

Supplementary Material

1 SUPPLEMENTARY FIGURES AND TABLES

1.1 Figures

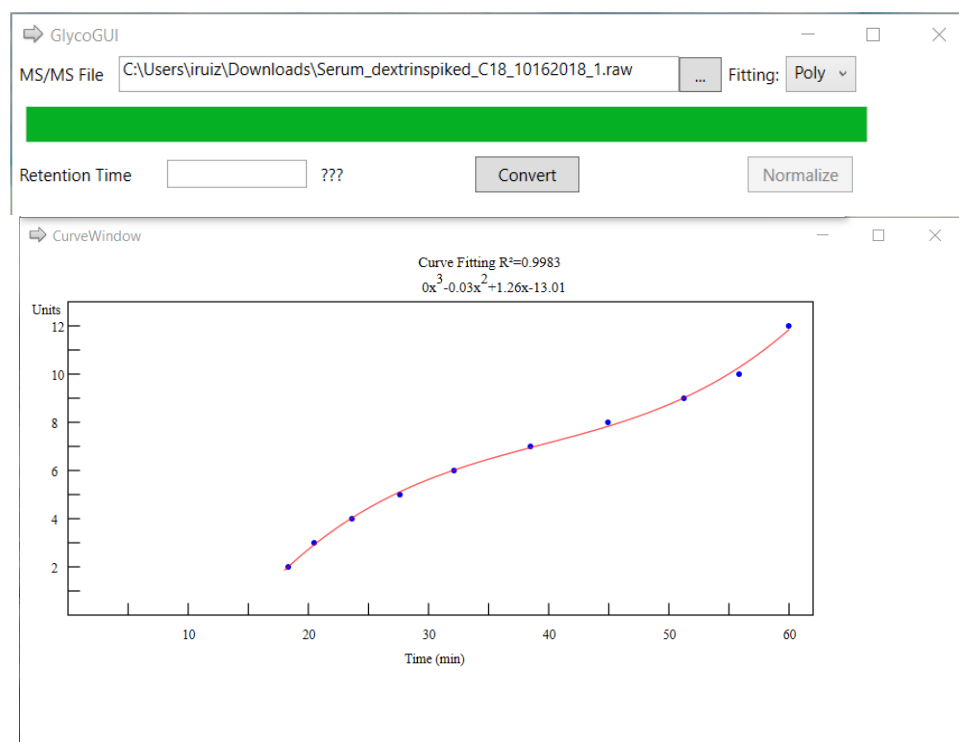


Figure S1. GlycanGUI interface for normalization of retention time.

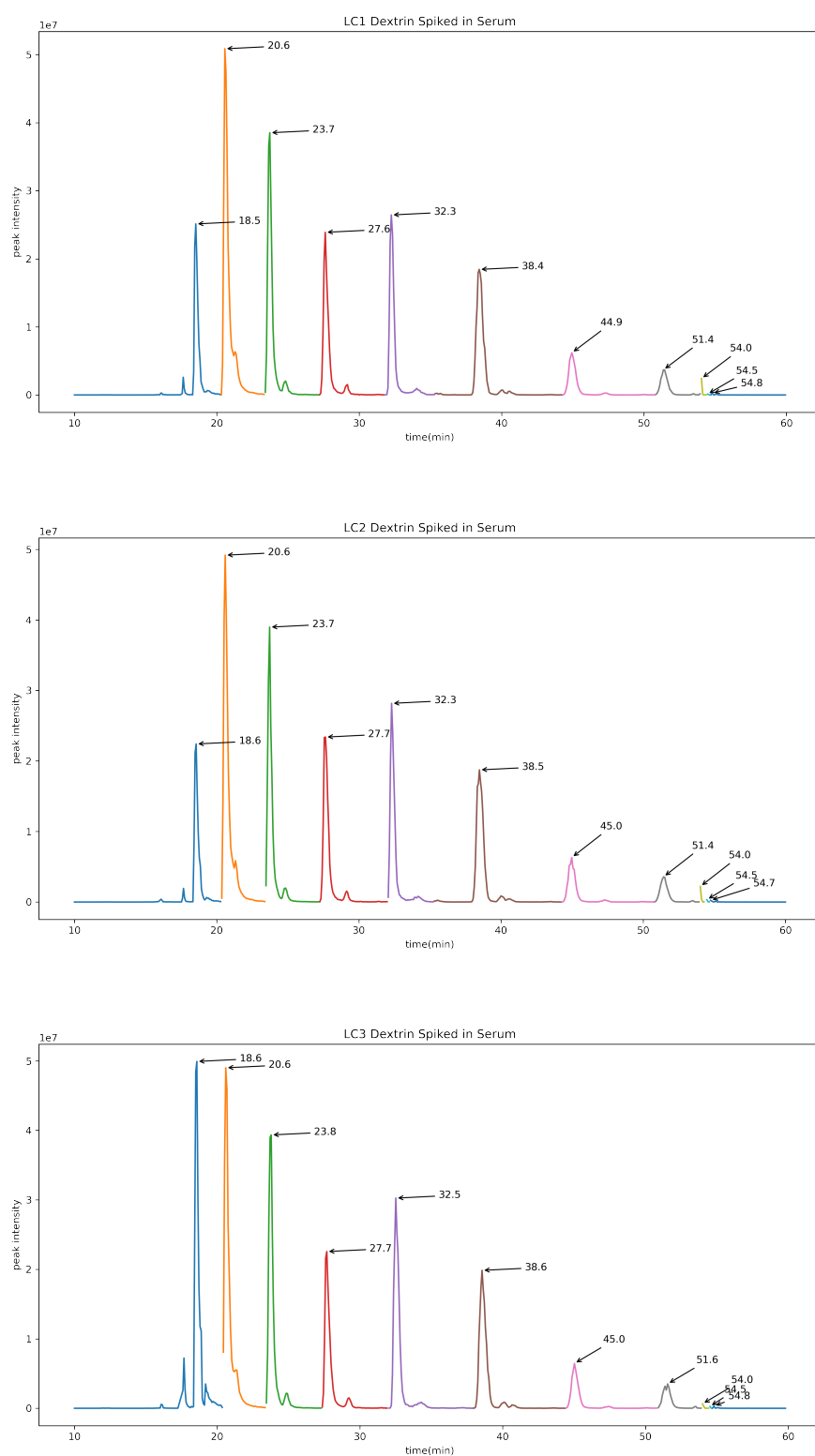


Figure S2. Chromatogram showing the retention time of dextrin identified by peak matching and dynamic programming.

