Supplementary information

Chemical modification of sialylated oligosaccharides to functionalize nanostructured lipid carriers: exploring two different strategies

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Characterization of linkers and glycoconjugates

p-Toluenesulfonyl PEG_4 (1)

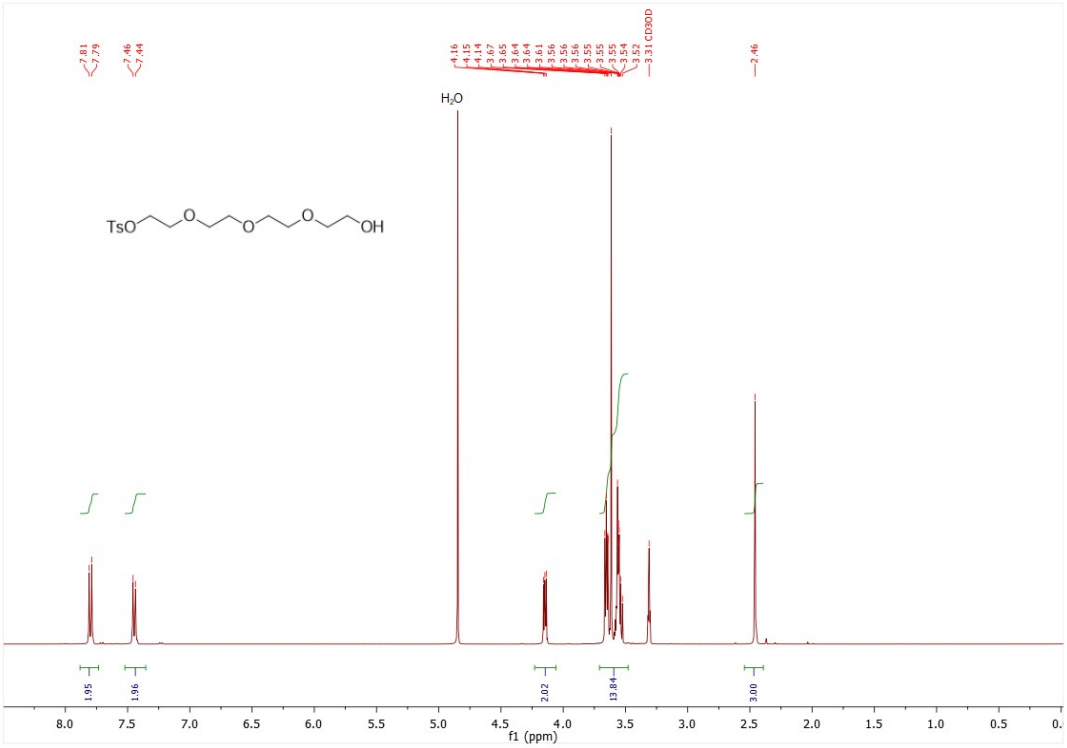

Figure S1. ^{1}H NMR spectrum of **1** (CD_3OD, 298K)

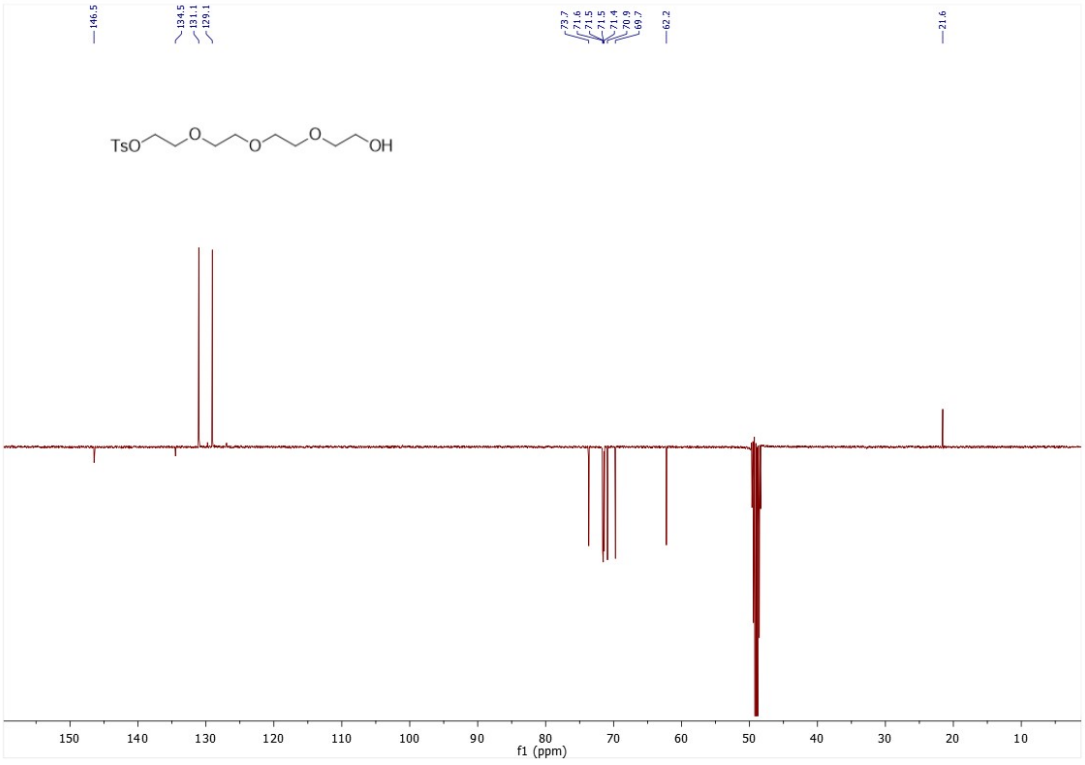

Figure S2. ^{13}C DEPTQ-135 NMR spectrum of **1** (CD_3OD, 298K)

***(N-t*-Butoxycarbonyl, *N*-methyl-hydroxylamine)-PEG$_4$ (2)**

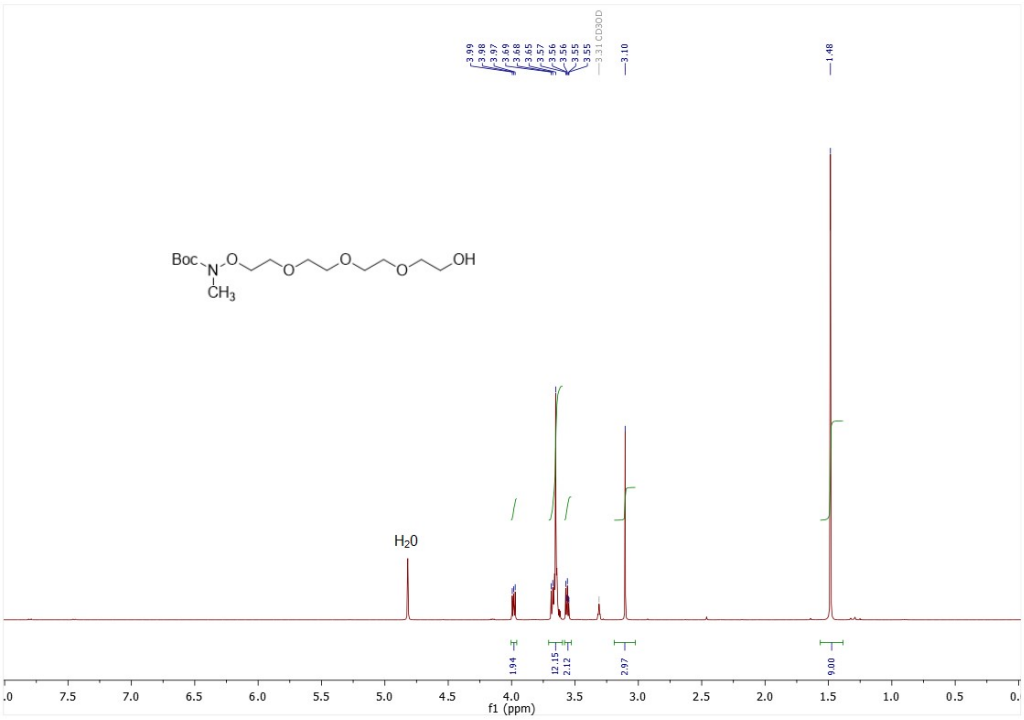

Figure S3. ^{1}H NMR spectrum of **2** (CD_3OD, 298K)

