Supporting information to

# Targeting extracellular lectins of *Pseudomonas aeruginosa* with glycomimetic liposomes

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**General experimental details.**

Commercial chemicals and solvents were used without further purification.

DPPC, DSPC, DPPE and 16:0 Glutaryl PE (DPPE-GA) were purchased from Avanti Polar Lipids (Alabama, USA). All silicone tubing (ID x OD, 1/16 x 1/8 inch) was purchased from Sigma-Aldrich (produced by Saint-Gobain, MI, USA). Polylactic acid (PLA) filament, 2.85 mm diameter, was purchased from Formfutura (Nijmegen, Netherlands). Polydimethylsiloxane as Slygard 184, and black Slygard 170 (Dow Chemical Co., Michigen, USA) was purchased from Sigma-Aldrich. UHU plus endfest 90 min (UHU GmbH & Co. KG, Bühl, Germany) was purchased from a commercial supplier. HC polycarboxylate hydrogel, NHS-activated glass slides were purchased from XanTec bioanalytics GmbH (Düsseldorf, Germany).

Thin layer chromatography (TLC) was performed using silica gel 60 aluminum plates containing fluorescence indicator (Merck KGaA, Darmstadt, Germany) and developed under UV light (254 nm) and using a molybdate solution (0.02 M solution of $(NH_4)Ce(SO_4)_4 \cdot 2H_2O$ and $(NH_4)_6Mo_7O_{24} \cdot 4H_2O$ in aqueous 10% $H_2SO_4$) or a potassium permanganate solution (3 g of $KMnO_4$, 20 g of $K_2CO_3$ in 5 mL of 5% NaOH and 300 mL of water) with heating.

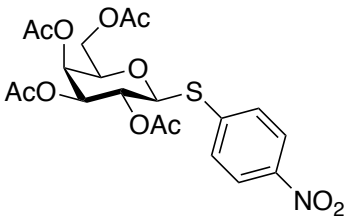
Medium pressure liquid chromatography (MPLC) was performed on a Teledyne Isco Combiflash Rf200 system using normal phase self-packed silica gel columns (60 Å, 400 mesh particle size, Fluka) or reversed-phase pre-packed silica gel 60 Å columns from Macherey-Nagel ($C_{18}$ ec, endcapped). Preparative high-pressure liquid chromatography (HPLC) was performed on Waters 2545 Binary Gradient Module with a Waters 2489 UV/Vis detector using a RP-18 column (250/21 Nucleodur C18 Gravity SB, 5 µm from Macherey-Nagel, Germany).

Analytical HPLC-MS was performed on a Thermo Dionex Ultimate 3000 HPLC coupled to a Bruker amaZon SL mass spectrometer, with UV detection at 254 nm using a RP-18 column (100/2 Nucleoshell RP18plus, 2.7 µm from Macherey-Nagel, Germany) as stationary phase. High resolution mass spectrometry (HRMS) was performed on an Ultimate 3000 UPLC system coupled to a Q Exactive Focus Orbitrap system with HESI source (Thermo Fisher, Dreieich, Germany). The UPLC was operated with a C18 column (EC 150/2 Nucleodur C18 Pyramid, 3 µm from Macherey-Nagel, Germany).

$^1$H- and $^{13}$C-NMR spectra were recorded on a Bruker Avance III 500 UltraShield spectrometer at 500 MHz and 126 MHz, respectively. Chemical shifts (δ) are given in ppm and were calibrated on residual solvent peaks: $CHCl_3$-*d1* ($^1$H-NMR δ = 7.26 ppm, $^{13}$C-NMR δ = 77.0

ppm), MeOH-*d4* ($^{1}$H -NMR δ = 3.31 ppm, $^{13}$C -NMR δ = 49.0 ppm), DMSO-*d*$_6$ ($^{1}$H -NMR δ = 2.50 ppm, $^{13}$C -NMR δ = 39.51 ppm). Deuterated solvents were purchased from Eurisotop (Saarbrücken, Germany). Multiplicities are specified as s = singlet, bs = broad singlet, d = doublet, dd = doublet of doublets, t = triplet, td = triplet of doublets, q = quartet, m = multiplet. The spectra were assigned with the help of $^{1}$H,$^{1}$H-COSY and $^{1}$H,$^{13}$C-HSQC experiments.

**Compound synthesis**




***p*-nitrophenyl 2,3,4,6-tetra-O-acetyl-β-D-thiogalactopyranoside (2)**.

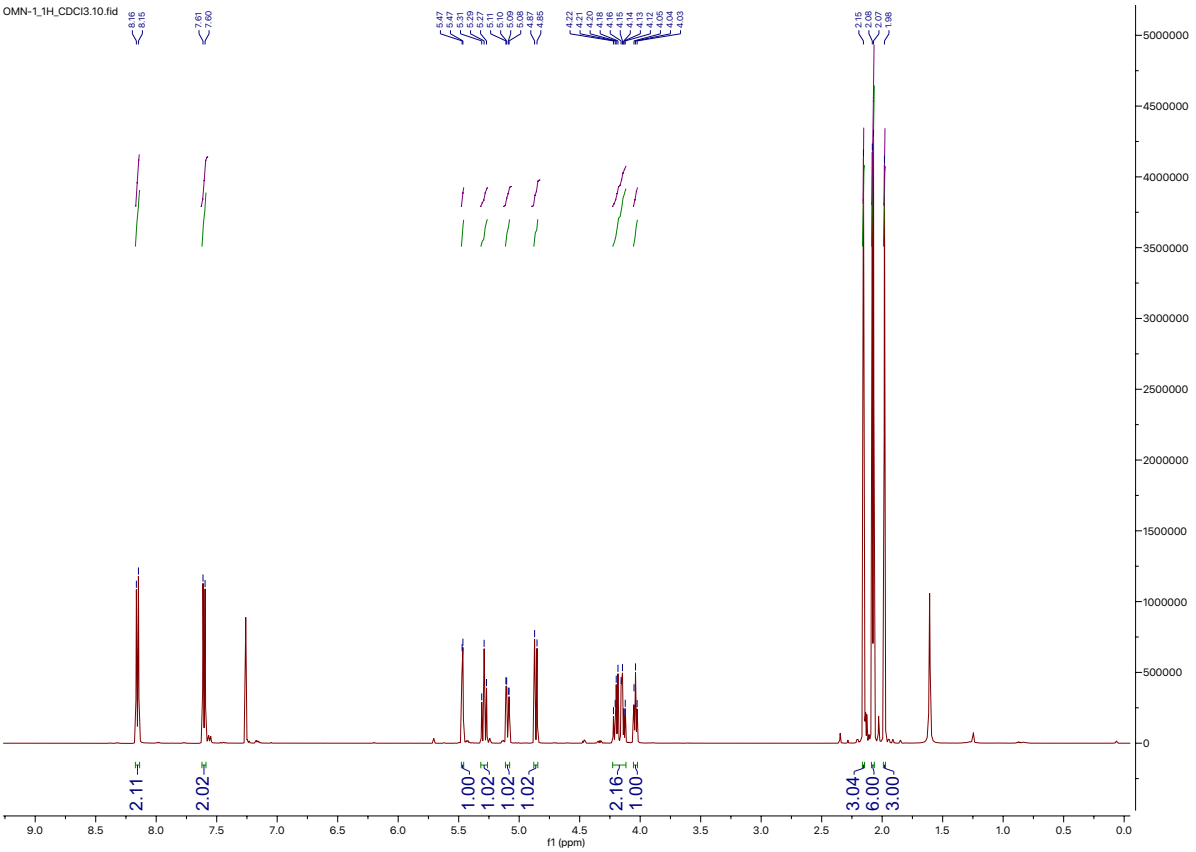
Compound **2** was synthesized according to Escopy *et al.*[1]: Penta-*O*-acetyl-β-D-galactopyranose (**1**, 2 g, 5.1 mmol) and para-nitro-thiophenol (1.5 g, 2 equiv., 10.2 mmol) were dissolved in 20 mL dry dichloromethane with 200 mg 3 Å activated molecular sieves under nitrogen. The mixture was cooled to 0 °C, triflic acid (360 µL, 0.8 equiv., 4.09 mmol) was added dropwise and the reaction was stirred for 30 min. The reaction was diluted with DCM, filtrated through celite, washed with aqueous sodium bicarbonate, water and brine consequentially, and dried over anhydrous sodium sulfate. After filtration the obtained organic phase was concentrated *in vacuo* and the residue was recrystallized twice from EtOAc to provide **2** as white crystals (1.65 g, 3.4 mmol, 66%).

$^{1}$H NMR (500 MHz, $CHCl_3$-*d1*) δ 8.16 (d, *J* = 8.5 Hz, 2H, ArH), 7.60 (d, *J* = 8.5 Hz, 2H, ArH), 5.47 (d, *J* = 3.3 Hz, 1H, H-4), 5.29 (t, *J* = 9.9 Hz, 1H, H-2), 5.10 (dd, *J* = 9.9, 3.2 Hz, 1H, H-3), 4.86 (d, *J* = 10.0 Hz, 1H, H-1), 4.23 – 4.12 (m, 2H, H-6), 4.04 (t, *J* = 6.5 Hz, 1H, H-5), 2.15 (s, 3H, $CH_3$), 2.08 (d, *J* = 5.1 Hz, 6H, $CH_3$), 1.98 (s, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, $CHCl_3$-*d1*) δ 170.33 ($CH_3\underline{C}(O)$), 170.04 ($CH_3\underline{C}(O)$), 169.97 ($CH_3\underline{C}(O)$), 169.39 ($CH_3\underline{C}(O)$), 146.85 (ArC), 142.41 (ArC), 130.41 (ArCH), 123.86 (ArCH), 84.85 (C-1), 74.86 (C-5), 71.73 (C-3), 67.08 (C-2), 66.72 (C-4), 61.68 (C-6), 20.76 ($CH_3$), 20.71 ($CH_3$), 20.66 ($CH_3$), 20.55 ($CH_3$).

HPLC-MS: $[C_{20}H_{23}NO_{11}S + Na]^+$ calcd. 508.09, found 508.08.
HRMS: $[C_{20}H_{23}NO_{11}S + Na]^+$ calcd. 508.0884, found 508.0873.

Spectroscopic data is in accordance with the literature[2].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5.08
4.87
4.85
4.22
4.21
4.20
4.18
4.16
4.15
4.14
4.13
4.12
4.06
4.04
4.03
2.15
2.08
2.07
1.98
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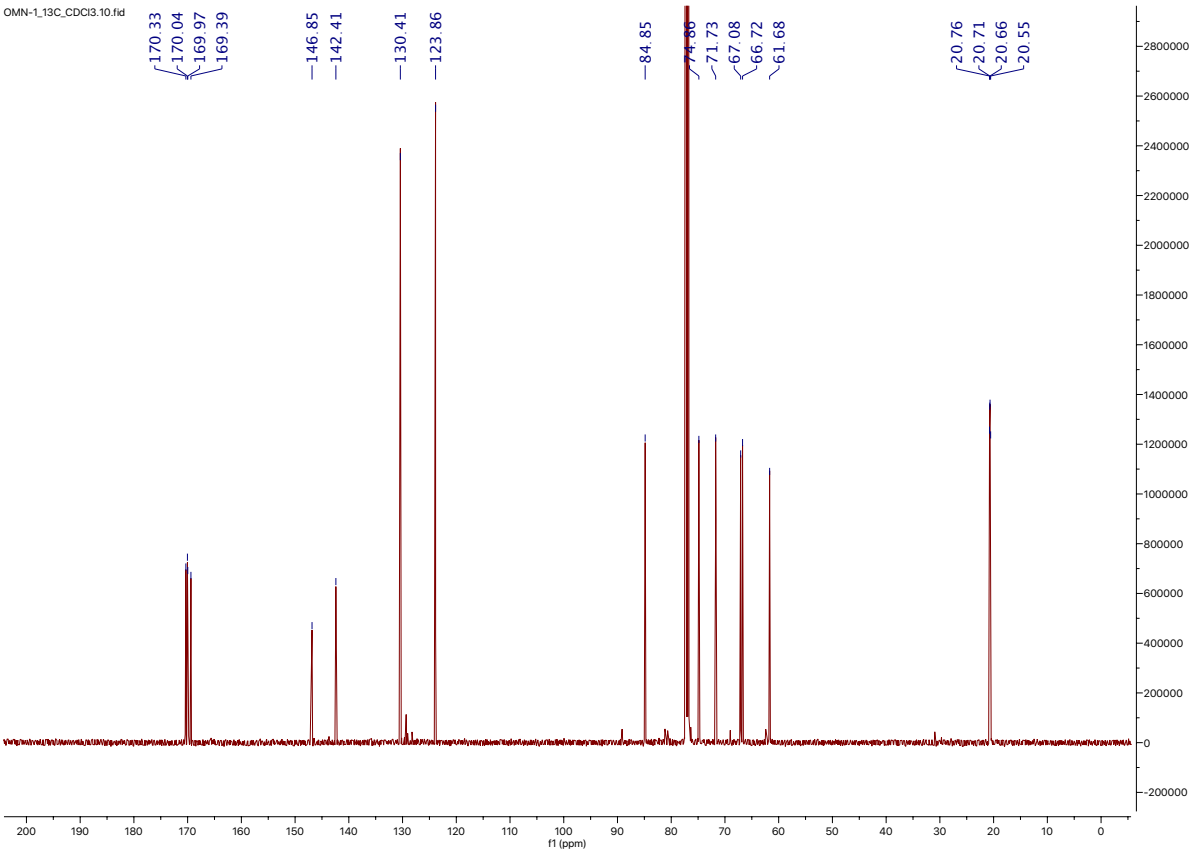
1.00
3.04
6.00
3.00
f1 (ppm)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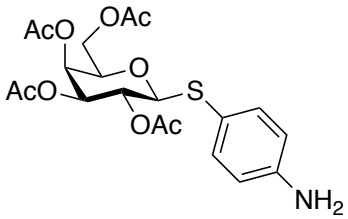
20.71
20.66
20.55
f1 (ppm)




**3**

***p*-Aminophenyl 2,3,4,6-tetra-O-acetyl-β-D-thiogalactopyranoside (3)**.

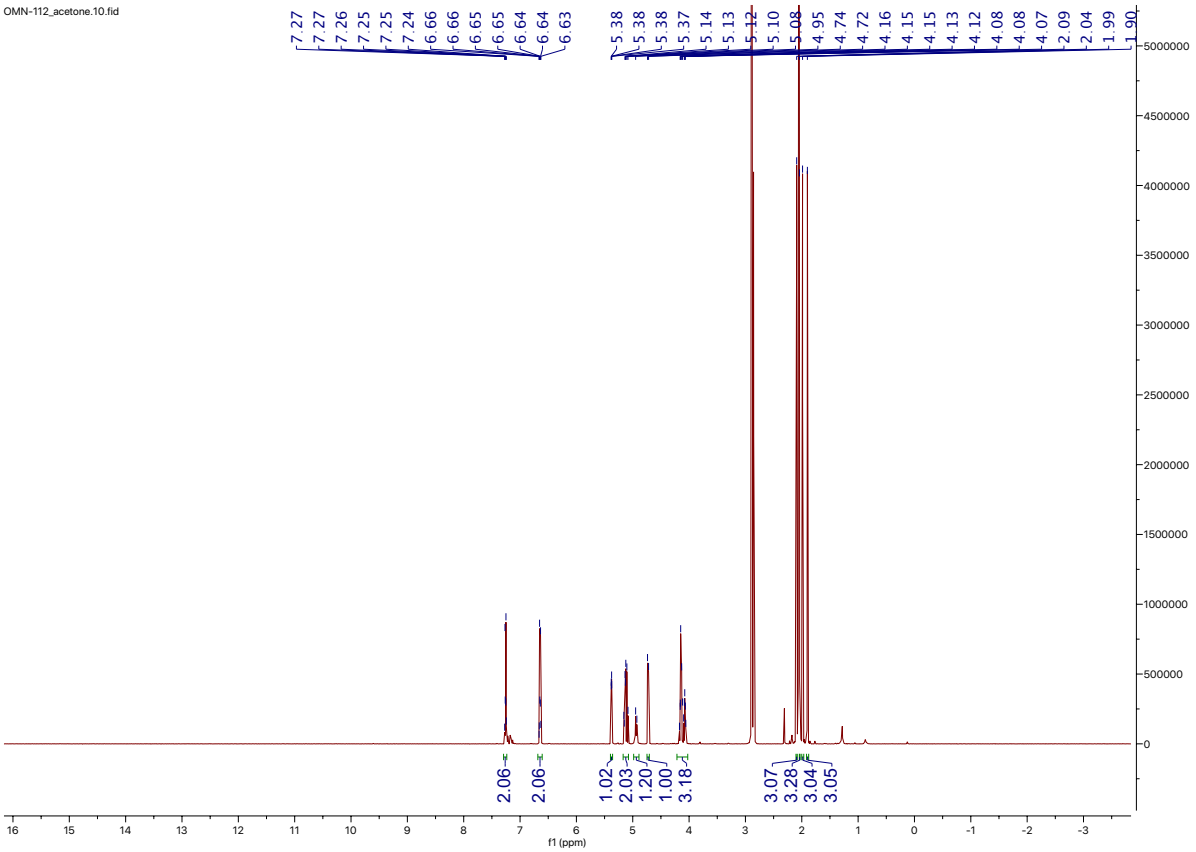
Compound **3** was synthesized according to Casoni *et al.*[2]: **2** (900 mg, 1.85 mmol) was suspended in dry DCM (40 mL) and 90 mg palladium on activated charcoal (10% Pd basis) was added under nitrogen atmosphere. The reaction flask was flushed with hydrogen and stirred overnight at r.t. under hydrogen atmosphere. The reaction mixture was filtered through celite and the solvent was removed *in vacuo.* The crude product was purified by normal phase MPLC (Toluene/EtOAc, 40–80% EtOAc). **3** was obtained as a light-pink solid (818 mg, 1.8 mmol, 97%).

$^{1}$H NMR (500 MHz, Acetone-$d_6$) δ 7.29 – 7.23 (m, 2H, ArH), 6.68 – 6.61 (m, 2H, ArH), 5.38 (dd, $J$ = 3.2, 0.9 Hz, 1H, H-4), 5.18 – 5.06 (m, 2H, H-2, H-3), 4.94 (br s, $J$ = 10.9 Hz, $NH_2$), 4.73 (d, $J$ = 9.3 Hz, 1H, H-1), 4.19 – 4.04 (m, 3H, H-5, H-6), 2.09 (s, 3H, $CH_3$), 2.04 (s, 3H, $CH_3$), 1.99 (s, 3H, $CH_3$), 1.90 (s, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, Acetone-$d_6$) δ 170.81 ($CH_3\underline{C}(O)$), 170.60 ($CH_3\underline{C}(O)$), 170.26 ($CH_3\underline{C}(O)$), 169.88 ($CH_3\underline{C}(O)$), 150.39 (ArC), 150.34 (ArC), 136.71 (ArCH), 129.86 (Toluene contamination), 129.14 (Toluene contamination), 117.95 (ArC), 115.38 (ArCH), 115.35 (ArCH), 88.19 (C-1), 75.01 (C-5), 72.82 (C-3), 68.68 (C-2), 68.42 (C-4), 62.63 (C-6), 20.92 ($CH_3$), 20.73 ($CH_3$), 20.64 ($CH_3$), 20.63 ($CH_3$).

HPLC-MS: $[C_{20}H_{25}NO_9S + H]^+$ calcd. 456.13, found 456.09.
HRMS: $[C_{20}H_{25}NO_9S + H]^+$ calcd. 456.1323, found 456.1311.

