

S2 Table. Weight (pq[1]) and its error (SE) of each *N*-glycan calculated using O-PLS

Var ID (Primary) ^{1, 2}	Var ID (Polarity)	Var ID (m/z)	pq[1]	SE	pq[1]/SE
dHex1 Hex5 HexNAc4	Positive	895.34	-0.2309	0.1004	2.2994
Hex5 HexNAc4 NeuNAc2(1)(N)	Negative	1111.39(1)	-0.2038	0.0893	2.2821
dHex1 Hex5 HexNAc4 NeuNAc2(N)	Negative	1184.43	-0.1908	0.1015	1.8791
dHex1 Hex5 HexNAc4 NeuNAc1(N)	Negative	1038.88	-0.1817	0.1001	1.8150
dHex1 Hex5 HexNAc4 NeuNAc1(P)	Positive	1040.89	-0.1765	0.0848	2.0820
Hex8 HexNAc2 (NH4)1	Positive	870.83	-0.1689	0.1412	1.1957
dHex1 Hex5 HexNAc5	Positive	996.88	-0.1398	0.1111	1.2589
Hex5 HexNAc4 NeuNAc1(N)	Negative	965.85	-0.1319	0.1412	0.9341
dHex2 Hex6 HexNAc5	Positive	1150.95	-0.1085	0.1422	0.7636
Hex5 HexNAc4 NeuNAc1(P)	Positive	967.86	-0.1078	0.1563	0.6894
dHex1 Hex5 HexNAc4 NeuNAc2(P)	Positive	1186.44	-0.1043	0.1444	0.7223
dHex1 Hex4 HexNAc4	Positive	814.32	-0.0843	0.0978	0.8619
Hex5 HexNAc4 NeuNAc2(2)(N)	Negative	1111.39(2)	-0.0733	0.1404	0.5222
Hex9 HexNAc2 (NH4)1	Positive	951.85	-0.0509	0.0922	0.5525
Hex5 HexNAc3 NeuNAc1	Positive	866.32	-0.0330	0.1343	0.2458
dHex1 Hex5 HexNAc5 NeuNAc1	Positive	1142.43	0.0087	0.1149	0.0761
Hex6 HexNAc5 NeuNAc3(2)(P)	Positive	961.35(2)	0.0300	0.1081	0.2772
Hex5 HexNAc2	Positive	1237.47	0.0324	0.1344	0.2410
Hex5 HexNAc4 NeuNAc2(2)(P)	Positive	1113.41(2)	0.0378	0.0867	0.4358
dHex1 Hex4 HexNAc5	Positive	915.86	0.0458	0.0969	0.4728
Hex6 HexNAc2	Positive	1399.53	0.0796	0.1267	0.6279
Hex6 HexNAc5 NeuNAc3 (2)(N)	Negative	1439.52(2)	0.0797	0.1084	0.7352
Hex5 HexNAc4 NeuNAc2(1)(P)	Positive	1113.41(1)	0.0848	0.1085	0.7818
Hex7 HexNAc6 NeuNAc4 (1)	Negative	1178.09(1)	0.0889	0.1232	0.7215
dHex1 Hex5 HexNAc5 NeuNAc2	Positive	1287.98	0.0991	0.1140	0.8695

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Hex4 HexNAc4 NeuNAc1	Positive	886.84	0.1007	0.1336	0.7534
Hex6 HexNAc5 NeuNAc1(1)	Positive	1150.44(1)	0.1026	0.0955	1.0747
dHex1 Hex3 HexNAc5	Positive	834.83	0.1104	0.1283	0.8610
Hex6 HexNAc5 NeuNAc2	Positive	1295.99	0.1177	0.0978	1.2032
Hex3 HexNAc5	Positive	761.8	0.1292	0.0898	1.4393
Hex6 HexNAc5 NeuNAc3(1)(P)	Positive	961.35(1)	0.1303	0.1192	1.0926
dHex2 Hex7 HexNAc6 NeuNAc4 (1)	Negative	1275.47(1)	0.1362	0.0915	1.4877
Hex5 HexNAc5 NeuNAc1	Positive	1069.4	0.1393	0.0668	2.0850
Hex4 HexNAc5	Positive	842.82	0.1466	0.0783	1.8736
dHex2 Hex6 HexNAc5 NeuNAc3	Negative	1585.58	0.1474	0.1331	1.1071
dHex2 Hex7 HexNAc6 NeuNAc4 (2)	Negative	1275.47(2)	0.1535	0.0818	1.8775
dHex1 Hex6 HexNAc5 NeuNAc3(1)(N)	Negative	1512.55(1)	0.1549	0.1151	1.3449
dHex1 Hex7 HexNAc6 NeuNAc4 (1)	Negative	1226.77(1)	0.1574	0.0789	1.9940
Hex7 HexNAc6 NeuNAc4 (2)	Negative	1178.09(2)	0.1608	0.0807	1.9926
dHex3 Hex7 HexNAc6 NeuNAc4	Negative	1324.14	0.1629	0.0960	1.6978
dHex1 Hex7 HexNAc6 NeuNAc4 (2)	Negative	1226.77(2)	0.1631	0.0718	2.2698
dHex1 Hex6 HexNAc5 NeuNAc3(2)(P)	Positive	1514.57(2)	0.1644	0.1104	1.4897
dHex1 Hex3 HexNAc4	Positive	1465.59	0.1674	0.1264	1.3240
dHex1 Hex7 HexNAc6 NeuNAc3	Negative	1695.12	0.1714	0.0712	2.4073
Hex6 HexNAc5 NeuNAc3 (1)(N)	Negative	1439.52(1)	0.1929	0.0592	3.2581
Hex4 HexNAc5 NeuNAc1	Positive	988.37	0.2006	0.0596	3.3625
dHex1 Hex4 HexNAc5 NeuNAc1	Positive	1061.41	0.2055	0.0683	3.0082
Hex6 HexNAc5 NeuNAc1(2)	Positive	1150.44(2)	0.2101	0.0368	5.7084
dHex1 Hex6 HexNAc5 NeuNAc3(2)(N)	Negative	1512.55(2)	0.2102	0.0921	2.2822
dHex1 Hex6 HexNAc5 NeuNAc3(1)(P)	Positive	1514.57(1)	0.2164	0.0570	3.7928

¹Numbers in parentheses represent isomers, and "N" or "P" in parentheses indicates data obtained from the negative or positive ion mode, respectively.

²Hex, hexose; HexNAc, *N*-acetylhexosamine; NeuNAc, *N*-acetylneuraminic acid; dHex, deoxyhexose; NH4, ammonium.