

Supporting Information

Molecular Motifs Encoding Self-Assembly for Peptide Fibers into Molecular Gels

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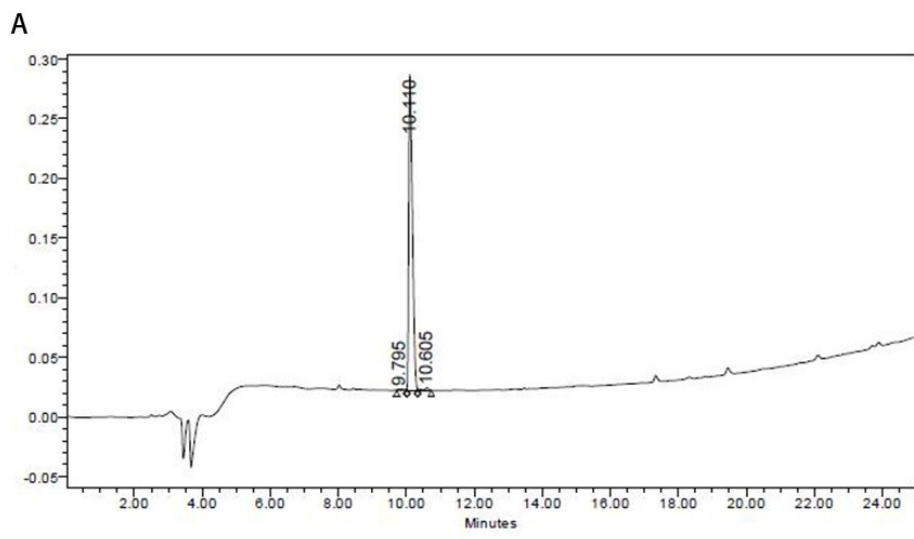
Scanning Colorimetry (DSC)

Methods:

DSC8000 differential scanning calorimeter (DSC) (Perkin-Elmer, Waltham, MA, USA) was utilized to measure the phase transition of the gels. The DSC chamber was pre-cooled to 20 °C with a nitrogen flush (50ml/min). 6 to 10 mg of gel was sealed in stainless steel pans (Perkin-Elmer, Waltham, MA, USA) with built-in torque for improved seals. Samples were heated to 180 °C at 5 °C/min, then held isothermally for 10 min, and then were cooled down to 20 °C at 5 °C/min. GraphWare software Pyris 11.0 was used to integrate the transition peaks to determine the onset melting temperature.

Table S1. Hansen coordinates ($\text{MP}_a^{1/2}$) for the center of the solution, gel and precipitate spheres, as well as the radius ($\text{MP}_a^{1/2}$) for each gelator sphere.

Gelator No.	Center of solution sphere				Center of gel sphere				Center of precipitate sphere			
	$2\delta_d$	δ_p	δ_h	R	$2\delta_d$	δ_p	δ_h	R	$2\delta_d$	δ_p	δ_h	R
L-LL	33.60	9.60	24.00	19.51	31.60	5.70	11.80	4.62	32.80	8.80	3.70	9.78
L-FF	35.40	13.70	17.90	8.65	32.80	8.70	11.50	5.61	31.10	8.00	21.15	22.62
L-YY	36.80	9.75	17.30	12.40	31.39	13.17	23.98	18.50	33.10	1.55	2.85	4.10
L-WW	35.20	11.70	23.80	19.33	NA	NA	NA	NA	30.86	7.86	6.43	10.15
D-FFF	36.10	7.80	8.20	3.95	32.10	15.75	14.65	8.97	31.10	8.00	21.15	22.62
D-FF	36.40	9.20	15.70	10.78	31.10	12.05	11.25	7.89	31.10	8.00	21.15	22.62
L-LLL	36.40	9.20	15.65	10.78	NA	NA	NA	NA	31.10	8.00	21.15	22.62
L-FFF	36.38	9.21	15.65	10.78	31.10	12.05	11.25	7.89	31.10	8.00	21.15	22.62
L-YYY	35.20	11.70	23.80	19.30	NA	NA	NA	NA	31.90	2.59	3.54	4.56
L-WWW	35.19	11.71	23.80	19.33	NA	NA	NA	NA	33.30	1.55	2.85	4.10
C-L-LL	35.90	11.80	9.43	4.68	34.70	7.30	13.10	13.44	31.30	8.23	21.06	22.62
C-L-FF	NA	NA	NA	NA	NA	NA	NA	NA	31.10	8.00	21.15	22.62
C-L-YY	35.90	11.80	9.43	4.68	31.61	11.10	29.34	13.90	32.29	5.65	12.94	14.22
C-L-WW	36.40	9.20	15.65	10.78	NA	NA	NA	NA	31.10	8.00	21.15	22.62
C-D-FF	NA	NA	NA	NA	NA	NA	NA	NA	31.10	8.00	21.15	22.62



	RT	Area	% Area	Height
1	9.795	12366	0.62	1175
2	10.110	1970510	98.29	269827
3	10.605	22006	1.10	1907

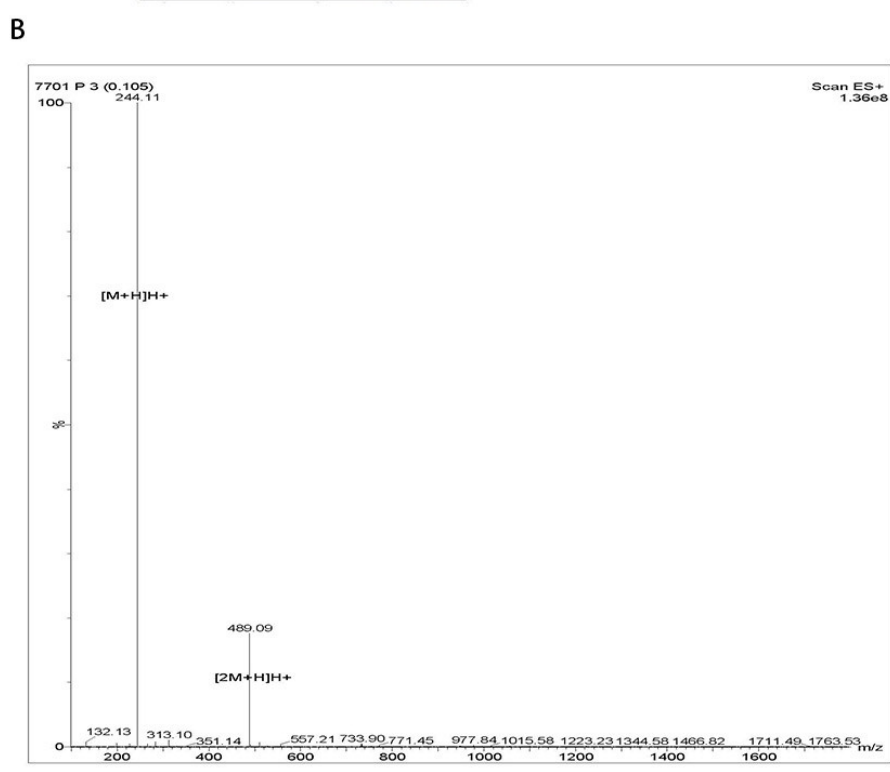
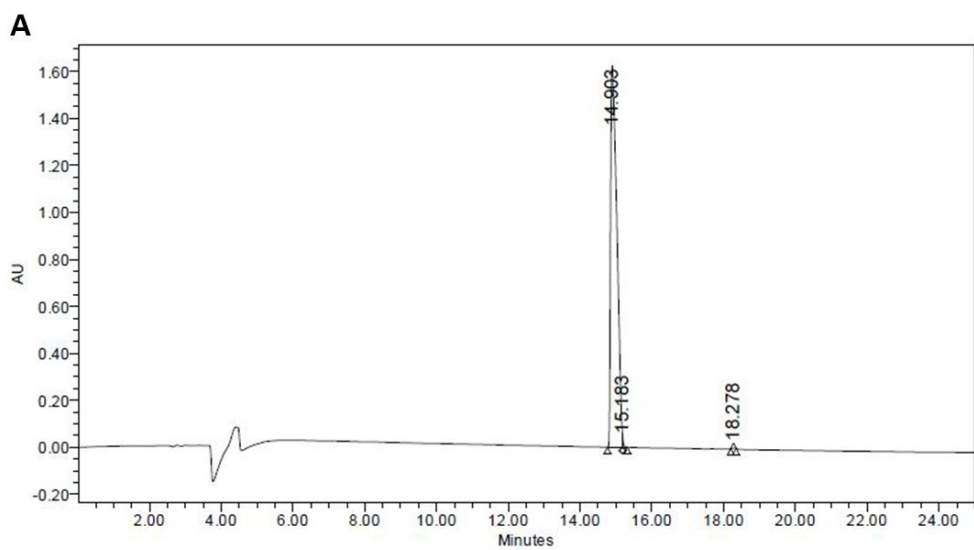


Figure S1. Analytical HPLC (A) and ESI-MS (B) of gelator_L-LL.



	RT	Area	% Area	Height
1	14.903	19496384	99.13	1630341
2	15.183	69267	0.35	47939
3	18.278	102335	0.52	20889

