SUPPORTING INFORMATION

Toward Sustainable Gel Chemistry: Supramolecular Gelation of Amino Acid Derivatives in Green Solvents

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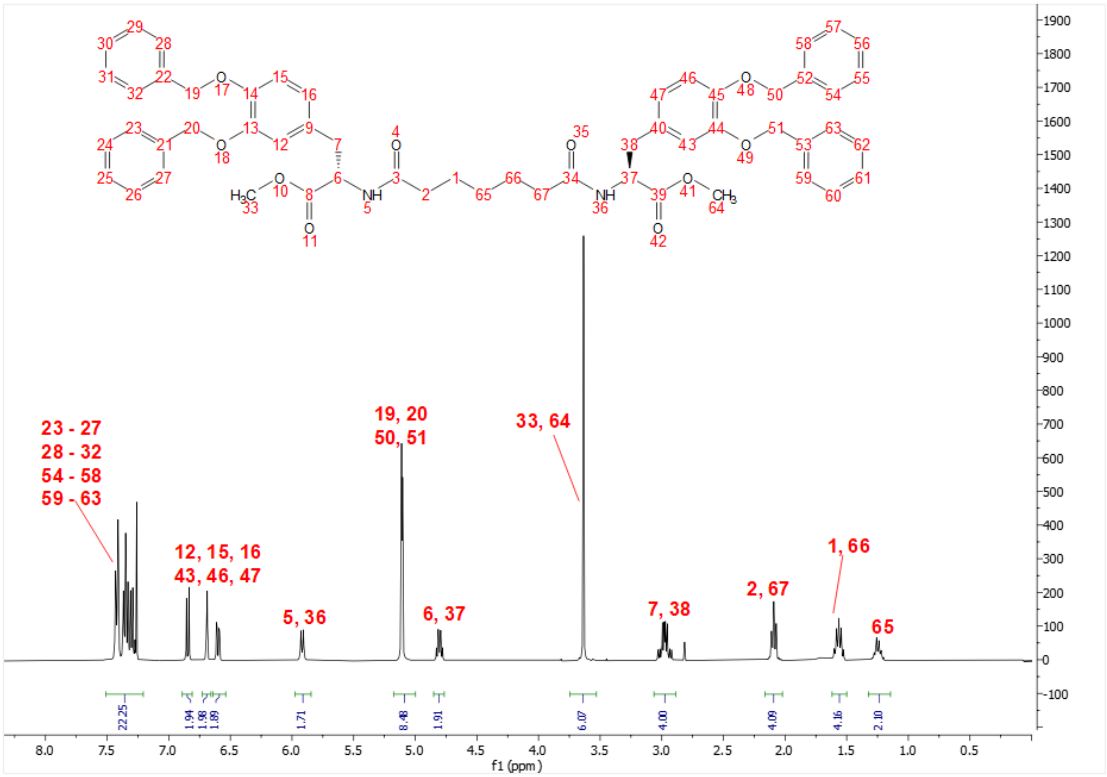
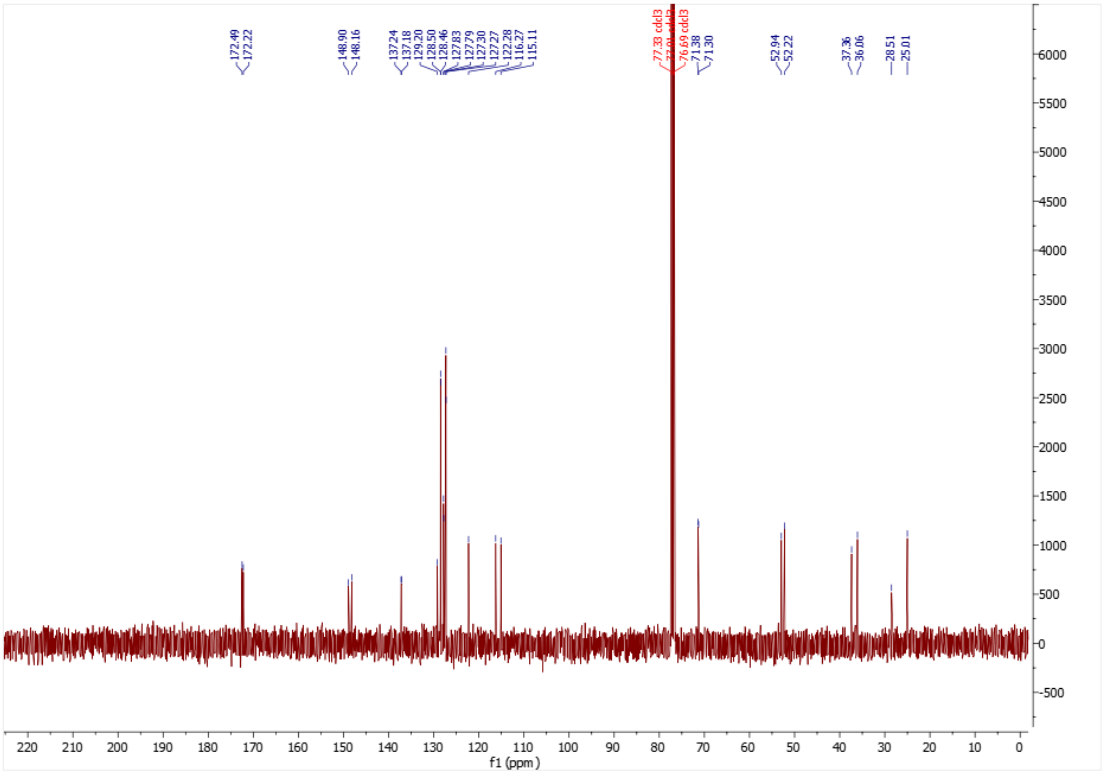
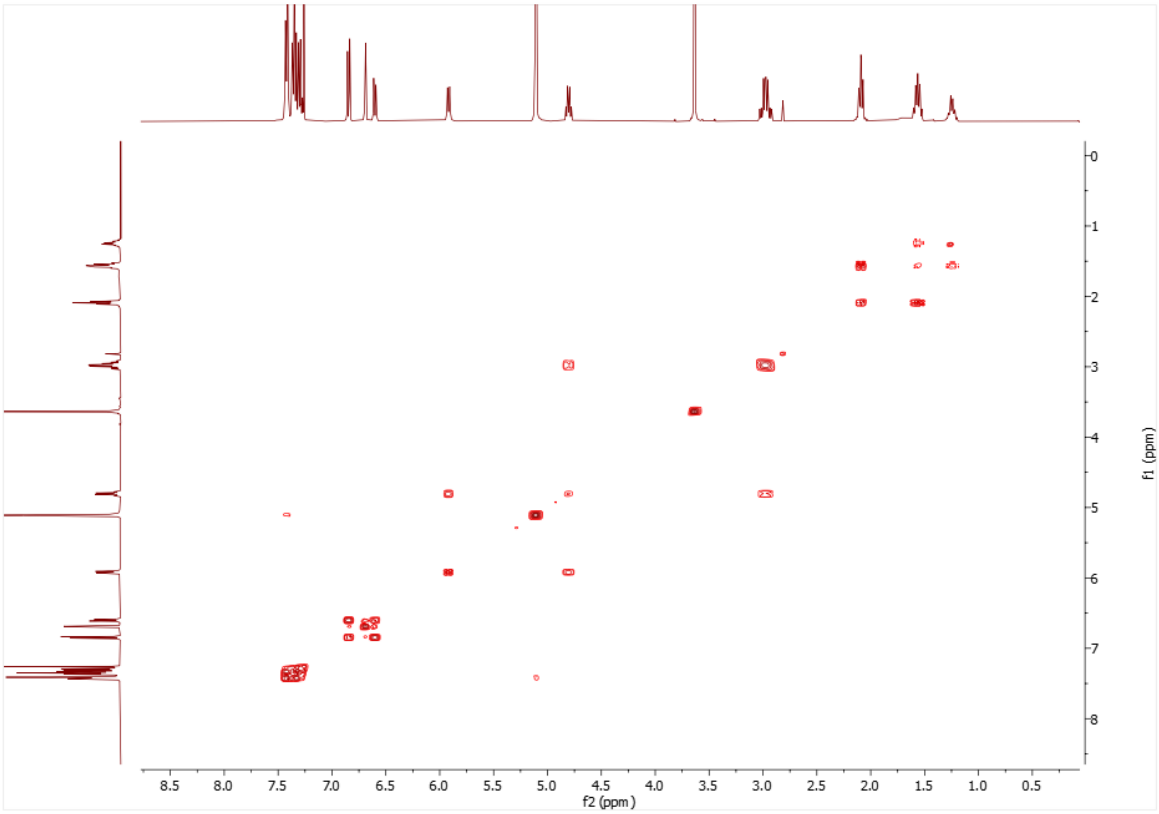
^{1}H NMR Gelator B