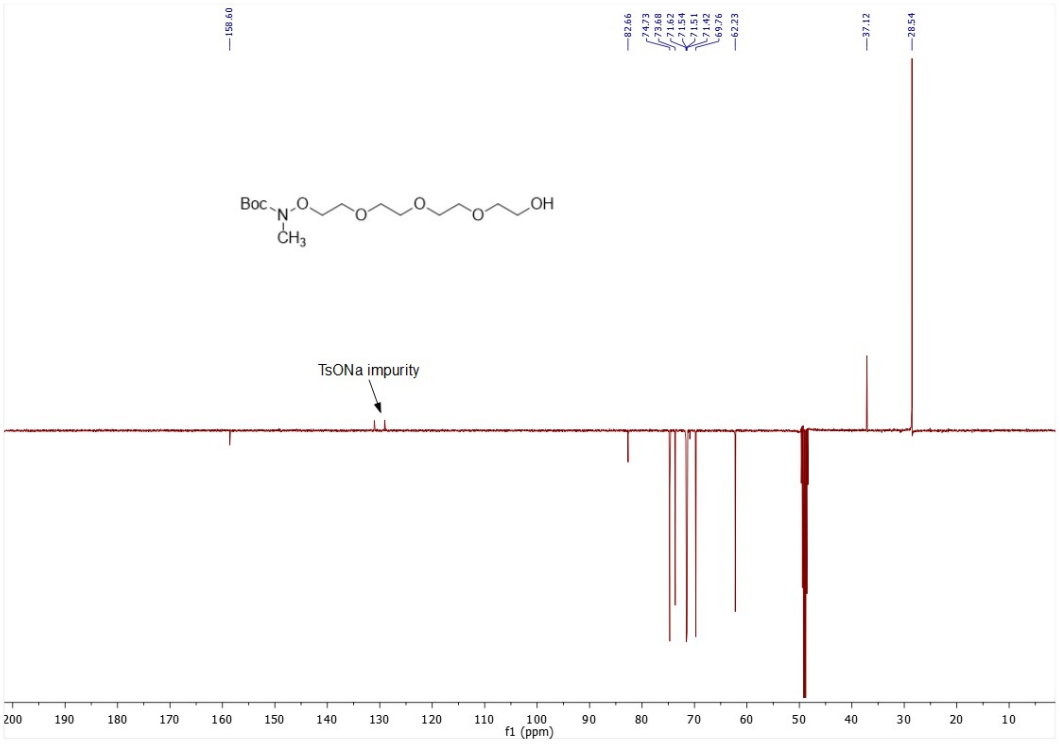

Figure S4. ^{13}C DEPTQ-135 NMR spectrum of **2** (CD_3OD, 298K)

***(N-t*-Butoxycarbonyl, *N*-methyl-hydroxylamine)-PEG$_4$-(*p*-toluenesulfonyl) (3)**

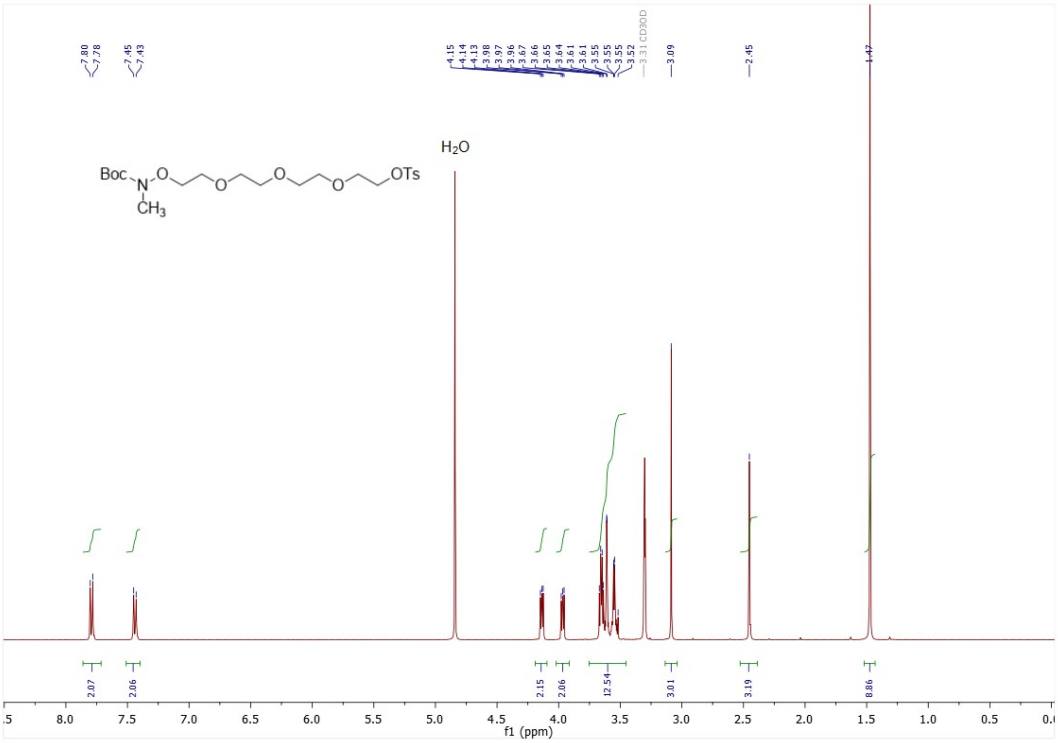

Figure S5. ^{1}H NMR spectrum of **3** (CD_3OD, 298K)

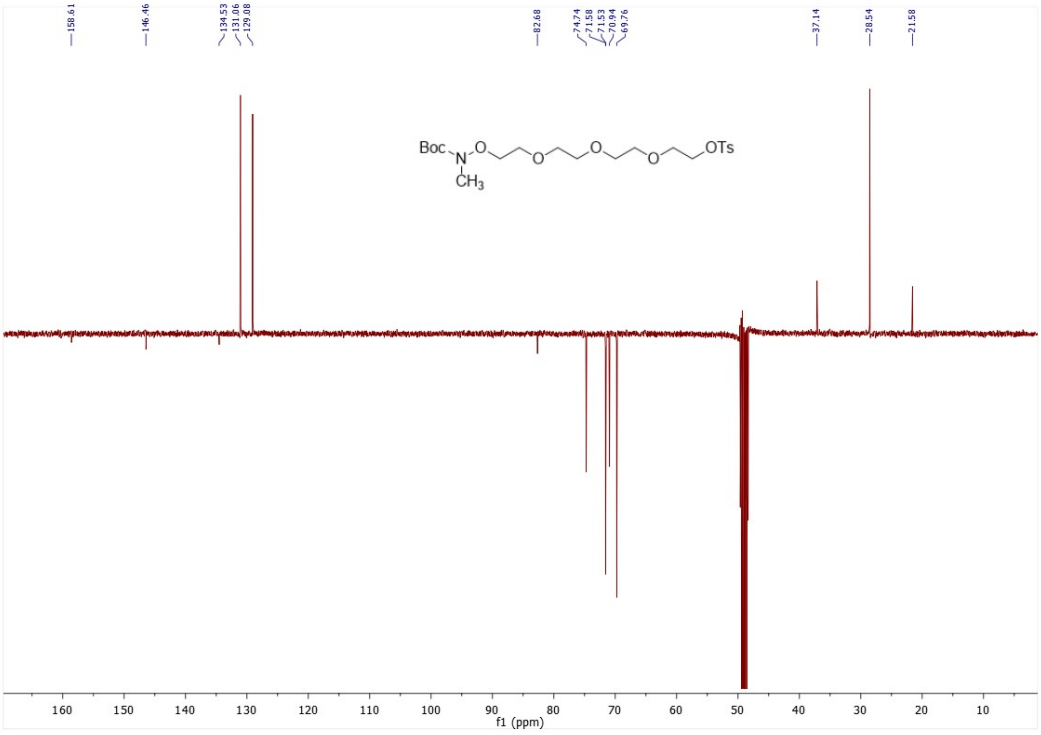

Figure S6. ^{13}C DEPTQ-135 NMR spectrum of **3** (CD_3OD, 298K)