Spectroscopic data is in accordance with the literature[2].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4.12
4.08
4.08
4.07
2.09
2.04
1.99
1.90
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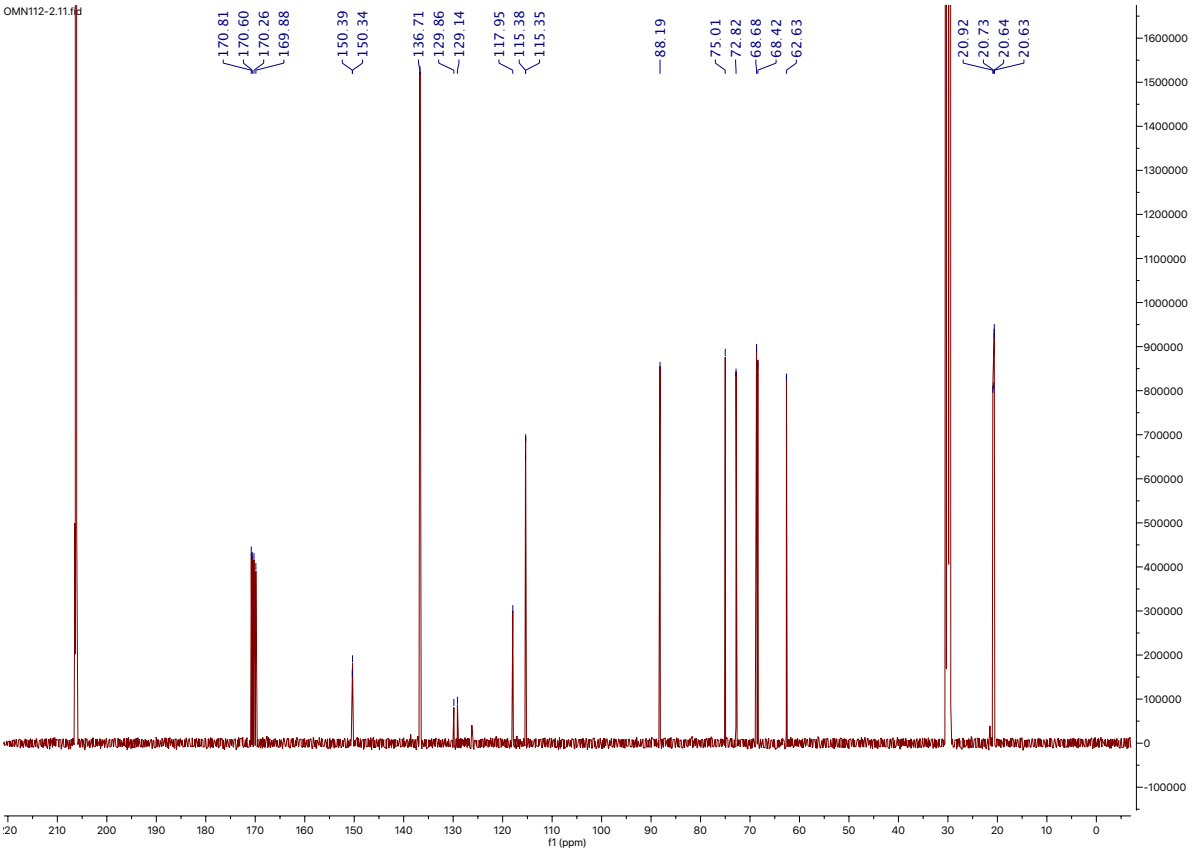
3.05
f1 (ppm)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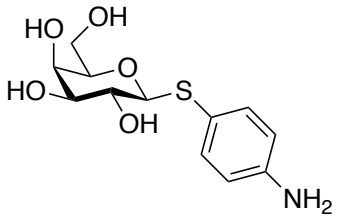
20.73
20.64
20.63
f1 (ppm)




***p*-Aminophenyl β-D-thiogalactopyranoside (4)**.

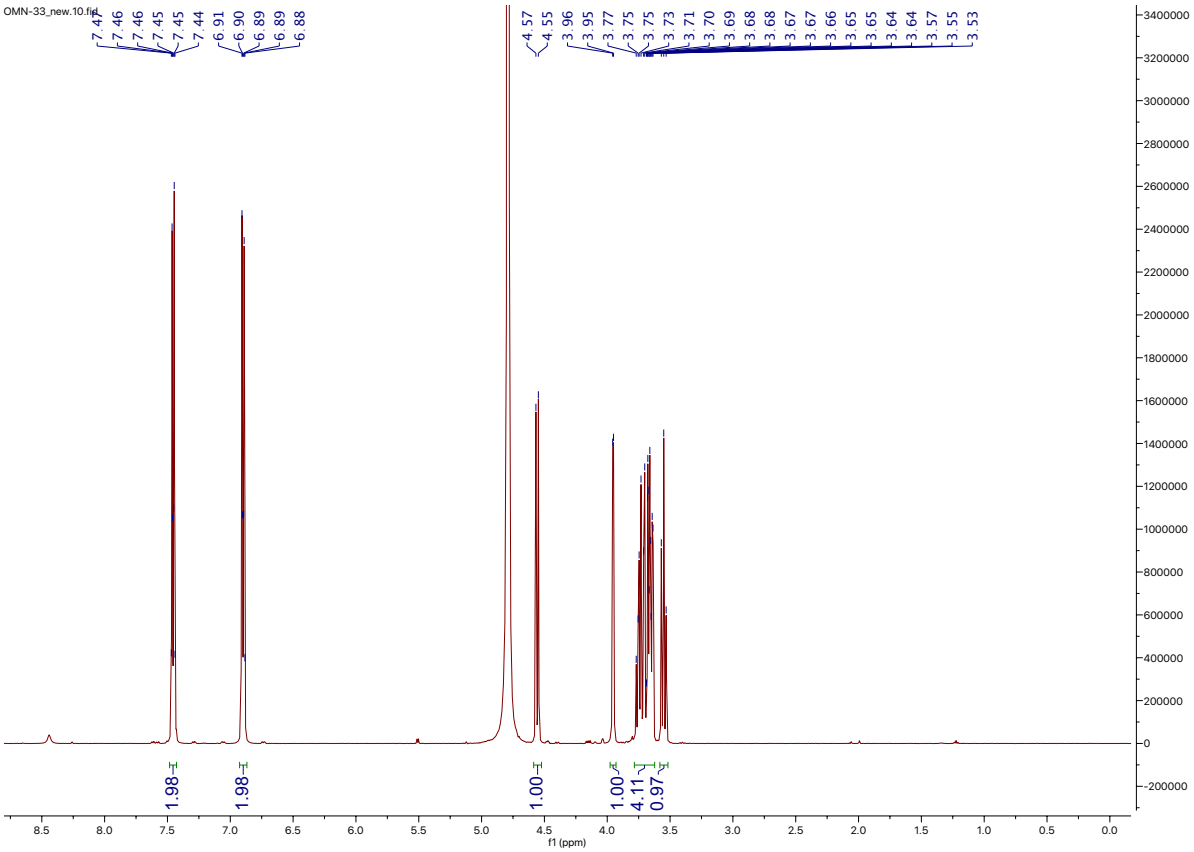
Compound **3** (300 mg, 0.66 mmol) was suspended in dry MeOH (5 mL) and 5.3 M NaOMe in MeOH (62 μL, 0.5 equiv., 0.33 mmol) was added. The reaction mixture was stirred for 30 min at r.t., when 0.1 M HCl was added to neutralize the reaction mixture to pH 7. The solvent was removed *in vacuo* and the residue was purified by reverse phase MPLC ($H_2O$/MeCN + 0.1% formic acid, 5-15% MeCN) to give **4** as a white solid (178 mg, 0.62 mmol, quant.).

$^1$H NMR (500 MHz, $D_2O$) δ 7.48 – 7.42 (m, 2H, ArH), 6.93 – 6.88 (m, 2H, ArH), 4.56 (d, $J$ = 9.8 Hz, 1H, H-1), 3.95 (d, $J$ = 3.3 Hz, 1H, H-4), 3.78 – 3.62 (m, 4H, H-2, H-5, H-6), 3.55 (t, $J$ = 9.6 Hz, 1H, H-3).

$^{13}$C NMR (126 MHz, $D_2O$) δ 144.74 (ArC), 134.54 (ArCH), 121.81 (ArC), 117.67 (ArCH), 88.83 (C-1), 78.93 (C-5), 73.96 (C-3), 69.08 (C-2), 68.67 (C-4), 60.91 (C-6).

HRMS: $[C_{12}H_{17}NO_5S + H]^+$ calcd. 288.0900, found 288.0891.

Spectroscopic data is in accordance with the literature[3].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3.95
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3.75
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3.73
3.71
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3.69
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3.65
3.65
3.64
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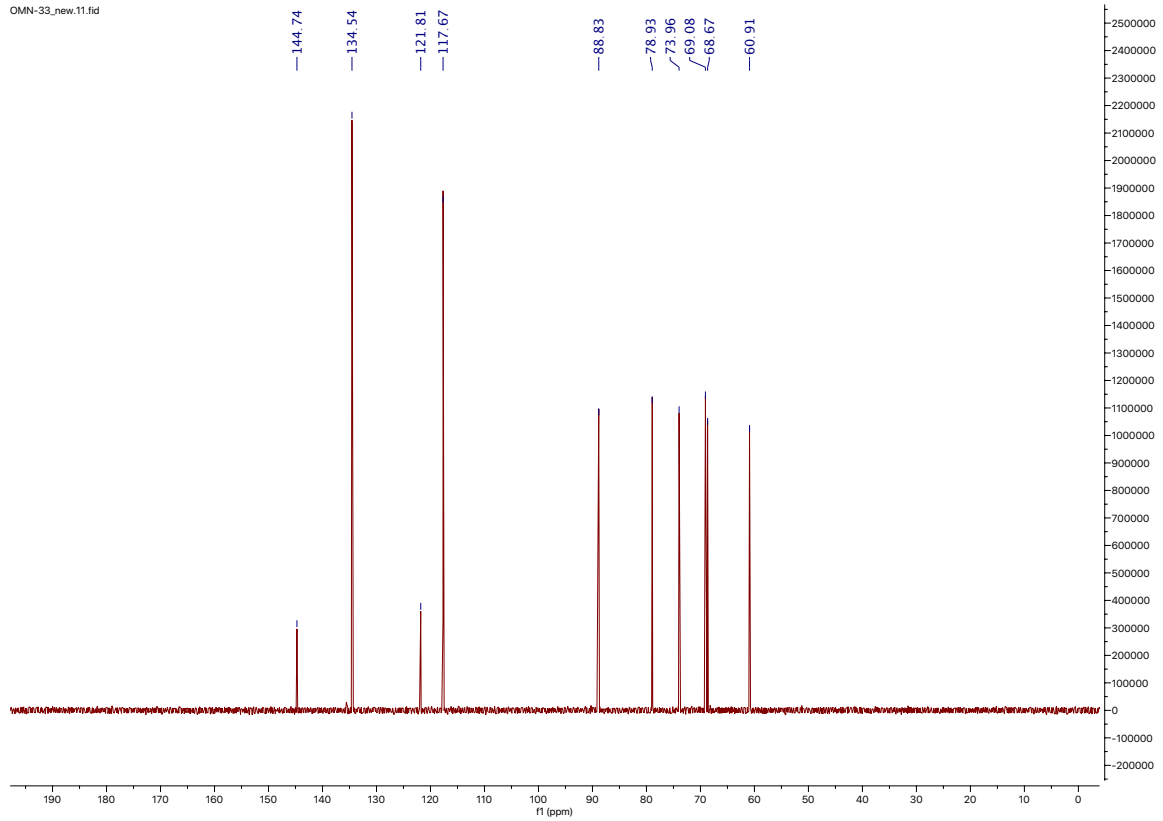
f1 (ppm)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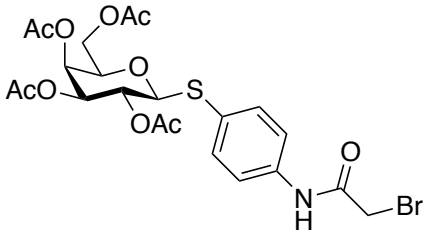
68.67
60.91
f1 (ppm)

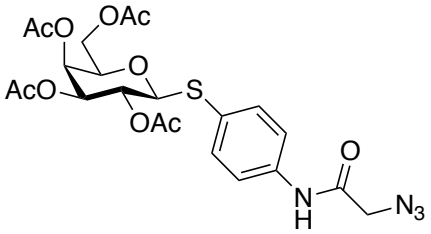



**5**

**4-(2-Bromoacetamido)phenyl 2,3,4,6-tetra-O-acetyl-β-D-thiogalactopyranoside (5)**.

Compound **5** was synthesized according to Casoni *et al.*[2]: **3** (400 mg, 0.88 mmol) was dissolved in dry DCM (10 mL) and triethylamine (194 µL, 1.6 equiv., 1.4 mmol) was added under nitrogen atmosphere. The reaction flask was cooled to 0 °C and bromoacetyl bromide (115 µL, 1.5 equiv, 1.32 mmol) was added dropwise under vigorous stirring. The reaction mixture was warmed to r.t. and stirred for 2 h. Then, the reaction was diluted with DCM and washed with aqueous saturated ammonium chloride, water and brine consequentially, and dried over anhydrous sodium sulfate. After filtration, the solvent was removed *in vacuo*. Crude **5** (551 mg) was used for further modification without purification.

HPLC-MS: $[C_{22}H_{26}BrNO_{10}S + H]^+$ calcd. 576.05, found 576.00.




**6**, 73% over two steps

**4-(2-Azidoacetamido)phenyl 2,3,4,6-tetra-O-acetyl-β-D-thiogalactopyranoside (6)**.

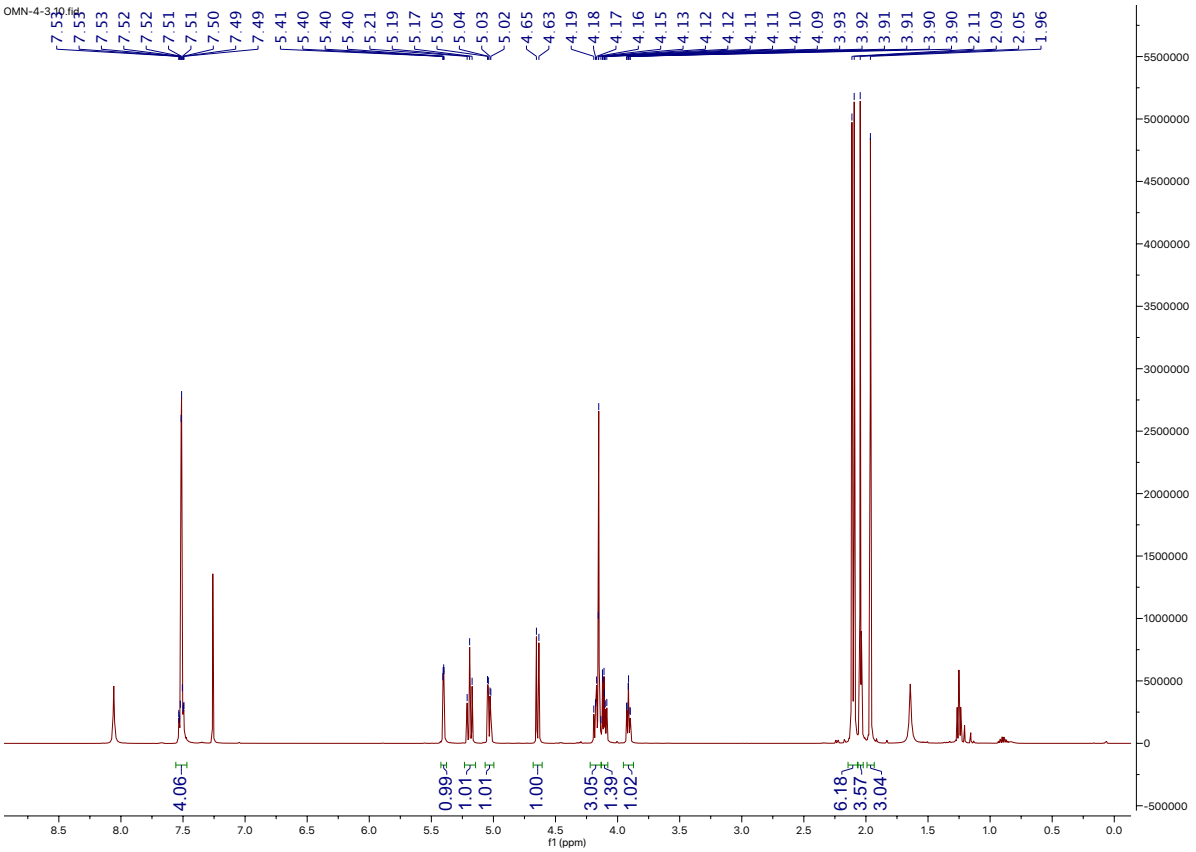
Compound **6** was synthesized according to Casoni *et al.*[2]: **5** (551 mg) was suspended in dry DMF (10 mL), sodium azide (285 mg, 5 equiv., 4.4 mmol) was added and the reaction was stirred for 3 h under nitrogen atmosphere. The reaction was diluted with water and extracted three times with EtOAc, combined organic phases were washed with water, brine and then dried over anhydrous sodium sulfate. After filtration, the solvent was removed *in vacuo.* The crude product was purified by normal phase MPLC (petroleum ether/EtOAc, 40–70% EtOAc). **6** was obtained as a white solid (341 mg, 0.64 mmol, 73% over two steps).

$^{1}$H NMR (500 MHz, $CHCl_3$-*d1*) δ 7.56 – 7.45 (m, 4H, ArH), 5.40 (dd, *J* = 3.4, 1.1 Hz, 1H, H-4), 5.19 (t, *J* = 10.0 Hz, 1H, H-2), 5.03 (dd, *J* = 9.9, 3.4 Hz, 1H, H-3), 4.64 (d, *J* = 9.9 Hz, 1H, H-1), 4.23 – 4.06 (m, 1H, H-$6_a$), 4.16 (s, 2H, $CH_2$) 3.95 – 3.86 (m, 1H, H-$6_b$), 2.11 (s, 3H, $CH_3$), 2.09 (s, 3H, $CH_3$), 2.05 (s, 3H, $CH_3$), 1.96 (s, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, $CHCl_3$-*d1*) δ 170.53 ($CH_3\underline{C}$(O)), 170.33 ($CH_3\underline{C}$(O)), 170.19 ($CH_3\underline{C}$(O)), 169.55 ($CH_3\underline{C}$(O)), 164.68 (NHC(O)), 137.21 (ArC), 134.26 (ArCH), 128.03 (ArC), 120.34 (ArCH), 86.76 (C-1), 74.58 (C-5), 72.10 (C-3), 67.32 (C-4, C-2), 61.71 (C-6), 53.08 ($CH_2$), 20.99 ($CH_3$), 20.84 ($CH_3$), 20.79 ($CH_3$), 20.71 ($CH_3$).

HRMS: $[C_{22}H_{26}N_4O_{10}S + H]^+$ calcd. 539.1442, found 539.1436.

Spectroscopic data is in accordance with the literature[2].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4.65 4.63 4.19 4.18 4.17 4.16 4.15 4.13 4.12 4.12 4.11 4.11 4.10 4.09
3.93 3.92 3.91 3.91 3.90 3.90 2.11 2.09 2.05 1.96
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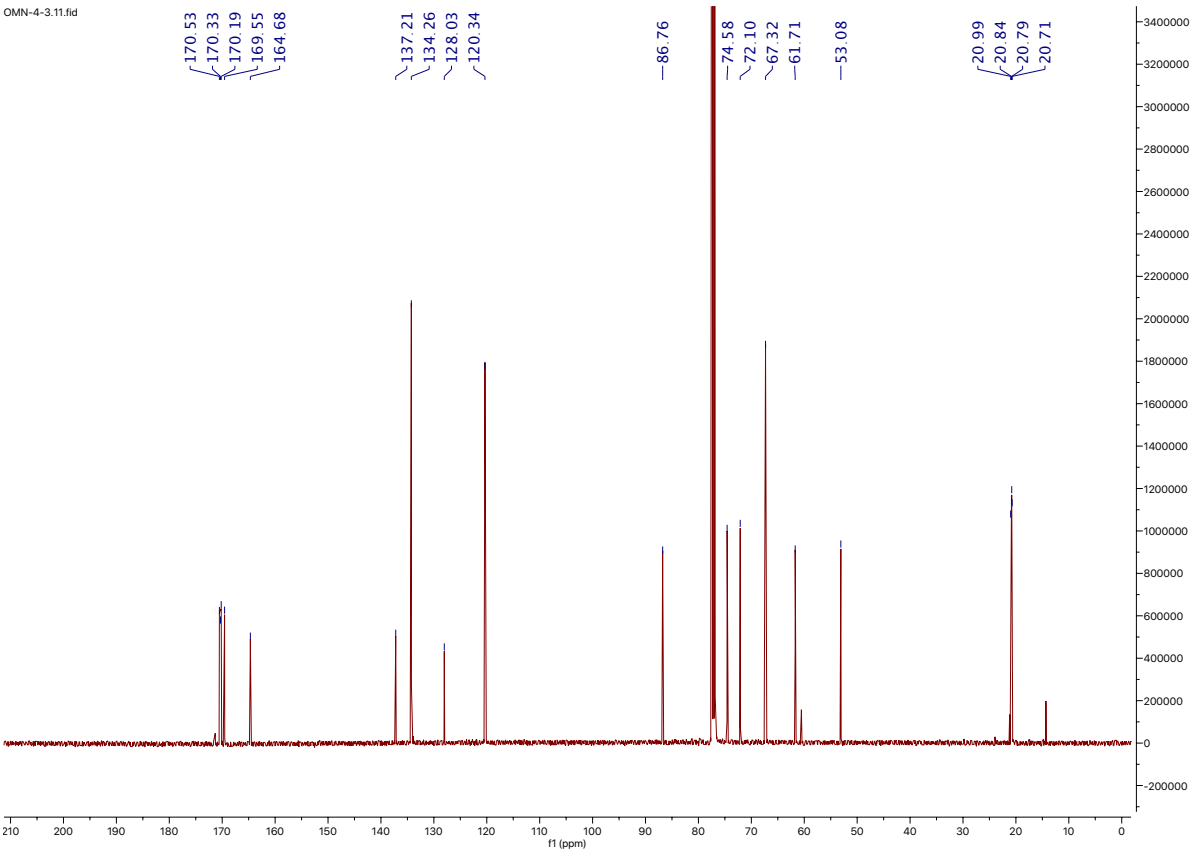
f1 (ppm)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86.76
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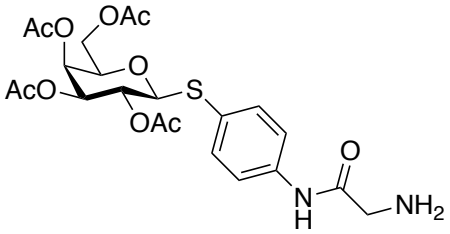
53.08
20.99 20.84 20.79 20.71
f1 (ppm)




