

McLean Group Collision Cross Section Database

MALDI Generated Data

Biomolecular Class	Name (parent name if fragmented)	species	m/z (Da)	Ω ($\text{\AA}^2$)	σ (# of measurements)
Carbohydrates ¹					
carbohydrate	B ₂ (LNFP1)	[M+Na] ⁺	331.0	118.6	0.5(7)
carbohydrate	Y ₂ (LNFP2)	[M+Na] ⁺	365.1	113.5	1.3(8)
carbohydrate	Y ₂ (LNFP1)	[M+Na] ⁺	365.1	112.8	1.3(12)
carbohydrate	B ₂ (P1 penta)	[M+Na] ⁺	388.0	114.1	1.1(5)
carbohydrate	^{2,4} A ₃ (H-type2-LN-LN)	[M+Na] ⁺	391.1	110.9	0.5(5)
carbohydrate	C ₂ (P1 penta)	[M+Na] ⁺	406.1	118.3	2.1(9)
carbohydrate	C ₂ (Lec-Lec)	[M+Na] ⁺	406.1	126.1	6.1(5)
carbohydrate	C ₂ (GNLNLN)	[M+Na] ⁺	406.1	115.3	0.1(5)
carbohydrate	C ₂ (LNT)	[M+Na] ⁺	406.1	119.4	1.5(5)
carbohydrate	^{2,4} A ₃ (P1 antigen)	[M+Na] ⁺	407.0	119.0	3.7(5)
carbohydrate	^{2,4} A ₃ (Gal α 3-type1)	[M+Na] ⁺	407.3	118.5	0.6(8)
carbohydrate	Y ₃ &C ₃ (LNFP1)	[M+Na] ⁺	409.4	125.6	1.4(9)
carbohydrate	Y ₃ &C ₂ (LNFP2)	[M+Na] ⁺	409.4	139.5	2.4(9)
carbohydrate	Y ₂ (P1 antigen)	[M+Na] ⁺	434.0	131.0	1.4(5)
carbohydrate	^{0,3} A ₃ (P1)	[M+Na] ⁺	437.0	135.3	0.9(5)
carbohydrate	Y ₂ -N ₂ (H-type2-LN-LN)	[M+Na] ⁺	438.5	135.4	1.2(5)
carbohydrate	Z _{1a} (Di-Le ^A)	[M+Na] ⁺	441.4	138.8	0.9(9)
carbohydrate	Y ₂ -N ₂ (Lec-Lec)	[M+Na] ⁺	447.4	134.5	2.1(12)
carbohydrate	Y ₂ -N ₂ (GNLNLN)	[M+Na] ⁺	447.4	131.2	1.4(5)
carbohydrate	Y ₂ -N ₂ (P1 penta)	[M+Na] ⁺	447.4	134.1	0.3(8)
carbohydrate	Y ₂ -N ₂ (P1)	[M+Na] ⁺	447.4	131.0	0.8(8)
carbohydrate	^{2,4} A ₃ (LNT)	[M+Na] ⁺	448.4	124.0	0.9(14)
carbohydrate	^{2,4} A ₃ (GNLNLN)	[M+Na] ⁺	448.4	115.1	0.5(8)
carbohydrate	^{1,3} A ₃ (Gal α 3-type1)	[M+Na] ⁺	448.4	128.0	2.0(5)