***(N-t*-Butoxycarbonyl, *N*-methyl-hydroxylamine)-PEG$_4$-(*S*-acetyl) (4)**

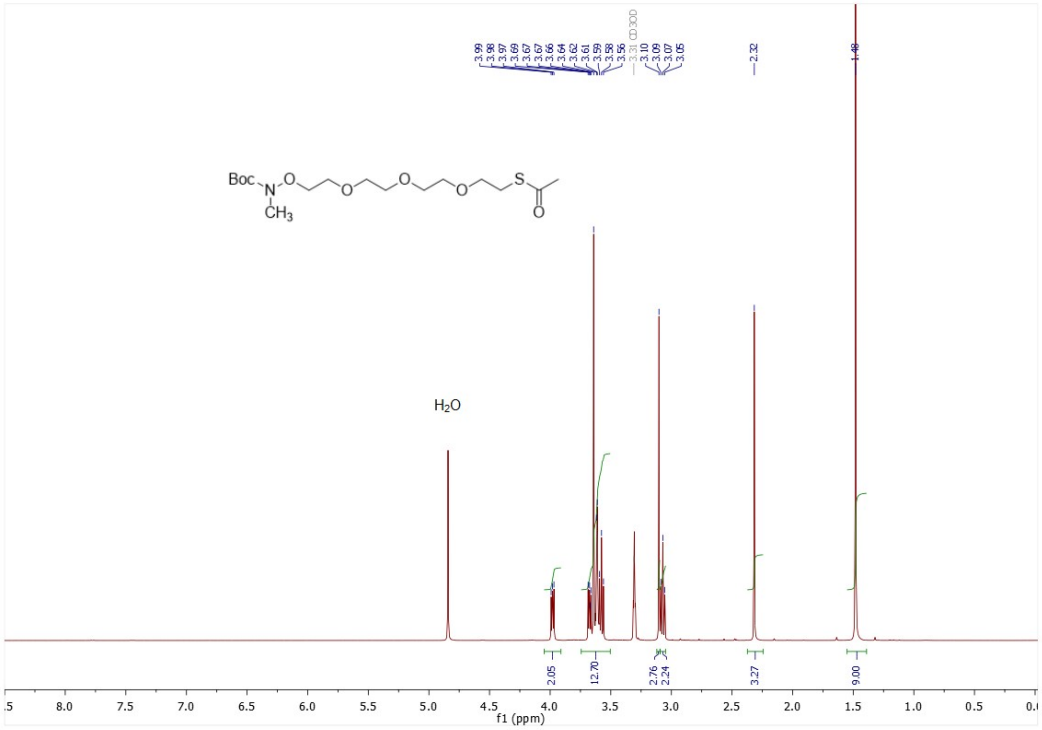

Figure S7. ^{1}H NMR spectrum of **4** (CD_3OD, 298K)

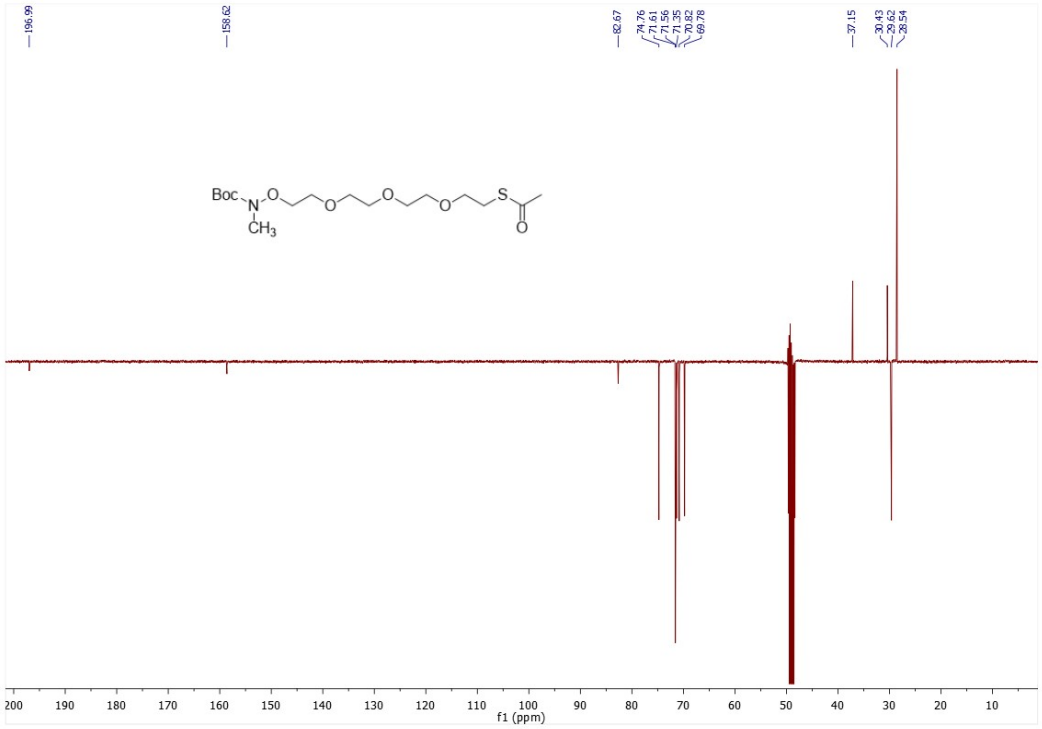

Figure S8. ^{13}C DEPTQ-135 NMR spectrum of **4** (CD_3OD, 298K)

***(N-t*-Butoxycarbonyl, *N*-methyl-hydroxylamine)-PEG$_4$-(orthopyridyl disulfide) (5)**

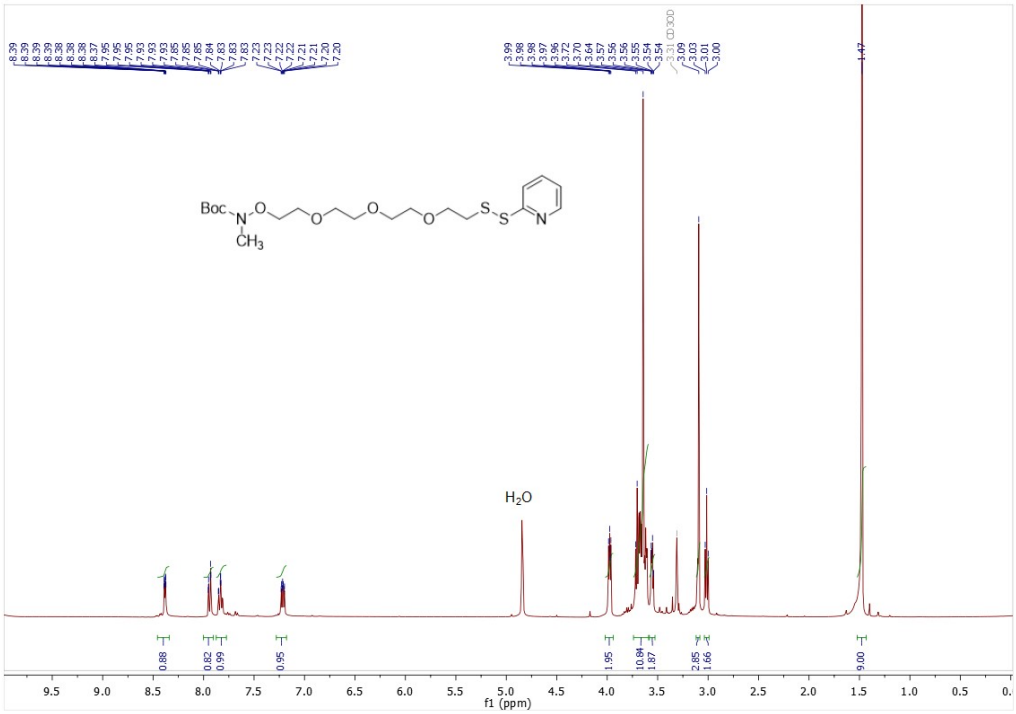

Figure S9. ^{1}H NMR spectrum of **5** (CD_3OD, 298K)