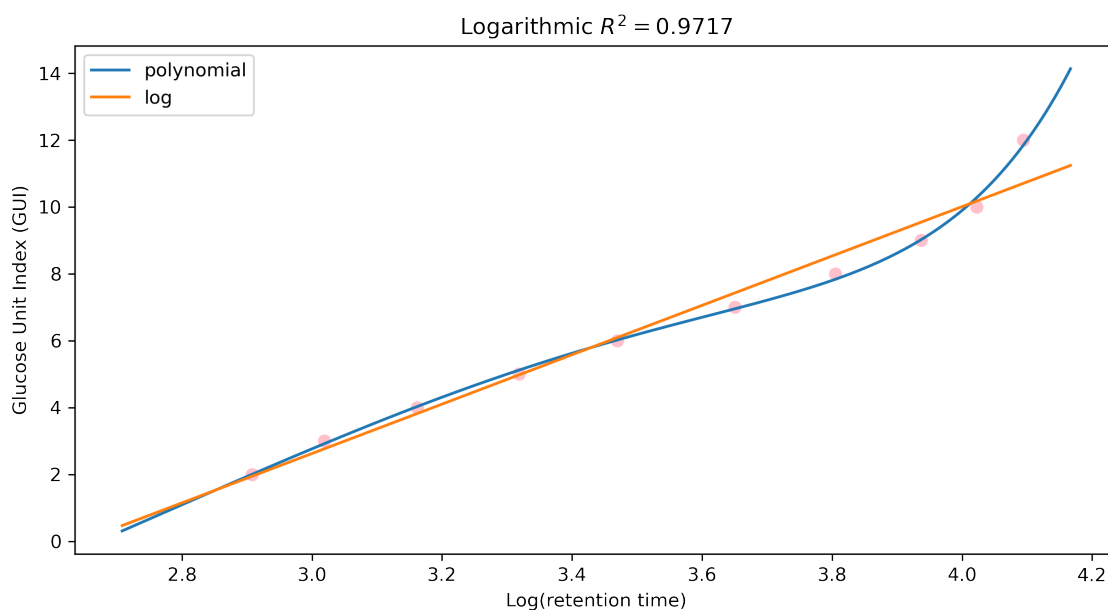


Figure S3. The curve fitting of GUI as a function of log retention time. The polynomial fitting is plotted in logarithmic scale to compare with that of logarithmic fitting.

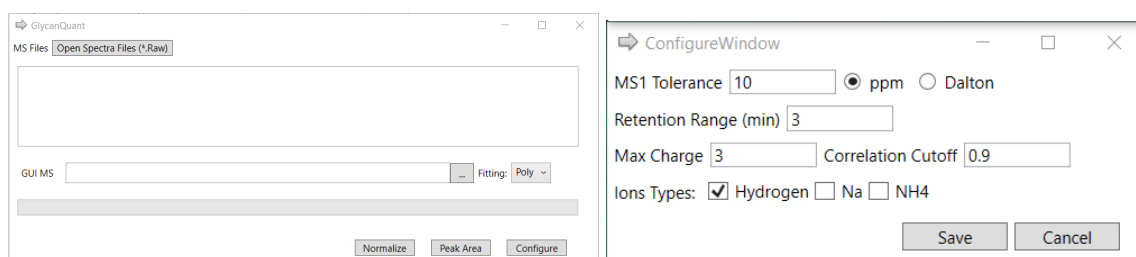


Figure S4. GlycanGUI interface for quantification of glycans.

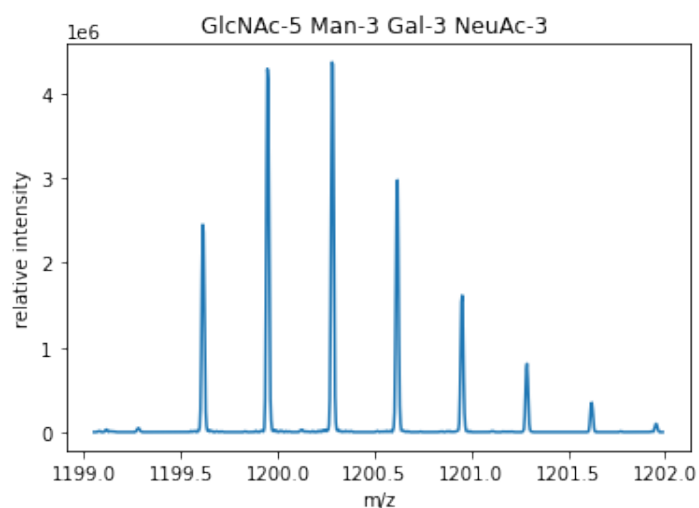


Figure S5. The example of an isotopic cluster of glycan $\text{GlcNAc}_5\text{Man}_3\text{Gal}_3\text{NeuAc}_3$.

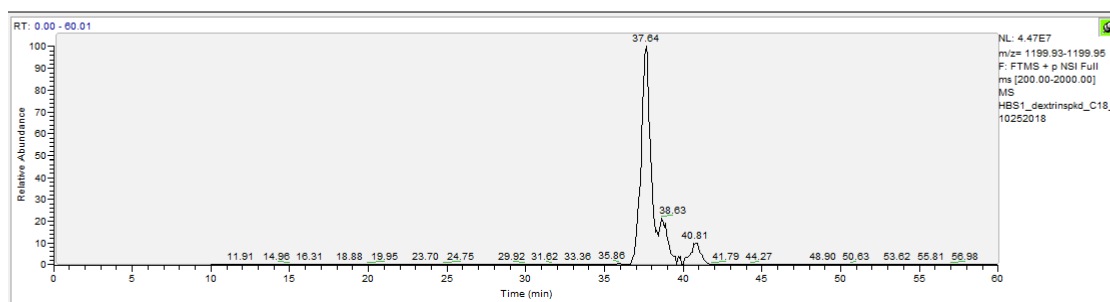


Figure S6. The snapshot of Xcalibur (Thermo Scientific) generated chromatograph.

1.2 Tables

Table S1: Glycan automatically annotated (including manual annotated were highlighted in bold).

