Supplementary Materials

Amphiphilic Low-Molecular-Weight Gelators Bearing β-S-N-Acetylglucosamine Linked to a Tartaric Acid Scaffold: Synthesis, Self-Assembly and Wheat Germ Agglutinin Binding

Vicente Leafar Peña García[1,2,3], Pablo Héctor Di Chenna[1,3,*] and Maria Laura Uhrig[1,2,*]

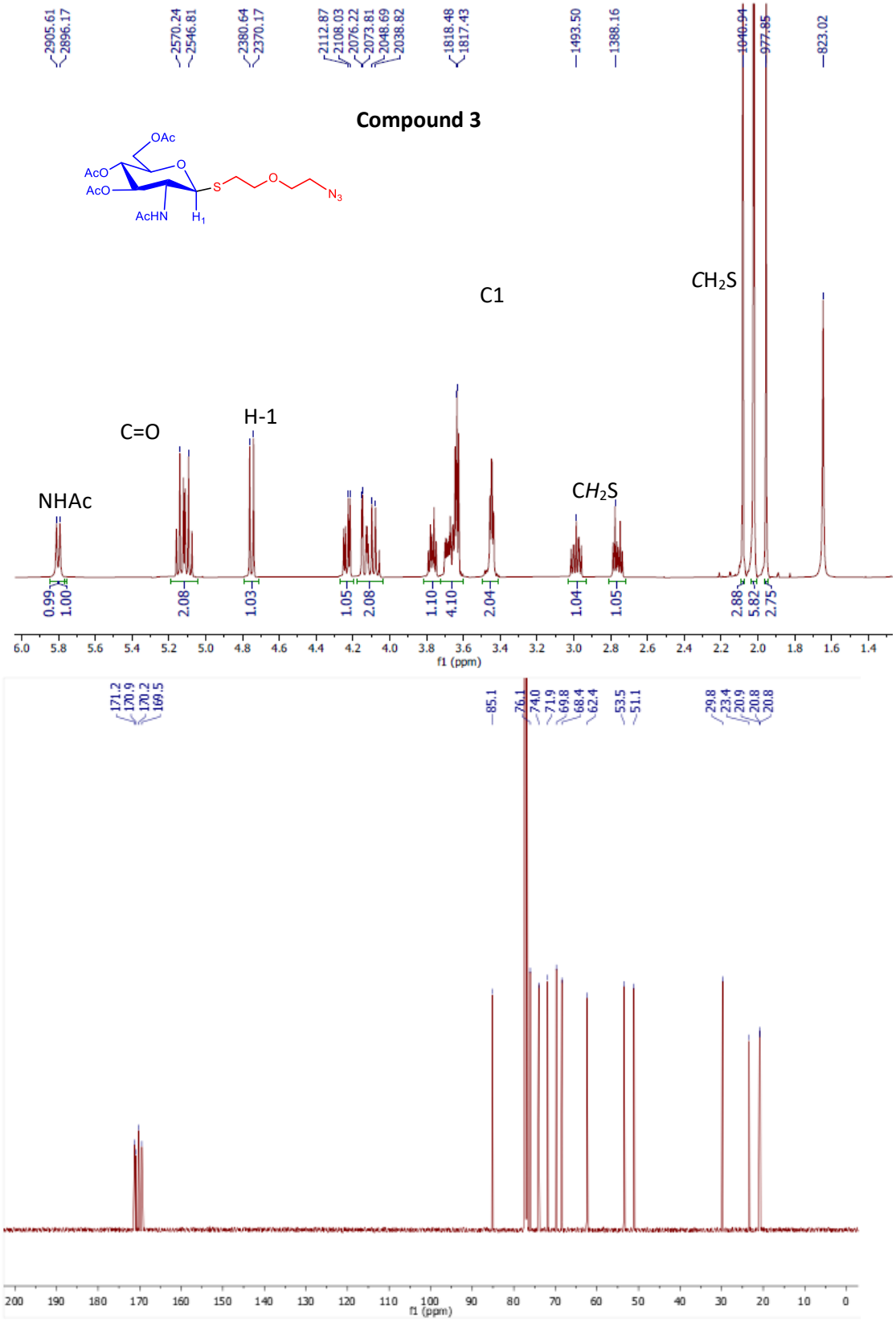
[1] Departamento de Química Orgánica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Intendente Güiraldes 2160, 3er piso, Pabellón 2, Ciudad Universitaria, Buenos Aires C1428EGA, Argentina; vicentepena@qo.fcen.uba.ar

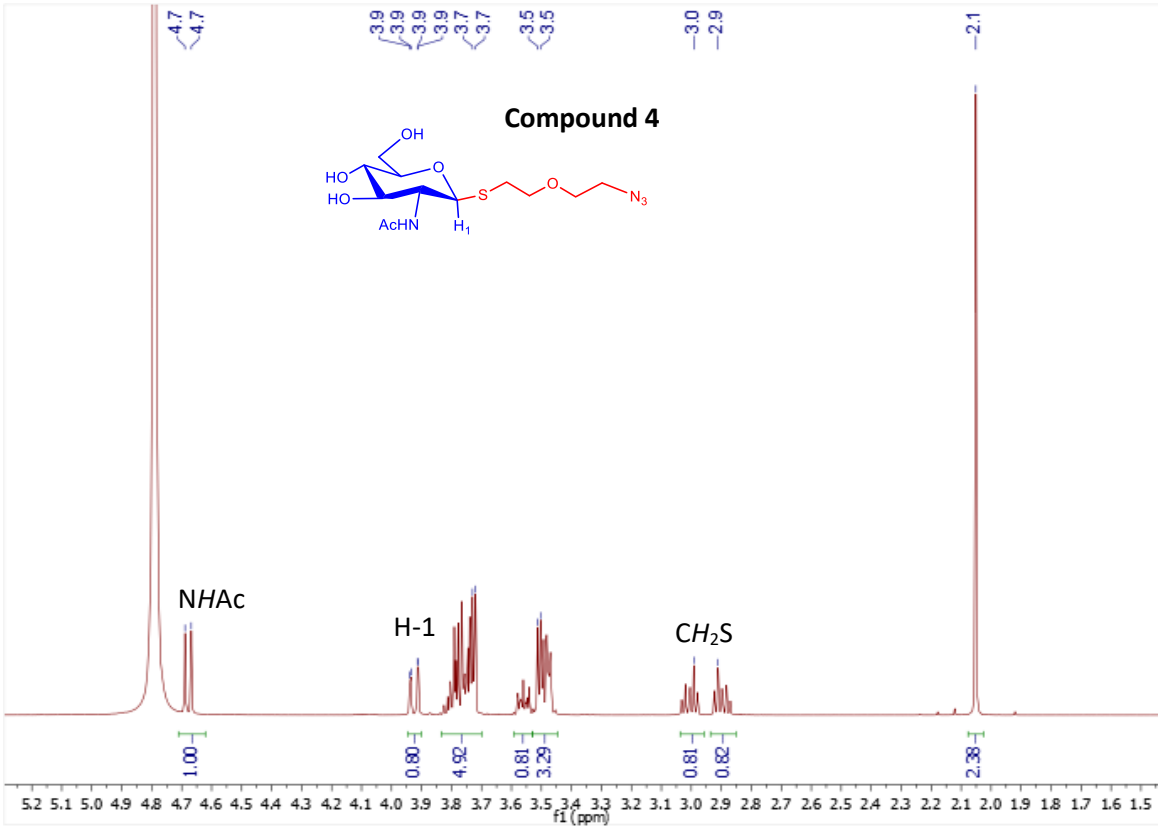
[2] Centro de Investigaciones en Hidratos de Carbono (CIHIDECAR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET)–Universidad de Buenos Aires, Buenos Aires C1428EGA, Argentina

