

*Analytical and Bioanalytical Chemistry*

**Electronic Supplementary Information**

**Characterizing Ion Mobility-Mass Spectrometry Conformation Space for the Analysis of Complex Biological Samples**

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**Table S1.** Biomolecular class species and collision cross sections reported in this work.

Biomolecular Class	Name (parent name if fragmented)	species	m/z (Da)	$\Omega$ ( $\text{\AA}^2$ )	$\sigma$ (# of measurements)
<b>Oligonucleotides<sup>1</sup></b>					
oligonucleotide	d2-G-H <sub>2</sub> O (GACT)	[M+H] <sup>+</sup>	492.1	129.2	0.3(6)
oligonucleotide	w2-G-H <sub>2</sub> O (TCAG)	[M+H] <sup>+</sup>	492.1	137.7	0.5(6)
oligonucleotide	w2-C-H <sub>2</sub> O (TGAC)	[M+H] <sup>+</sup>	492.6	135.5	0.4(6)
oligonucleotide	d2-C-H <sub>2</sub> O or x2-T-H <sub>2</sub> O (CAGT)	[M+H] <sup>+</sup>	492.9	125.7	0.5(6)
oligonucleotide	a2 (TCGA)	[M+H] <sup>+</sup>	514.1	134.3	0.5(6)
oligonucleotide	a2 (TCAG)	[M+H] <sup>+</sup>	514.1	138.2	0.3(6)
oligonucleotide	a2 (TCG)	[M+H] <sup>+</sup>	514.1	150.9	0.4(6)
oligonucleotide	a2-T (ACTG)	[M+H] <sup>+</sup>	524.1	137.9	0.5(6)
oligonucleotide	z2 or a2 (GCAT)	[M+H] <sup>+</sup>	539.1	141.6	0.4(6)
oligonucleotide	w2 (GCT)	[M+H] <sup>+</sup>	610.1	154.9	0.6(6)
oligonucleotide	w2 (GTC)	[M+H] <sup>+</sup>	612.1	145.5	0.4(6)
oligonucleotide	c2 (GCT)	[M+H] <sup>+</sup>	618.1	163.1	0.5(6)
oligonucleotide	w2 (TGAC)	[M+H] <sup>+</sup>	621.1	153.2	0.6(6)
oligonucleotide	w2 (TGCA)	[M+H] <sup>+</sup>	621.1	156.7	0.3(6)
oligonucleotide	w2 (CGTA)	[M+H] <sup>+</sup>	636.1	163.5	0.1(6)
oligonucleotide	w2 (GCTA)	[M+H] <sup>+</sup>	636.1	165.1	0.4(6)
oligonucleotide	w2 (CGAT)	[M+H] <sup>+</sup>	636.1	152	0.4(6)
oligonucleotide	w2 (GCAT)	[M+H] <sup>+</sup>	636.1	153.7	0.2(6)
oligonucleotide	w2 (ACTG)	[M+H] <sup>+</sup>	652.1	142.1	0.7(6)
oligonucleotide	w2 (CTG)	[M+H] <sup>+</sup>	652.1	161.9	0.2(6)
oligonucleotide	w2 (TCAG)	[M+H] <sup>+</sup>	661.1	158.4	0.2(6)
oligonucleotide	TGC-G (TGC)	[M+H] <sup>+</sup>	710.2	171	1.3(6)
oligonucleotide	GTC-G (GTC)	[M+H] <sup>+</sup>	710.2	172.5	0.2(6)
oligonucleotide	GCT-G (GCT)	[M+H] <sup>+</sup>	710.2	176	0.9(6)
oligonucleotide	a3-G (ATGC)	[M+H] <sup>+</sup>	716.2	171.7	0.3(6)
oligonucleotide	a3-C (TACG)	[M+H] <sup>+</sup>	716.2	170.5	0.4(6)
oligonucleotide	a3-G (TAGC)	[M+H] <sup>+</sup>	716.2	173.7	0.3(6)