Glycan Annotated	GUI
HexNAc ₁₀ Hex ₇ Fuc ₂	1.98,6.3,6.54,7.68
HexNAc ₆ Hex ₄ Fuc ₁ NeuAc ₁	0.59,1.37,1.67,2.84,3.33 4.16,5.78,6.31,6.63,1.23 6.56
HexNAc ₆ Hex ₆ Fuc ₁	0.23,1.12,2.28,2.6,3.23 3.77,4.52,5.13,5.55,6.33 6.7,7.15,5.44,6.66
HexNAc ₆ Hex ₇ Fuc ₂ NeuAc ₂	0.34,1.37,2.46,4.88,6.42 8.14,10.58
HexNAc ₉ Hex ₉ Fuc ₂	3.57,8.06,9.13,10.46
HexNAc₅Hex₆NeuAc₂	0.36,6.31,6.61,7.09,6.02 6.68
HexNAc₆Hex₇Fuc₁NeuAc₃	7.64,7.86,8.01
HexNAc ₆ Hex ₇ Fuc ₃ NeuAc ₂	1.36,5.24,5.98,6.74,6.99 8.01
HexNAc₅Hex₆Fuc₁NeuAc₁	0.21,1.45,6.2,6.37,6.5 6.62,7.02,1.7,6.01,6.56
HexNAc ₉ Hex ₇ Fuc ₁	1.29,3.67,4.06,6.74,7.67
HexNAc ₆ Hex ₄ Fuc ₂	0.2,0.65,1.41,1.9,2.64 3.1,3.58,4.13,4.52,4.84 5.55,6.74,14.06,1.53,5.71 6.49,10.5
HexNAc ₈ Hex ₈ Fuc ₂	0.72,1.74,3.83,6.42,7.97
HexNAc ₆ Hex ₅ Fuc ₂	0.13,0.34,0.94,1.33,3.36 3.68,4.18,4.92,5.19,5.77 6.61,1.29,6.29,6.51,7.0
HexNAc₅Hex₄NeuAc₁	0.26,1.12,1.86,4.58,4.9 5.58,6.0,0.28,1.33,4.58 5.54,5.94,6.28,9.51,10.56

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₁₀ Hex ₈ Fuc ₁	0.2,2.2,4.37,6.27,10.54
HexNAc ₁₀ Hex ₉ Fuc ₁	4.08,4.87,5.29,6.65,6.98 8.1
HexNAc ₆ Hex ₅ Fuc ₃	0.22,0.76,2.13,3.38,3.57 3.98,4.3,4.64,5.3,5.47 5.83,6.24,6.81,7.68
HexNAc₅Hex₄Fuc₁	0.39,1.33,5.29,0.3,1.07 4.55,5.32,5.79,6.1,7.04
HexNAc₆Hex₇NeuAc₄	7.74,7.91
HexNAc ₆ Hex ₇ Fuc ₅ NeuAc ₃	8.12,9.42
HexNAc₆Hex₇NeuAc₂	0.23,2.17,2.31,5.64,6.22 6.8,7.18,10.49
HexNAc ₅ Hex ₆ Fuc ₂ NeuAc ₂	0.22,1.36,1.94,2.89,4.27 5.47,5.86,7.73,7.93,10.46 11.72,5.93,6.19,6.43,6.64 7.07,7.28
HexNAc ₉ Hex ₉ Fuc ₁	1.44,5.11,8.29,9.27,10.54
HexNAc ₉ Hex ₇ Fuc ₃	7.64,7.86,8.01
HexNAc ₆ Hex ₆ Fuc ₃ NeuAc ₁	1.24,2.35,3.02,7.63
HexNAc ₄ Hex ₅ Fuc ₃ NeuAc ₁	0.05,0.3,0.65,1.65,2.92 3.94,5.1,5.99,6.58,6.76 7.02,7.49,7.74,10.77,3.86 5.21,5.63,5.93,6.23,6.48 6.95,7.29,7.66
HexNAc ₅ Hex ₅ Fuc ₂	0.46,1.35,5.5,5.8,6.37 1.57,2.89,3.83,5.16,5.61 5.76,6.02,6.41,6.92,7.04
HexNAc ₉ Hex ₉	1.66,3.54,7.54,8.88
HexNAc ₆ Hex ₅ Fuc ₂ NeuAc ₂	0.76,1.96,3.47,4.28,6.08 6.25,10.51,2.06
HexNAc ₁₀ Hex ₉ NeuAc ₁	4.46,9.84
HexNAc ₆ Hex ₅ Fuc ₅ NeuAc ₂	0.24,1.16,4.01,6.11,7.86 8.63
HexNAc ₆ Hex ₅ Fuc ₁ NeuAc ₁	0.5,2.28,5.2,6.6,8.36 2.89,6.74,7.42
HexNAc ₈ Hex ₇ Fuc ₃	0.57,2.67,2.96,4.22,6.45 7.27,7.62,8.02,11.87
HexNAc ₅ Hex ₃ Fuc ₄	0.27,1.41,1.97,4.4,0.37 0.98,1.62,3.2,6.32,10.42
HexNAc ₆ Hex ₅ Fuc ₃ NeuAc ₂	0.47,1.61,2.4,4.56,6.7 9.93,10.58,11.42,2.67
HexNAc ₆ Hex ₆ Fuc ₁ NeuAc ₁	0.44,1.86,2.56,6.81,7.14