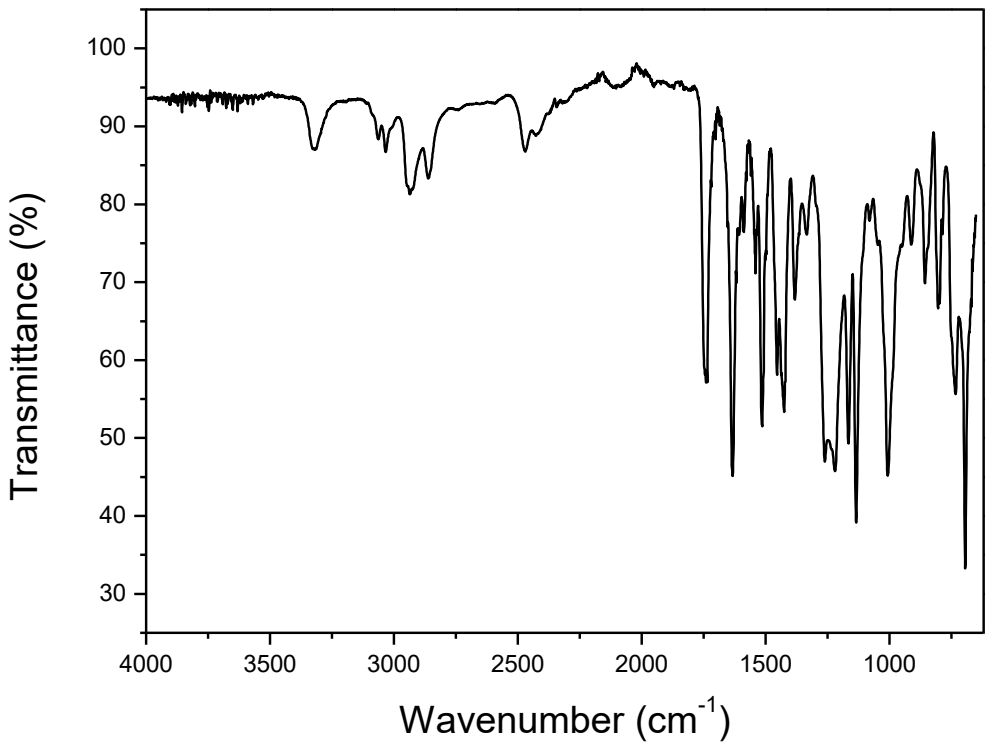
^{13}C NMR Gelator B



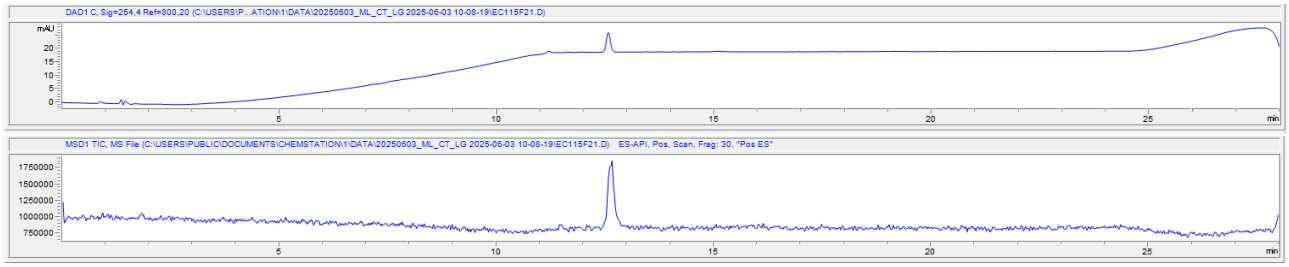
COSY NMR Gelator B

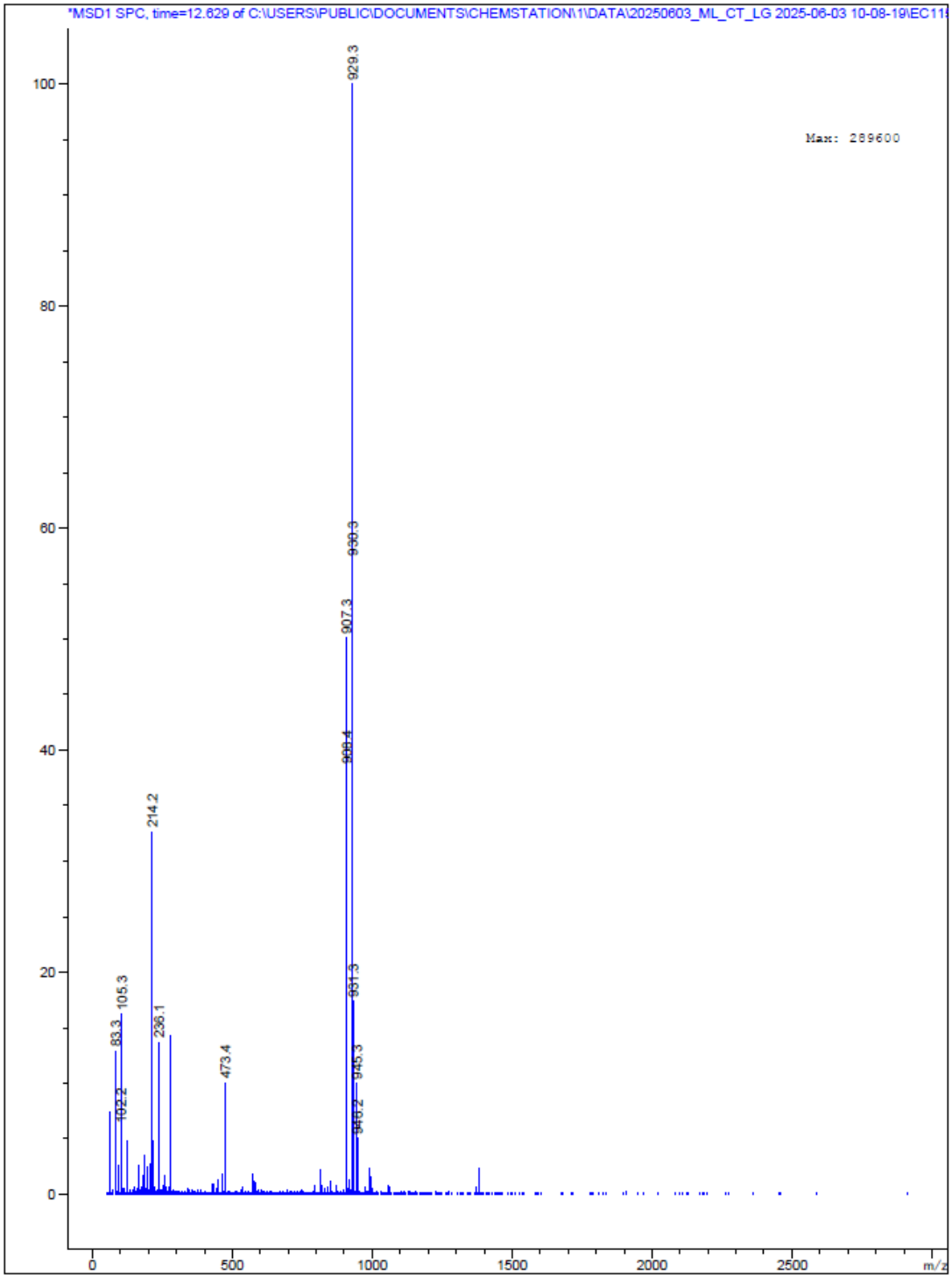


FT-IR spectrum of Gelator B

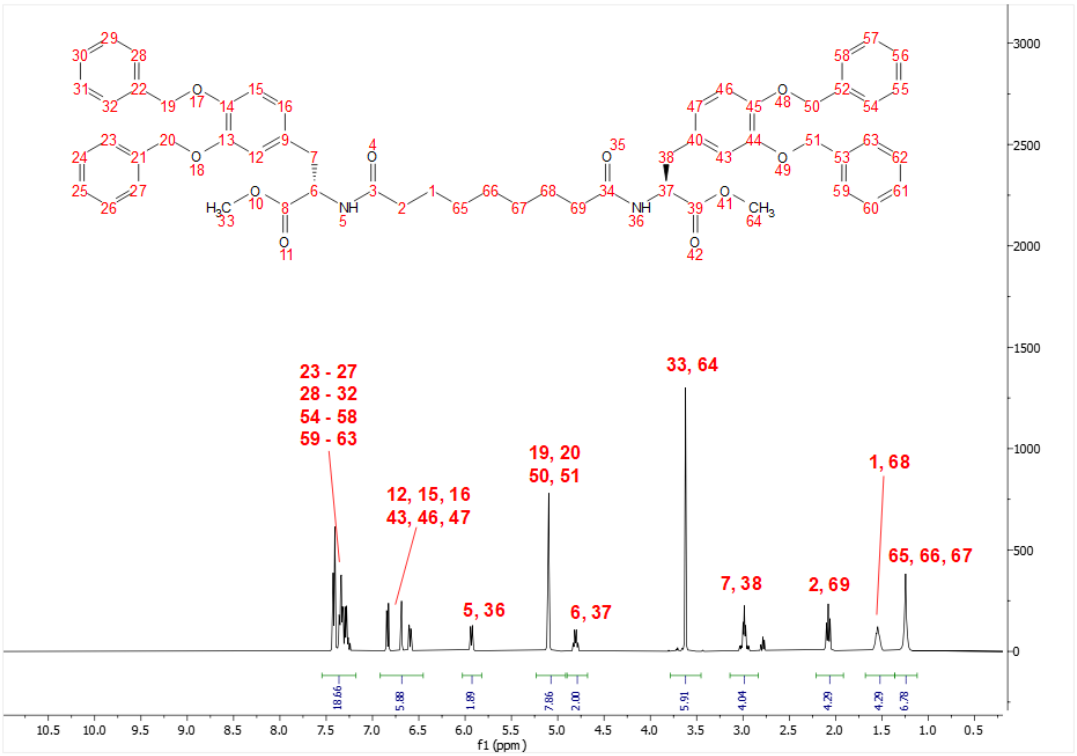


HPLC-MS of gelator B





^{1}H NMR of gelator C



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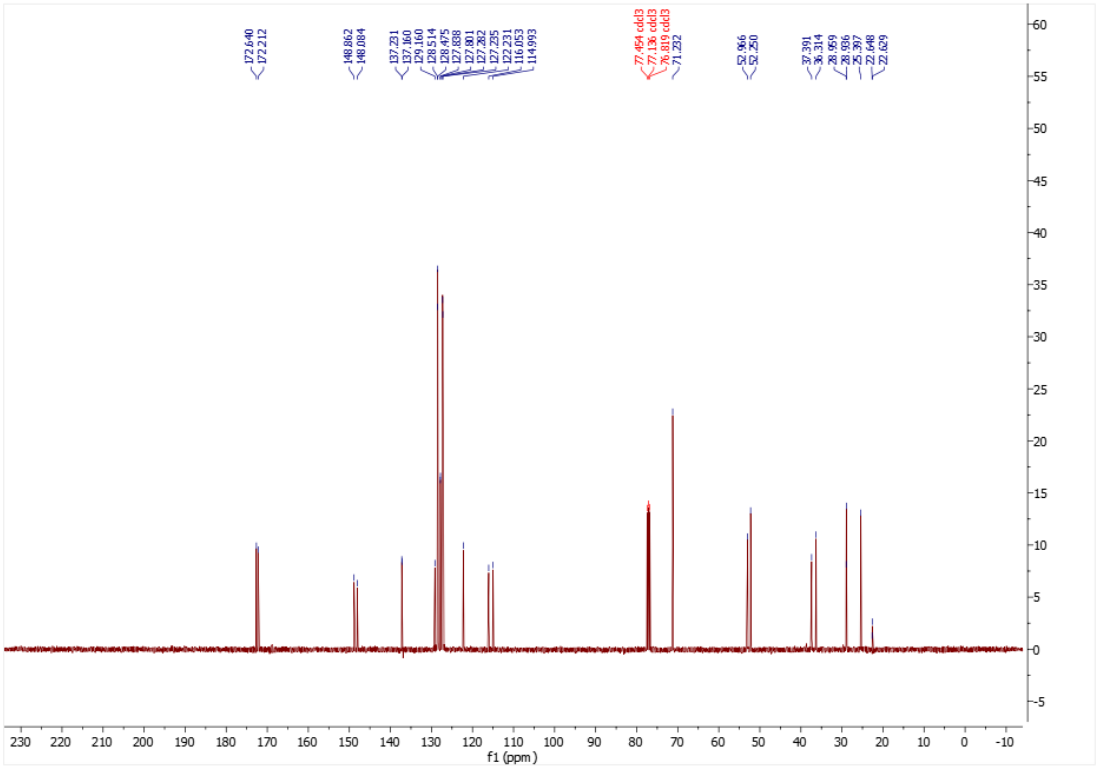

