Supporting Information

Sulfonamide as amide isostere for fine-tuning the gelation properties of physical gels

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1. Tabular data of gelation ability and gel properties

Table S1 Gelation ability and typical gel properties of **Sulfo-Glu** in H_2O and diverse organic solvents.[a]

Solvent	CGC (g/L)	Gelation time (min)	T_{gel} (ºC)	Appearance
CH_2Cl_2	32.5±3.9	2.77±0.10	50.7±2.4	OG
$CHCl_3$	45.0±5.0	1.95±0.18	57.0±2.2	OG
CH_3CN	3.5±0.2	20.8±0.3	35.5±0.5	OG
H_2O	33.3	>12h	55.5±1.5	OG
MeOH	PG at ≤ 200 g/L			
Glycerol	5.5±0.6	15±2	32	OG
Et_2O	PG at ≤ 200 g/L			
Hexane	PG at ≤ 200 g/L			
Xylene	23.6±1.4	3.58±0.41	50.5±1.5	OG
Benzene	18.2	0.78±0.11	66.7±1.8	OG
Toluene	13.8±0.5	7.37±0.19	72±2	OG
EtOH	PG at ≤ 200 g/L			
*i*PrOH	PG at ≤ 200 g/L			
2-Butanol	PG at ≤ 200 g/L			
1-Hexanol	PG at ≤ 200 g/L			
DMSO	Soluble			
DMF	Soluble			
THF	PG at ≤ 200 g/L			
AcOEt	47.2±2.8	6.29±0.21	42	OG
Acetone	PG at ≤ 200 g/L			
Chlorobenzene	26.8±1.8	85±5	58.5±0.5	TLG/OG
Benzonitrile	47.2±2.8	4.20±0.33	58±1	TLG/OG

[a] Error values reported as STDV were estimated from at least two randomized experiments. Abbreviations: CS = clear solution resulting after heating a mixture of the compound and the corresponding solvent; I = insolubility of the compound in the corresponding solvent; room temperature ionic liquid); OG = opaque gel; P = precipitation of the compound from isotropic solutions of **Sulfo-Glu** and the corresponding solvent; PG = partial gel (phase separation between gel and sol after time); TLG = translucent gel.

Table S2 Gel properties of **Sulfo-Glu** in H_2O and diverse organic solvents at the maximum CGC of the three isosteres.[a]

Solvent	Concentration (g/L)	Gelation time (min)	T_{gel} (ºC)
CH_2Cl_2	180	28±6	72±2
$CHCl_3$	100	46±4	62±1
CH_3CN	110	23±5	71±1
Glycerol	20	239±16	61±1
Xylene	95	51±1	83±2
Benzene	200	21±3	80±1
Toluene	135	37±5	82±1

[a] Error values reported as STDV were estimated from at least two randomized experiments.

2. Concentration dependence of gelation time and T_{gel}

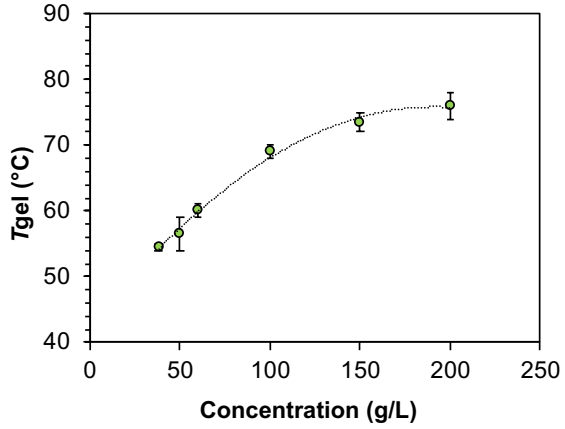


Fig. S1 T_{gel} evolution of **Sulfo-Glu** hydrogels depending on gelator concentration.

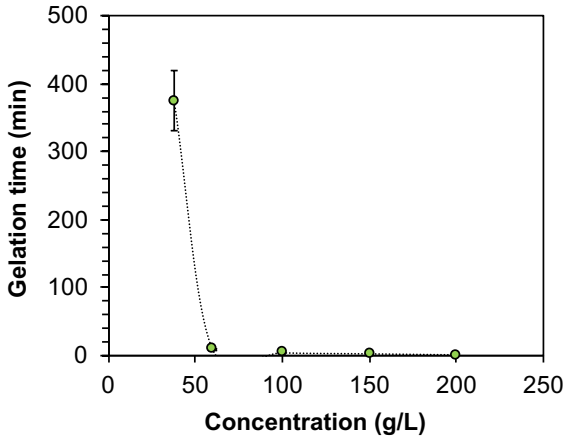
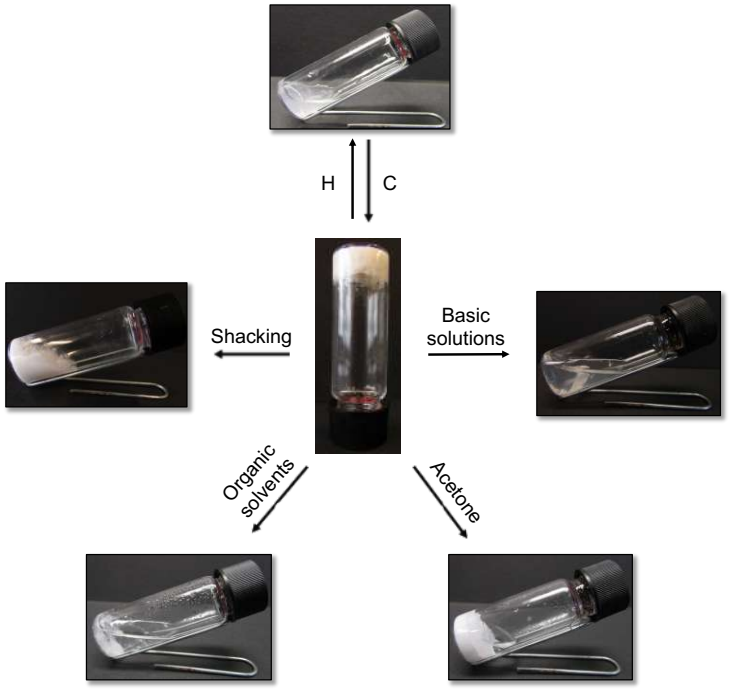


Fig. S2 Gelation time of **Sulfo-Glu** hydrogels depending on the gelator concentration.

3. External stimuli-responsive behavior

A)



B)

Fig S3 A) Representative diagram showing the external stimuli response map of **Sulfo-Glu** hydrogels. Abbreviations: C = cooling; H = heating. B) Appearance of **Sulfo-Glu** hydrogels in the presence of different additives and stimuli.