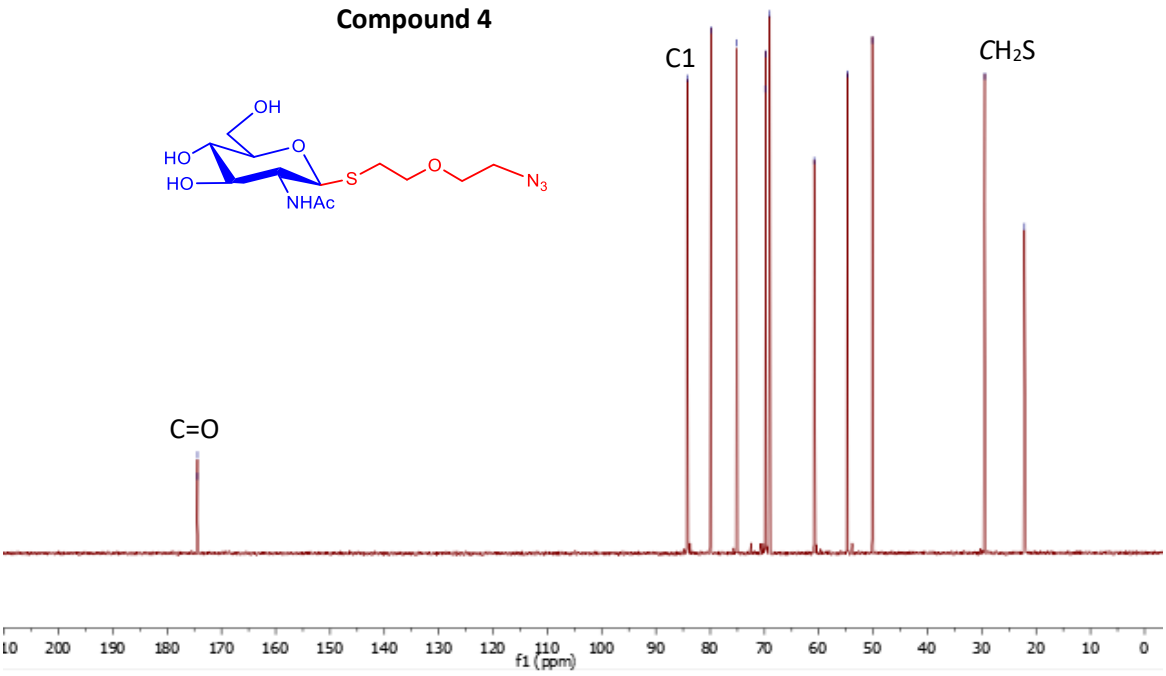
[3] Unidad de Microanálisis y Métodos Físicos en Química Orgánica (UMYMFOR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET)–Universidad de Buenos Aires, Buenos Aires C1428EGA, Argentina

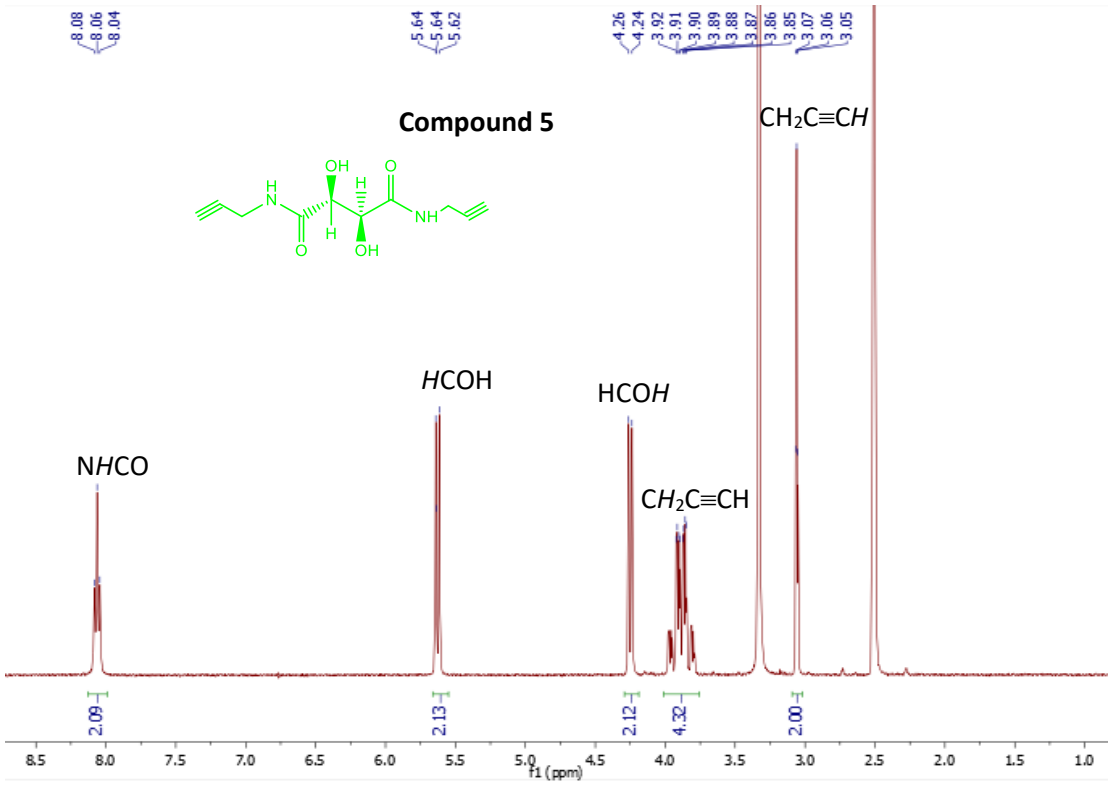
* Correspondence: dichenna@qo.fcen.uba.ar (P.H.D.C.); mluhrig@qo.fcen.uba.ar (M.L.U.)

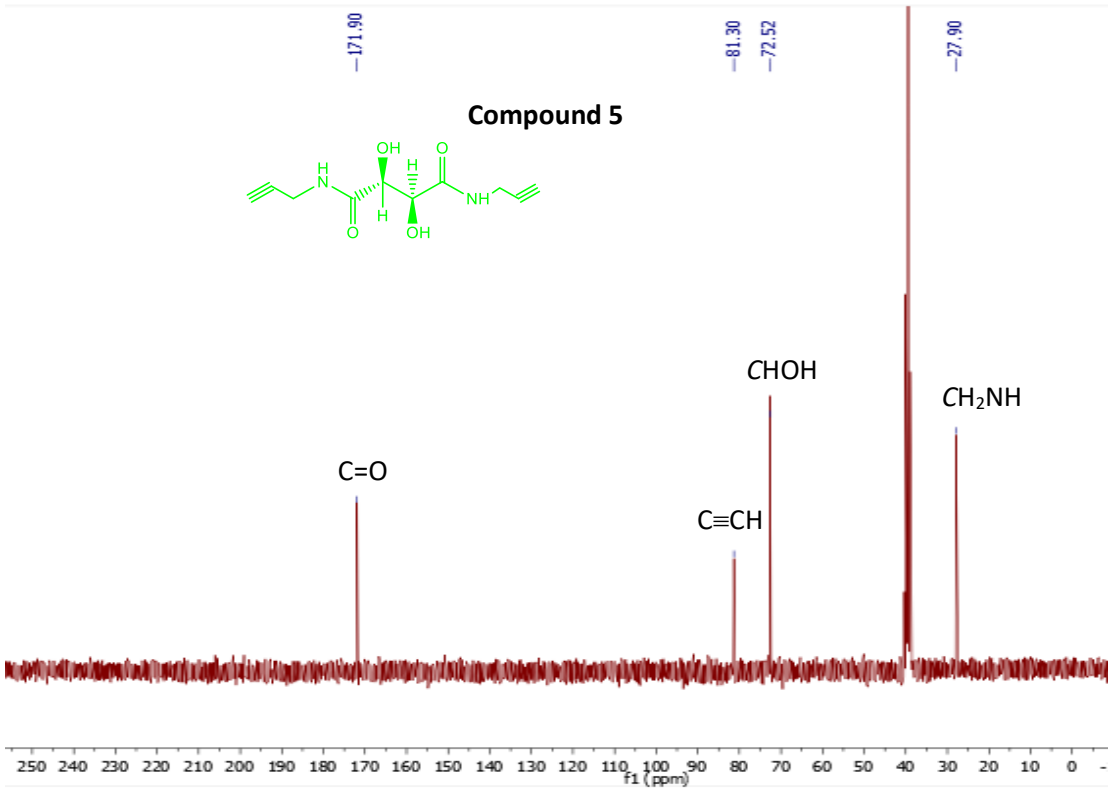
Figure S1. ^{1}H and ^{13}C NMR spectra (500 and 125 MHz respectively).

