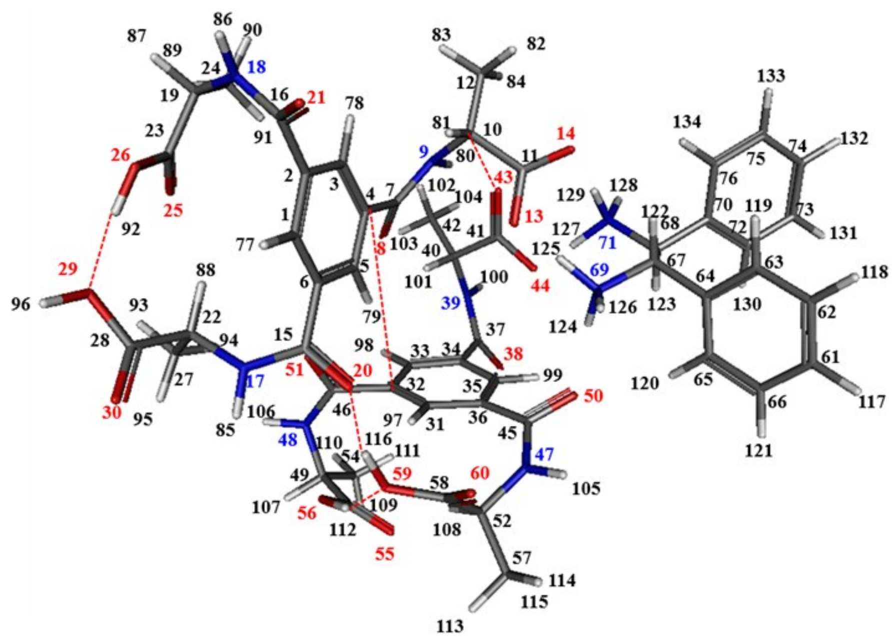


Fig. S7 Molecular structures and atom numbering of (A) **1L+2R** and (B) **1L+2S** as predicted using DFT calculations.

Table S1. Calculated relative energy (kcal/mol), bond lengths (Å) and bond angles (°) of **1L+2R** and **1L+2S** based on optimization at the B3LYP/6-31+G(d) level.

Relative energy (kcal/mol)	1L-2R	1L-2S
	10.09	0
Bond length (Å)	**1L-2R**	**1L-2S**
H124-N109	1.53	
O14-H128	1.18	
O70-H127	1.8	
H96-O79	1.8	
O29-H46	1.76	
O25-H90	1.96	
C52-C4	4.27	
O70-H123	2.61	
O50-H124		1.81
O14-H129		1.68
O20-H116		1.57
O43-H80		1.91
O59-H112		1.71
029-H92		1.78
C32-C4		5.12
O14-H123		4.45
Bond angles (°)	**1L-2R**	**1L-2S**
O14-H128-N111	167.69	
O70-H127-N111	146.39	
H124-N109-H126	107.78	
H46-O29-H50	116.08	
O25-H90-N68	148.92	
H96-O79-H100	118.21	
O14-H129-N71		173.33
O50-H124-N69		145.41
H92-O29-H96		117.51
O20-H116-O59		154.75
O43-C10-H81		152.8
O59-H112-O56		153.72

