

Supporting Information **for**

Synthesis of aminoxy glycoside derivatives of the outer core domain of *Pseudomonas aeruginosa* lipopolysaccharide

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¹H and ¹³C NMR of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-
(1 \rightarrow 3)-[4,6-*O*-acetyl-2-*O*-benzoyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-azido-4,6-*O*-
acetyl-2-deoxy- α -D-galactopyranoside (**20**) S29

HRMS data of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[4,6-
O-acetyl-2-*O*-benzoyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-*N*-
tertbutyloxycarbonylalanine-4,6-*O*-acetyl-2-deoxy- α -D-galactopyranoside (**21**) S30

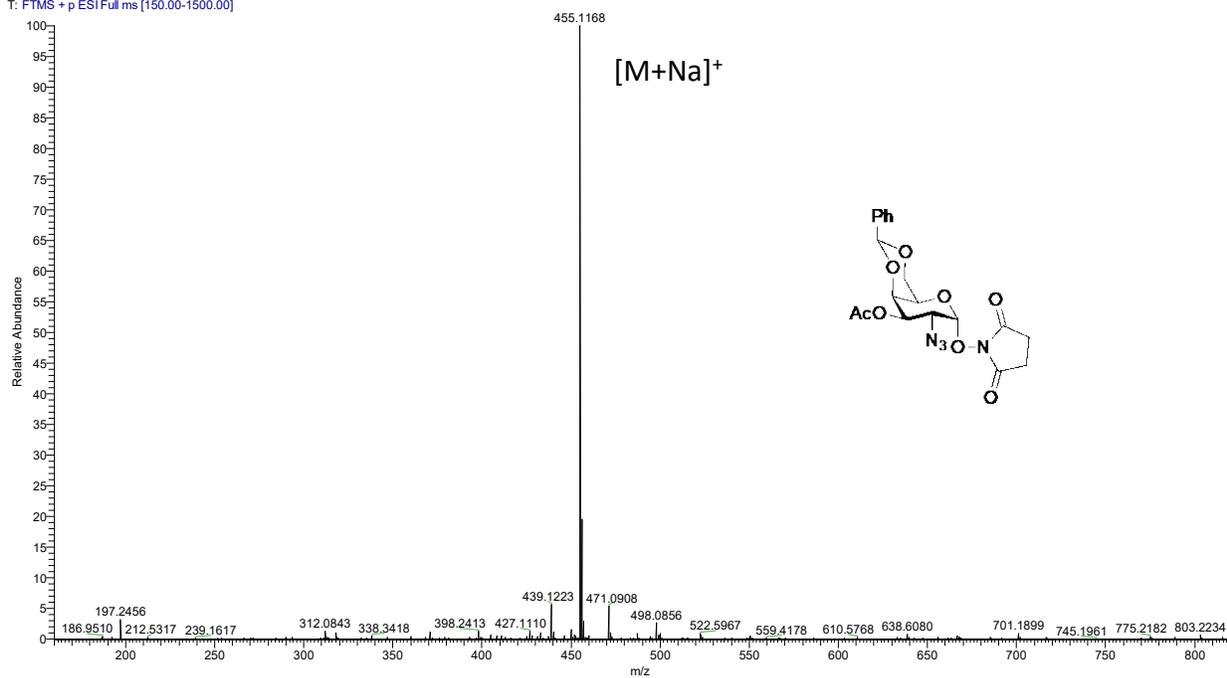
¹H and ¹³C NMR of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-
(1 \rightarrow 3)-[4,6-*O*-acetyl-2-*O*-benzoyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-*N*-
tertbutyloxycarbonylalanine-4,6-*O*-acetyl-2-deoxy- α -D-galactopyranoside (**21**) S31

HRMS data of Aminoxy [α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[β -D-glucopyranosyl]-
(1 \rightarrow 3)-2-*N*-alanine-2-deoxy- α -D-galactopyranoside (**4**) S32

¹H and ¹³C NMR of Aminoxy [α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[β -D-
glucopyranosyl]-(1 \rightarrow 3)-2-*N*-alanine-2-deoxy- α -D-galactopyranoside (**4**) S33

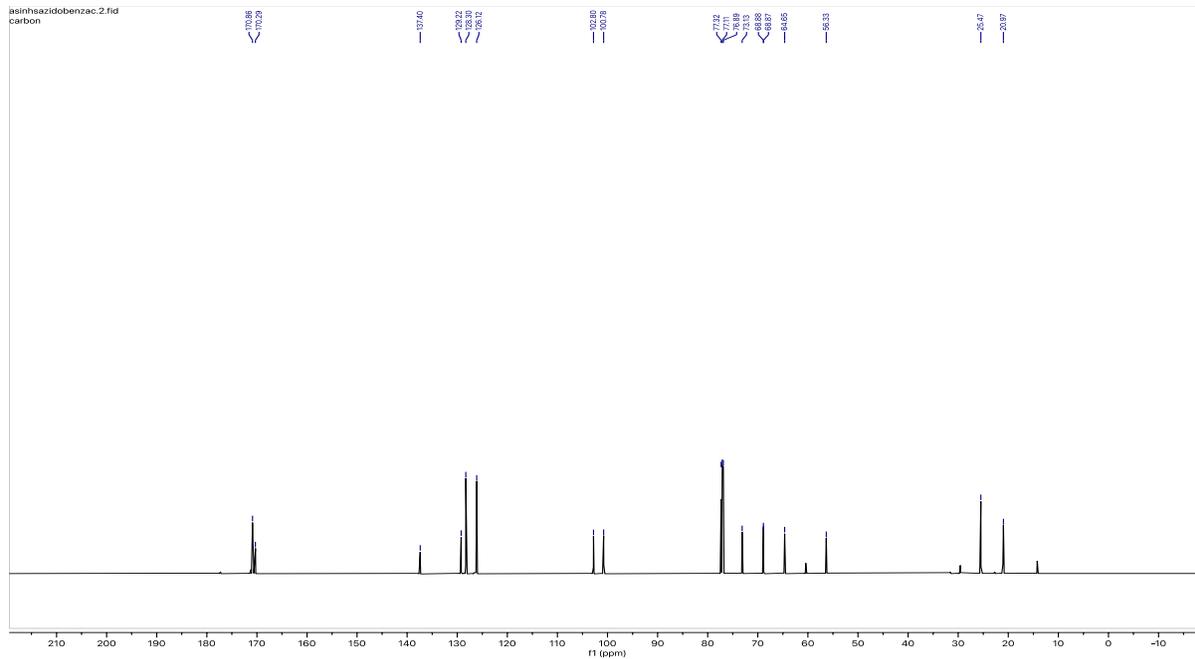
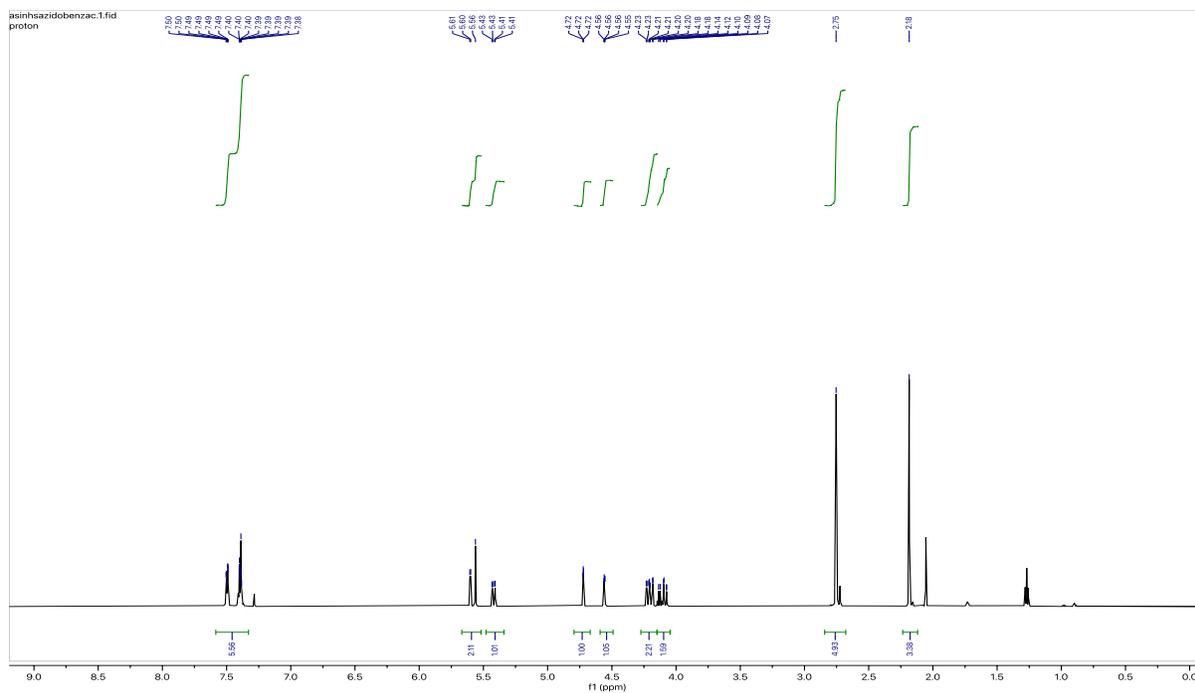
HRMS data of Succinimidyl 2-azido-3-O-acetate-4,6-O-benzylidene-2-deoxy- α -D-galactopyranoside (**8**)

40011 AS38 #2-116 RT: 0.01-0.91 AV: 115 NL: 1.64E8
T: FTMS + p ESI Full ms [150.00-1500.00]



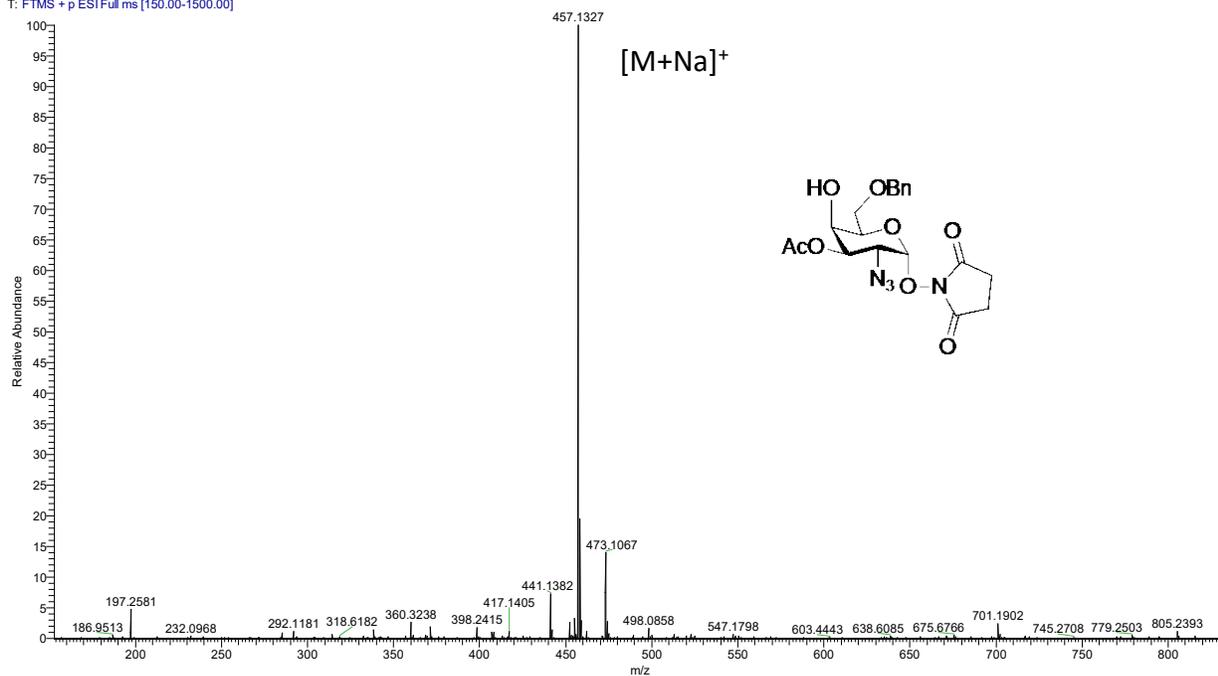
$$\text{Mass accuracy} = (455.1168 - 455.1173)/455.1173 * 10^6 = 1.1 \text{ ppm}$$