oligonucleotide	a3-C (ATCG)	[M+H] <sup>+</sup>	716.2	172.2	0.1(6)
oligonucleotide	CGT-C (CGT)	[M+H] <sup>+</sup>	750.2	170.9	0.3(6)
oligonucleotide	TCG-C (TCG)	[M+H] <sup>+</sup>	750.2	182.9	1.0(6)
oligonucleotide	CTG-C (CTG)	[M+H] <sup>+</sup>	750.2	176.3	1.3(6)
oligonucleotide	x3-G or w3-G-H <sub>2</sub> O (CATG)	[M+H] <sup>+</sup>	796.1	179.8	0.4(6)
oligonucleotide	x3-G or w3-G-H <sub>2</sub> O (CTAG)	[M+H] <sup>+</sup>	796.1	181.6	0.8(6)
oligonucleotide	c3-G or x3-C (GATC)	[M+H] <sup>+</sup>	796.1	181.8	0.3(6)
oligonucleotide	c3-G (GTAC)	[M+H] <sup>+</sup>	796.1	179.2	0.3(6)
oligonucleotide	w3-C (GACT)	[M+H] <sup>+</sup>	814.1	156.1	0.4(6)
oligonucleotide	w3-G or d3-C (CATG)	[M+H] <sup>+</sup>	814.1	179.5	0.7(6)
oligonucleotide	w3-G or d3-C (CTAG)	[M+H] <sup>+</sup>	814.1	186.4	1.3(6)
oligonucleotide	d3-G or w3-C (GATC)	[M+H] <sup>+</sup>	814.1	182	0.3(6)
oligonucleotide	d3-G or w3-C (GTAC)	[M+H] <sup>+</sup>	814.1	183.1	0.3(6)
oligonucleotide	w3-G (CTGA)	[M+H] <sup>+</sup>	814.1	170.4	0.8(6)
oligonucleotide	w3-C (GCAT)	[M+H] <sup>+</sup>	814.1	180.3	0.4(6)
oligonucleotide	w3-C (GTCA)	[M+H] <sup>+</sup>	814.1	172.1	0.8(6)
oligonucleotide	w3-G (CAGT)	[M+H] <sup>+</sup>	814.3	172	0.7(6)
oligonucleotide	CGT	[M+H] <sup>+</sup>	861.2	187.6	0.6(6)
oligonucleotide	TCG	[M+H] <sup>+</sup>	861.2	186.1	0.4(6)
oligonucleotide	TGC	[M+H] <sup>+</sup>	861.2	190.2	0.3(6)
oligonucleotide	GTC	[M+H] <sup>+</sup>	861.2	187.2	0.1(6)
oligonucleotide	GCT	[M+H] <sup>+</sup>	861.2	198.3	0.1(6)
oligonucleotide	CTG	[M+H] <sup>+</sup>	861.2	190.5	0.2(6)
oligonucleotide	w3 (GCTA)	[M+H] <sup>+</sup>	925.2	187.8	0.1(6)
oligonucleotide	w3 (GACT)	[M+H] <sup>+</sup>	925.2	191.4	0.3(6)
oligonucleotide	w3 (GATC)	[M+H] <sup>+</sup>	925.2	193.8	0.2(6)
oligonucleotide	w3 (GTAC)	[M+H] <sup>+</sup>	925.2	197.3	0.1(6)
oligonucleotide	w3 (GCAT)	[M+H] <sup>+</sup>	925.2	200.6	0.5(6)
oligonucleotide	w3 (GTCA)	[M+H] <sup>+</sup>	925.2	202.3	0.2(6)
oligonucleotide	w3 (CAGT)	[M+H] <sup>+</sup>	965.2	197.9	0.5(6)
oligonucleotide	w3 (CGTA)	[M+H] <sup>+</sup>	965.2	193	0.6(6)
oligonucleotide	W3 (ACTG)	[M+H] <sup>+</sup>	965.2	199.1	0.3(6)

oligonucleotide	w3 (CTAG)	[M+H] <sup>+</sup>	965.2	191.2	0.5(6)
oligonucleotide	w3 (CGAT)	[M+H] <sup>+</sup>	965.2	200.5	0.3(6)
oligonucleotide	w3 (CTGA)	[M+H] <sup>+</sup>	965.2	202.6	0.3(6)
oligonucleotide	GACT-G (GACT)	[M+H] <sup>+</sup>	1023.2	211.9	0.4(6)
oligonucleotide	GCTA-G (GCTA)	[M+H] <sup>+</sup>	1023.2	209.2	0.8(6)
oligonucleotide	GATC-G (GATC)	[M+H] <sup>+</sup>	1023.2	212.5	0.4(6)
oligonucleotide	GTAC-G (GTAC)	[M+H] <sup>+</sup>	1023.2	211.4	0.5(6)
oligonucleotide	GCAT-G (GCAT)	[M+H] <sup>+</sup>	1023.2	215	0.6(6)
oligonucleotide	GTCA-G (GTCA)	[M+H] <sup>+</sup>	1023.2	216.3	0.7(6)
oligonucleotide	ATGC-C (ATGC)	[M+H] <sup>+</sup>	1063.2	213.2	0.6(6)
oligonucleotide	CAGT-C (CAGT)	[M+H] <sup>+</sup>	1063.2	214.4	0.8(6)
oligonucleotide	CGTA-C (CGTA)	[M+H] <sup>+</sup>	1063.2	215.7	0.8(6)
oligonucleotide	CGAT-C (CGAT)	[M+H] <sup>+</sup>	1063.2	216.3	0.7(6)
oligonucleotide	CGTA	[M+H] <sup>+</sup>	1174.2	234	0.5(6)
oligonucleotide	ACGT	[M+H] <sup>+</sup>	1174.3	219.3	0.3(6)
oligonucleotide	AGTC	[M+H] <sup>+</sup>	1174.3	214.3	0.4(6)
oligonucleotide	ATGC	[M+H] <sup>+</sup>	1174.3	232.3	0.3(6)
oligonucleotide	CAGT	[M+H] <sup>+</sup>	1174.3	220.7	0.5(6)
oligonucleotide	GCTA	[M+H] <sup>+</sup>	1174.3	223.1	0.7(6)
oligonucleotide	TACG	[M+H] <sup>+</sup>	1174.3	231.9	0.5(6)
oligonucleotide	GACT	[M+H] <sup>+</sup>	1174.3	228.6	0.2(6)
oligonucleotide	GCTA	[M+H] <sup>+</sup>	1174.3	223.3	0.6(6)
oligonucleotide	TCGA	[M+H] <sup>+</sup>	1174.3	217.2	0.5(6)
oligonucleotide	ACTG	[M+H] <sup>+</sup>	1174.3	227.4	0.4(6)
oligonucleotide	CATG	[M+H] <sup>+</sup>	1174.3	216.7	0.4(6)
oligonucleotide	CTAG	[M+H] <sup>+</sup>	1174.3	231.6	0.3(6)
oligonucleotide	GATC	[M+H] <sup>+</sup>	1174.3	210.7	0.4(6)
oligonucleotide	GTAC	[M+H] <sup>+</sup>	1174.3	224.1	0.3(6)
oligonucleotide	TAGC	[M+H] <sup>+</sup>	1174.3	220.3	0.4(6)
oligonucleotide	TGAC	[M+H] <sup>+</sup>	1174.3	224.3	0.4(6)
oligonucleotide	AGCT	[M+H] <sup>+</sup>	1174.3	232.4	0.5(6)
oligonucleotide	ATCG	[M+H] <sup>+</sup>	1174.3	226.2	0.6(6)
oligonucleotide	CGAT	[M+H] <sup>+</sup>	1174.3	215.4	0.4(6)