4. Additional electron microscopy images

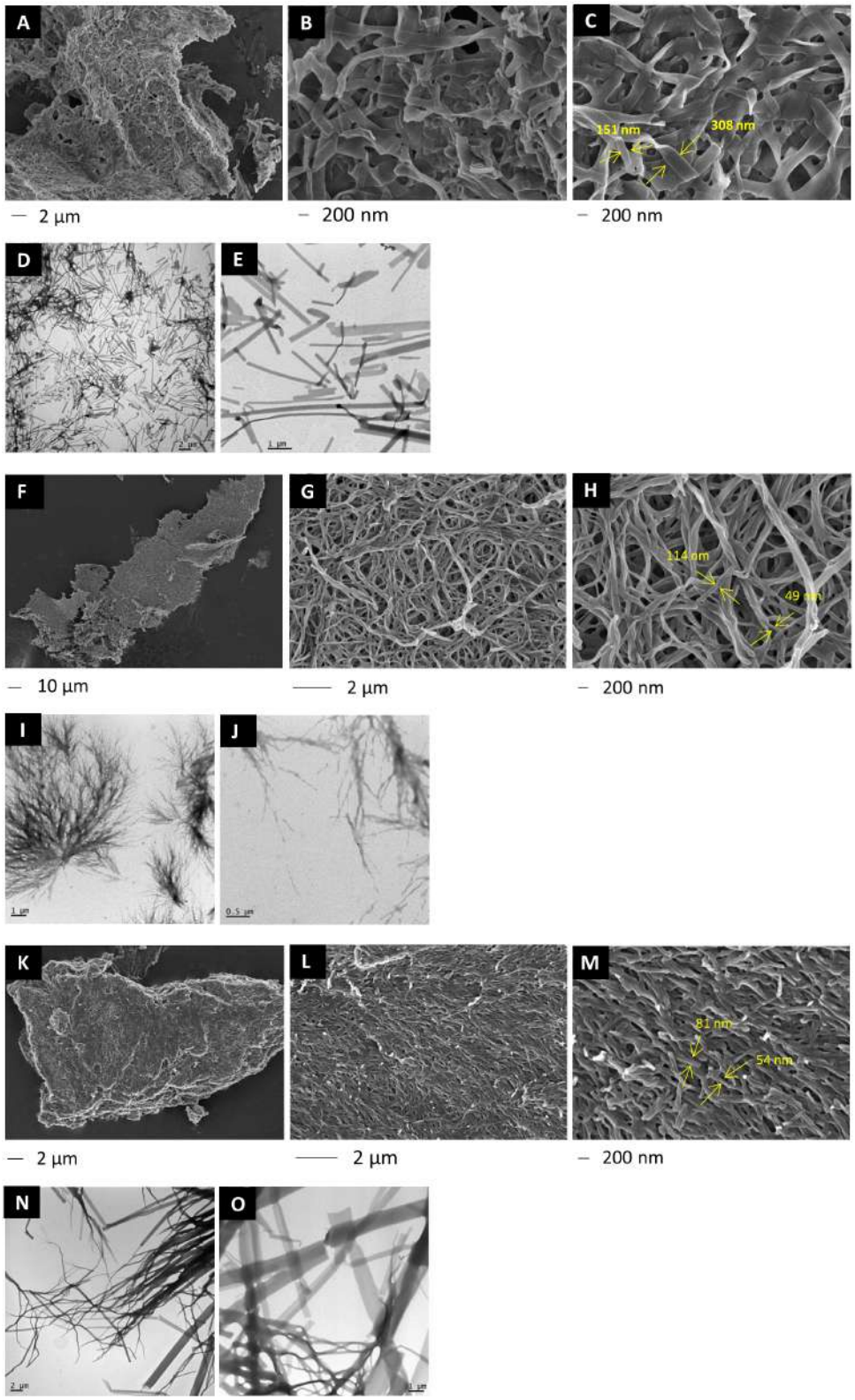


Fig. S4 FESEM (**A**-**C**, **F**-**H** and **K**-**M**) and TEM (**D**-**E**, **I**-**J** and **N**-**O**) images of materials derived from **Sulfo-Glu** at the CGC of gels made in different solvents. **A**-**E**: H_2O (33.3 g/L); **F**-**J**: CH_3CN (3.5 g/L); **K**-**O**: toluene (13.8 g/L).

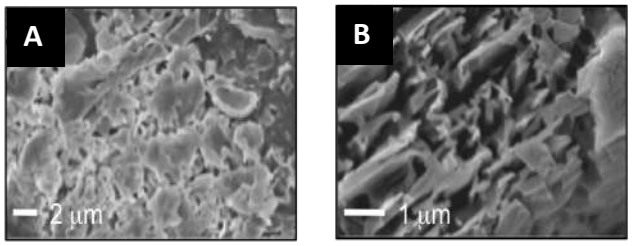
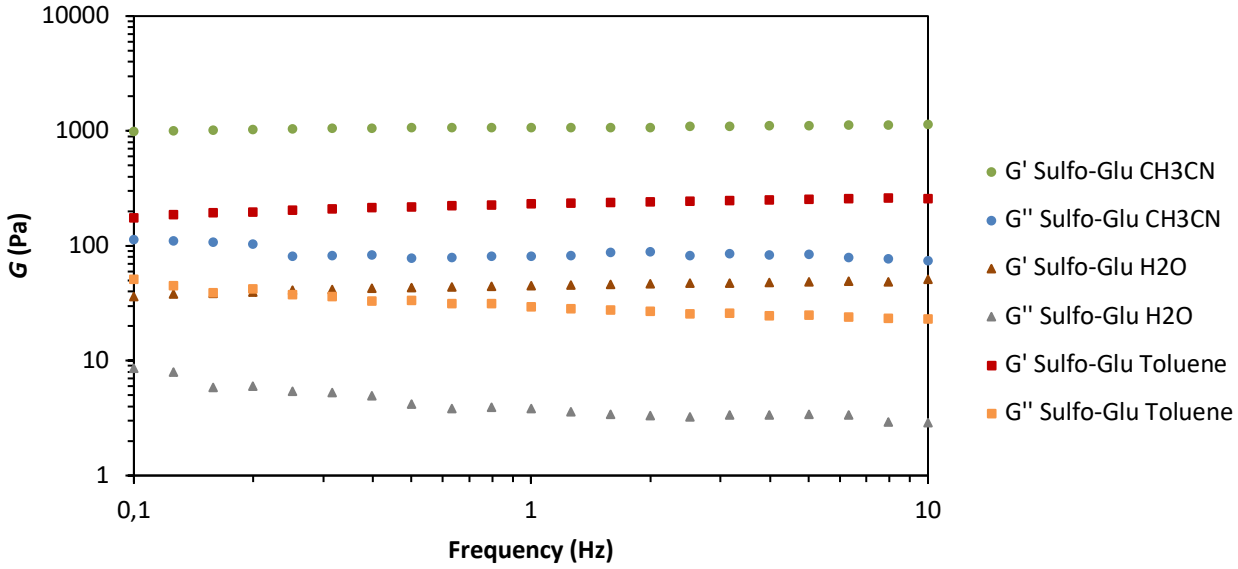
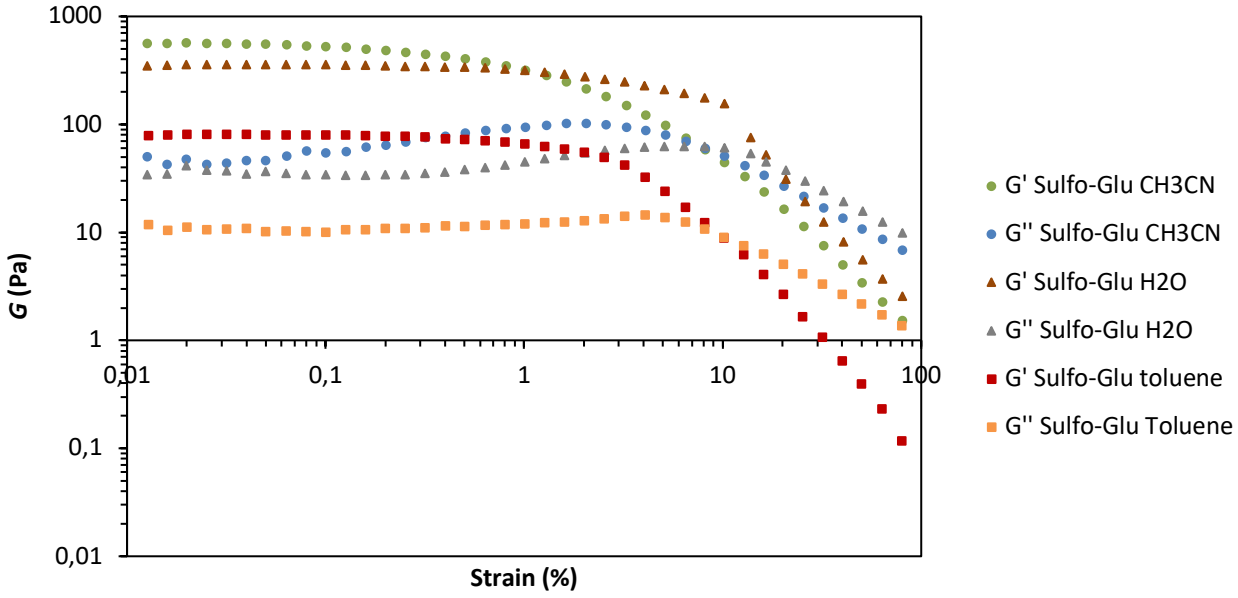


Fig. S5 FESEM images of the xerogels prepared from the hydrogels made of A) **C_{18}-Glu** (c = 25 g L^{-1}) and B) **Click-Glu** (c = 25 g L^{-1}).