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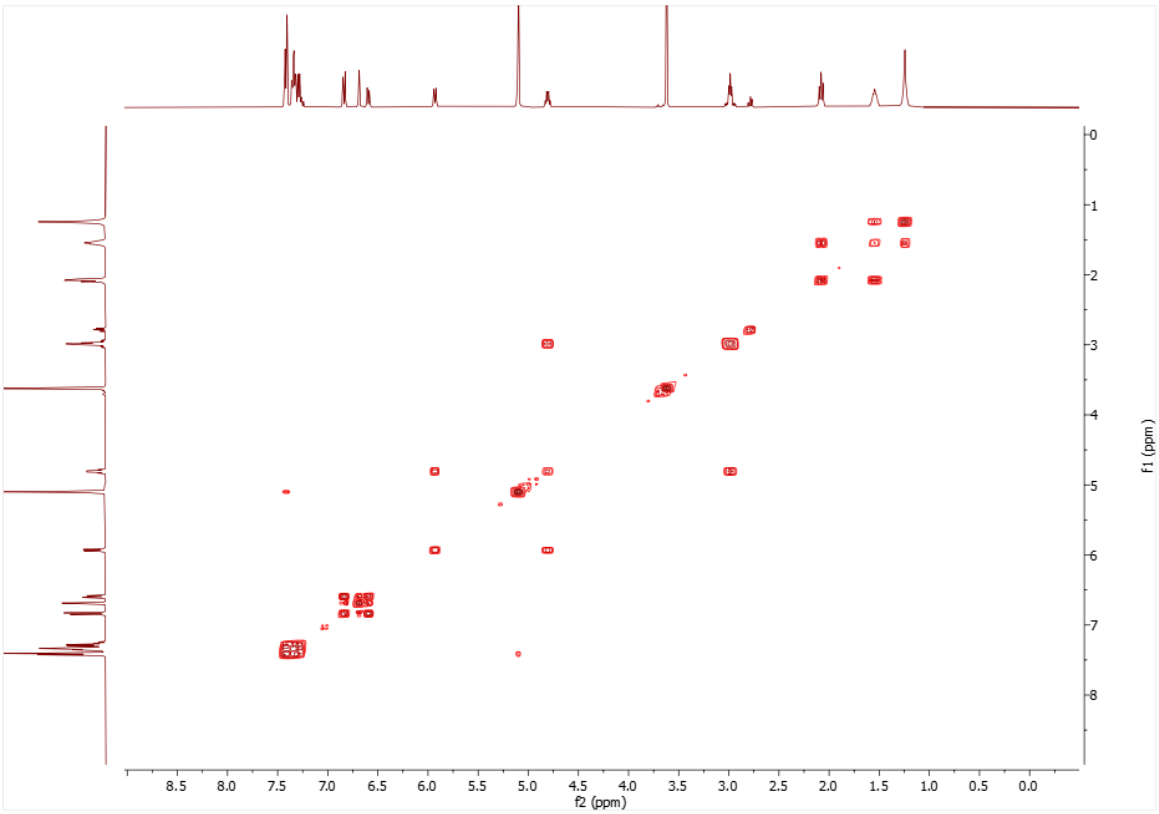
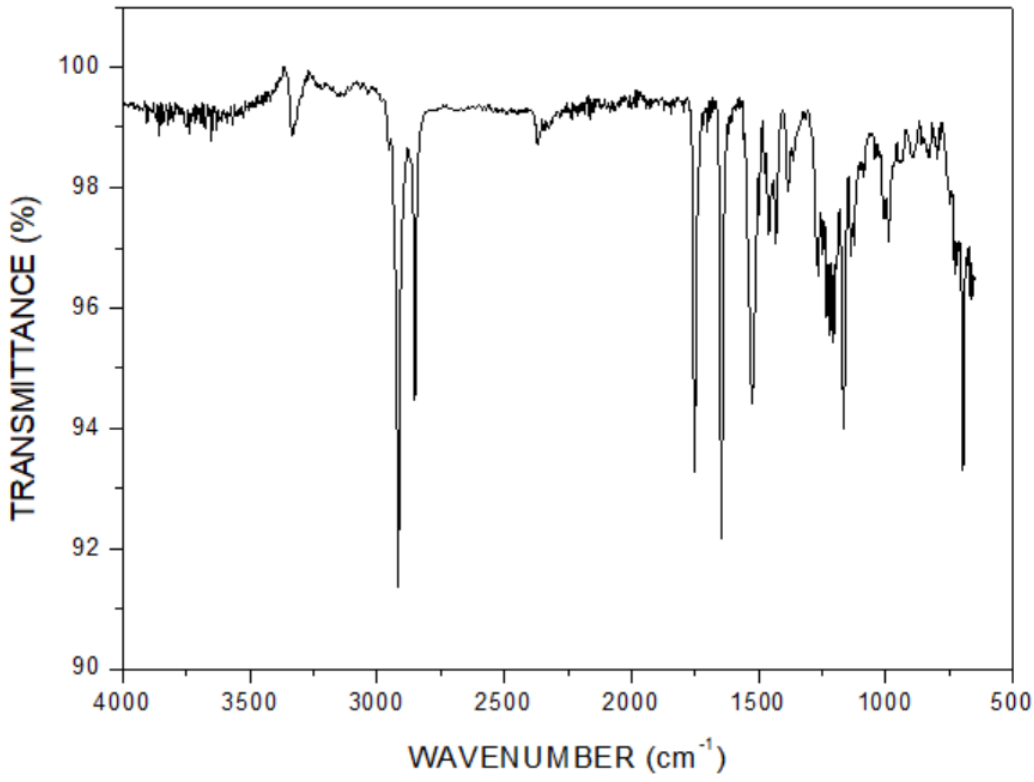


FT-IR spectrum of Gelator C



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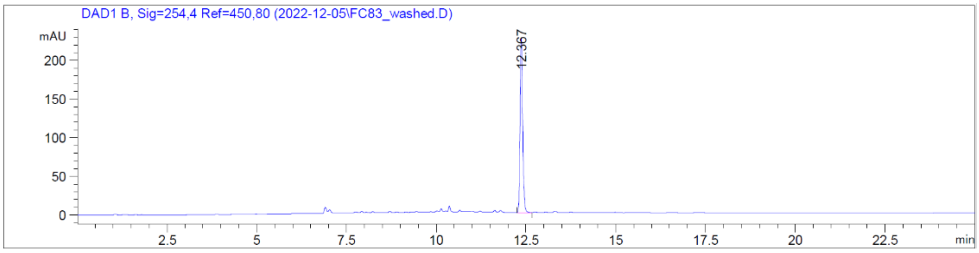
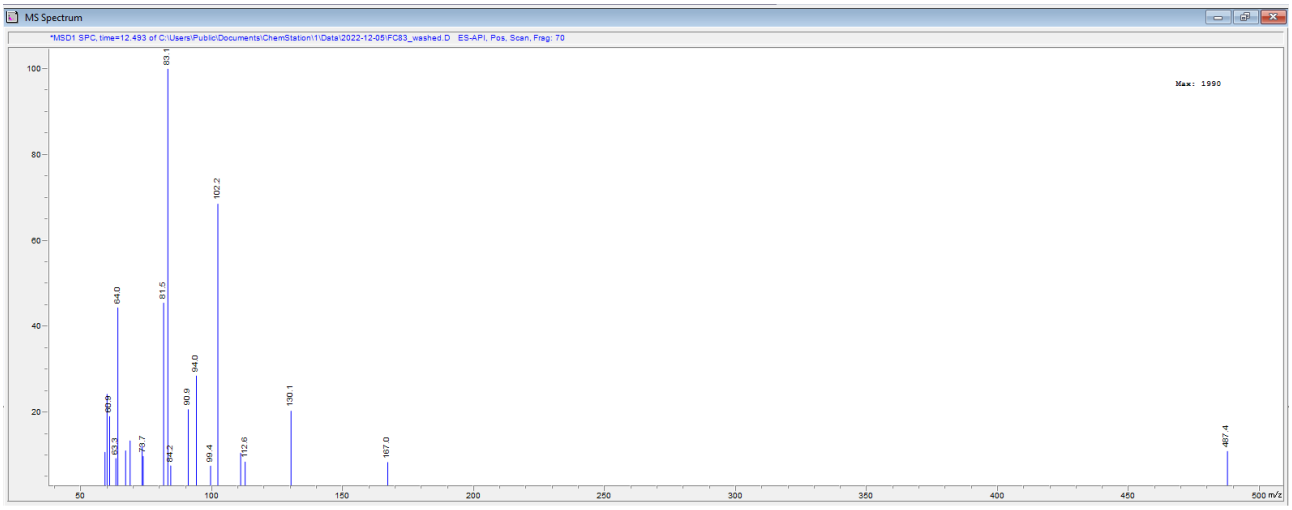
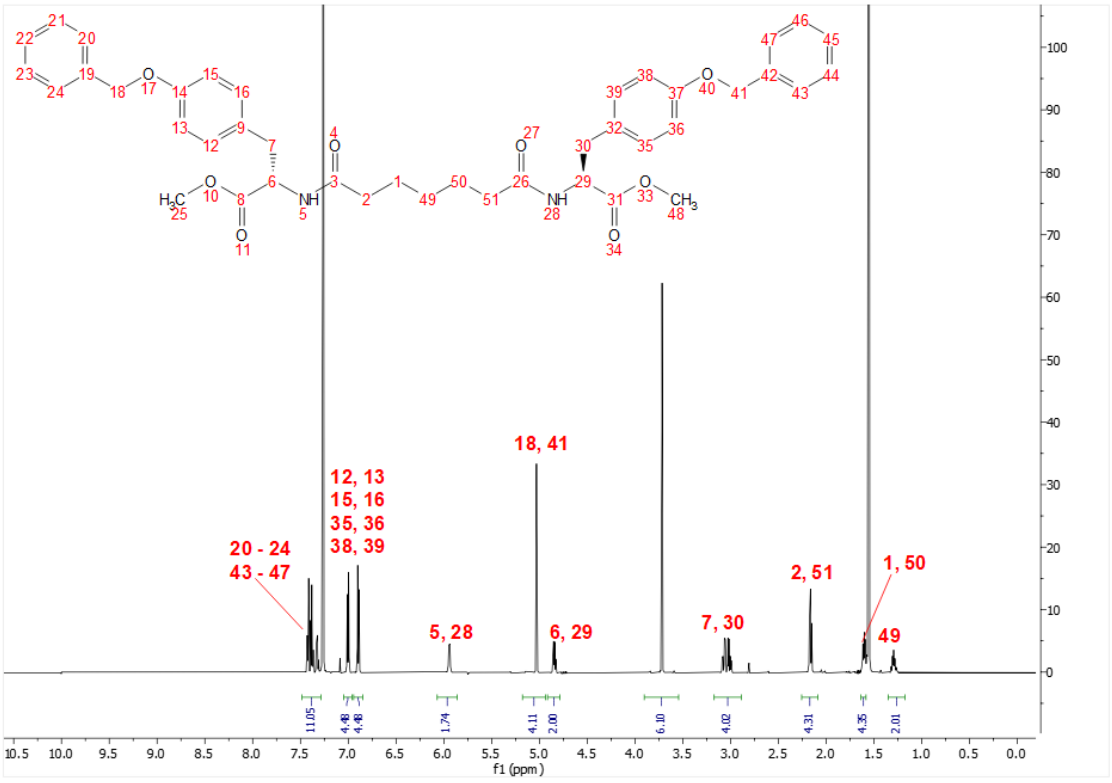




^{1}H NMR of gelator E



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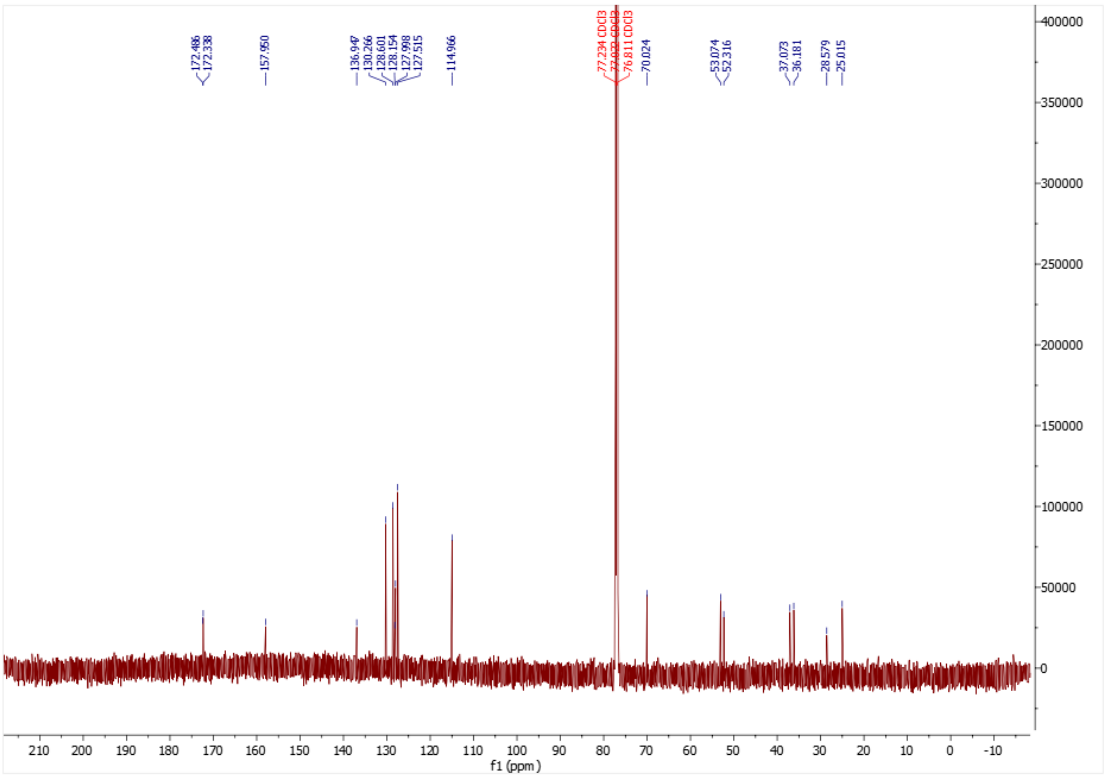