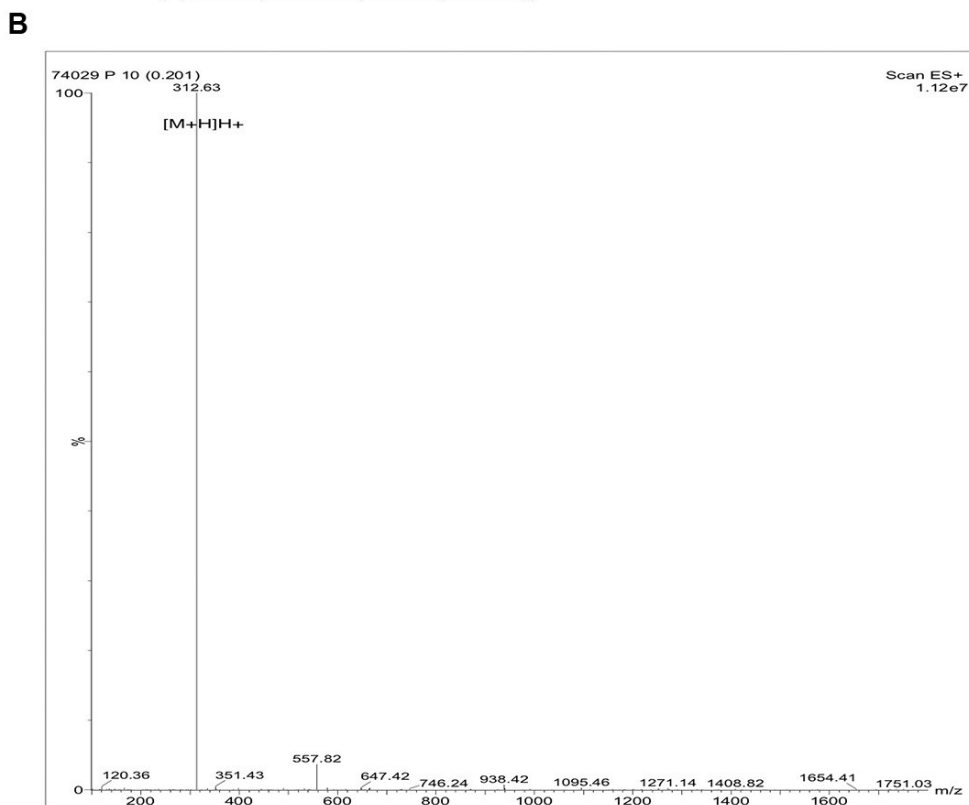
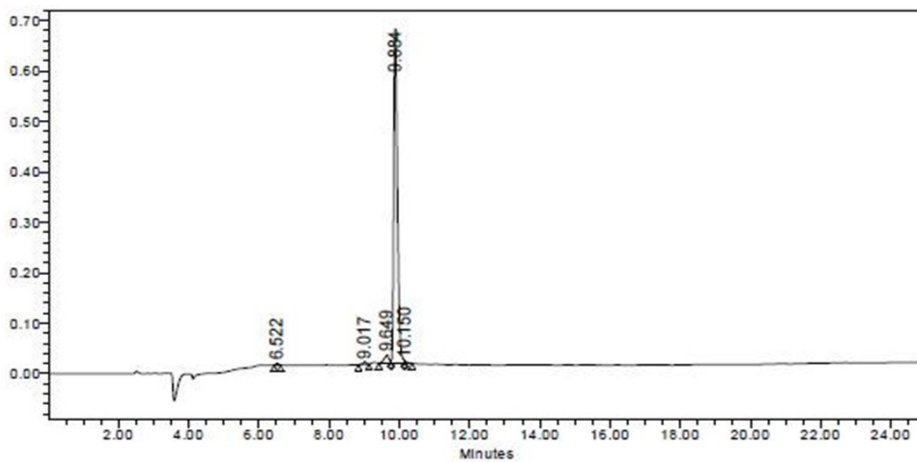


Figure S2. Analytical HPLC (A) and ESI-MS (B) of gelator _L-FF.

A

	RT	Area	% Area	Height
1	6.522	21328	0.43	4277
2	9.017	29322	0.59	4330
3	9.649	154966	3.11	16479
4	9.884	4756005	95.44	661624
5	10.150	21416	0.43	4976

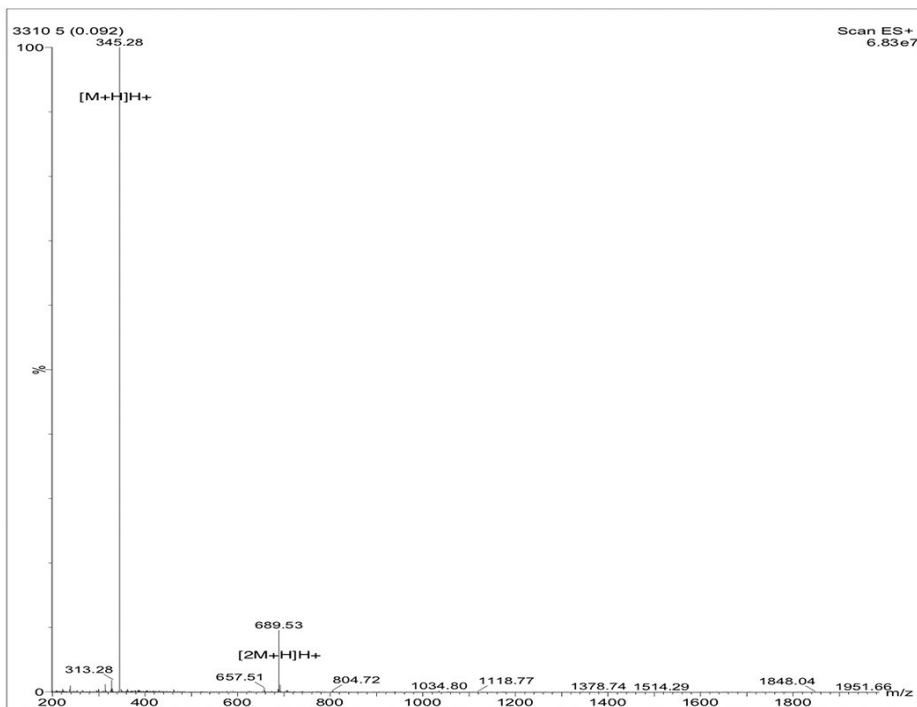
B

Figure S3. Analytical HPLC (A) and ESI-MS (B) of gelator _L-YY.

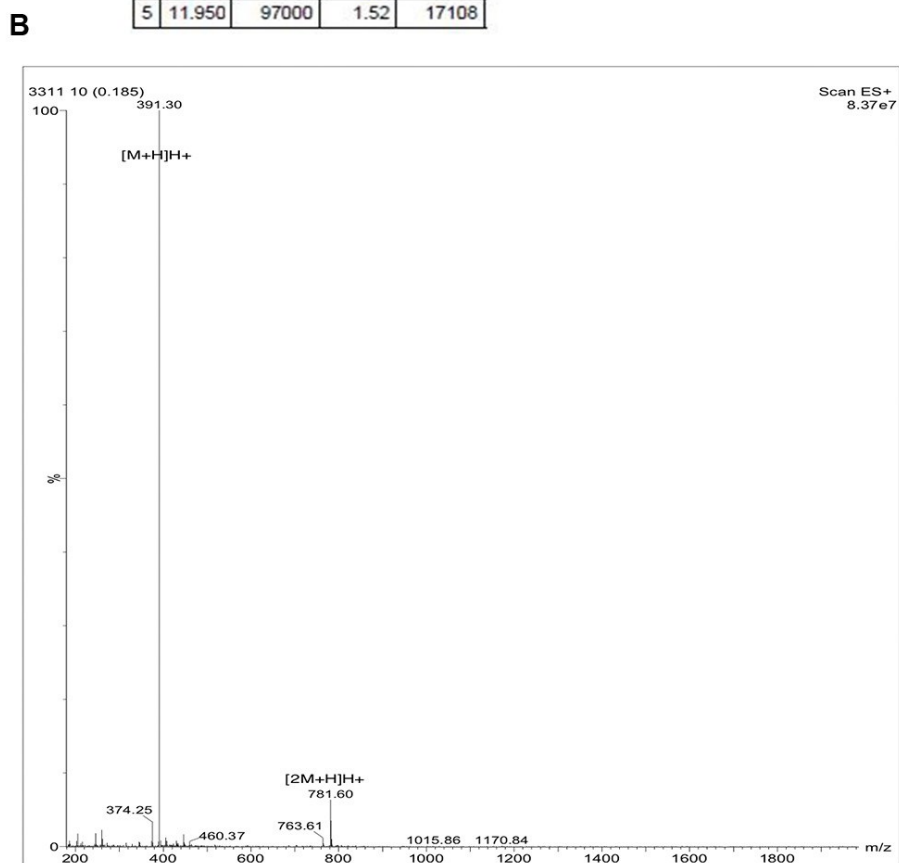
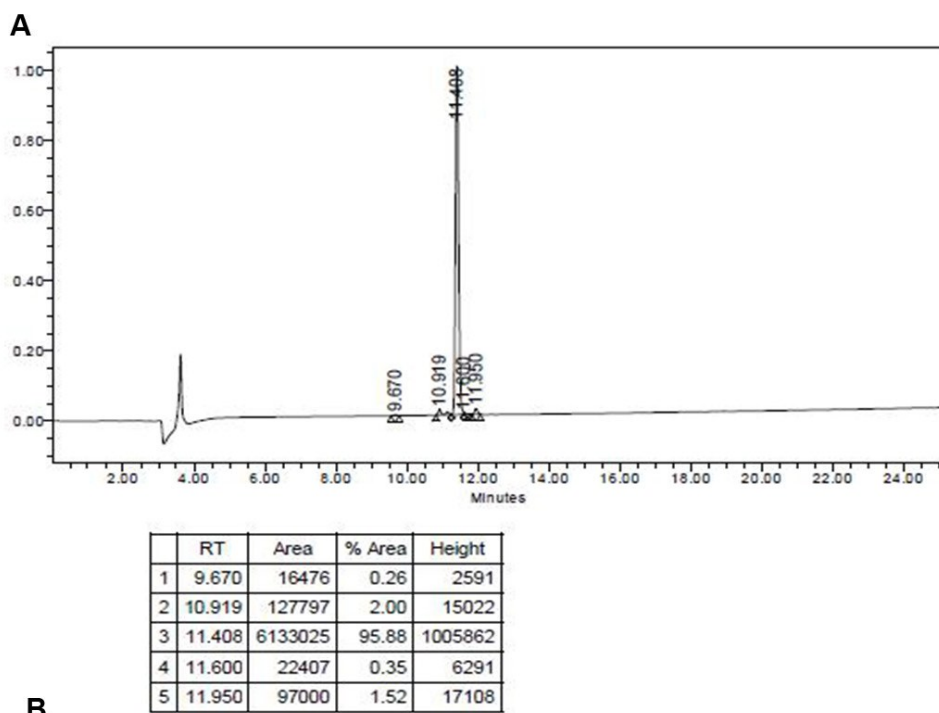
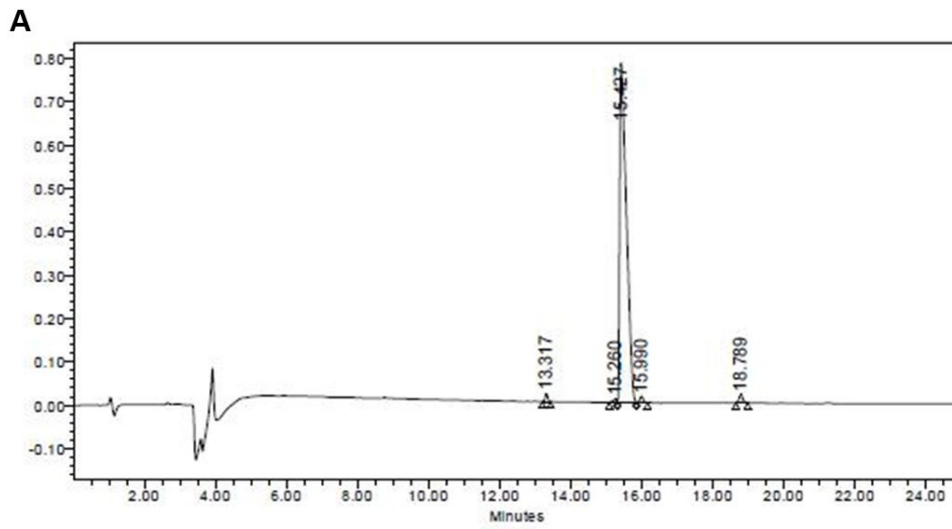


Figure S4. Analytical HPLC (A) and ESI-MS (B) of gelator_L-WW.



