Supplementary Material

An improved method for the purification of milk oligosaccharides by graphitised carbon-solid phase extraction

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Table S1. *p*-Values from Tukey's post-hoc test for pairwise comparisons of OS and lactose abundances after washing the PGC SPE sorbent with water, 2%, 4%, 6%, or 8% acetonitrile

Fig. S1. LC-MS chromatogram of a bovine milk oligosaccharide sample.

Table S1

p-Values from Tukey's post-hoc test for pairwise comparisons of OS and lactose abundances after washing the PGC SPE sorbent with water, 2%, 4%, 6%, or 8% acetonitrile. [a]

Compound	0% vs 2%	0% vs 4%	0% vs 6%	0% vs 8%	2% vs 4%	2% vs 6%	2% vs 8%	4% vs 6%	4% vs 8%	6% vs 8%
Acidic										
1_1_0_1_0	0.002	0.004	0.098	0.006	0.492	0.0004	0.001	0.0008	0.002	0.086
2_0_0_1_0 (6'-SL)	2.2×10^{-5}	1.2×10^{-5}	0.0006	0.350	0.031	0.0006	3.2×10^{-5}	0.0001	1.6×10^{-5}	0.002
2_0_0_1_0 (3'-SL)	0.042	0.007	0.381	0.038	0.296	0.008	0.002	0.002	0.0006	0.278
2_0_0_2_0	0.001	3.4×10^{-5}	0.004	0.997	0.0009	0.297	0.001	0.0003	3.7×10^{-5}	0.005
2_0_0_0_1	0.0003	0.0001	0.206	0.058	0.110	0.001	8.4×10^{-5}	0.0003	3.5×10^{-5}	0.007
3_0_0_1_0	0.0003	0.0002	0.330	0.0008	0.371	0.0009	2×10^{-5}	0.0004	1.5×10^{-5}	0.0004
3_1_0_1_0	0.002	0.005	0.002	0.195	0.414	0.998	0.009	0.546	0.040	0.011
4_2_0_1_0	0.592	0.020	0.030	0.328	0.078	0.126	0.965	0.986	0.146	0.240
Neutral										
2_1_0_0_0	0.106	0.999	0.002	0.0002	0.129	0.0004	6.6×10^{-5}	0.001	0.0002	0.026
3_0_0_0_0 isomer 1	0.702	0.268	0.001	0.0003	0.071	0.0006	0.0002	0.004	0.0007	0.118
3_0_0_0_0 isomer 2	0.038	0.561	0.0002	4.9×10^{-5}	0.179	0.001	0.0002	0.0004	7.8×10^{-5}	0.038
3_1_0_0_0 isomer 1	0.0004	0.0004	0.002	10^{-4}	0.998	2.9×10^{-5}	1.1×10^{-5}	2.8×10^{-5}	1.1×10^{-5}	0.004
3_1_0_0_0 isomer 2	0.002	0.003	0.001	0.0006	0.988	0.756	0.232	0.530	0.144	0.709
3_1_0_0_0 isomer 3	0.0006	0.001	6.3×10^{-5}	1.2×10^{-5}	0.582	0.009	0.0001	0.003	7×10^{-5}	0.001
3_1_0_0_0 isomer 4	0.008	0.008	0.731	0.0002	0.046	0.001	0.073	0.021	0.003	0.0003
3_2_0_0_0	0.007	0.135	0.950	0.032	0.086	0.012	0.394	0.277	0.607	0.061
3_3_0_0_0	0.802	0.752	0.627	0.532	1.000	0.996	0.978	0.999	0.990	1.000
3_6_1_0_0	0.718	0.317	0.116	0.714	0.883	0.426	1	0.856	0.886	0.429
4_1_0_0_0	0.072	0.031	0.012	0.006	0.886	0.347	0.142	0.758	0.361	0.899
4_5_1_0_0	0.020	0.275	0.154	0.969	0.177	0.314	0.033	0.977	0.500	0.288
5_4_1_0_0	0.004	0.006	0.009	0.688	0.978	0.823	0.011	0.982	0.016	0.025
Summed OS	0.011	0.003	0.029	0.001	0.406	0.001	0.0001	0.0003	6.1×10^{-5}	0.023
Lactose	0.129	0.001	0.001	0.001	0.008	0.008	0.007	1.000	0.997	0.997

[a] All acetonitrile washes also contained 0.1% TFA. Oligosaccharides are represented by their monosaccharide compositions, denoted as Hex_HexNAc_Fuc_NeuAc_NeuGc, with each number representing the quantity of the respective monosaccharide type. Hex: hexose, HexNAc: *N*-acetylhexosamine, Fuc: fucose, NeuAc: *N*-acetylneuraminic acid, NeuGc: N-glycolylneuraminic acid.