oligonucleotide	CTGA	[M+H] <sup>+</sup>	1174.3	231.4	0.4(6)
oligonucleotide	GCAT	[M+H] <sup>+</sup>	1174.3	229.1	0.5(6)
oligonucleotide	TCAG	[M+H] <sup>+</sup>	1174.3	233	0.1(6)
oligonucleotide	TGCA	[M+H] <sup>+</sup>	1174.3	230	0.3(6)
<b>Carbohydrates<sup>2</sup></b>					
carbohydrate	B <sub>2</sub> (LNFP1)	[M+Na] <sup>+</sup>	331.0	118.6	0.5(7)
carbohydrate	Y <sub>2</sub> (LNFP2)	[M+Na] <sup>+</sup>	365.1	113.5	1.3(8)
carbohydrate	Y <sub>2</sub> (LNFP1)	[M+Na] <sup>+</sup>	365.1	112.8	1.3(12)
carbohydrate	B <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	388.0	114.1	1.1(5)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	391.1	110.9	0.5(5)
carbohydrate	C <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	406.1	118.3	2.1(9)
carbohydrate	C <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	406.1	126.1	6.1(5)
carbohydrate	C <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	406.1	115.3	0.1(5)
carbohydrate	C <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	406.1	119.4	1.5(5)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (P1 antigen)	[M+Na] <sup>+</sup>	407.0	119.0	3.7(5)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	407.3	118.5	0.6(8)
carbohydrate	Y <sub>3</sub> &C <sub>3</sub> (LNFP1)	[M+Na] <sup>+</sup>	409.4	125.6	1.4(9)
carbohydrate	Y <sub>3β</sub> &C <sub>2</sub> (LNFP2)	[M+Na] <sup>+</sup>	409.4	139.5	2.4(9)
carbohydrate	Y <sub>2</sub> (P1 antigen)	[M+Na] <sup>+</sup>	434.0	131.0	1.4(5)
carbohydrate	<sup>0,3</sup> A <sub>3</sub> (P1)	[M+Na] <sup>+</sup>	437.0	135.3	0.9(5)
carbohydrate	Y <sub>2</sub> -N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	438.5	135.4	1.2(5)
carbohydrate	Z <sub>1α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	441.4	138.8	0.9(9)
carbohydrate	Y <sub>2</sub> -N <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	447.4	134.5	2.1(12)
carbohydrate	Y <sub>2</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	447.4	131.2	1.4(5)
carbohydrate	Y <sub>2</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	447.4	134.1	0.3(8)
carbohydrate	Y <sub>2</sub> -N <sub>2</sub> (P1)	[M+Na] <sup>+</sup>	447.4	131.0	0.8(8)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (LNT)	[M+Na] <sup>+</sup>	448.4	124.0	0.9(14)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	448.4	115.1	0.5(8)
carbohydrate	<sup>1,3</sup> A <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	448.4	128.0	2.0(5)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (P1 penta)	[M+Na] <sup>+</sup>	448.4	135.1	1.3(5)

carbohydrate	<sup>0,2</sup> A <sub>2α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	451.0	132.2	3.1(5)
carbohydrate	<sup>0,2</sup> A <sub>3</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	451.0	131.1	0.6(5)
carbohydrate	Z <sub>2</sub> (P1)	[M+Na] <sup>+</sup>	457.0	137.6	2.1(5)
carbohydrate	Z <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	457.0	122.3	1.0(7)
carbohydrate	Z <sub>2</sub> (P1)	[M+Na] <sup>+</sup>	457.0	106.7	0.5(5)
carbohydrate	Z <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	457.0	107.7	1.3(5)
carbohydrate	Y <sub>1α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	459.4	110.7	0.8(5)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (P1 antigen)	[M+Na] <sup>+</sup>	462.0	131.2	0.8(5)
carbohydrate	<sup>0,2</sup> A <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	467.4	132.5	0.6(5)
carbohydrate	Y <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	475.4	102.5	0.5(5)
carbohydrate	Y <sub>2</sub> (P1)	[M+Na] <sup>+</sup>	475.4	136.9	0.8(5)
carbohydrate	Y <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	475.4	138.0	1.3(5)
carbohydrate	Y <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	475.4	133.8	0.6(7)
carbohydrate	Y <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	475.4	135.3	3.5(7)
carbohydrate	<sup>1,5</sup> X <sub>1α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	487.4	132.0	2.5(8)
carbohydrate	<sup>0,2</sup> X <sub>2</sub> -N <sub>2</sub> (P1 antigen)	[M+Na] <sup>+</sup>	489.0	151.9	3.1(5)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	503.4	144.8	3.5(8)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	503.4	152.3	3.8(5)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	503.4	127.0	18.6(5)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	503.4	108.1	0.7(5)
carbohydrate	<sup>1,5</sup> X <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	503.4	137.9	2.6(5)
carbohydrate	<sup>1,5</sup> A <sub>3</sub> (P1)	[M+Na] <sup>+</sup>	522.5	135.9	0.1(5)
carbohydrate	<sup>1,5</sup> A <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	522.5	135.2	1.3(5)
carbohydrate	<sup>0,2</sup> X <sub>2</sub> -N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	531.0	122.1	1.5(5)
carbohydrate	B <sub>3</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	534.5	142.9	0.3(5)
carbohydrate	B <sub>2</sub> (LNFP2)	[M+Na] <sup>+</sup>	534.5	152.2	0.6(5)
carbohydrate	B <sub>3</sub> (LNFP1)	[M+Na] <sup>+</sup>	534.5	151.5	0.7(9)
carbohydrate	B <sub>2α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	534.5	145.8	2(8)
carbohydrate	<sup>3,5</sup> X <sub>1</sub> -N <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	535.0	145.5	1.8(5)
carbohydrate	<sup>0,3</sup> X <sub>0</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	547.5	153.5	3.9(6)