^1H and ^{13}C NMR of Succinimidyl 2-azido-3-*O*-acetate-4,6-*O*-benzylidene-2-deoxy- α -D-galactopyranoside (**8**)



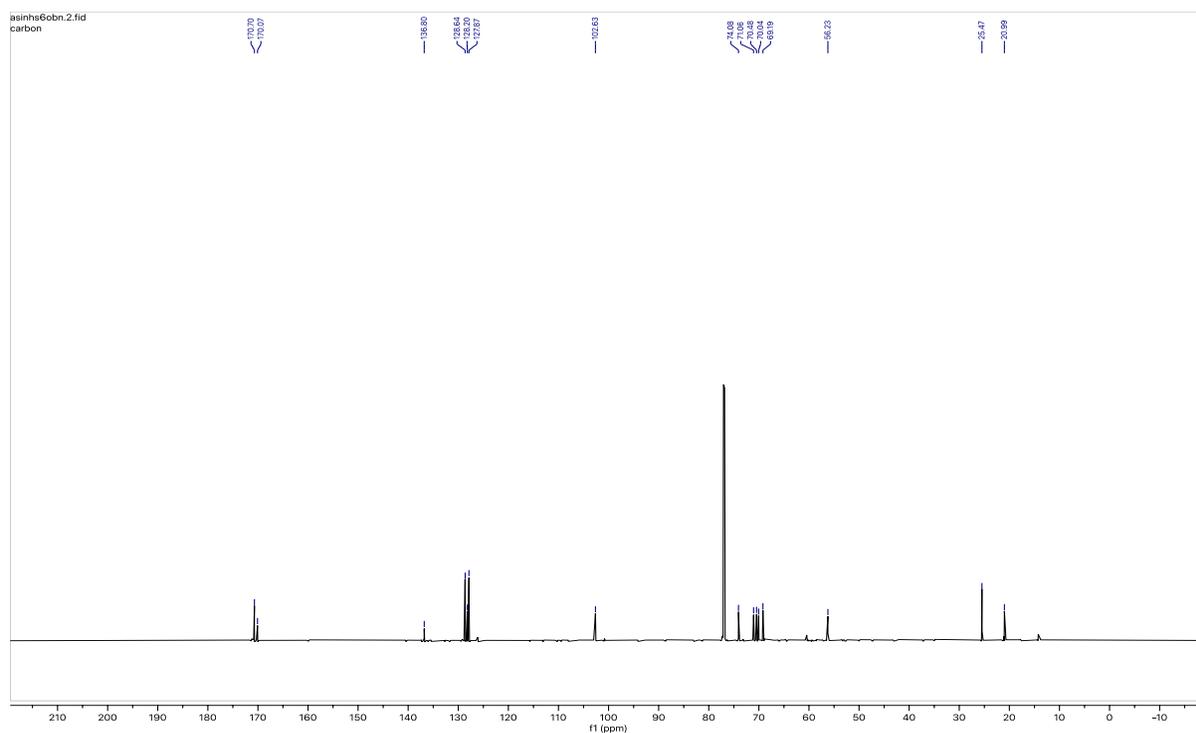
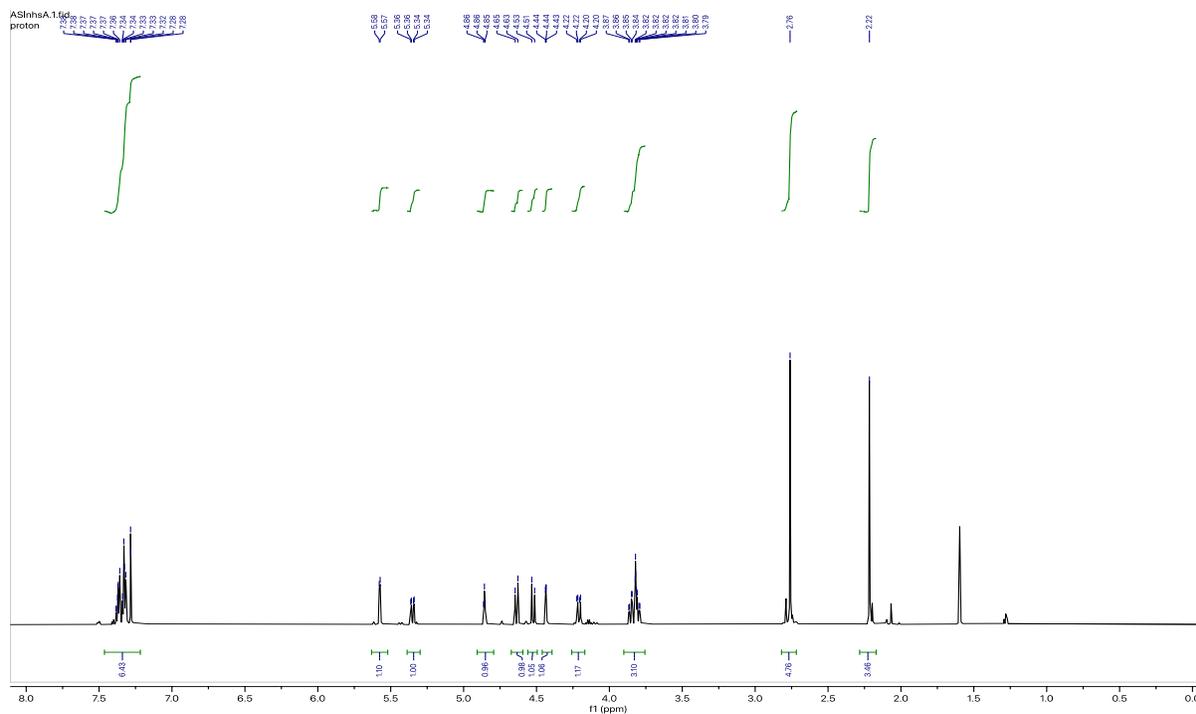
HRMS data of Succinimidyl 2-azido-3-O-acetate-6-O-benzyl-2-deoxy- α -D-galactopyranoside (**9**)

40011 AS39 #1-115 RT: 0.00-0.90 AV: 115 NL: 1.22E8
T: FTMS + p ESI Full ms [150.00-1500.00]

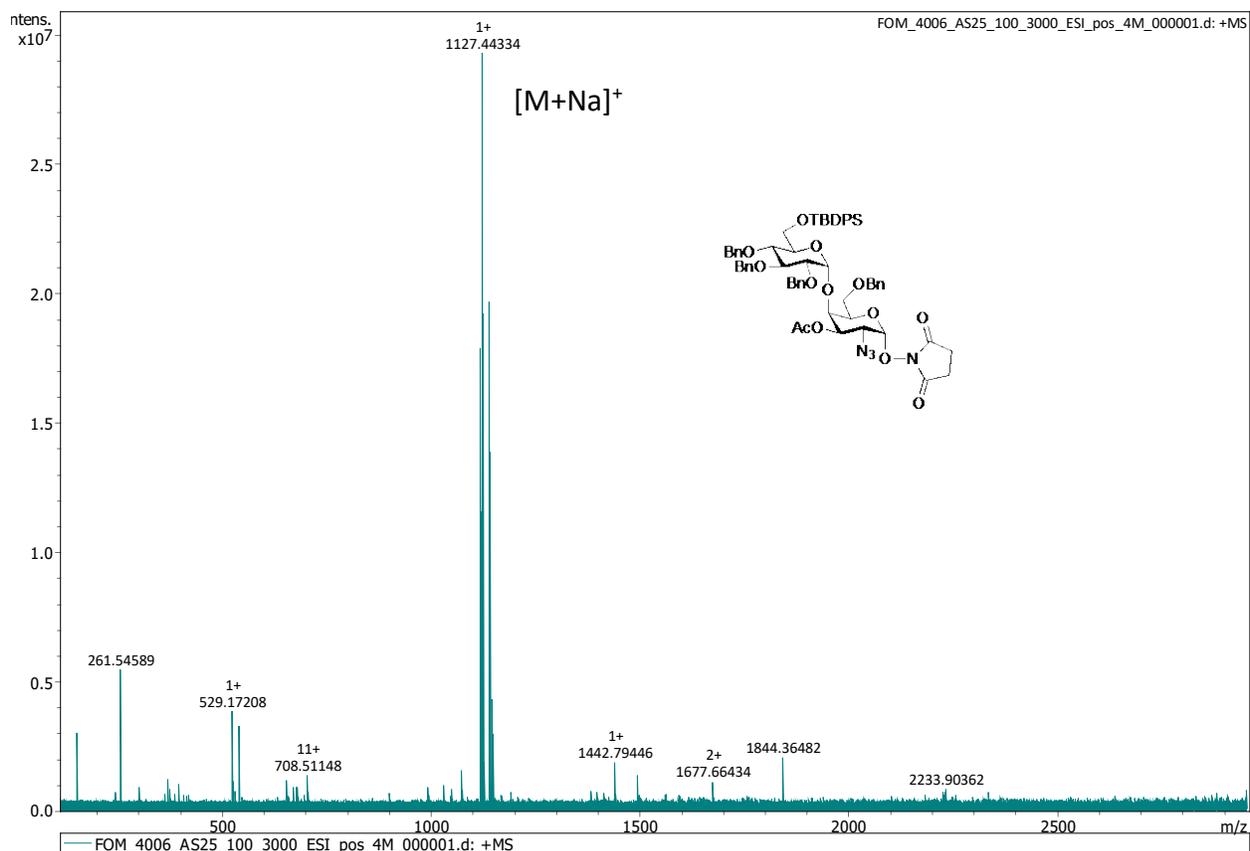


$$\text{Mass accuracy} = (457.1327 - 457.1330)/457.1330 * 10^6 = 0.7 \text{ ppm}$$

^1H and ^{13}C NMR of Succinimidyl 2-azido-3-O-acetate-6-O-benzyl-2-deoxy- α -D-galactopyranoside (9)

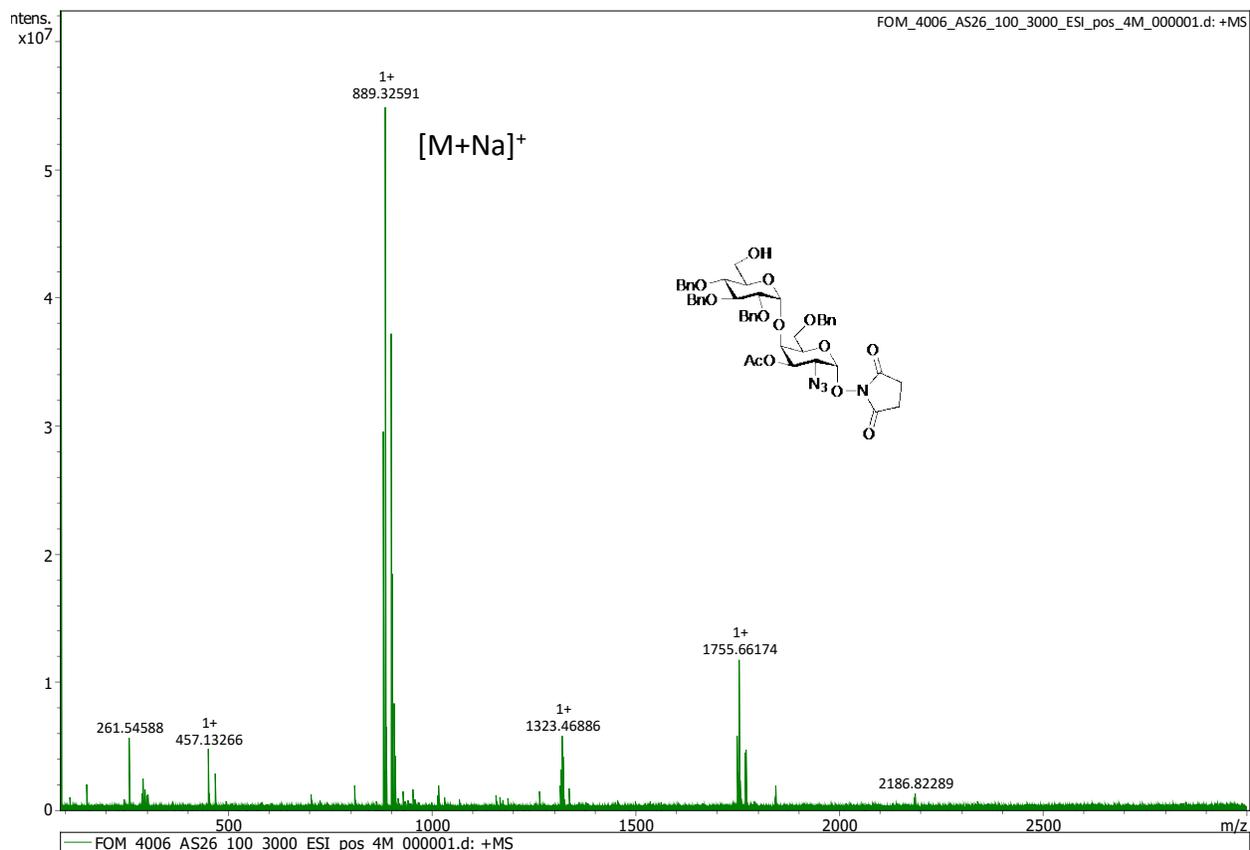


HRMS data of Succinimidyl [2,3,4-tri-*O*-benzyl-6-tertbutyldiphenylsilyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-azido-3-*O*-acetate-6-*O*-benzyl-2-deoxy- α -D-galactopyranoside (**10**)