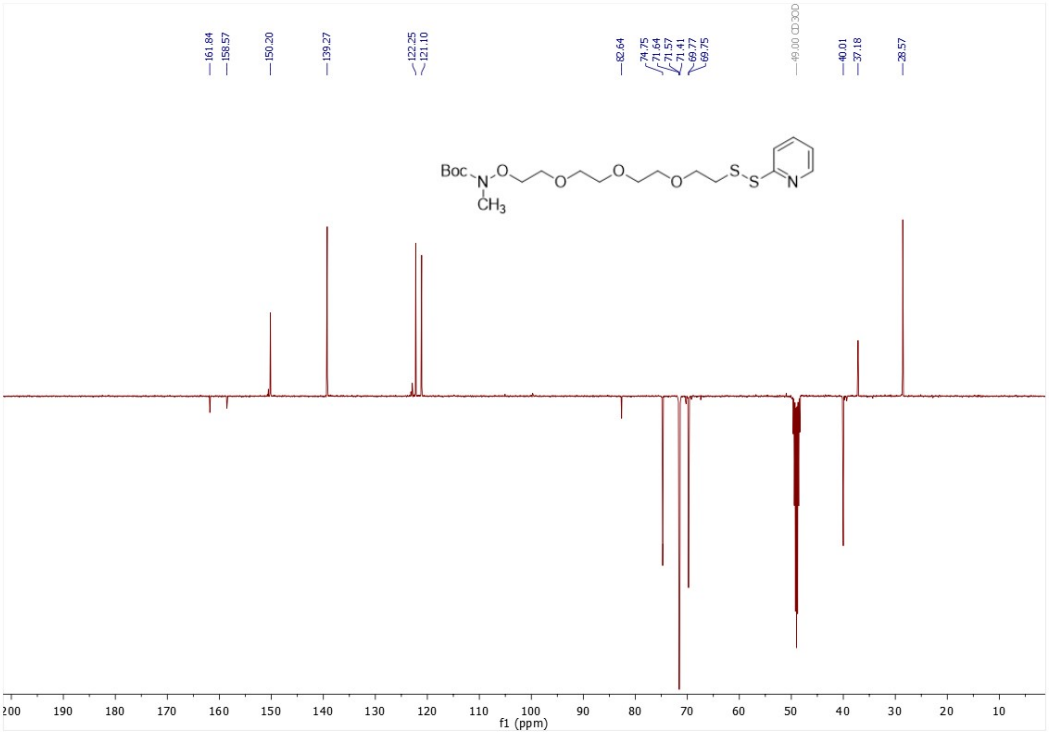

Figure S10. ^{13}C DEPTQ-135 NMR spectrum of **5** (CD_3OD, 298K)

α-2,6'-Sialyllactose-PEG$_4$-(orthopyridyl disulfide) (6)

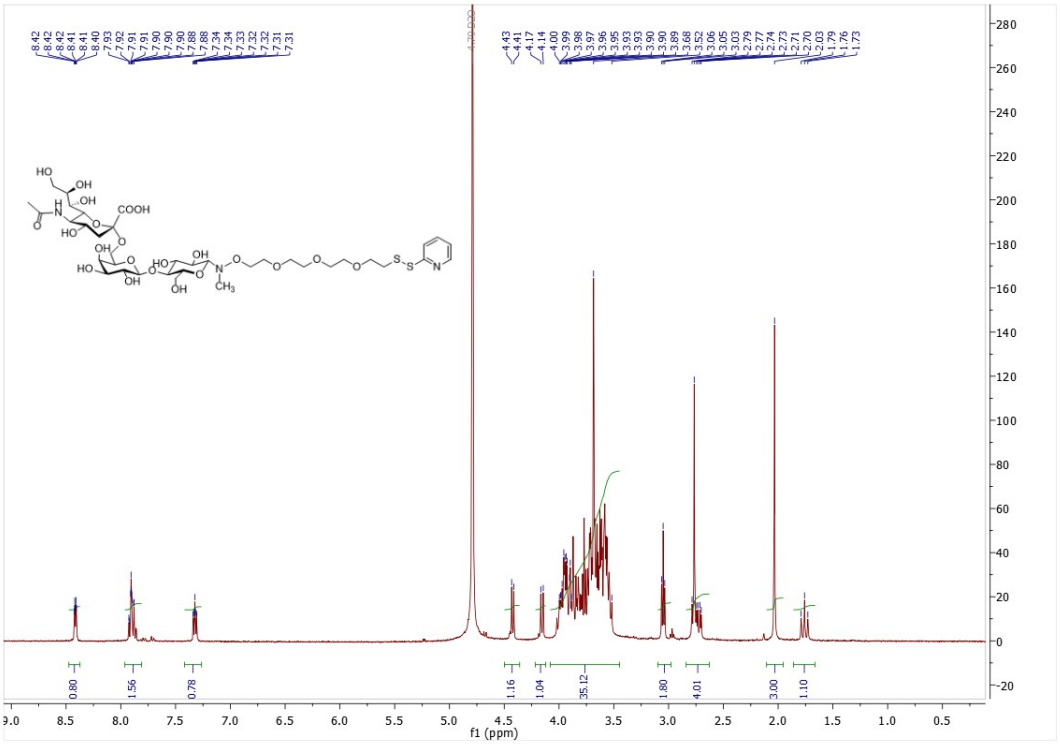

Figure S11. ^{1}H NMR spectrum of **6** (D_2O, 298K)

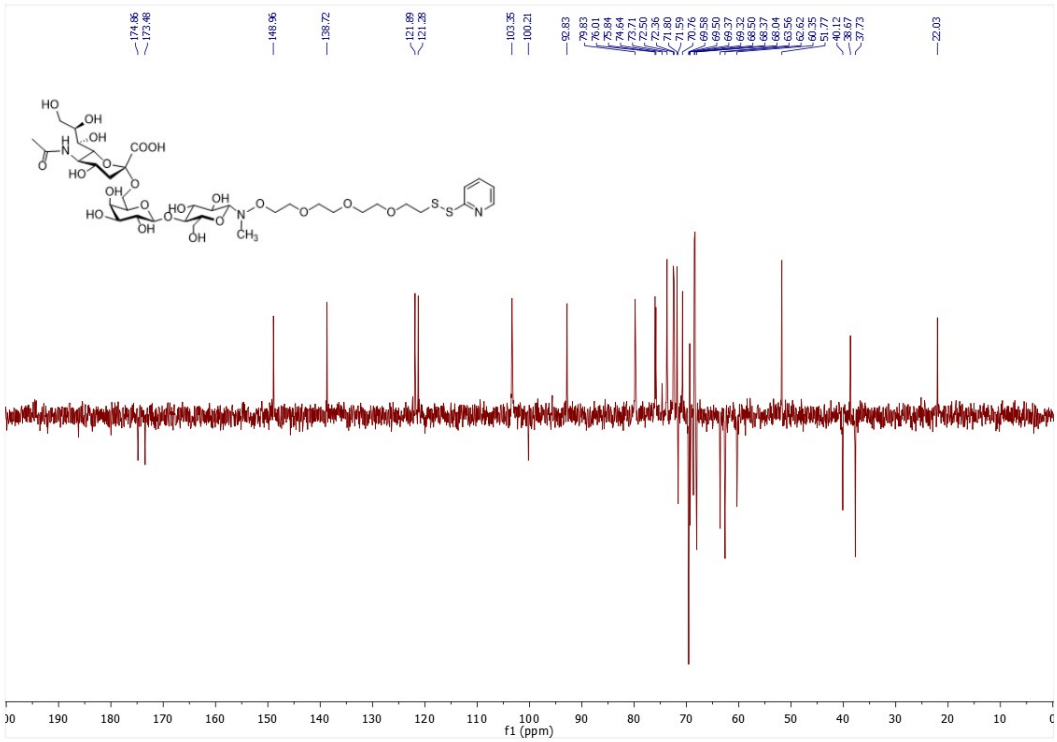

Figure S12. ^{13}C DEPTQ-135 NMR spectrum of **6** (D_2O, 298K)