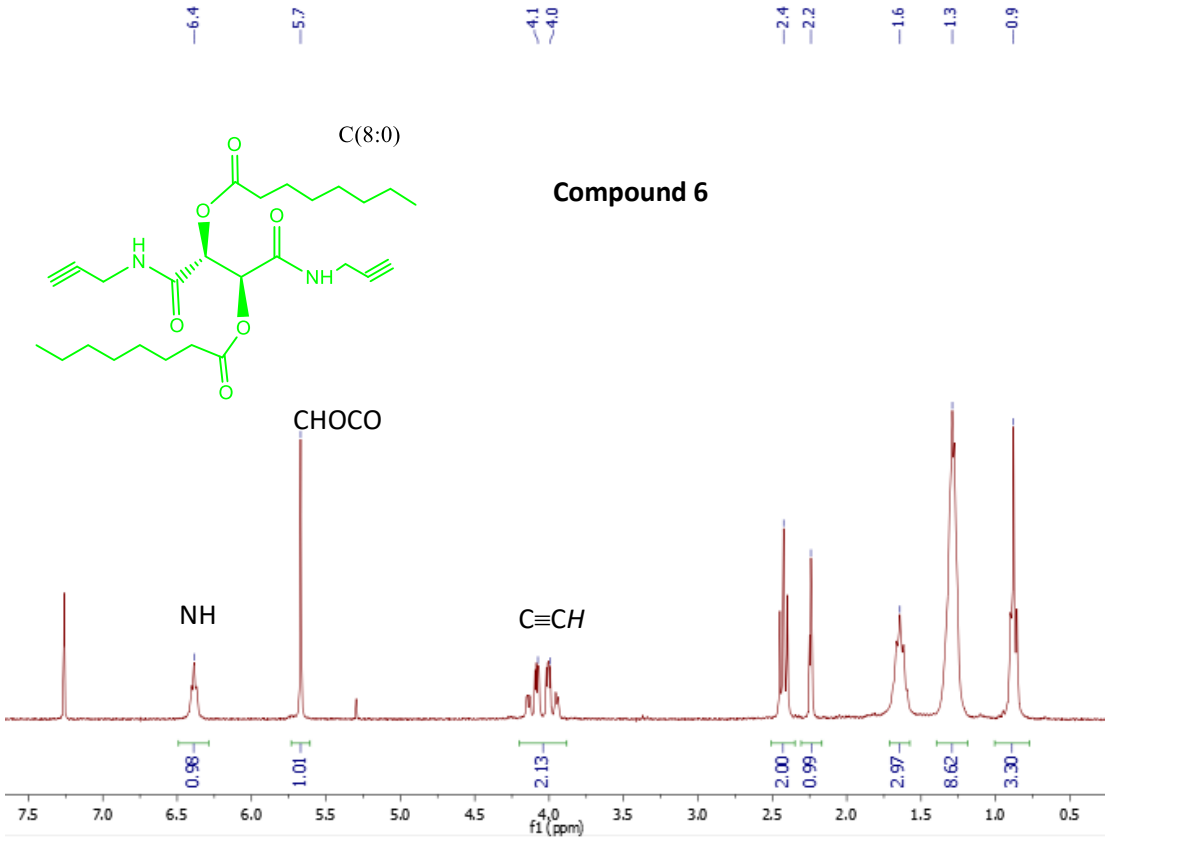


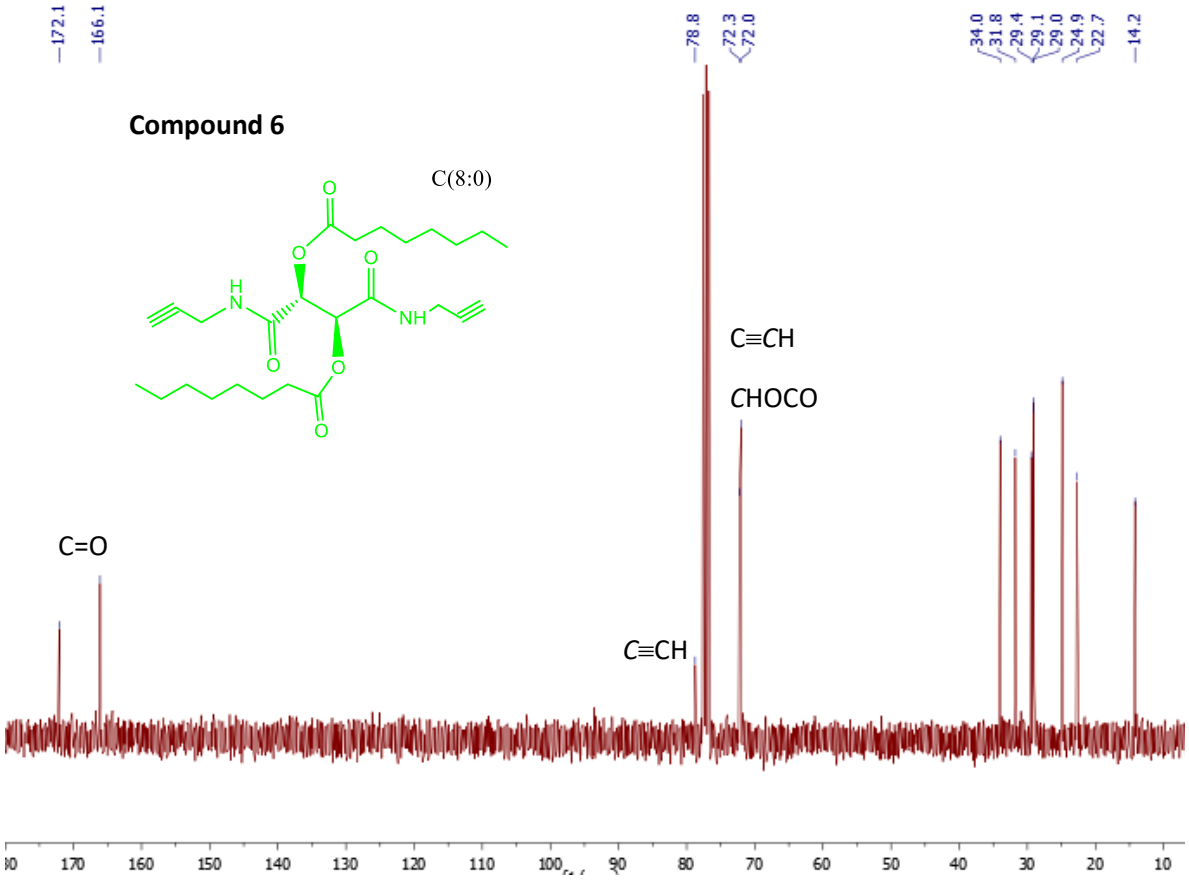

Compound 4
NHAc
H-1
CH2S

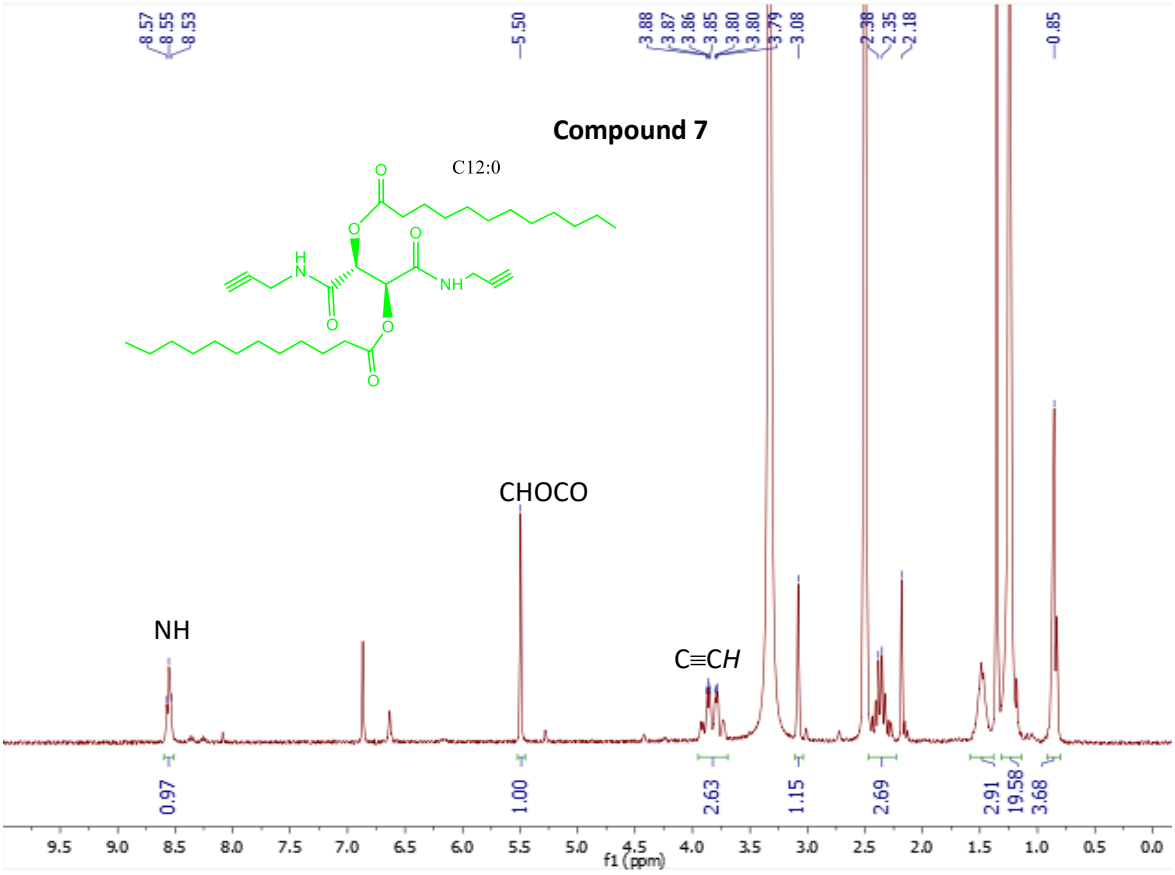

Compound 4
C1
CH2S
C=O

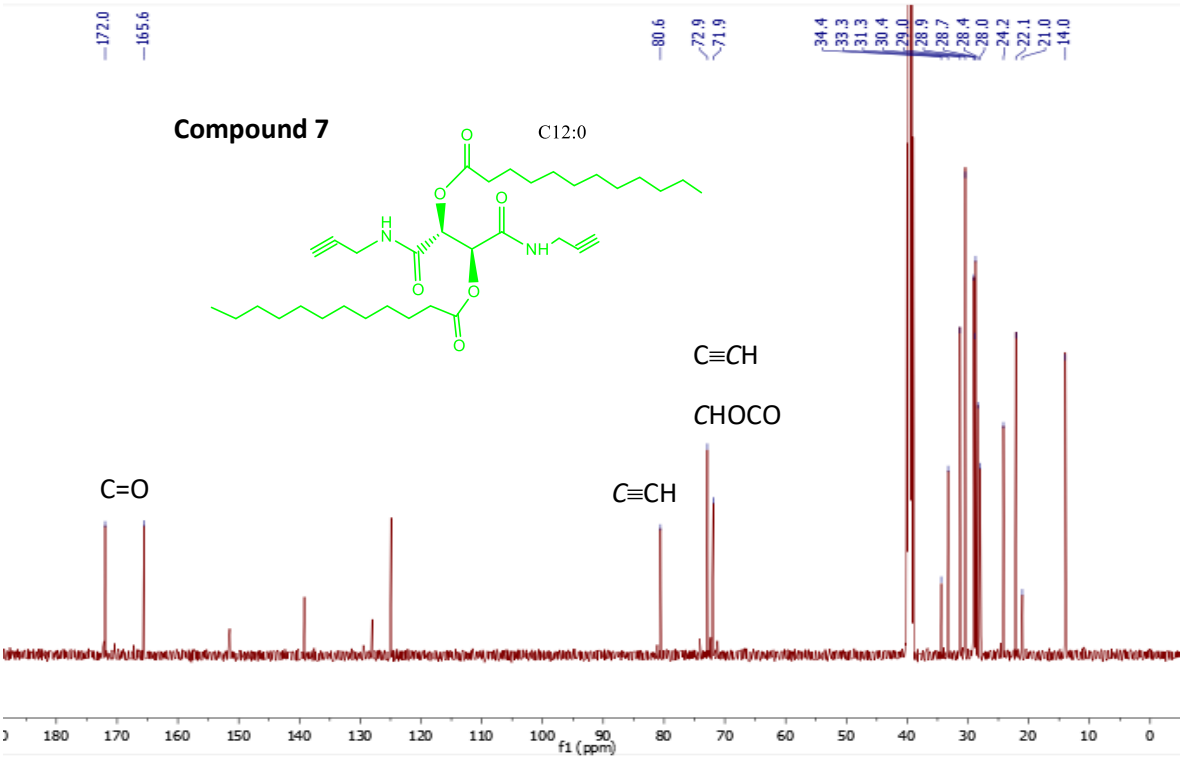

8.08
8.06
8.04
5.64
5.64
5.62