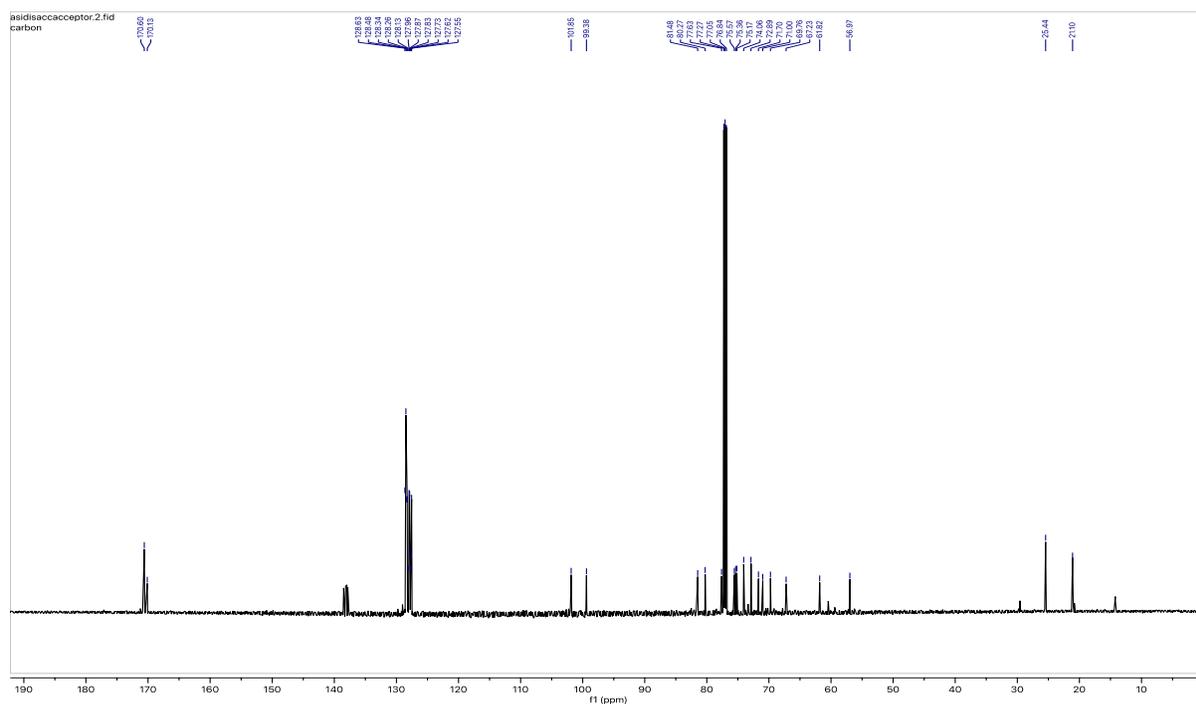
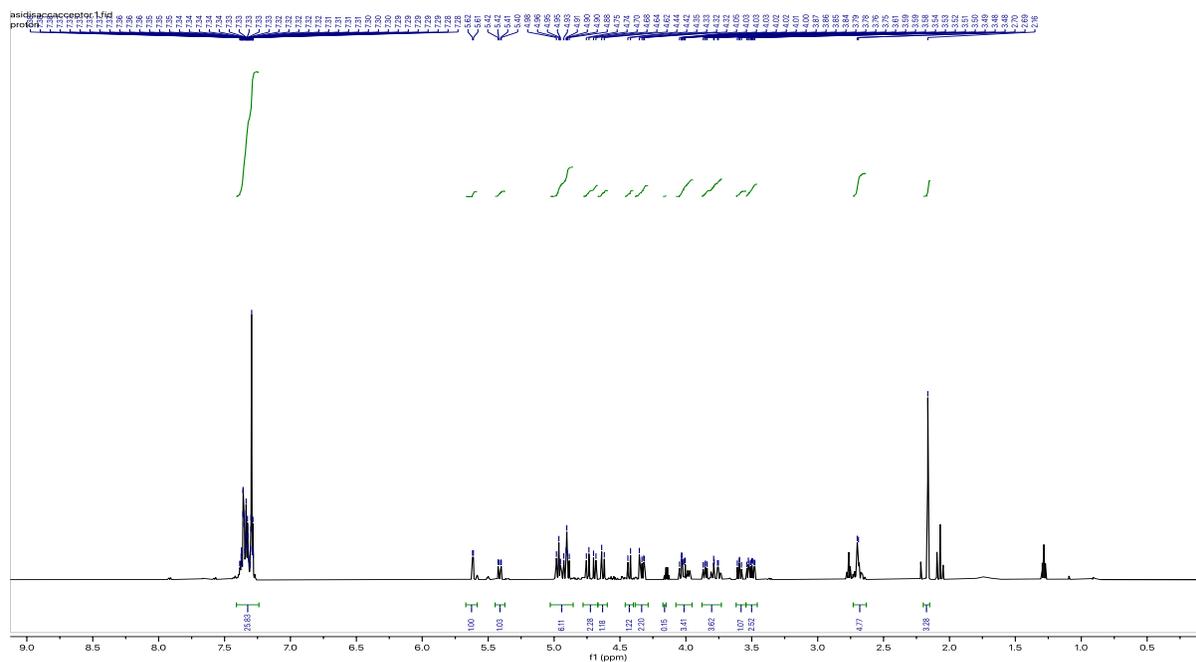
$$\text{Mass accuracy} = (1127.4434 - 1127.4552)/1127.4552 * 10^6 = 0.9 \text{ ppm}$$

HRMS data of Succinimidyl [2,3,4-tri-*O*-benzyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-azido-3-*O*-acetate-6-*O*-benzyl-2-deoxy α -D-galactopyranoside (**11**)

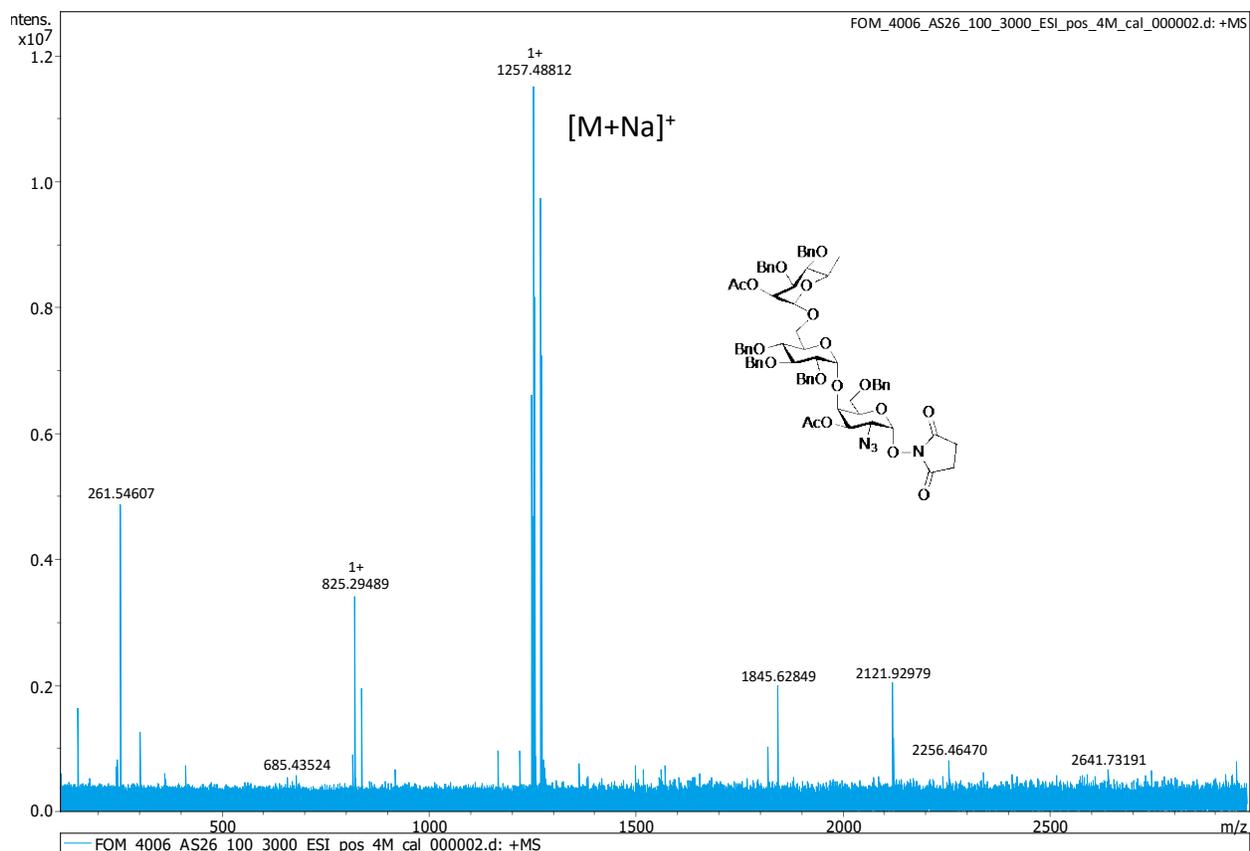


$$\text{Mass accuracy} = (889.3259 - 889.3374)/889.3374 * 10^6 = 0.8 \text{ ppm}$$

¹H and ¹³C NMR of Succinimidyl [2,3,4-tri-*O*-benzyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-azido-3-*O*-acetate-6-*O*-benzyl-2-deoxy α -D-galactopyranoside (**11**)