α-2,3'-Sialyllactose-PEG$_4$-(orthopyridyl disulfide) (7)

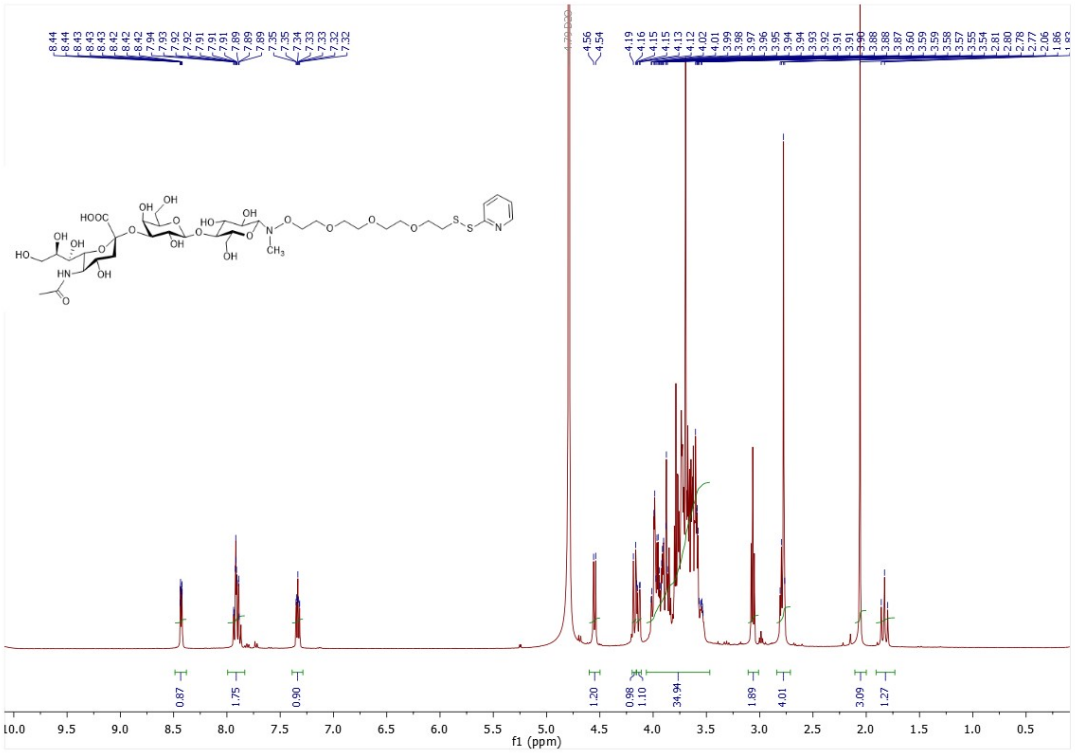

Figure S13. ^{1}H NMR spectrum of **7** (D_2O, 298K)

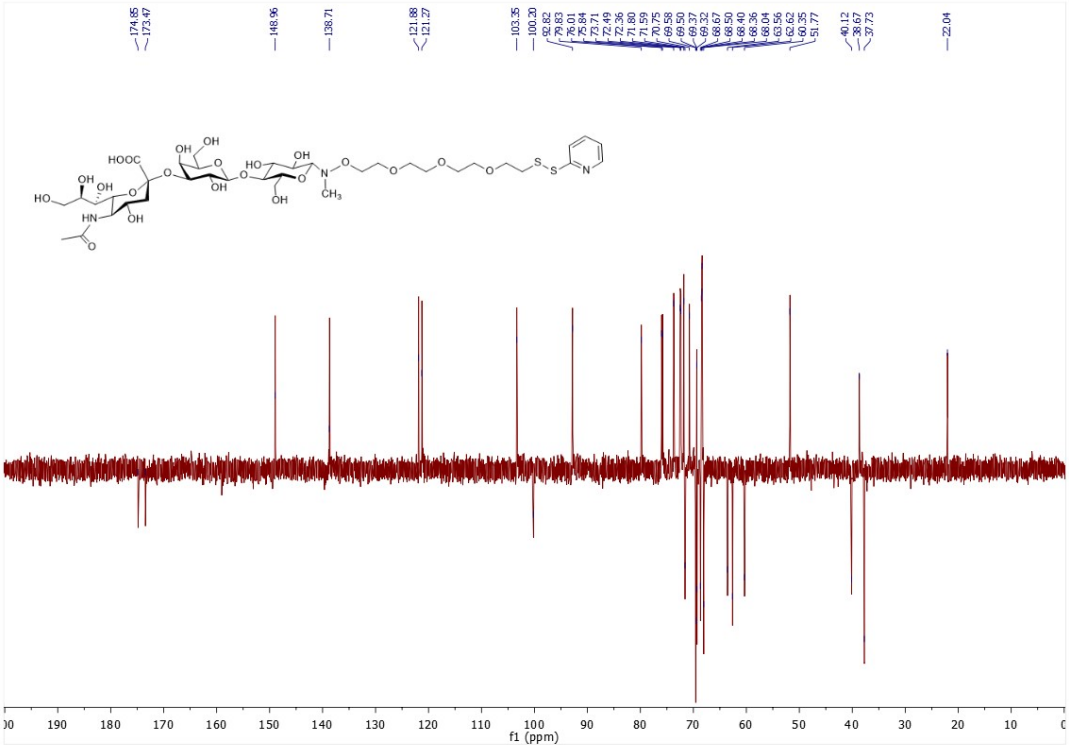

Figure S14. ^{13}C DEPTQ-135 NMR spectrum of **7** (D_2O, 298K)

***N*-(α-2,6'-sialyl-1-deoxylactitol-1-yl)dodecylamine (8)**

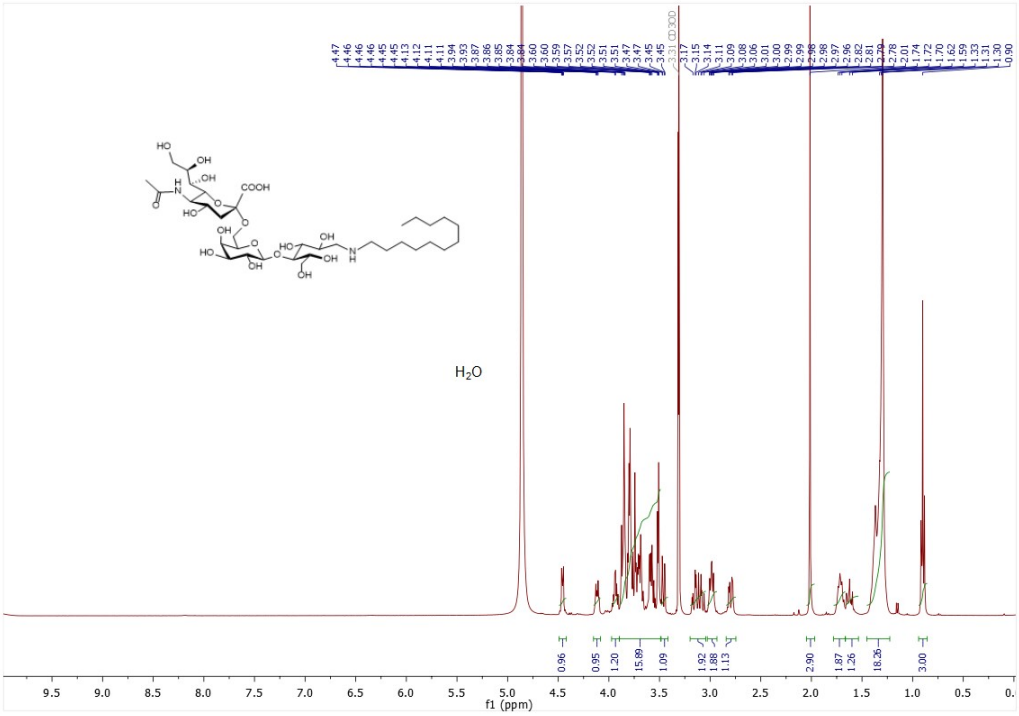

Figure S15. ^{1}H NMR spectrum of **8** (CD_3OD, 298K)