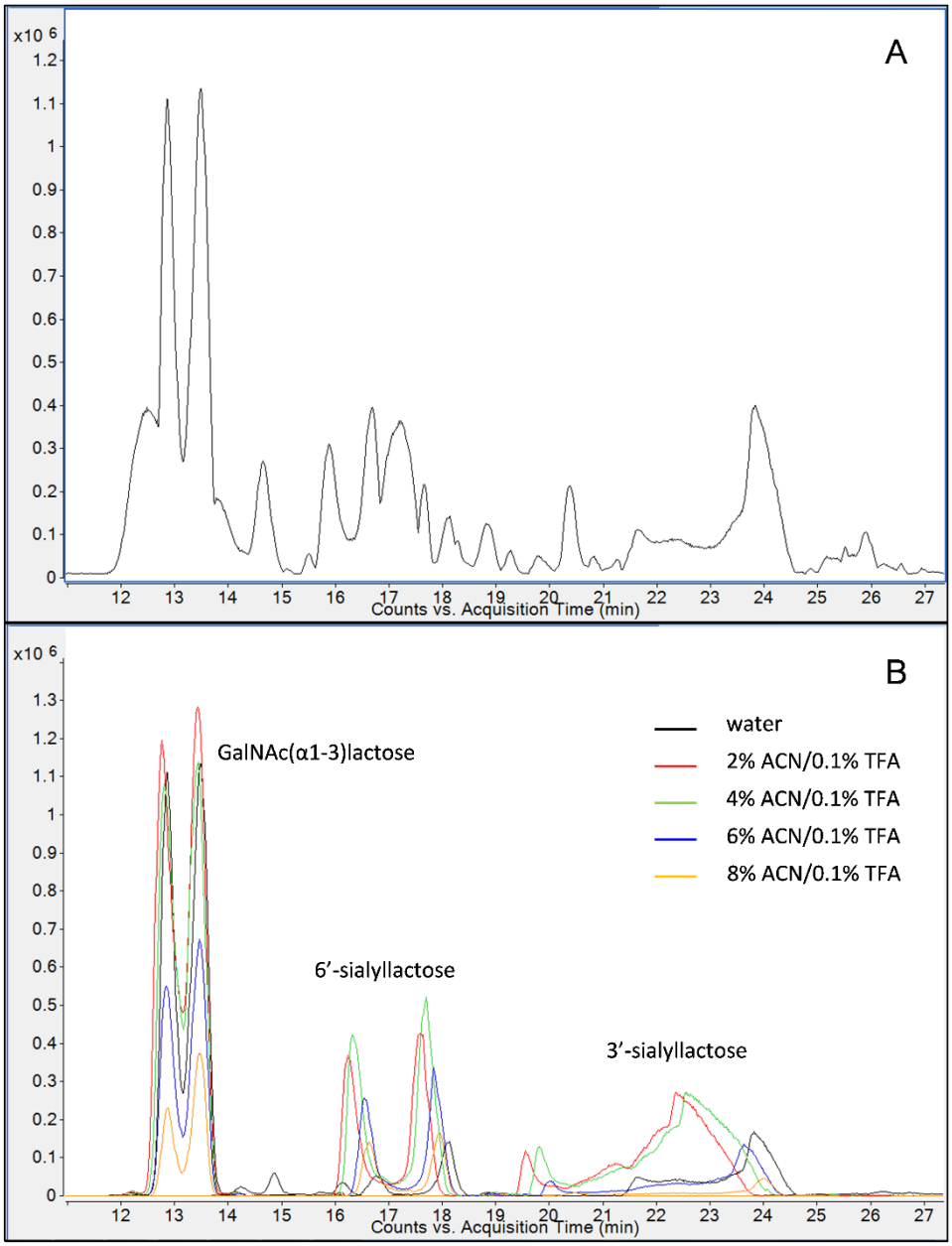

Fig. S1. LC-MS chromatogram of a bovine milk oligosaccharide sample (A). The effect of varying the solid phase extraction sorbent wash solution can be seen in the varying peak heights of the most abundant oligosaccharides, which are annotated in (B) as extracted ion chromatograms.