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₈ Hex ₉ Fuc ₁	7.1,10.51
HexNAc ₆ Hex ₄ Fuc ₅	0.77,1.78,6.69
	0.0,0.2,1.16,1.57,2.28
	2.96,4.5,5.18,6.09,6.66
	7.24,7.78,6.64,7.25
HexNAc₆Hex₇NeuAc₃	7.25
HexNAc ₆ Hex ₆ Fuc ₂ NeuAc ₂	0.43,1.16,2.28,3.06,3.26
	4.15,6.2,6.48,6.72,7.07
	8.22,8.63,10.42
HexNAc ₈ Hex ₉ Fuc ₁ NeuAc ₁	1.9,4.0,4.34,4.54,5.41
	6.38,6.63,6.8,7.04
HexNAc ₆ Hex ₆	0.63,1.94,4.59,5.59,5.85
	6.15,6.48,7.04,7.25,7.77
	0.0,0.38,1.07,2.01,2.46
	3.38,4.25,4.68,5.02,5.16
	5.88,6.11,6.76,8.06
HexNAc₃Hex₄Fuc₁	0.8,1.49,2.42,2.82,4.01
	4.44,4.97,0.0,0.34
HexNAc ₆ Hex ₅ Fuc ₄ NeuAc ₁	0.28,2.92,3.98,6.27,7.32
	8.08,2.25
HexNAc ₉ Hex ₁₀ NeuAc ₁	9.27
HexNAc₃Hex₃Fuc₁	0.46,3.56,3.92
HexNAc ₈ Hex ₈ Fuc ₁	0.45,1.37,7.4,7.62
HexNAc₅Hex₆Fuc₁NeuAc₂	6.59,6.75,6.96,7.15,7.61
	6.58,7.08
HexNAc ₉ Hex ₈ Fuc ₁ NeuAc ₁	7.87,8.06,8.22
HexNAc ₄ Hex ₄ Fuc ₂	0.29,0.81,1.45,2.46,3.63
	4.38,5.0,5.13,5.28,5.96
	6.64,7.27,0.54,4.32
HexNAc ₆ Hex ₃	0.0,1.7,1.07,4.02,5.24
	6.09
HexNAc ₁₀ Hex ₇ Fuc ₁	1.23,1.41,4.66,6.08,6.74
	7.11
HexNAc ₅ Hex ₅ Fuc ₂ NeuAc ₁	0.34,1.03,1.71,5.2,5.7
	6.22,6.63,7.06,7.46,1.9
	6.32,6.62,7.04
HexNAc ₆ Hex ₃ Fuc ₄	0.0,0.34,1.17,2.69,3.9
	5.54,7.06,7.63,1.33,1.69
HexNAc ₉ Hex ₈ Fuc ₃	7.74,7.93
HexNAc ₆ Hex ₄ Fuc ₄ NeuAc ₁	0.32,1.49,2.33,2.82,4.4
HexNAc₃Hex₃	0.0,3.22,3.66
HexNAc ₉ Hex ₈ Fuc ₃ NeuAc ₁	4.89,10.05

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₅ Hex ₄ Fuc ₄ NeuAc ₁	0.38,1.28,5.39,6.49,6.66 6.38
HexNAc₄Hex₄Fuc₁	0.8,3.12,4.31,4.6,4.86 5.38,5.78,6.68,7.18,13.52
HexNAc ₄ Hex ₅ Fuc ₂	0.24,0.45,1.29,4.3,4.53 5.64,6.4,0.25,4.11,4.83 5.02,5.66,5.98
HexNAc ₉ Hex ₉ NeuAc ₁	6.16,8.25,9.57,10.46
HexNAc ₆ Hex ₃ Fuc ₅	0.25,0.42,1.49,2.71,3.98 5.26,5.54,6.28,6.45,6.72 7.0,1.74,3.09,6.68
HexNAc₅Hex₆NeuAc₃	2.13,6.64,6.92,7.4,2.18
HexNAc ₆ Hex ₇ Fuc ₂	6.98,0.41,0.77,1.47,3.84 4.08,4.33,4.56,4.98,5.22 5.44,5.77,6.01,6.32,6.62 6.85,7.16,7.71,7.9
HexNAc ₆ Hex ₄ Fuc ₃	0.3,0.54,1.24,2.24,2.82 3.06,3.36,4.3,5.14,6.0 6.96,1.57,1.9,2.89
HexNAc ₈ Hex ₉ Fuc ₃	1.53,4.3,7.19
HexNAc ₁₀ Hex ₇	1.21,1.74,2.77,3.29,5.94 6.53
HexNAc ₆ Hex ₄ Fuc ₅ NeuAc ₁	0.29,2.29,3.23,5.85,6.45 7.61,8.11,8.33,8.98,2.38 6.51,7.02,7.91
HexNAc ₇ Hex ₇ Fuc ₂	0.4,1.62,3.19,4.23,5.45 6.55,7.01,7.86,2.02,5.53
HexNAc₄Hex₅NeuAc₂	0.0,4.56,5.98,6.22,6.53 6.81,7.7,8.48,12.94,13.3 13.84,1.12,4.54,4.97,5.3 6.39,6.63,7.01
HexNAc ₆ Hex ₆ Fuc ₅ NeuAc ₁	0.52,2.94,3.61,5.6
HexNAc ₁₀ Hex ₉ Fuc ₄	9.59,10.58
HexNAc ₆ Hex ₇ Fuc ₃ NeuAc ₃	4.52,7.44,10.38
HexNAc ₆ Hex ₆ Fuc ₃ NeuAc ₂	1.04,2.89,3.47,4.01,5.48 5.76,6.15,6.48,6.79,6.95 7.59,9.52,9.88
HexNAc ₆ Hex ₅ Fuc ₄	0.17,0.9,1.43,1.94,3.2 3.83,4.48,4.77,5.07,5.31 5.59,5.81,6.06,6.42,6.83 7.16,8.12,7.03
HexNAc ₉ Hex ₈ Fuc ₂	2.56,7.85,8.12

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₁₀ Hex ₁₁	4.9,6.06
HexNAc ₅ Hex ₄ Fuc ₂ NeuAc ₁	1.03,1.45,1.94,5.24,5.51 6.04,0.29,1.74,2.24,2.69 3.29,4.09,5.36,6.79
HexNAc ₁₀ Hex ₉	1.4,1.7,3.47,4.18,4.75 6.23,7.3,7.8,8.68
HexNAc ₂ Hex ₃	0.0,2.25
HexNAc ₆ Hex ₄ NeuAc ₁	1.36,2.28,3.77,4.54,4.89 5.46,5.69,6.06,6.64,7.1 0.42,1.32,2.78,3.44,5.98 6.43,8.63
HexNAc ₁₀ Hex ₇ Fuc ₅	7.02,8.7
HexNAc ₆ Hex ₆ Fuc ₂ NeuAc ₁	1.03,2.01,2.82,5.79,6.7 6.92
HexNAc ₆ Hex ₅ Fuc ₁ NeuAc ₂	0.41,2.36,3.75,5.13,6.81 7.58
HexNAc₆Hex₆Fuc₁NeuAc₃	0.71,2.99,6.62,7.69,7.99
HexNAc ₇ Hex ₈ Fuc ₁ NeuAc ₁	1.45,2.62,3.16,7.11,11.39
HexNAc ₁₀ Hex ₁₁ Fuc ₁	7.13,7.89,8.46
HexNAc ₈ Hex ₉ Fuc ₃ NeuAc ₁	8.8,10.47
HexNAc₆Hex₇NeuAc₁	0.22,1.57,2.25,2.64,6.02 6.32,6.71,7.02,10.58,11.94
HexNAc ₆ Hex ₆ Fuc ₂	0.34,0.57,1.66,2.6,5.55 6.34,6.74,7.19,2.36
HexNAc₆Hex₇Fuc₁NeuAc₄	8.39,8.63
HexNAc ₉ Hex ₁₀ Fuc ₂	1.97,9.08
HexNAc ₆ Hex ₇ Fuc ₁	0.25,1.36,2.81,3.1,3.54 3.94,4.3,4.5,4.99,5.24 5.51,5.83,6.18,6.68,7.03 6.86
HexNAc ₆ Hex ₅ Fuc ₁	2.06,5.98,6.24,6.78,7.05 0.28,0.67,3.47,4.0,4.36 4.6,4.76,4.95,5.35,6.06 6.51
HexNAc ₁₀ Hex ₇ Fuc ₄	1.12,6.33
HexNAc ₆ Hex ₄ Fuc ₂ NeuAc ₁	0.24,0.63,1.61,2.06,3.76 5.74,6.98,10.48
HexNAc ₅ Hex ₆ Fuc ₃ NeuAc ₂	0.42,1.57,2.14,4.01,5.96 6.34,6.38,6.78,12.21
HexNAc ₆ Hex ₆ Fuc ₅ NeuAc ₂	1.36,3.47,4.18,4.75,6.19 6.6,6.86,7.4,7.85,8.71
HexNAc₆Hex₇Fuc₁NeuAc₁	1.41,2.17,2.56,5.4,5.82