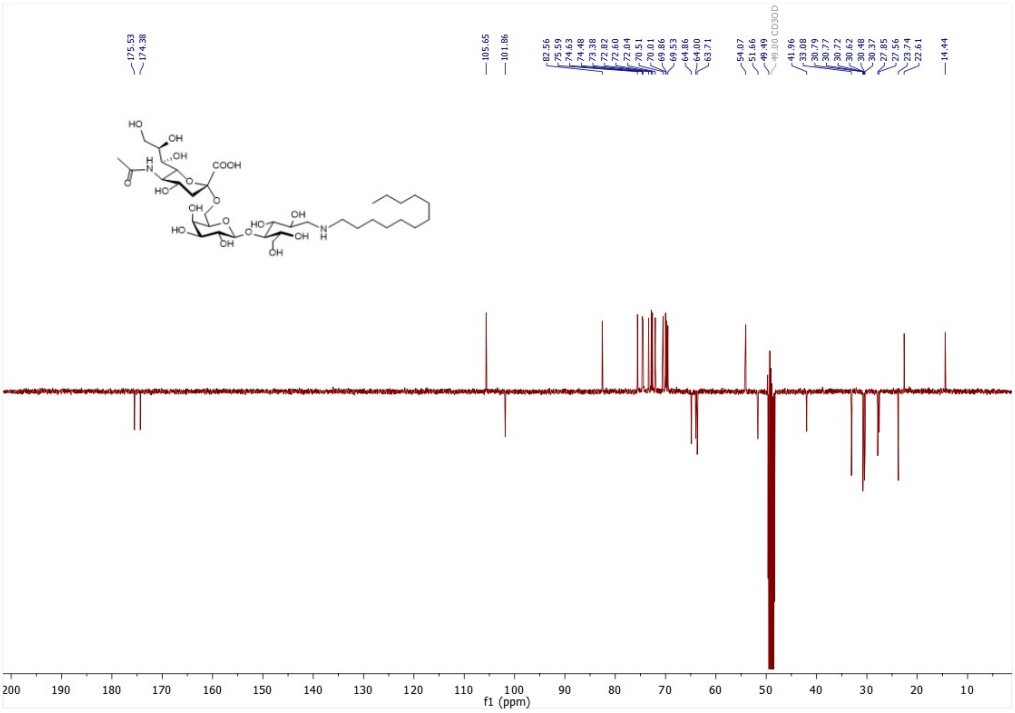

Figure S16. ^{13}C DEPTQ-135 NMR spectrum of **8** (CD_3OD, 298K)

***N*-(α-2,6'-sialyl-1-deoxylactitol-1-yl)hexadecylamine (9)**

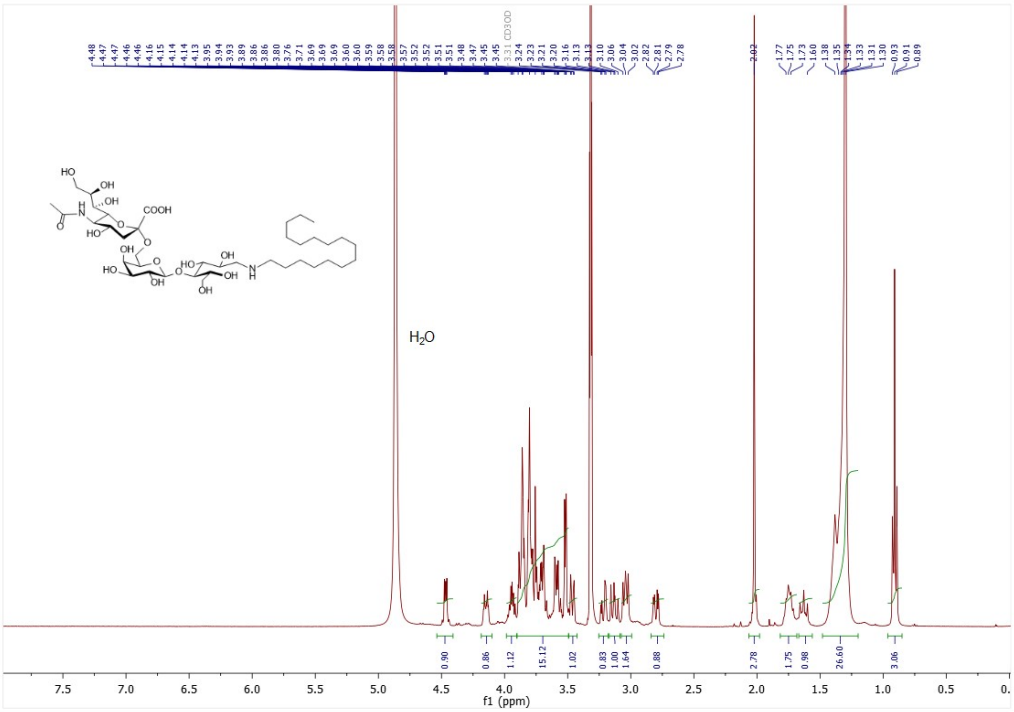

Figure S17. ^{1}H NMR spectrum of **9** (MeOD, 298K)

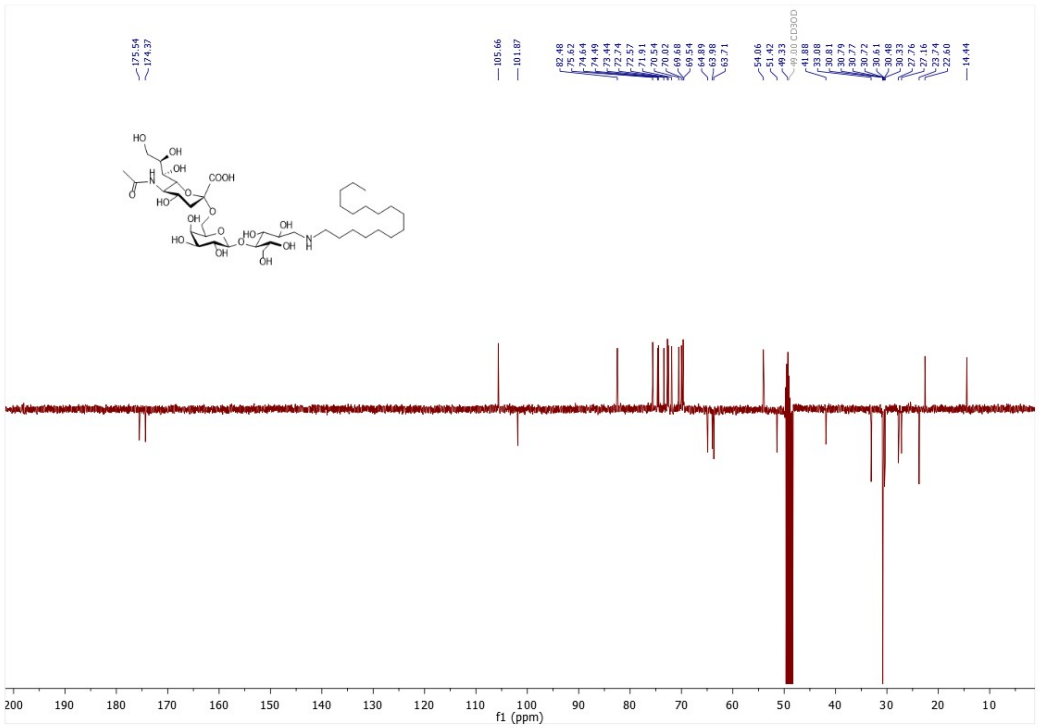

Figure S18. ^{13}C DEPTQ-135 NMR spectrum of **9** (CD_3OD, 298K)