	RT	Area	% Area	Height
1	13.317	90768	0.86	18677
2	15.260	56514	0.54	8614
3	15.427	10187362	96.49	799034
4	15.990	92962	0.88	14082
5	18.789	130512	1.24	18537

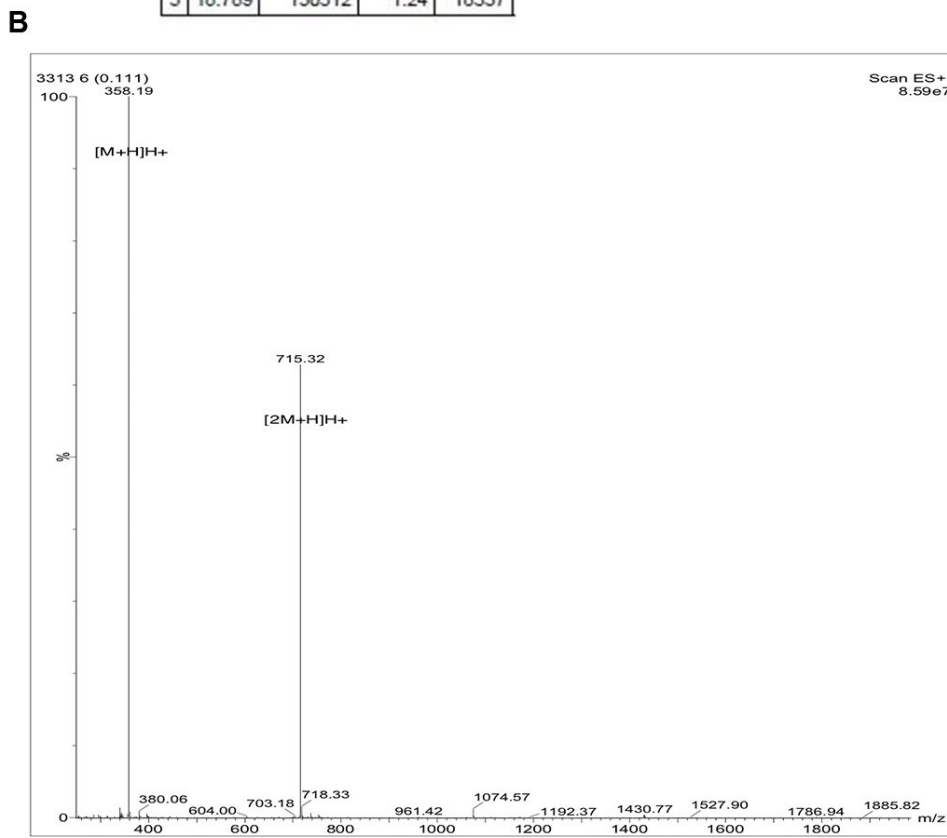
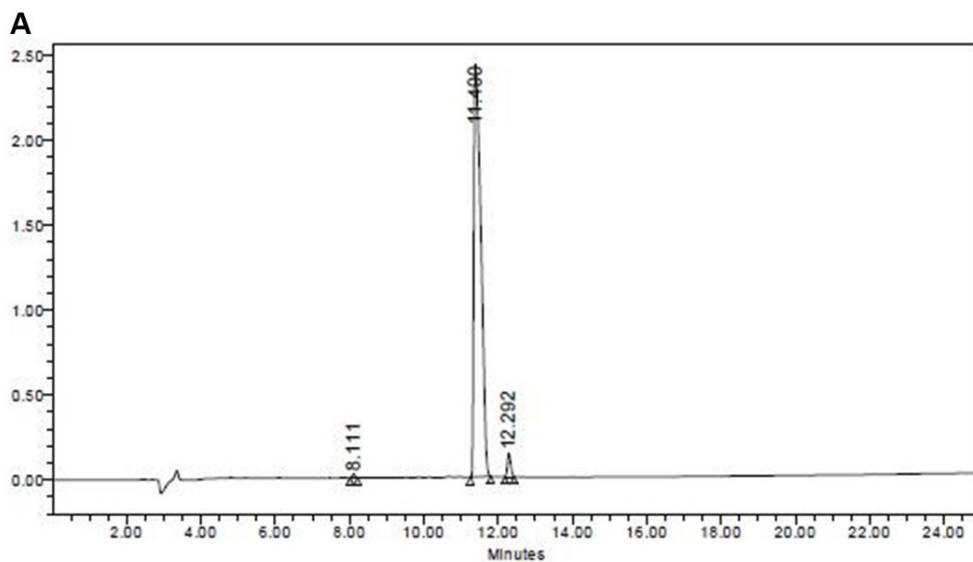


Figure S5. Analytical HPLC (A) and ESI-MS (B) of gelator _L-LLL.



RT	Area	% Area	Height
1	107216	0.32	20939
2	32057953	97.12	2430203
3	844792	2.56	139884

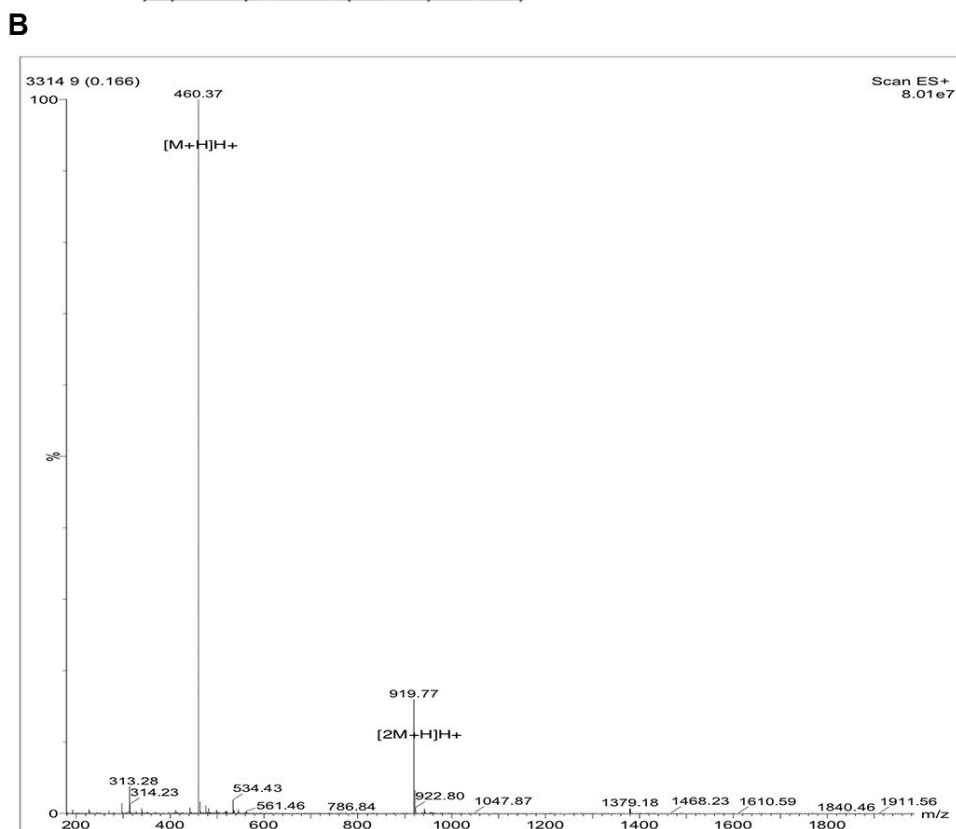
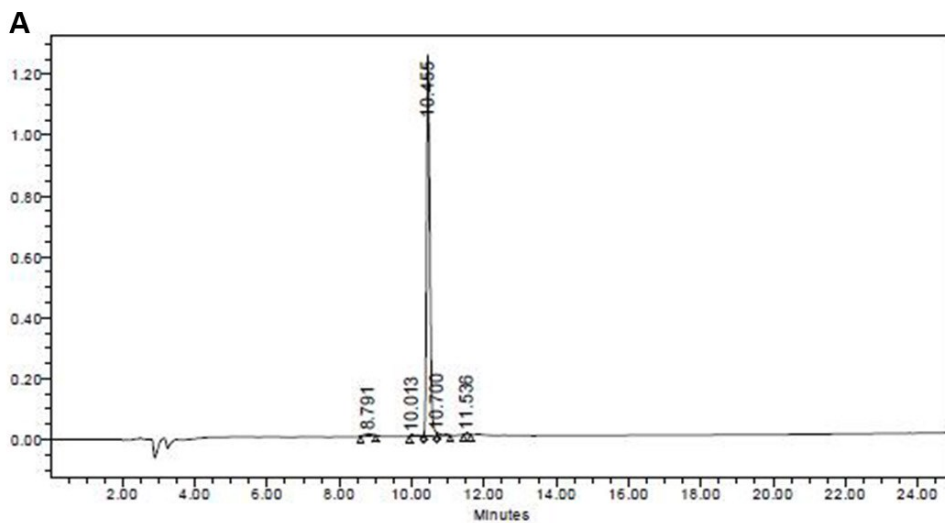


Figure S6. Analytical HPLC (A) and ESI-MS (B) of gelator _L-FFF.