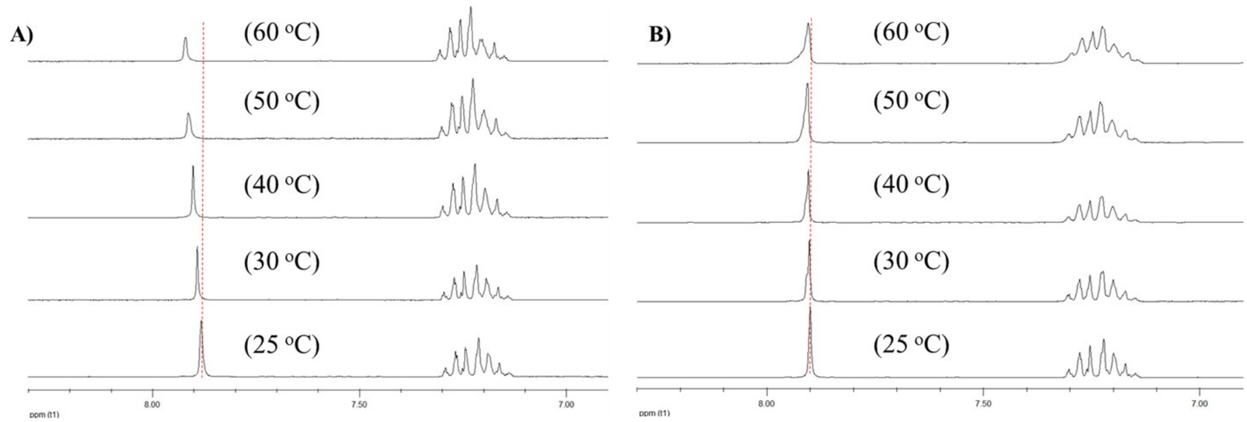


Fig. S8 Variable temperature (VT) ^{1}H NMR spectra of (A) **1L** with **2R** and (B) **1L** with **2S** as temperature increases in D_2O and DMSO-d_6 mixtures. The left singlet correspond to the aromatic protons of gelator **1L** which experience shielding upon aggregation at lower temperatures, while the complex multiplet on the right corresponds to the aromatic protons of **2R** (for sub-figure A) or **2S** (for sub-figure B).

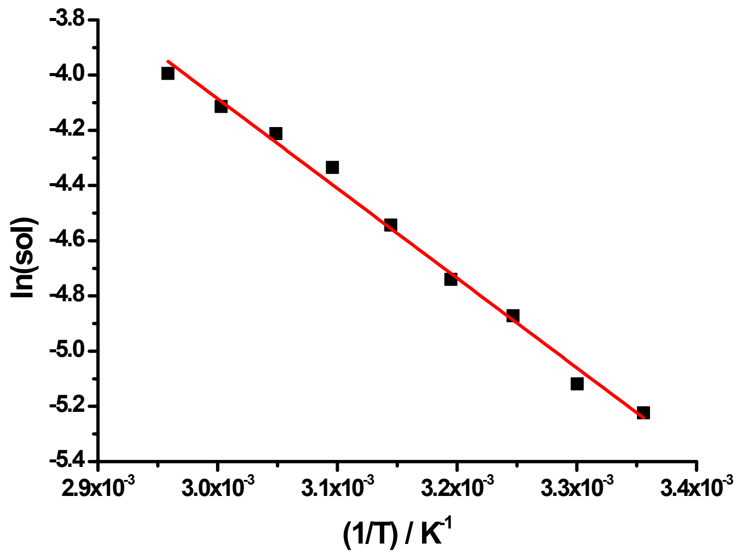


Fig. S9 Van‘t Hoff plots of hydrogel (**1L**+**2R**).

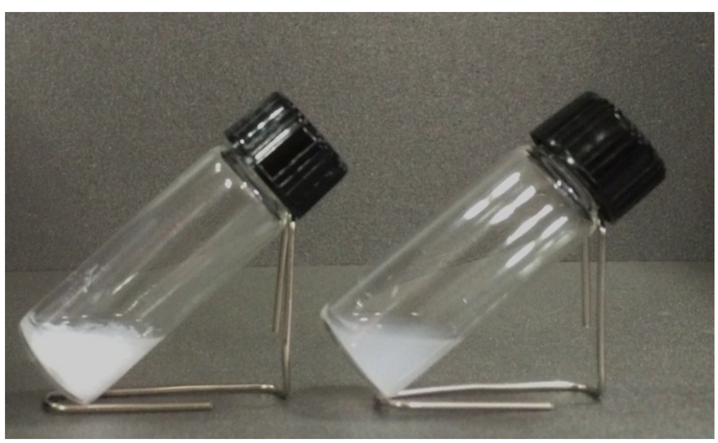


Fig. S10 Photograph of gelation test of (left) gelator **1L** and (right) **1L** with racemic mixture of **2R** (0.75 equiv.) and **2S** (0.75 equiv.) in water (0.1 wt%).