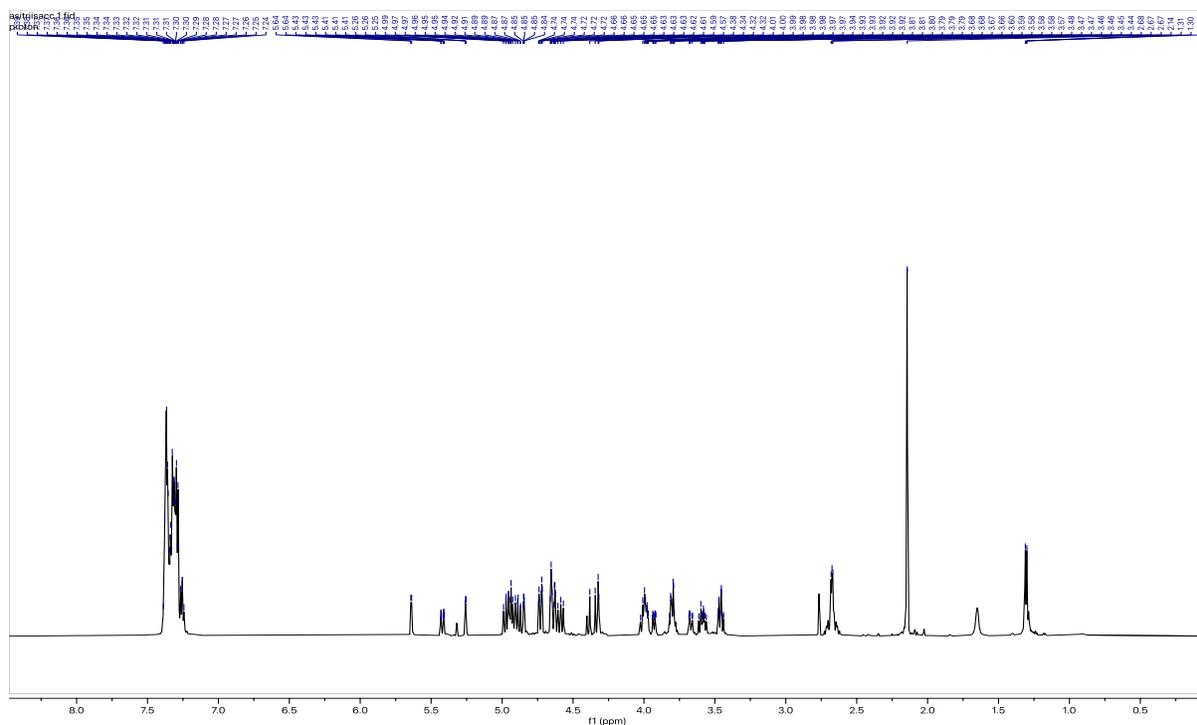


HRMS data of Succinimidyl [2-*O*-acetyl-3,4-di-*O*-benzyl- α -L-rhamnopyranosyl]-(1 \rightarrow 6)-[2,3,4-tri-*O*-benzyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-azido-3-*O*-acetate-6-*O*-benzyl-2-deoxy- α -D-galactopyranoside (**12**)

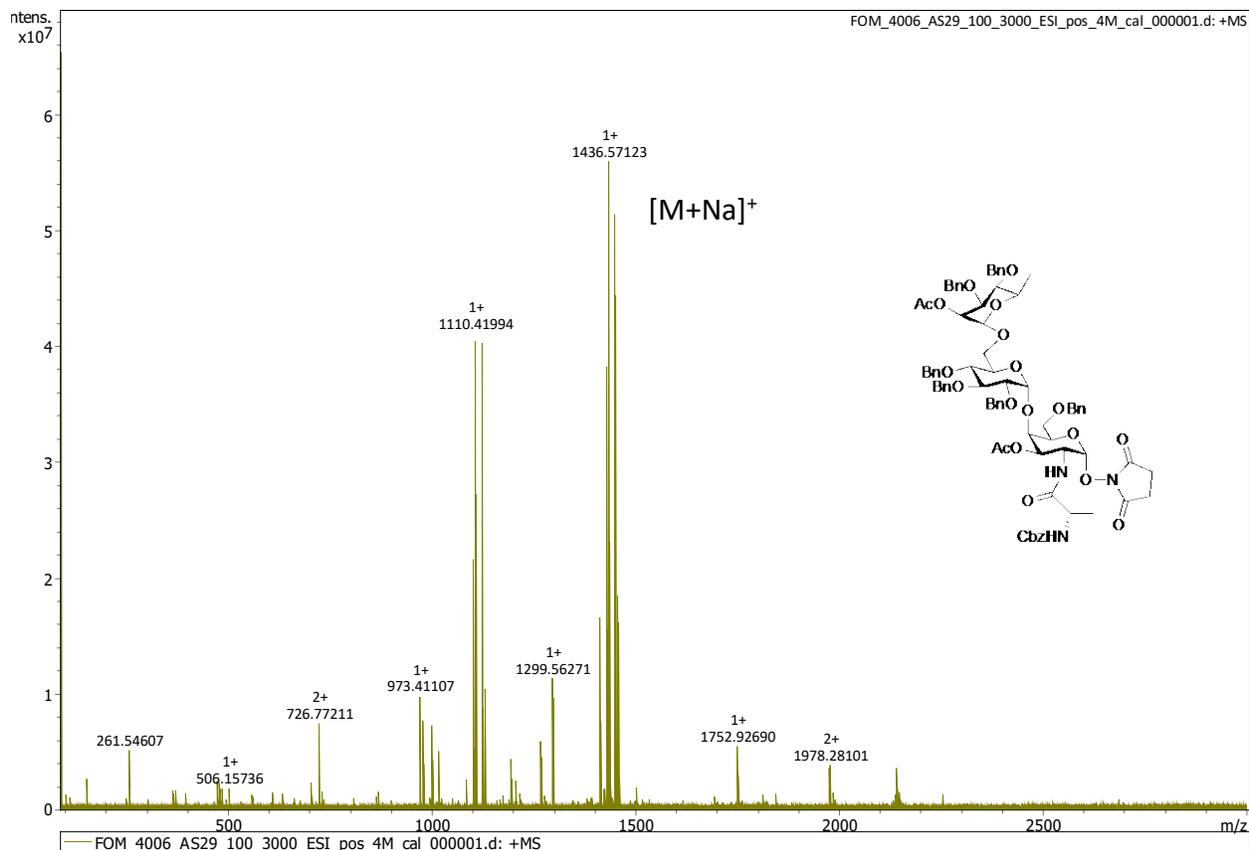


$$\text{Mass accuracy} = (1257.4881 - 1257.4998)/1257.4998 * 10^6 = 0.7 \text{ ppm}$$

¹H and ¹³C NMR of Succinimidyl [2-*O*-acetyl-3,4-di-*O*-benzyl- α -L-rhamnopyranosyl]-(1 \rightarrow 6)-[2,3,4-tri-*O*-benzyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-azido-3-*O*-acetate-6-*O*-benzyl-2-deoxy- α -D-galactopyranoside (**12**)

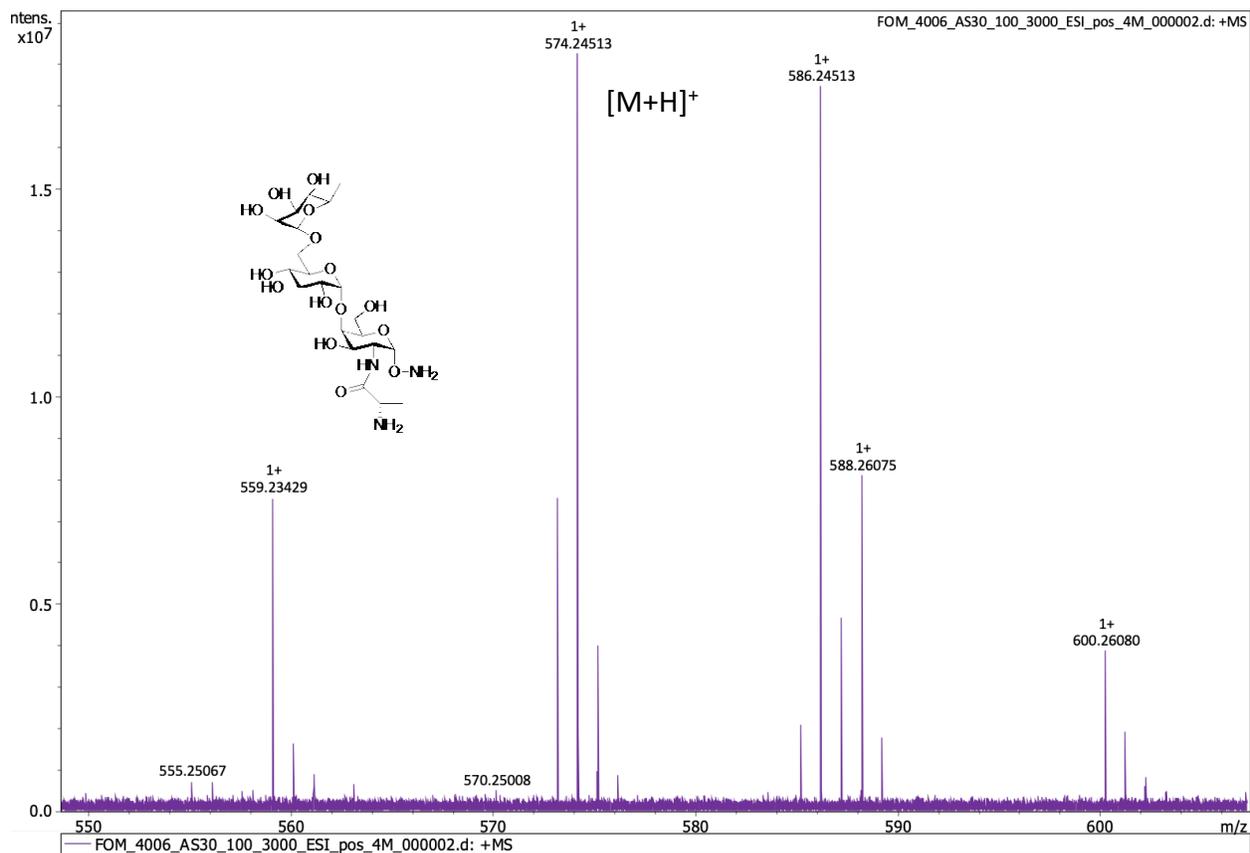


HRMS data of Succinimidyl [2-*O*-acetyl-3,4-di-*O*-benzyl- α -L-rhamnopyranosyl]-(1 \rightarrow 6)-[2,3,4-tri-*O*-benzyl- α -D-glucopyranosyl]-(1 \rightarrow 4)-2-*N*-benzyloxycarbonylalanine-3-*O*-acetate-6-*O*-benzyl-2-deoxy- α -D-galactopyranoside (**13**)



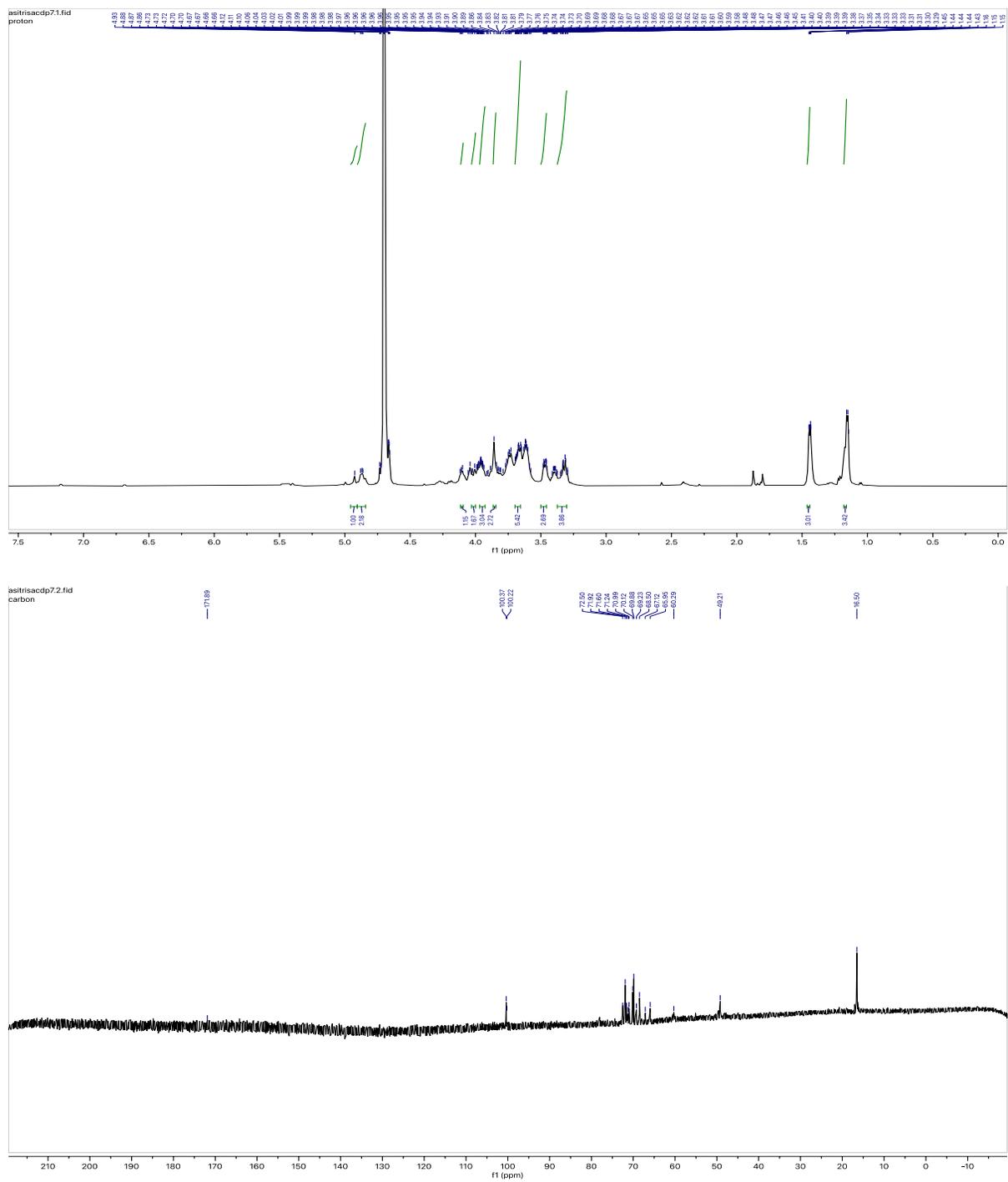
$$\text{Mass accuracy} = (1436.5712 - 1436.5832)/1436.5832 * 10^6 = 8.4 \text{ ppm}$$