	RT	Area	% Area	Height
1	8.791	103237	1.28	6963
2	10.013	59962	0.75	5689
3	10.455	7755915	96.49	1249279
4	10.700	83807	1.04	10249
5	11.536	35346	0.44	6126

B

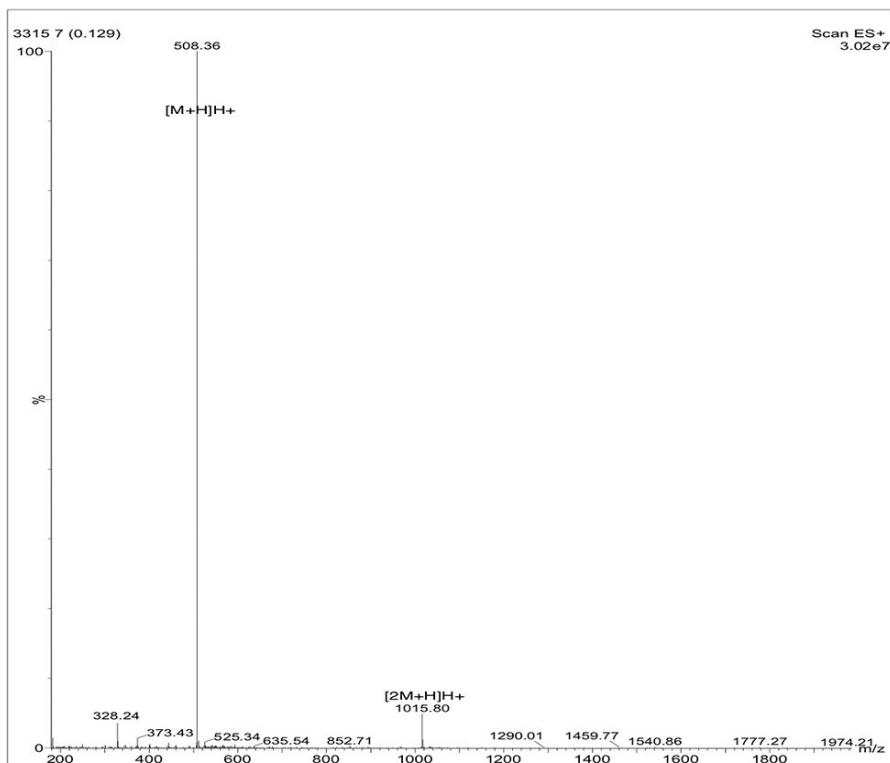
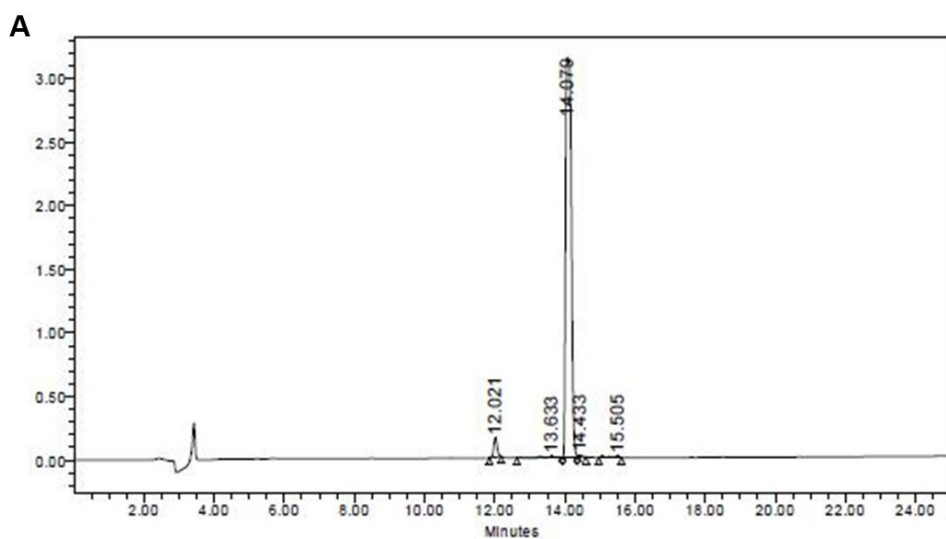


Figure S7. Analytical HPLC (A) and ESI-MS (B) of gelator L -YYY.



	RT	Area	% Area	Height
1	12.021	1037008	2.78	155080
2	13.633	216373	0.58	12166
3	14.079	35714726	95.61	3192719
4	14.433	131372	0.35	14714
5	15.505	255131	0.68	17334

B

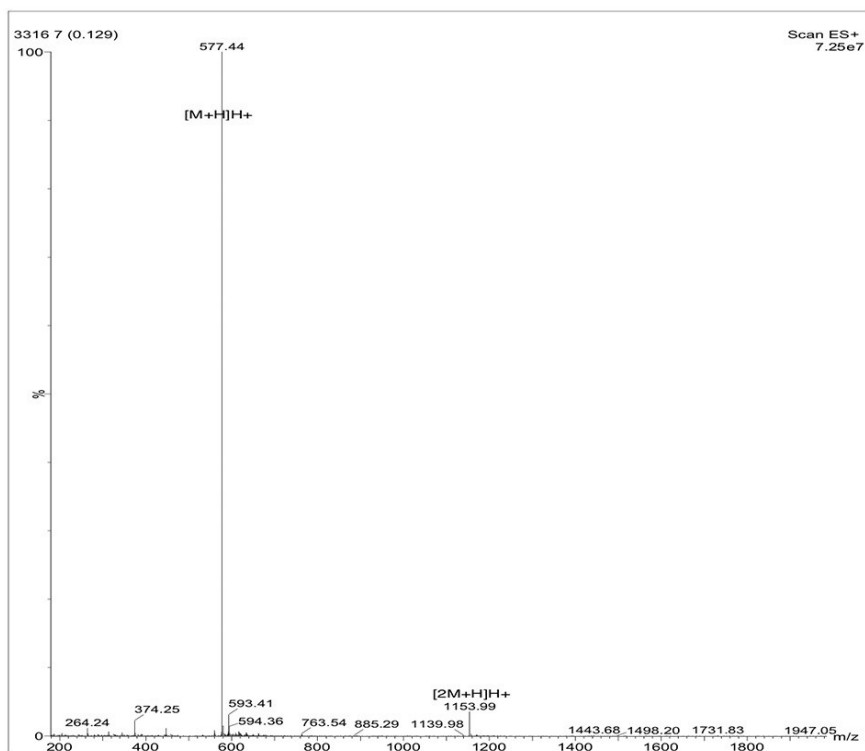
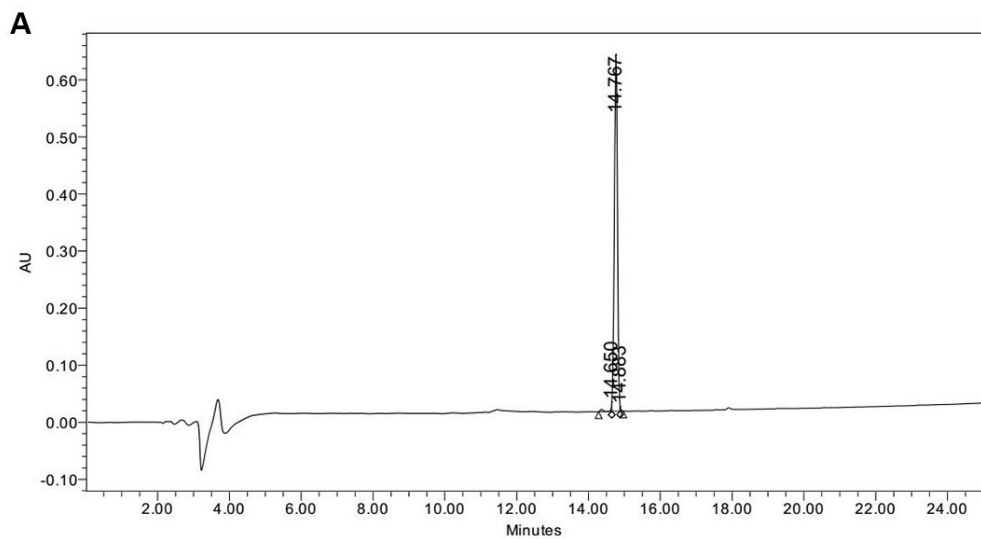


Figure S8. Analytical HPLC (A) and ESI-MS (B) of gelator_L-WWW.



	RT	Area	% Area	Height
1	14.650	37943	1.01	16438
2	14.767	3724240	98.75	621500
3	14.883	9270	0.25	7907

B

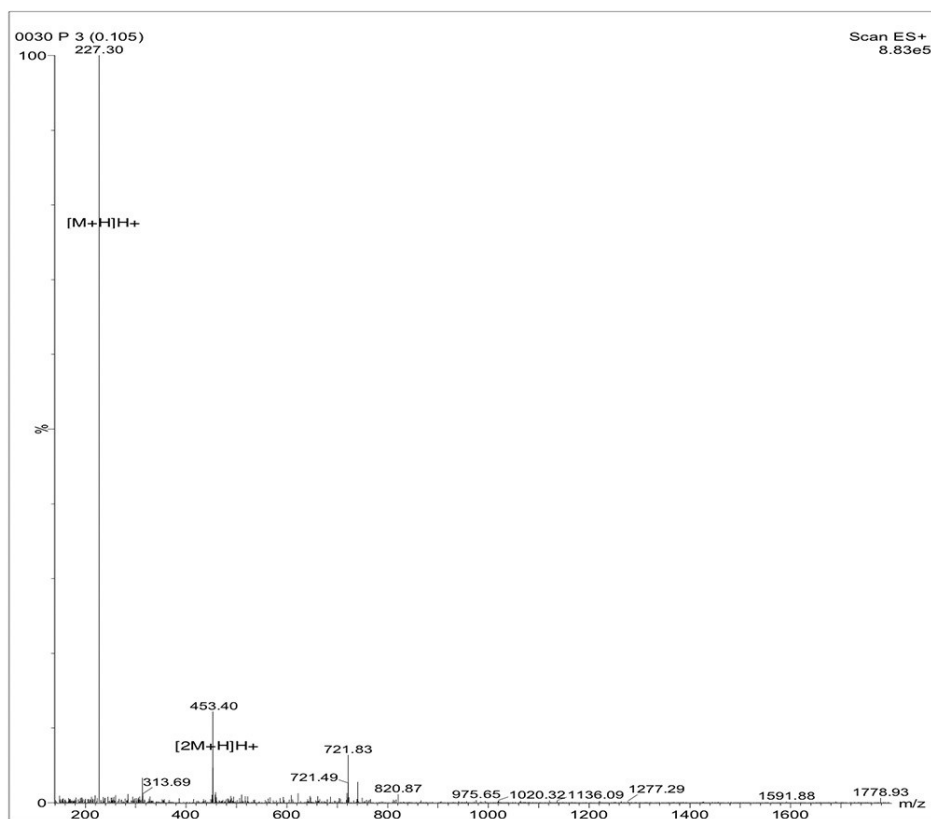
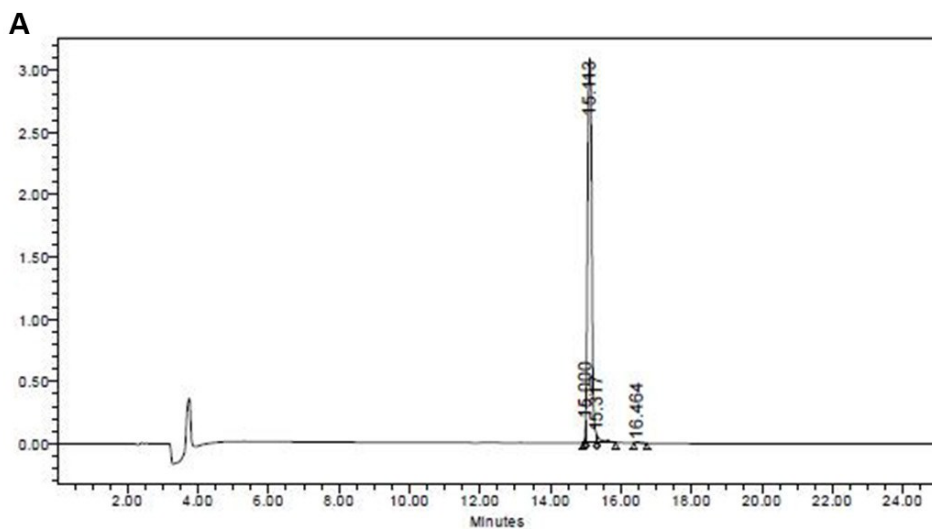


Figure S9. Analytical HPLC (A) and ESI-MS (B) of gelator C_L-LL.