**7**, 97%

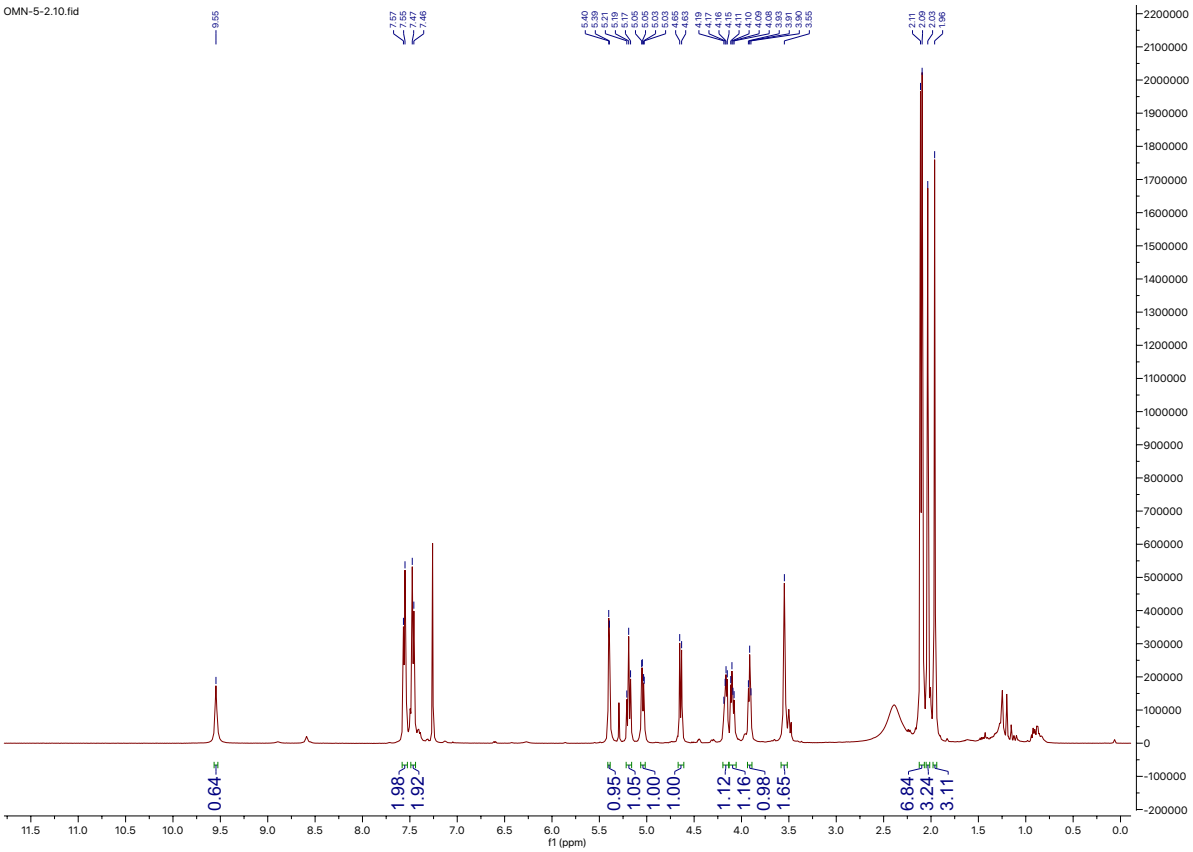
**4-(2-Aminoacetamido)phenyl 2,3,4,6-tetra-O-acetyl-β-D-thiogalactopyranoside (7)**.

Compound **6** (320 mg, 0.6 mmol) was suspended in dry DCM (10 mL) and 32 mg palladium on activated charcoal (10% Pd basis) was added under nitrogen atmosphere. The flask was flushed with hydrogen and the reaction was stirred for 2 h at r.t. under hydrogen atmosphere. The reaction mixture was filtered through celite and the solvent was removed *in vacuo*. **7** was obtained as a white solid (308 mg, 1.8 mmol, 97%.).

$^{1}$H NMR (500 MHz, $CHCl_3$-*d1*) δ 9.55 (br s, 1H, $NH_2$), 7.56 (d, *J* = 8.2 Hz, 2H, ArH), 7.47 (d, *J* = 8.3 Hz, 2H, ArH), 5.40 (d, *J* = 3.4 Hz, 1H, H-4), 5.19 (t, *J* = 9.9 Hz, 1H, H-2), 5.04 (dd, *J* = 10.0, 3.4 Hz, 1H, H-3), 4.64 (d, *J* = 10.0 Hz, 1H), 4.17 (dd, *J* = 11.4, 6.6 Hz, 1H, H-$6_a$), 4.10 (dd, *J* = 11.4, 6.2 Hz, 1H, H-$6_b$), 3.91 (t, *J* = 6.7 Hz, 1H, H-5), 3.55 (s, 2H, $CH_2$), 2.11 (s, 3H, $CH_3$), 2.09 (s, 3H, $CH_3$), 2.03 (s, 3H, $CH_3$), 1.96 (s, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, $CHCl_3$-*d1*) δ 170.61 ($CH_3\underline{C}(O)$), 170.38 ($CH_3\underline{C}(O)$), 170.20 ($CH_3\underline{C}(O)$), 169.61 (NHC(O)), 138.10 (ArC), 134.29 (ArCH), 126.93 (ArC), 119.86 (ArCH), 86.98 (C-1), 74.52 (C-5), 72.12 (C-3), 67.40 (C-2), 67.36 (C-4), 61.72 (C-6), 44.88 ($CH_2$), 21.01 ($CH_3$), 20.85 ($CH_3$), 20.80 ($CH_3$), 20.72 ($CH_3$).

HRMS: $[C_{22}H_{28}N_2O_{10}S + H]^+$ calcd. 513.1537, found 513.1535.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4.08
3.93
3.91
3.90
3.55
2.11
2.09
2.03
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0.64
1.98
1.92
0.95
1.05
1.00
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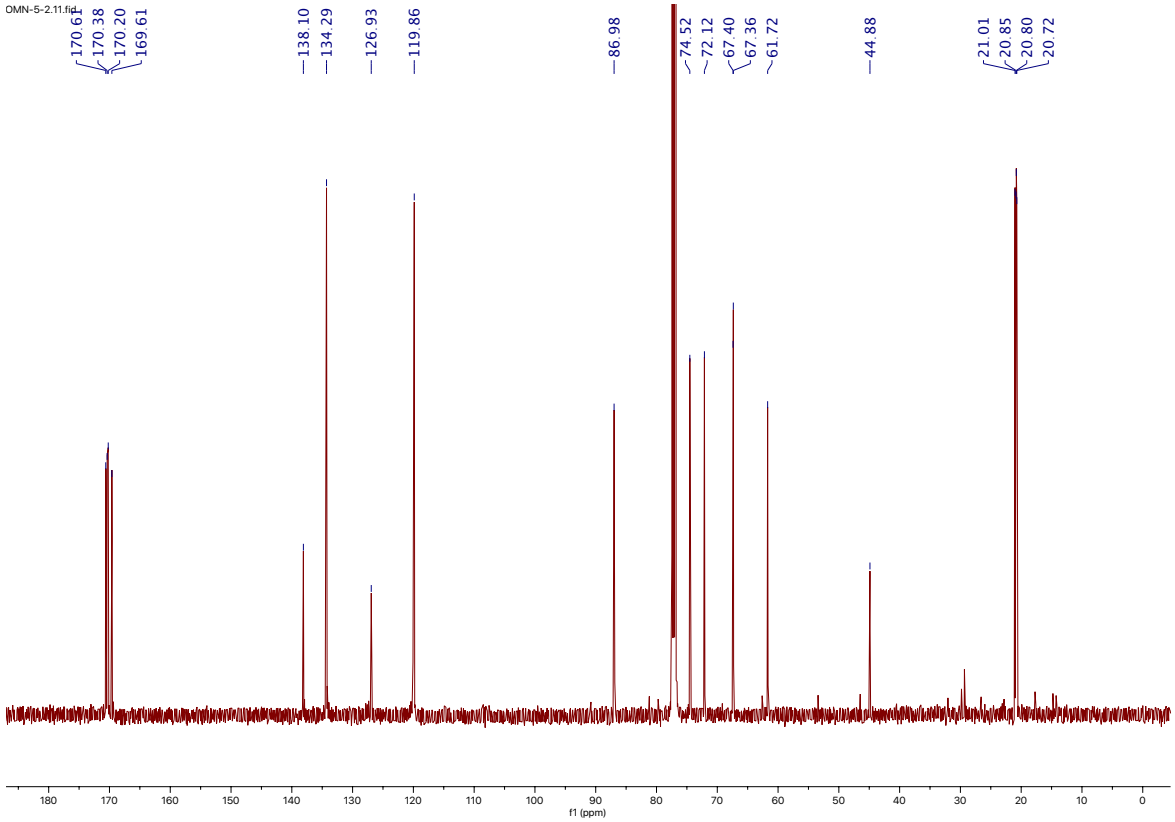
f1 (ppm)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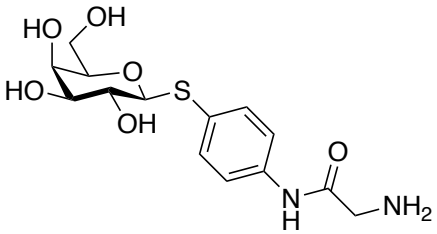
21.01
20.85
20.80
20.72
f1 (ppm)




**8**, 96%

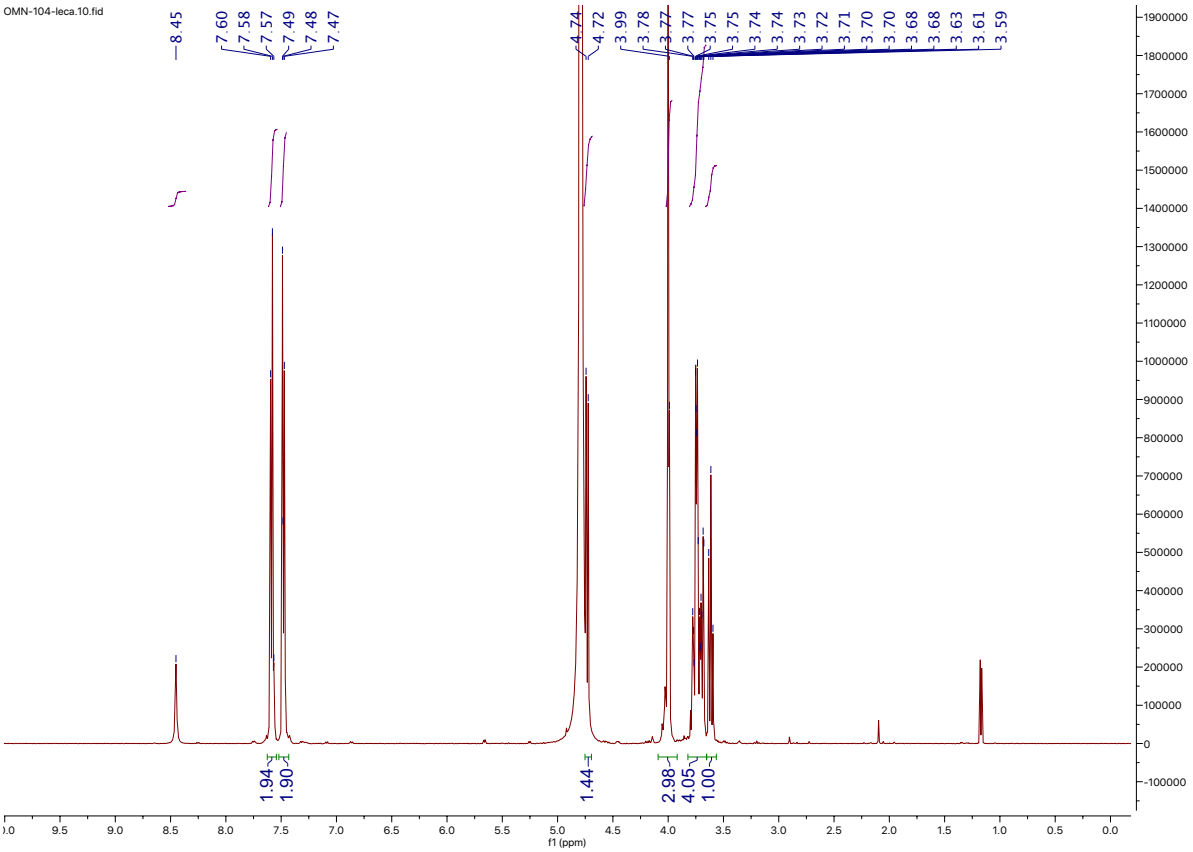
**4-(2-Aminoacetamido)phenyl β-D-thiogalactopyranoside (8)**.

Compound **7** (220 mg, 0.429 mmol) was suspended in dry MeOH (3 mL) and 5.3 M NaOMe in MeOH (40 µL, 0.5 equiv., 0.214 mmol) was added. The reaction mixture was stirred for 15 min at r.t.. Then, 0.1 M HCl was added to neutralize the reaction mixture to pH 7. The solvent was removed *in vacuo* and crude product was purified by reverse phase MPLC ($H_2O$/MeCN + 0.1% formic acid, 5-20% MeCN) to give **8** as a white solid (148 mg, 4.28 mmol, quant.).

$^1$H NMR (500 MHz, $D_2O$) δ 7.59 (d, J = 8.3 Hz, 2H, ArH), 7.48 (d, J = 8.5 Hz, 2H, ArH), 4.73 (d, J = 9.7 Hz, 1H, H-1), 3.99 (m, 3H, H-4, $CH_2$), 3.81 – 3.66 (m, 4H, H-3, H-5, H-6), 3.61 (t, J = 9.6 Hz, 1H, H-2).

$^{13}$C NMR (126 MHz, $D_2O$) δ 165.43 (NHC(O)), 136.15 (ArC), 132.39 (ArCH), 128.96 (ArC), 121.69 (ArCH), 88.14 (C-1), 78.99 (C-5), 73.93 (C-3), 69.12 (C-2), 68.66 (C-4), 60.95 (C-6), 40.99 ($CH_2$).

HRMS: $[C_{14}H_{20}N_2O_6S + H]^+$ calcd. 345.1115, found 345.1105.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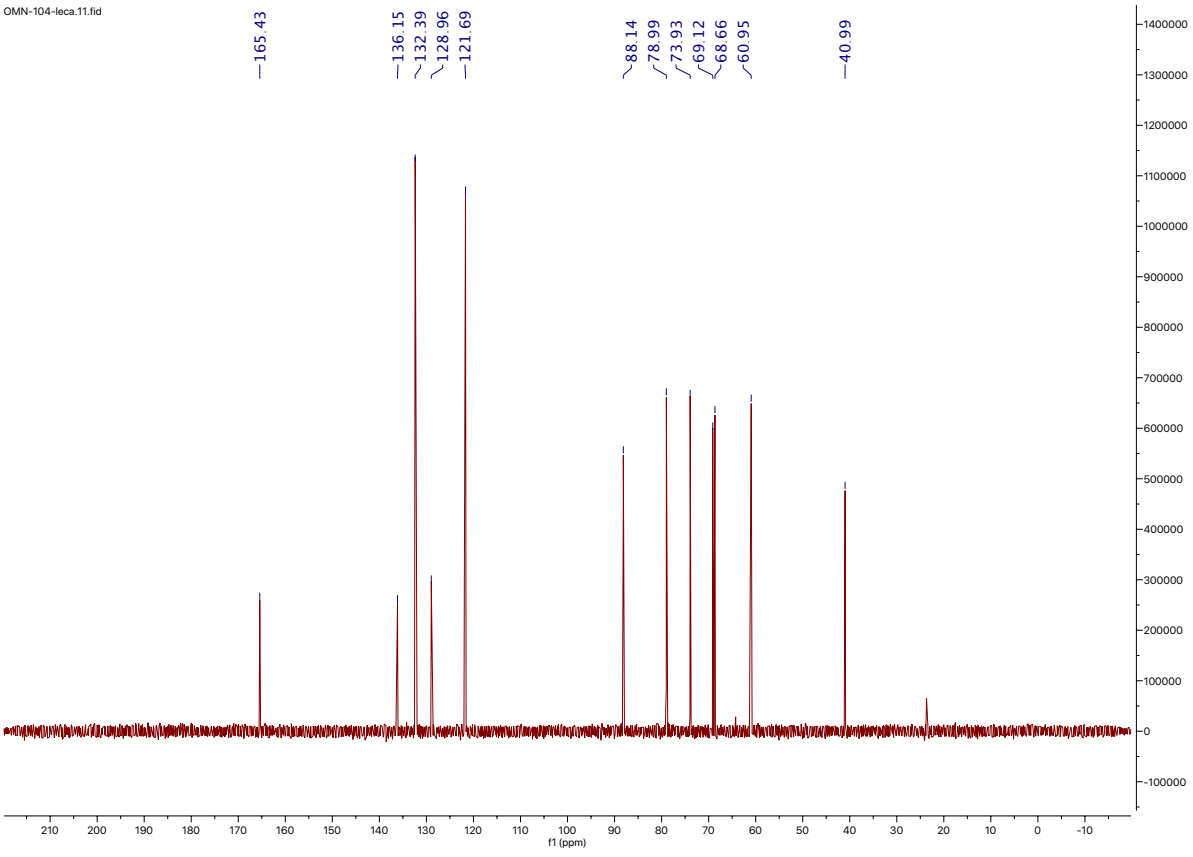
1.00
f1 (ppm)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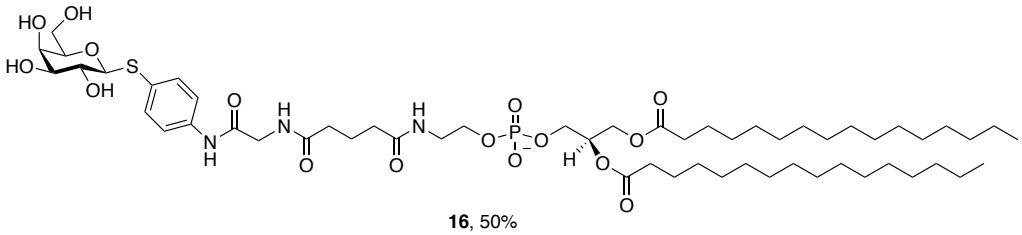
68.66
60.95
40.99
f1 (ppm)



**16**, 50%

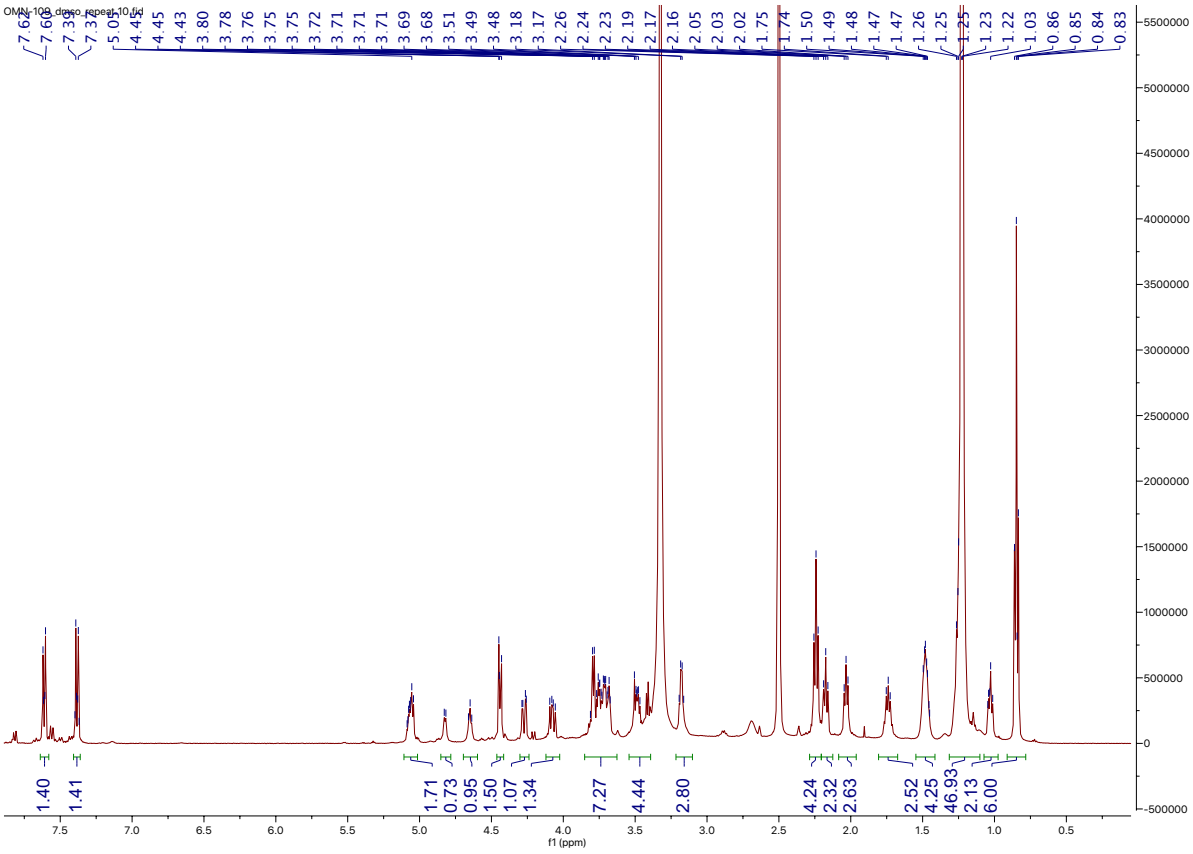
**Glycolipid 16**

16:0 Glutaryl PE (50 mg, 60 µmol) was suspended in a mixture of $CHCl_3$/DMF 1:1 (5 mL) and HBTU (28 mg, 1.2 equiv., 72 µmol), HOBt (8 mg, 1.2 equiv., 72 µmol) and $Et_3N$ (42 µL, 5 equiv., 0.3 mmol) was added and stirred for 30 min under nitrogen atmosphere at 40 °C until phospholipid was completely dissolved. Then, **8** (32 mg, 1.55 equiv., 0.093 mmol) was added and the reaction was stirred at 40 °C for 48 h. The solvent was removed *in vacuo* and the crude product was purified by reverse phase MPLC ($^{i}$PrOH:$H_2O$:MeOH (5:4:1) / $^{i}$PrOH + 0.2% formic acid, 10-50%). **16** was obtained as a beige solid (34 mg, 0.03 mmol, 50%).