carbohydrate	Z <sub>3β</sub> &C <sub>3</sub> (LNFP2)	[M+Na] <sup>+</sup>	547.6	165.6	4.1(5)
carbohydrate	B <sub>3</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	550.0	148.0	2.3(16)
carbohydrate	B <sub>3</sub> (LNT)	[M+Na] <sup>+</sup>	550.0	145.5	0.4(5)
carbohydrate	B <sub>3</sub> (P1 penta)	[M+Na] <sup>+</sup>	550.0	150.6	0.3(13)
carbohydrate	B <sub>3</sub> (P1 antigen)	[M+Na] <sup>+</sup>	550.0	145.2	4.0(10)
carbohydrate	B <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	552.5	142.7	0.6(5)
carbohydrate	C <sub>2α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	552.5	149.4	1.3(9)
carbohydrate	C <sub>2</sub> (LNFP2)	[M+Na] <sup>+</sup>	552.5	151.3	0.9(5)
carbohydrate	C <sub>3</sub> (LNFP1)	[M+Na] <sup>+</sup>	552.5	134.1	1.6(9)
carbohydrate	B <sub>3</sub> (P1)	[M+Na] <sup>+</sup>	552.5	109.0	1.0(5)
carbohydrate	C <sub>3</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	552.5	148.3	2.2(5)
carbohydrate	<sup>3,5</sup> X <sub>1</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	563.0	126.8	0.7(5)
carbohydrate	C <sub>3</sub> (LNT)	[M+Na] <sup>+</sup>	568.5	150.7	1.9(5)
carbohydrate	C <sub>3</sub> (P1 antigen)	[M+Na] <sup>+</sup>	568.5	148.6	1.2(6)
carbohydrate	C <sub>3</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	568.5	152.9	2.9(15)
carbohydrate	Y <sub>3</sub> (LNFP1)	[M+Na] <sup>+</sup>	568.5	157.4	0.4(5)
carbohydrate	C <sub>3</sub> (P1 penta)	[M+Na] <sup>+</sup>	568.5	153.4	0.8(5)
carbohydrate	C <sub>3</sub> (P1)	[M+Na] <sup>+</sup>	568.5	154.3	0.8(5)
carbohydrate	C <sub>3</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	568.5	153.5	3.2(7)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> (P1 antigen)	[M+Na] <sup>+</sup>	577.5	165.3	1.0(5)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	577.5	160.5	0.8(11)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	577.5	163.0	15.3(5)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> -N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	591.0	153.7	1.8(7)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> -N <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	591.0	158.1	1.5(5)
carbohydrate	B <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	591.5	155.8	0.4(10)
carbohydrate	Z <sub>3</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	591.5	146.3	0.5(5)
carbohydrate	<sup>2,4</sup> A <sub>3α</sub> (Di-LeA)	[M+Na] <sup>+</sup>	594.5	159.8	2.2(15)
carbohydrate	<sup>2,4</sup> A <sub>3</sub> (LNFP2)	[M+Na] <sup>+</sup>	594.5	173.6	1.0(5)
carbohydrate	Y <sub>3</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	609.0	160.1	1.7(10)
carbohydrate	M-N <sub>2</sub> (Galα3-type1)	[M+Na] <sup>+</sup>	609.6	135.4	1.4(7)

carbohydrate	M-N <sub>2</sub> (P1)	[M+Na] <sup>+</sup>	609.6	155.2	0.9(8)
carbohydrate	C <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	610.5	161.7	0.3(5)
carbohydrate	<sup>2,4</sup> A <sub>4</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	610.5	162.2	0.5(5)
carbohydrate	<sup>2,4</sup> A <sub>4</sub> (LNT)	[M+Na] <sup>+</sup>	610.5	163.4	1.3(7)
carbohydrate	<sup>2,4</sup> A <sub>4</sub> (P1 antigen)	[M+Na] <sup>+</sup>	610.5	156.7	0.3(5)
carbohydrate	<sup>2,4</sup> X <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	619.0	169.9	2.3(5)
carbohydrate	<sup>3,5</sup> A <sub>4</sub> (LNT)	[M+Na] <sup>+</sup>	624.0	123.6	0.8(5)
carbohydrate	Z <sub>3</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	633.1	170.1	2.1(5)
carbohydrate	Z <sub>3</sub> -N <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	633.1	166.2	1.3(5)
carbohydrate	Z <sub>3</sub> -N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	633.1	131.9	2.1(5)
carbohydrate	Galα3-type1	[M+Na] <sup>+</sup>	637.6	160.2	1.4(45)
carbohydrate	P1	[M+Na] <sup>+</sup>	637.6	166.9	1.2(70)
carbohydrate	Y <sub>3</sub> (P1 penta)	[M+Na] <sup>+</sup>	637.6	170.1	1.4(8)
carbohydrate	Y <sub>3</sub> (P1 antigen)	[M+Na] <sup>+</sup>	637.6	168.2	0.6(5)
carbohydrate	Y <sub>3</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	651.0	173.0	1.8(9)
carbohydrate	Y <sub>3</sub> -N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	651.0	176.2	0.6(5)
carbohydrate	Y <sub>3</sub> -N <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	651.0	171.1	2.0(18)
carbohydrate	Z <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	661.0	108.8	0.4(5)
carbohydrate	<sup>0,2</sup> A <sub>4</sub> (LNT)	[M+Na] <sup>+</sup>	670.9	170.1	1.6(7)
carbohydrate	<sup>0,2</sup> A <sub>4</sub> (P1 penta)	[M+Na] <sup>+</sup>	670.9	172.2	0.1(5)
carbohydrate	Y <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	678.7	179.0	2.9(5)
carbohydrate	Y <sub>3</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	678.7	176.5	1.9(8)
carbohydrate	<sup>1,5</sup> A <sub>4</sub> (P1 penta)	[M+Na] <sup>+</sup>	684.0	175.7	0.5(5)
carbohydrate	<sup>0,2</sup> X <sub>3</sub> -N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	692.5	111.9	2.3(5)
carbohydrate	<sup>0,2</sup> X <sub>3</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	692.5	145.6	0.4(5)
carbohydrate	B <sub>4</sub> (LNFP1)	[M+Na] <sup>+</sup>	696.6	180.4	0.5(10)
carbohydrate	B <sub>3α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	696.6	175.9	1.4(14)
carbohydrate	B <sub>3</sub> (LNFP2)	[M+Na] <sup>+</sup>	696.6	182.5	0.5(5)
carbohydrate	B <sub>4</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	696.6	176.9	2.5(5)
carbohydrate	<sup>1,5</sup> X <sub>3</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	707.0	145.9	4.1(5)