	RT	Area	% Area	Height
1	15.000	159591	0.61	171024
2	15.113	25477484	97.17	3103086
3	15.317	506389	1.93	62345
4	16.464	75694	0.29	9654

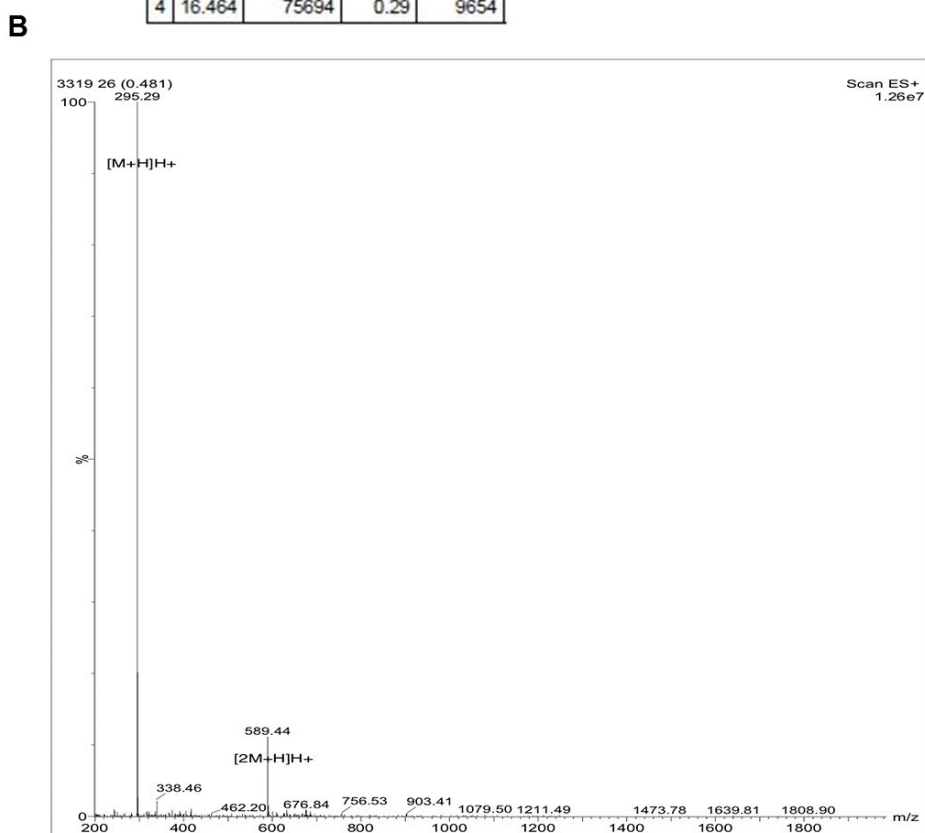
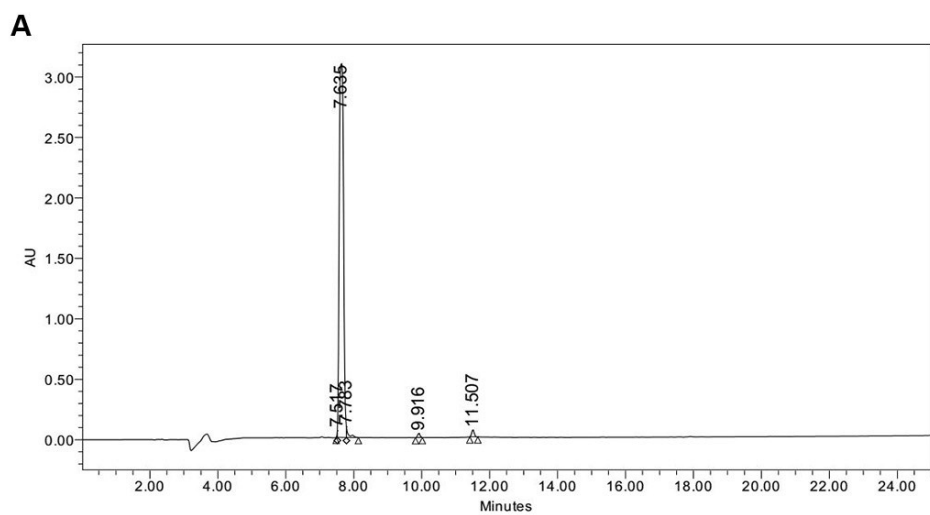


Figure S10. Analytical HPLC (A) and ESI-MS (B) of gelator C_L-FF.



	RT	Area	% Area	Height
1	7.517	38809	0.14	55461
2	7.635	26905773	96.97	3099128
3	7.783	333382	1.20	87193
4	9.916	168348	0.61	33623
5	11.507	299331	1.08	57173

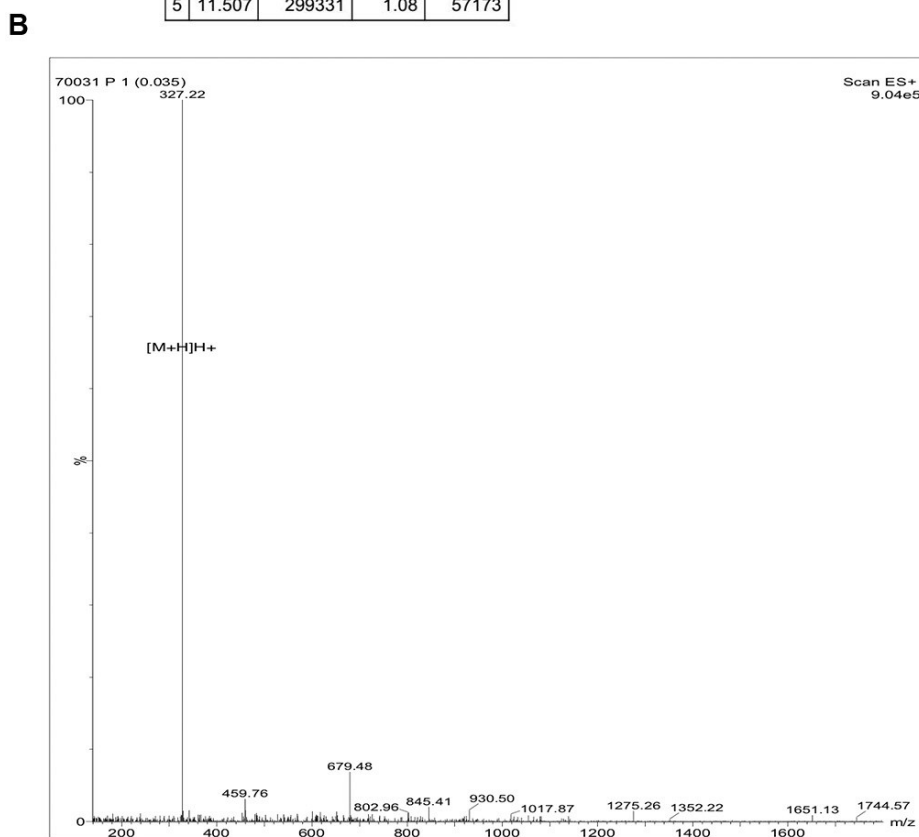
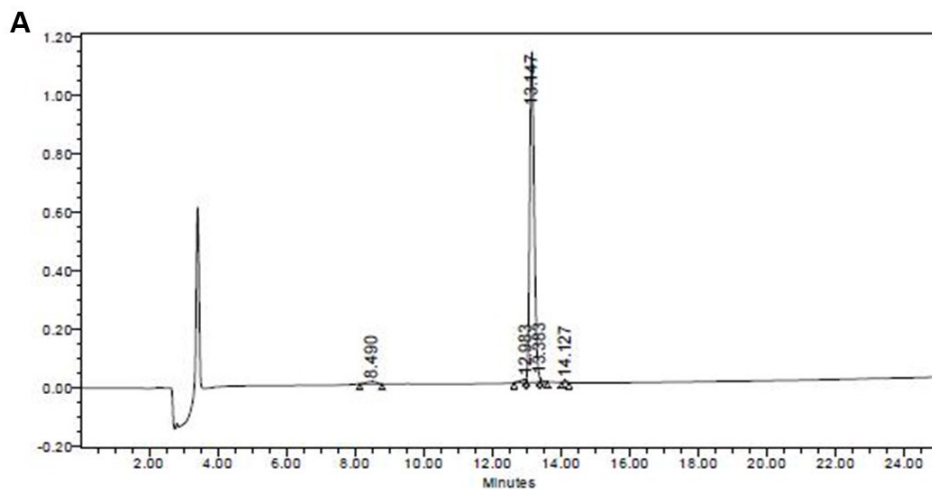


Figure S11. Analytical HPLC (A) and ESI-MS (B) of gelator C_L-YY.



	RT	Area	% Area	Height
1	8.490	167156	1.56	8345
2	12.983	117286	1.10	11202
3	13.147	10314699	96.42	1126074
4	13.383	52911	0.49	15540
5	14.127	45298	0.42	7875

B

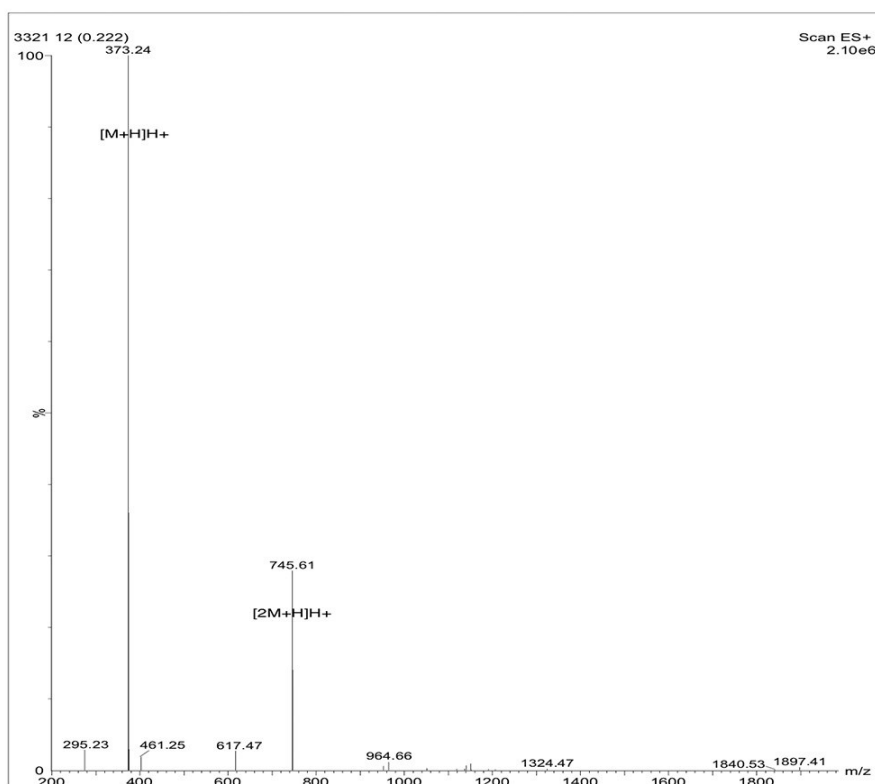


Figure S12. Analytical HPLC (A) and ESI-MS (B) of gelator C_L-WW.