HRMS data of Aminoxy [α -L-rhamnopyranosyl]-(1 \rightarrow 6)-[α -D-glucopyranosyl]-(1 \rightarrow 4)-2-N-alanine-2-deoxy- α -D-galactopyranoside (**3**)



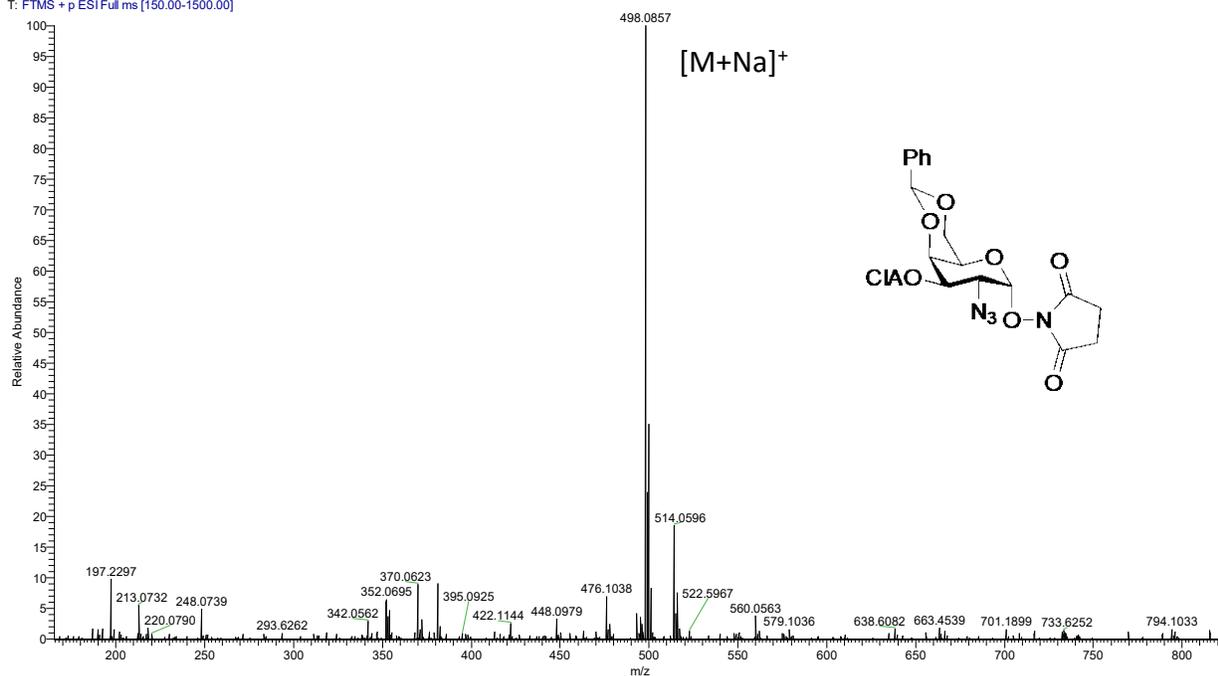
$$\text{Mass accuracy} = (574.2451 - 574.2381) / 574.2381 * 10^6 = 0.5 \text{ ppm}$$

^1H and ^{13}C NMR of Aminoxy [α -L-rhamnopyranosyl]-(1 \rightarrow 6)-[α -D-glucopyranosyl]-(1 \rightarrow 4)-2-N-alanine-2-deoxy- α -D-galactopyranoside (**3**)



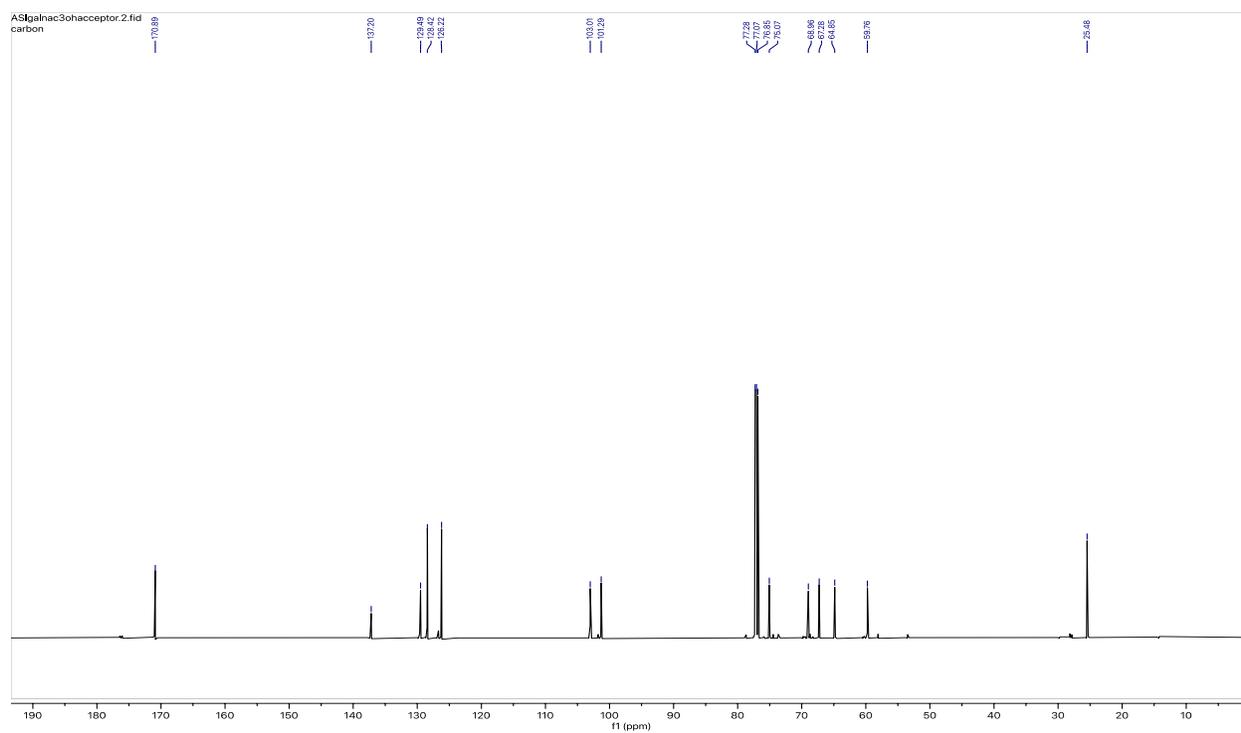
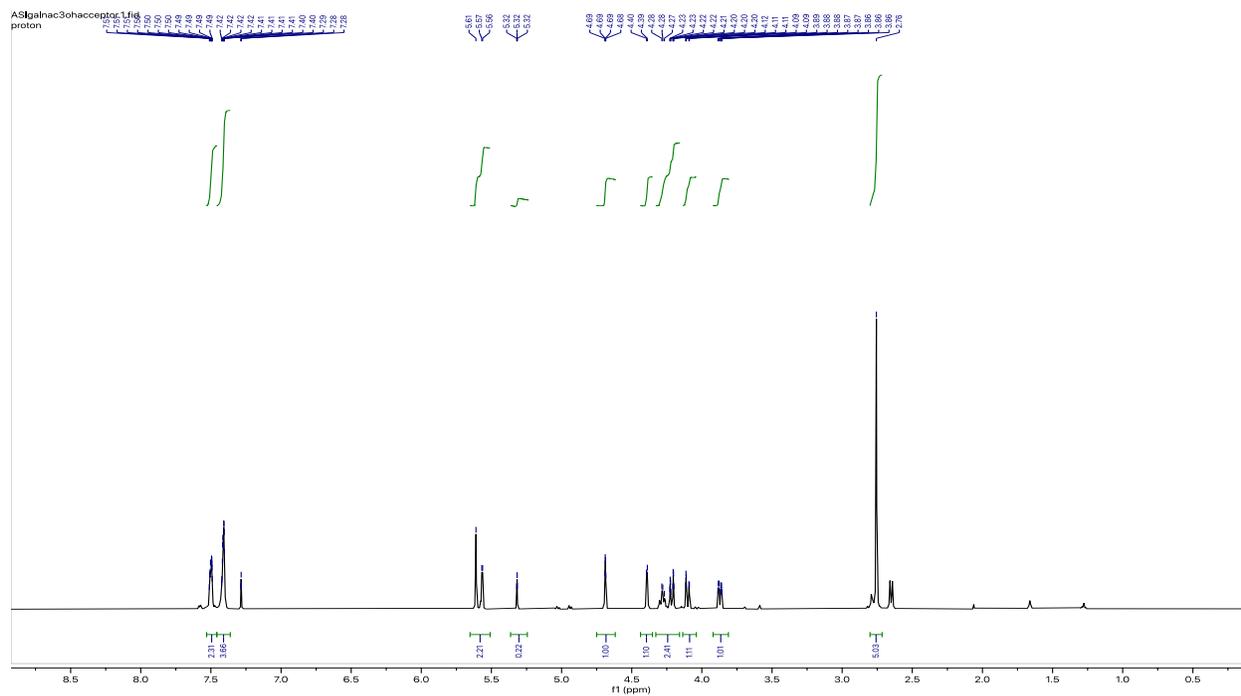
HRMS data of Succinimidyl 2-azido-4,6-O-benzylidene-3-O-chloroacetyl-2-deoxy- α -D-galactopyranoside (**15**)

40011 AS37 #2-129 RT: 0.01-1.01 AV: 128 NL: 3.65E7
T: FTMS + p ESI Full ms [150.00-1500.00]



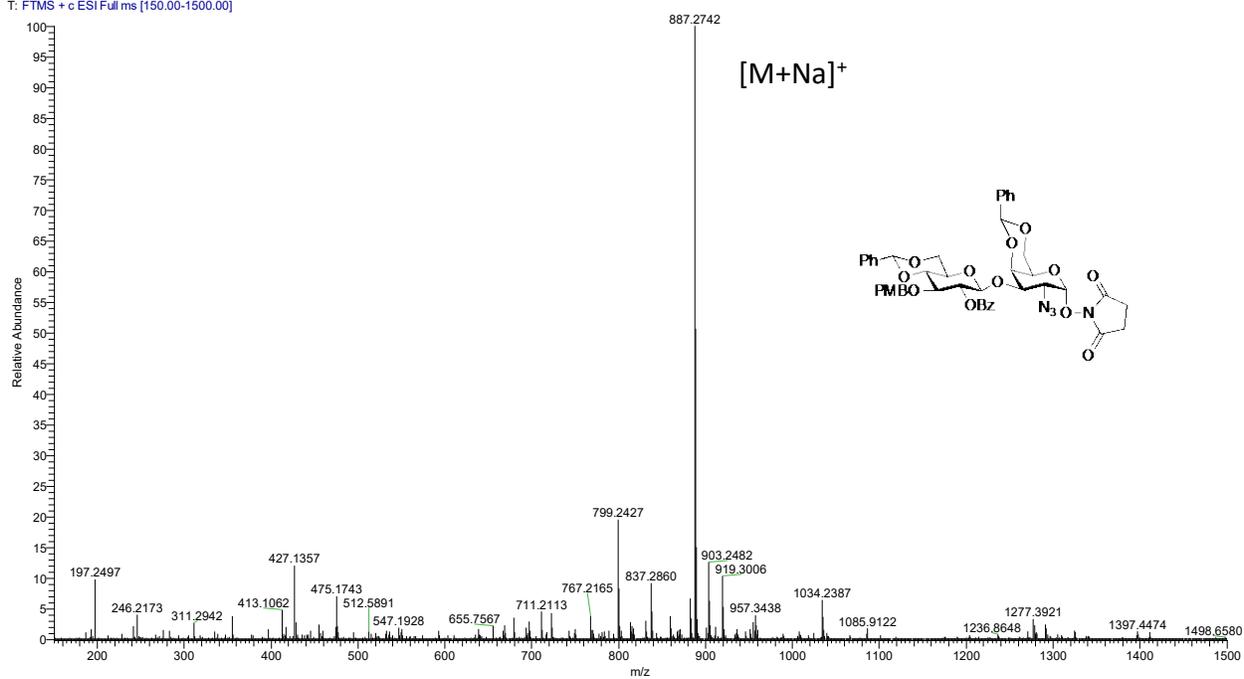
$$\text{Mass accuracy} = (498.0857 - 498.0784)/498.0784 * 10^6 = 14.6 \text{ ppm}$$