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc₅Hex₆Fuc₂NeuAc₃	6.66,6.96,7.16,7.04
HexNAc ₆ Hex ₆ NeuAc ₃	7.49,7.72,7.83,8.34,11.52
HexNAc ₅ Hex ₆ Fuc ₄ NeuAc ₃	1.12,2.82,7.07
HexNAc ₁₀ Hex ₉ Fuc ₃ NeuAc ₂	2.24,5.39,8.07,8.45,9.32
HexNAc ₁₀ Hex ₇ Fuc ₃	12.05
	1.7,2.81,6.12,6.41,7.22
	7.82,9.73
HexNAc ₅ Hex ₅ Fuc ₃ NeuAc ₂	1.05,1.49,2.31,2.96,3.21
	3.57,3.77,4.18,5.01,5.88
	6.59,7.1,9.05,9.27,2.09
HexNAc₆Hex₄Fuc₁	0.57,1.37,6.22,6.42,0.0
	0.29,1.21,1.36,2.74,4.3
	5.94
HexNAc ₆ Hex ₆ Fuc ₄ NeuAc ₁	0.29,2.28,3.54,6.59,7.36
HexNAc ₆ Hex ₅ Fuc ₄ NeuAc ₂	0.85,1.97,2.99,4.12,6.45
	7.01,7.36,8.6
HexNAc ₆ Hex ₃ Fuc ₂	0.38,1.41,5.07,5.92,6.53
	0.0,0.88,1.32,4.67,6.33
HexNAc ₇ Hex ₈ Fuc ₂ NeuAc ₁	0.82,7.11,7.66
HexNAc ₆ Hex ₇ Fuc ₄ NeuAc ₂	1.57,3.9,6.81,7.3,7.75
	8.94,9.96,10.57
HexNAc ₆ Hex ₇ Fuc ₃	0.26,0.63,1.78,2.21,3.74
	4.35,5.67,6.37,6.74,6.98
	7.32,7.59,8.04,8.92
HexNAc₄Hex₅NeuAc₁	0.26,0.98,1.49,2.05,2.43
	2.99,3.73,4.25,4.96,5.19
	5.44,6.04,6.48,7.04,8.09
	0.0,0.37,1.32,1.82,4.54
	5.06,5.5,5.65,5.8,6.11
	6.29,6.5,13.52,14.06
HexNAc ₅ Hex ₄ Fuc ₃ NeuAc ₁	0.43,1.99,2.89,5.23,5.75
	8.25,1.45,1.94
HexNAc ₃ Hex ₃ Fuc ₂	0.72,2.44,2.94,3.3,4.78
	5.1,5.59,6.09,0.01
HexNAc ₈ Hex ₈	0.71,2.49,3.77,5.9,6.47
	6.9,7.35
HexNAc ₄ Hex ₅ Fuc ₂ NeuAc ₂	0.67,2.51,6.86,2.78,6.96
HexNAc₅Hex₃Fuc₁	0.47,0.5,1.4,2.31,5.21
	5.48,5.74
HexNAc ₅ Hex ₅ Fuc ₄ NeuAc ₂	1.33,2.21,4.12,5.73,6.19
	6.56,6.98,7.42,7.7,11.47
	12.47

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₅ Hex ₅ Fuc ₂ NeuAc ₂	0.37,1.81,2.53,2.9,4.5 4.85,5.27,5.88,6.16,6.73 7.08,7.57,8.92,11.43,11.62
HexNAc ₆ Hex ₇ Fuc ₃ NeuAc ₁	0.69,2.85,4.06,6.83,7.44
HexNAc ₉ Hex ₇ Fuc ₂	7.23
HexNAc ₁₀ Hex ₉ Fuc ₃	4.36,8.84
HexNAc ₆ Hex ₇ Fuc ₄ NeuAc ₁	1.35,5.91,6.54,7.28,8.01
HexNAc₄Hex₅Fuc₁NeuAc₂	0.28,1.49,6.26,6.49,6.79 7.28,6.18,6.78,7.28
HexNAc ₁₀ Hex ₈	0.94,1.57,4.41,4.86,7.07 7.89
HexNAc ₆ Hex ₇ Fuc ₂ NeuAc ₃	8.63,8.95
HexNAc ₆ Hex ₅ NeuAc ₂	0.3,1.25,1.86,4.57,5.54 6.16,6.31,6.65,9.8
HexNAc ₆ Hex ₆ NeuAc ₂	0.43,2.13,2.81,5.56,6.58 7.15
HexNAc ₅ Hex ₆ Fuc ₂ NeuAc ₁	0.3,1.61,2.05,5.17,5.46 6.39,7.01,7.34,7.89,5.76 5.99,6.4,6.62,7.14,7.83
HexNAc ₆ Hex ₇ Fuc ₄ NeuAc ₃	3.96,8.47,9.59
HexNAc ₁₀ Hex ₈ Fuc ₃	4.54,8.43,8.79,9.44
HexNAc₆Hex₇Fuc₁NeuAc₂	0.28,1.41,3.44,5.59,7.3 7.67
HexNAc ₆ Hex ₆ Fuc ₃	0.0,0.34,1.04,1.77,3.74 4.05,5.32,6.88,7.24,7.66
HexNAc ₅ Hex ₃ Fuc ₃	0.4,1.15,2.05,2.6,0.29 1.2,1.94,2.28,6.59,7.42
HexNAc ₆ Hex ₆ NeuAc ₁	2.92,6.11,0.62,4.42,6.09 6.4,7.48
HexNAc ₈ Hex ₇ Fuc ₂	7.19,7.52,7.79,7.11
HexNAc₅Hex₅NeuAc₂	0.33,1.29,2.71,2.92,3.61 4.13,4.51,5.18,5.29,6.06 6.62,5.98,6.43,6.75
HexNAc ₆ Hex ₃ Fuc ₁	0.32,1.49,5.67,0.52,2.32 3.36,4.8,5.69,6.64
HexNAc ₅ Hex ₆ Fuc ₂	0.42,2.05,4.98,5.48,6.17 6.5,6.74,1.55,5.86,6.26 6.55,6.82
HexNAc ₈ Hex ₈ NeuAc ₁	0.16,2.77,3.4,4.06,4.56 4.94,5.4,5.87,6.17,6.61 6.97,7.41
HexNAc ₁₀ Hex ₈ Fuc ₃ NeuAc ₁	9.7