carbohydrate	<sup>1,5</sup> X <sub>3</sub> (GNLNLN)	[M+Na] <sup>+</sup>	707.0	145.7	0.3(5)
carbohydrate	<sup>1,5</sup> X <sub>3</sub> (LNT)	[M+Na] <sup>+</sup>	707.0	148.1	0.5(5)
carbohydrate	B <sub>4</sub> (P1 antigen)	[M+Na] <sup>+</sup>	713.0	166.0	1.6(5)
carbohydrate	B <sub>4</sub> (P1 penta)	[M+Na] <sup>+</sup>	713.0	171.4	1.9(5)
carbohydrate	C <sub>3α</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	715.0	179.1	1.4(8)
carbohydrate	C <sub>3</sub> (LNFP2)	[M+Na] <sup>+</sup>	715.0	183.8	1.2(5)
carbohydrate	C <sub>4</sub> (LNFP1)	[M+Na] <sup>+</sup>	715.0	180.5	1.9(8)
carbohydrate	C <sub>4</sub> (P1 antigen)	[M+Na] <sup>+</sup>	731.0	169.9	1.7(5)
carbohydrate	Y <sub>4</sub> (LNFP1)	[M+Na] <sup>+</sup>	731.1	179.7	0.6(5)
carbohydrate	Y <sub>3α</sub> (LNFP2)	[M+Na] <sup>+</sup>	731.0	179.6	0.2(5)
carbohydrate	<sup>1,5</sup> X <sub>3α</sub> (LNFP2)	[M+Na] <sup>+</sup>	742.0	191.3	1.1(5)
carbohydrate	<sup>2,4</sup> X <sub>3</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	752.0	175.4	1.1(5)
carbohydrate	<sup>2,4</sup> X <sub>3</sub> -N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	752.0	180.0	1.0(5)
carbohydrate	B <sub>4</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	754.0	178.7	2.2(14)
carbohydrate	B <sub>4</sub> (LNT)	[M+Na] <sup>+</sup>	754.0	179.2	1.1(5)
carbohydrate	B <sub>4</sub> (GNLNLN)	[M+Na] <sup>+</sup>	754.0	183.9	0.9(5)
carbohydrate	<sup>0,2</sup> X <sub>3α</sub> (LNFP2)	[M+Na] <sup>+</sup>	756.7	190.3	0.7(5)
carbohydrate	<sup>2,4</sup> A <sub>5</sub> (LNFP1)	[M+Na] <sup>+</sup>	756.7	192.6	0.6(7)
carbohydrate	<sup>1,5</sup> X <sub>4</sub> (LNFP1)	[M+Na] <sup>+</sup>	758.6	195.9	1.3(5)
carbohydrate	C <sub>4</sub> (LNT)	[M+Na] <sup>+</sup>	772.0	180.1	1.6(10)
carbohydrate	C <sub>4</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	772.0	176.4	1.6(10)
carbohydrate	<sup>2,4</sup> A <sub>5</sub> (P1 penta)	[M+Na] <sup>+</sup>	772.0	173.6	1.6(5)
carbohydrate	<sup>2,4</sup> A <sub>5</sub> (P1 antigen)	[M+Na] <sup>+</sup>	773.0	176.8	0.4(5)
carbohydrate	Z <sub>4</sub> (P1 antigen)	[M+Na] <sup>+</sup>	782.0	150.1	1.1(5)
carbohydrate	Y <sub>4</sub> (P1 antigen)	[M+Na] <sup>+</sup>	800.0	111.9	1.2(5)
carbohydrate	M-N <sub>2</sub> (LNT)	[M+Na] <sup>+</sup>	812.8	189.3	0.3(7)
carbohydrate	M-N <sub>2</sub> (Lec-Lec)	[M+Na] <sup>+</sup>	812.8	180.2	1.9(20)
carbohydrate	Y <sub>4</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	813.0	191.5	0.9(8)
carbohydrate	Y <sub>4</sub> -N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	813.0	191.0	1.6(7)
carbohydrate	Y <sub>4</sub> -N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	813.0	178.1	0.7(8)