***N*-(α-2,3'-sialyl-1-deoxylactitol-1-yl)dodecylamine (10)**

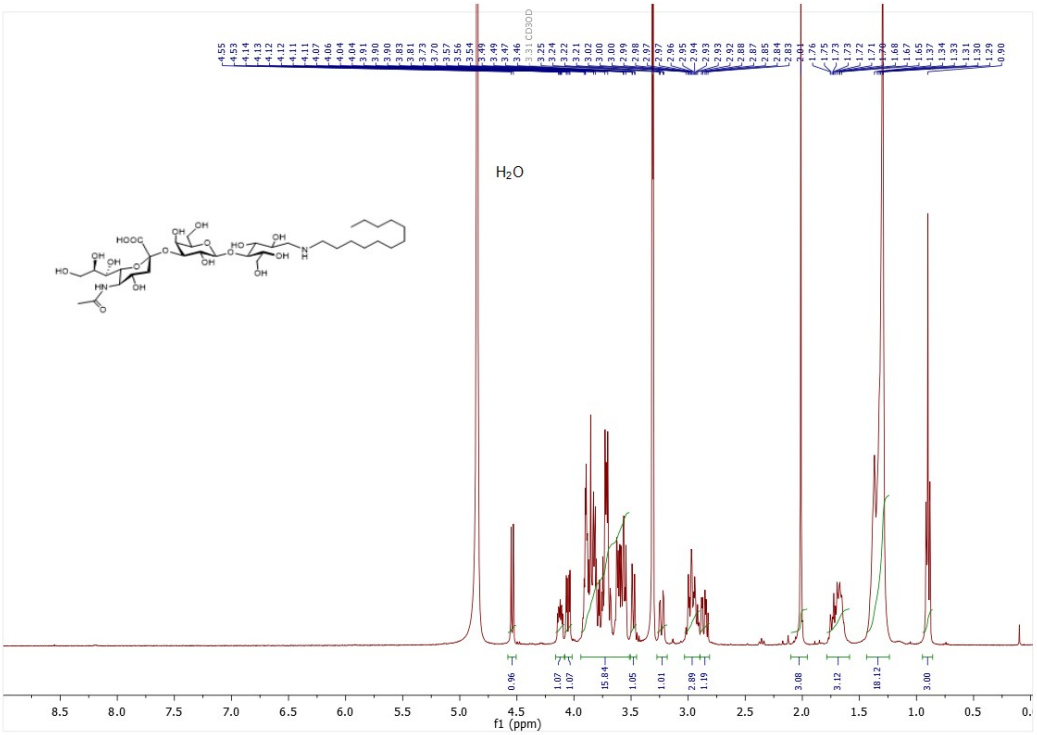

Figure S19. ^{1}H NMR spectrum of **10** (CD_3OD, 298K)

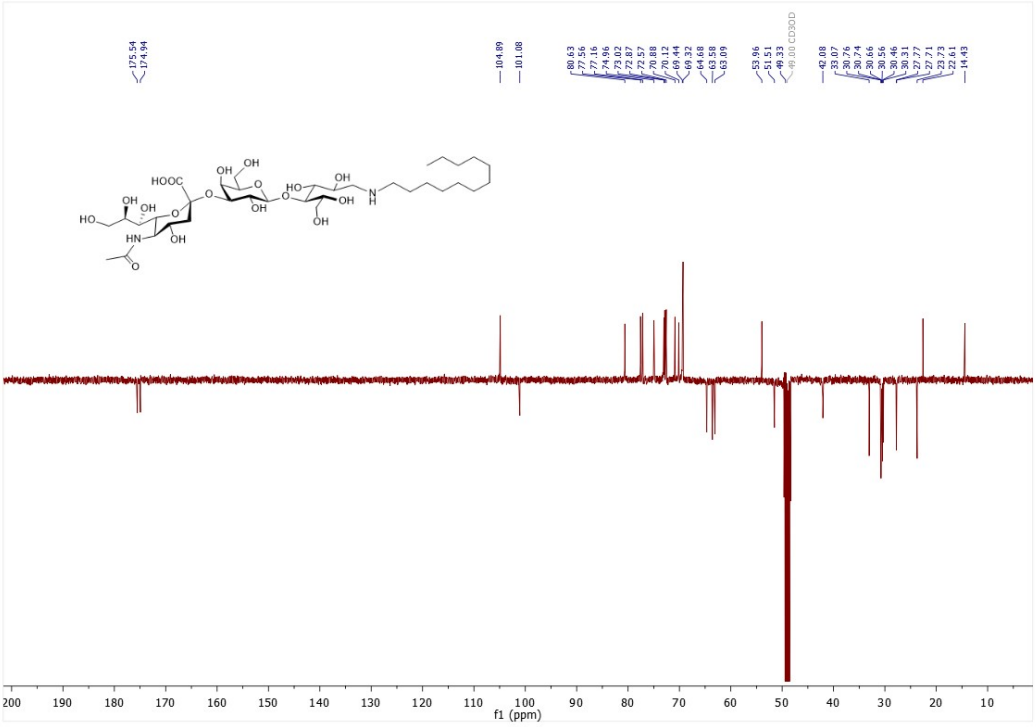

Figure S20. ^{13}C DEPTQ-135 NMR spectrum of **10** (CD_3OD, 298K)

***N*-(α-2,6'-sialyl-1-deoxylactitol-1-yl)hexadecylamine (11)**

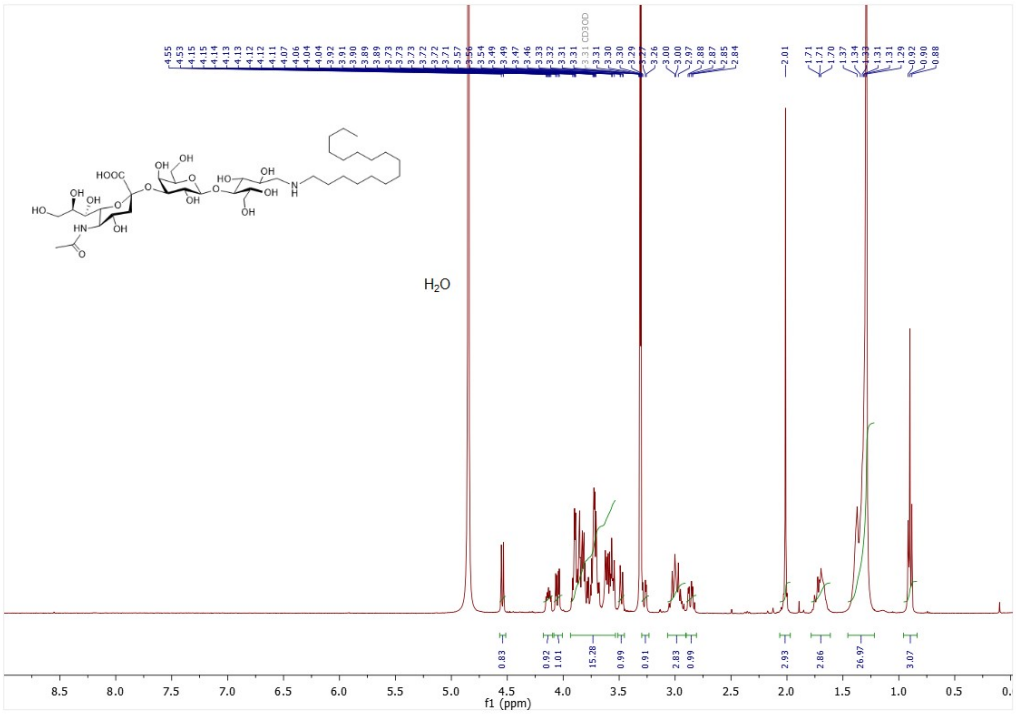

Figure S21. ^{1}H NMR spectrum of **11** (CD_3OD, 298K)