We would like to acknowledge the use of Servicio General de Apoyo a la Investigación-SAI and the Laboratorio de Microscopías Avanzadas at Instituto de Nanociencia de Aragón, Universidad de Zaragoza, for FESEM and TEM imaging.

4. Rheological measurements





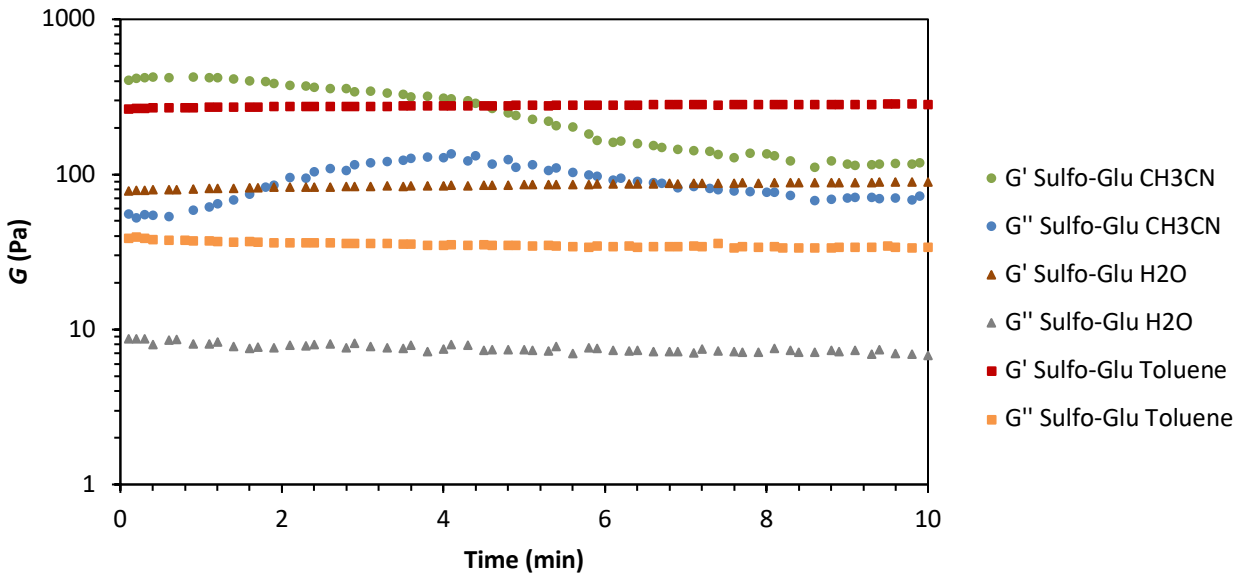
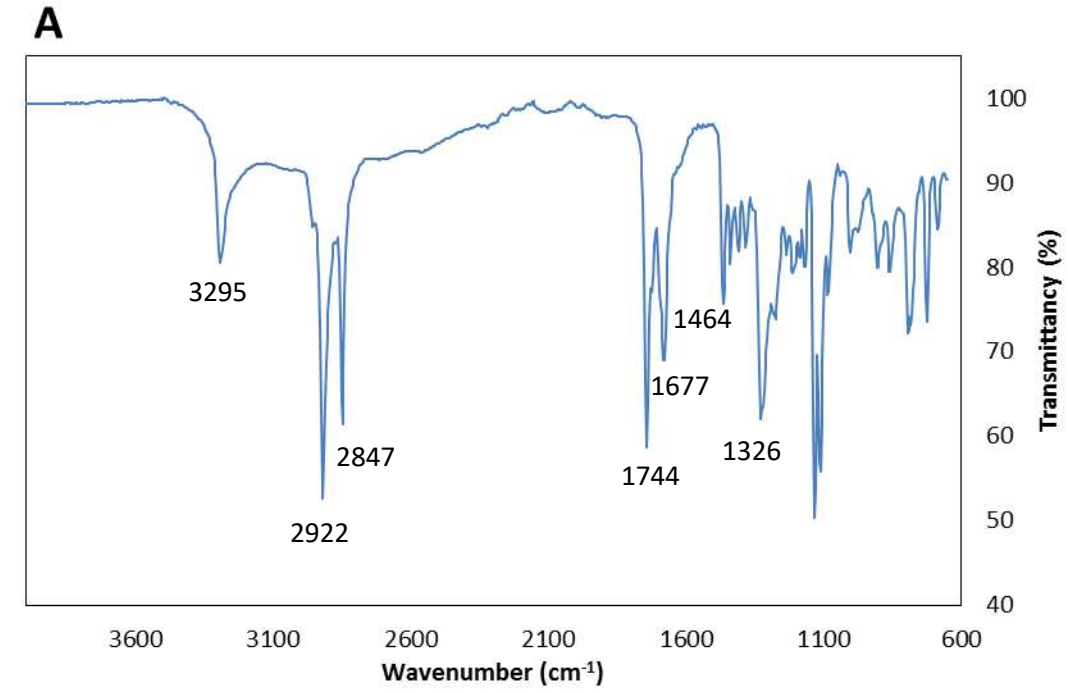
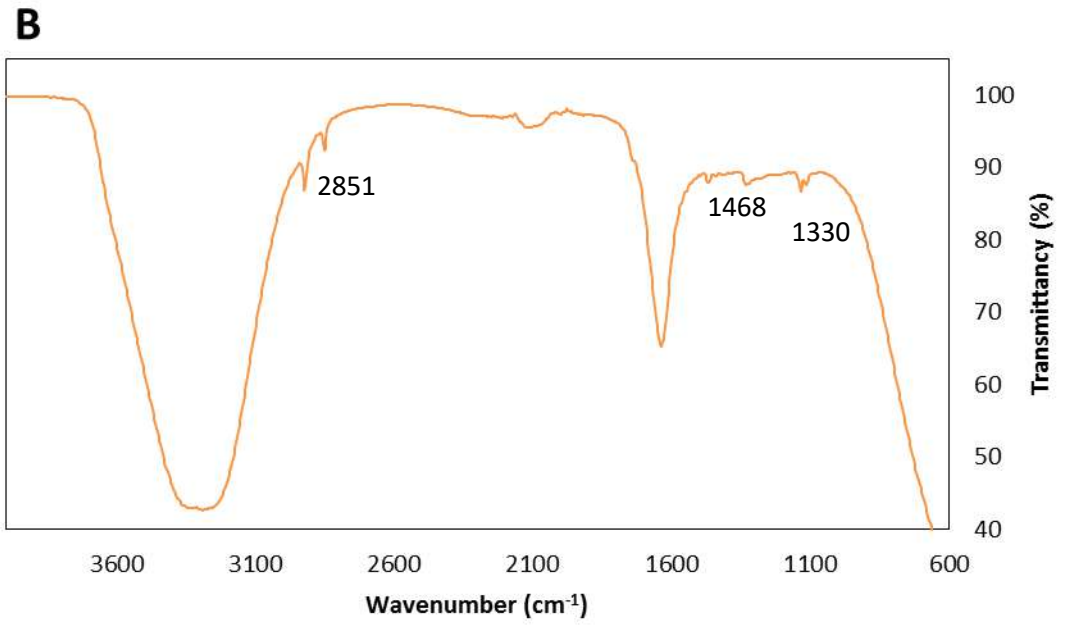
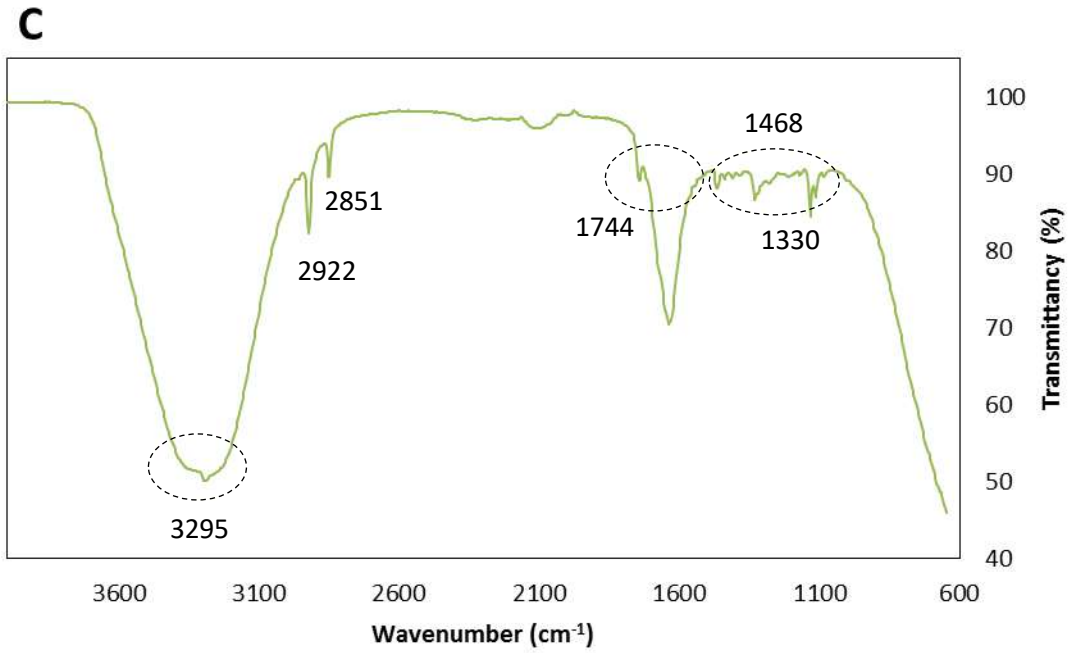