carbohydrate	<sup>2,4</sup> A <sub>5</sub> (GNLNLN)	[M+Na] <sup>+</sup>	814.0	191.5	1.8(5)
carbohydrate	<sup>0,2</sup> A <sub>5</sub> (P1 penta)	[M+Na] <sup>+</sup>	833.5	182.9	0.4(5)
carbohydrate	<sup>0,2</sup> A <sub>5</sub> (P1 antigen)	[M+Na] <sup>+</sup>	833.5	185.0	1.2(5)
carbohydrate	B <sub>1</sub> (3'SLN-Lec)	[M+Na] <sup>+</sup>	840.8	188.0	0.9(5)
carbohydrate	LNT	[M+Na] <sup>+</sup>	840.8	195.9	1.4(42)
carbohydrate	Lec-Lec	[M+Na] <sup>+</sup>	840.8	183.2	1.6(51)
carbohydrate	Y <sub>4</sub> (GNLNLN)	[M+Na] <sup>+</sup>	841.2	198.5	1.0(5)
carbohydrate	Y <sub>4</sub> (P1 penta)	[M+Na] <sup>+</sup>	841.2	184.2	0.7(10)
carbohydrate	Y <sub>4</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	841.2	199.3	0.5(5)
carbohydrate	<sup>0,2</sup> A <sub>5</sub> (GNLNLN)	[M+Na] <sup>+</sup>	874.0	172.6	2.0(8)
carbohydrate	B <sub>5</sub> (P1 antigen)	[M+Na] <sup>+</sup>	875.0	188.1	1.7(5)
carbohydrate	LNFP1	[M+Na] <sup>+</sup>	876.8	204.4	1.4(162)
carbohydrate	LNFP2	[M+Na] <sup>+</sup>	876.8	201.3	1.2(181)
carbohydrate	LNFP3	[M+Na] <sup>+</sup>	876.8	199.2	1.0(17)
carbohydrate	LNFP5	[M+Na] <sup>+</sup>	876.8	201.8	0.7(18)
carbohydrate	C <sub>5</sub> (P1 antigen)	[M+Na] <sup>+</sup>	893.0	194.4	0.8(7)
carbohydrate	<sup>0,2</sup> X <sub>4</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	896.0	147.4	0.6(5)
carbohydrate	B <sub>5</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	900.0	207.7	0.7(5)
carbohydrate	B <sub>5</sub> (P1 penta)	[M+Na] <sup>+</sup>	915.0	197.0	2.1(8)
carbohydrate	C <sub>5</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	918.0	201.4	4.0(5)
carbohydrate	C <sub>5</sub> (P1 penta)	[M+Na] <sup>+</sup>	933.0	192.3	0.7(8)
carbohydrate	M-N <sub>2</sub> (P1 antigen)	[M+Na] <sup>+</sup>	933.8	195.8	1.3(15)
carbohydrate	<sup>2,4</sup> X <sub>4</sub> -N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	956.0	214.4	1.2(5)
carbohydrate	Y <sub>3ja</sub> -N <sub>2</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	959.0	211.7	1.5(12)
carbohydrate	P1 antigen	[M+Na] <sup>+</sup>	961.8	203.4	0.9(18)
carbohydrate	M-N <sub>2</sub> (P1 penta)	[M+Na] <sup>+</sup>	974.5	202.6	0.7(15)
carbohydrate	C <sub>5</sub> (GNLNLN)	[M+Na] <sup>+</sup>	975.1	215.3	1.3(11)
carbohydrate	Y <sub>3ja</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	987.0	217.5	1.8(20)
carbohydrate	α-cyclodextrin	[M+Na] <sup>+</sup>	995.6	200.7	0.5(5)
carbohydrate	P1 penta	[M+Na] <sup>+</sup>	1002.4	206.2	0.6(30)

carbohydrate	M-N <sub>2</sub> (GNLNLN)	[M+Na] <sup>+</sup>	1015.9	220.6	2.3(24)
carbohydrate	Y <sub>5</sub> -N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1016.0	220.3	2.7(5)
carbohydrate	LNDFH1	[M+Na] <sup>+</sup>	1022.9	225.6	1.1(18)
carbohydrate	LNDFH2	[M+Na] <sup>+</sup>	1022.9	220.6	1.0(18)
carbohydrate	GNLNLN	[M+Na] <sup>+</sup>	1043.9	230.5	0.8(25)
carbohydrate	B <sub>4</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	1046.8	234.9	3.0(6)
carbohydrate	C <sub>4</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	1064.4	230.2	3.3(11)
carbohydrate	M-N <sub>2</sub> (Di-Le <sup>A</sup> )	[M+Na] <sup>+</sup>	1105.1	231.5	0.5(10)
carbohydrate	Di-Le <sup>A</sup>	[M+Na] <sup>+</sup>	1133.4	241.9	0.56(23)
carbohydrate	β-cyclodextrin	[M+Na] <sup>+</sup>	1157.0	231.4	0.6(5)
carbohydrate	Y <sub>6</sub> -N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1178.0	232.3	0.7(5)
carbohydrate	<sup>0,2</sup> A <sub>7</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1182.0	231.7	2.0(5)
carbohydrate	Tri-LacNAc	[M+Na] <sup>+</sup>	1206.0	232.6	0.6(5)
carbohydrate	Y <sub>6</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1206.4	239.3	0.3(5)
carbohydrate	C <sub>7</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1283.2	243.8	0.7(5)
carbohydrate	M-N <sub>2</sub> (H-type2-LN-LN)	[M+Na] <sup>+</sup>	1324.2	245.5	0.4(7)
carbohydrate	H-type2-LN-LN	[M+Na] <sup>+</sup>	1352.2	252.1	0.6(7)
<b>Lipids<sup>3</sup></b>					
lipid	PE 34:2	[M+H] <sup>+</sup>	716.5	206.9	2.0(29)
lipid	PE 34:1	[M+H] <sup>+</sup>	718.5	205.8	4.3(29)
lipid	SM (36:1)	[M+H] <sup>+</sup>	731.6	221.1	2.0(33)
lipid	PE 34:2	[M+Na] <sup>+</sup>	738.5	213.5	2.1(29)
lipid	PE 34:1	[M+Na] <sup>+</sup>	740.5	214.7	1.5(29)
lipid	SM (36:1)	[M+Na] <sup>+</sup>	753.6	221.3	2.6(33)
lipid	PC 34:2	[M+H] <sup>+</sup>	758.6	217.4	3.2(33)
lipid	SM (38:1)	[M+H] <sup>+</sup>	759.7	229.8	3.4(33)
lipid	PC 34:1	[M+H] <sup>+</sup>	760.6	219.1	2.7(33)
lipid	PE 36:4	[M+Na] <sup>+</sup>	762.5	214.4	1.6(29)
lipid	PE 36:2	[M+Na] <sup>+</sup>	766.5	220.9	2.7(29)
lipid	PE 36:1	[M+Na] <sup>+</sup>	768.6	221.7	4.8(29)