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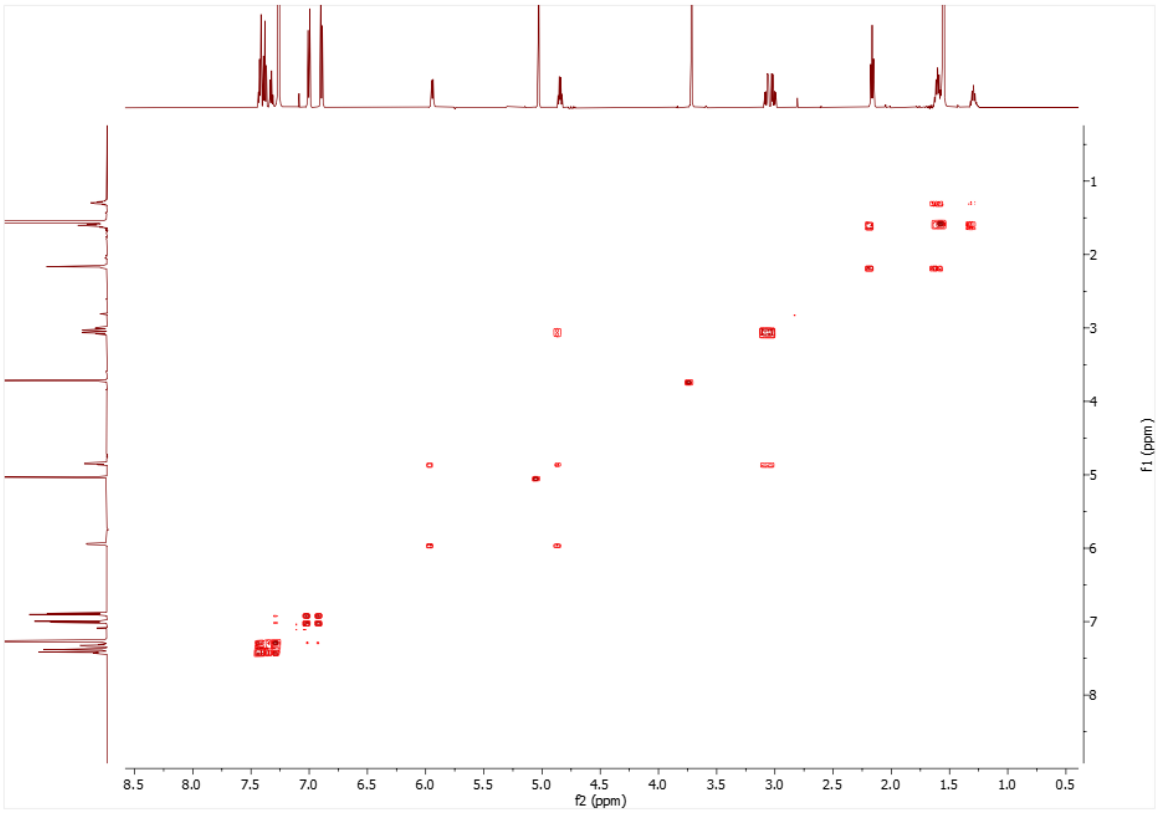
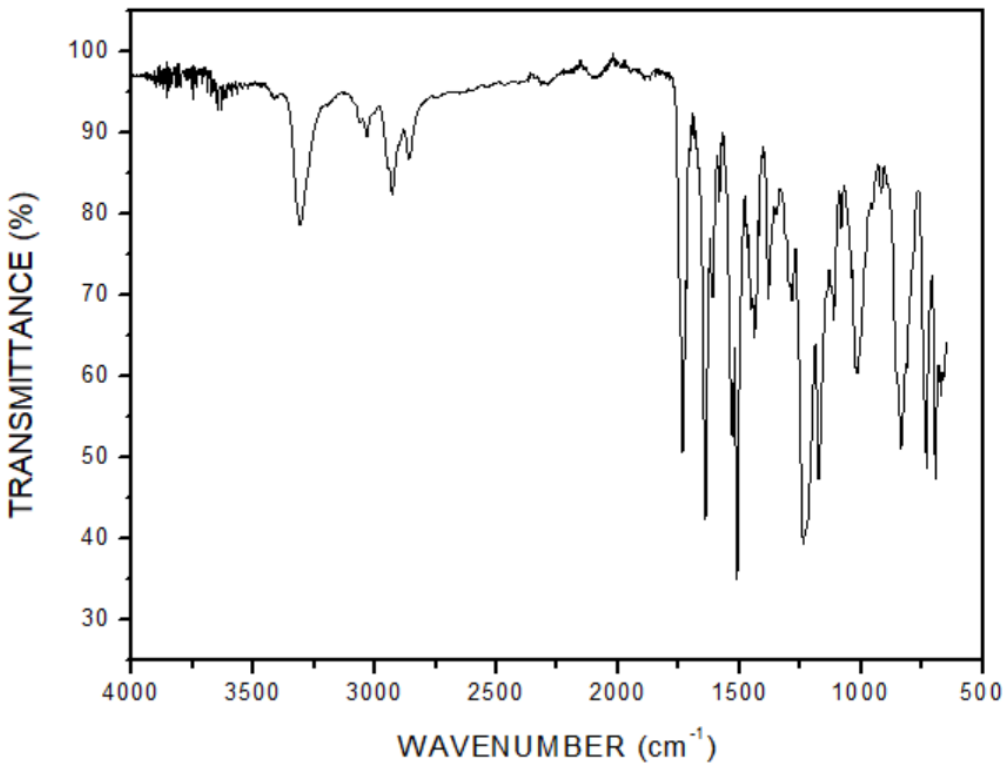


FT-IR spectrum of gelator E



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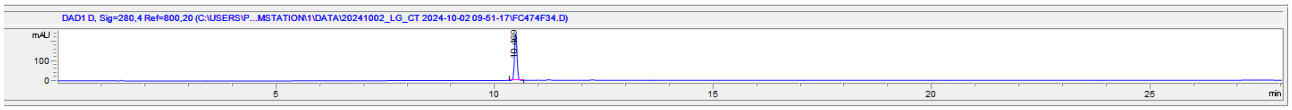
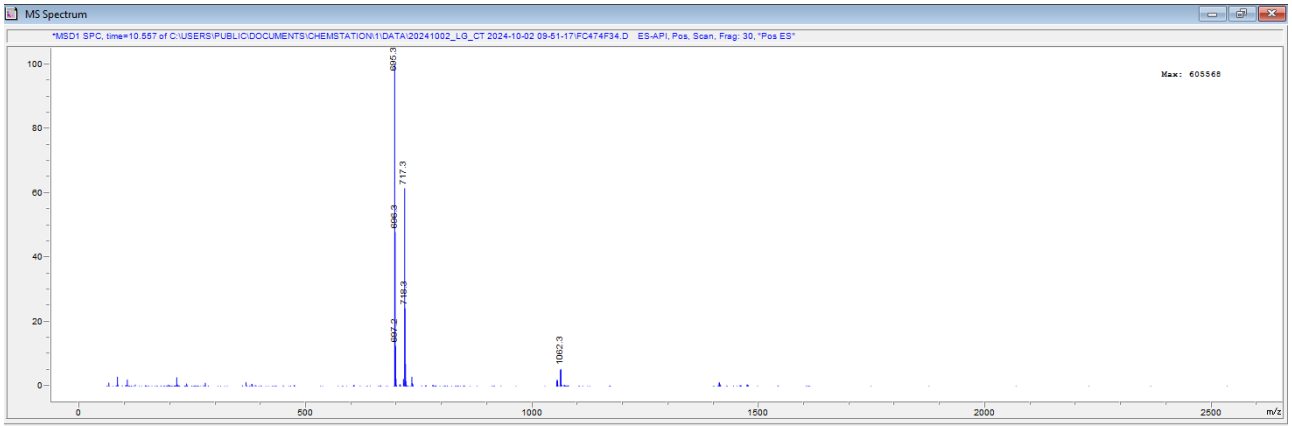
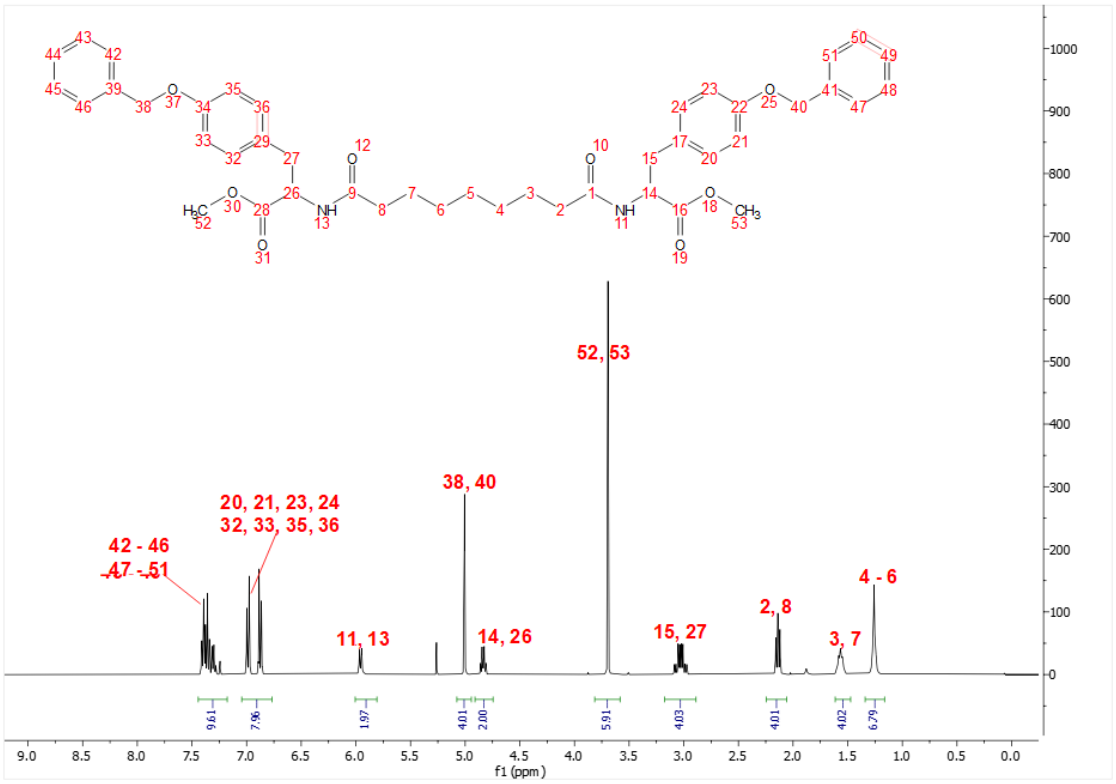