Fig. S6 Oscillatory rheological experiments of model gels prepared from **Sulfo-Glu** in water and toluene at 33.3 g/L. *Top*: DFS-plots. *Middle*: DSS-plots. *Bottom*: DTS-plots.

6. FT-IR spectra of gel and xerogel materials






C
3295
2922
2851
1744
1468
1330
100
90
80
70
60
50
40
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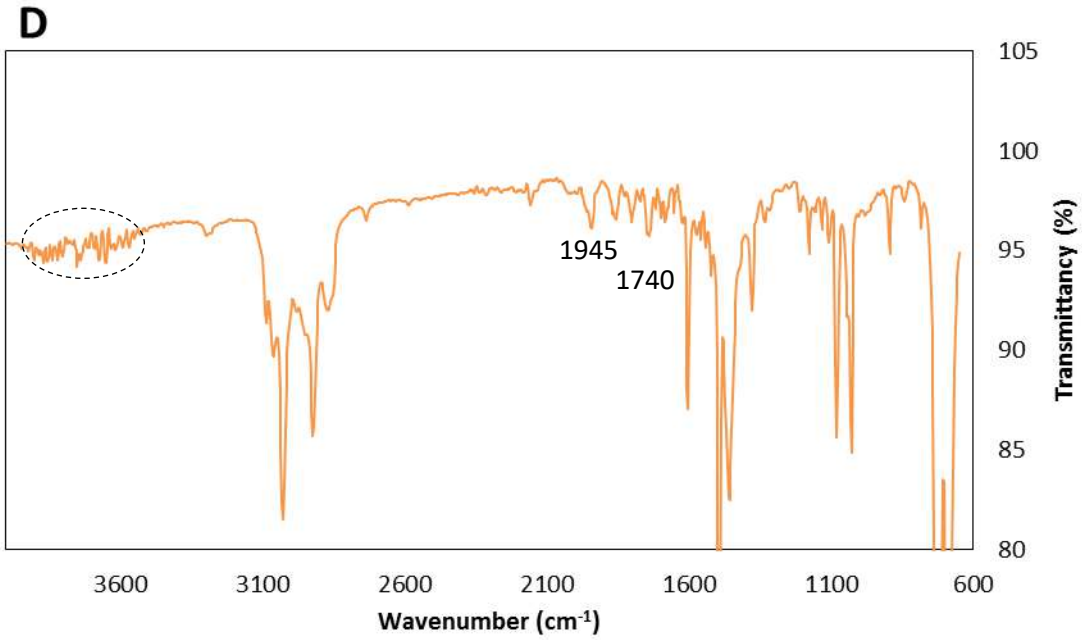
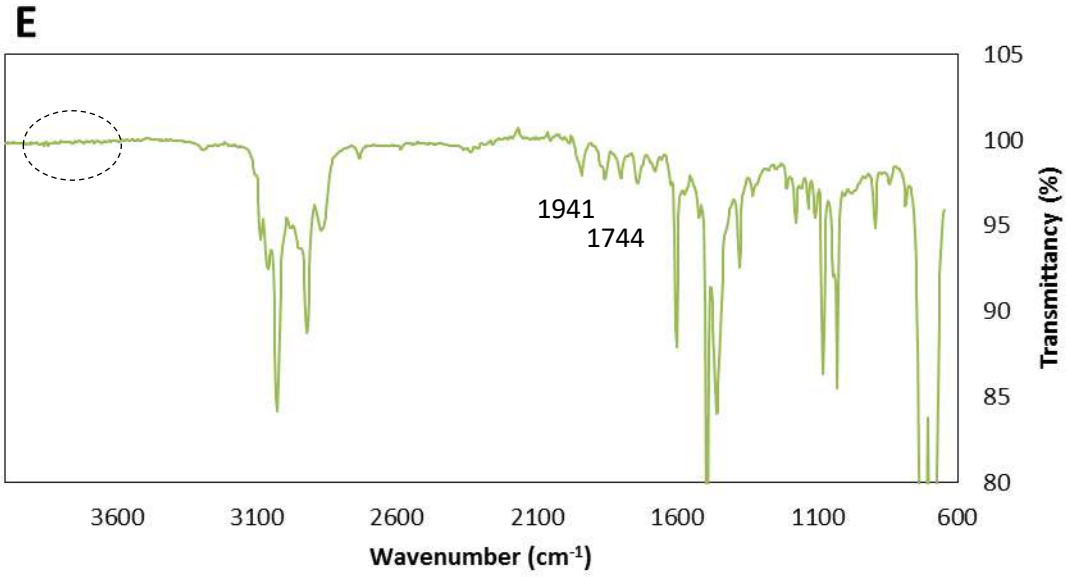
3100
2600
2100
1600
1100
600
Wavenumber (cm-1)


D
1945
1740
105
100
95
90
85
80
Transmittancy (%)
3600
3100
2600
2100
1600
1100
600
Wavenumber (cm-1)


E
1941
1744
105
100
95
90
85
80
Transmittancy (%)
3600
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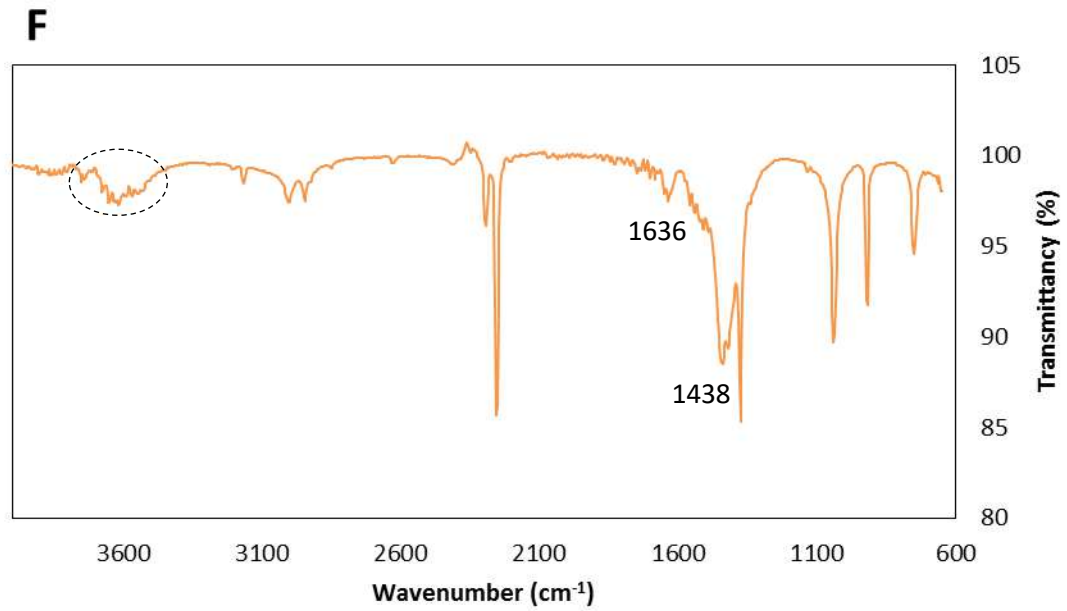
2600
2100
1600
1100
600
Wavenumber (cm-1)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1438
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Transmittancy (%)
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1100
600
Wavenumber (cm-1)