4.26
4.24
3.92
3.91
3.90
3.89
3.88
3.87
3.86
3.85
3.07
3.06
3.05
Compound 5
CH2C≡CH
HCOH
HCOH
NHCO
CH2C≡CH
2.09
2.13
2.12
4.32
2.00
f1 (ppm)

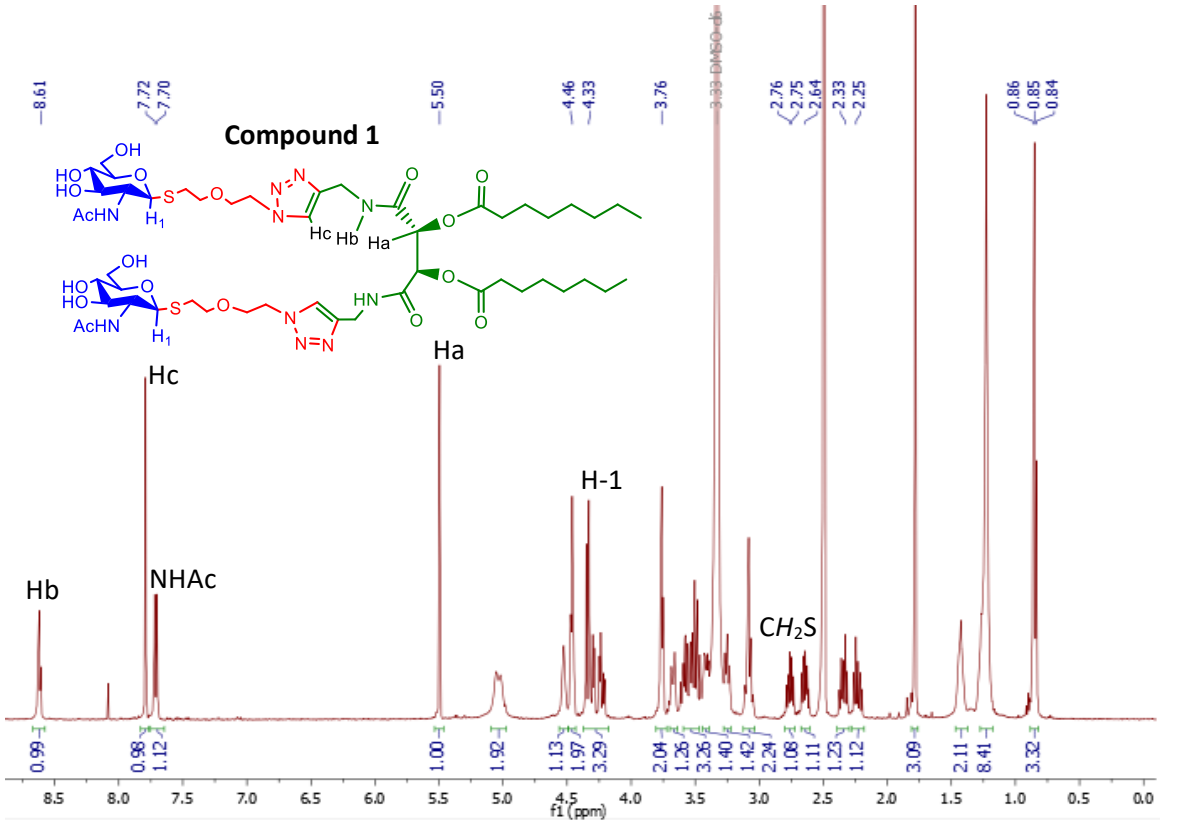

171.90
81.30
72.52
27.90
Compound 5
CHOH
CH2NH
C=O
C≡CH
f1 (ppm)

