

Supplemental Table

1

Quantitation of N-linked glycans from murine embryonic stem cells and embroid bodies

m/z	Charge state	Glycan structure	EB(¹³ C)/ES(D) Run 1	EB(¹³ C)/ES(D) Run 2	EB(¹³ C)/ES(D) Run 3	EB(¹³ C)/ES(D) %SDEV
1188.65	[M+1Na] ¹⁺		0.18	-0.32	-0.04	24.96
1395.75	[M+1Na] ¹⁺		0.60	0.17	0.10	27.23
812.93, 1602.86	[M+2Na] ²⁺ , [M+1Na] ¹⁺		0.16	-0.17	0.01	16.48
916.48, 1809.97	[M+2Na] ²⁺ , [M+1Na] ¹⁺		-0.56	-1.03	-0.80	23.61
1020.04	[M+2Na] ²⁺		-0.27	-0.74	-0.44	23.99
756.73, 1123.59	[M+3Na] ³⁺ , [M+2Na] ²⁺		-1.54	-1.32	-1.12	21.35
825.76, 1227.15	[M+3Na] ³⁺ , [M+2Na] ²⁺		-0.47	-0.93	-0.41	28.12
1330.71	[M+2Na] ²⁺		-1.29	-1.53	-1.16	18.77
1365.75	[M+1Na] ¹⁺		0.93	0.37	0.50	29.42
1572.85	[M+1Na] ¹⁺		0.19	0.08	0.25	8.58
1779.96	[M+1Na] ¹⁺		-0.32	-0.64	-0.34	17.80
1005.03, 1987.07	[M+2Na] ²⁺ , [M+1Na] ¹⁺		0.08	-0.07	0.32	19.69
942.51	[M+2Na] ²⁺		-0.06	0.05	-0.18	11.60
957.51	[M+2Na] ²⁺		0.15	0.51	-0.06	29.03
1046.06	[M+2Na] ²⁺		-0.38	-0.64	-0.36	15.75

Mass	Formula	Structure	$\Delta_{\text{H}}^{\text{H}}/\text{eV}$	$\Delta_{\text{H}}^{\text{H}}/\text{eV}$	$\Delta_{\text{H}}^{\text{H}}/\text{eV}$	Relative Abundance (%)
1046.06	$[\text{M}+2\text{Na}]^{2+}$		-0.38	-0.64	-0.36	15.75
1061.07	$[\text{M}+2\text{Na}]^{2+}$		-0.74	-1.27	-0.77	29.72
1149.62	$[\text{M}+2\text{Na}]^{2+}$		-0.57	-0.99	-0.69	21.67
978.02	$[\text{M}+2\text{Na}]^{2+}$		-0.90	-0.95	-0.95	2.77
1066.57	$[\text{M}+2\text{Na}]^{2+}$		-0.84	-1.30	-1.21	24.12
1081.58	$[\text{M}+2\text{Na}]^{2+}$		-0.86	-1.00	-1.00	7.90
1170.13	$[\text{M}+2\text{Na}]^{2+}$		-0.94	-1.27	-1.18	17.11
1258.68	$[\text{M}+2\text{Na}]^{2+}$		-0.91	-1.15	-1.00	12.35
1185.13	$[\text{M}+2\text{Na}]^{2+}$		0.37	0.41	0.39	2.00
1273.68	$[\text{M}+2\text{Na}]^{2+}$		-1.12	-0.94	-0.80	16.15
1362.24	$[\text{M}+2\text{Na}]^{2+}$		-1.61	-1.86	-1.49	18.91
1264.67	$[\text{M}+2\text{Na}]^{2+}$		-0.68	-0.89	-0.50	19.11
1368.23	$[\text{M}+2\text{Na}]^{2+}$		-0.84	-1.18	-1.09	17.90
1427.26	$[\text{M}+2\text{Na}]^{2+}$		0.29	0.14	-0.03	15.80

All expression ratios calculated as Log_2 ; %SDEV calculated as the relative percent standard deviation taken from the average expression ratio.