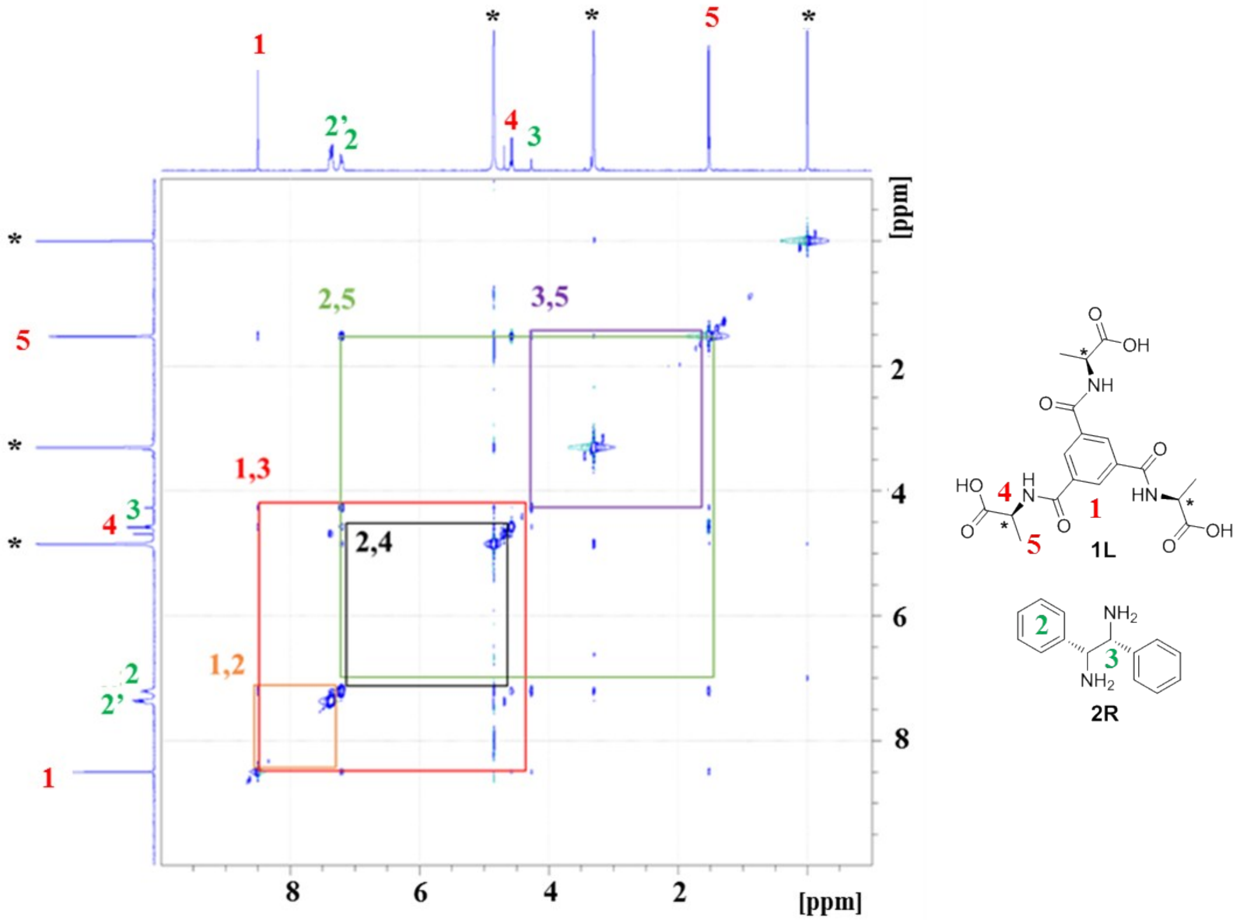


Fig. S11 2D NOESY spectrum (500 MHz, CD_3OD, 323 K) of **1L** (2.0 mM) with **2R** (1.5 equiv.).