$^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.64 – 7.58 (m, 2H, ArH), 7.41 – 7.35 (m, 2H, ArH), 5.07 (ddd, $J$ = 14.1, 7.5, 4.3 Hz, 1H, C(O)C<u>H</u>$CH_2OPO_3$), 4.82 (d, $J$ = 5.7 Hz, 1H, NH), 4.65 (t, $J$ = 5.7 Hz, 1H, NH), 4.44 (d, $J$ = 9.4 Hz, 1H, H-1), 4.27 (dd, $J$ = 12.0, 3.1 Hz, 1H, C(O)OC<u>$H_{2a}$</u>CH), 4.07 (dd, $J$ = 12.1, 7.1 Hz, 1H, C(O)OC<u>$H_{2b}$</u>CH), 3.85 – 3.62 (m, 6H, C(O)C<u>$H_2$</u>NH, $CH_2$<u>C</u>$H_2OPO_3$, CH<u>C</u>$H_2OPO_3$), 3.55 – 3.44 (m, 2H, H-6), 3.18 (q, $J$ = 5.2 Hz, 2H, C<u>$H_2$</u>$CH_2OPO_3$), 2.24 (t, $J$ = 7.3 Hz, 4H, C<u>$H_2$</u>C(O)O), 2.17 (t, $J$ = 7.4 Hz, 2H, $CH_2CH_2$C<u>$H_2$</u>C(O)NH), 2.03 (t, $J$ = 6.6 Hz, 2H, NHC(O)C<u>$H_2$</u>$CH_2CH_2$), 1.79 – 1.69 (m, 2H, NHC(O)$CH_2$C<u>$H_2$</u>), 1.54 – 1.40 (m, 4H, C<u>$H_2$</u>$CH_2$C(O)O), 1.30 – 1.16 (m, 46H, $CH_2$), 1.08 – 0.98 (m, 2H, $CH_2$), 0.85 (t, $J$ = 6.8 Hz, 6H).

$^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 172.55 (OC(O)), 172.35 (OC(O)), 172.29 (NHC(O)), 171.77 (NHC(O)), 168.56 (NHC(O)), 138.01 (ArC), 131.06 (ArCH), 128.21 (ArC), 119.61 (ArCH), 88.36 (C-1), 79.14 (C-5), 74.75 (C-3), 70.45 (d, $J$ = 8.1 Hz, C(O)C<u>H</u>$CH_2OPO_3$), 69.18 (C-2), 68.30 (C-4), 62.82 (d, $J$ = 4.6 Hz, $CH_2$<u>C</u>$H_2OPO_3$), 62.55 (d, $J$ = 5.4 Hz, CH<u>C</u>$H_2OPO_3$), 62.30 (C(O)O<u>C</u>$H_2$CH), 60.48 (C-6), 45.63, 43.45 (C(O)<u>C</u>$H_2$NH), 34.84 (NHC(O)<u>C</u>$H_2CH_2CH_2$), 33.92 ($CH_2CH_2$<u>C</u>$H_2$C(O)NH), 33.59 (<u>C</u>$H_2$C(O)O), 33.42 (<u>C</u>$H_2$C(O)O), 31.31, 29.08, 29.03, 28.95, 28.78, 28.76, 28.73, 28.45, 28.42, 24.48 (<u>C</u>$H_2CH_2$C(O)O), 24.43 (<u>C</u>$H_2CH_2$C(O)O), 22.11, 21.52 (NHC(O)$CH_2$<u>C</u>$H_2$), 13.95 ($CH_3$).

HRMS: $[C_{56}H_9N_3O_{16}PS + H]^+$ calcd. 1132.6478, found 1132.6442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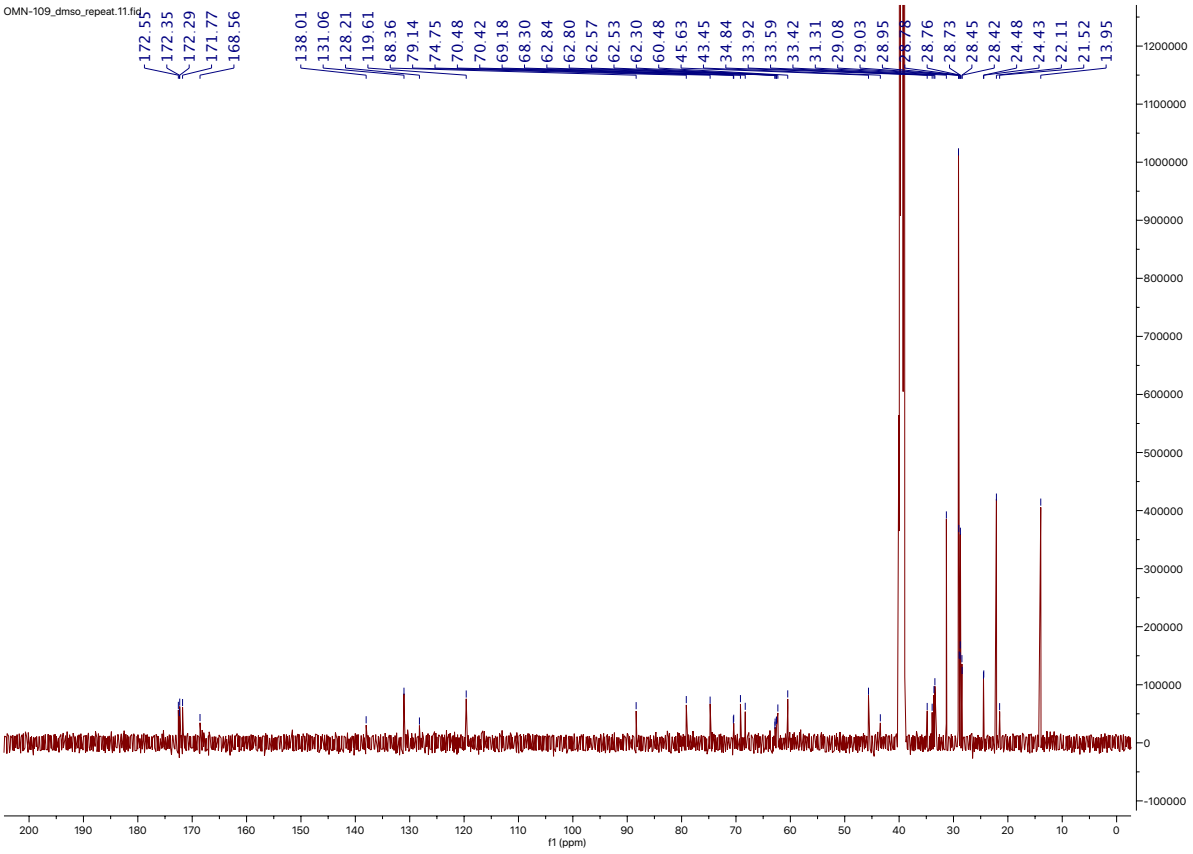
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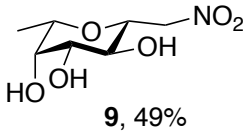



**9**, 49%

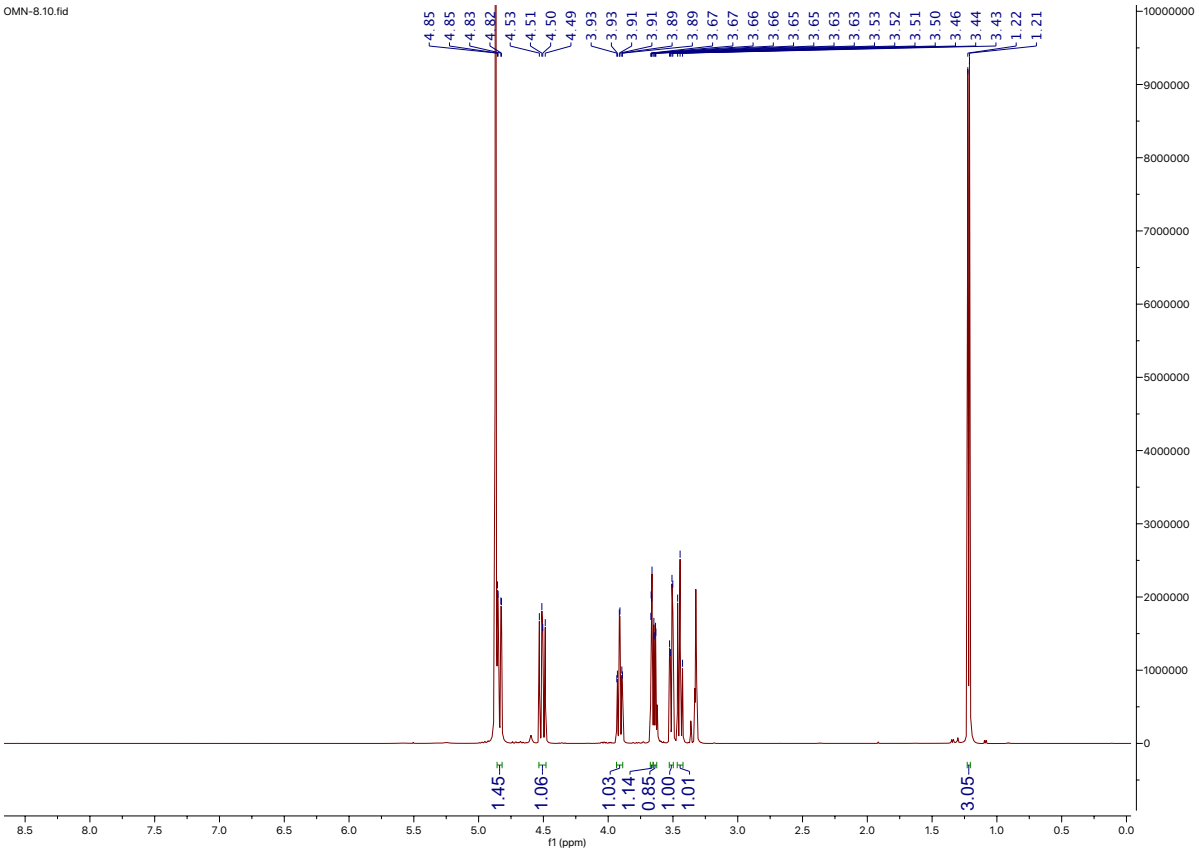
**β-L-Fucopyranosyl nitromethane (9)**.

Compound **9** was synthesized according to Hauck *et al.*[4]: L-Fucose (2 g, 12.1 mmol) was dissolved in 12 mL dry DMSO and then nitromethane (8 mL, 12 equiv., 145.2 mmol) and 1 M sodium methoxide in MeOH (2.4 mL, 0.2 equiv., 2.4 mmol) were added under nitrogen dropwisely. The reaction mixture was stirred for 6 h and was then quenched by pouring the solution on ice-cold water premixed with 0.2 equiv. 1 M HCl. The obtained solution was adjusted to pH 4 by adding 1 M HCl and stirred o.n. under reflux. After cooling to r.t., the pH was adjusted to 6 by adding 1 M NaOH. The obtained solution was extracted with $CHCl_3$ to remove excess DMSO and then the aqueous phase was lyophilized. Crude product was purified by normal phase MPLC (DCM/MeOH, 0-15% MeOH) and then recrystallized from ethanol to give **9** (1268 mg, 6.12 mmol, 50%).

$^1$H NMR (500 MHz, MeOH-$d_4$) δ 4.84 (dd, $J$ = 13.1, 2.3 Hz, 1H, $CH_{2a}$), 4.51 (dd, $J$ = 13.1, 9.6 Hz, 1H, $CH_{2b}$), 3.91 (td, $J$ = 9.6, 2.3 Hz, 1H, H-1), 3.67 (dd, $J$ = 3.3, 1.1 Hz, 1H, H-4), 3.64 (dd, $J$ = 6.4, 1.1 Hz, 1H, H-5), 3.51 (dd, $J$ = 9.3, 3.2 Hz, 1H, H-3), 3.45 (t, $J$ = 9.5 Hz, 1H, H-2), 1.22 (d, $J$ = 6.5 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 78.44 (C-1), 78.28 ($CH_2$), 76.24 (C-3), 75.72 (C-5), 73.42 (C-4), 69.27 (C-2), 16.92 ($CH_3$).

Spectroscopic data is in accordance with the literature[5].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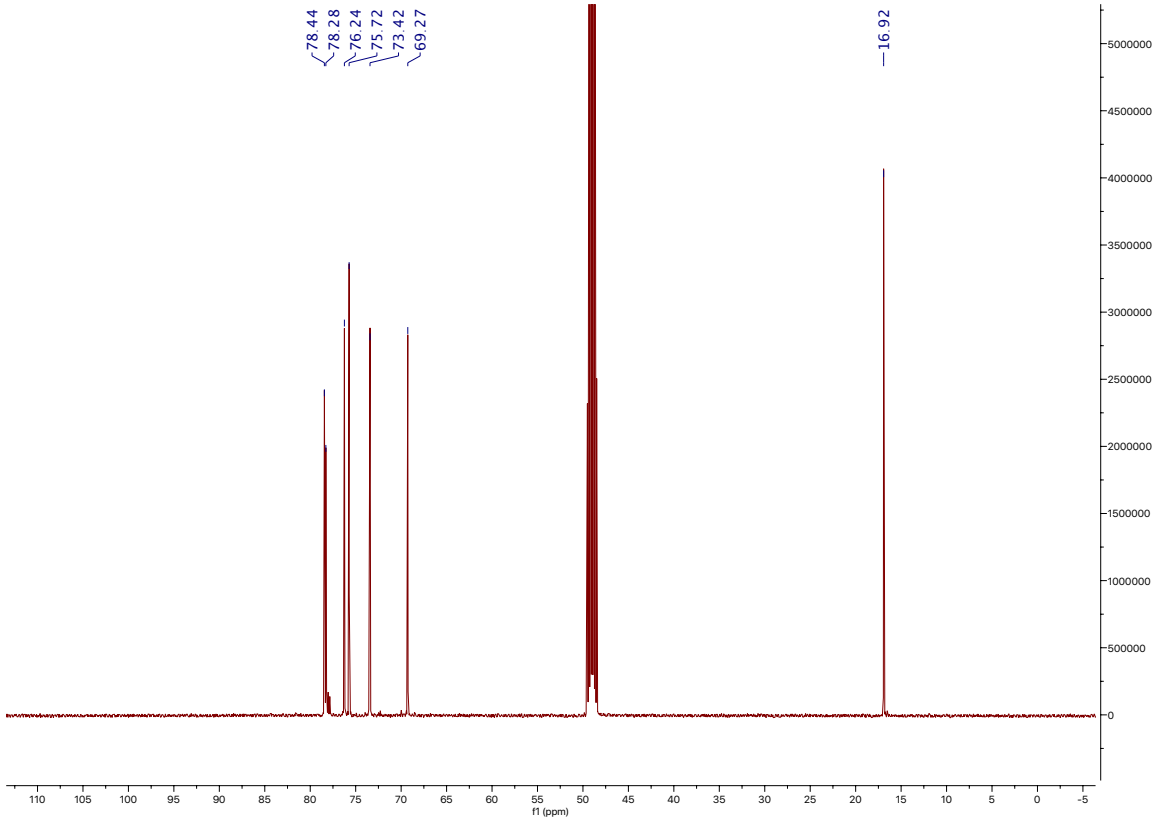
f1 (ppm)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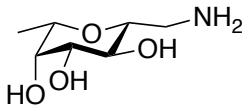
f1 (ppm)




**10**, 98%

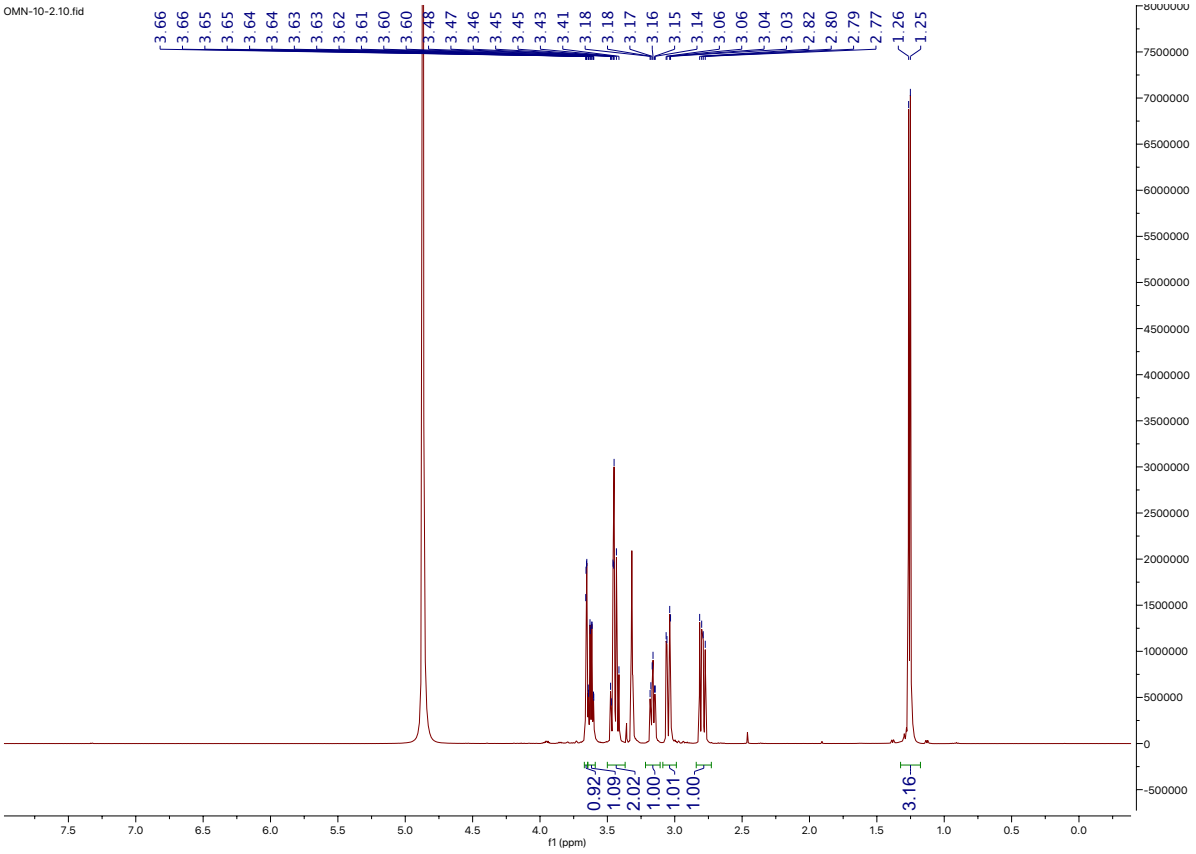
**β-L-Fucopyranosyl methylamine (10)**.