carbohydrate	^{2,4} A ₃ (P1 penta)	[M+Na] ⁺	448.4	135.1	1.3(5)
carbohydrate	^{0,2} A _{2α} (Di-Le ^A)	[M+Na] ⁺	451.0	132.2	3.1(5)
carbohydrate	^{0,2} A ₃ (H-type2-LN-LN)	[M+Na] ⁺	451.0	131.1	0.6(5)
carbohydrate	Z ₂ (P1)	[M+Na] ⁺	457.0	137.6	2.1(5)
carbohydrate	Z ₂ (Galα3-type1)	[M+Na] ⁺	457.0	122.3	1.0(7)
carbohydrate	Z ₂ (P1)	[M+Na] ⁺	457.0	106.7	0.5(5)
carbohydrate	Z ₂ (GNLNLN)	[M+Na] ⁺	457.0	107.7	1.3(5)
carbohydrate	Y _{1α} (Di-Le ^A)	[M+Na] ⁺	459.4	110.7	0.8(5)
carbohydrate	^{1,5} X ₂ (P1 antigen)	[M+Na] ⁺	462.0	131.2	0.8(5)
carbohydrate	^{0,2} A ₃ (Galα3-type1)	[M+Na] ⁺	467.4	132.5	0.6(5)
carbohydrate	Y ₂ (LNT)	[M+Na] ⁺	475.4	102.5	0.5(5)
carbohydrate	Y ₂ (P1)	[M+Na] ⁺	475.4	136.9	0.8(5)
carbohydrate	Y ₂ (Lec-Lec)	[M+Na] ⁺	475.4	138.0	1.3(5)
carbohydrate	Y ₂ (Galα3-type1)	[M+Na] ⁺	475.4	133.8	0.6(7)
carbohydrate	Y ₂ (P1 penta)	[M+Na] ⁺	475.4	135.3	3.5(7)
carbohydrate	^{1,5} X _{1α} (Di-Le ^A)	[M+Na] ⁺	487.4	132.0	2.5(8)
carbohydrate	^{0,2} X ₂ -N ₂ (P1 antigen)	[M+Na] ⁺	489.0	151.9	3.1(5)
carbohydrate	^{1,5} X ₂ (Galα3-type1)	[M+Na] ⁺	503.4	144.8	3.5(8)
carbohydrate	^{1,5} X ₂ (Lec-Lec)	[M+Na] ⁺	503.4	152.3	3.8(5)
carbohydrate	^{1,5} X ₂ (GNLNLN)	[M+Na] ⁺	503.4	127.0	18.6(5)
carbohydrate	^{1,5} X ₂ (LNT)	[M+Na] ⁺	503.4	108.1	0.7(5)
carbohydrate	^{1,5} X ₂ (H-type2-LN-LN)	[M+Na] ⁺	503.4	137.9	2.6(5)
carbohydrate	^{1,5} A ₃ (P1)	[M+Na] ⁺	522.5	135.9	0.1(5)
carbohydrate	^{1,5} A ₃ (Galα3-type1)	[M+Na] ⁺	522.5	135.2	1.3(5)
carbohydrate	^{0,2} X ₂ -N ₂ (LNT)	[M+Na] ⁺	531.0	122.1	1.5(5)
carbohydrate	B ₃ (H-type2-LN-LN)	[M+Na] ⁺	534.5	142.9	0.3(5)
carbohydrate	B ₂ (LNFP2)	[M+Na] ⁺	534.5	152.2	0.6(5)
carbohydrate	B ₃ (LNFP1)	[M+Na] ⁺	534.5	151.5	0.7(9)
carbohydrate	B _{2α} (Di-Le ^A)	[M+Na] ⁺	534.5	145.8	2(8)
carbohydrate	^{3,5} X ₁ -N ₂ (Galα3-type1)	[M+Na] ⁺	535.0	145.5	1.8(5)