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc ₆ Hex ₃ Fuc ₃	0.0,0.33,1.9,2.36,2.58 4.95,5.49,0.58,1.98,4.08 6.46
HexNAc ₆ Hex ₇	0.17,0.3,0.79,2.22,4.75 5.03,5.19,5.83,6.07,7.48 7.73,7.86,1.74,6.13,6.68 7.01
HexNAc ₆ Hex ₆ Fuc ₄ NeuAc ₃	3.06,7.53,9.41
HexNAc₅Hex₄Fuc₁NeuAc₁	0.6,5.19,5.37,6.22,6.37 1.11,1.86,5.26,6.28
HexNAc₆Hex₇Fuc₂NeuAc₄	9.27,9.7
HexNAc ₉ Hex ₁₀ NeuAc ₂	9.0
HexNAc ₆ Hex ₅ Fuc ₅ NeuAc ₁	0.76,4.65,6.41,8.8,6.98
HexNAc ₆ Hex ₇ Fuc ₅ NeuAc ₁	0.59,4.23,6.25
HexNAc ₁₀ Hex ₈ Fuc ₂	0.94,8.0
HexNAc ₇ Hex ₈ Fuc ₁	0.32,1.32,2.24,2.93,5.68 6.45,6.73,8.53,5.9,6.35 7.96
HexNAc ₁₀ Hex ₁₀ NeuAc ₁	8.12,9.53
HexNAc₄Hex₅Fuc₁NeuAc₁	0.0,0.24,1.1,1.92,3.06 3.57,4.89,5.43,5.88,6.2 6.52,6.74,7.34,13.99,0.26 1.86,5.48,5.9,6.42,6.74 6.93
HexNAc₃Hex₄	0.3,0.47,3.74,4.14,4.3 4.52
HexNAc ₈ Hex ₈ Fuc ₂ NeuAc ₁	1.61,4.83,6.28,6.92,7.27 7.57,8.73,9.08,9.73,10.63
HexNAc ₆ Hex ₅ Fuc ₅	0.71,1.16,2.35,2.96,4.4 5.78,6.25,7.08,7.25
HexNAc ₇ Hex ₈ NeuAc ₁	1.44,3.44,6.43,6.74,6.79 7.11
HexNAc ₃ Hex ₄ Fuc ₂ NeuAc ₁	0.71,1.81,6.32,0.24,0.99 1.36,1.82,3.06,6.08,10.95
HexNAc ₄ Hex ₅ Fuc ₂ NeuAc ₁	0.27,1.16,2.2,4.86,6.48 6.72,7.24,0.8,1.37,1.98 2.17,4.4,4.85,5.65,6.06 6.76,7.23,7.48
HexNAc ₇ Hex ₈	1.03,2.28,4.06,5.39,6.43 8.34,9.85,6.74,7.06
HexNAc₅Hex₆NeuAc₁	0.2,2.92,5.74,6.08,6.3 6.69,1.32,2.29,5.44,6.14

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Glycan Annotated	GUI
	6.66,6.84
HexNAc ₂ Hex ₃ Fuc ₁	0.0,0.34
HexNAc ₆ Hex ₄ Fuc ₃ NeuAc ₁	0.34,2.22,2.78,2.22
HexNAc₄Hex₅	0.36,4.65,5.1,5.35,5.88
	0.32,1.94
HexNAc ₅ Hex ₆ Fuc ₄ NeuAc ₂	0.24,3.06,6.56,6.95,9.22
	11.44
HexNAc ₉ Hex ₈ Fuc ₂ NeuAc ₁	8.66,8.9
HexNAc ₄ Hex ₄ Fuc ₃	0.22,0.58,0.9,4.85,5.22
	5.38,6.09,6.38,6.69,6.97
	7.15,0.28,0.94,4.88,5.58
HexNAc₄Hex₃	0.42,0.63,1.18,3.7,4.06
	4.25
HexNAc ₈ Hex ₉	1.45,2.21,7.0,8.7
HexNAc₆Hex₆Fuc₁NeuAc₂	0.76,2.46,6.16,7.1,7.24
	7.38,7.7
HexNAc₅Hex₅NeuAc₁	0.22,1.25,5.43,5.76,6.18
	6.47,1.82,4.42,5.77,6.08
	6.43
HexNAc ₁₀ Hex ₈ Fuc ₅	5.41,10.58
HexNAc ₈ Hex ₇	0.43,0.71,2.85,4.01,5.4
	6.56
HexNAc ₅ Hex ₆ Fuc ₄	1.92,5.03,5.32,5.54,6.33
	6.64,7.45,6.09,7.29,7.9
HexNAc₃Hex₄Fuc₁NeuAc₁	0.57,1.16,5.44,1.02,1.37
	4.3,5.36
HexNAc₅Hex₆Fuc₁NeuAc₃	6.91,7.17,7.56,6.83,11.74
HexNAc ₁₀ Hex ₉ Fuc ₂	4.3,4.86,6.09,6.88
HexNAc ₉ Hex ₈ Fuc ₄	8.4,8.63
HexNAc ₆ Hex ₄ Fuc ₄	0.32,0.76,0.99,1.86,2.29
	2.85,3.44,3.75,4.52,4.91
	5.22,5.86,7.2,2.33,10.58
HexNAc ₅ Hex ₅ Fuc ₄ NeuAc ₁	0.37,1.16,2.35,3.23,3.47
	5.49,6.45,6.73,7.11,7.75
HexNAc₅Hex₅Fuc₁NeuAc₁	0.57,1.51,2.92,5.94,6.45
	6.77,0.94,1.44,1.98,2.75
	5.05,5.9,6.18,6.51,6.81
	7.02,7.65
HexNAc ₁₀ Hex ₁₀ Fuc ₁	7.48,10.58
HexNAc₅Hex₅	0.28,0.58,5.86,0.21,3.09
	5.12,5.51,5.9
HexNAc ₉ Hex ₉ NeuAc ₂	1.11,7.61