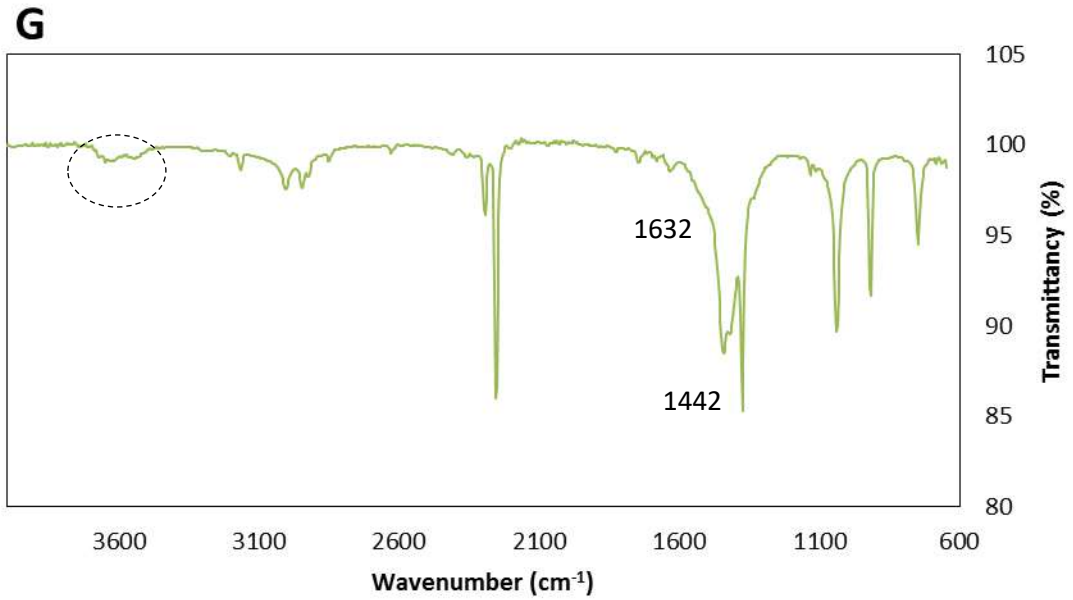
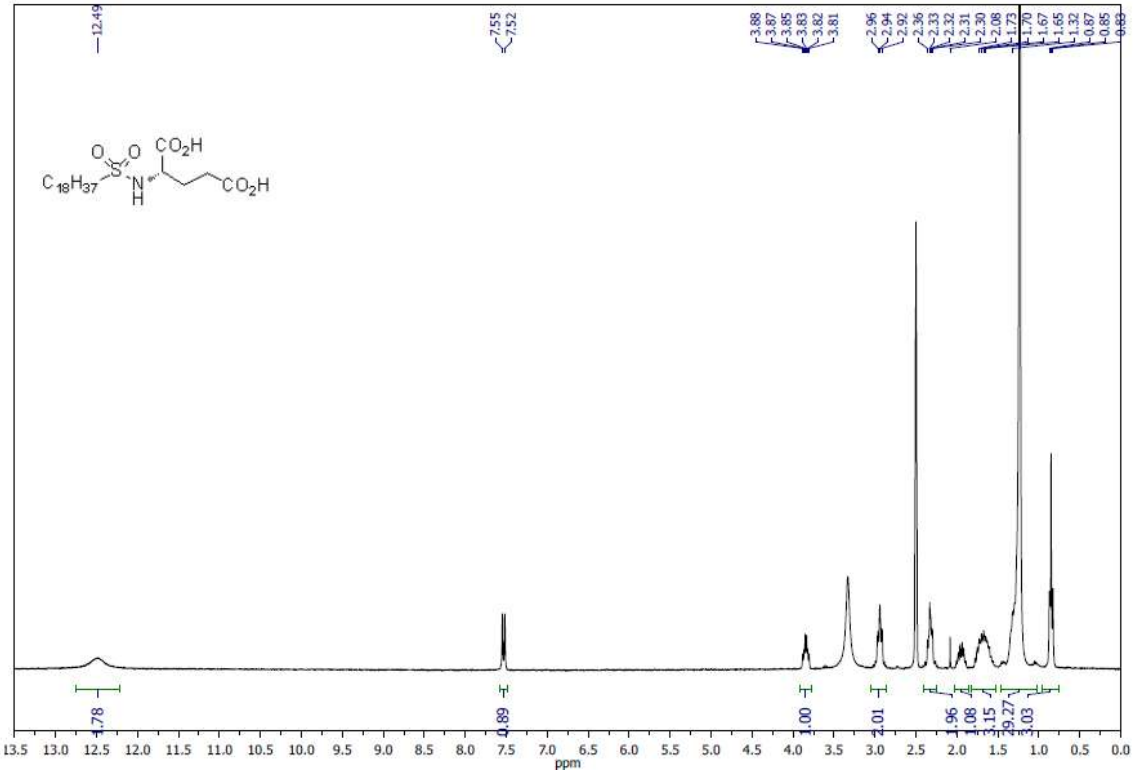
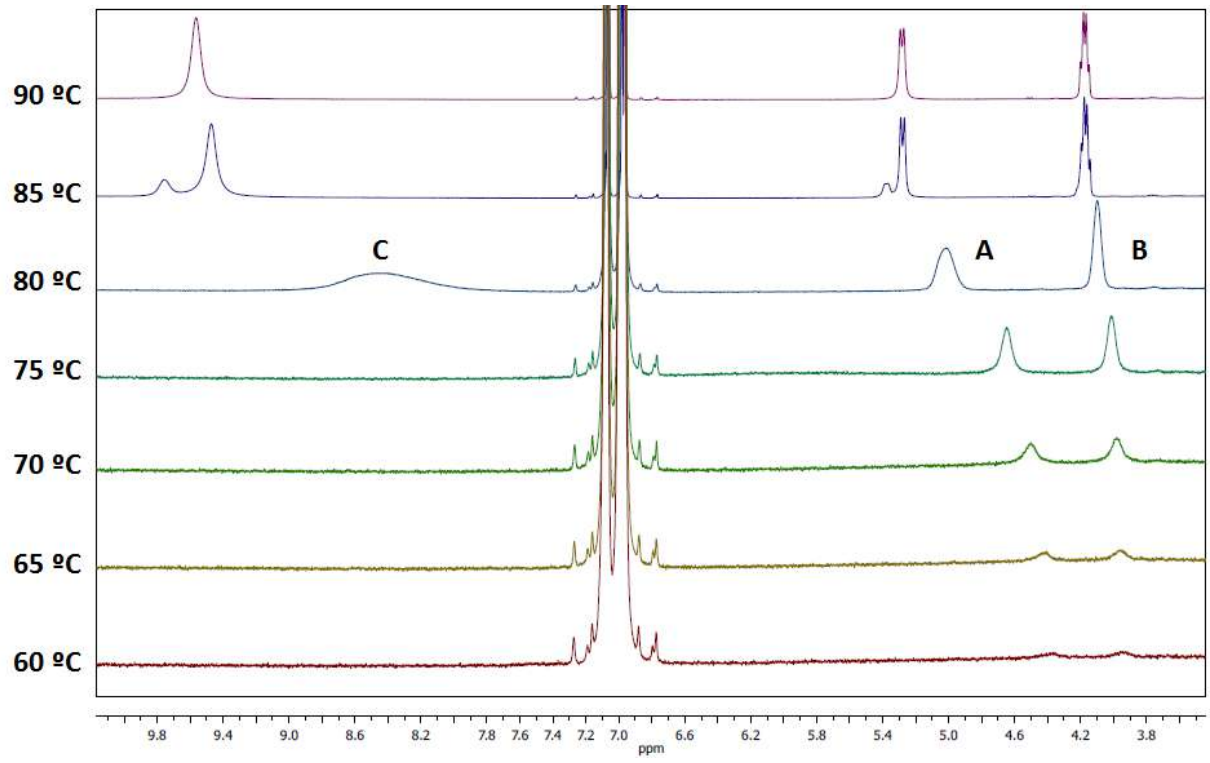


Fig. S7 FT-IR spectra of solid **Sulfo-Glu** and selected isotropic solutions/gels at the CGC of such gels. The measurements of the solutions were conducted at rt after all the **Sulfo-Glu** was dissolved and before the gel was formed. (A) solid **Sulfo-Glu**; (B) **Sulfo-Glu** dissolved in H_2O; (C) **Sulfo-Glu** gel in H_2O; (D) **Sulfo-Glu** dissolved in toluene; (E) **Sulfo-Glu** gel in toluene; (F) **Sulfo-Glu** dissolved in CH_3CN; (G) **Sulfo-Glu** gel in CH_3CN.