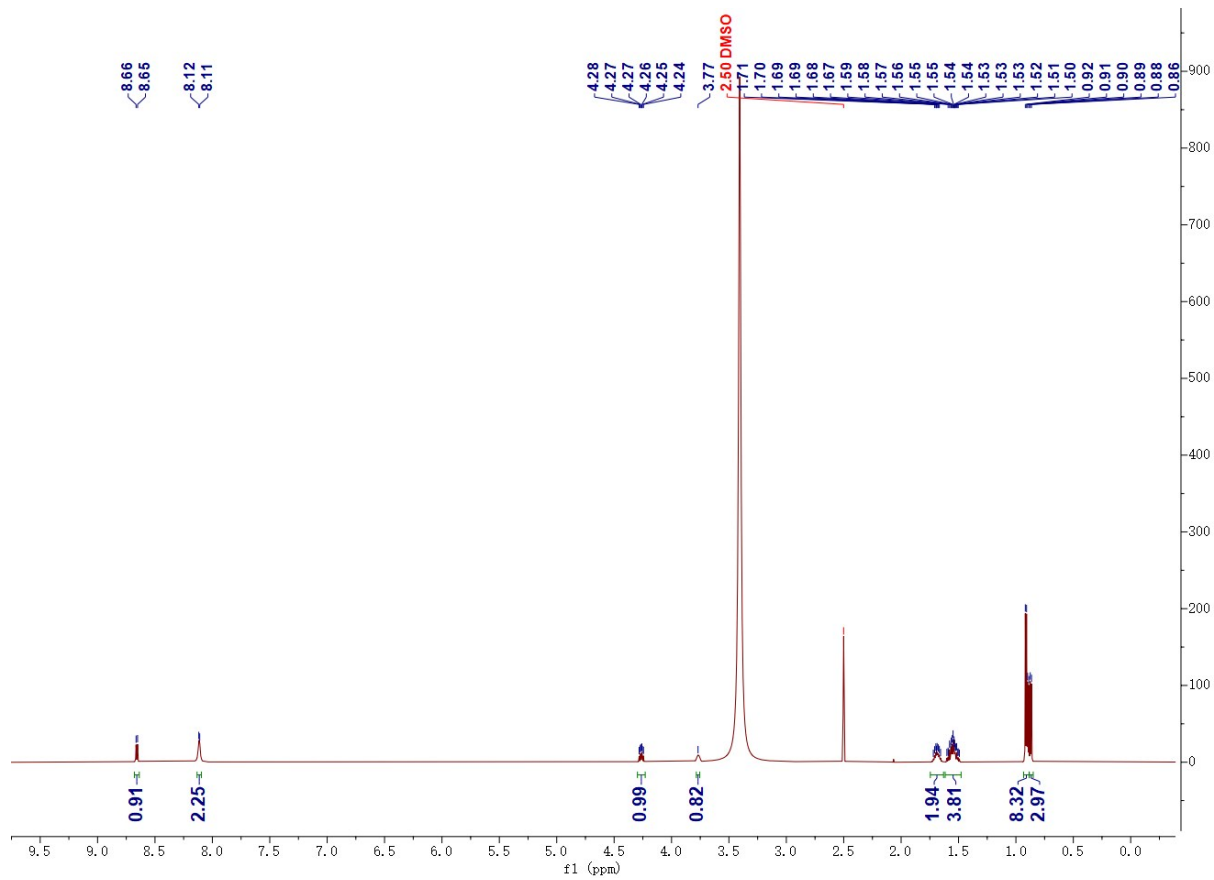


Figure S13: ¹H-NMR (600 MHz, DMSO-*d*₆) of L-LL.

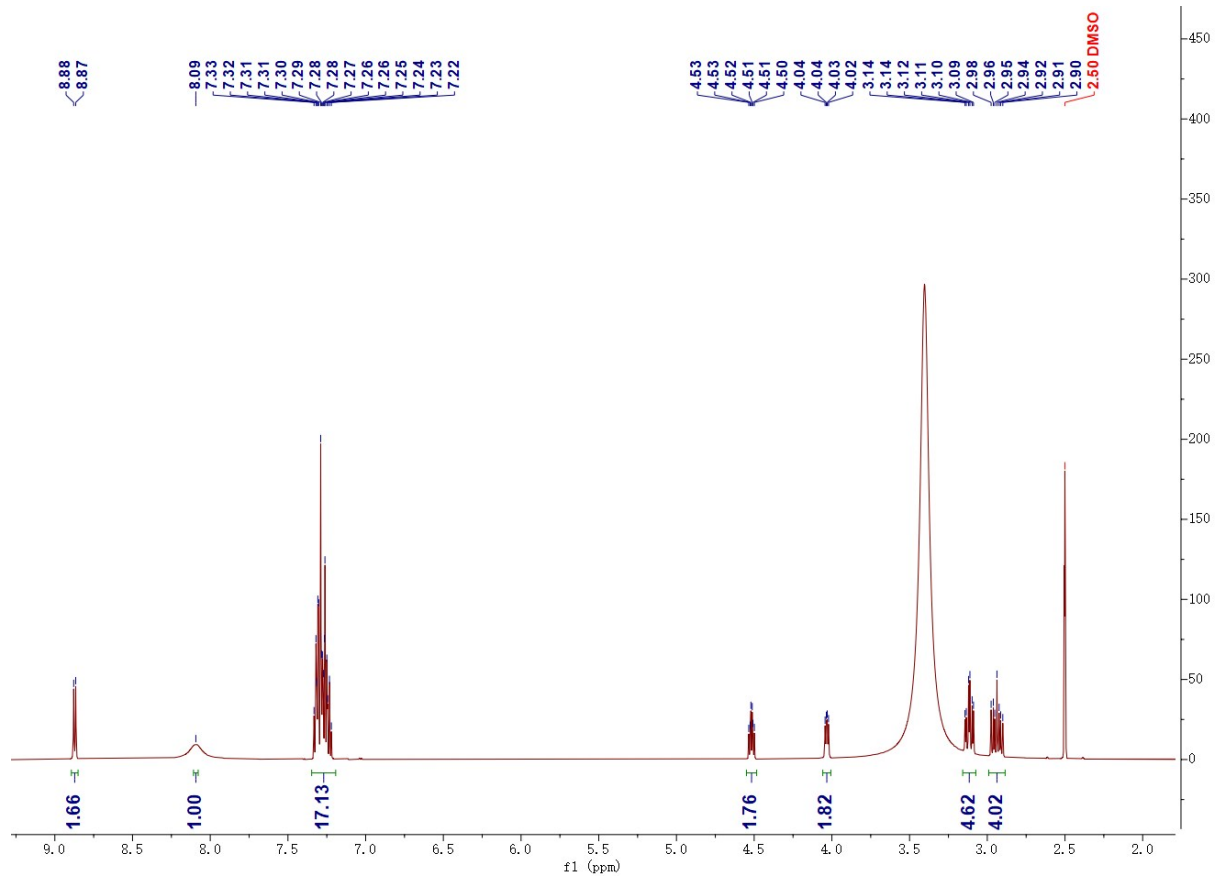


Figure S14: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of L-FF .

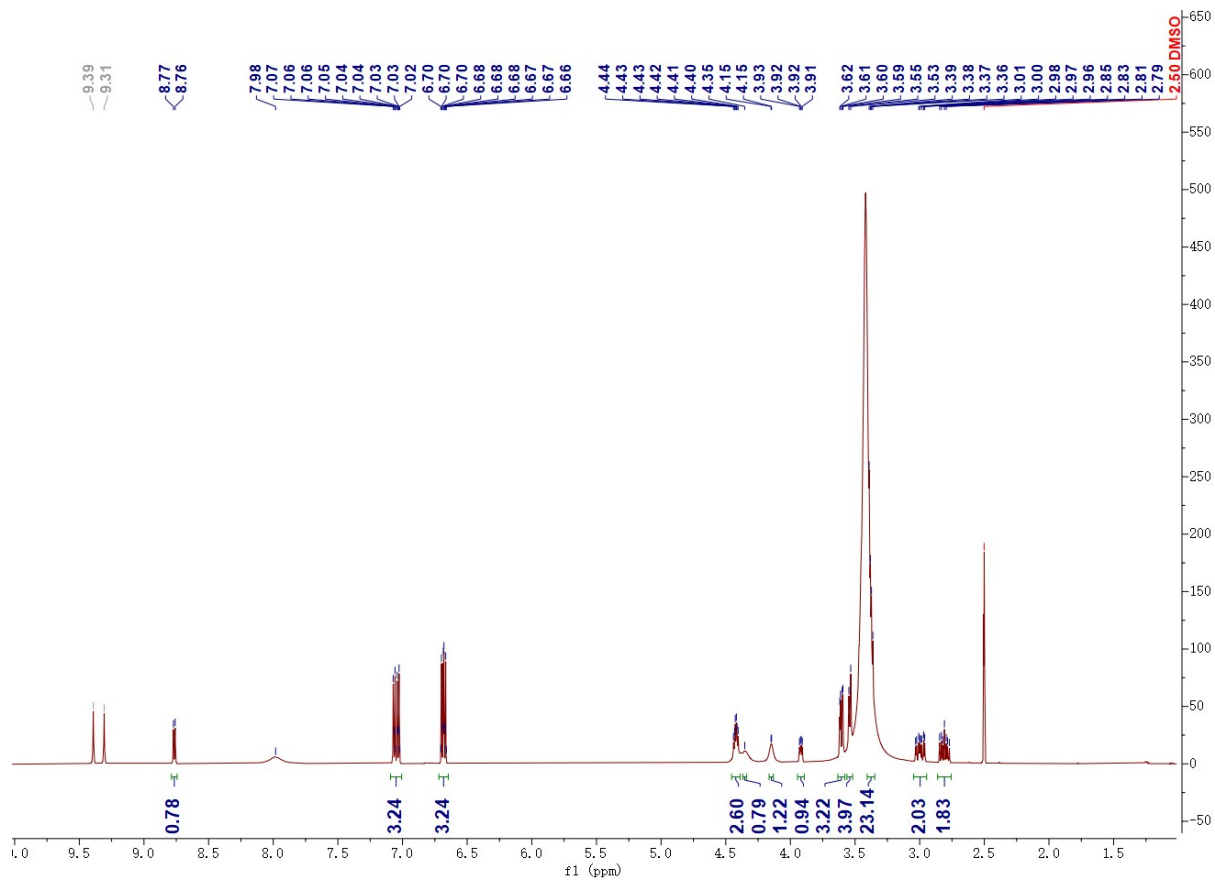


Figure S15: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of L-YY .