Supplemental Figure 1

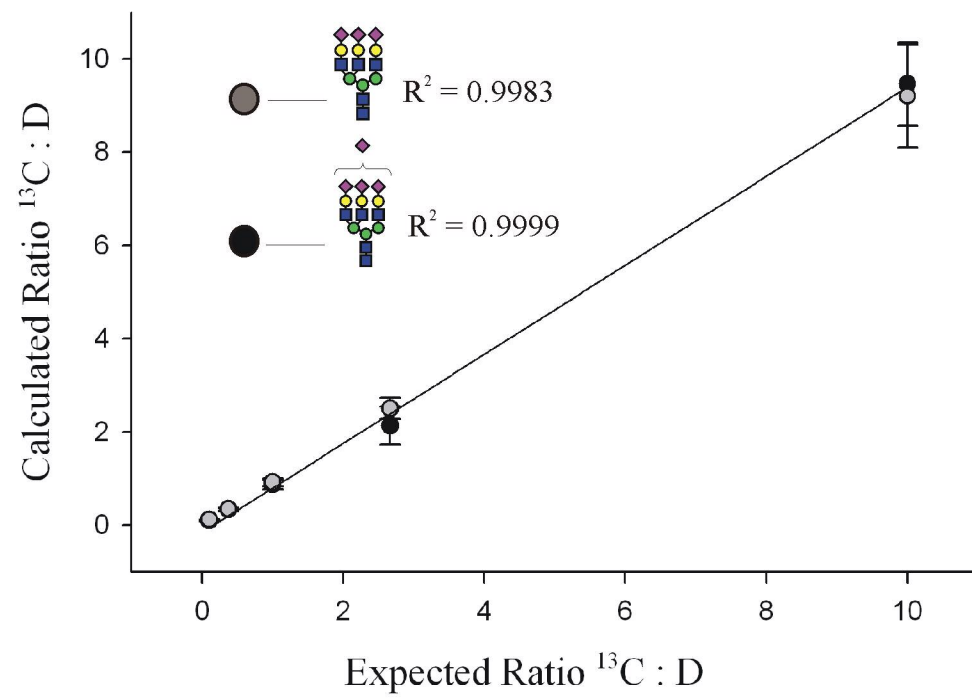
Correlation between calculated and expected ratios for quantitation of two fetuin glycans by QUIBL. In each experiment the $^{13}\text{CH}_3$ and $^{12}\text{CH}_2\text{D}$ labeled glycans were mixed together at the ratios 10:1, 8:3, 1:1, 3:8, and 1:10 ($^{13}\text{CH}_3$: $^{12}\text{CH}_2\text{D}$) and analyzed by FTICR. The calculated expression ratios were determined by comparing the sum of the peak intensities for all isotopes between $^{13}\text{CH}_3$ and $^{12}\text{CH}_2\text{D}$ labeled precursor ions for each glycan. For both glycans a linear correlation was observed between the calculated and the expected ratios with a minimum R^2 of 0.9983.

Supplemental Figure 2

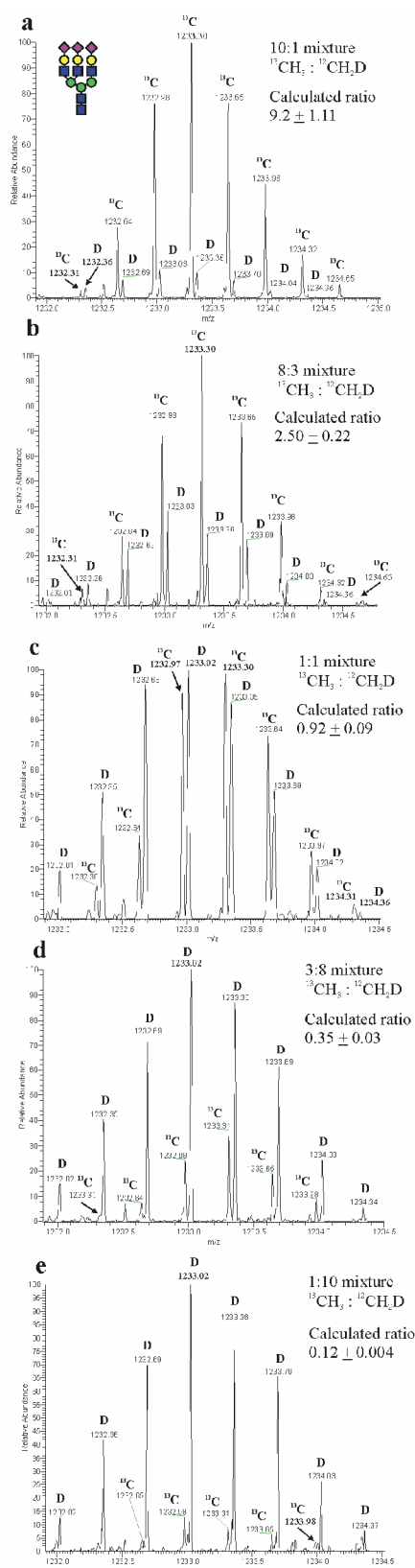
QUIBL analysis of a differently labeled fetuin glycan mixed at five different ratios. Two fetuin glycan mixtures were permethylated in either $^{13}\text{CH}_3\text{I}$ or $^{12}\text{CH}_2\text{DI}$. The two differentially labeled glycan mixtures were then mixed together at the ratios 10:1, 8:3, 1:1, 3:8, and 1:10 ($^{13}\text{CH}_3$: $^{12}\text{CH}_2\text{D}$) and analyzed by FTICR (a,b,c,d,e). Accurate quantitation was achieved at all ratios over two orders of magnitude.

Supplemental Figure 3

MS^n analysis of two di-fucosylated (Lewis X type) N-linked glycans from ES and EB cells. (a, b) MS^2 of the two Lewis X type N-linked glycans. (c) MS^3 of the fragment ion at 1846.00 m/z from MS^2 of the glycan in shown in (a). (d) MS^3 of the fragment ion at 1126.18 m/z from MS^2 of the glycan in shown in (b).



Supplemental Figure 1.



Supplemental Figure 2.