7. Variable temperature NMR experiments





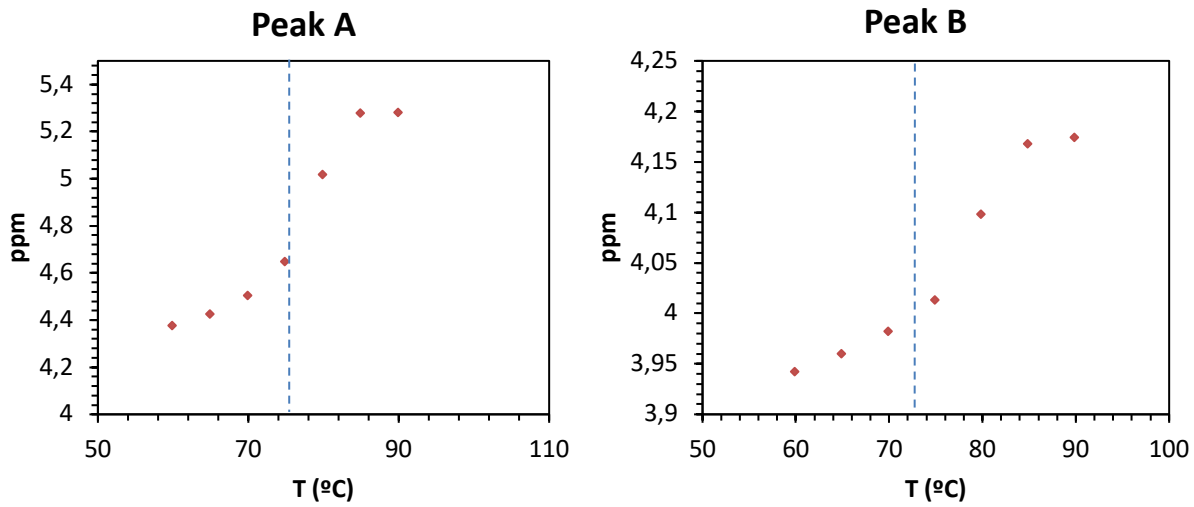


Fig. S8 1H-NMR spectrum of **Sulfo-Glu** in toluene (c = 30.2 g L^{-1}) and plot of chemical shifts of peaks **A** and **B** against temperature. The dotted line represents the middle of the curve.

8. Cartesian coordinates

Table S3 Cartesian coordinates for the structures of the lowest energy minima in chloroform.

C_{18}-Glu

6	14.341697	8.482035	-2.207525
6	13.472191	7.858921	-1.129595
6	14.267112	7.405022	0.085935
6	13.412004	6.778952	1.176195
6	14.206565	6.324097	2.390408
6	13.350287	5.697612	3.479786
6	14.143253	5.240184	4.694058
6	13.284641	4.614630	5.782090
6	14.074782	4.152633	6.996533
6	13.211039	3.532628	8.083665
6	13.995756	3.062438	9.298526
6	13.122405	2.456545	10.386092
6	13.898911	1.976602	11.602331
6	13.013350	1.395995	12.694331
6	13.785728	0.907938	13.909771
6	12.892770	0.365257	15.015186
6	13.686774	-0.105608	16.222386
6	12.834753	-0.650258	17.345420
7	13.366520	-0.520622	18.587698
6	12.674552	-0.995379	19.765895
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6	12.258943	-2.445034	19.590769
8	12.963638	-3.324835	19.128877
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6	16.270121	-4.287201	18.141712
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6	18.318923	1.985757	11.718121
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6	18.381130	3.042876	9.402570
6	17.585048	3.495609	8.188637
6	18.442283	4.104167	7.089891
6	17.648596	4.554253	5.873377
6	18.506841	5.169099	4.778903
6	17.715664	5.619212	3.560676
6	18.576715	6.234775	2.468812
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1	18.940339	0.143627	13.737821
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1	18.904005	2.829216	12.114051
1	19.058192	1.233276	11.405594
1	16.768940	3.184130	10.823707
1	16.946297	1.598752	10.105514
1	18.949772	3.895381	9.803804

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1	17.021054	2.641497	7.782240
1	16.820498	4.223315	8.502231
1	19.001092	4.960493	7.496910
1	19.206102	3.375857	6.777730
1	16.878568	5.277054	6.184829
1	17.091195	3.697560	5.463234
1	19.060995	6.026602	5.189808
1	19.274561	4.444583	4.467411
1	17.159994	4.762266	3.148659
1	16.944322	6.341297	3.870490
1	19.129854	7.091994	2.881665
1	19.345258	5.510294	2.159237
1	17.019742	7.410425	1.554607
1	17.232981	5.829765	0.835378
1	19.211643	8.152481	0.572205
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1	17.318249	6.895657	-1.480856
1	17.108572	8.478025	-0.764023
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1	17.428628	7.965535	-3.828723

Click-Glu

7	0.470235	2.957404	0.191852
7	-0.652258	2.687812	0.890678
6	-1.318100	3.823939	1.201322
6	-0.542278	4.835163	0.670483
7	0.535600	4.258479	0.060503
6	-1.016560	1.320837	1.201305
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6	-0.148406	7.058507	-0.467740
6	-0.272014	8.568916	-0.350876
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6	0.724961	11.537184	-2.688118
6	0.602830	13.051059	-2.616436
6	1.180909	13.763913	-3.828868
6	1.055280	15.278017	-3.766837
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6	1.515956	17.501181	-4.920854
6	2.109867	18.206600	-6.130022
6	1.982845	19.721063	-6.079065
6	2.589804	20.424091	-7.283114
6	2.442013	21.938008	-7.246066
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6	-2.308686	1.200934	-0.967183
6	-3.505556	0.580660	-1.656956
8	-3.495917	-0.563838	-2.070846
8	-4.601216	1.334874	-1.768752
8	-0.491848	1.920726	3.485486
7	-4.398749	3.697465	-0.353443
6	-4.069673	5.015935	-0.444236
6	-4.318918	5.582619	0.788903
7	-4.769645	4.559409	1.560157