Compound **10** was synthesized according to Sommer *et al.*[5]: Compound **9** (800 mg, 3.86 mmol) was suspended in dry MeOH (20 mL) and 80 mg palladium on activated charcoal (10% Pd basis) was added under nitrogen atmosphere. The reaction flask was flushed with hydrogen and stirred overnight at r.t. under hydrogen atmosphere. The reaction mixture was filtered through celite and the solvent was removed *in vacuo*. **10** was obtained as a white solid (682 mg, 3.85 mmol, quant.).

$^{1}$H NMR (500 MHz, MeOH-$d_4$) δ 3.66 (dd, $J$ = 3.0, 1.1 Hz, 1H, H-4), 3.62 (qd, $J$ = 6.4, 1.1 Hz, 1H, H-5), 3.48 – 3.41 (m, 2H, H-2, H-3), 3.16 (td, $J$ = 8.0, 2.9 Hz, 1H, H-1), 3.05 (dd, $J$ = 13.3, 3.0 Hz, 1H, $CH_{2a}$), 2.79 (dd, $J$ = 13.3, 7.5 Hz, 1H, $CH_{2b}$), 1.26 (d, $J$ = 6.5 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 80.96 (C-1), 76.45 (C-3), 75.60 (C-5), 73.62 (C-4), 70.12 (C-2), 43.50 ($CH_2$), 17.13 ($CH_3$).

Spectroscopic data is in accordance with the literature[5].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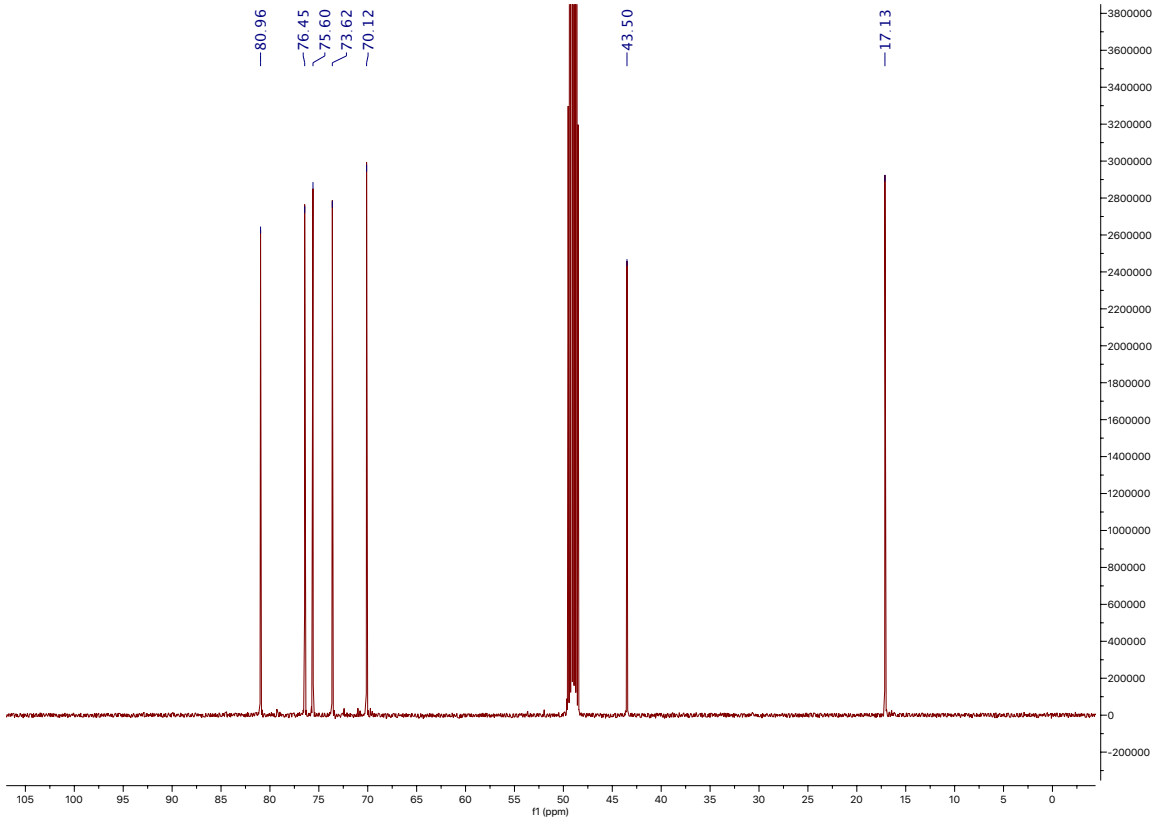
f1 (ppm)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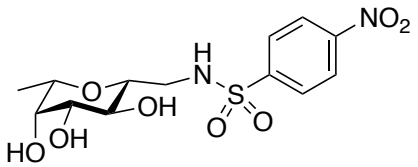
f1 (ppm)



**11**, 62%

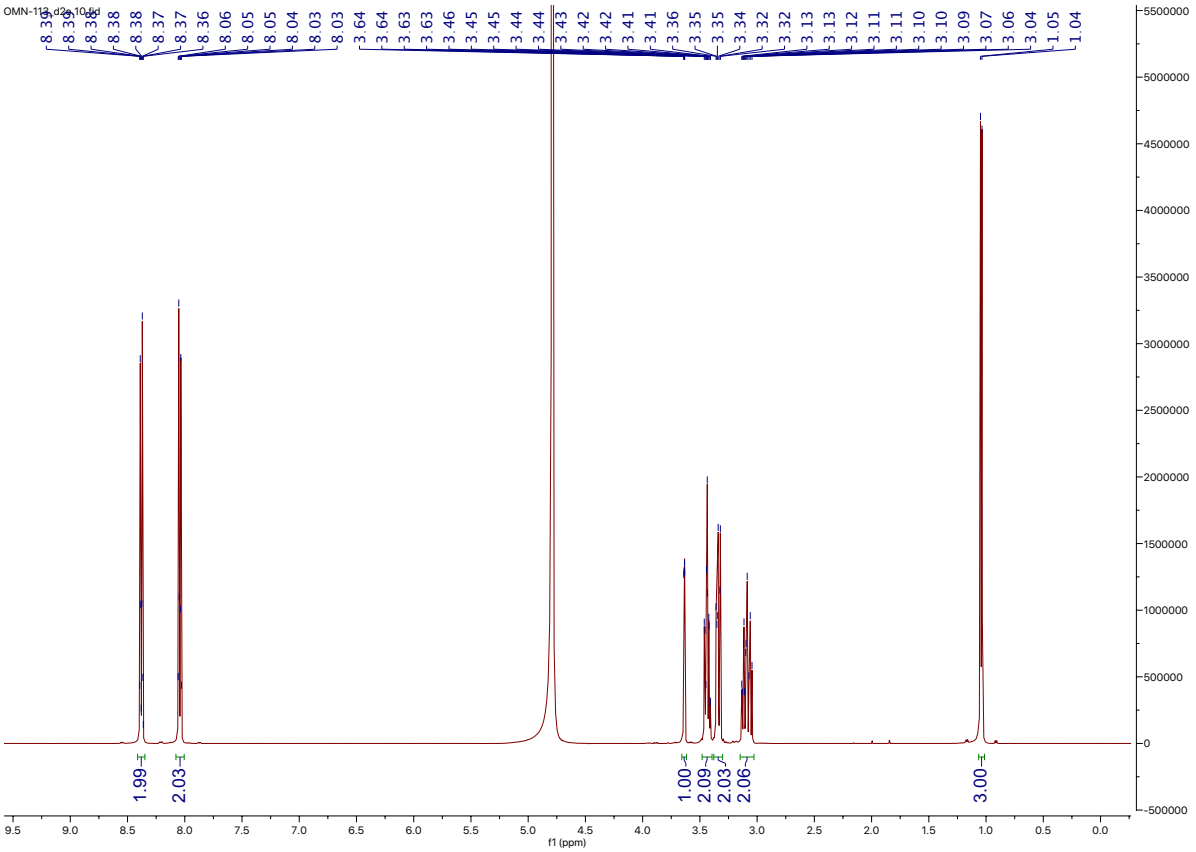
**β-L-Fucopyranosylmethyl 4-nitrobenzenesulfonamide (11).**

Amine **10** (480 mg, 2.24 mmol) was dissolved in dry DMF (10 mL) and triethylamine (465 µL, 1.5 equiv., 3.36 mmol) was added and stirred for 5 min under nitrogen atmosphere. The reaction flask was cooled down 0 °C and 4-nitro-benzenesulfonyl chloride (544 mg, 1.1 equiv, 2.46 mmol) in 10 mL of dry DMF was added dropwise under vigorous stirring. The reaction mixture was warmed to r.t. and stirred for 3 h. The reaction was quenched with ice-cold satd. sodium hydrogencarbonate, stirred for 5 min, then diluted with ice-cold water and lyophilized. Crude product was purified by reverse phase MPLC ($H_2O$/MeCN + 0.1% formic acid, 10-40% MeCN) to obtain **11** (502 mg, 1.38 mmol, 62%).

$^1$H NMR (500 MHz, $D_2O$) δ 8.44 – 8.32 (m, 2H, ArH), 8.09 – 7.99 (m, 2H, ArH), 3.64 (dd, $J$ = 3.4, 1.0 Hz, 1H, H-4), 3.47 – 3.40 (m, 2H, H-3, H-5), 3.37 – 3.30 (m, 2H, H-2, $CH_{2a}$), 3.15 – 3.03 (m, 2H, H-1, $CH_{2b}$), 1.04 (d, $J$ = 6.5 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, $D_2O$) δ 150.04 (ArC), 144.57 (ArC), 128.04 (ArCH), 124.61 (ArCH), 77.44 (C-1), 74.06 (C-3), 73.81 (C-5), 71.56 (C-4), 67.84 (C-2), 43.80 ($CH_2$), 15.60 ($CH_3$).

HRMS: $[C_{13}H_{18}N_2O_8S + H]^+$ calcd. 363.0857, found 363.0844.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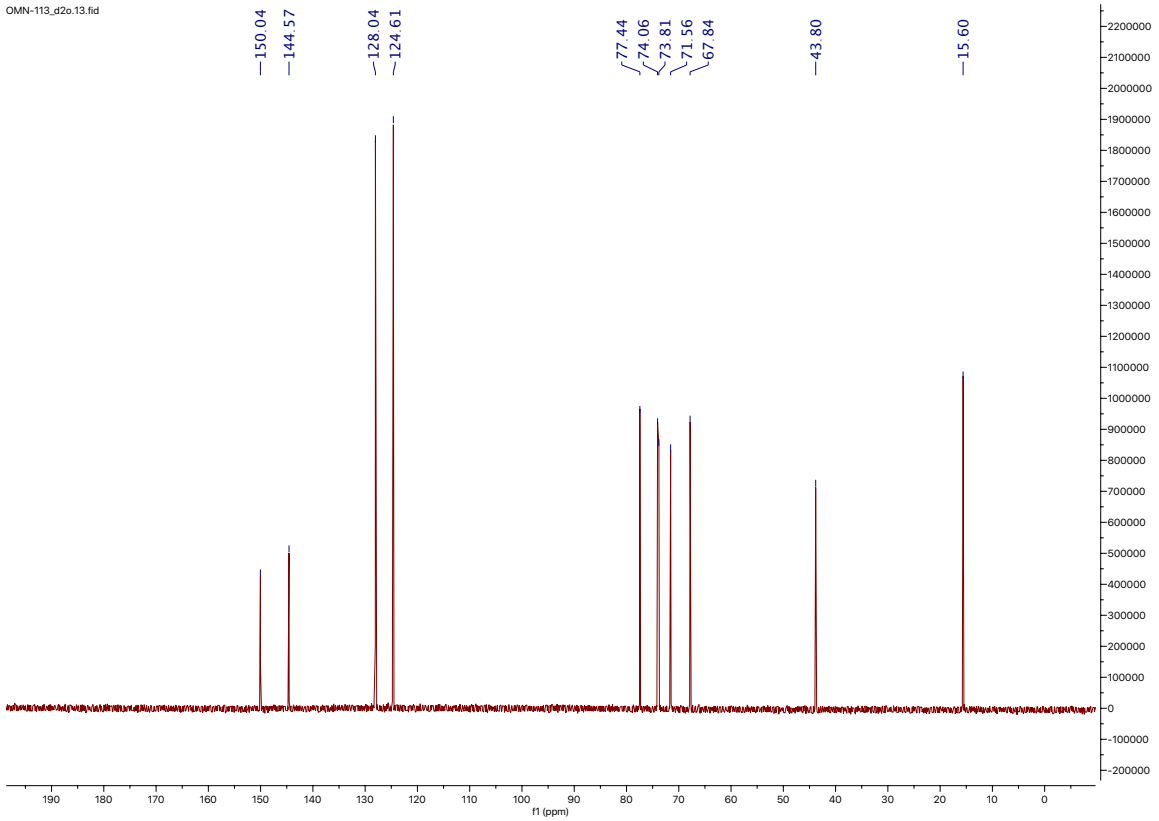
1.99 2.03 1.00 2.09 2.03 2.06 3.00
f1 (ppm)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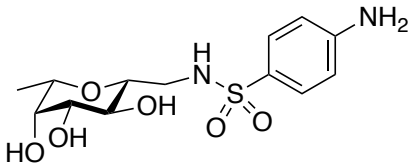
f1 (ppm)



**12**, 98%

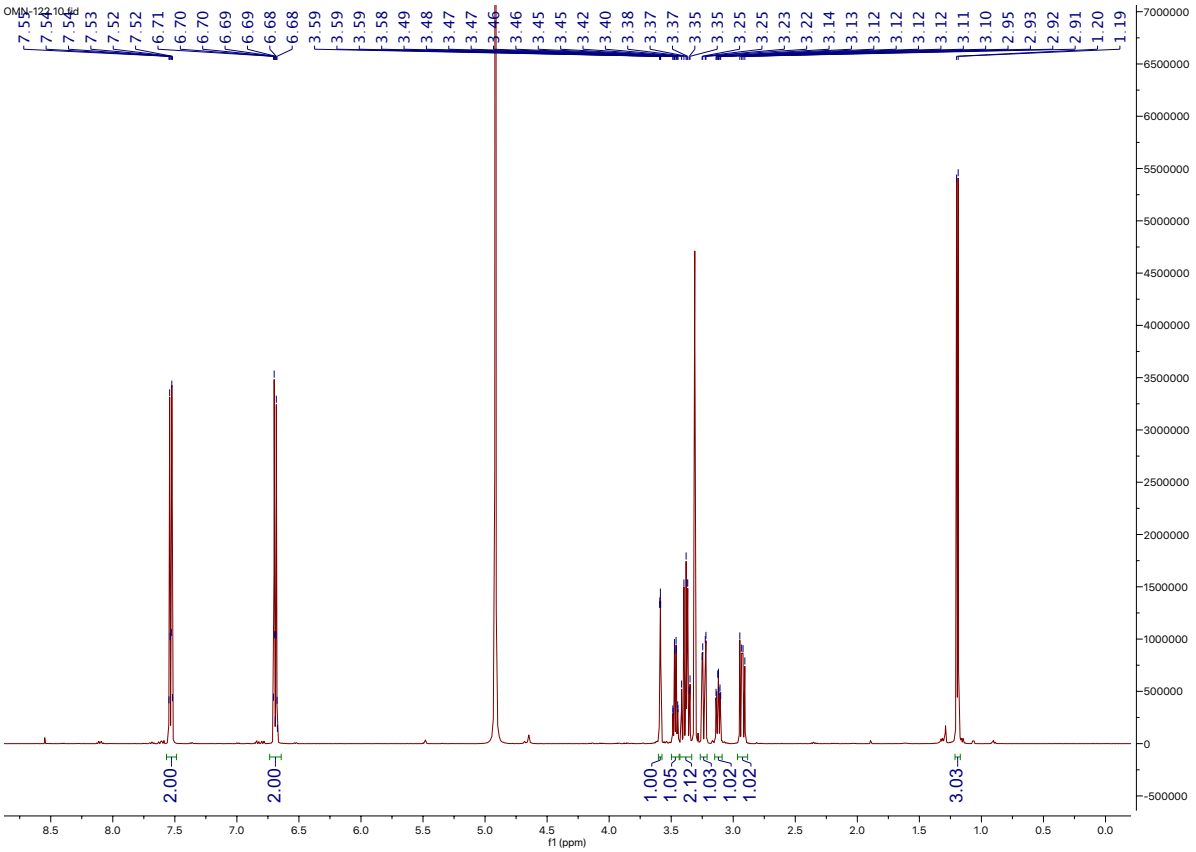
**β-L-Fucopyranosylmethyl 4-aminobenzenesulfonamide (12)**.

Compound **11** (280 mg, 0.77 mmol) was suspended in dry MeOH (12 mL) and 9 mg palladium on activated charcoal (10% Pd basis) was added under nitrogen atmosphere. The reaction flask was flushed with hydrogen and stirred 2 h at r.t. under hydrogen atmosphere. The reaction mixture was filtered through celite and the solvent was removed *in vacuo*. **12** was obtained as a white solid (250 mg, 0.753 mmol, quant.).

$^{1}$H NMR (500 MHz, MeOH-$d_4$) δ 7.56 – 7.51 (m, 2H, ArH), 6.73 – 6.66 (m, 2H, ArH), 3.59 (dd, $J$ = 3.0, 1.0 Hz, 1H, H-4), 3.47 (qd, $J$ = 6.5, 1.1 Hz, 1H, H-5), 3.42 – 3.33 (m, 2H, H-3, H-2), 3.24 (dd, $J$ = 12.9, 2.7 Hz, 1H, $CH_{2a}$), 3.12 (ddd, $J$ = 8.9, 7.3, 2.7 Hz, 1H, H-1), 2.93 (dd, $J$ = 12.9, 7.3 Hz, 1H, $CH_{2b}$), 1.19 (d, $J$ = 6.5 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 154.07 (ArC), 130.01 (ArCH), 127.39 (ArC), 114.39 (ArCH), 79.55 (C-1), 76.31 (C-3), 75.52 (C-5), 73.60 (C-4), 69.78 (C-2), 45.52 ($CH_2$), 17.06 ($CH_3$).