^{1}H NMR of gelator F



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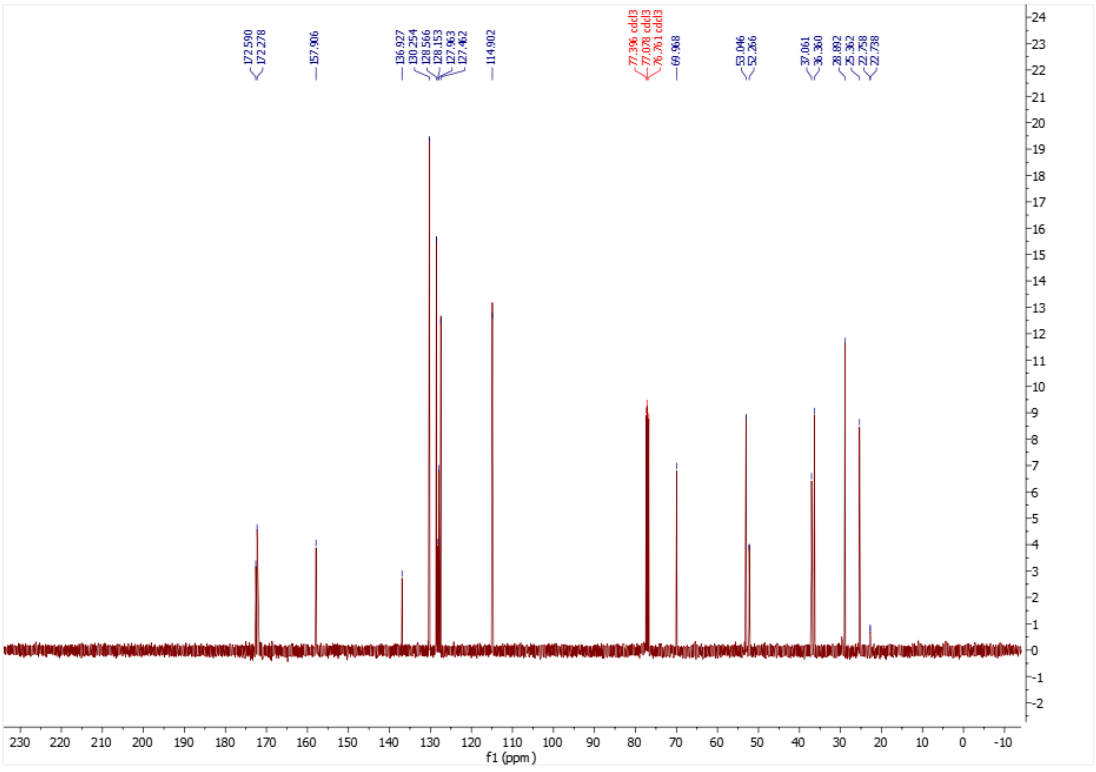
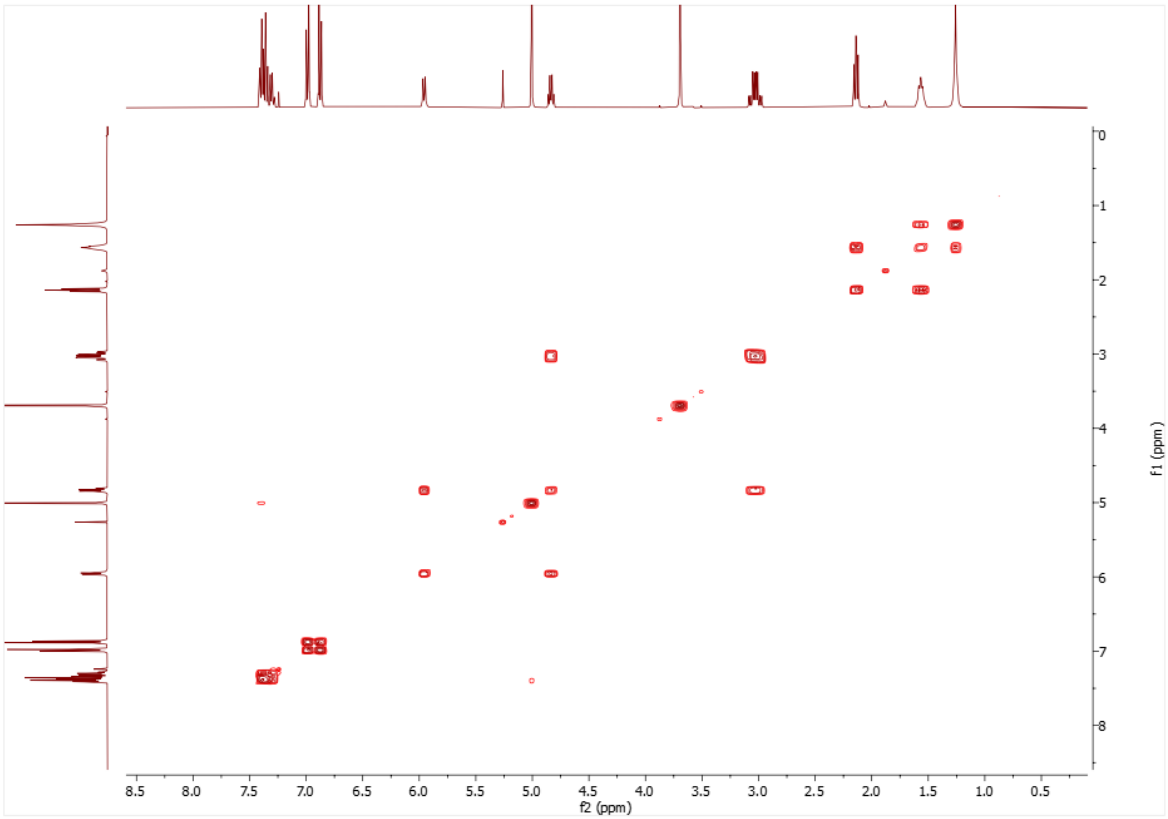
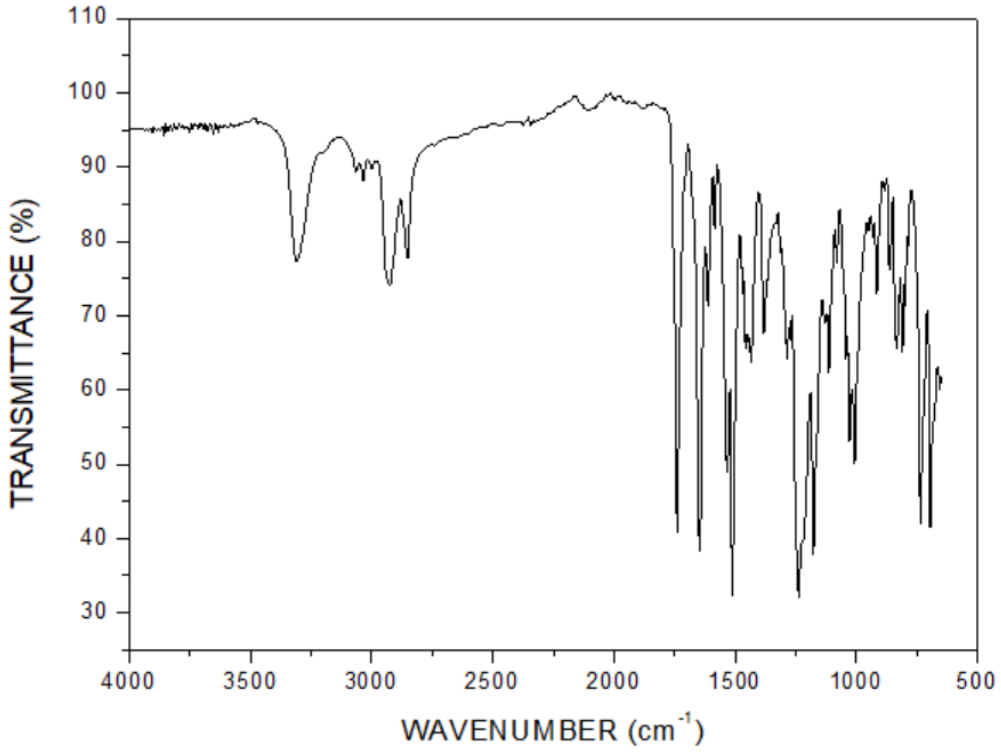


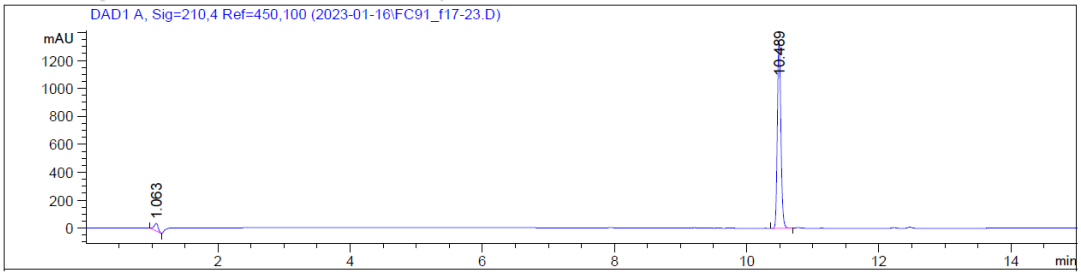
COSY NMR of gelator F



FT-IR spectrum of gelator F



HPLC-MS of gelator F



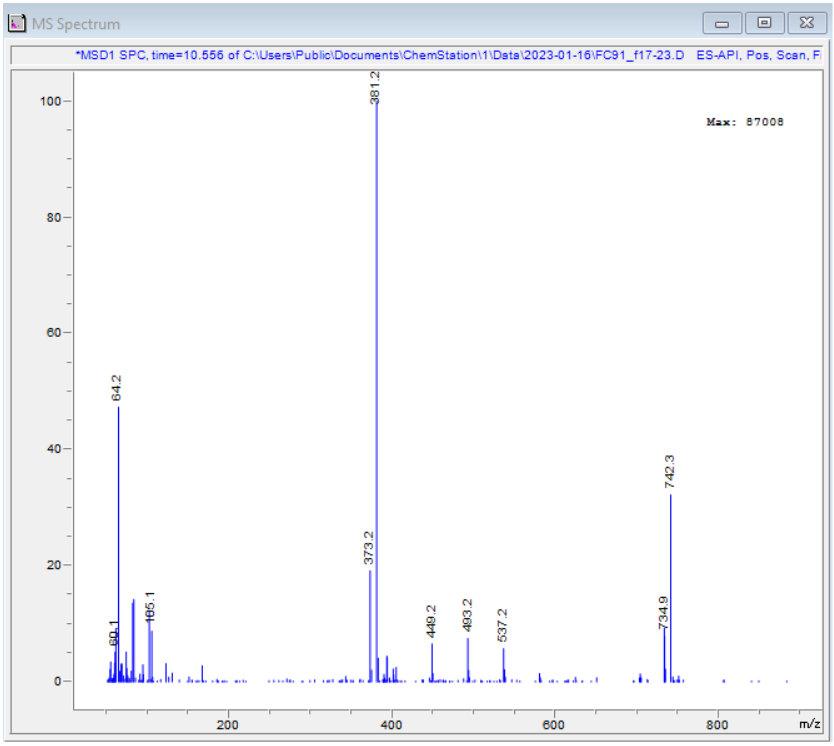


Table S1. List of the properties of the green solvents used (T_b, dielectric constant and density) taken from *stenutz.eu*; the LogP were calculated using *molinspiration* (https://www.molinspiration.com). Hansen solubility parameters (δ_d, δ_p, δ_h) calculated with the free software ZoomLab® from BASF, according to Hoy's method[1] (https://pharmaceutical.basf.com/global/en/pharma-solutions/about-basf-pharma/digitalization/zoomlab).

Solvent	T_b (°C)	Log*P*	Dielectric Constant	Density (g/mL)	δ_d	δ_p	δ_h
GVL	207	-0.46	36.14	1.103	16.86	11.30	10.29
DMC	90.3	0.15	3.09	1.07	14.52	10.84	14.79
DEC	127	0.90	3.10	0.976	15.11	9.29	12.34
^{i}PrOH	82	0.42	19.92	0.786	14.87	4.65	16.22
^{i}AmOH	131	1.33	15.20	0.812	14.19	9.22	15.79

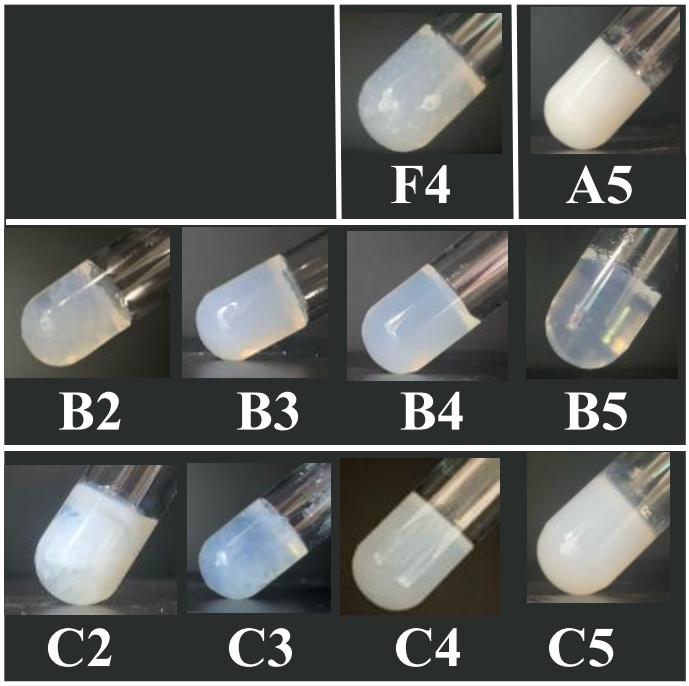


Figure S1. Photos of the gels obtained at their MGC.

Table S2. Gelation tests with the indication of T_d, the temperature necessary to dissolve the gelator.

Gelator	Gel	SOLVENT	T_d (°C)
D	-	All	-
A	**A5**	^{i}AmOH	60
	A7	GVL:H_2O 1:1	60
E	**E8**	GVL:H_2O 3:7	40
B	**B2**	DMC	60
	B3	DEC	90
	B4	^{i}PrOH	90
	B5	^{i}AmOH	90
	B6	GVL:H_2O 7:3	40
F	**F4**	^{i}PrOH	70
	F7	GVL:H_2O 1:1	60
C	**C2**	DMC	80
	C3	DEC	90
	C4	^{i}PrOH	90
	C5	^{i}AmOH	90
	C6	GVL:H_2O 7:3	60
	C7	GVL:H_2O 1:1	60
	C8	GVL:H_2O 3:7	60

Table S3. Maximum temperature (Tmax) and duration of the plateau for the temperature sweep tests on the different molecule/solvent samples.