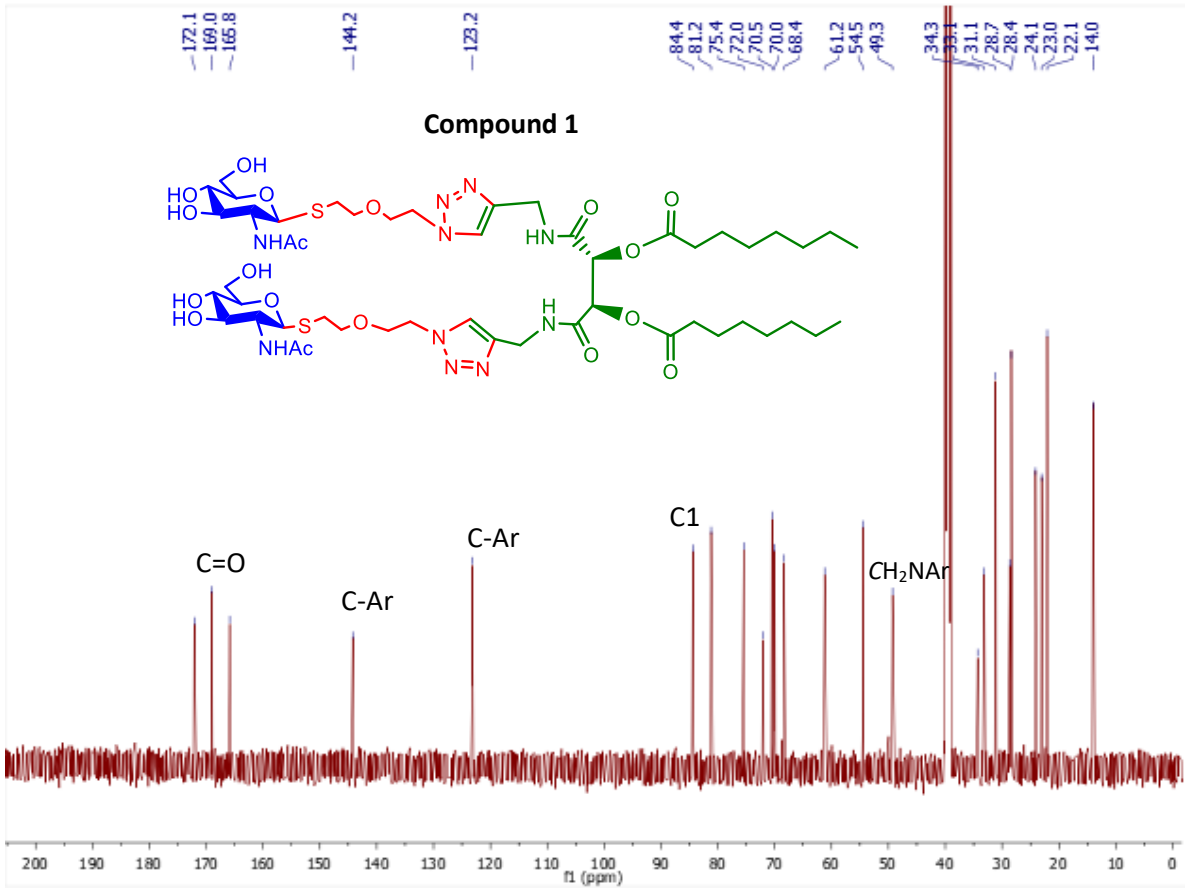

6.4
5.7
4.1
4.0
2.4
2.2
1.6
1.3
0.9
C(8:0)
Compound 6
CHOCO
NH
C≡CH
0.98
1.01
2.13
2.00
0.99
2.97
8.62
3.30
f1 (ppm)

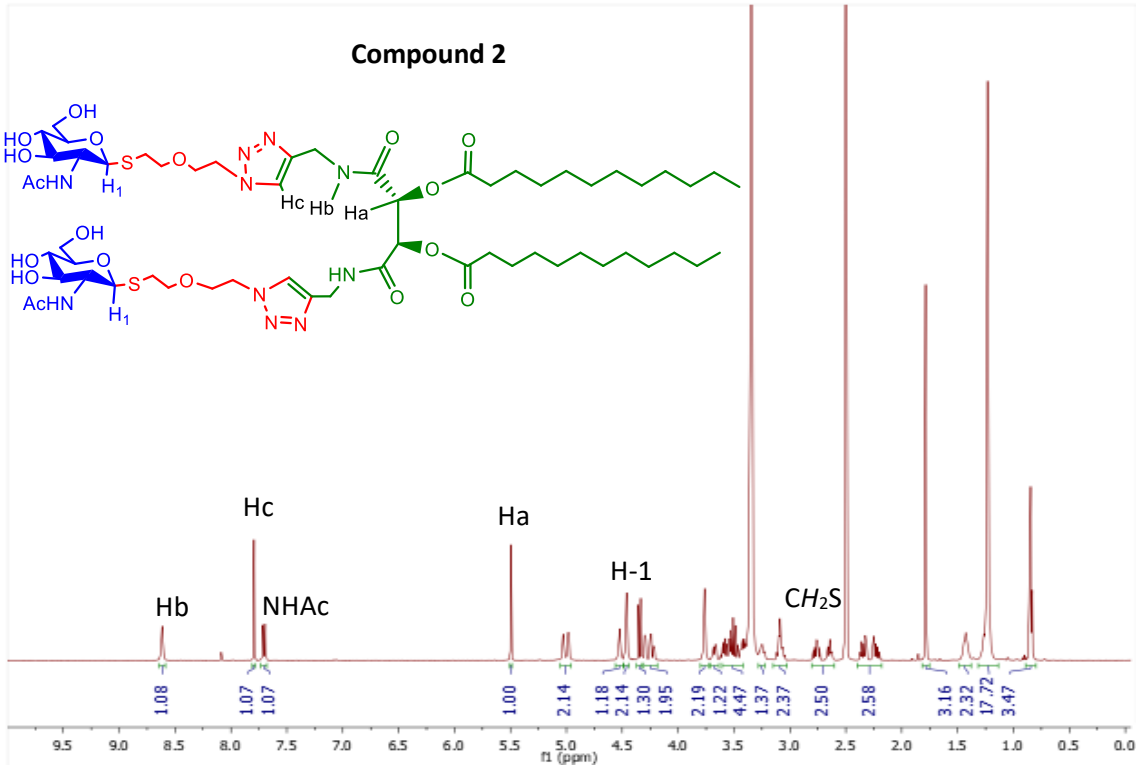

172.1
166.1
78.8
72.3
72.0
34.0
31.8
29.4
29.1
29.0
24.9
22.7
14.2
Compound 6
C(8:0)
C≡CH
CHOCO
C=O
C≡CH

