Supporting Information

Enhanced Carbohydrate Structural Selectivity in Ion Mobility-Mass Spectrometry Analyses by Boronic Acid Derivatization

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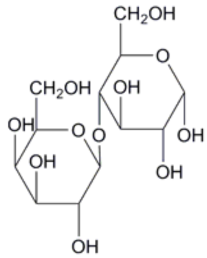
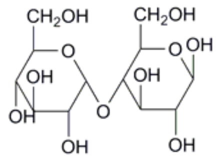
Abstract: Boronic acid derivatization of carbohydrates and glycans is demonstrated as an ion mobility shift strategy to improve confidence in the identification and characterization of carbohydrate assignments using ion mobility-mass spectrometry.

Table S1. Common names, systematic names, average molecular weights, and derivatized mass of the carbohydrates reported in this work.

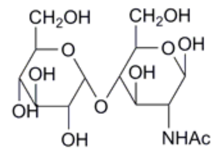
Common name or abbreviation	Systematic name	Molecular weight (M_r, Da)	$[M+Na]^+$ (Da)	$[M+FBA+Na]^+$ (Da)	$[M+PBA+Na]^+$ (Da)
Maltose	4-O-α-D-Glucose-D-glucose	342.3	365.3	559.1	641.5
Lactose	β-D-galactose-(1→4)-α-D-glucose	342.3	365.3	559.1	641.5
LN	β-D-Galactose-(1→4)-D-*N*-acetylglucosamine	383.4	383.4	600.2	682.5
Gala3-type1	Galactose-α-(1→3)-galactose-β-(1→3)-N-acetylglucosamine-β-azide	614.6	637.6	831.4	913.7
P1	Galactose-α-(1→4)-galactose-β-(1→4)-N-acetylglucosamine-β-azide	614.6	637.6	831.4	913.7
Lec-Lec	Galactose-β-(1→3)-N-acetylglucosamine-β-(1→3)-galactose-β-(1→3)-N-acetylglucosamine-β-azide	817.8	840.8	1034.6	1116.9
LNT	Galactose-β-(1→3)-N-acetylglucosamine-β-(1→3)-galactose-β(1→4)-N-acetylglucosamine-β-azide	817.8	840.8	1034.6	1116.9
LNFP1	α-L-fucose-(1→2)-β-D-galactose-(1→3)-β-D-N-acetylglucosamine-(1→3)-β-D-galactose-(1→4)-D-glucose	853.8	876.8	1070.6	1152.9
LNFP2	β-D-Galactose-(1→3)-(α-L-fucose-[1→4])-β-D- N-acetylglucosamine-(1→3)-β-D-galactose-(1→4)-D-glucose	853.8	876.8	1070.6	1152.9



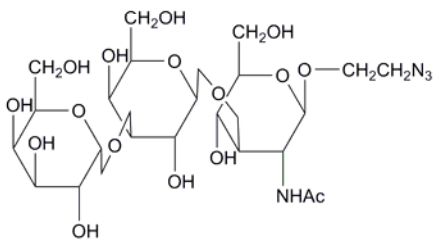
Lactose
MW= 342.30



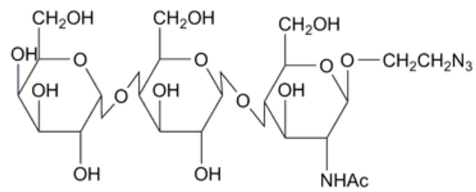
Maltose
MW= 342.30



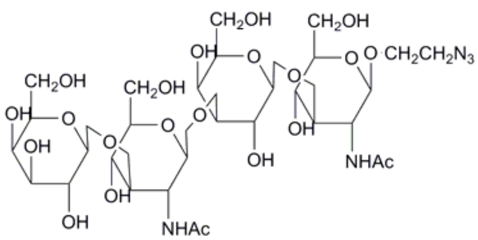
N-Acetyllactosamine
MW= 383.35



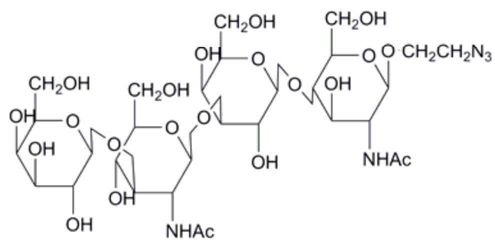
Gala3-type1
MW= 614.55



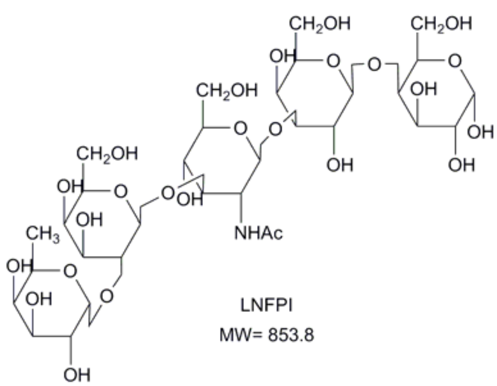
P1
MW= 614.55



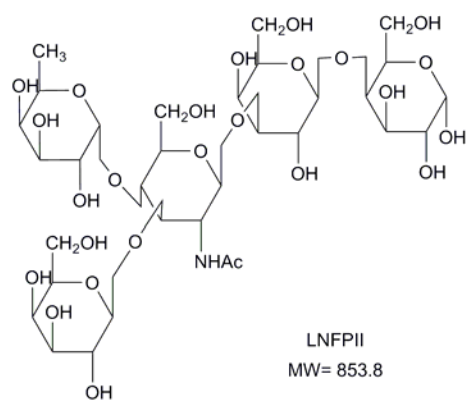
Lec-Lec
MW= 817.75



LNT
MW= 817.75



LNFPI
MW= 853.8



LNFPII
MW= 853.8

Figure S1 Structures of the underivatized carbohydrates studied.

Table S2 Collision cross sections determined for protonated and/or sodium coordinated carbohydrates prior to and following boronic acid derivatization.

	Collision cross section (Å^2)^a		
Carbohydrate	$[M+Na]^+$	$[M+FBA+Na]^+$	$[M+PBA+Na]^+$
Maltose	103.1 ± 4.1 (21)	140.3 ± 7.7 (5)	156.3 ± 5.7 (16)
Lactose	106.8 ± 5.1 (35)	151.5 ± 8.4 (16)	163.7 ± 3.4 (30)
LN	117.4 ± 1.8 (23)	156.7 ± 3.4 (15)	195.0 ± 1.5 (30)
Gala3-type1	160.2 ± 2.1 (26)	197.9 ± 4.4 (31)	229.8 ± 7.3 (18)
P1	166.9 ± 1.2 (70)	200.5 ± 2.8 (39)	255.4 ± 2.3 (40)
Lec-Lec	183.2 ± 1.6 (51)	220.0 ± 2.6 (15)	252.2 ± 2.1 (21)
LNT	195.9 ± 1.4 (42)	217.9 ± 2.8 (19)	254.8 ± 8.3 (19)
LNFP1	204.3 ± 1.4 (147)	222.5 ± 3.4 (9)	230.2 ± 6.1 (26)
LNFP2	201.4 ± 1.0 (166)	226.1 ± 2.3 (11)	233.7 ± 3.1 (21)

a. Error represents ± 1σ for *n* measurements indicated in parenthesis. The protonated form of PBA derivatized carbohydrates is not included as the relative abundance for [M+PBA+H]+ species was <2% of the base peak ($[M+PBA+Na]^+$) in the spectra.