HRMS: $[C_{13}H_{20}N_2O_6S + H]^+$ calcd. 333.1115, found 333.1104.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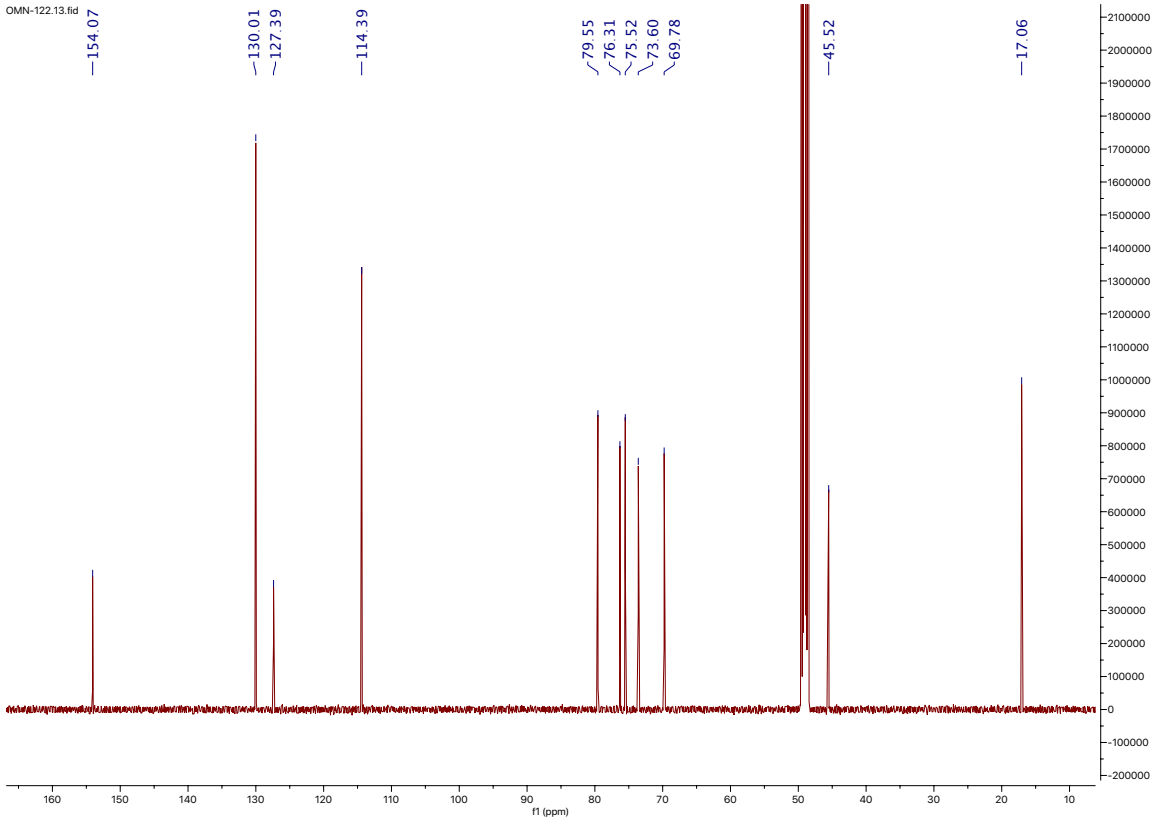
3.59 3.59 3.59 3.58 3.49 3.48 3.47 3.47 3.46 3.46 3.45 3.45 3.42 3.40 3.38 3.37 3.37 3.35 3.35 3.25 3.25 3.23 3.22 3.14 3.13 3.12 3.12 3.12 3.12 3.11 3.10 2.95 2.93 2.92 2.91 1.20 1.19
2.00 2.00 1.00 1.05 2.12 1.03 1.02 1.02 3.03
f1 (ppm)


OMN-122.13.fid
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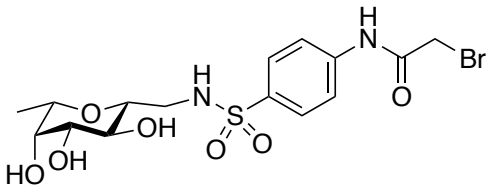
f1 (ppm)



**13**

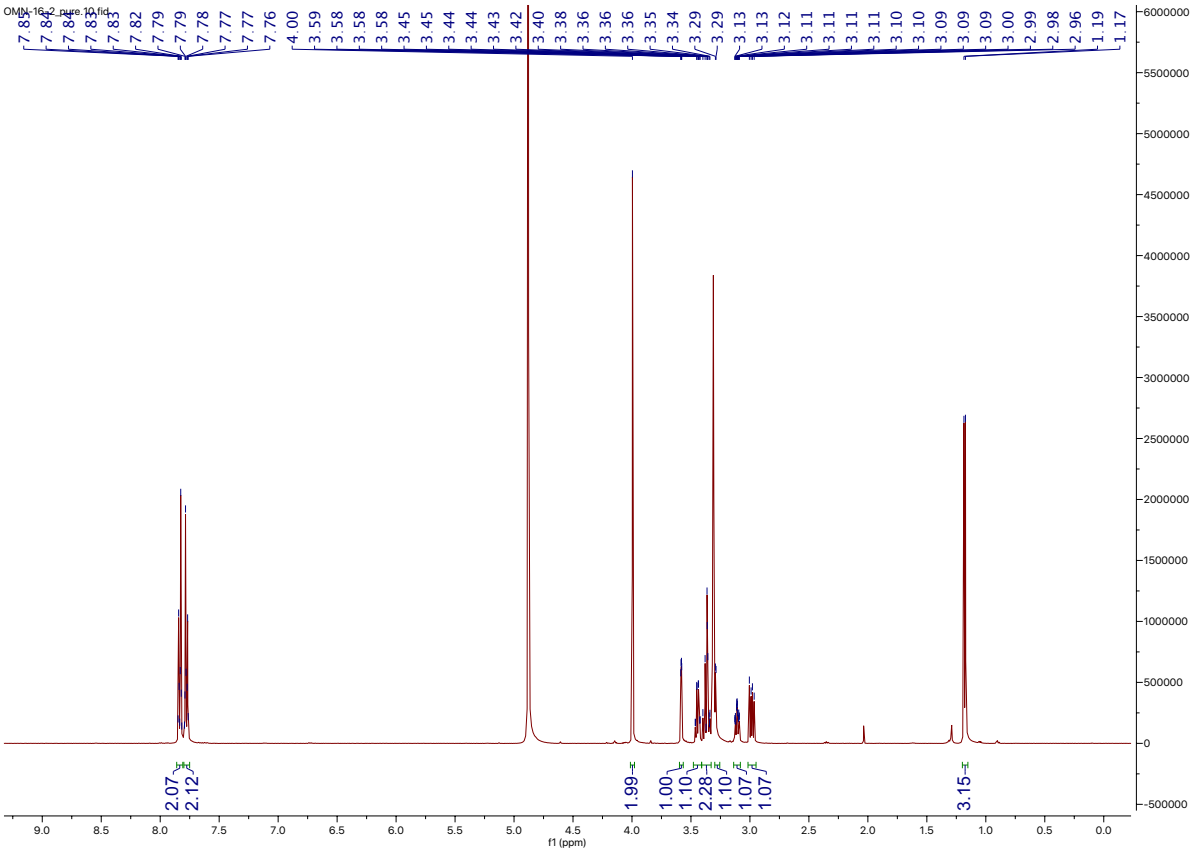
**β-L-Fucopyranosylmethyl 4-(2-bromoacetamido)-benzenesulfonamide (13)**.

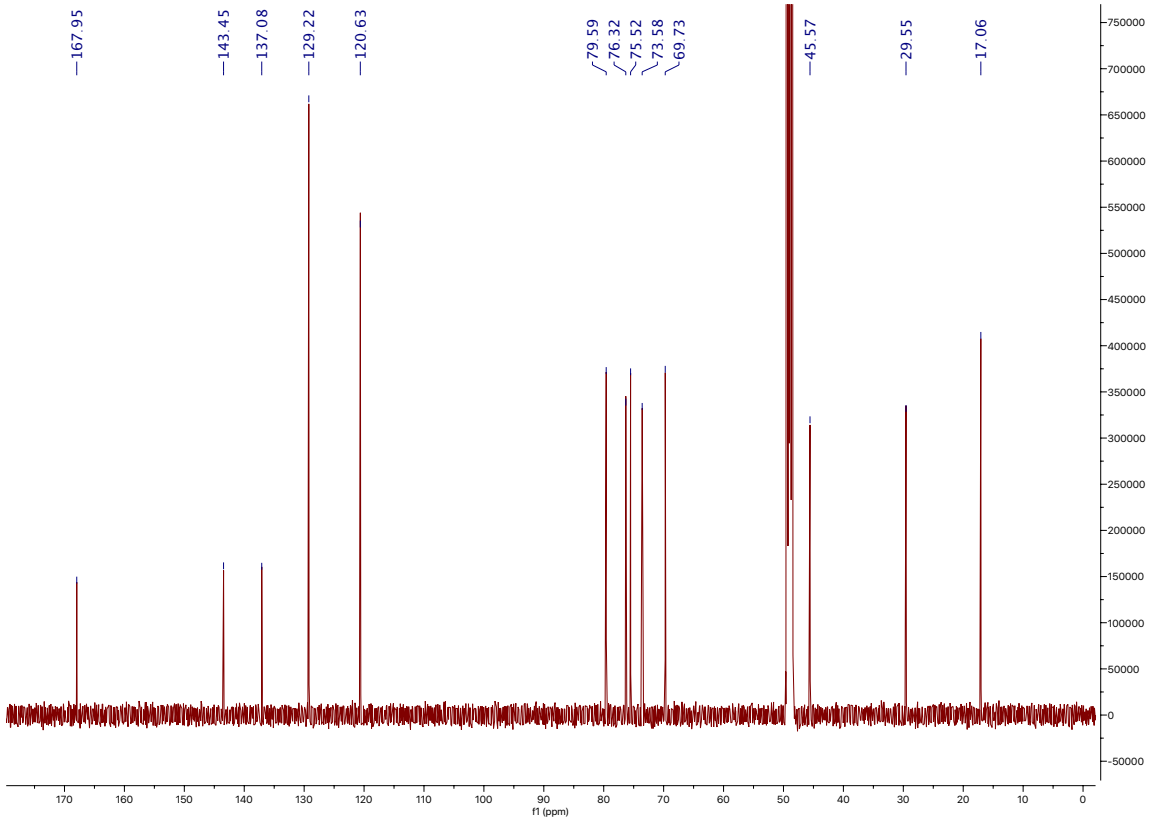
**12** (275 mg, 0.83 mmol) was dissolved in dry DMF (5 mL) and triethylamine (252 µL, 2.2 equiv., 1.82 mmol) was added and stirred for 5 min under nitrogen atmosphere. The reaction flask was cooled down 0 °C and bromoacetyl bromide (48 µL, 1.1 equiv, 0.91 mmol) was added dropwise under vigorous stirring. The reaction mixture was warmed to r.t. and stirred for 4 h. The reaction was diluted with EtOAc and washed with satd. ammonium chloride, water and brine sequentially, then dried over anhydrous sodium sulfate. After filtration, the solvent was removed *in vacuo*. The crude product was purified by reverse phase MPLC ($H_2O$/MeCN + 0.1% formic acid, 15-50% MeCN). **13** was obtained as a white solid (293 mg, 0.645 mmol, 78%)

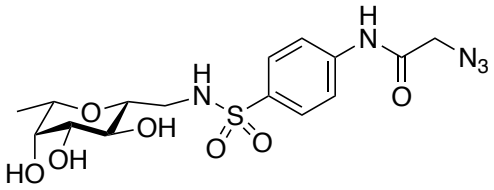
$^1$H NMR (500 MHz, MeOH-$d_4$) δ 7.86 – 7.81 (m, 2H, ArH), 7.80 – 7.75 (m, 2H, ArH), 4.00 (s, 2H, $CH_2Br$), 3.58 (dd, $J$ = 2.9, 1.1 Hz, 1H, H-4), 3.44 (qd, $J$ = 6.4, 1.1 Hz, 1H, H-5), 3.41 – 3.33 (m, 2H, H-2, H-3), 3.29 (d, $J$ = 2.6 Hz, 1H, $CH_{2a}$), 3.11 (dddd, $J$ = 8.2, 7.3, 2.6, 1.0 Hz, 1H, H-1), 2.98 (dd, $J$ = 13.0, 7.3 Hz, 1H, $CH_{2b}$), 1.18 (d, $J$ = 6.5 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 167.95 NHC(O)), 143.45 (ArC), 137.08 (ArC), 129.22 (ArCH), 120.63 (ArCH), 79.59 (C-1), 76.32 (C-2), 75.52 (C-5), 73.58 (C-4), 69.73 (C-3), 45.57 ($CH_2N_3$), 29.55 ($CH_2$), 17.06 ($CH_3$).

HRMS: $[C_{15}H_{21}BrN_2O_7S + H]^+$ calcd. 455.0305, found 455.0292.


OMN-16-2_pure 10.fid
7.85 7.84 7.84 7.83 7.83 7.82 7.79 7.79 7.78 7.77 7.77 7.76
4.00 3.59 3.58 3.58 3.58 3.45 3.45 3.44 3.44 3.43 3.42 3.40 3.38 3.36 3.36 3.35 3.34 3.29 3.29 3.13 3.13 3.12 3.11 3.11 3.11 3.11 3.10 3.10 3.09 3.09 3.09 3.00 2.99 2.98 2.96 1.19 1.17
2.07 2.12 1.99 1.00 1.10 2.28 1.10 1.07 1.07 3.15
f1 (ppm)


167.95
143.45
137.08
129.22
120.63
79.59
76.32
75.52
73.58
69.73
45.57
29.55
17.06
f1 (ppm)



**14**, 56% over two steps

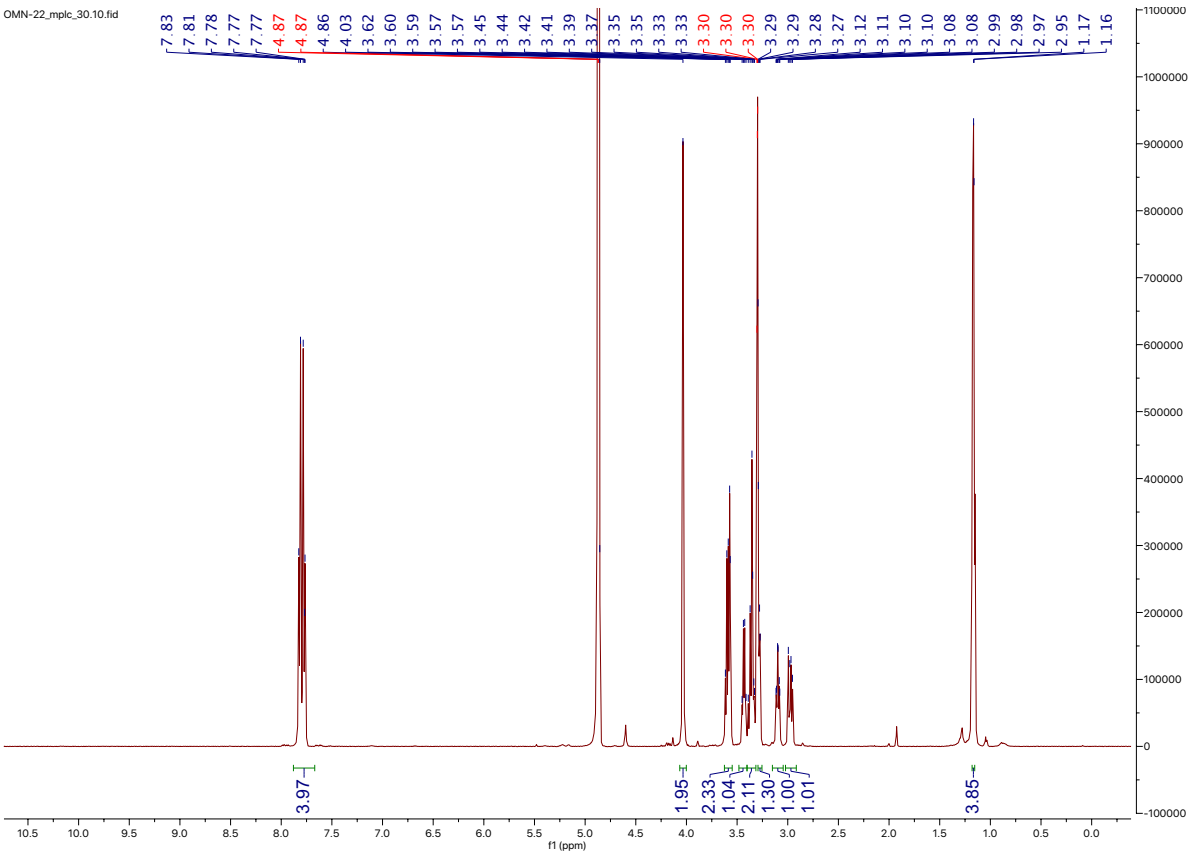
**β-L-Fucopyranosylmethyl 4-(2-azidoacetamido)-benzenesulfonamide (14)**.

**13** (262 mg, 0.58 mmol) was suspended in dry DMF (15 mL), sodium azide (114 mg, 3 equiv., 1.74 mmol) was added and the mixture was stirred for 2 h under nitrogen atmosphere. The reaction was diluted with water and extracted three times with EtOAc, combined organic phases were washed with satd. ammonium chloride, water, brine and then dried over anhydrous sodium sulfate. After filtration, the solvent was removed *in vacuo*. The crude product was purified by normal phase MPLC (DCM/MeOH, 10–45% EtOAc). **6** was obtained as a white solid (173 mg, 0.42 mmol, 72%).

$^{1}$H NMR (500 MHz, MeOH-$d_4$) δ 7.90 – 7.52 (m, 4H, ArH), 4.03 (s, 2H, $CH_2N_3$), 3.63 – 3.55 (m, 2H, NH, H-4), 3.43 (q, $J$ = 6.4 Hz, 1H, H-5), 3.39 – 3.31 (m, 2H, H-2, H-3), 3.28 (dd, $J$ = 8.1, 2.1 Hz, 1H, $CH_{2a}$), 3.10 (td, $J$ = 8.5, 8.0, 2.5 Hz, 1H, H-1), 2.97 (dd, $J$ = 13.0, 7.2 Hz, 1H, $CH_{2b}$), 1.16 (d, $J$ = 2.3 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 168.86 (NHC(O)), 143.18 (ArC), 136.85 (ArC), 129.17 (ArCH), 120.76 (ArCH), 79.52 (C-1), 76.27 (C-2), 75.48 (C-5), 73.54 (C-4), 69.70 (C-3), 53.20 ($CH_2N_3$), 45.53 ($CH_2$), 17.05 ($CH_3$).

HRMS: $[C_{15}H_{23}N_5O_7S + H]^+$ calcd. 416.1234, found 416.1223.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7.77
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4.87
4.86
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3.29
3.29
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3.27
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3.11
3.10
3.10
3.08
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2.97
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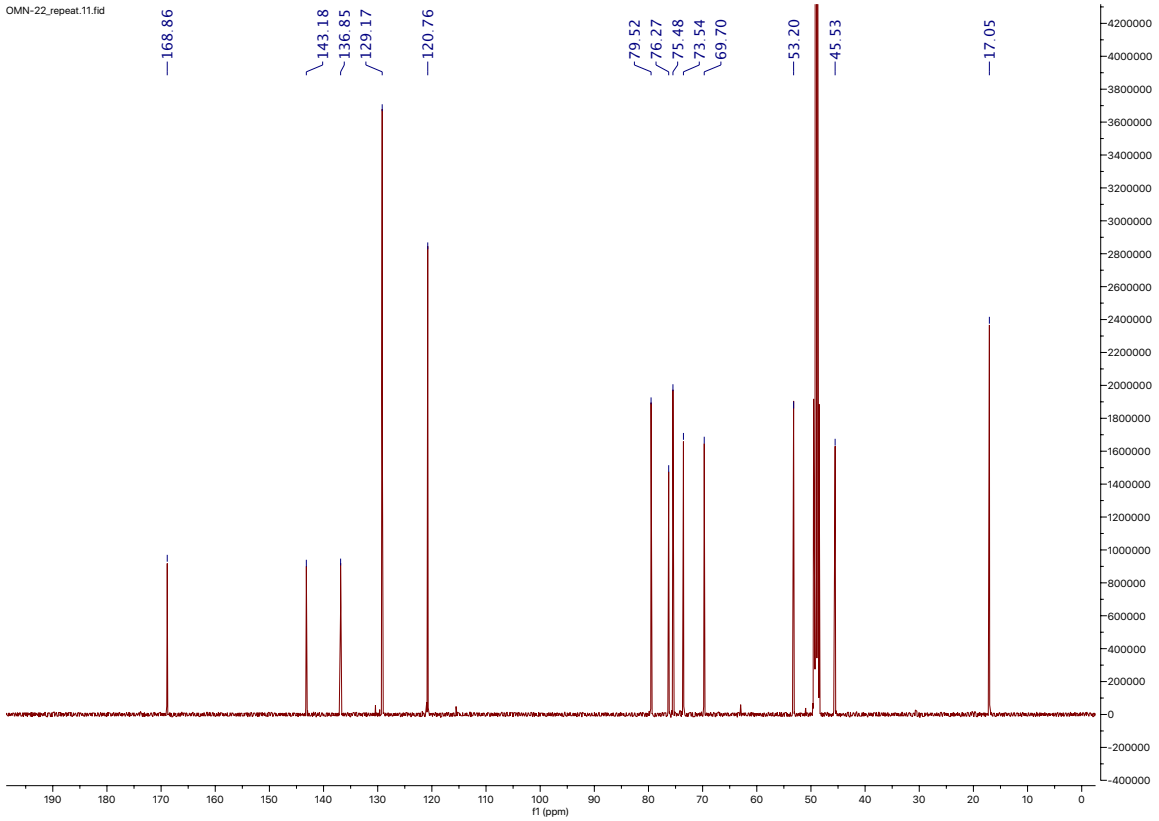
2.11
1.30
1.00
1.01
3.85
f1 (ppm)


OMN-22_repeat.11.fid
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143.18
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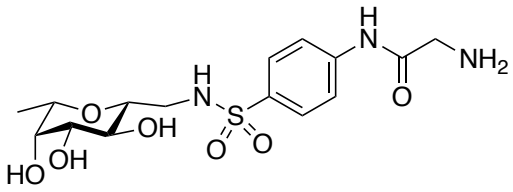
129.17
120.76
79.52
76.27
75.48
73.54
69.70
53.20
45.53
17.05
f1 (ppm)



**15**, 97%

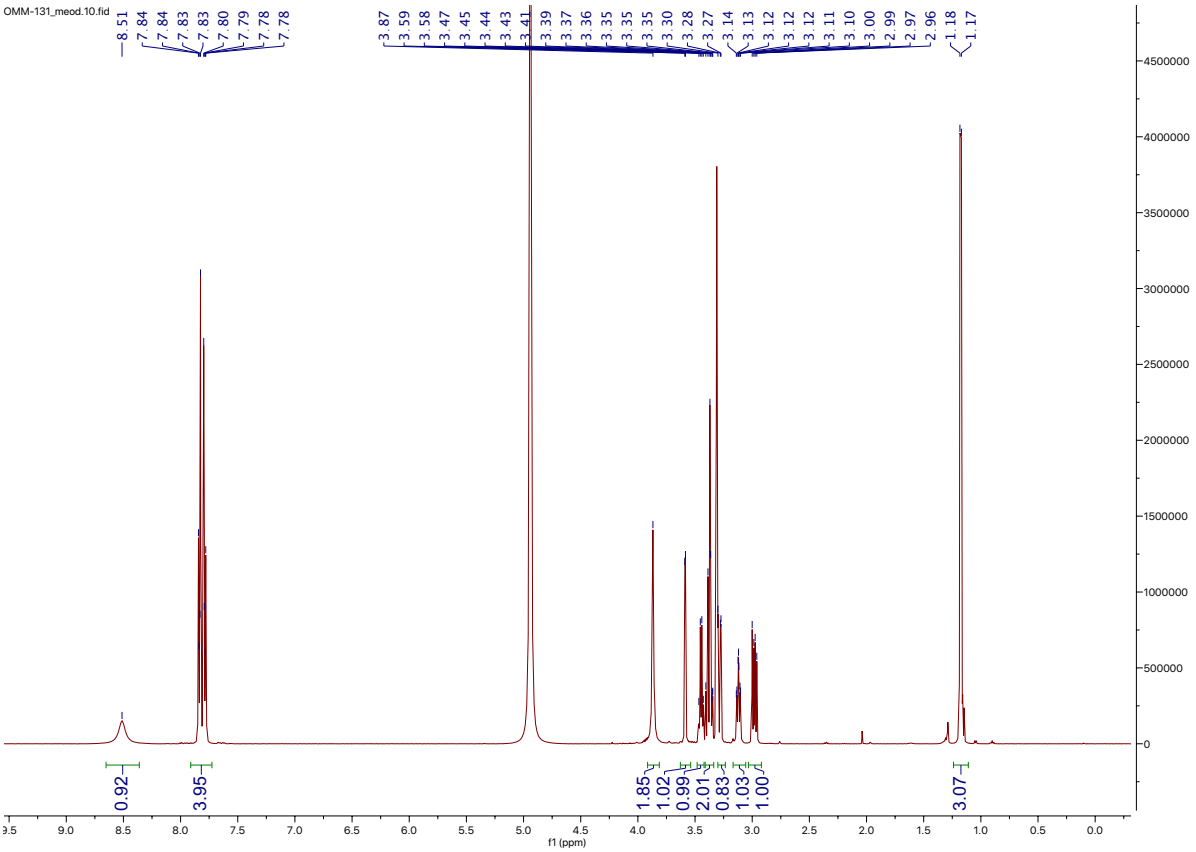
**β-L-Fucopyranosylmethyl 4-(2-aminoacetamido)-benzenesulfonamide (15)**.