carbohydrate	^{0,3} X ₀ (Galα3-type1)	[M+Na] ⁺	547.5	153.5	3.9(6)
carbohydrate	Z _{3β} &C ₃ (LNFP2)	[M+Na] ⁺	547.6	165.6	4.1(5)
carbohydrate	B ₃ (Lec-Lec)	[M+Na] ⁺	550.0	148.0	2.3(16)
carbohydrate	B ₃ (LNT)	[M+Na] ⁺	550.0	145.5	0.4(5)
carbohydrate	B ₃ (P1 penta)	[M+Na] ⁺	550.0	150.6	0.3(13)
carbohydrate	B ₃ (P1 antigen)	[M+Na] ⁺	550.0	145.2	4.0(10)
carbohydrate	B ₃ (Galα3-type1)	[M+Na] ⁺	552.5	142.7	0.6(5)
carbohydrate	C _{2α} (Di-Le ^A)	[M+Na] ⁺	552.5	149.4	1.3(9)
carbohydrate	C ₂ (LNFP2)	[M+Na] ⁺	552.5	151.3	0.9(5)
carbohydrate	C ₃ (LNFP1)	[M+Na] ⁺	552.5	134.1	1.6(9)
carbohydrate	B ₃ (P1)	[M+Na] ⁺	552.5	109.0	1.0(5)
carbohydrate	C ₃ (H-type2-LN-LN)	[M+Na] ⁺	552.5	148.3	2.2(5)
carbohydrate	^{3,5} X ₁ (Galα3-type1)	[M+Na] ⁺	563.0	126.8	0.7(5)
carbohydrate	C ₃ (LNT)	[M+Na] ⁺	568.5	150.7	1.9(5)
carbohydrate	C ₃ (P1 antigen)	[M+Na] ⁺	568.5	148.6	1.2(6)
carbohydrate	C ₃ (Lec-Lec)	[M+Na] ⁺	568.5	152.9	2.9(15)
carbohydrate	Y ₃ (LNFP1)	[M+Na] ⁺	568.5	157.4	0.4(5)
carbohydrate	C ₃ (P1 penta)	[M+Na] ⁺	568.5	153.4	0.8(5)
carbohydrate	C ₃ (P1)	[M+Na] ⁺	568.5	154.3	0.8(5)
carbohydrate	C ₃ (Galα3-type1)	[M+Na] ⁺	568.5	153.5	3.2(7)
carbohydrate	^{2,4} X ₂ (P1 antigen)	[M+Na] ⁺	577.5	165.3	1.0(5)
carbohydrate	^{2,4} X ₂ (P1 penta)	[M+Na] ⁺	577.5	160.5	0.8(11)
carbohydrate	^{2,4} X ₂ (Galα3-type1)	[M+Na] ⁺	577.5	163.0	15.3(5)
carbohydrate	^{2,4} X ₂ -N ₂ (LNT)	[M+Na] ⁺	591.0	153.7	1.8(7)
carbohydrate	^{2,4} X ₂ -N ₂ (Lec-Lec)	[M+Na] ⁺	591.0	158.1	1.5(5)
carbohydrate	B ₃ (GNLNLN)	[M+Na] ⁺	591.5	155.8	0.4(10)
carbohydrate	Z ₃ -N ₂ (P1 penta)	[M+Na] ⁺	591.5	146.3	0.5(5)
carbohydrate	^{2,4} A _{3α} (Di-LeA)	[M+Na] ⁺	594.5	159.8	2.2(15)
carbohydrate	^{2,4} A ₃ (LNFP2)	[M+Na] ⁺	594.5	173.6	1.0(5)
carbohydrate	Y ₃ -N ₂ (P1 penta)	[M+Na] ⁺	609.0	160.1	1.7(10)

carbohydrate	M-N ₂ (Galα3-type1)	[M+Na] ⁺	609.6	135.4	1.4(7)
carbohydrate	M-N ₂ (P1)	[M+Na] ⁺	609.6	155.2	0.9(8)
carbohydrate	C ₃ (GNLNLN)	[M+Na] ⁺	610.5	161.7	0.3(5)
carbohydrate	^{2,4} A ₄ (Lec-Lec)	[M+Na] ⁺	610.5	162.2	0.5(5)
carbohydrate	^{2,4} A ₄ (LNT)	[M+Na] ⁺	610.5	163.4	1.3(7)
carbohydrate	^{2,4} A ₄ (P1 antigen)	[M+Na] ⁺	610.5	156.7	0.3(5)
carbohydrate	^{2,4} X ₂ (LNT)	[M+Na] ⁺	619.0	169.9	2.3(5)
carbohydrate	^{3,5} A ₄ (LNT)	[M+Na] ⁺	624.0	123.6	0.8(5)
carbohydrate	Z ₃ -N ₂ (GNLNLN)	[M+Na] ⁺	633.1	170.1	2.1(5)
carbohydrate	Z ₃ -N ₂ (Lec-Lec)	[M+Na] ⁺	633.1	166.2	1.3(5)
carbohydrate	Z ₃ -N ₂ (LNT)	[M+Na] ⁺	633.1	131.9	2.1(5)
carbohydrate	Galα3-type1	[M+Na] ⁺	637.6	160.2	1.4(45)
carbohydrate	P1	[M+Na] ⁺	637.6	166.9	1.2(70)
carbohydrate	Y ₃ (P1 penta)	[M+Na] ⁺	637.6	170.1	1.4(8)
carbohydrate	Y ₃ (P1 antigen)	[M+Na] ⁺	637.6	168.2	0.6(5)
carbohydrate	Y ₃ -N ₂ (GNLNLN)	[M+Na] ⁺	651.0	173.0	1.8(9)
carbohydrate	Y ₃ -N ₂ (LNT)	[M+Na] ⁺	651.0	176.2	0.6(5)
carbohydrate	Y ₃ -N ₂ (Lec-Lec)	[M+Na] ⁺	651.0	171.1	2.0(18)
carbohydrate	Z ₃ (GNLNLN)	[M+Na] ⁺	661.0	108.8	0.4(5)
carbohydrate	^{0,2} A ₄ (LNT)	[M+Na] ⁺	670.9	170.1	1.6(7)
carbohydrate	^{0,2} A ₄ (P1 penta)	[M+Na] ⁺	670.9	172.2	0.1(5)
carbohydrate	Y ₃ (GNLNLN)	[M+Na] ⁺	678.7	179.0	2.9(5)
carbohydrate	Y ₃ (Lec-Lec)	[M+Na] ⁺	678.7	176.5	1.9(8)
carbohydrate	^{1,5} A ₄ (P1 penta)	[M+Na] ⁺	684.0	175.7	0.5(5)
carbohydrate	^{0,2} X ₃ -N ₂ (LNT)	[M+Na] ⁺	692.5	111.9	2.3(5)
carbohydrate	^{0,2} X ₃ -N ₂ (P1 penta)	[M+Na] ⁺	692.5	145.6	0.4(5)
carbohydrate	B ₄ (LNFP1)	[M+Na] ⁺	696.6	180.4	0.5(10)
carbohydrate	B _{3α} (Di-Le ^A)	[M+Na] ⁺	696.6	175.9	1.4(14)
carbohydrate	B ₃ (LNFP2)	[M+Na] ⁺	696.6	182.5	0.5(5)
carbohydrate	B ₄ (H-type2-LN-LN)	[M+Na] ⁺	696.6	176.9	2.5(5)