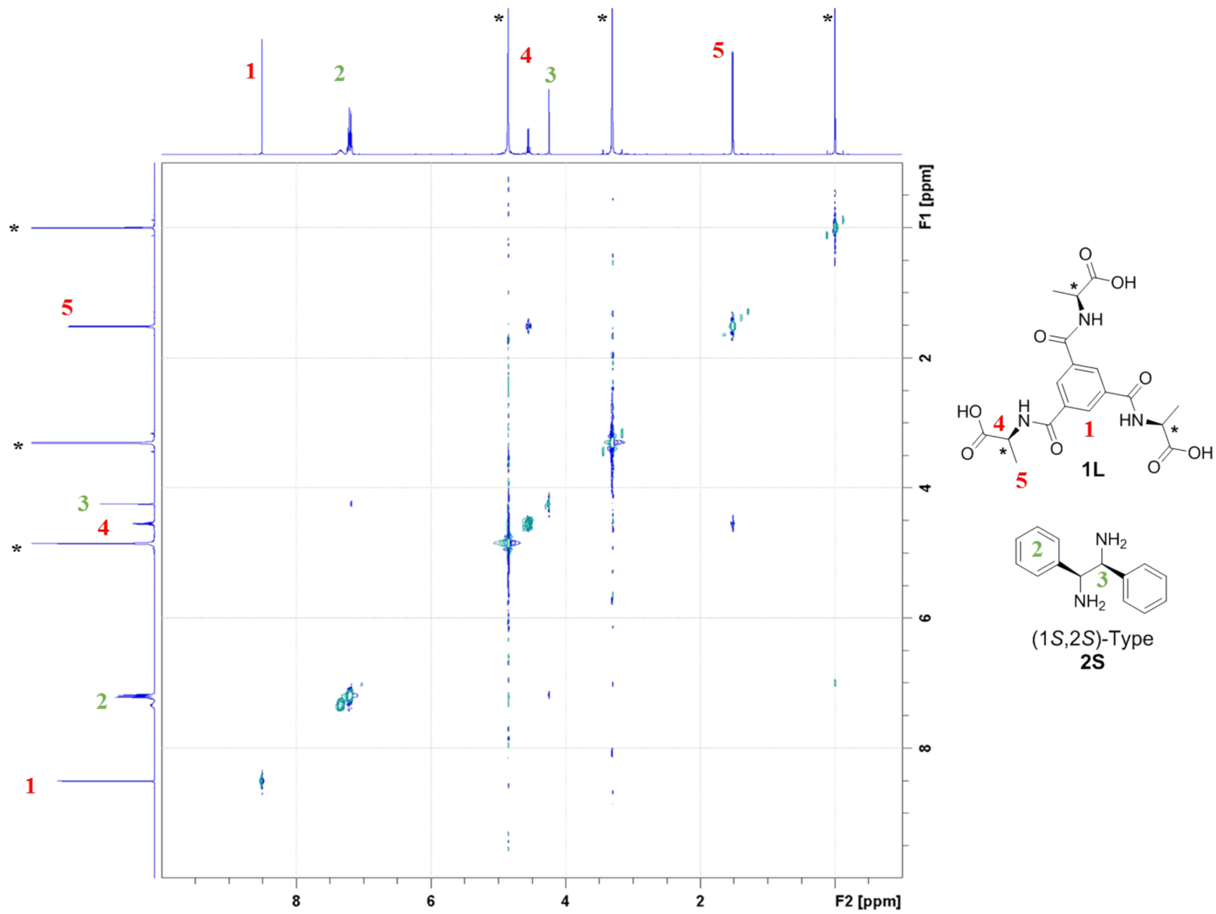


Fig. S12 2D NOESY spectrum (500 MHz, CD_3OD, 323 K) of **1L** (2.0 mM) with **2S** (1.5 equiv.) showing no significant through space coupling between the gelator and the diamine.