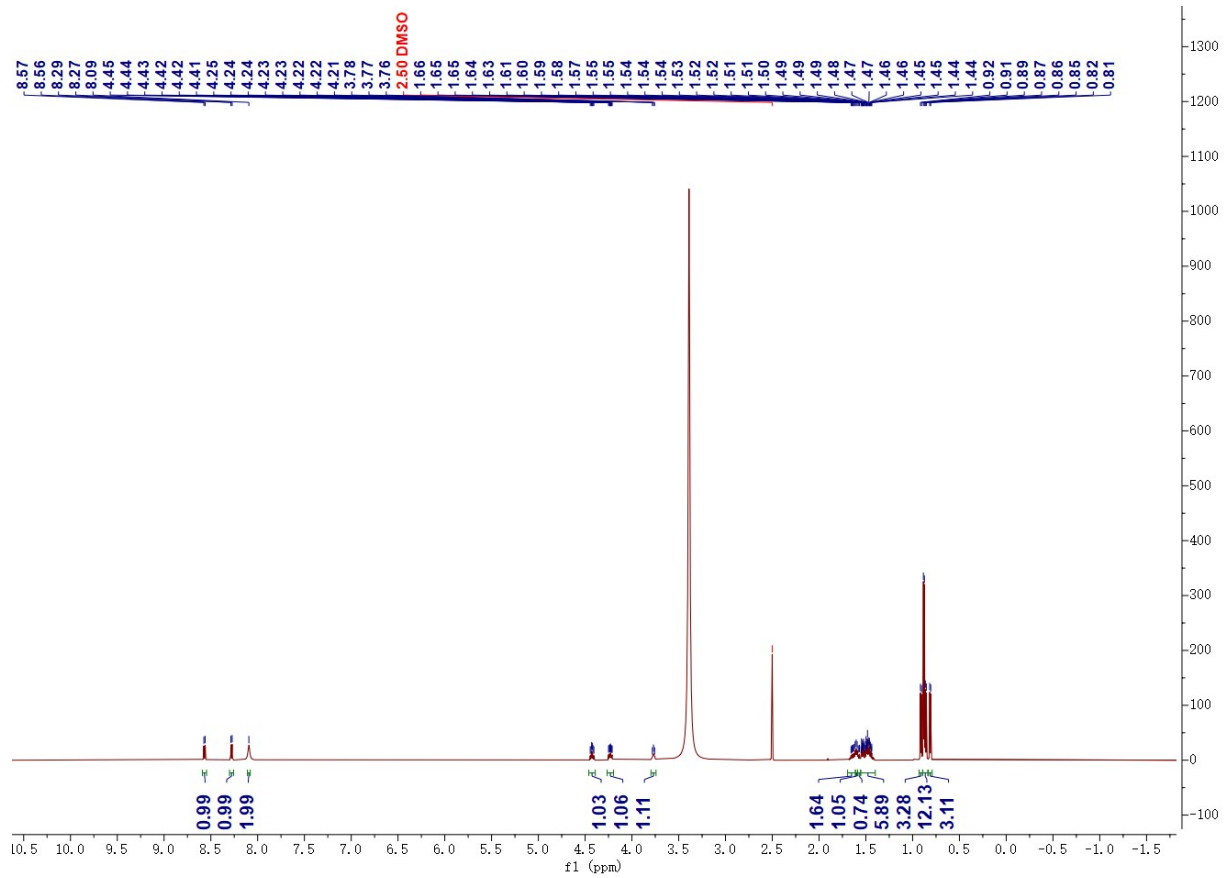


Figure S16: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of L-LLL .

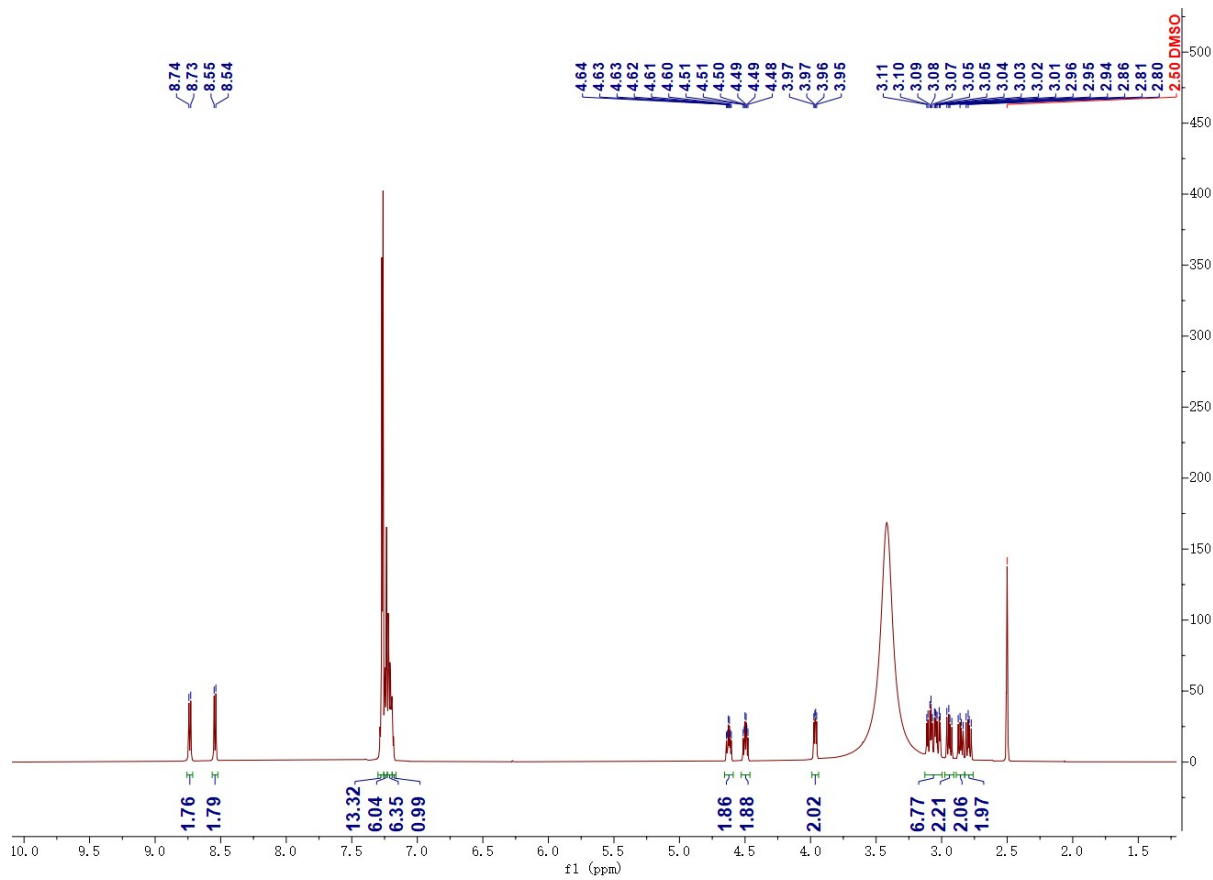


Figure S17: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of L-FFF .

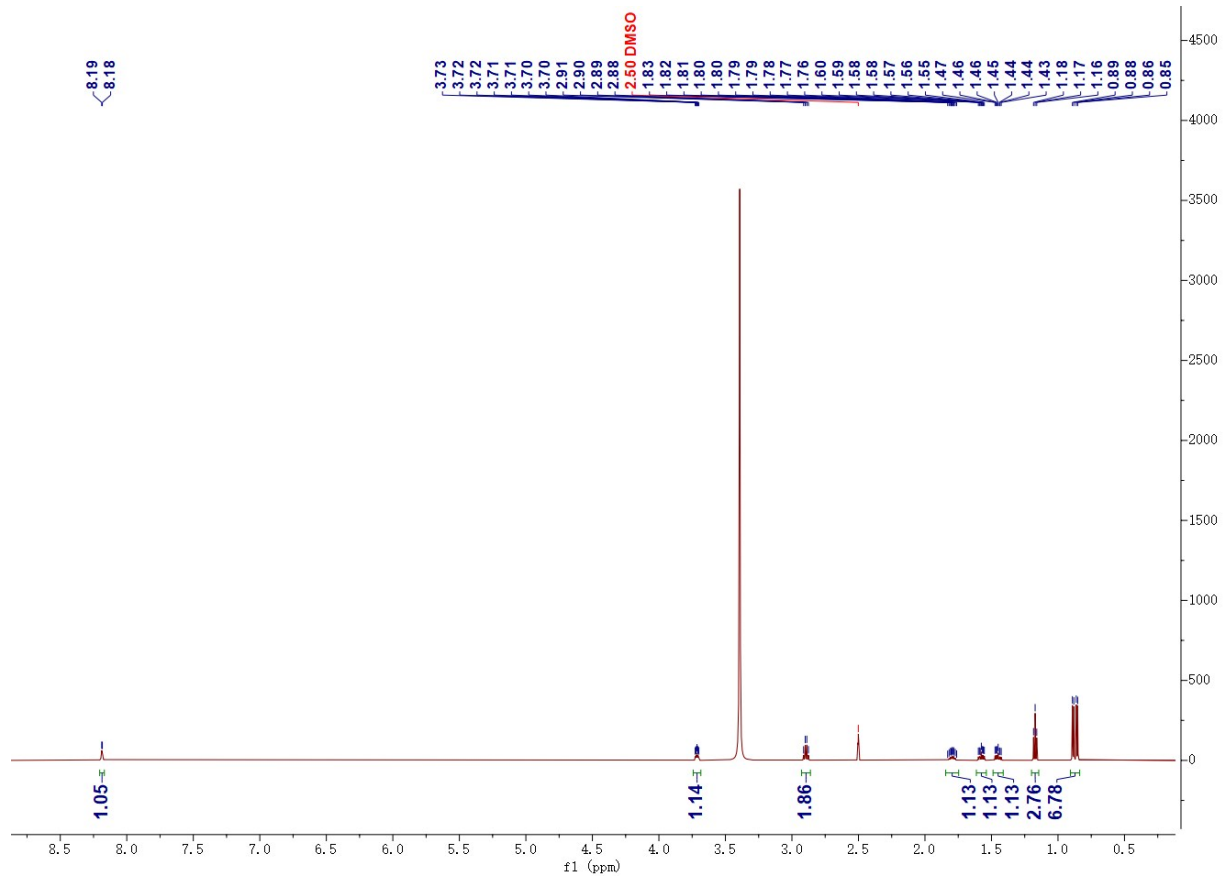


Figure S18: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of $c\text{-L-LL}$.