Gel	Tmax (°C)	Plateau (min)
B2	75	5
B3	93	10
B5	93	10
C2	93	10
C3	93	10
C5	93	10
F4	75	10

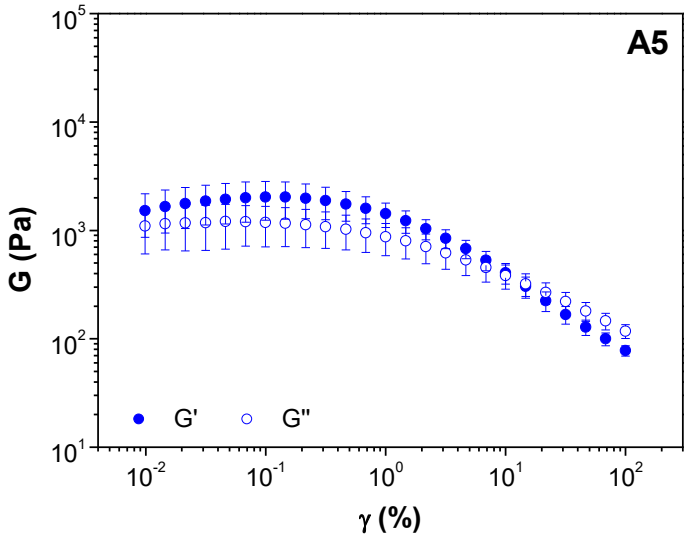


Figure S2. Amplitude sweep of the gel **A5**. The tests were performed in triplicate, and the results are reported as mean ± standard deviation.

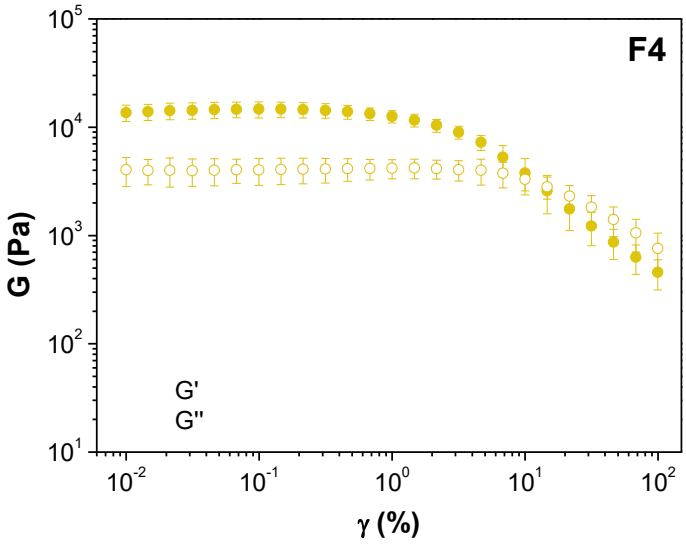


Figure S3. Amplitude sweep of the gel **F4**. The tests were performed in triplicate, and the results are reported as mean ± standard deviation.

Table S4. Values of G′ of the gels obtained at their MGC, taken from the amplitude sweeps at γ=0.03%

GEL	MGC	G′ (KPa)
A5	1.0%	1.9 ± 0.7
B2	1.0%	24.1 ± 1.3
B3	1.2%	36.3 ± 17.3
B4	0.4%	5.6 ± 0.4
B5	0.6%	3.0 ± 0.4
C2	1.0%	15.0 ± 3.7
C3	1.2%	6.6 ± 2.2
C4	0.6%	7.9 ± 3.4
C5	0.4%	4.1 ± 0.5
F4	1.0%	14.3 ± 2.4

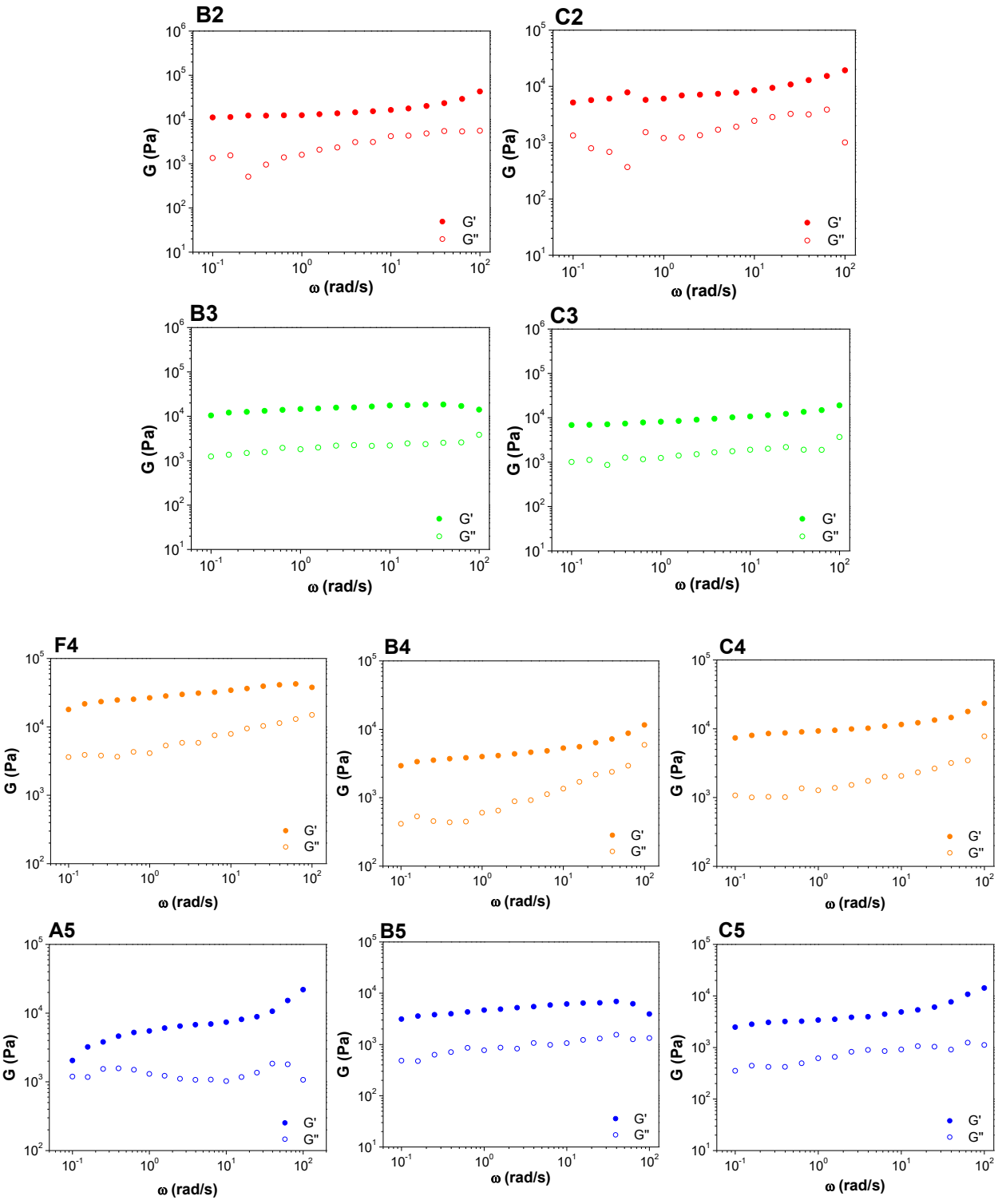


Figure S4. Frequency sweep of the gels obtained at their MGC (γ=0.01%).

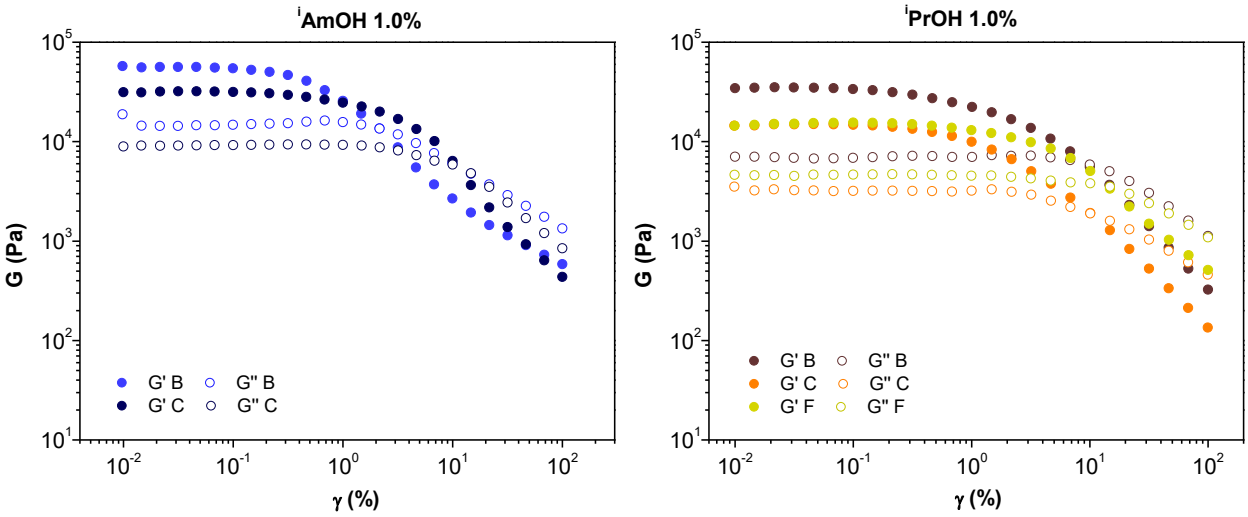


Figure S5. Comparison of the amplitude sweep of the gels obtained in ^{i}AmOH and ^{i}PrOH at 1.0% w/v concentration.

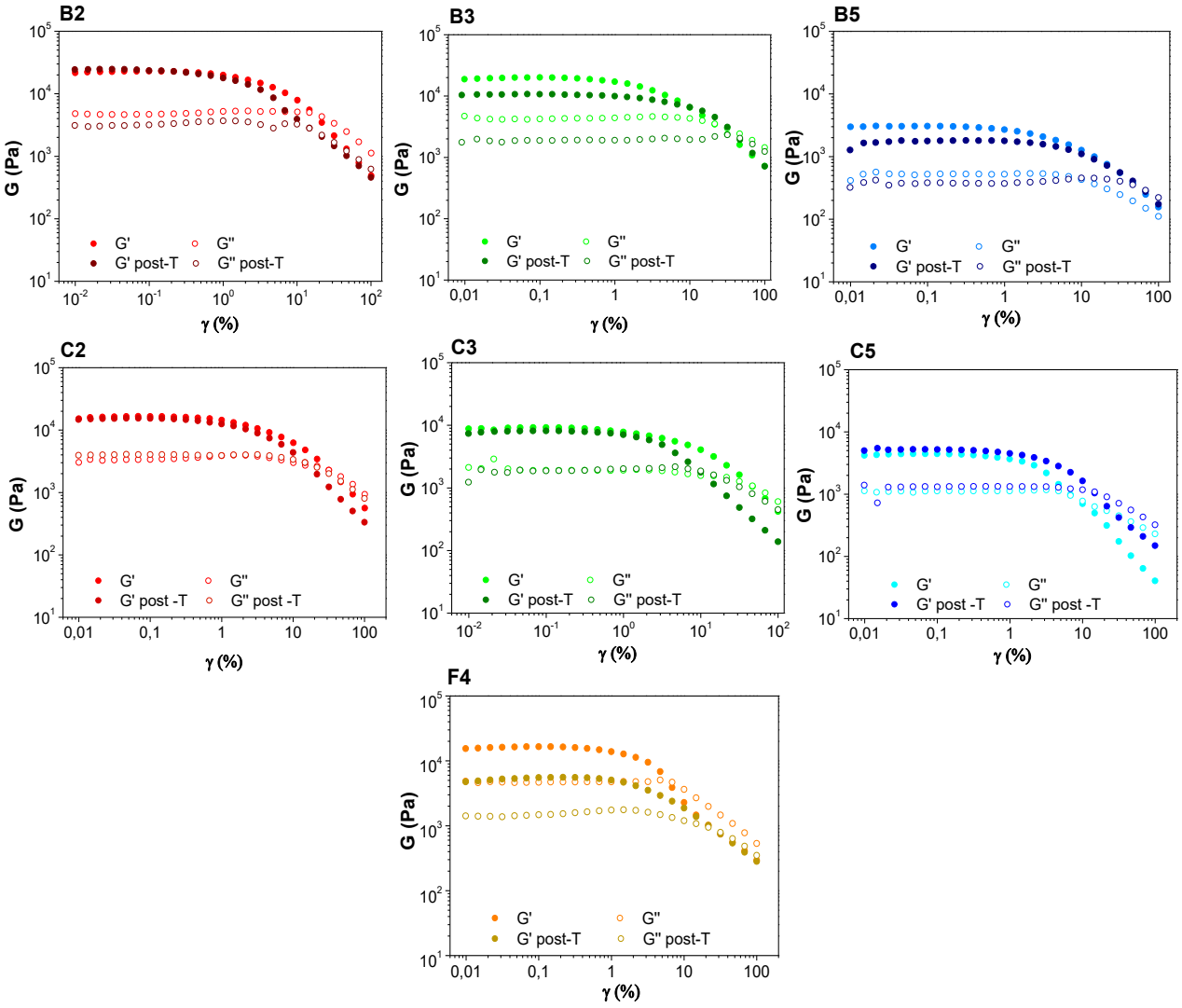


Figure S6. Comparison of the amplitude sweep of the gels before and after the temperature sweep analysis (complete dissolution and reformation of the gels).