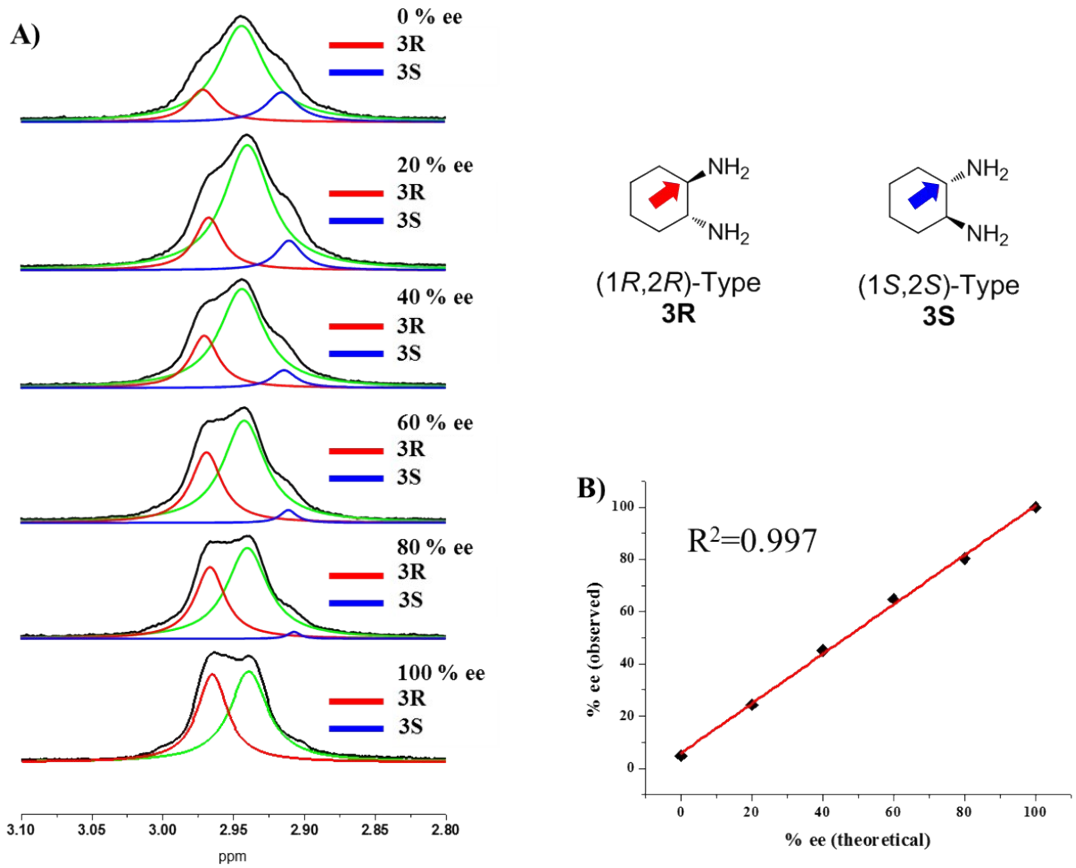


Fig. S13 (A) A selected region of 300 MHz ^{1}H NMR of gelator **1L** (20 mM) with various enantiomeric excess (% ee) in the presence of various mixtures of **3R** and **3S** (30 mM) in D_2O/DMSO-d_6 (5/1 v/v%); green curves present mixture of proton of **3R** and **3S** amines. (B) Correlation between the theoretical and observed % ee values.