Compound **14** (150 mg, 0.36 mmol) was suspended in dry MeOH (5 mL) and 15 mg palladium on activated charcoal (10% Pd basis) was added under a nitrogen atmosphere. The reaction flask was flushed with hydrogen and stirred overnight at r.t. under hydrogen. The reaction mixture was filtered through celite and the solvent was removed *in vacuo*. **15** was obtained as a white solid (135 mg, 0.347 mmol, quant.).

$^{1}$H NMR (500 MHz, MeOH-$d_4$) δ 8.51 (s, 2H, $NH_2$), 7.87 – 7.76 (m, 4H, ArH), 3.87 (s, 2H, $CH_2$), 3.59 (d, $J$ = 2.7 Hz, 1H, H-4), 3.45 (q, $J$ = 6.4 Hz, 1H, H-5), 3.41 – 3.34 (m, 2H, H-2, H-3), 3.30 – 3.27 (m, 1H, $CH_{2a}$), 3.12 (ddd, $J$ = 9.1, 7.6, 2.5 Hz, 1H, H-1), 2.98 (dd, $J$ = 12.9, 7.3 Hz, 1H, $CH_{2b}$), 1.18 (d, $J$ = 6.4 Hz, 3H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 166.64 (NHC(O)), 143.10 (ArC), 136.93 (ArC), 129.30 (ArCH), 120.41 (ArCH), 79.60 (C-1), 76.29 (C-2), 75.50 (C-5), 73.56 (C-4), 69.68 (C-3), 45.54 ($CH_2$NH), 42.51 ($CH_2NH_2$), 17.08 ($CH_3$).

HRMS: $[C_{15}H_{23}N_3O_7S + H]^+$ calcd. 390.1329, found 390.1327.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7.78
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3.37
3.36
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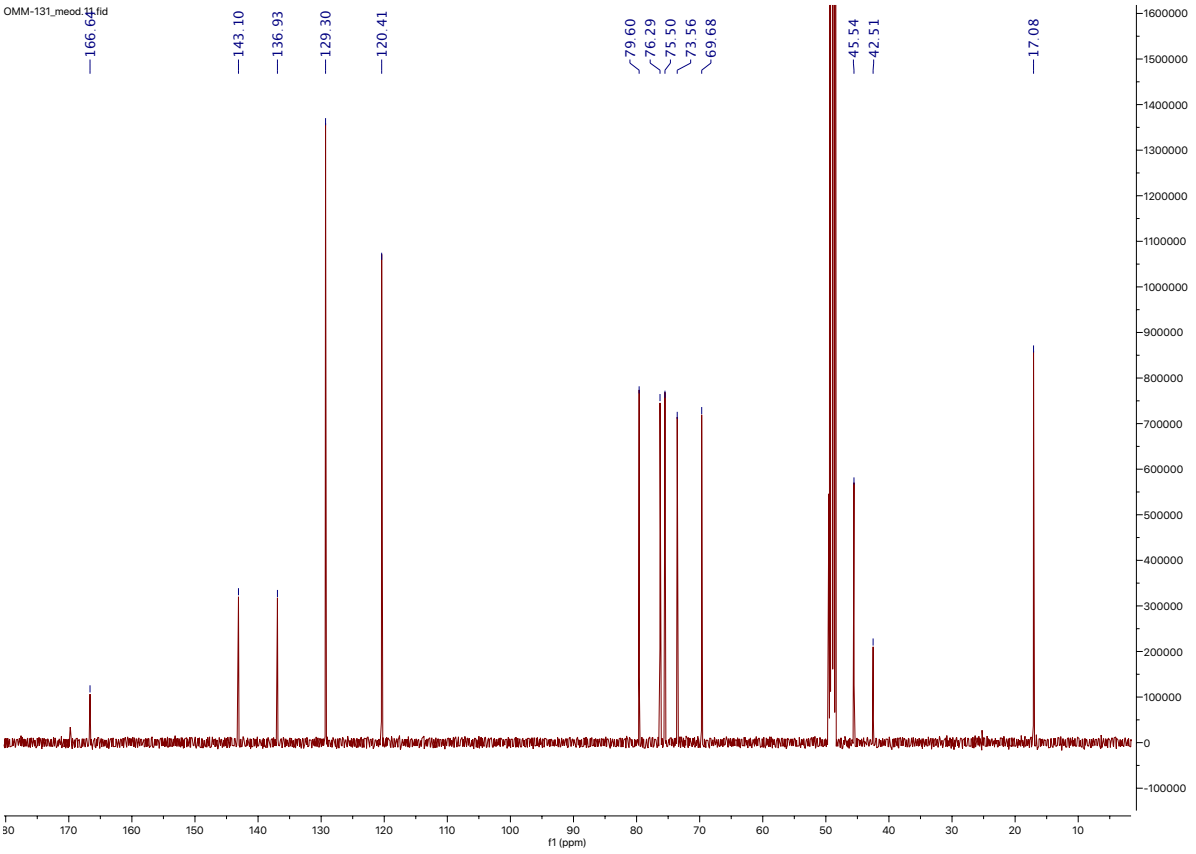
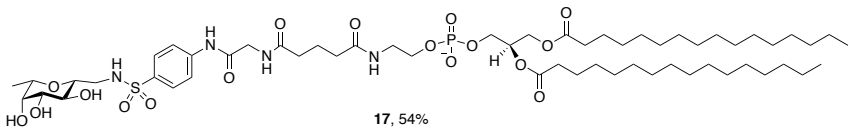
3.28
3.27
3.14
3.13
3.12
3.12
3.12
3.11
3.10
3.00
2.99
2.97
2.96
1.18
1.17
0.92
3.95
1.85
1.02
0.99
2.01
0.83
1.03
1.00
3.07
f1 (ppm)


OMM-131_meod.11.fid
166.64
143.10
136.93
129.30
120.41
79.60
76.29
75.50
73.56
69.68
45.54
42.51
17.08
f1 (ppm)



**17**, 54%

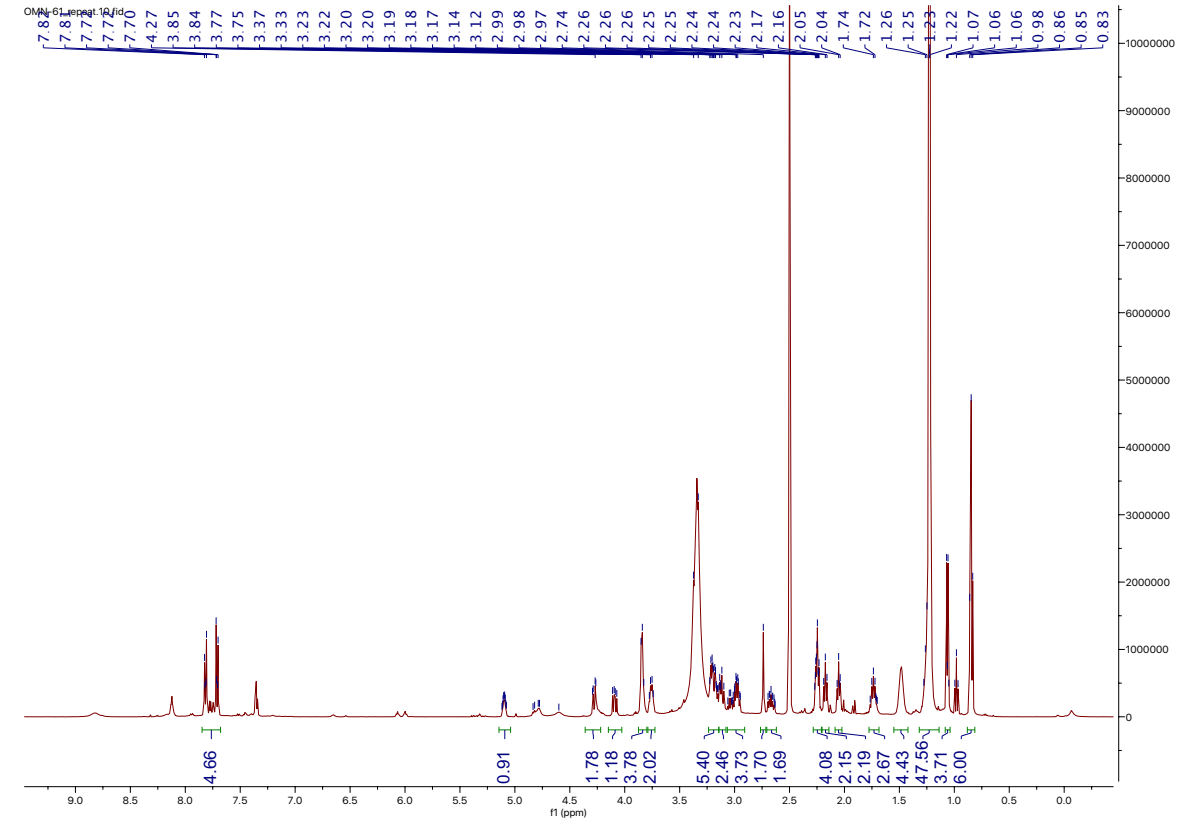
**Glycolipid 17**.

16:0 Glutaryl PE (50 mg, 60 µmol) was suspended in mixture $CHCl_3$/DMF 1:1 (5 mL) and HBTU (28 mg, 1.2 equiv., 72 µmol), HOBt (8 mg, 1.2 equiv., 72 µmol) and $Et_3N$ (42 µL, 5 equiv., 0.3 mmol) was added and stirred for 30 min under a nitrogen atmosphere at 40 °C until the phospholipid was completely dissolved. Then, **8** (32 mg, 1.55 equiv., 93 µmol) was added and reaction was stirred at 40 °C for 48 h. The solvent was removed *in vacuo* and the crude product was purified by reverse phase MPLC ($^{i}$PrOH:$H_2O$:MeOH (5:4:1) / $^{i}$PrOH + 0.2% formic acid, 10-50%). **17** was obtained as a white solid (39 mg, 33 µmol, 54%).

$^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.87 – 7.68 (m, 4H, ArH), 5.16 – 5.05 (m, 1H, C(O)C<u>H</u>$CH_2OPO_3$), 4.86 – 4.71 (m, 1H, NH), 4.60 (br s, 1H, NH), 4.28 (dd, *J* = 12.0, 3.1 Hz, 1H, C(O)OC<u>$H_{2a}$</u>CH), 4.09 (dd, *J* = 12.0, 7.1 Hz, 1H, C(O)OC<u>$H_{2b}$</u>CH), 3.84 (m, 3H, C(O)OCHC<u>$H_{2a}$</u>$OPO_3$, $CH_2C$<u>$H_2$</u>$OPO_3$), 3.78 – 3.71 (m, 2H, CHC<u>$H_2$</u>$OPO_3$), 3.39 – 3.37 (m, H-4, H-5, HDO), 3.24 – 3.15 (m, 4H, H-2, C<u>$H_{2a}$</u>$NHSO_2$, C<u>$H_2$</u>$CH_2OPO_3$), 3.15 – 3.09 (m, 3H, H-3, $CH_2$), 3.06 – 2.94 (m, 3H, H-1, $CH_2$), 2.74 (s, 2H, C(O)<u>C</u>$H_2$NH), 2.71 – 2.62 (m, 1H, C<u>$H_{2b}$</u>$NHSO_2$), 2.25 (m, 4H, C<u>$H_2$</u>C(O)O), 2.17 (t, *J* = 7.5 Hz, 2H, NHC(O)C<u>$H_2$</u>$CH_2$), 2.05 (m, 2H, NHC(O)C<u>$H_2$</u>$CH_2$), 1.78 – 1.69 (m, 2H, NHC(O)$CH_2$C<u>$H_2$</u>), 1.29 – 1.18 (m, 40H), 1.06 (d, *J* = 6.4 Hz, 3H, C<u>$H_3$</u>CHO), 0.85 (t, *J* = 6.9 Hz, 6H, $CH_3$)

$^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 172.54 (OC(O)), 172.41 (OC(O)), 172.30 (NHC(O)), 171.87 (NHC(O)), 169.04 (NHC(O)), 158.45, 142.44 (ArC), 134.52 (ArC), 127.54 (ArCH), 118.83 (ArCH), 78.32 (C-1), 74.64 (C-2), 73.61 (C-5), 71.55 (C-4), 70.19 (d, *J* = 5.0 Hz, C(O)O<u>C</u>$HCH_2OPO_3$), 68.29 (C-3), 63.36 (d, *J* = 5.5 Hz, $CH_2$<u>C</u>$H_2OPO_3$), 63.02 (d, *J* = 7.1 Hz, CH<u>C</u>$H_2OPO_3$), 62.13 (C(O)O<u>C</u>$H_2$CH), 54.55, 44.52 ($CH_2NHSO_2$), 43.34, 42.15 (C(O)<u>C</u>$H_2$NH), 39.95 (m, <u>C</u>$H_2CH_2OPO_3$), 34.78 (NHC(O)C<u>$H_2$</u>$CH_2$), 34.11 (d, *J* = 11.1 Hz, $CH_2$<u>C</u>$H_2OPO_3$), 33.57 (<u>C</u>$H_2$C(O)O), 33.40 (<u>C</u>$H_2$C(O)O), 31.31, 29.08 ($CH_2$), 29.04, 28.96, 28.95, 28.79, 28.76, 28.73, 28.45, 28.42, 24.47 (<u>C</u>$H_2CH_2$C(O)O), 24.42 (<u>C</u>$H_2CH_2$C(O)O), 22.11, 21.46 (NHC(O)$CH_2$C<u>$H_2$</u>), 16.91 (<u>C</u>$H_3$CHO), 15.64, 13.95 ($CH_3$).

HRMS: $[C_{57}H_{101}N_4O_{17}PS + H]^+$ calcd. 1177.6693, found 1177.6654.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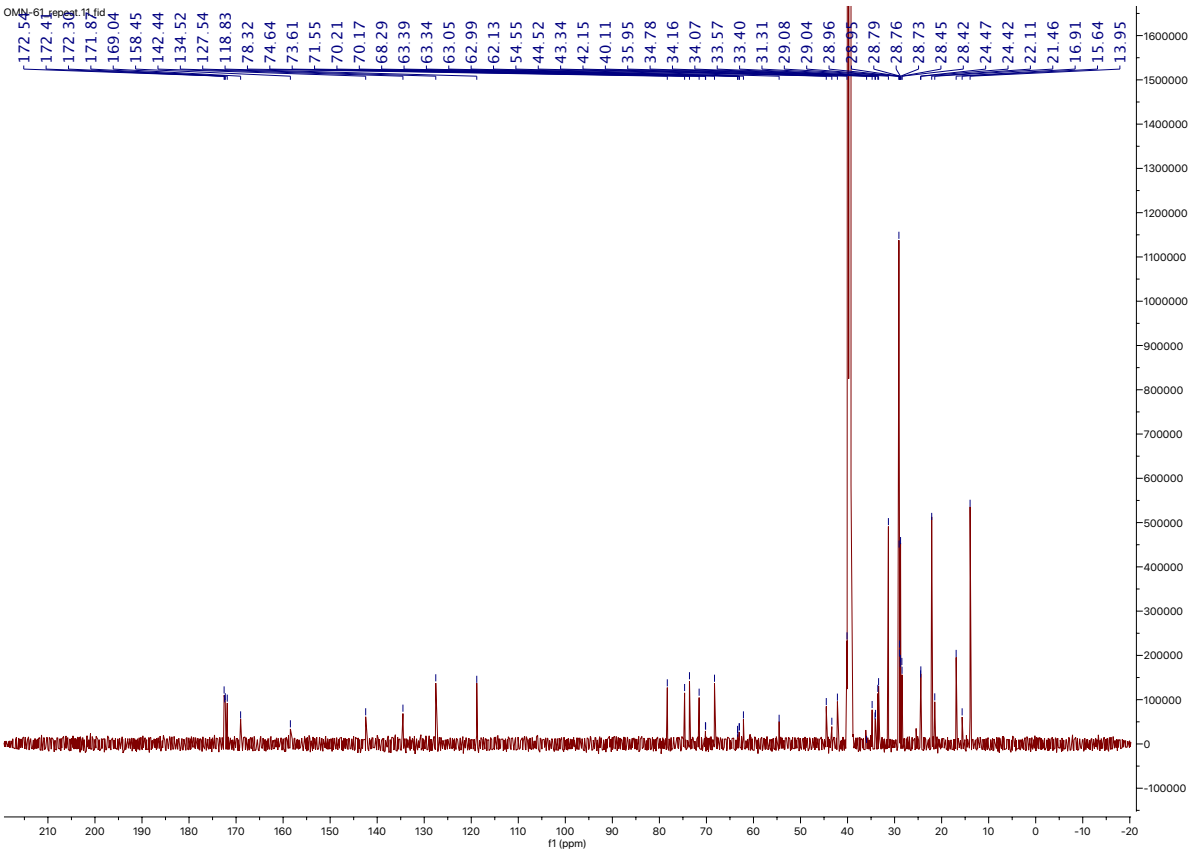
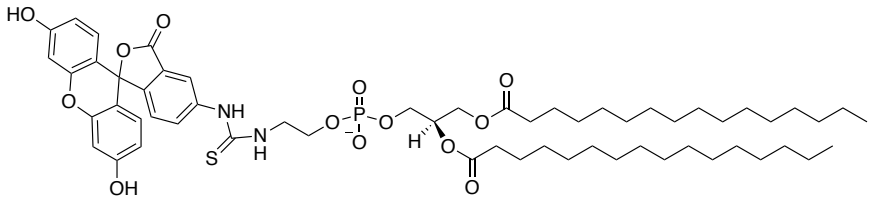
4.66 0.91 1.78 1.18 3.78 2.02 5.40 2.46 3.73 1.70 1.69 4.08 2.15 2.19 2.67 4.43 47.56 3.71 6.00
f1 (ppm)


OMN-61_repeat 11.fid
172.54 172.41 172.30 171.85 169.04 158.45 142.44 134.52 127.54 118.83 78.32 74.64 73.61 71.55 70.21 70.17 68.29 63.39 63.34 63.05 62.99 62.13 54.55 44.52 43.34 42.15 40.11 35.95 34.78 34.16 34.07 33.57 33.40 31.31 29.08 29.04 28.96 28.95 28.79 28.76 28.73 28.45 28.42 24.47 24.42 22.11 21.46 16.91 15.64 13.95
f1 (ppm)



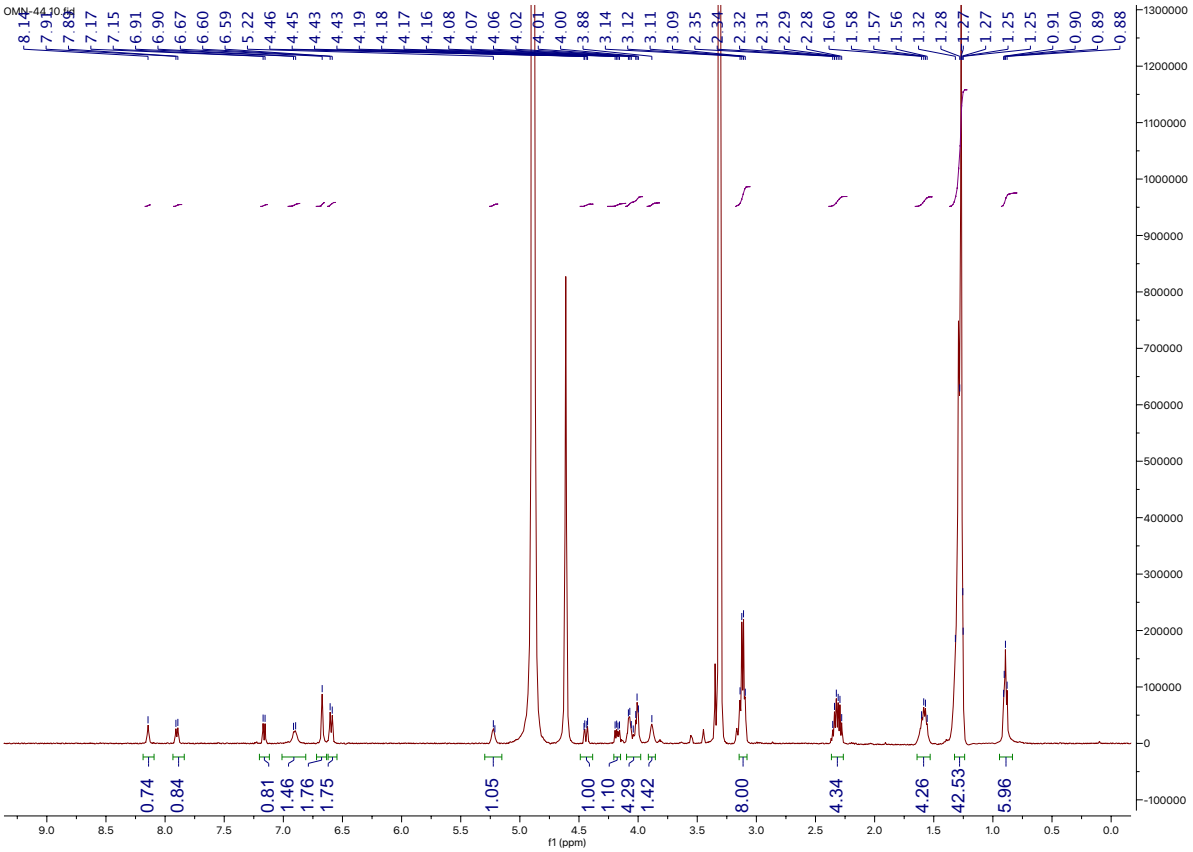
**Fluorescein-conjugated DPPE (18)**.