Table S5. T_{gel} of the gels obtained at their MGC, grouped by solvent, compared with their solvent boiling point.

SAMPLE	Solvent	T_{gel} (°C)	Solvent b.p. (°C)	Termoreversible
A5	5 – ^{i}AmOH	-	130-132	NO
F4	4 – ^{i}PrOH	70	81-83	YES

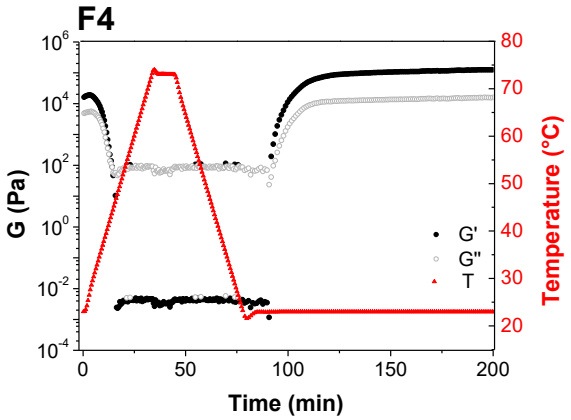


Figure S7. Temperature sweep tests of gel **F4**. G' (black, full circles), G'' (grey, empty circles), temperature ramp (red triangles).

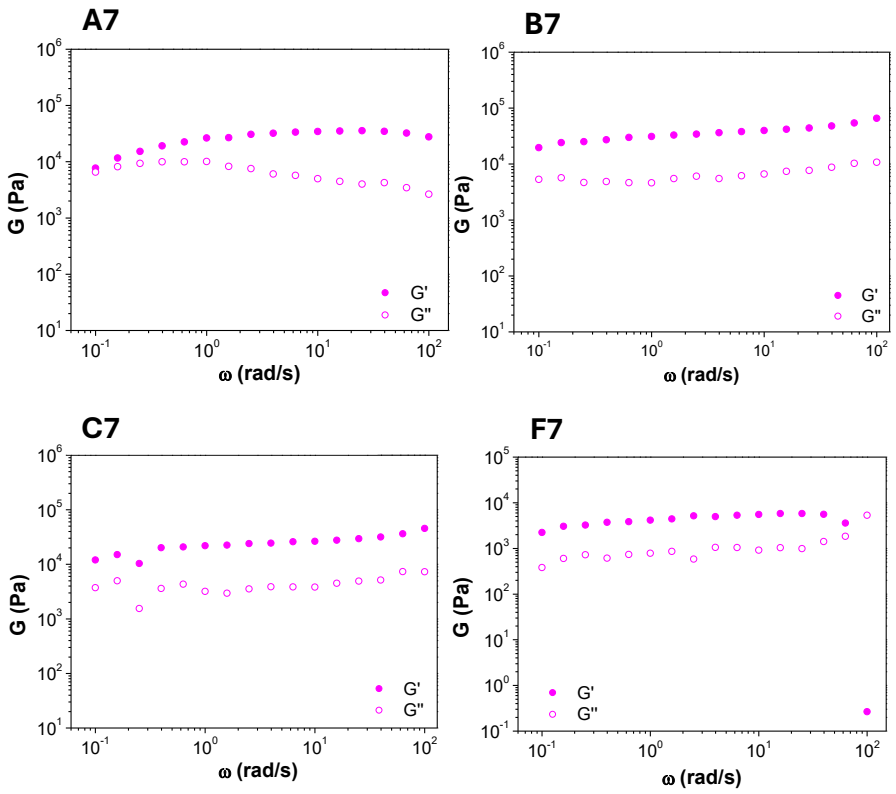


Figure S8. Frequency sweep of the gels obtained at their MGC (γ=0.01%).

Table S6. Values of G′ of the gels obtained at their MGC, taken from the amplitude sweeps at γ=0.03%

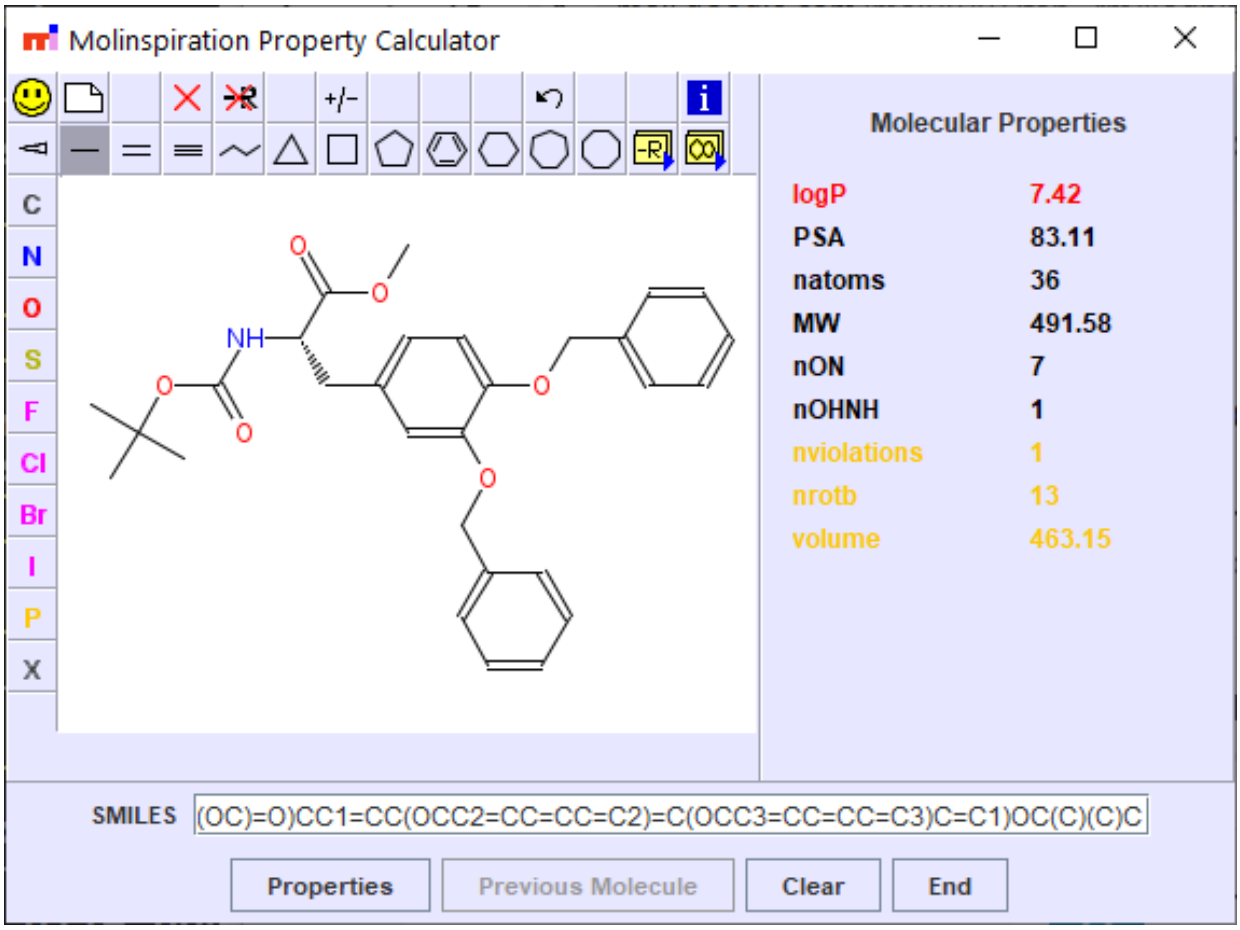
GEL	MGC	G′ (KPa)
A7	1.2%	27.2 ± 12.7
F7	0.6%	1.0 ± 0.3
B7	1.6%	39.1 ± 21.9
C7	1.0%	36.7 ± 2.6

Table S7. Data extracted from the X-ray diffraction analysis. For each peak the maximum angle (2θ), the angular spacing associated (d), and the crystallite size (D) are reported.

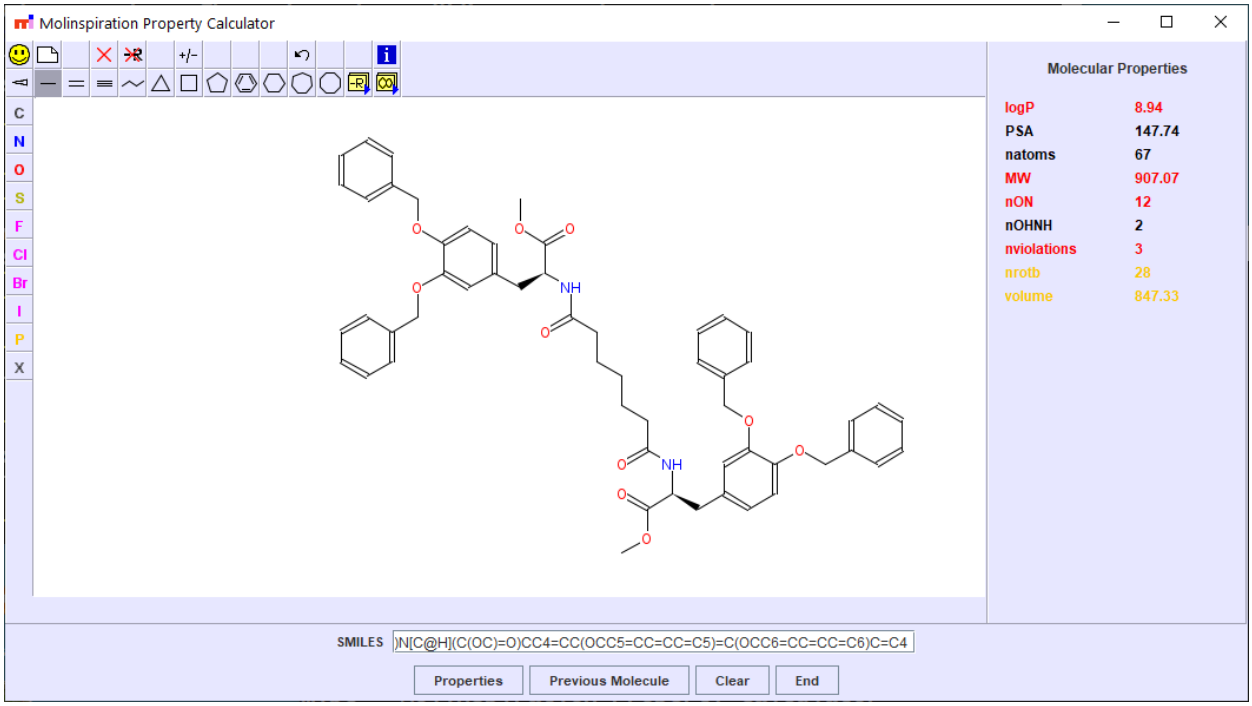
		A	B	C
Peak 1	**2θ (°)**	5.6	5.8	4.7
	d (Å)	15.8	15.1	18.7
	D (nm)	36.2	5.4	9.9
Peak 2	**2θ (°)**	6.2		6.5
	d (Å)	14.3		13.6
	D (nm)	34.6		12.2
Peak 3	**2θ (°)**	9.5		9.3
	d (Å)	9.3		9.6
	D (nm)	29.5		11.2
Peak 4	**2θ (°)**	10.7		
	d (Å)	8.3		
	D (nm)	21.6		