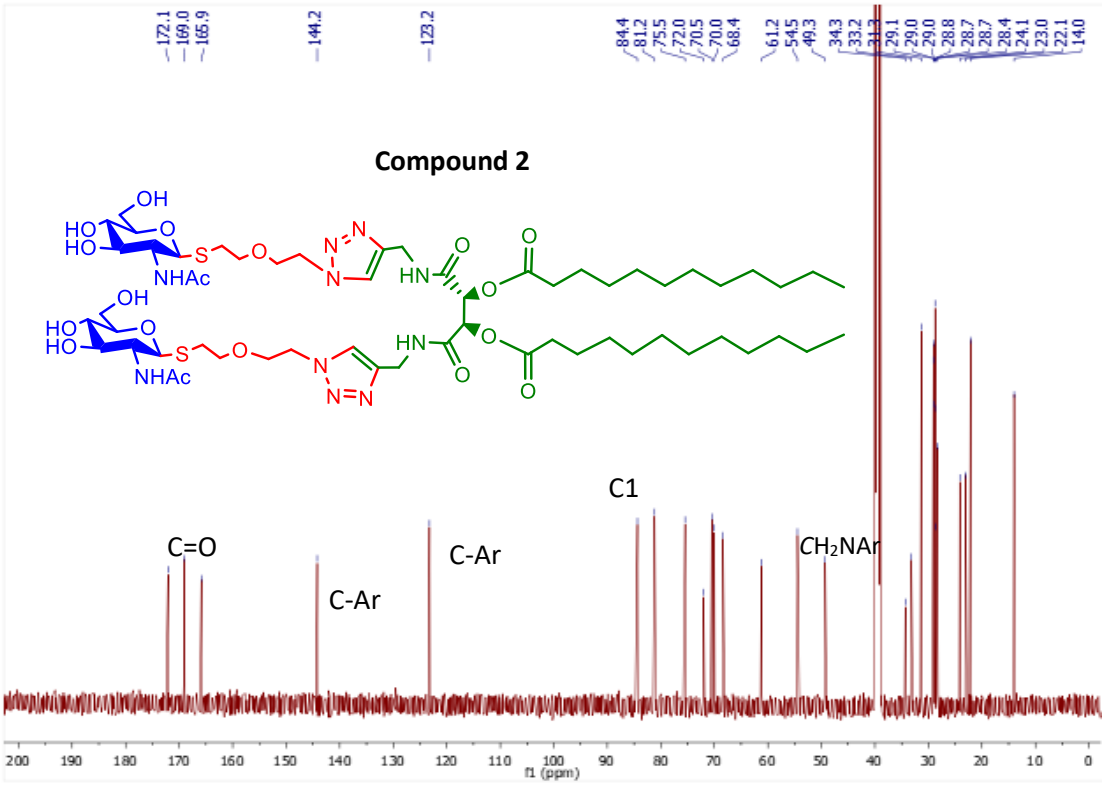

Compound 7
C12:0
CHOCO
NH
C≡CH
f1 (ppm)

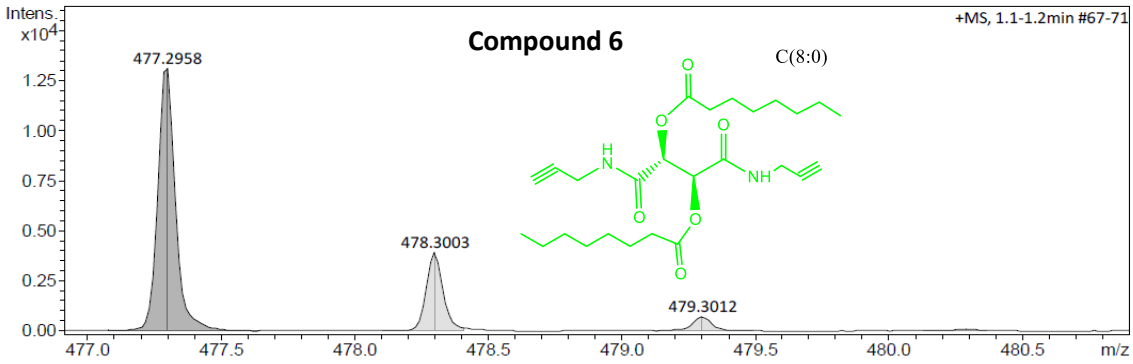

Compound 7
C12:0
C=O
C≡CH
CHOCO
f1 (ppm)


Compound 1
Hc
Ha
H-1
Hb
NHAc
CH2S
f1 (ppm)

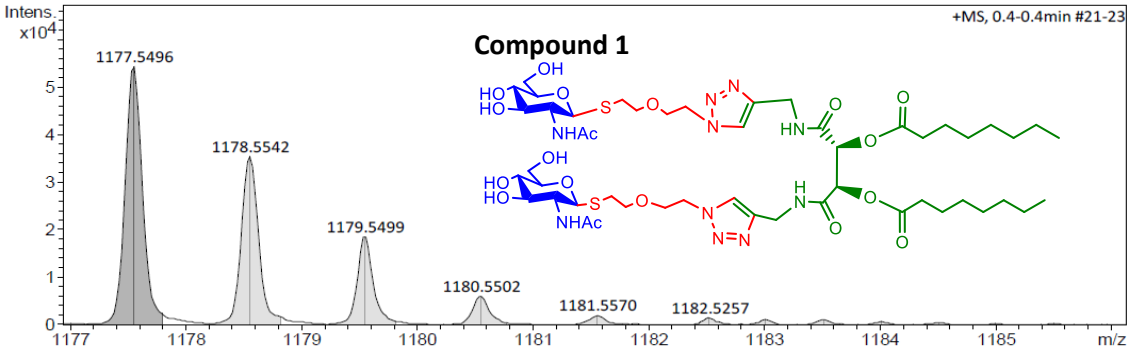

Compound 1
C=O
C-Ar
C-Ar
C1
CH2NAr
f1 (ppm)


Compound 2
Hb
Hc
NHAc
Ha
H-1
CH2S
f1 (ppm)

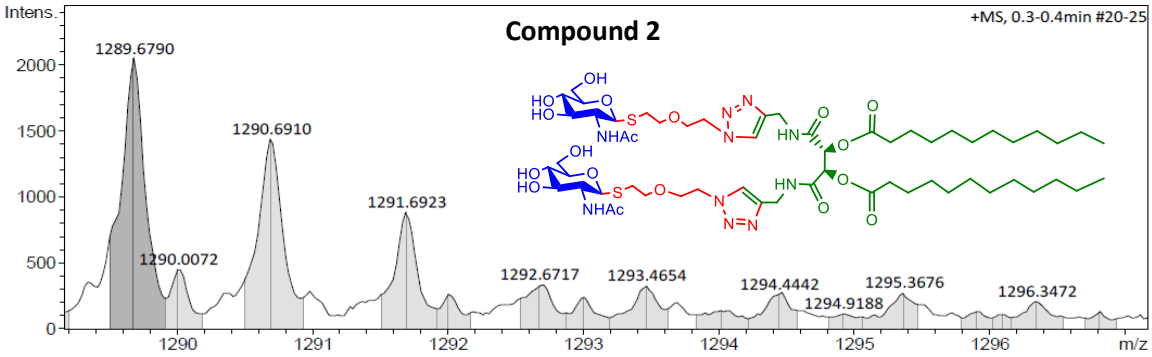

Compound 2
C=O
C-Ar
C-Ar
C1
CH2NAr
f1 (ppm)



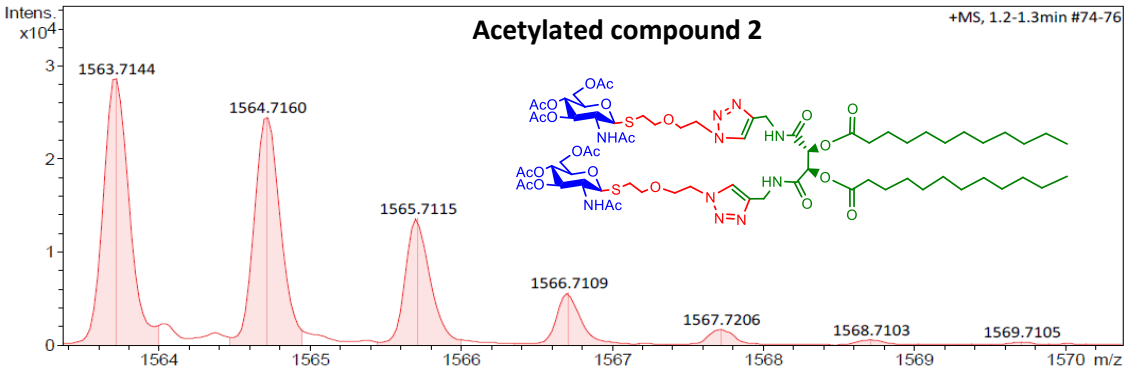
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
477.2958	1	C26H41N2O6	477.2959	0.2	4.1	1	100.00	7.5	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1177.5496	1	C50H85N10O18S2	1177.5479	-1.4	22.1	1	100.00	13.5	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1289.6790	1	C58H101N10O18S2	1289.6731	-4.6	34.1	1	20.56	13.5	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1563.7144	1	C70H112N10NaO24S2	1563.7185	2.6	11.8	1	100.00	19.5	even	ok