^1H and ^{13}C NMR of Succinimidyl 2-azido-4,6-*O*-benzylidene-2-deoxy- α -D-galactopyranoside (16)



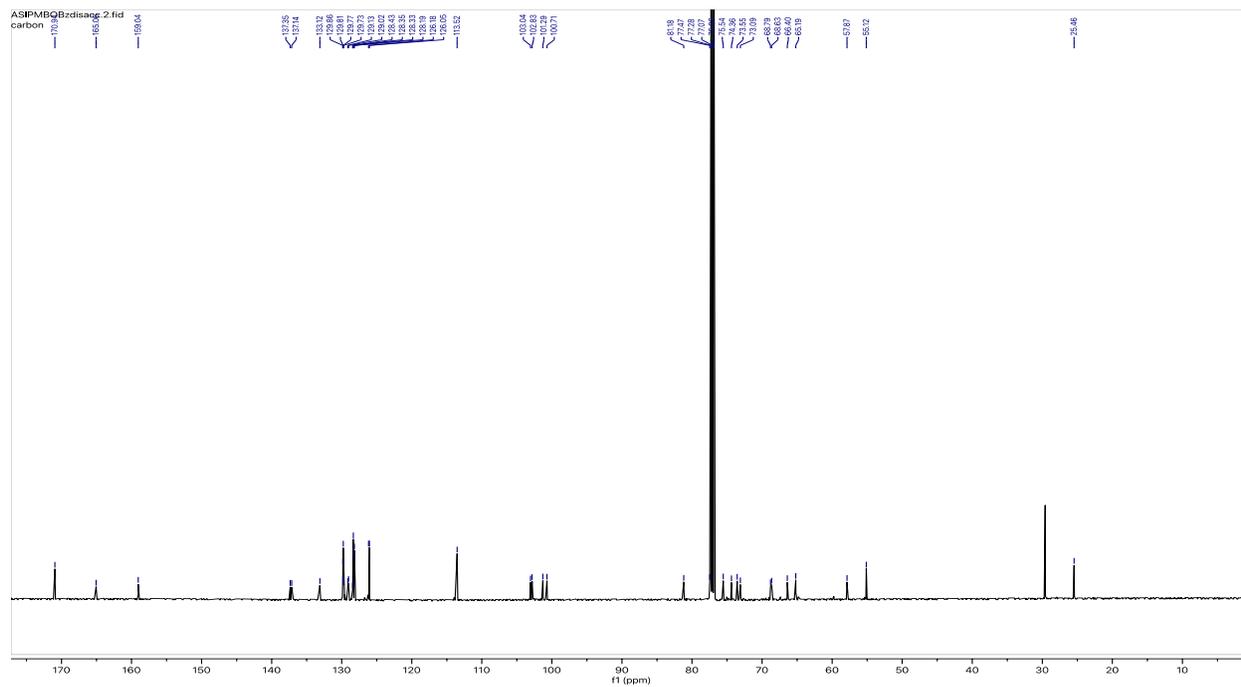
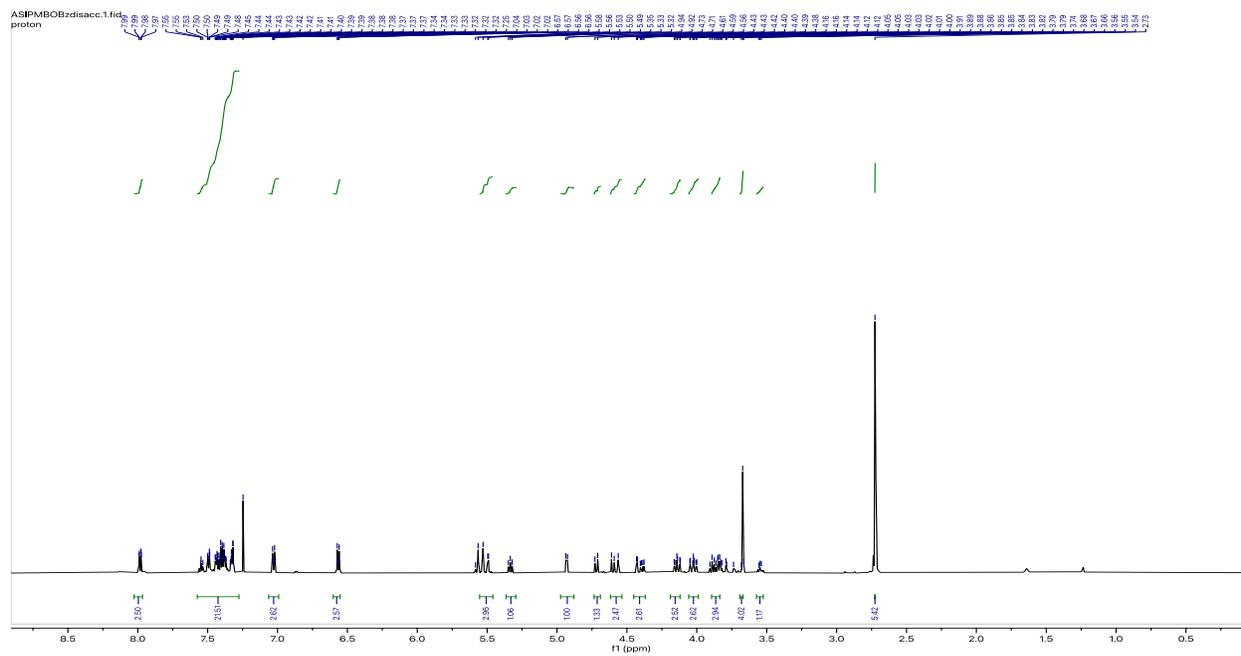
HRMS data of Succinimidyl [2-*O*-benzoyl-4,6-*O*-benzylidene-3-*O*-(*p*-methoxy)benzyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-azido-4,6-*O*-benzylidene-2-deoxy- α -D-galactopyranoside (**17**)

40009 AS31 #3-124 RT: 0.02-0.97 AV: 122 NL: 2.89E7
T: FTMS + c ESI Full ms [150.00-1500.00]



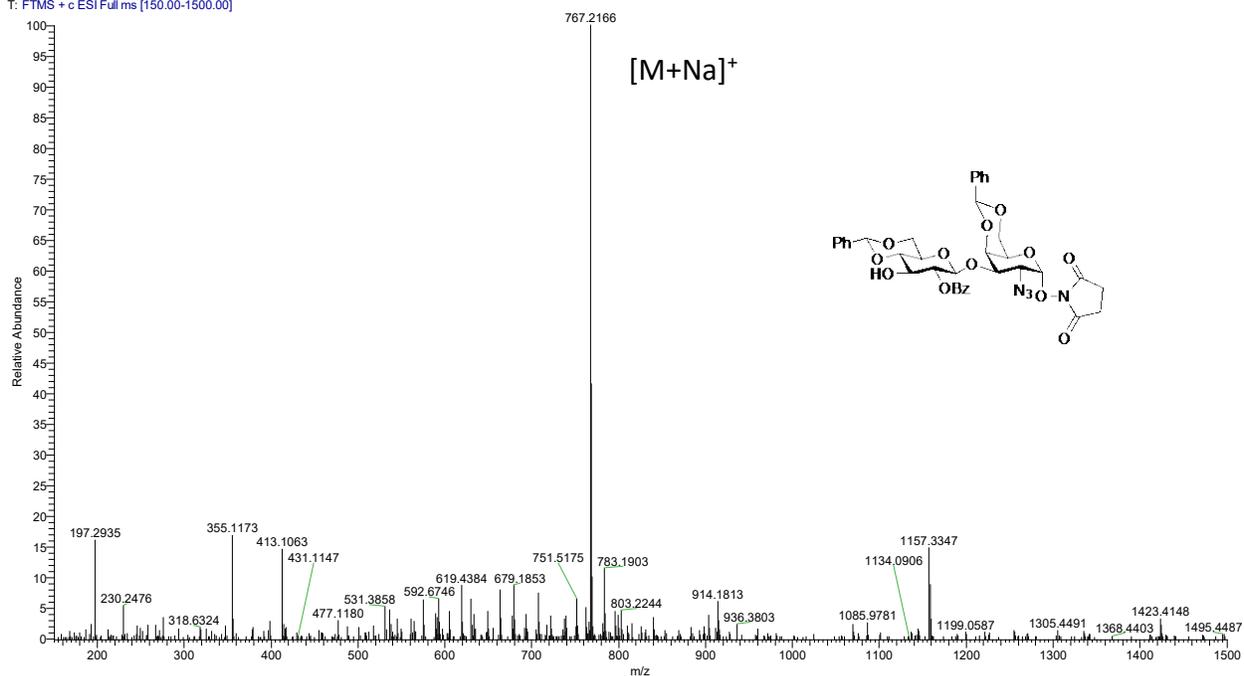
$$\text{Mass accuracy} = (887.2742 - 887.2746)/887.2746 * 10^6 = 0.5 \text{ ppm}$$

¹H and ¹³C NMR of Succinimidyl [2-*O*-benzoyl-4,6-*O*-benzylidene-3-*O*-(*p*-methoxy)benzyl-β-D-glucopyranosyl]-(1→3)-2-azido-4,6-*O*-benzylidene-2-deoxy-α-D-galactopyranoside (17)