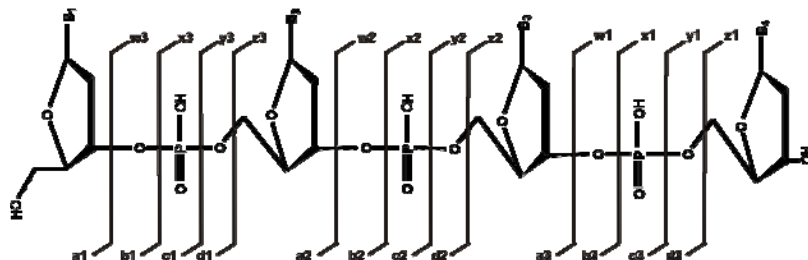
lipid	PC 34:2	[M+Na] <sup>+</sup>	780.6	218.9	2.8(33)
lipid	SM (38:1)	[M+Na] <sup>+</sup>	781.6	231.3	2.5(33)
lipid	PC 34:1	[M+Na] <sup>+</sup>	782.6	221.7	3.2(33)
lipid	PC 36:2	[M+H] <sup>+</sup>	786.6	222.6	2.2(33)
lipid	SM (40:1)	[M+H] <sup>+</sup>	787.7	232.2	5.0(33)
lipid	PE 38:5	[M+Na] <sup>+</sup>	788.5	220.6	5.2(29)
lipid	PC 36:1	[M+H] <sup>+</sup>	788.6	227.4	4.3(33)
lipid	PE 38:4	[M+Na] <sup>+</sup>	790.5	228.1	3.6(29)
lipid	CB (40:1)	[M+Na] <sup>+</sup>	806.6	232.9	2.4(33)
lipid	PC 36:2	[M+Na] <sup>+</sup>	808.6	226.7	4.6(33)
lipid	CB (39:1)h	[M+Na] <sup>+</sup>	808.6	236.6	2.9(33)
lipid	PS 36:2	[M+Na] <sup>+</sup>	810.5	217.1	5.5(29)
lipid	PC 36:1	[M+Na] <sup>+</sup>	810.6	228.1	2.0(33)
lipid	PS 36:1	[M+Na] <sup>+</sup>	812.5	222.6	2.4(29)
lipid	SM (42:2)	[M+H] <sup>+</sup>	813.7	241.8	2.5(33)
lipid	SM (42:1)	[M+H] <sup>+</sup>	815.7	242.1	6.3(33)
lipid	CB (40:2)h	[M+Na] <sup>+</sup>	820.6	236.2	5.6(33)
lipid	CB (40:1)h	[M+Na] <sup>+</sup>	822.6	234.6	5.3(33)
lipid	CB (42:6)	[M+Na] <sup>+</sup>	824.6	237.9	1.9(33)
lipid	CB (42:2)	[M+Na] <sup>+</sup>	832.7	238.8	1.7(33)
lipid	PS 38:4	[M+Na] <sup>+</sup>	834.5	225.5	2.1(29)
lipid	CB (42:1)	[M+Na] <sup>+</sup>	834.7	239.3	2.6(33)
lipid	SM (42:2)	[M+Na] <sup>+</sup>	835.7	239.4	2.8(33)
lipid	CB (41:1)h	[M+Na] <sup>+</sup>	836.7	240.2	3.4(33)
lipid	SM (42:1)	[M+Na] <sup>+</sup>	837.7	239.3	4.7(33)
lipid	PS 38:1	[M+Na] <sup>+</sup>	840.6	222.6	5.5(29)
lipid	CB (42:3)h	[M+Na] <sup>+</sup>	846.6	238.8	2.2(33)
lipid	CB (42:2)h	[M+Na] <sup>+</sup>	848.7	240.3	2.7(33)
lipid	CB (44:7)	[M+Na] <sup>+</sup>	850.6	242.8	1.9(33)
lipid	CB (44:6)	[M+Na] <sup>+</sup>	852.6	243.3	3.7(33)
lipid	PS 40:6	[M+Na] <sup>+</sup>	858.5	231.9	2.8(29)
lipid	CB (44:2)	[M+Na] <sup>+</sup>	860.7	245.9	5.2(33)
lipid	CB (44:1)	[M+Na] <sup>+</sup>	862.7	244.3	5.5(33)