DPPE (30 mg, 1.1 equiv., 43 µmol) was suspended in mixture $CHCl_3$/DMF 1:1 (5 mL) and FITC (15 mg, 39 µmol) and $Et_3N$ (18 µL, 3 equiv., 123 µmol) were added and stirred overnight under nitrogen atmosphere at 40 °C. Then, **8** (32 mg, 1.55 equiv., 93 µmol) was added and reaction was stirred at 40 °C for 48 h. The solvent was removed *in vacuo* and the crude product was purified by reverse phase MPLC (iPrOH:$H_2O$:MeOH (5:4:1) + 0.2% formic acid/ iPrOH + 0.2% formic acid, 10-80% PrOH + 0.2% formic acid). **18** was obtained as an orange solid (33 mg, 0.03 mmol, 72%).

$^1$H NMR (500 MHz, MeOH-$d_4$) δ 8.14 (s, 1H, ArH), 7.90 (d, J = 8.2 Hz, 1H, ArH), 7.16 (d, J = 8.3 Hz, 1H, ArH), 6.90 (d, J = 8.9 Hz, 2H, ArH), 6.67 (s, 2H, ArH), 6.60 (m, 2H, ArH), 5.22 (s, 1H, CHOC(O)), 4.44 (dd, J = 11.8, 3.1 Hz, 1H, C(O)OC$\underline{H}_{2a}$CH), 4.18 (dd, J = 12.1, 6.5 Hz, 1H, C(O)OC$\underline{H}_{2b}$CH), 4.04 (dt, J = 30.1, 5.8 Hz, 4H, $CH_2C\underline{H}_2OPO_3$, $CHC\underline{H}_2OPO_3$), 3.88 (s, 2H, NH), 3.12 (q, J = 7.4 Hz, 6H, $CH_2$), 2.32 (dq, J = 14.9, 7.4 Hz, 4H, $C\underline{H}_2CH_2OPO_3$, $C\underline{H}_2C(O)O$), 1.66 – 1.51 (m, 4H, $C\underline{H}_2CH_2C(O)O$), 1.28 (m, 42 H, $CH_2$, ), 0.89 (t, J = 6.1 Hz, 6H, $CH_3$).

$^{13}$C NMR (126 MHz, MeOH-$d_4$) δ 181.76 (CS), 174.52 (C(O)O), 174.19 (C(O)O), 169.41 (C(O)O), 152.89 (ArCOH), 130.87, 119.88, 112.25, 103.21, 87.28, 78.11, 70.94, 63.04, 34.67, 34.50, 32.34, 30.11, 30.09, 30.07, 29.96, 29.94, 29.77, 29.74, 29.56, 29.54, 25.35, 25.29, 23.07, 14.28 ($CH_3$).

HPLC-MS: $[C_{58}H_{85}N_2O_{13}PS + H]^+$ calcd. 1081.5583, found 1081.5540.


OMN-44.10.fid
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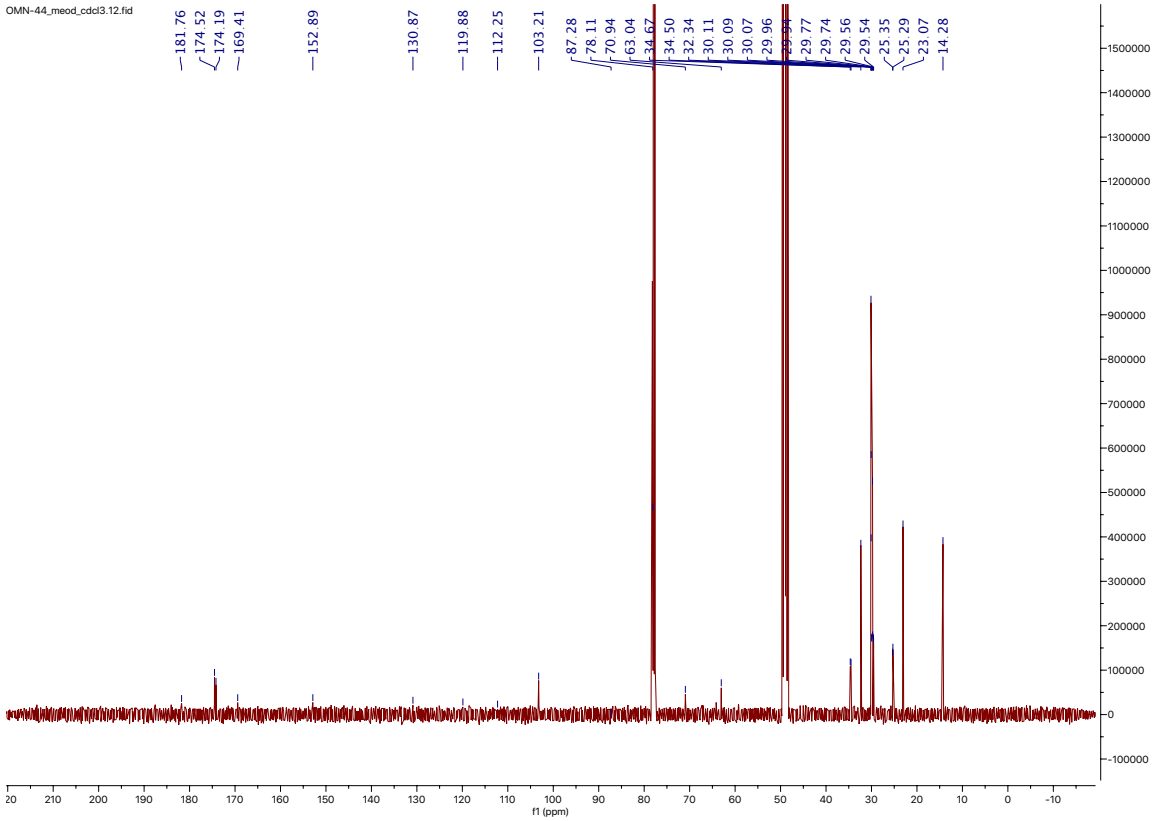
0.74 0.84 0.81 1.46 1.76 1.75 1.05 1.00 1.10 4.29 1.42 8.00 4.34 4.26 42.53 5.96
f1 (ppm)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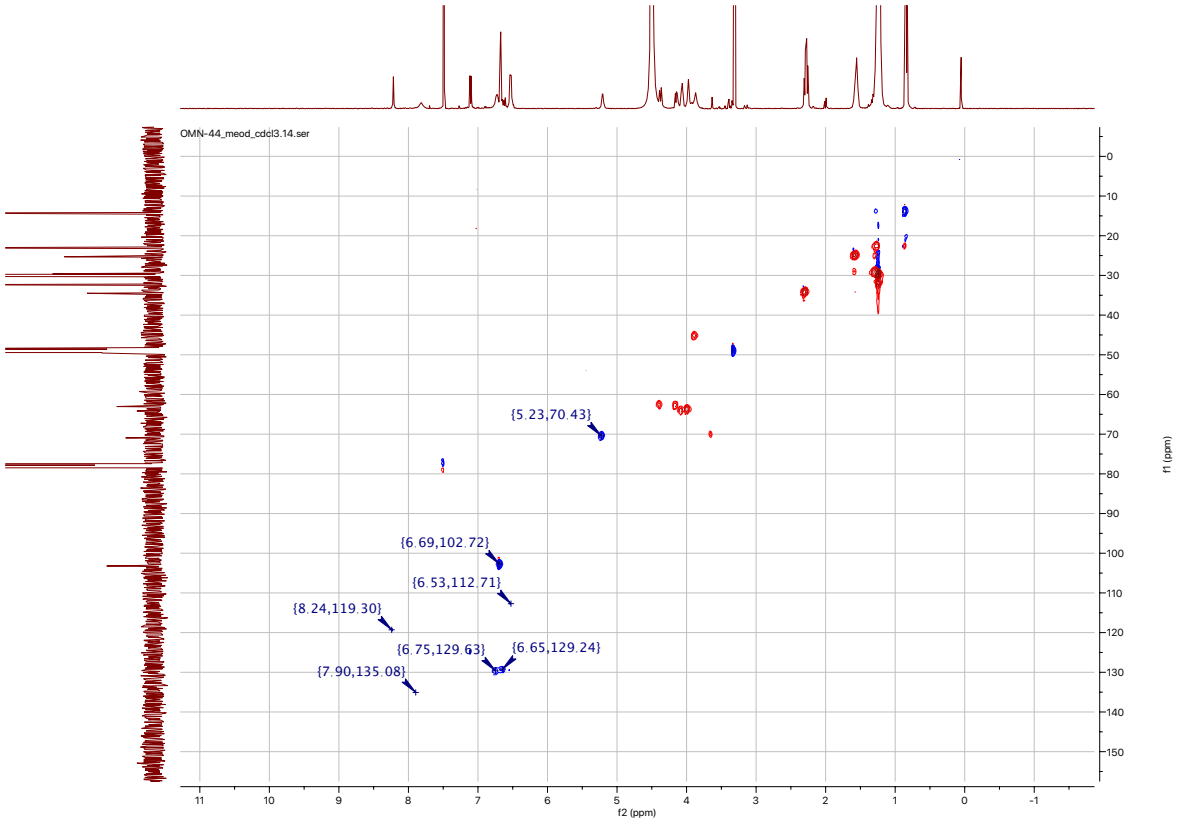
181.76 174.52 174.19 169.41 152.89 130.87 119.88 112.25 103.21 87.28 78.11 70.94 63.04 34.67 34.50 32.34 30.11 30.09 30.07 29.96 29.94 29.77 29.74 29.56 29.54 25.35 25.29 23.07 14.28
f1 (ppm)


OMN-44_meod_cdcl3.14.ser
{5.23,70.43}
{6.69,102.72}
{6.53,112.71}
{8.24,119.30}
{6.75,129.63}
{6.65,129.24}
{7.90,135.08}
f2 (ppm)
f1 (ppm)

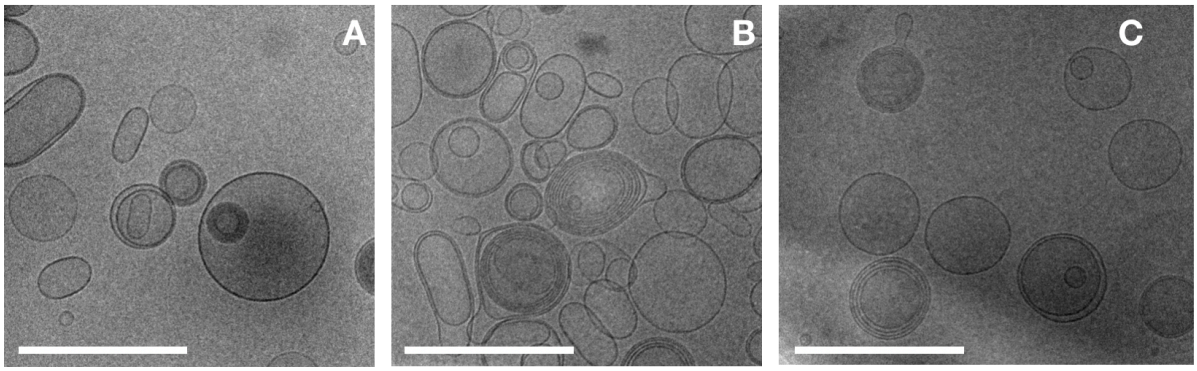



**Figure S1.** Transmission electron micrograph for the fluorescent liposomes produced by extrusion: plain liposomes (A), 15%-LecA-targeted ligand **16** (B), 15%-LecB-targeted ligand **17** (C).

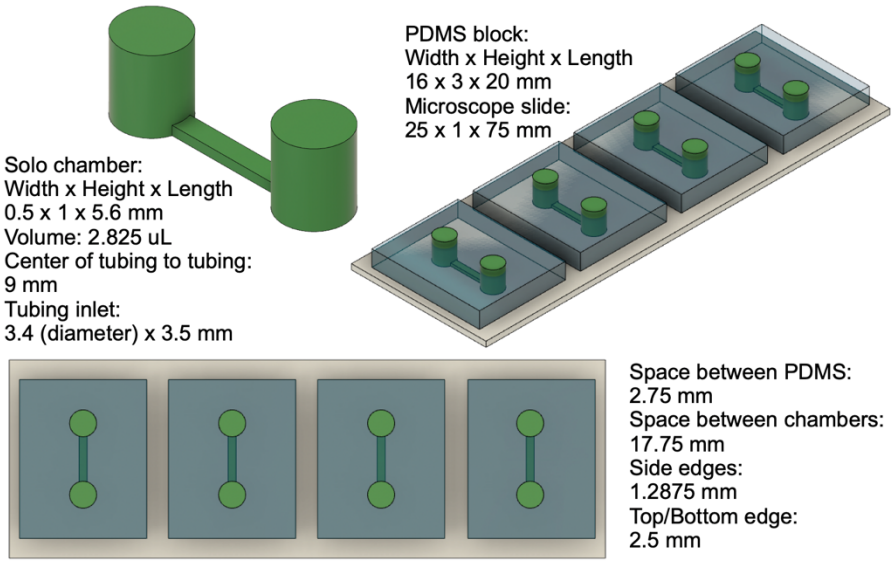



**Figure S2.** Detailed representation of the flow chamber.

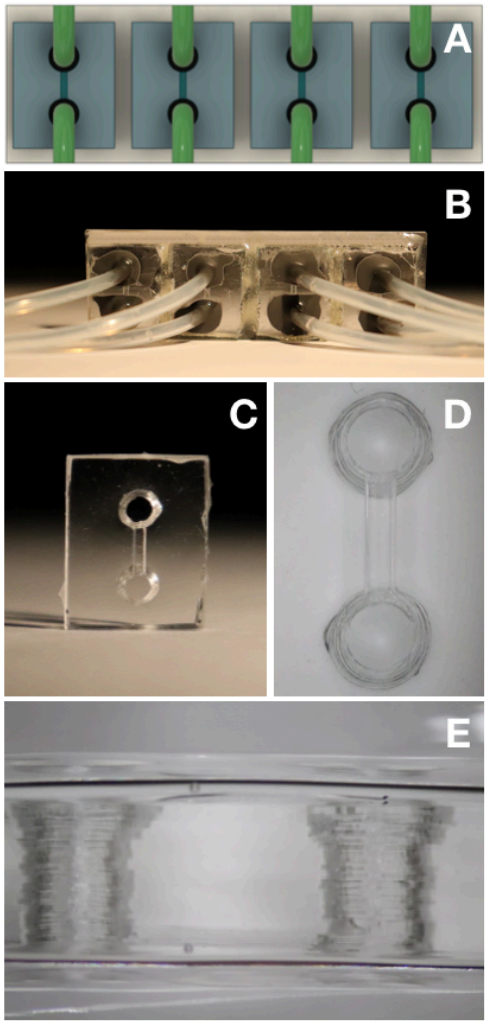



**Figure S3.** Flow chamber. Tube side: graphic representation (A) and photo (B); single flow chamber (C and D); profile of the outlet (E).

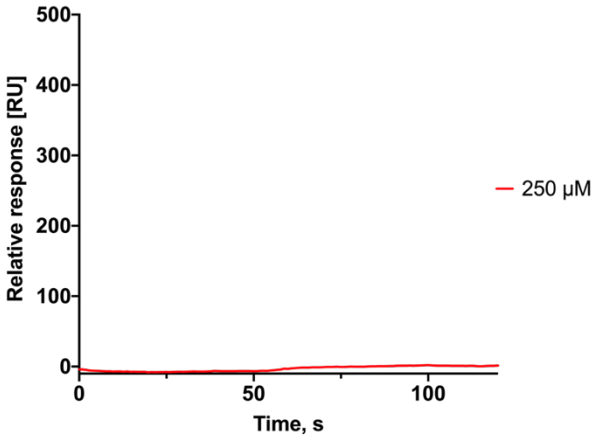



**Figure S4**: SPR sensorgram for LecB-targeted liposomes injected on the LecA-coupled chip demonstrates lectin-specificity of binding.

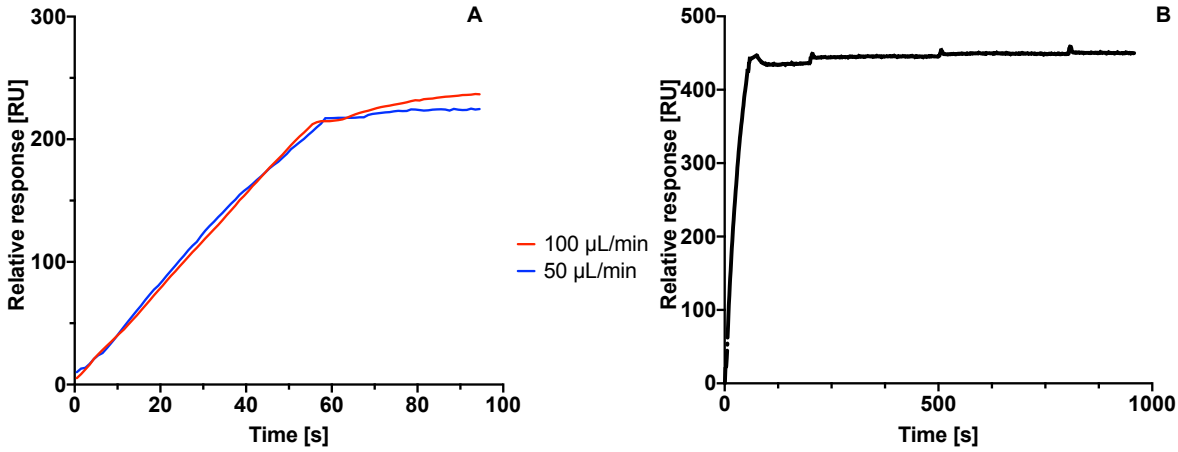



**Figure S5. Sensograms of LecA interactions** with: 15% LecA-targeted non-fluorescent liposomes (32 µM of LecA-ligand **16**) at different flow rates to reveal an impact of mass transfer effect (A), 15% LecA-targeted non-fluorescent liposomes (250 µM of LecA-ligand **16**) with 15 min dissociation time (B).

## Supporting Information References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