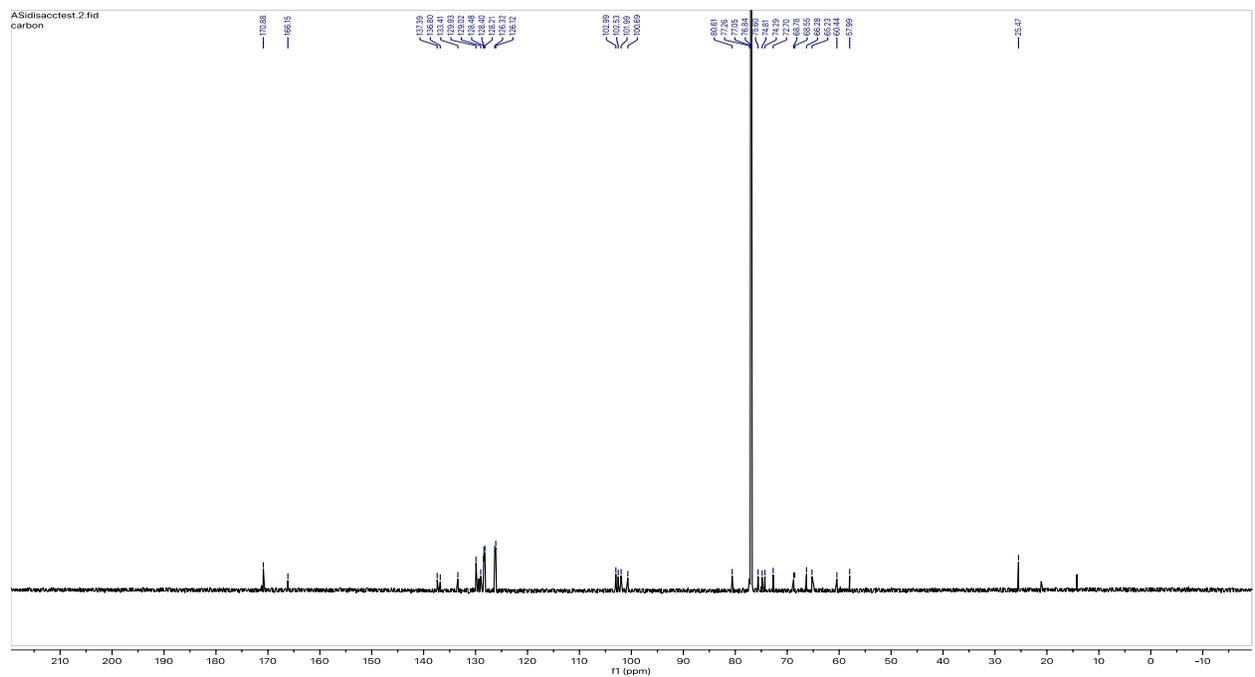
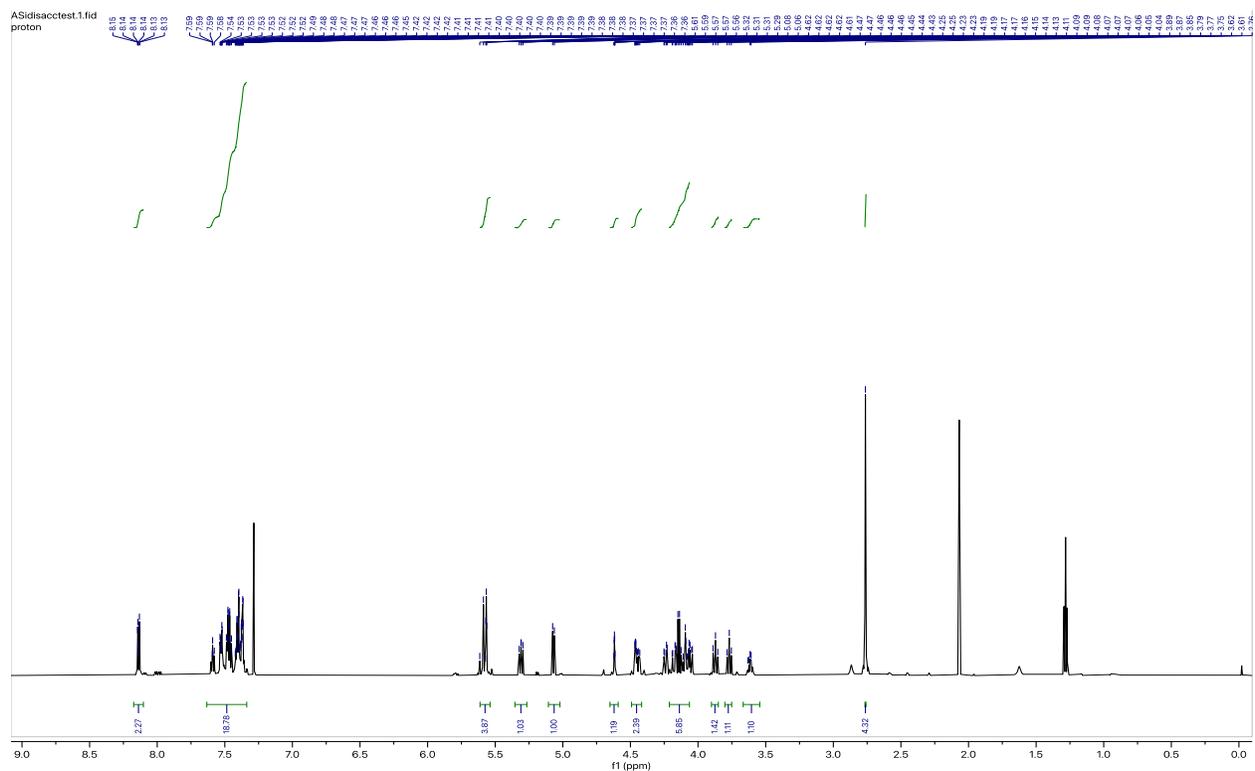
HRMS data of Succinimidyl [2-*O*-benzoyl-4,6-*O*-benzylidene-β-D-glucopyranosyl]-(1→3)-2-azido-4,6-*O*-benzylidene-2-deoxy-α-D-galactopyranoside (**18**)

40009 AS32 #1 RT: 0.01 AV: 1 NL: 2.20E7
T: FTMS + c ESI Full ms [150.00-1500.00]



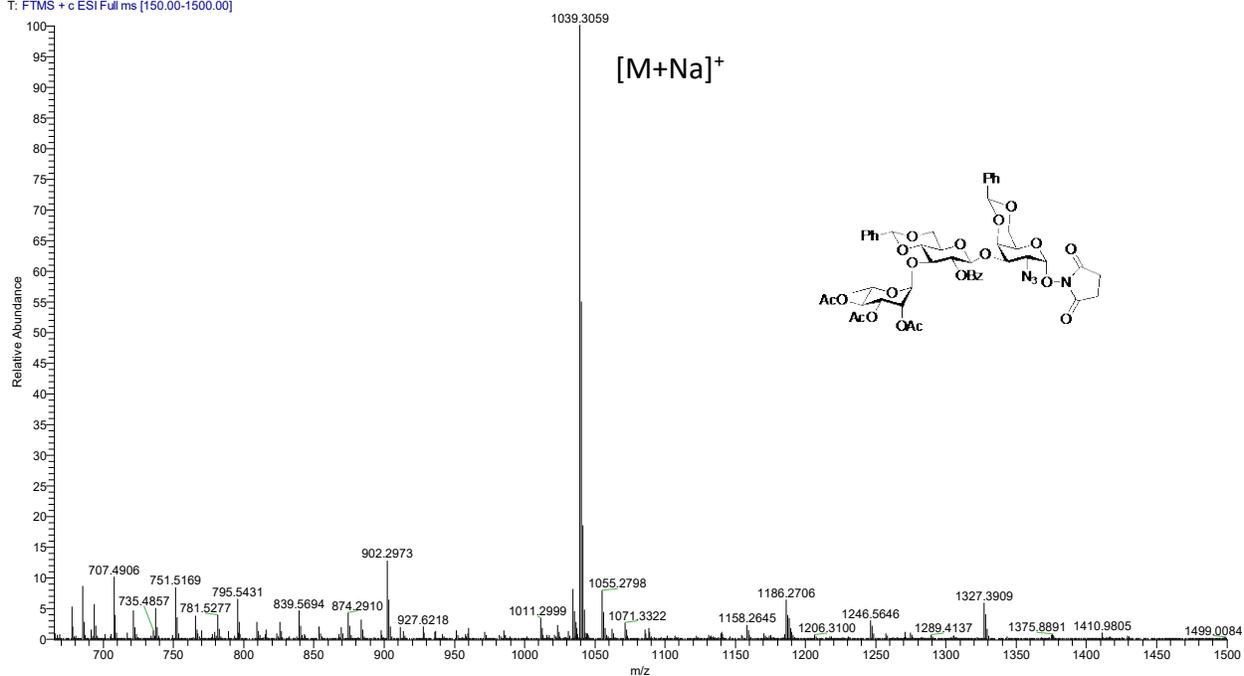
$$\text{Mass accuracy} = (767.2166 - 767.2171) / 767.2171 * 10^6 = 0.7 \text{ ppm}$$

¹H and ¹³C NMR of Succinimidyl [2-*O*-benzoyl-4,6-*O*-benzylidene-β-D-glucopyranosyl]-(1→3)-2-azido-4,6-*O*-benzylidene-2-deoxy-α-D-galactopyranoside (**18**)



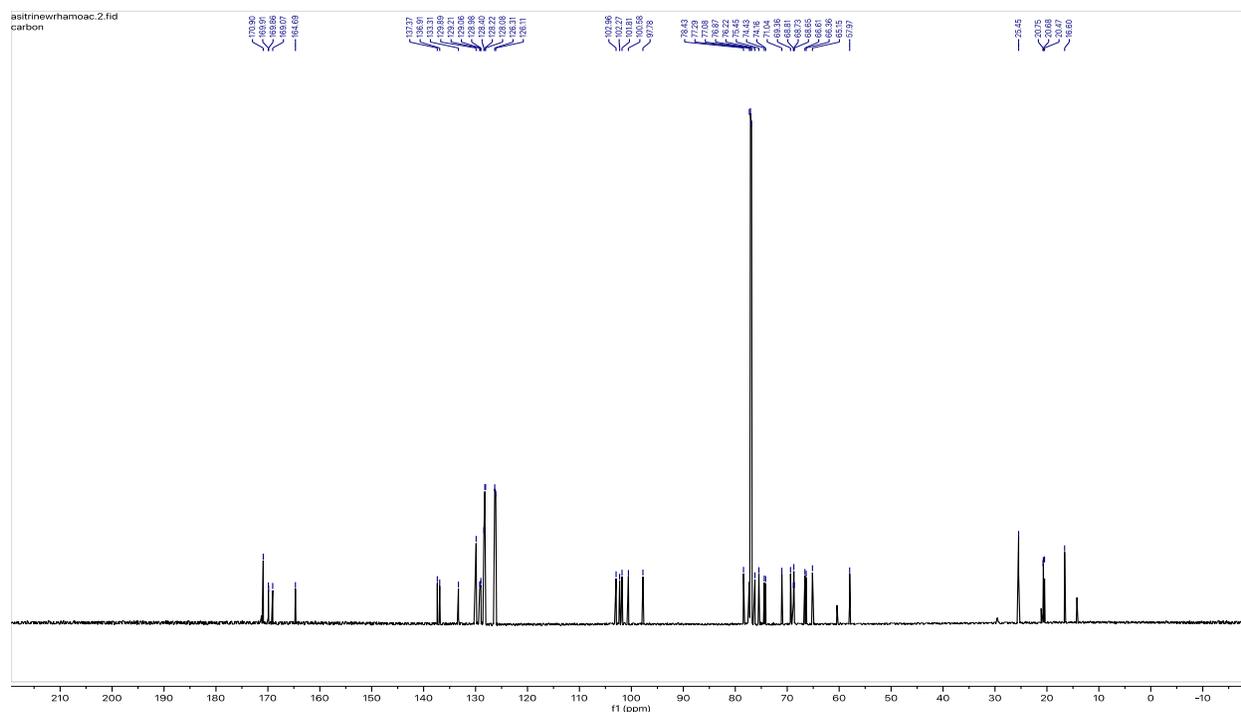
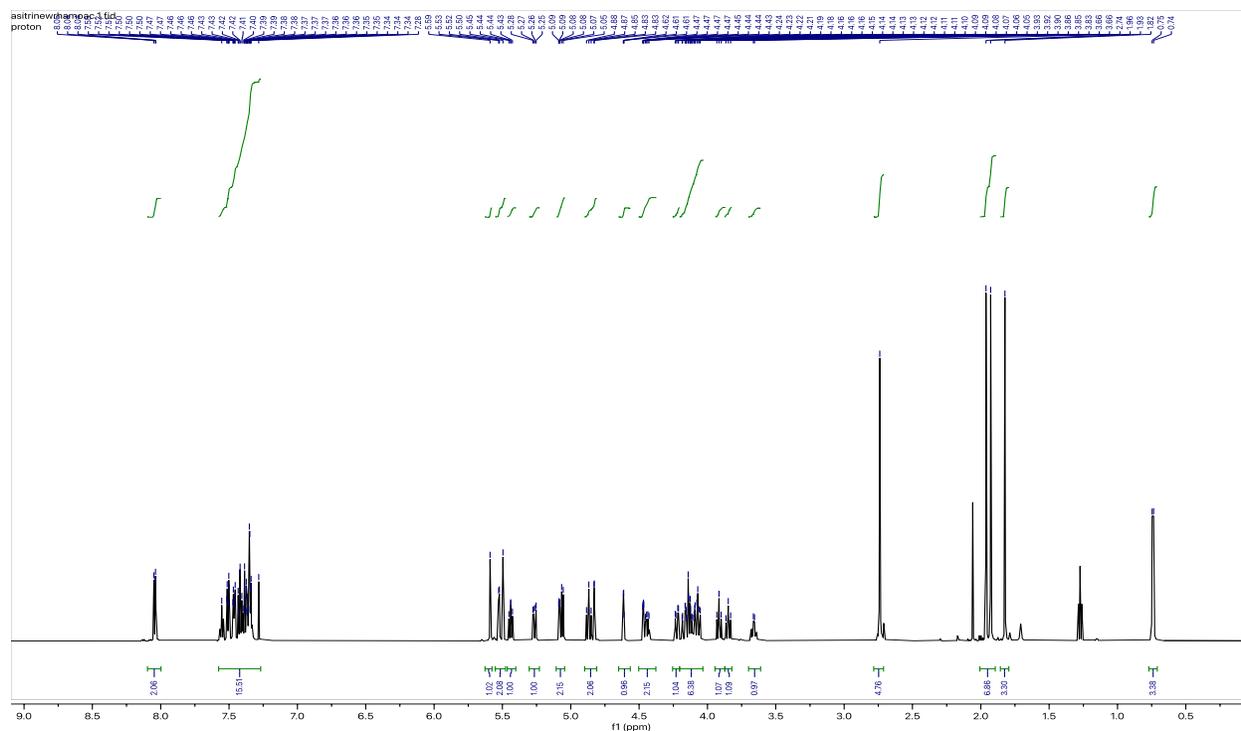
HRMS data of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[2-*O*-benzoyl-4,6-*O*-benzylidene- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-azido-4,6-*O*-benzylidene-2-deoxy- α -D-galactopyranoside (**19**)