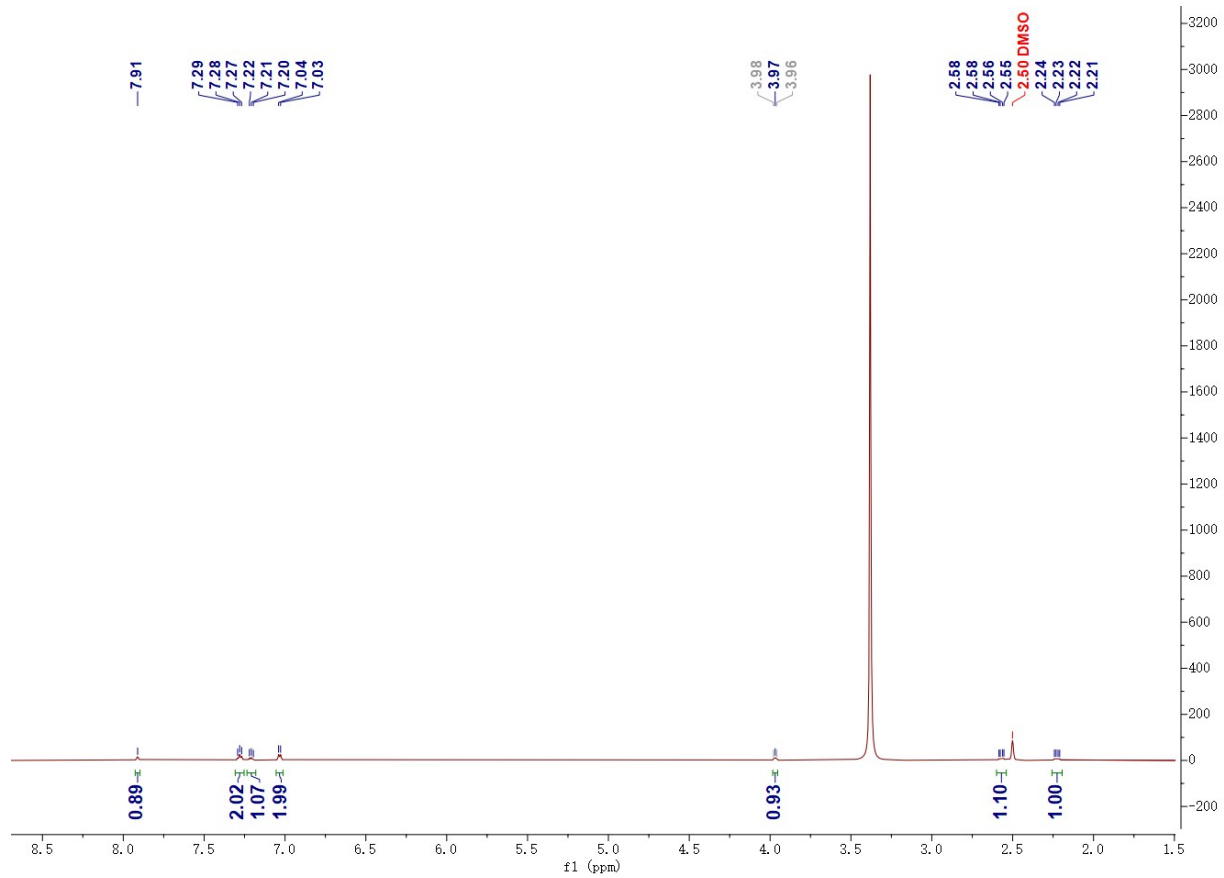


Figure S19: ¹H-NMR (600 MHz, DMSO-*d*₆) of c-L-FF.

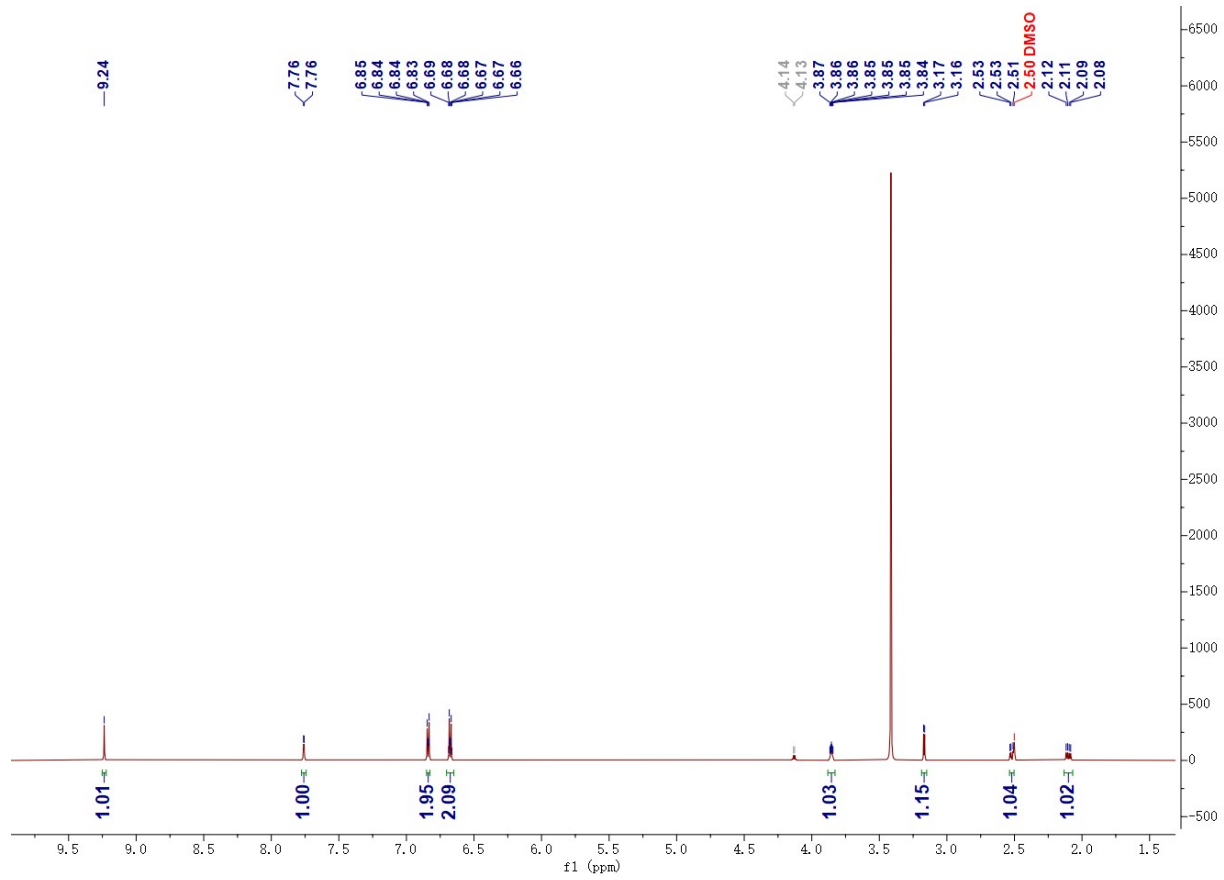


Figure S20: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of $c\text{-L-YY}$.

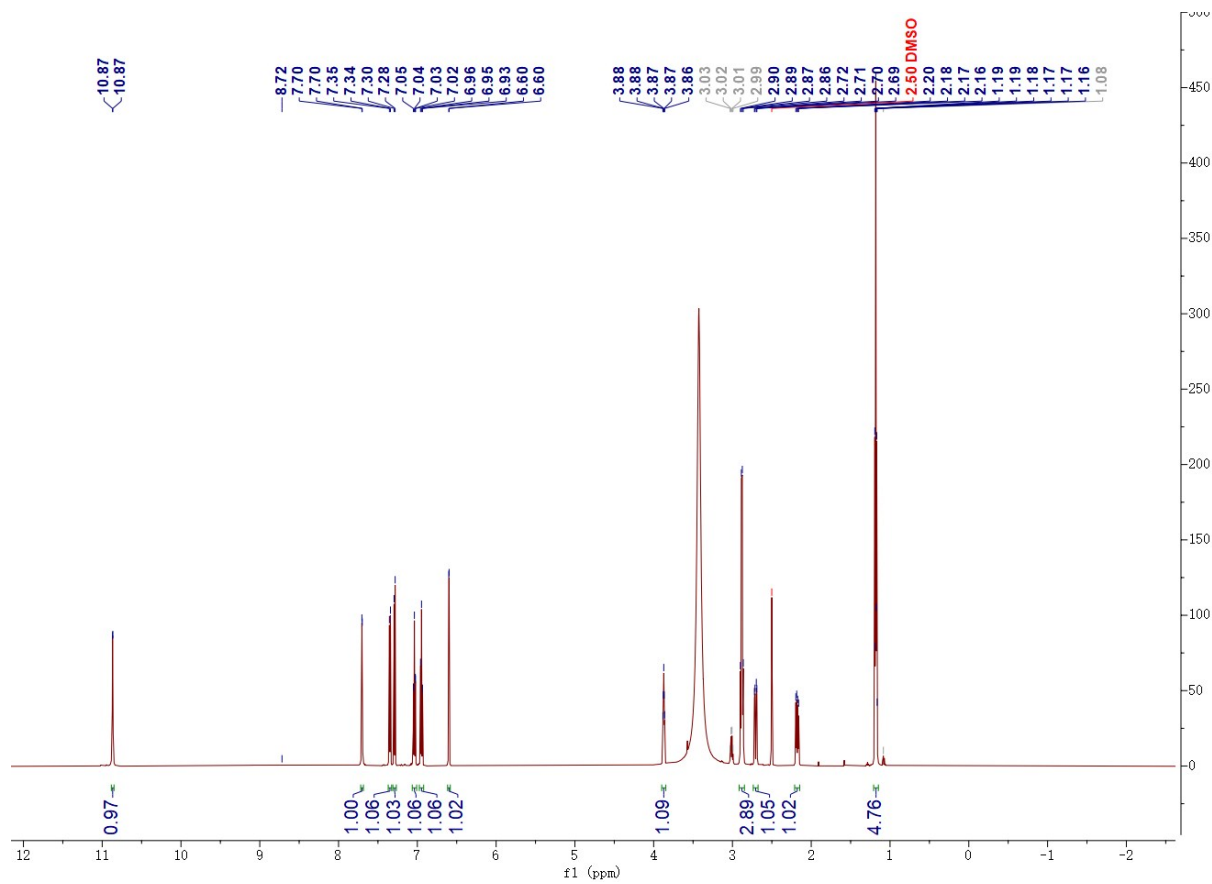


Figure S21: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) of $c\text{-L-WW}$.