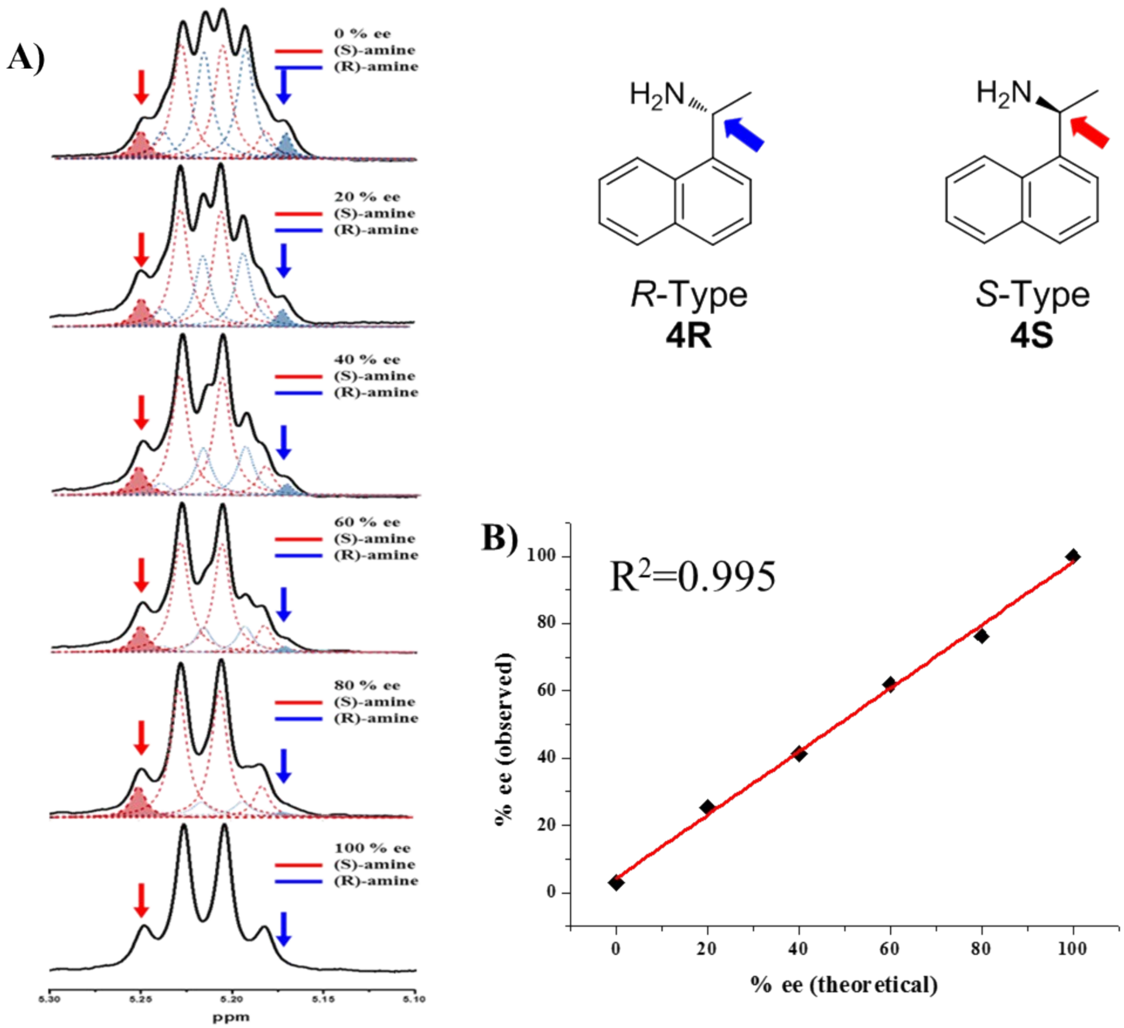


Fig. S14 (A) A selected region of 300 MHz ^{1}H NMR of gelator **1L** (20 mM) with various enantiomeric excess (% ee) in the presence of various mixtures of **4S** and **4R** (30 mM) in D_2O/DMSO-d_6 (5/1 v/v%). (B) Correlation between the theoretical and observed % ee values.

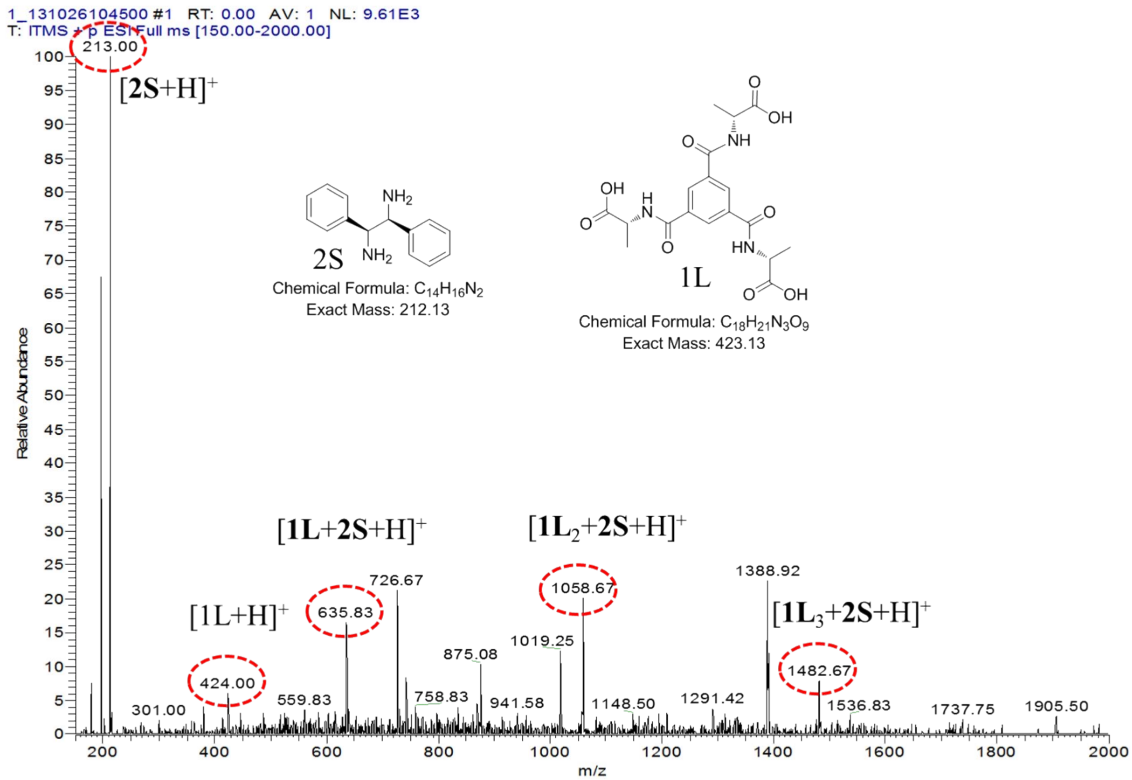


Fig. S15 ESI-mass spectrum of obtained precipitation from mixtures of **1L** with **2S**.