carbohydrate	^{1,5} X ₃ (Lec-Lec)	[M+Na] ⁺	707.0	145.9	4.1(5)
carbohydrate	^{1,5} X ₃ (GNLNLN)	[M+Na] ⁺	707.0	145.7	0.3(5)
carbohydrate	^{1,5} X ₃ (LNT)	[M+Na] ⁺	707.0	148.1	0.5(5)
carbohydrate	B ₄ (P1 antigen)	[M+Na] ⁺	713.0	166.0	1.6(5)
carbohydrate	B ₄ (P1 penta)	[M+Na] ⁺	713.0	171.4	1.9(5)
carbohydrate	C _{3α} (Di-Le ^A)	[M+Na] ⁺	715.0	179.1	1.4(8)
carbohydrate	C ₃ (LNFP2)	[M+Na] ⁺	715.0	183.8	1.2(5)
carbohydrate	C ₄ (LNFP1)	[M+Na] ⁺	715.0	180.5	1.9(8)
carbohydrate	C ₄ (P1 antigen)	[M+Na] ⁺	731.0	169.9	1.7(5)
carbohydrate	Y ₄ (LNFP1)	[M+Na] ⁺	731.1	179.7	0.6(5)
carbohydrate	Y _{3α} (LNFP2)	[M+Na] ⁺	731.0	179.6	0.2(5)
carbohydrate	^{1,5} X _{3α} (LNFP2)	[M+Na] ⁺	742.0	191.3	1.1(5)
carbohydrate	^{2,4} X ₃ -N ₂ (P1 penta)	[M+Na] ⁺	752.0	175.4	1.1(5)
carbohydrate	^{2,4} X ₃ -N ₂ (H-type2-LN-LN)	[M+Na] ⁺	752.0	180.0	1.0(5)
carbohydrate	B ₄ (Lec-Lec)	[M+Na] ⁺	754.0	178.7	2.2(14)
carbohydrate	B ₄ (LNT)	[M+Na] ⁺	754.0	179.2	1.1(5)
carbohydrate	B ₄ (GNLNLN)	[M+Na] ⁺	754.0	183.9	0.9(5)
carbohydrate	^{0,2} X _{3α} (LNFP2)	[M+Na] ⁺	756.7	190.3	0.7(5)
carbohydrate	^{2,4} A ₅ (LNFP1)	[M+Na] ⁺	756.7	192.6	0.6(7)
carbohydrate	^{1,5} X ₄ (LNFP1)	[M+Na] ⁺	758.6	195.9	1.3(5)
carbohydrate	C ₄ (LNT)	[M+Na] ⁺	772.0	180.1	1.6(10)
carbohydrate	C ₄ (Lec-Lec)	[M+Na] ⁺	772.0	176.4	1.6(10)
carbohydrate	^{2,4} A ₅ (P1 penta)	[M+Na] ⁺	772.0	173.6	1.6(5)
carbohydrate	^{2,4} A ₅ (P1 antigen)	[M+Na] ⁺	773.0	176.8	0.4(5)
carbohydrate	Z ₄ (P1 antigen)	[M+Na] ⁺	782.0	150.1	1.1(5)
carbohydrate	Y ₄ (P1 antigen)	[M+Na] ⁺	800.0	111.9	1.2(5)
carbohydrate	M-N ₂ (LNT)	[M+Na] ⁺	812.8	189.3	0.3(7)
carbohydrate	M-N ₂ (Lec-Lec)	[M+Na] ⁺	812.8	180.2	1.9(20)
carbohydrate	Y ₄ -N ₂ (GNLNLN)	[M+Na] ⁺	813.0	191.5	0.9(8)
carbohydrate	Y ₄ -N ₂ (H-type2-LN-LN)	[M+Na] ⁺	813.0	191.0	1.6(7)