lipid	CB (44:8)h	[M+Na] <sup>+</sup>	864.6	245.2	2.9(33)
lipid	CB (44:7)h	[M+Na] <sup>+</sup>	866.6	252.2	5.1(33)
lipid	SM (44:1)	[M+Na] <sup>+</sup>	866.7	247.9	4.3(33)
lipid	CB (44:2)h	[M+Na] <sup>+</sup>	876.7	246.7	3.7(33)
lipid	PS 42:9	[M+Na] <sup>+</sup>	880.5	238	1.7(29)
lipid	PS 42:8	[M+Na] <sup>+</sup>	882.5	230.8	3.0(29)
lipid	PC 42:1	[M+Na] <sup>+</sup>	894.7	238.2	2.3(33)
lipid	PC 42:0	[M+Na] <sup>+</sup>	896.7	246.3	2.1(33)

Footnotes on table nomenclature:

1. Oligonucleotide nomenclature:

G - Guanine  
 A - Adenine  
 C - Cytosine  
 T - Thymine



**Scheme S1.** Oligonucleotide fragmentation is specified in McLuckey nomenclature (McLuckey SA, Habibi-Goudarzi S. (1993) J. Am. Chem. Soc. 115: 12085-12095). In this table, tentative fragment ion assignments are given by the predominant fragmentation channels observed previously.

## 2. Carbohydrate nomenclature:

LNFP1	Fuca1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glc
LNFP2	Galβ1-3[Fuca1-4]GlcNAcβ1-3Galβ1-4Glc
LNFP3	Galβ1-4[Fuca1-3]GlcNAcβ1-3Galβ1-4Glc
LNFP5	Galβ1-3GlcNAcβ1-3Galβ1-4[Fuca1-3]Glc
LNDFH1	Fuca1-2Galβ1-3[Fuca1-4]GlcNAcβ1-3Galβ1-4Glc
LNDFH2	Galβ1-3[Fuca1-4]GlcNAcβ1-3Galβ1-4[Fuca1-3]Glc
Galα3-type1	Galα1-3Galβ1-3GlcNAcβ-Sp
P1	Galα1-4Galβ1-4GlcNAcβ-Sp
P1 penta	Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4GlcNAcβ-Sp
H-type2-LN-LN	Fuca1-2(Galβ1-4GlcNAcβ1-3) <sub>3</sub> β-Sp
Lec-Lec	Galβ1-3GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp
GNLNLN	GlcNAcβ1-3(Galβ1-4GlcNAcβ1-3) <sub>2</sub> β-Sp
LNT	Galβ1-3GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp
P1 antigen	Galα1-4Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp
Di-Le <sup>A</sup>	Galβ1-3[Fuca1-4]GlcNAcβ1-3Galβ1-3[Fuca1-4]GlcNAcβ-Sp
3'SLN-Lec	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp
Tri-LacNAc	(Galβ1-4GlcNAcβ1-3) <sub>3</sub> β-Sp
α-cyclodextrin	Cyclomaltohexaose
β-cyclodextrin	Cyclomaltoheptaose

Fuc - Fucose

Gal - Galactose

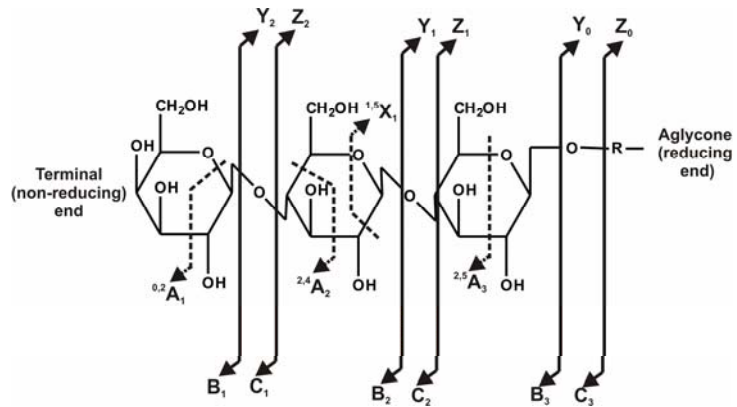
Glc - Glucose

GlcNAc - N-acetylglucosamine

GalNAc - N-acetylgalactosamine

Neu5Ac - N-Acetylneuraminic Acid

Sp – alkyne spacer not utilized in these studies but which readily loses N<sub>2</sub> in the MS accounting for some carbohydrate fragment peaks



**Scheme S2.** Carbohydrate fragmentation is specified in Domon-Costello nomenclature (Domon B, Costello CE (1988) Glycoconjugate J 5: 397-409)

### 3. Lipid nomenclature :

Glycerophospholipids:

Ex. PC X:Y

PC, PE, PS = abbreviated names phosphatidylcholine, phosphatidylethanolamine, phosphatidylserine.

X = total number of carbons in fatty acid chains

Y = total number of double bonds in fatty acid chains

Sphingolipids:

Ex. SM (x:y)

SM, CB = abbreviated names sphingomyelin, cerebroside

x = total number of carbons in the amide linked fatty acid of the ceramide plus eighteen carbons from the sphingosine backbone  
y = total number of double bonds, one trans double bond in the sphingosine backbone plus the number of double bonds in the amide linked fatty acid of the ceramide

( ) = used to distinguish sphingolipid from glycerophospholipid nomenclature in the table

Hydroxylation on Cerebrosides:

Ex. CB (x:y)h

h = denotes hydroxylation on the number two carbon (from carbonyl) of the amide linked fatty acid.