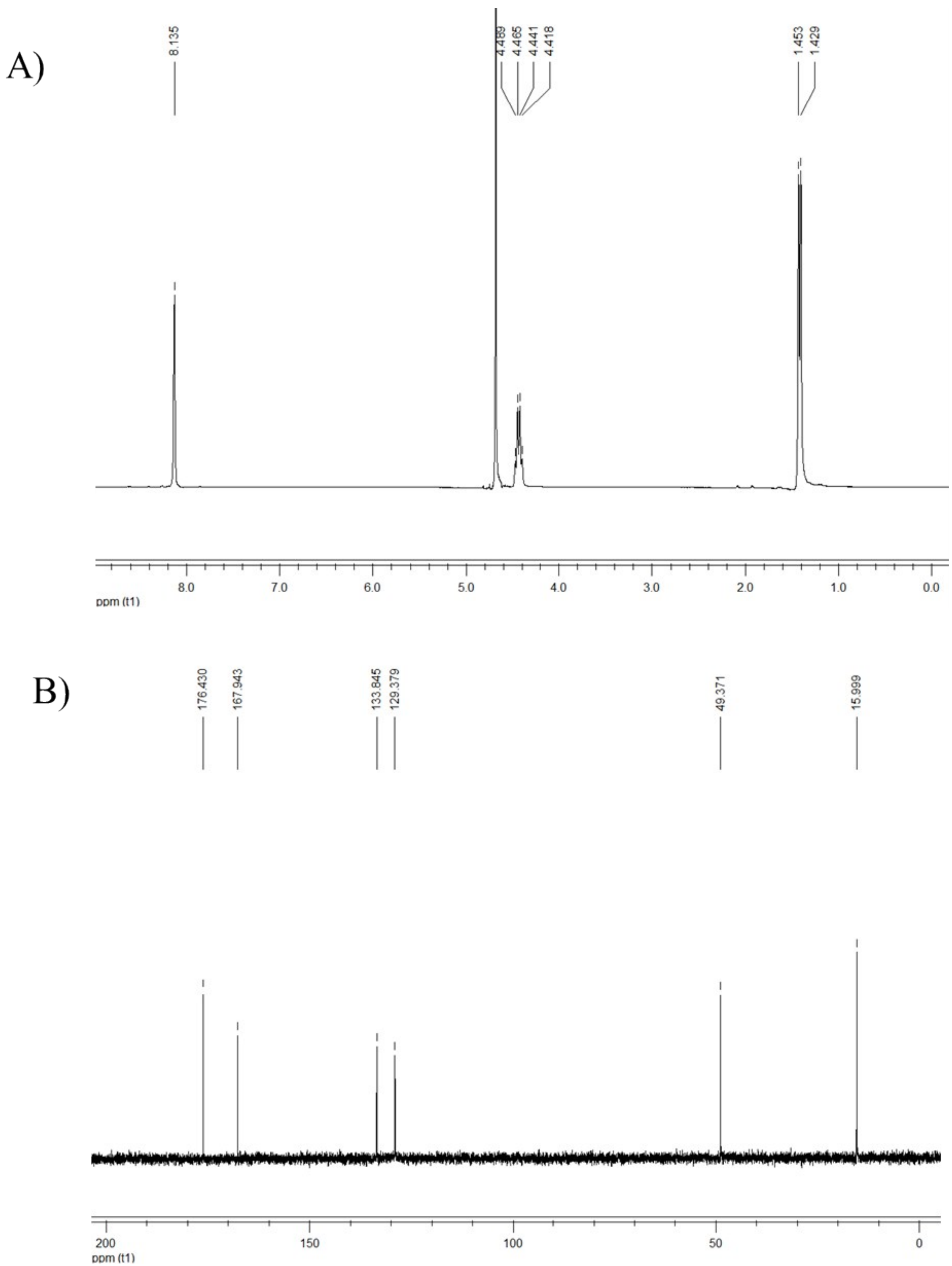
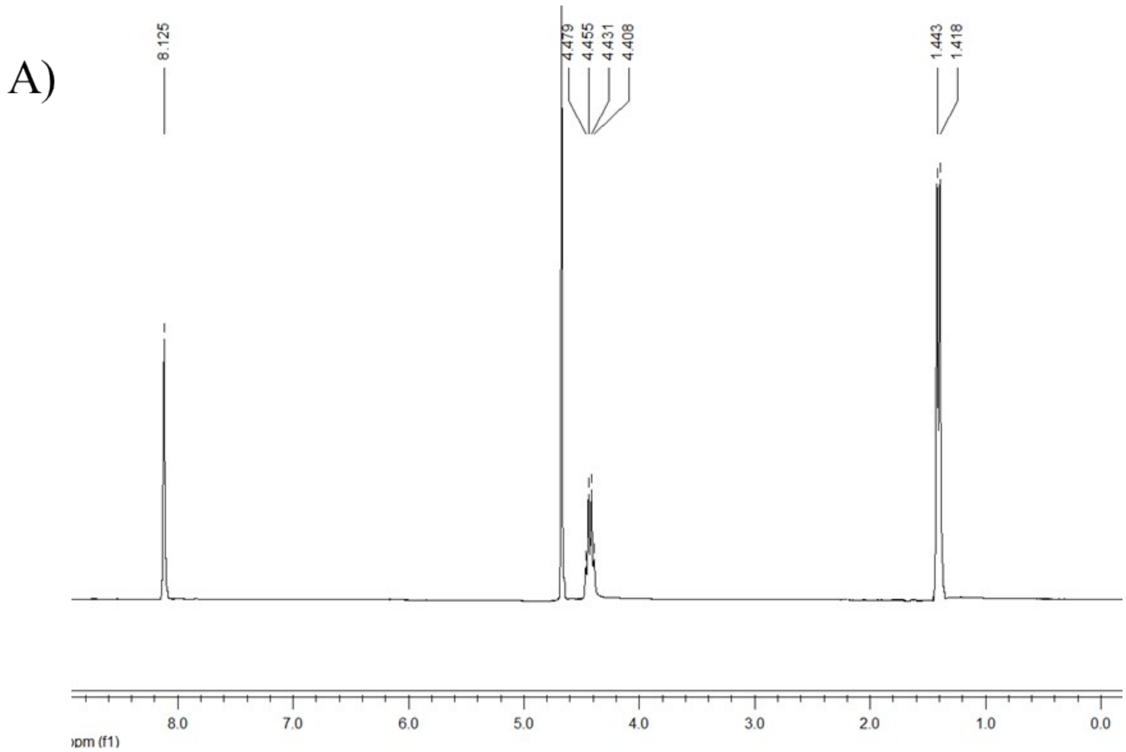