carbohydrate	Y ₄ -N ₂ (P1 penta)	[M+Na] ⁺	813.0	178.1	0.7(8)
carbohydrate	^{2,4} A ₅ (GNLNLN)	[M+Na] ⁺	814.0	191.5	1.8(5)
carbohydrate	^{0,2} A ₅ (P1 penta)	[M+Na] ⁺	833.5	182.9	0.4(5)
carbohydrate	^{0,2} A ₅ (P1 antigen)	[M+Na] ⁺	833.5	185.0	1.2(5)
carbohydrate	B ₁ (3'SLN-Lec)	[M+Na] ⁺	840.8	188.0	0.9(5)
carbohydrate	LNT	[M+Na] ⁺	840.8	195.9	1.4(42)
carbohydrate	Lec-Lec	[M+Na] ⁺	840.8	183.2	1.6(51)
carbohydrate	Y ₄ (GNLNLN)	[M+Na] ⁺	841.2	198.5	1.0(5)
carbohydrate	Y ₄ (P1 penta)	[M+Na] ⁺	841.2	184.2	0.7(10)
carbohydrate	Y ₄ (H-type2-LN-LN)	[M+Na] ⁺	841.2	199.3	0.5(5)
carbohydrate	^{0,2} A ₅ (GNLNLN)	[M+Na] ⁺	874.0	172.6	2.0(8)
carbohydrate	B ₅ (P1 antigen)	[M+Na] ⁺	875.0	188.1	1.7(5)
carbohydrate	LNFP1	[M+Na] ⁺	876.8	204.4	1.4(162)
carbohydrate	LNFP2	[M+Na] ⁺	876.8	201.3	1.2(181)
carbohydrate	LNFP3	[M+Na] ⁺	876.8	199.2	1.0(17)
carbohydrate	LNFP5	[M+Na] ⁺	876.8	201.8	0.7(18)
carbohydrate	C ₅ (P1 antigen)	[M+Na] ⁺	893.0	194.4	0.8(7)
carbohydrate	^{0,2} X ₄ -N ₂ (GNLNLN)	[M+Na] ⁺	896.0	147.4	0.6(5)
carbohydrate	B ₅ (H-type2-LN-LN)	[M+Na] ⁺	900.0	207.7	0.7(5)
carbohydrate	B ₅ (P1 penta)	[M+Na] ⁺	915.0	197.0	2.1(8)
carbohydrate	C ₅ (H-type2-LN-LN)	[M+Na] ⁺	918.0	201.4	4.0(5)
carbohydrate	C ₅ (P1 penta)	[M+Na] ⁺	933.0	192.3	0.7(8)
carbohydrate	M-N ₂ (P1 antigen)	[M+Na] ⁺	933.8	195.8	1.3(15)
carbohydrate	^{2,4} X ₄ -N ₂ (GNLNLN)	[M+Na] ⁺	956.0	214.4	1.2(5)
carbohydrate	Y _{3ja} -N ₂ (Di-Le ^A)	[M+Na] ⁺	959.0	211.7	1.5(12)
carbohydrate	P1 antigen	[M+Na] ⁺	961.8	203.4	0.9(18)
carbohydrate	M-N ₂ (P1 penta)	[M+Na] ⁺	974.5	202.6	0.7(15)
carbohydrate	C ₅ (GNLNLN)	[M+Na] ⁺	975.1	215.3	1.3(11)
carbohydrate	Y _{3ja} (Di-Le ^A)	[M+Na] ⁺	987.0	217.5	1.8(20)
carbohydrate	α-cyclodextrin	[M+Na] ⁺	995.6	200.7	0.5(5)