LogP calculations from https://molinspiration.com/docu/mipc/:

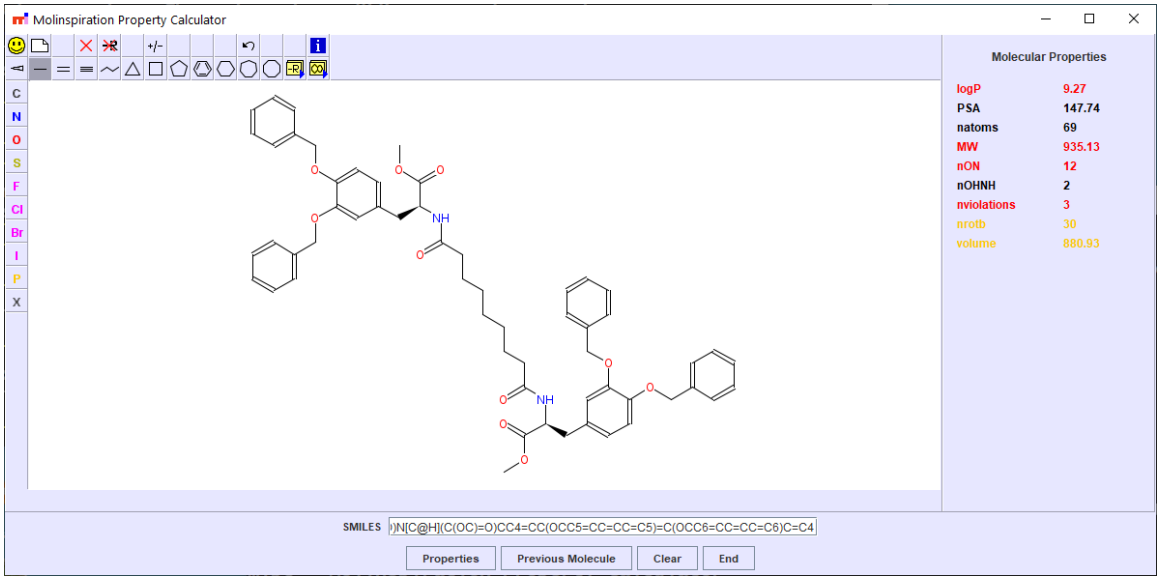
Compound A



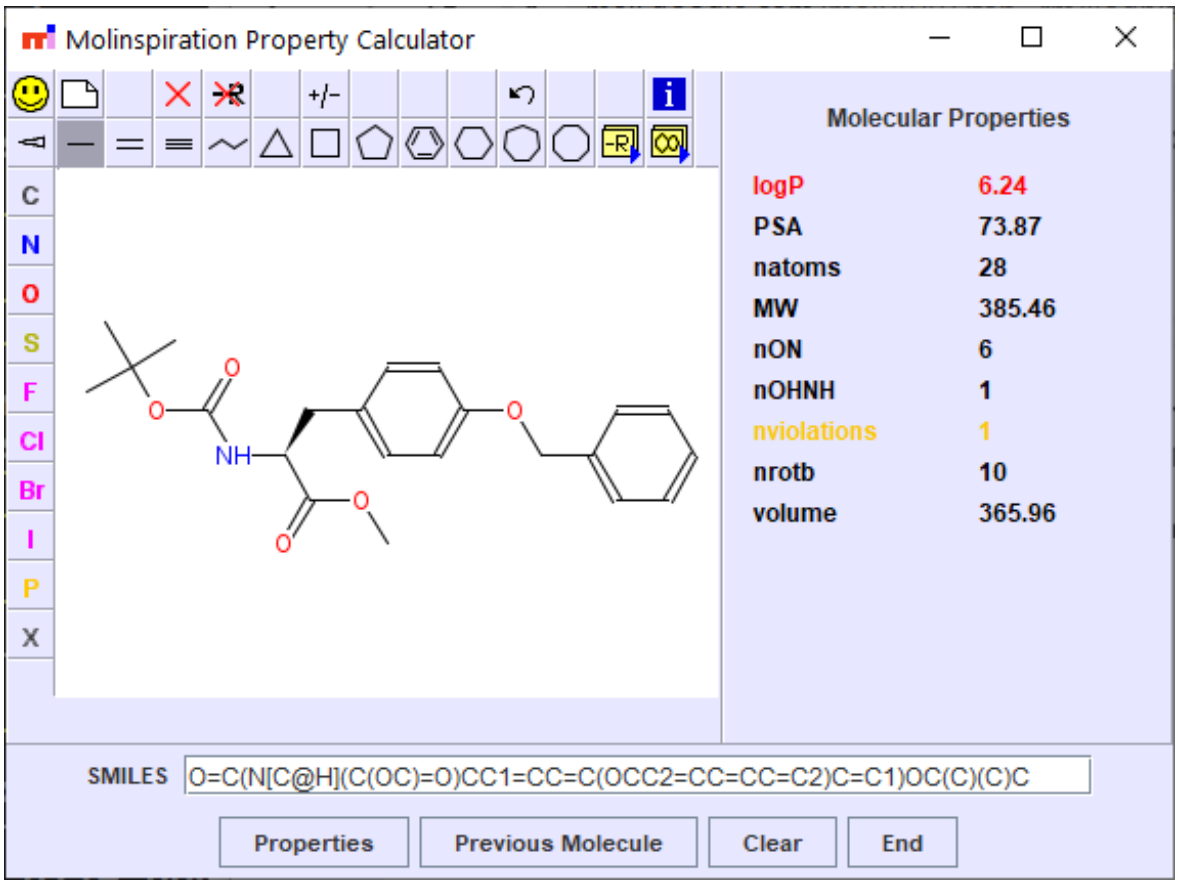
Compound B



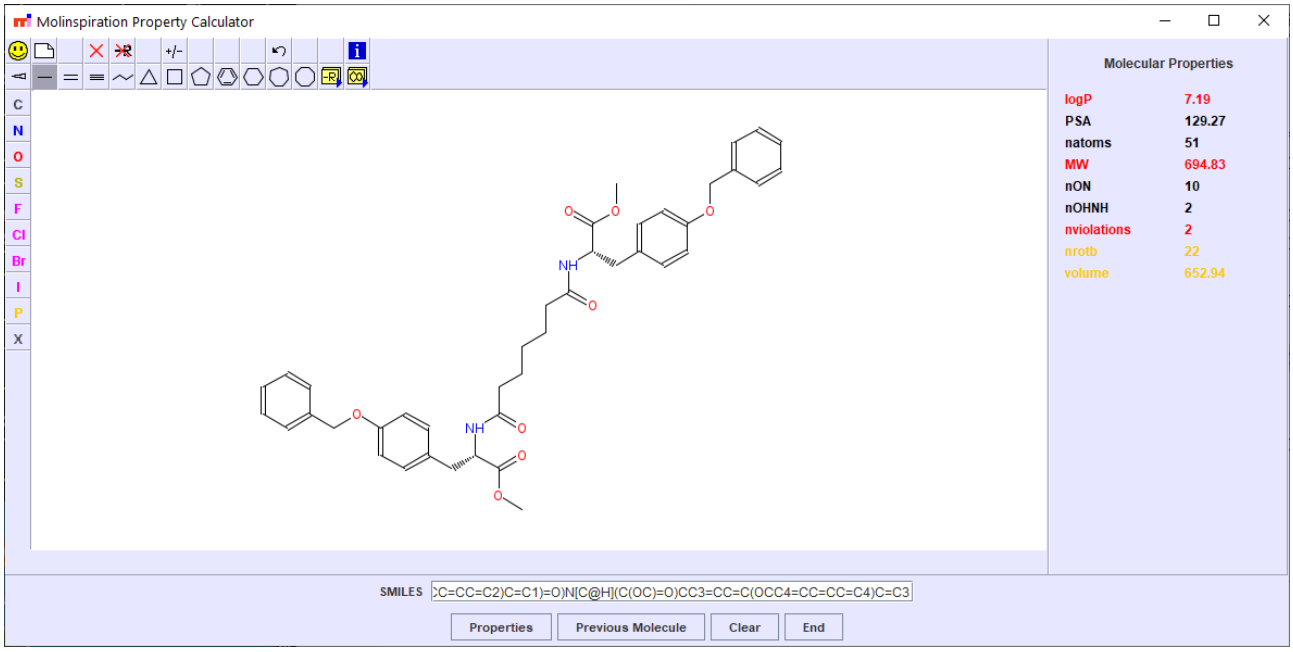
Compound C



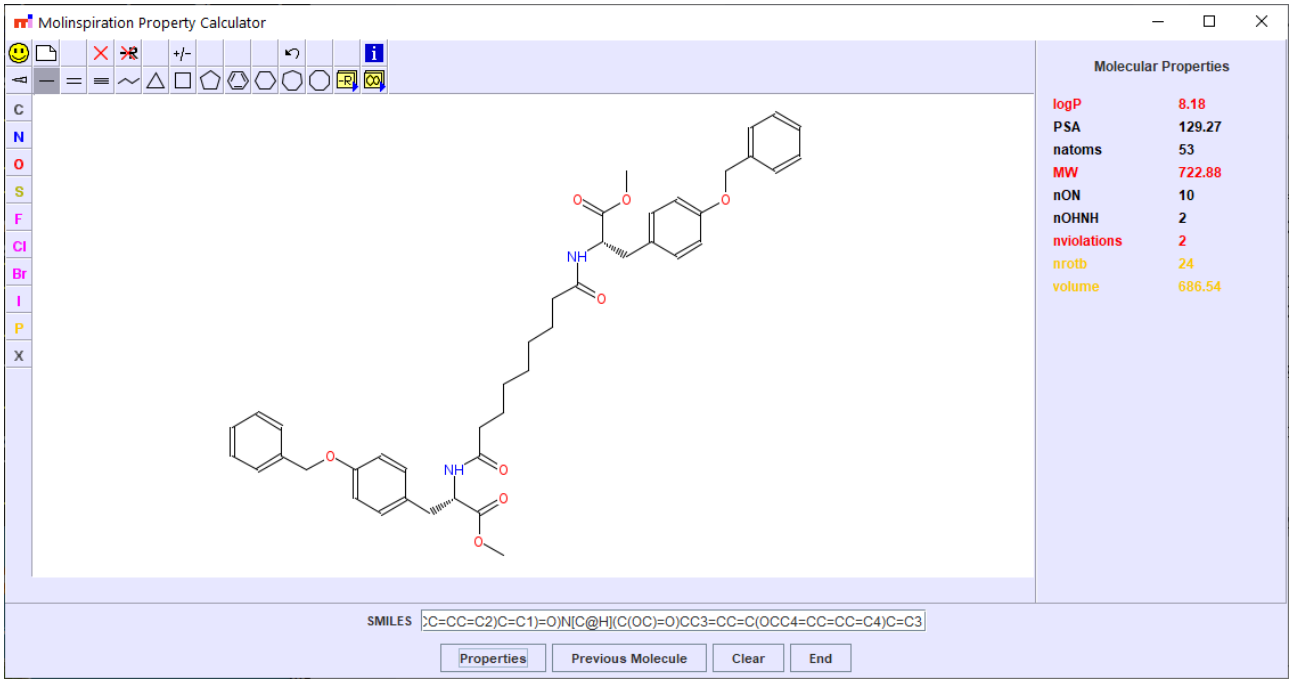
Compound D



Compound E



Compound F



References.

(1) Hoy, K. L. Tables of Solubility Parameters, Union Carbide Corp., Research and Development Dept., South Charleston, WV, 1985.