Fig. S16 (a) ^{1}H NMR spectrum of **1D** (300 MHz, D_2O). (b) ^{13}C NMR spectrum of **1D** (75 MHz, D_2O).



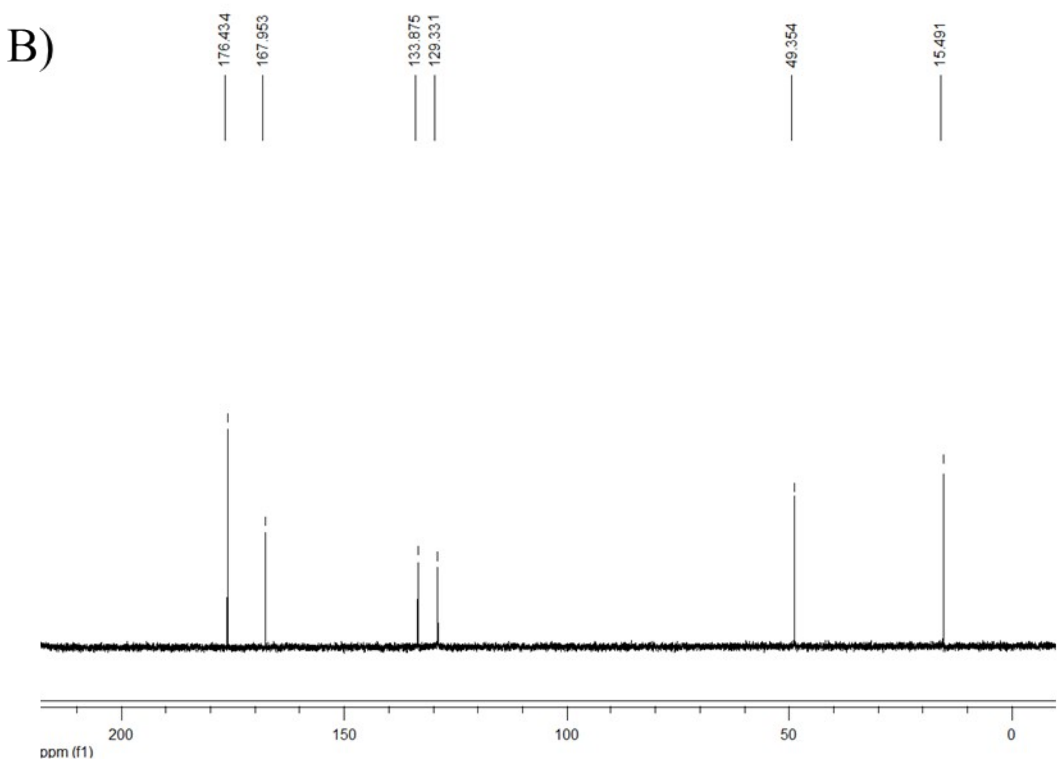


Fig. S17 (a) ^{1}H NMR spectrum of **1L** (300 MHz, D_2O). (b) ^{13}C NMR spectrum of **1L** (75 MHz, D_2O).