7	-4.825617	3.418772	0.855496
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6	-3.572712	7.145085	-1.684468
6	-3.017449	7.776387	-2.951038
6	-3.092855	9.295150	-2.928800
6	-2.520691	9.963701	-4.168783
6	-2.616535	11.480961	-4.127027
6	-2.032670	12.170594	-5.350003
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6	-1.678924	15.902112	-6.458469
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6	-1.220937	18.124009	-7.610090
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6	-0.334295	22.577507	-9.893683
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6	-4.672257	3.290441	3.625194
8	-3.576460	2.815745	3.408403
6	-4.713447	5.790620	3.709765
6	-3.199327	5.873355	3.869280
6	-2.683644	5.080493	5.052372
8	-1.372606	4.786561	5.056430
8	-3.377161	4.755791	5.991894
8	-5.539039	2.834459	4.528738
1	-0.212145	0.709957	0.769469
1	-2.541644	-0.124727	0.705360
1	-3.168635	1.493941	1.013232
1	-2.259546	2.279741	-1.156543
1	-1.411635	0.744799	-1.395692
1	-4.478765	2.230480	-1.350093
1	-1.781590	-0.606547	2.449793
1	-1.782090	6.550463	0.853230
1	-0.230976	6.696298	1.649785
1	0.904187	6.781341	-0.598290
1	-0.656719	6.713414	-1.380482
1	-1.328422	8.847359	-0.202829
1	0.251432	8.910700	0.554341
1	-0.244914	8.952401	-2.467654
1	1.331589	9.026255	-1.708193
1	-0.896280	11.096829	-1.340799
1	0.674811	11.170898	-0.566524
1	1.782400	11.262130	-2.815799
1	0.215513	11.173361	-3.594730
1	-0.457969	13.327236	-2.502149
1	1.100815	13.416014	-1.705615
1	0.683528	13.394207	-4.739798
1	2.240483	13.490051	-3.941464
1	-0.007060	15.552194	-3.662785
1	1.544538	15.648664	-2.853548
1	2.702248	15.712658	-5.082044
1	1.150650	15.614562	-5.890734
1	0.453030	17.775574	-4.823889
1	1.999721	17.874479	-4.005716
1	1.624104	17.831645	-7.045088
1	3.170908	17.932214	-6.227244
1	0.918612	19.994655	-5.995259
1	2.455560	20.097374	-5.159400
1	3.655754	20.162349	-7.360240
1	2.125138	20.036527	-8.203968
1	1.373209	22.191652	-7.181527
1	2.891788	22.323107	-6.320338

1	2.622273	22.268124	-9.383630
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1	-2.676718	5.569664	2.953855
1	-2.902824	6.915062	4.041035
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1	-2.464314	5.293354	-1.793716
1	-4.039710	5.216201	-2.549579
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1	-3.018209	7.537732	-0.817879
1	-1.971699	7.461510	-3.092079
1	-3.563083	7.390941	-3.824174
1	-2.562701	9.670522	-2.038789
1	-4.140551	9.604591	-2.798936
1	-1.466964	9.666581	-4.292097
1	-3.039341	9.586841	-5.062656
1	-3.670262	11.775620	-4.011090
1	-2.106741	11.851752	-3.223260
1	-0.973724	11.886189	-5.459270
1	-2.532242	11.795896	-6.255854
1	-1.648382	14.057670	-4.388916
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1	-0.494465	14.110465	-6.615766
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1	-2.738992	16.178278	-6.355309
1	-1.188157	16.273793	-5.544700
1	-0.025849	16.339385	-7.767291
1	-1.573475	16.235898	-8.582988
1	-0.735007	18.496489	-6.694060
1	-2.282890	18.393908	-7.509709
1	0.435806	18.577568	-8.907911
1	-1.105078	18.458207	-9.734166
1	-1.843656	20.611511	-8.681901
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1	-0.618512	20.681454	-10.879355
1	0.118486	22.988478	-8.983665
1	0.134356	23.077323	-10.746751
1	-1.393121	22.858586	-9.884710
1	-4.218821	6.593667	1.152260

Sulfo-Glu

6	13.300686	-1.288916	-10.571068
6	12.663631	-2.293392	-9.628335
6	11.347435	-1.803588	-9.045260
6	10.633822	-2.833121	-8.184363
6	9.342863	-2.307196	-7.578679
6	8.541328	-3.345486	-6.810592
6	7.265582	-2.773804	-6.214663
6	6.369764	-3.790602	-5.525388
6	5.086511	-3.162519	-5.006759
6	4.108441	-4.120979	-4.344921
6	2.822275	-3.416060	-3.946168
6	1.775151	-4.275427	-3.253824
6	0.498050	-3.484758	-3.019807

6	-0.609390	-4.191009	-2.251994
6	-1.862222	-3.327939	-2.238592
6	-3.016471	-3.819298	-1.374762
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7	-5.102590	-3.211515	0.979067
6	-5.940602	-3.922636	1.960010
6	-7.379219	-3.407296	2.062909
6	-8.037742	-3.731203	3.397369
6	-9.395514	-3.131777	3.617235
8	-10.018188	-2.811202	2.465038
8	-6.590180	-2.095773	-0.865295
8	-6.116100	-4.582829	-0.870188
6	-5.865607	-5.432329	1.781947
8	-6.829237	-6.151392	2.026716
8	-4.671084	-5.880904	1.462704
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8	-6.915950	-8.836909	2.007352
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6	-4.658920	-10.937157	-0.920379
7	-4.371077	-9.530105	-1.226739
16	-5.602714	-8.674558	-1.992315
8	-6.454712	-7.995133	-1.009203
6	-4.651548	-11.794803	-2.179059
8	-5.344738	-12.778189	-2.335738
8	-3.713298	-11.404801	-3.057173
6	-4.689464	-7.422938	-2.910796
6	-3.432909	-7.954900	-3.573051
6	-2.704711	-6.928952	-4.434677
6	-1.369866	-7.491341	-4.905366
6	-0.488584	-6.544774	-5.705872
6	0.813194	-7.214137	-6.125197
6	1.814833	-6.305090	-6.820538
6	3.088172	-7.037464	-7.218702
6	4.148854	-6.157608	-7.862249
6	5.399058	-6.927419	-8.262423
6	6.464186	-6.082272	-8.945867
6	7.697456	-6.881865	-9.340999
6	8.739981	-6.088046	-10.116005
6	9.973718	-6.907050	-10.469216
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6	12.244853	-6.985580	-11.612062
6	13.233729	-6.283725	-12.528390
8	-6.202007	-9.630467	-2.932091
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1	-4.532780	-2.817489	-2.572493
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1	-3.318972	-4.831789	-1.673292
1	-2.216928	-3.213634	-3.274677
1	-1.587767	-2.314209	-1.912114
1	-0.279603	-4.407369	-1.225921
1	-0.829958	-5.168160	-2.708926

1	0.746244	-2.550489	-2.494021
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1	2.169696	-4.657600	-2.300941
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1	2.375715	-2.970961	-4.849760
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1	6.124719	-4.599314	-6.233409
1	6.689788	-2.279203	-7.013635
1	7.523281	-1.973894	-5.504435
1	9.162562	-3.781794	-6.014583
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1	9.571187	-1.458984	-6.916048
1	8.711337	-1.890480	-8.379841
1	11.306148	-3.177442	-7.384588
1	10.417423	-3.726515	-8.791471
1	10.680128	-1.496528	-9.866301
1	11.523468	-0.891064	-8.455950
1	13.357995	-2.530691	-8.810746
1	12.491770	-3.244120	-10.153823
1	13.518046	-0.345889	-10.057270
1	14.239115	-1.658587	-10.995597
1	12.629665	-1.054154	-11.406000
1	-3.766735	-11.262423	-0.364050
1	-6.067678	-12.306307	-0.103975
1	-6.778816	-10.764071	-0.523676
1	-6.647912	-11.242987	1.945935
1	-4.880961	-11.257360	1.838991
1	-4.101329	-9.035104	-0.377550
1	-6.830799	-7.846232	2.098685
1	-3.754175	-12.024350	-3.802444
1	-4.489805	-6.622722	-2.189608
1	-5.428903	-7.044043	-3.624466
1	-2.751481	-8.312247	-2.792891
1	-3.679637	-8.838073	-4.174688
1	-3.322184	-6.636864	-5.295147
1	-2.537014	-6.006172	-3.857872
1	-0.803349	-7.828089	-4.022966
1	-1.553501	-8.401897	-5.494771
1	-0.267598	-5.650811	-5.102048
1	-1.026049	-6.180754	-6.593570
1	1.292644	-7.648508	-5.233561
1	0.583807	-8.071274	-6.776022
1	1.354599	-5.851090	-7.710594
1	2.067753	-5.465241	-6.154133
1	3.516425	-7.525272	-6.328517
1	2.832443	-7.858889	-7.904985
1	4.423777	-5.346919	-7.168485
1	3.725598	-5.659682	-8.747591
1	5.830705	-7.408928	-7.370493
1	5.114068	-7.754214	-8.930609
1	6.032602	-5.611291	-9.841885
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1	9.040218	-5.201049	-9.535024
1	8.284859	-5.696272	-11.037996
1	10.463821	-7.242178	-9.541325
1	9.660403	-7.828846	-10.982391