carbohydrate	P1 penta	[M+Na] ⁺	1002.4	206.2	0.6(30)
carbohydrate	M-N ₂ (GNLNLN)	[M+Na] ⁺	1015.9	220.6	2.3(24)
carbohydrate	Y ₅ -N ₂ (H-type2-LN-LN)	[M+Na] ⁺	1016.0	220.3	2.7(5)
carbohydrate	LNDFH1	[M+Na] ⁺	1022.9	225.6	1.1(18)
carbohydrate	LNDFH2	[M+Na] ⁺	1022.9	220.6	1.0(18)
carbohydrate	GNLNLN	[M+Na] ⁺	1043.9	230.5	0.8(25)
carbohydrate	B ₄ (Di-Le ^A)	[M+Na] ⁺	1046.8	234.9	3.0(6)
carbohydrate	C ₄ (Di-Le ^A)	[M+Na] ⁺	1064.4	230.2	3.3(11)
carbohydrate	M-N ₂ (Di-Le ^A)	[M+Na] ⁺	1105.1	231.5	0.5(10)
carbohydrate	Di-Le ^A	[M+Na] ⁺	1133.4	241.9	0.56(23)
carbohydrate	β-cyclodextrin	[M+Na] ⁺	1157.0	231.4	0.6(5)
carbohydrate	Y ₆ -N ₂ (H-type2-LN-LN)	[M+Na] ⁺	1178.0	232.3	0.7(5)
carbohydrate	^{0,2} A ₇ (H-type2-LN-LN)	[M+Na] ⁺	1182.0	231.7	2.0(5)
carbohydrate	Tri-LacNAc	[M+Na] ⁺	1206.0	232.6	0.6(5)
carbohydrate	Y ₆ (H-type2-LN-LN)	[M+Na] ⁺	1206.4	239.3	0.3(5)
carbohydrate	C ₇ (H-type2-LN-LN)	[M+Na] ⁺	1283.2	243.8	0.7(5)
carbohydrate	M-N ₂ (H-type2-LN-LN)	[M+Na] ⁺	1324.2	245.5	0.4(7)
carbohydrate	H-type2-LN-LN	[M+Na] ⁺	1352.2	252.1	0.6(7)

Footnotes on table nomenclature:

1. 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

Gal α 3-type1	Gal α 1-3Gal β 1-3GlcNAc β -Sp
P1	Gal α 1-4Gal β 1-4GlcNAc β -Sp
P1 penta	Galb1-3GalNAc β 1-3Gal α 1-4Gal β 1-4GlcNAc β -Sp
H-type2-LN-LN	Fuc α 1-2(Gal β 1-4GlcNAc β 1-3) ₃ β -Sp
Lec-Lec	Gal β 1-3GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp
GNLNLN	GlcNAc β 1-3(Gal β 1-4GlcNAc β 1-3) ₂ β -Sp
LNT	Gal β 1-3GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp
P1 antigen	Gal α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp
Di-Le ^A	Gal β 1-3[Fuc α 1-4]GlcNAc β 1-3Gal β 1-3[Fuc α 1-4]GlcNAc β -Sp
3'SLN-Lec	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp
Tri-LacNAc	(Gal β 1-4GlcNAc β 1-3) ₃ β -Sp
α -cyclodextrin	Cyclomaltohexaose
β -cyclodextrin	Cyclomaltoheptaose

Fuc - Fucose

Gal - Galactose

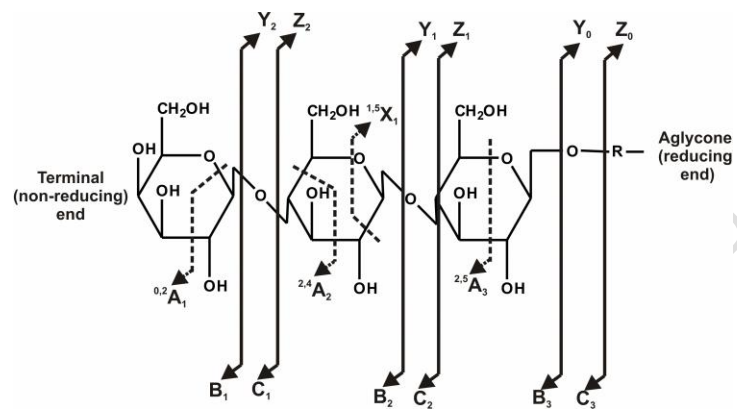
Glc - Glucose

GlcNAc - N-acetylglucosamine

GalNAc - N-acetylgalactosamine

Neu5Ac - N-Acetylneuraminic Acid

Sp – alkyne spacer not utilized in these studies but which readily loses N₂ 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)