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc₆Hex₇Fuc₃NeuAc₄	9.53
HexNAc ₈ Hex ₉ Fuc ₂	1.98,7.58,10.37
HexNAc₄Hex₄NeuAc₁	0.88,4.48,5.08,5.57,6.02
	6.54,7.74,0.0,0.38,4.58
	4.7,5.28,5.55,6.56
HexNAc ₅ Hex ₆	0.0,0.57,1.94,5.48,6.12
	0.3,2.17,2.38,2.76,5.5
	6.04,6.75,7.08,7.47,7.61
	8.06
HexNAc ₆ Hex ₆ Fuc ₂ NeuAc ₃	0.28,3.7,4.22,6.96,7.27
	7.61,7.89,8.13,8.74
HexNAc ₈ Hex ₉ NeuAc ₁	1.37,2.21,6.18,6.9,7.07
HexNAc ₁₀ Hex ₁₀	6.61,7.14,8.94,9.73,10.58
HexNAc ₆ Hex ₆ Fuc ₄ NeuAc ₂	1.07,1.29,2.28,3.77,4.56
	5.18,5.91,6.1,6.4,6.66
	6.91,7.19,7.5,7.83,8.3
	9.22,10.54
HexNAc ₄ Hex ₃ Fuc ₂	0.3,0.72,1.21,1.59,2.19
	4.59,0.77
HexNAc ₉ Hex ₈	1.16,3.21,3.67,4.4,7.99
HexNAc ₇ Hex ₈ Fuc ₂	0.22,2.01,2.43,3.92,6.32
	6.66,7.09,7.36,9.84
HexNAc ₅ Hex ₆ Fuc ₃	0.77,1.15,6.02,6.37,6.78
	5.08,6.6,7.13,8.27
HexNAc ₁₀ Hex ₈ Fuc ₂ NeuAc ₁	8.31,8.79
HexNAc ₉ Hex ₁₀	2.92,7.89
HexNAc₄Hex₅Fuc₁	0.42,1.61,4.8,5.1,5.29
	5.5,5.75,6.09,6.31,0.54
	4.65,5.17
HexNAc ₄ Hex ₅ Fuc ₃	0.3,1.07,2.06,4.59,4.85
	5.18,5.4,5.9,6.66,6.92
	7.66,0.21,1.29,1.78,2.96
	4.52,5.05,5.49,6.28,6.51
HexNAc ₉ Hex ₁₀ Fuc ₁	2.1,8.35
HexNAc ₅ Hex ₄ Fuc ₂	0.38,0.81,1.94,4.83,5.38
	0.16,1.25,3.54,5.13,6.38
HexNAc ₄ Hex ₄ Fuc ₃ NeuAc ₁	0.38,1.41,2.1,2.67,2.85
	3.09,3.3,4.3,4.5,5.27
	5.51,5.79,6.19,6.42,6.97
	0.36,1.2,2.01,2.24,5.55
	6.29,6.76,7.04,7.52,7.79
HexNAc₅Hex₄	0.34,0.49,1.65,5.26,5.62

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Glycan Annotated	GUI
HexNAc ₄ Hex ₃ Fuc ₃	5.87,6.77,0.28,0.72,5.38 0.81,1.11,4.01,4.9,5.95 7.01,0.17
HexNAc ₁₁ Hex ₁₁ Fuc ₂	11.83
HexNAc₅Hex₅Fuc₁NeuAc₂	5.46,6.41,6.81,0.2,0.68 1.78,2.24,5.58,5.95,6.5 6.84,7.0,7.27,7.59
HexNAc ₉ Hex ₉ Fuc ₁ NeuAc ₂	6.4,8.8,11.59
HexNAc ₉ Hex ₈ Fuc ₁	7.44
HexNAc₅Hex₆Fuc₁	0.76,1.73,5.85,6.17,6.56 8.87,0.53,2.6,4.67,6.13
HexNAc ₁₀ Hex ₈ Fuc ₄	6.71,8.31
HexNAc ₆ Hex ₇ Fuc ₂ NeuAc ₁	0.59,1.16,6.11,6.58,7.04
HexNAc ₆ Hex ₇ Fuc ₅ NeuAc ₂	4.58,7.0,7.27,9.73
HexNAc ₉ Hex ₉ Fuc ₁ NeuAc ₁	3.67,8.93,10.5
HexNAc ₆ Hex ₆ Fuc ₄	0.52,2.88,4.18,5.8,6.58 6.88,7.11,10.42
HexNAc ₈ Hex ₇ Fuc ₁	0.71,1.53,1.82,4.8,6.93 7.18,7.54,6.74
HexNAc₄Hex₄	0.28,0.63,1.12,1.91,2.35 4.19,4.58,4.91,5.04,5.34 5.98,0.0
HexNAc ₁₀ Hex ₁₁ Fuc ₁ NeuAc ₂	10.54
HexNAc ₈ Hex ₉ NeuAc ₂	6.51,7.59,9.54
HexNAc ₁₀ Hex ₁₀ Fuc ₅ NeuAc ₁	12.16
HexNAc ₆ Hex ₅	0.0,0.35,1.08,2.16,2.51 3.08,5.9,6.19,0.54,1.4 2.49,5.68,6.28,6.64,10.44
HexNAc ₅ Hex ₄ Fuc ₃	0.5,2.77,3.7,5.27,5.76 6.98,1.33,4.01,5.79,6.97
HexNAc ₈ Hex ₉ Fuc ₁ NeuAc ₂	4.76,8.92
HexNAc ₅ Hex ₄ Fuc ₄	0.99,2.21,6.4,6.67,6.88 0.59,1.69,2.77,3.8,6.6
HexNAc ₅ Hex ₆ Fuc ₄ NeuAc ₁	0.68,2.54,5.23,5.65,6.2 6.72,7.09,7.73,2.1,6.03
HexNAc₄Hex₃Fuc₁	0.0,0.67,1.06,1.82,2.57 3.36,4.06,4.38,4.78,5.08 5.41,7.71,13.5,14.17
HexNAc₃Hex₄NeuAc₁	0.0,0.9,4.72,0.32,1.02 1.33,1.62,2.15,4.74,5.04 5.21,6.21,6.5,6.89,7.48 7.76