1	10.512221	-5.898323	-12.293571
1	11.261600	-5.219468	-10.862746
1	12.728269	-7.225024	-10.653358
1	11.959316	-7.952934	-12.048835
1	13.558172	-5.324568	-12.109517
1	14.131263	-6.885547	-12.699341
1	12.785720	-6.072506	-13.505642

9. NMR spectra

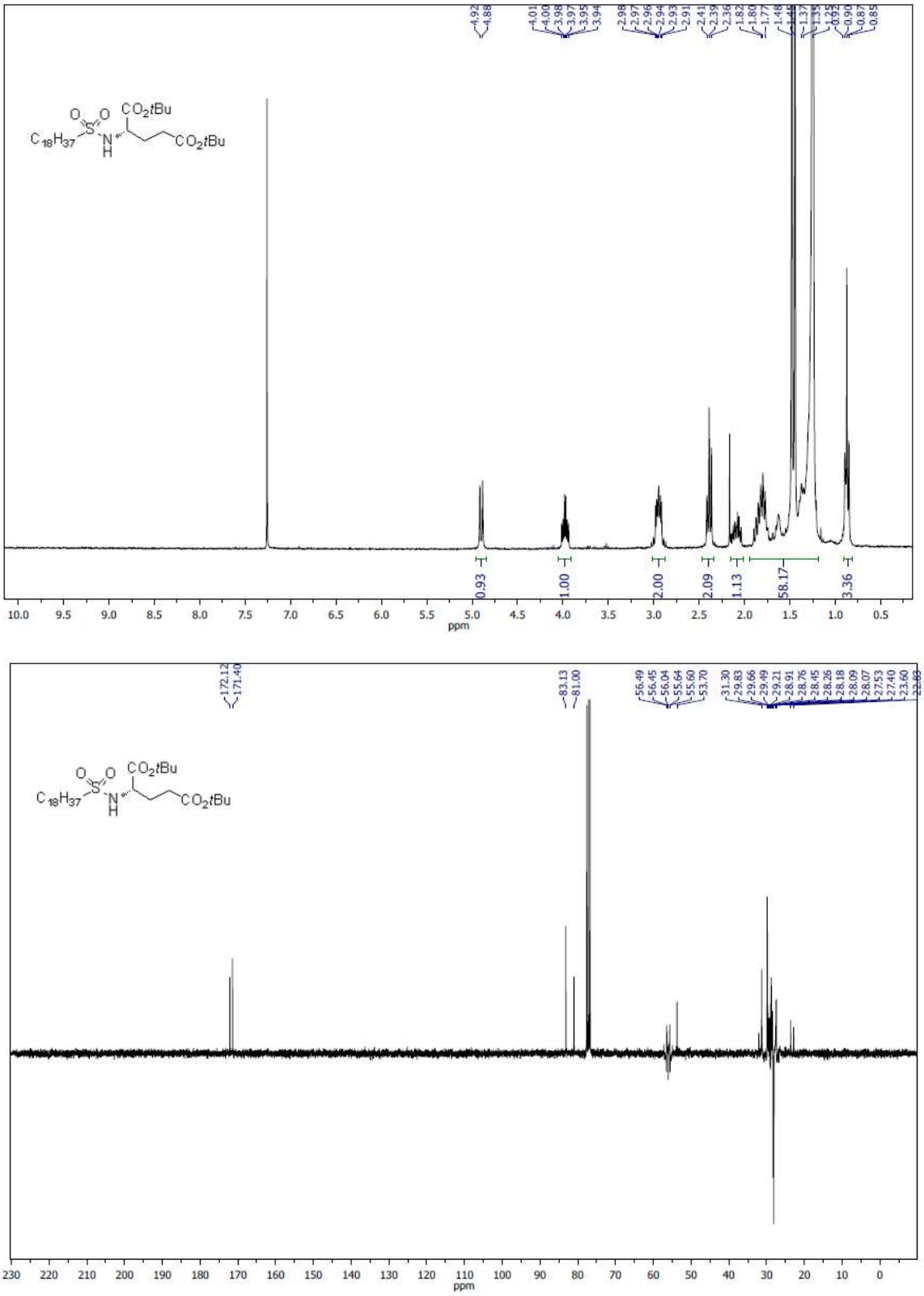

Fig. S9 ^{1}H NMR and ^{13}C-NMR-APT spectra of **Sulfo-Glu ester**.

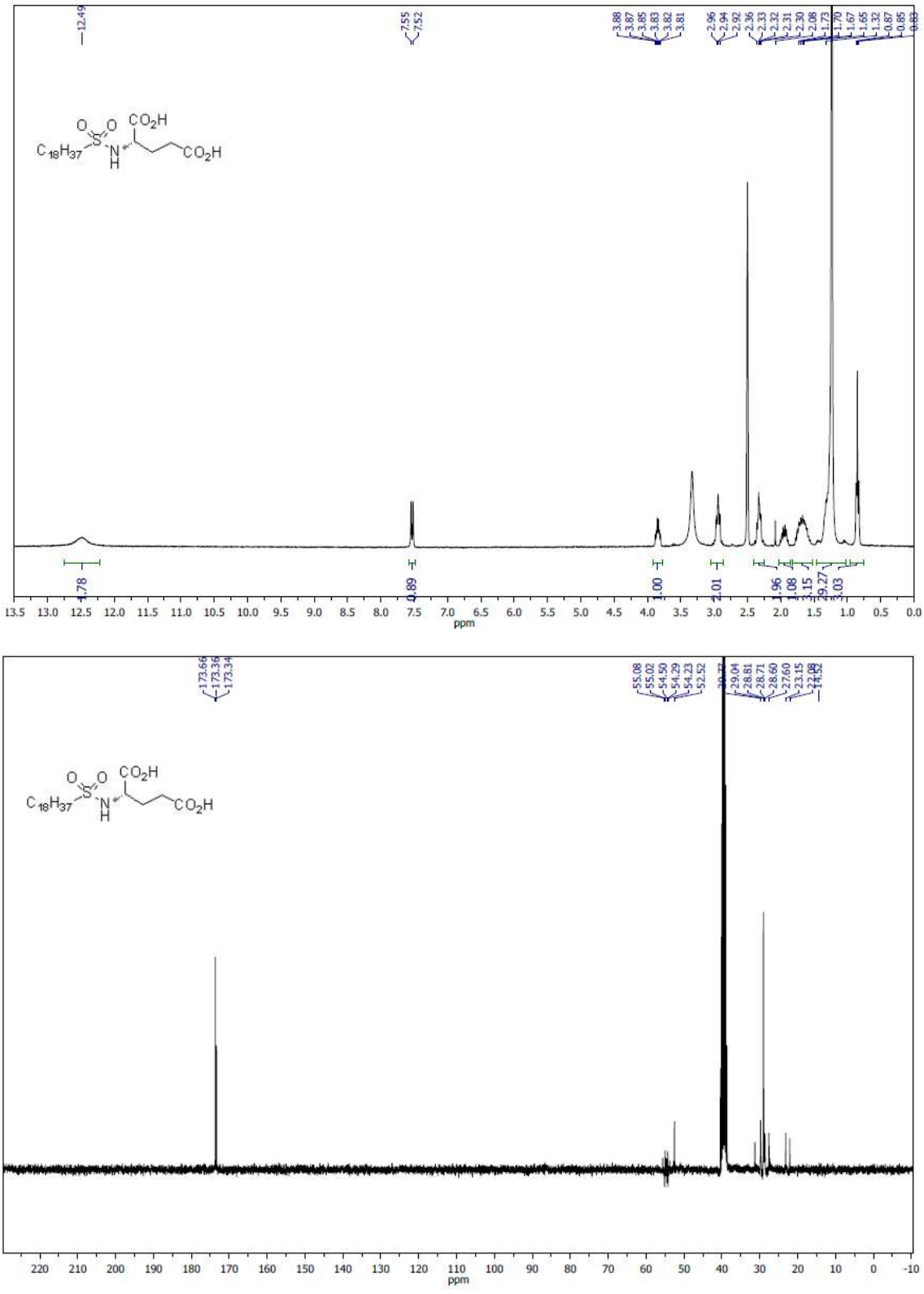

Fig. S10 ^{1}H NMR and ^{13}C-NMR-APT spectra of **Sulfo-Glu**.