40009 AS33 #1-97 RT: 0.00-0.77 AV: 97 NL: 1.92E7
T: FTMS + c ESI Full ms [150.00-1500.00]



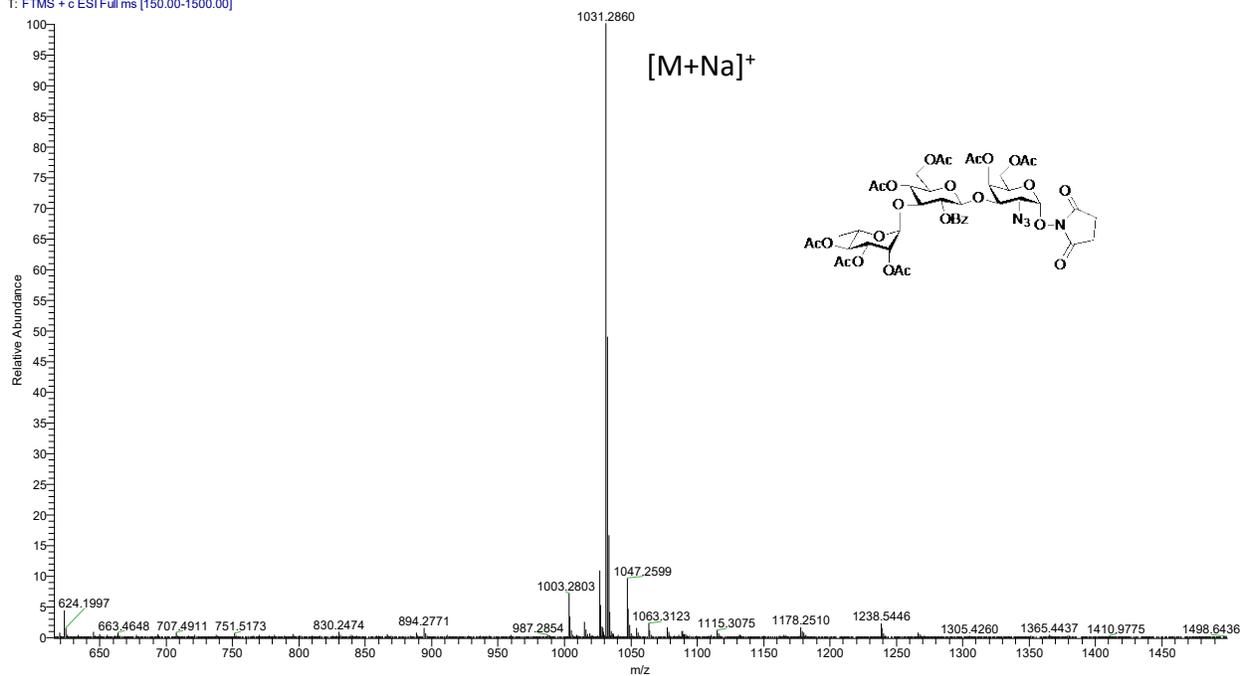
$$\text{Mass accuracy} = (1039.3059 - 1039.3067)/1039.3067 * 10^6 = 0.8 \text{ ppm}$$

¹H and ¹³C NMR of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[2-*O*-benzoyl-4,6-*O*-benzylidene- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-azido-4,6-*O*-benzylidene-2-deoxy- α -D-galactopyranoside (**19**)



HRMS data of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[4,6-*O*-acetyl-2-*O*-benzoyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-azido-4,6-*O*-acetyl-2-deoxy- α -D-galactopyranoside (20)

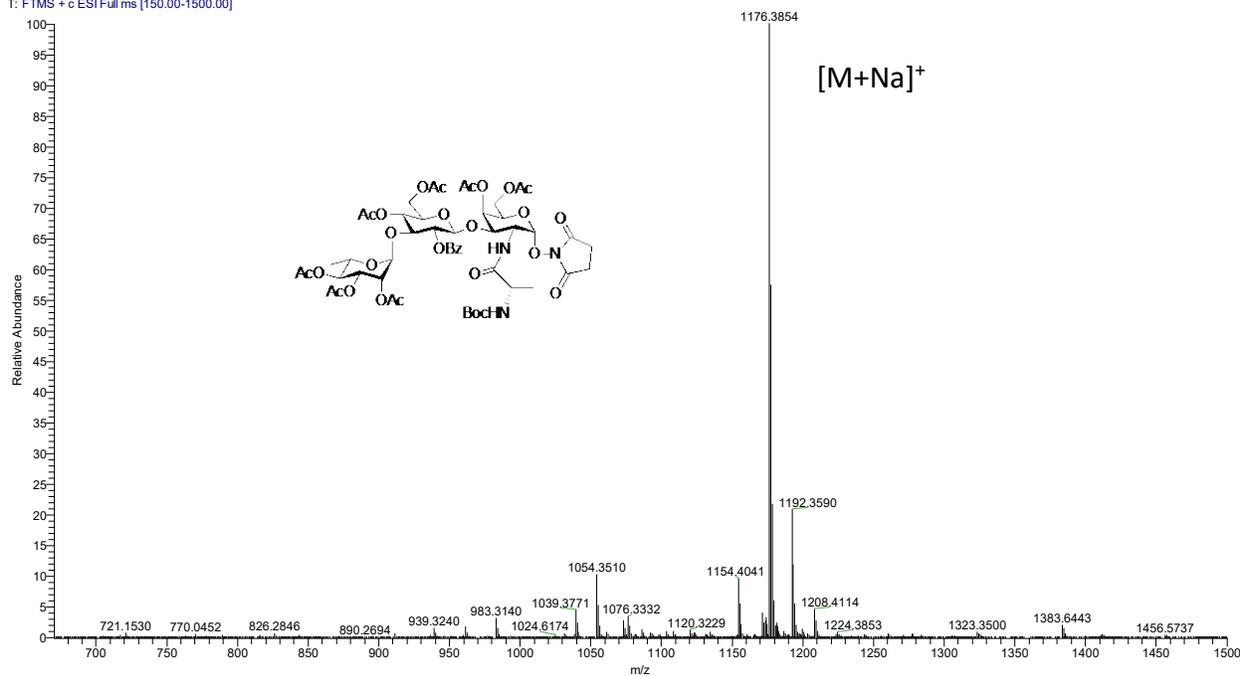
40009 AS34 #19-113 RT: 0.15-0.88 AV: 95 NL: 4.06E8
T: FTMS + c ESI Full ms [150.00-1500.00]



$$\text{Mass accuracy} = (1031.2860 - 1031.2864) / 1031.2864 * 10^6 = 0.4 \text{ ppm}$$

HRMS data of Succinimidyl [2,3,4-tri-*O*-acetyl- α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[4,6-*O*-acetyl-2-*O*-benzoyl- β -D-glucopyranosyl]-(1 \rightarrow 3)-2-*N*-tertbutyloxycarbonylalanine-4,6-*O*-acetyl-2-deoxy- α -D-galactopyranoside (**21**)

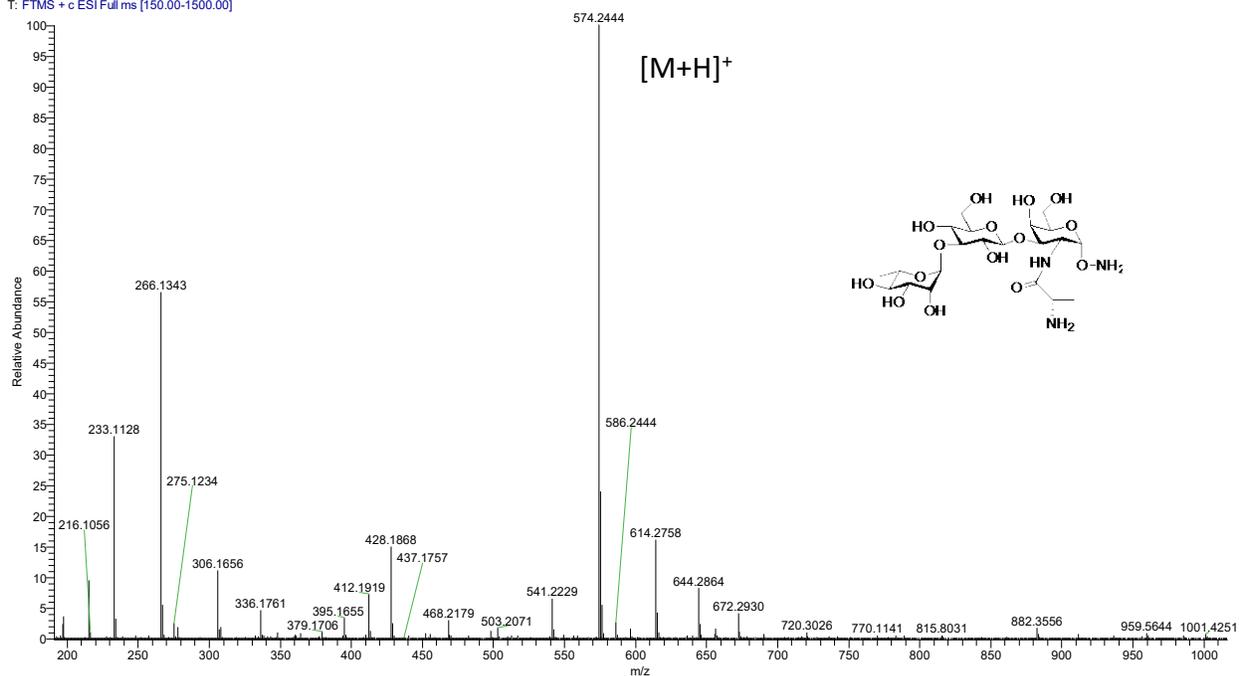
40009 AS35 #13-124 RT: 0.10-0.97 AV: 112 NL: 2.29E8
T: FTMS + c ESI Full ms [150.00-1500.00]



$$\text{Mass accuracy} = (1176.3854 - 1176.3854)/1176.3854 * 10^6 = 0.0 \text{ ppm}$$

HRMS data of Aminoxy [α -L-rhamnopyranosyl]-(1 \rightarrow 3)-[β -D-glucopyranosyl]-(1 \rightarrow 3)-2-N-alanine-2-deoxy- α -D-galactopyranoside (**4**)

40009 AS36 #3-128 RT: 0.02-0.99 AV: 126 NL: 3.31E8
T: FTMS + c ESI Full ms [150.00-1500.00]



$$\text{Mass accuracy} = (574.2444 - 574.2453) / 574.2453 * 10^6 = 1.6 \text{ ppm}$$