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Table S1 – Continued from previous page

Glycan Annotated	GUI
HexNAc₅Hex₃	0.0,0.18,1.16,4.9,0.18 1.61,2.66,3.04,4.92,5.14
HexNAc ₅ Hex ₆ Fuc ₃ NeuAc ₃	0.26,2.2,5.99,7.49,8.36 9.27
HexNAc ₆ Hex ₅ Fuc ₂ NeuAc ₁	1.79,6.99,1.65
HexNAc ₁₀ Hex ₈ NeuAc ₁	5.75,8.95
HexNAc ₇ Hex ₇	0.38,0.8,1.61,2.31,5.1 5.36,5.58,5.97,6.35,6.81 1.78,6.43,6.86,7.9
HexNAc ₅ Hex ₅ Fuc ₄	0.29,1.57,2.28,2.58,5.76 6.32,7.11,3.47,6.81,8.66
HexNAc ₆ Hex ₆ Fuc ₅	0.17,0.37,1.44,2.53,3.47 4.91,6.11,6.45,6.98,7.55 7.82,6.78
HexNAc ₉ Hex ₉ Fuc ₃	2.77,8.82
HexNAc ₆ Hex ₆ Fuc ₅ NeuAc ₃	6.65,10.42
HexNAc ₁₀ Hex ₉ Fuc ₁ NeuAc ₁	9.01
HexNAc ₈ Hex ₈ Fuc ₃ NeuAc ₁	4.52,7.05,7.48,9.8,10.58
HexNAc ₄ Hex ₄ Fuc ₂ NeuAc ₁	0.22,0.67,1.96,2.34,3.36 4.61,5.75,7.21,7.88,1.12 4.56,6.26,6.68,9.81
HexNAc ₉ Hex ₇	0.32,2.24,4.85,7.04,7.27
HexNAc ₅ Hex ₃ Fuc ₂	0.39,1.41,2.71,0.5,1.03 2.42,6.67
HexNAc ₉ Hex ₇ Fuc ₄	7.18,7.52,8.63,8.95
HexNAc ₆ Hex ₇ Fuc ₅	0.57,1.07,6.54,7.06,7.28 8.68
HexNAc ₅ Hex ₆ Fuc ₃ NeuAc ₁	0.32,1.29,3.16,4.42,5.11 6.06,7.77,8.49,6.5,7.18 8.65
HexNAc ₁₀ Hex ₈ Fuc ₁ NeuAc ₁	5.05,6.74
HexNAc ₄ Hex ₅ Fuc ₃ NeuAc ₂	0.27,6.63,6.8
HexNAc ₆ Hex ₇ Fuc ₄	0.3,1.12,1.45,2.53,3.0 5.14,5.75,6.18,6.37,6.62 6.97,7.4,7.71
HexNAc ₆ Hex ₅ NeuAc ₁	0.4,1.66,2.13,4.04,4.73 5.52,6.7,1.37,2.05,6.33 7.04,7.74,7.87,10.54
HexNAc ₈ Hex ₈ Fuc ₁ NeuAc ₁	0.22,1.53,6.23,6.78,6.95 7.88,8.69,10.46
HexNAc ₆ Hex ₅ Fuc ₃ NeuAc ₁	0.36,1.33,2.06,2.78
HexNAc ₃ Hex ₄ Fuc ₂	0.0,0.28,0.77,1.31,2.31

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Glycan Annotated	GUI
HexNAc₅Hex₅Fuc₁	3.54,3.83,4.06,4.36,4.5 4.84,5.08,5.73,6.16,6.66 7.16,7.82,8.92,9.21,9.7 0.2,1.29,2.81,5.54,5.94 6.11,6.32,0.17,0.76,1.21 2.06,5.46,5.94,6.32
HexNAc ₆ Hex ₆ Fuc ₃ NeuAc ₃	1.94,4.35,6.42,6.96,7.52 8.61
HexNAc ₇ Hex ₇ Fuc ₁	0.63,1.69,2.4,2.92,5.31 5.83,6.29,6.66,7.04,7.22 7.39
HexNAc ₉ Hex ₈ NeuAc ₁	1.08,4.18,5.34,9.03
HexNAc ₅ Hex ₅ Fuc ₃ NeuAc ₁	0.38,1.78,3.92,5.65,5.87 6.18,6.6,7.03,7.6,5.7 6.54,7.02
HexNAc ₅ Hex ₅ Fuc ₃	0.53,0.89,1.53,1.78,2.28 5.78,6.45,7.0,7.28,3.75 5.28,6.38,6.9
HexNAc ₆ Hex ₄	0.28,1.04,5.6,0.44,1.25 2.67,4.45,5.18,5.53,6.59
HexNAc₄Hex₄Fuc₁NeuAc₁	0.17,0.38,1.04,1.49,1.82 2.12,2.51,5.6,5.91,6.78 0.0,0.67,1.74,4.5,5.4 5.64
HexNAc ₉ Hex ₁₀ Fuc ₄ NeuAc ₁	6.69
HexNAc ₁₀ Hex ₁₀ Fuc ₂	8.42
HexNAc ₉ Hex ₁₀ Fuc ₁ NeuAc ₂	4.18
HexNAc ₉ Hex ₈ Fuc ₄ NeuAc ₁	10.58
HexNAc ₉ Hex ₁₀ Fuc ₂ NeuAc ₂	10.63
HexNAc ₁₀ Hex ₈ Fuc ₅ NeuAc ₁	10.58
HexNAc ₉ Hex ₁₀ Fuc ₃ NeuAc ₁	10.5
HexNAc ₈ Hex ₉ Fuc ₂ NeuAc ₁	6.54
HexNAc ₉ Hex ₁₀ Fuc ₁ NeuAc ₁	8.96,10.38
HexNAc ₁₀ Hex ₈ Fuc ₄ NeuAc ₁	10.54
HexNAc ₉ Hex ₉ Fuc ₂ NeuAc ₁	9.92
HexNAc ₈ Hex ₉ Fuc ₂ NeuAc ₂	9.02,9.74
HexNAc ₉ Hex ₉ Fuc ₄	7.6
HexNAc ₁₀ Hex ₉ Fuc ₂ NeuAc ₁	7.44