Figure S2. T_{gel} *vs* concentration plot for hydrogels of **1**

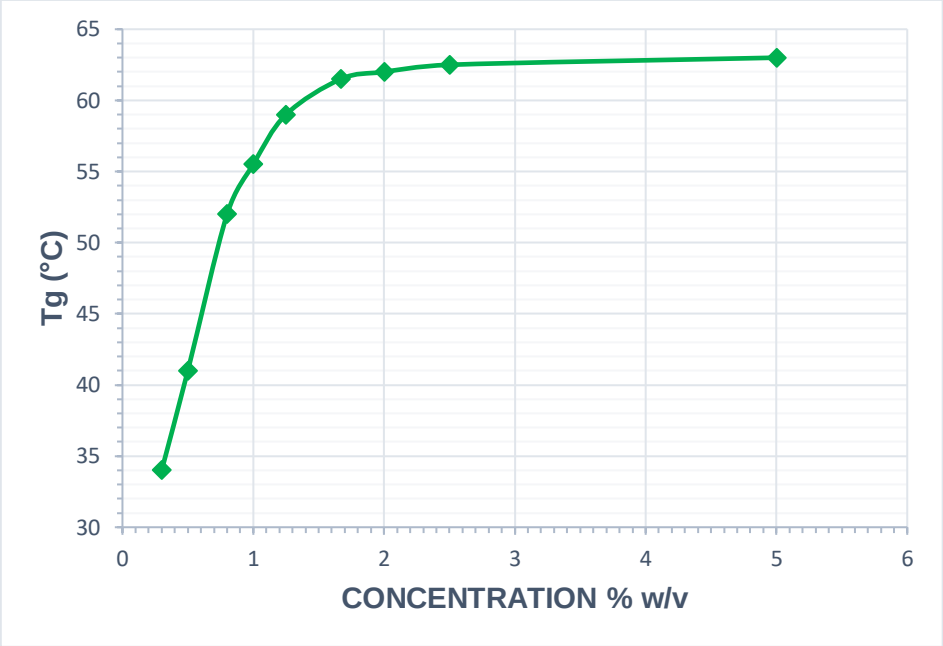


Figure S3. T_{gel} *vs* concentration plot for DMSO gels of **2**

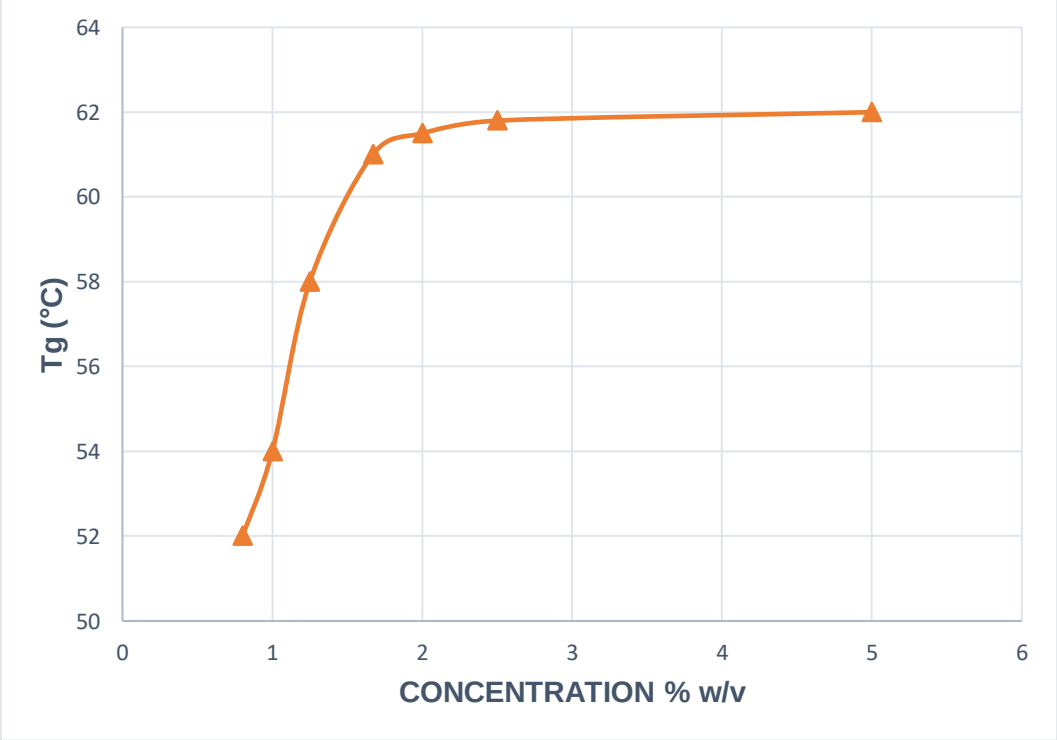


Figure S4. Reology. Dynamic strain sweep experiment of a hydrogel of **1** an DMSO gel of **2** at 25ºC.