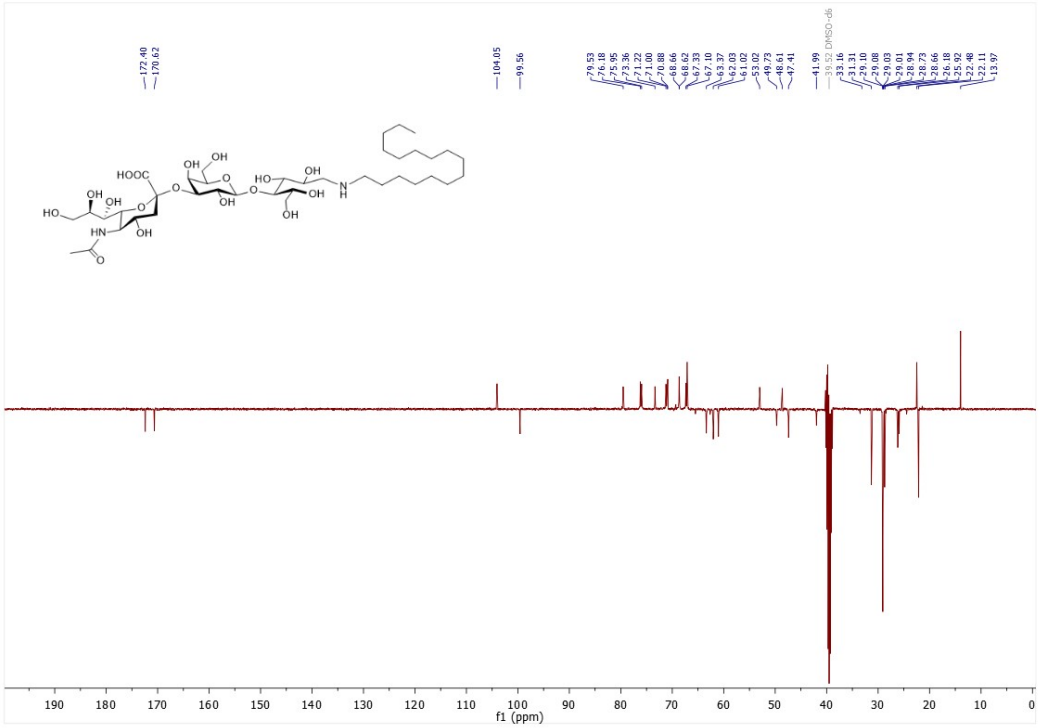

Figure S22. ^{13}C DEPTQ-135 NMR spectrum of **11** (DMSO-*d6*, 298K)

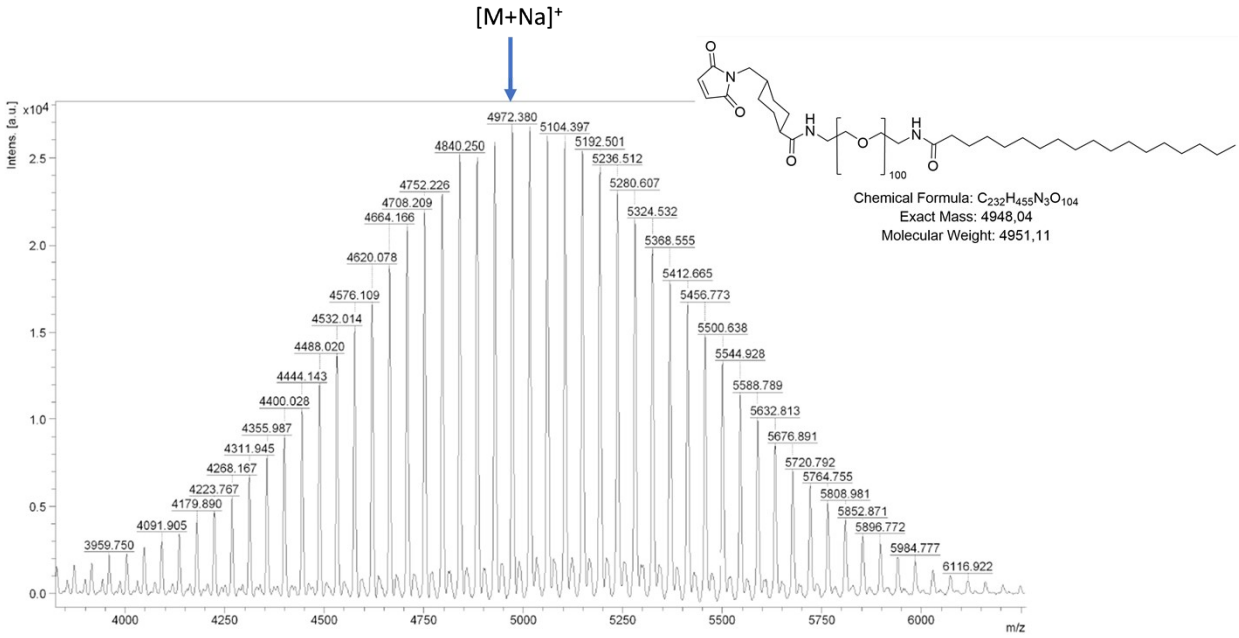

Figure S23. MALDI-TOF spectrum of **Mal-PEG$_{100}$-stearate**

Composition and characterization of NLC

		Control PEG-NLC	**Maleimide-PEG-NLC**		
			3% mol maleimide	5% mol maleimide	9% mol maleimide
Lipid phase	Lipoid S75	100 mg	50 mg	50 mg	50 mg
	Soybean Oil	205 mg	103 mg	103 mg	103 mg
	Suppocire™ NC	615 mg	308 mg	308 mg	308 mg
Aqueous phase	PEG$_{40}$-stearate	600 mg	270 mg	240 mg	210 mg
	Mal-PEG$_{100}$-stearate		30 mg	60 mg	90 mg
	1X PBS	2480 mg	1800 mg	1800 mg	1800 mg

Table S1. Composition of grafted-NLC formulations.

		C_{12} (**8** or **10**)	C_{16} (**9** or **11**)
Lipid phase	Lecithin compound	Lipoid™ SPC3 11.3 mg	Lipoid™ S75 5 mg
	Eldew™ SL-205	44.6 mg	32.6 mg
	Suppocire™ NC	14.8 mg	10.9 mg
Aqueous phase	Glycolipid	**8** or **10** 28 mg	**9** or **11** 8.3 mg
	Glycerol	1000 mg	1000 mg
	1X PBS	1800 mg	1800 mg

Table S2. Composition of glycolipid NLC formulations.

Particle	**Average hydrodynamic diameter** (nm)	**PDI**	**Zeta potential** (mV)
6'-SL-g-NLC	96±7	0.22±0.01	-21±4
	102±1	0.24±0.01	-27±1
	104±1	0.20±0.01	-27±1
3'-SL-g-NLC	102±1	0.22±0.01	-26±0.4
	101±1	0.23±0.01	-27±0.6
	107±1	0.20±0.01	-28±0.6
6'-SL-C16-NLC	62±1	0.20±0.02	-41±4
3'-SL-C16-NLC	84±2	0.17±0.01	-42±5

Table S3. Characteristics of grafted NLC and glycolipid NLC formulations after 2 months storage at 4°C.