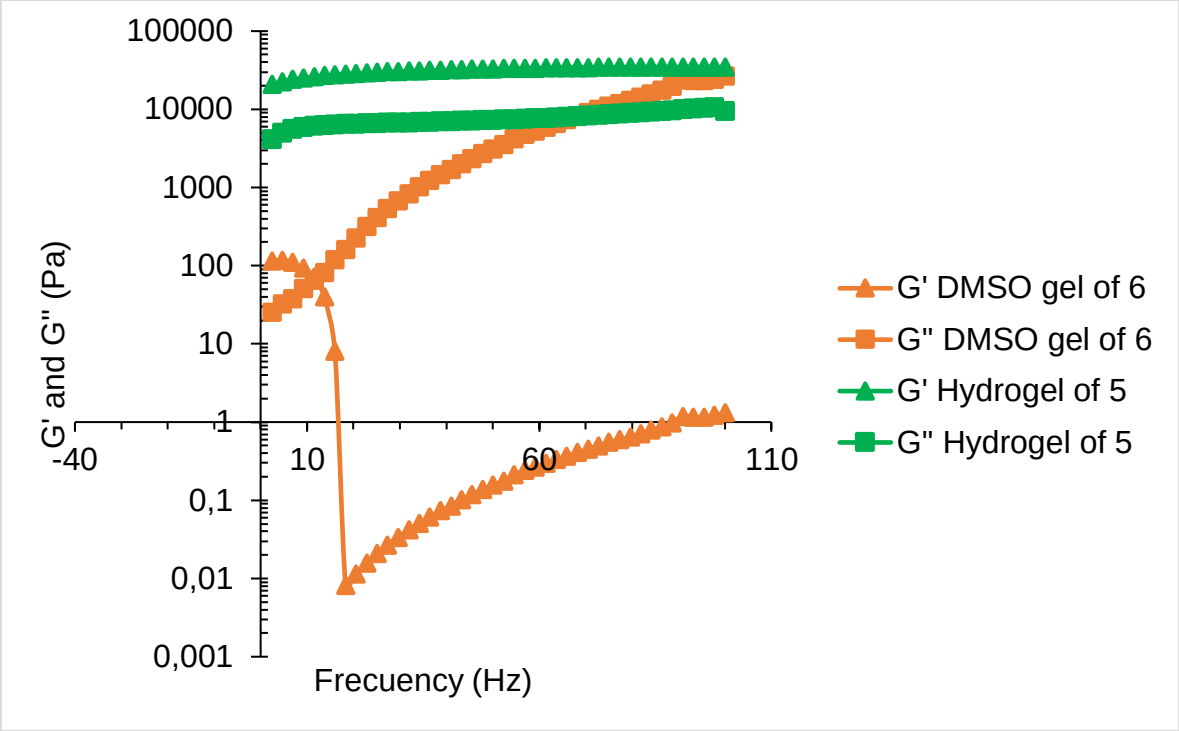


Figure S5. Powder XRD experiments

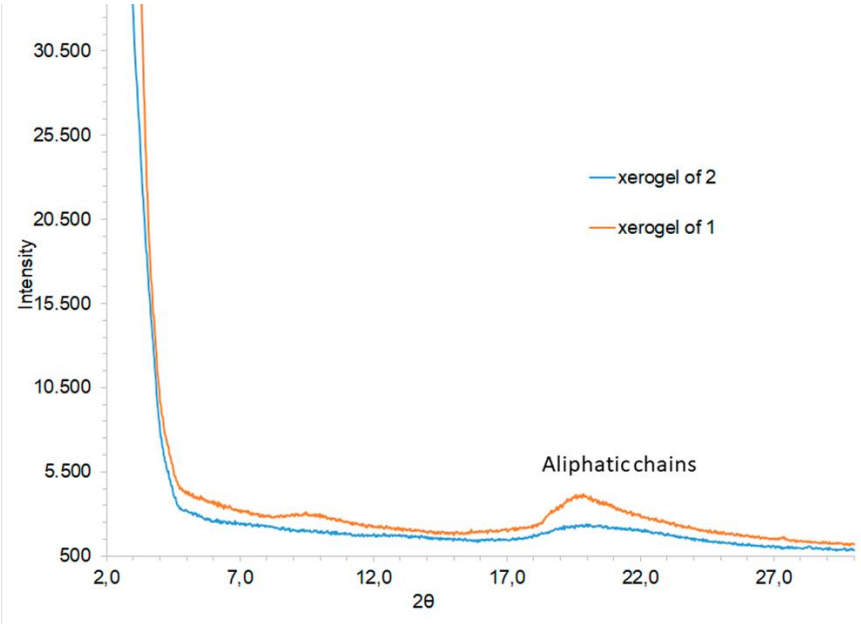
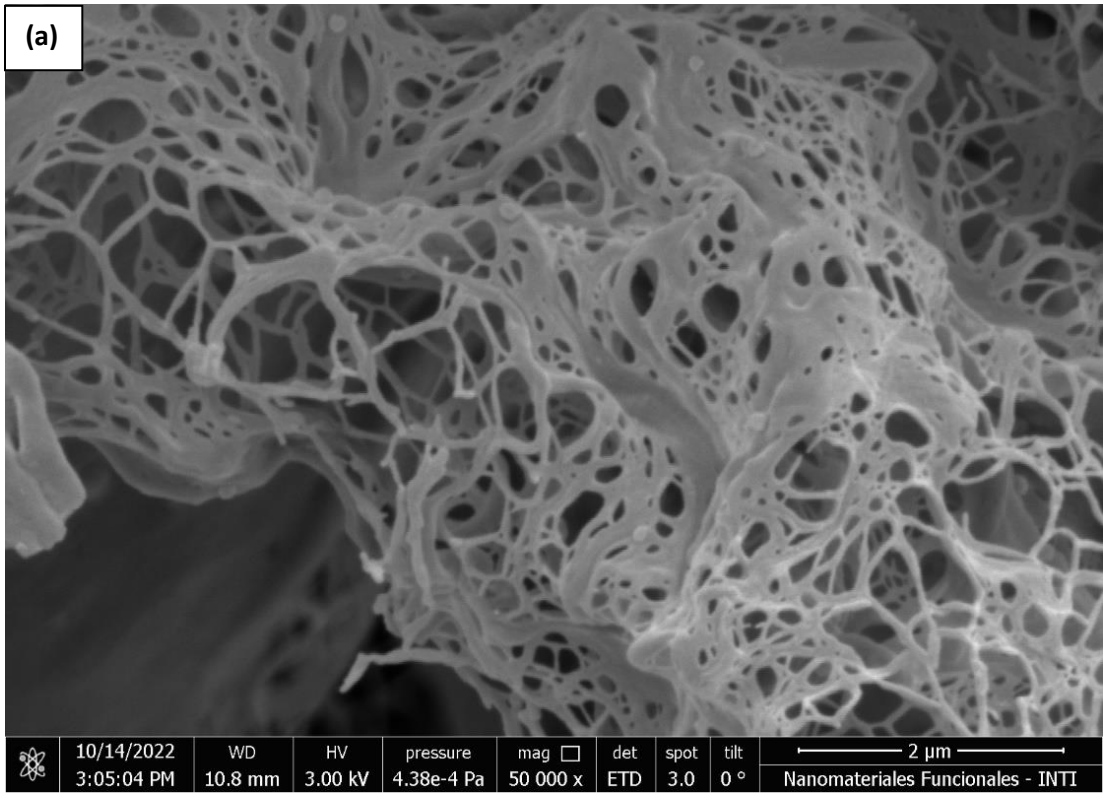


Figure S6. SEM images obtained from xerogels of a hydrogel of **1** (a) and a DMSO gel of **2** (b)



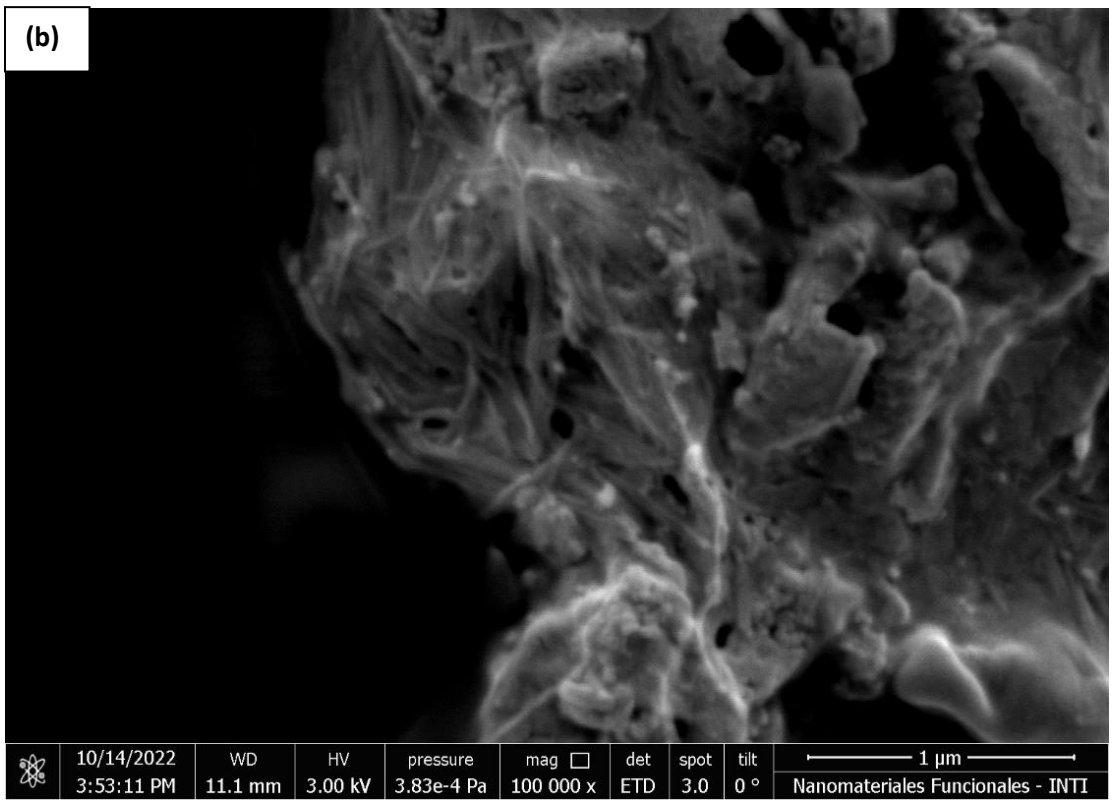


Figure S7. TEM image of the xerogel obtained from **2**