Human Milk Glycomics and Gut Microbial Genomics in Infant Feces Shows Correlation between Human Milk Oligosaccharides and Gut Microbiota: A Proof-of-Concept Study

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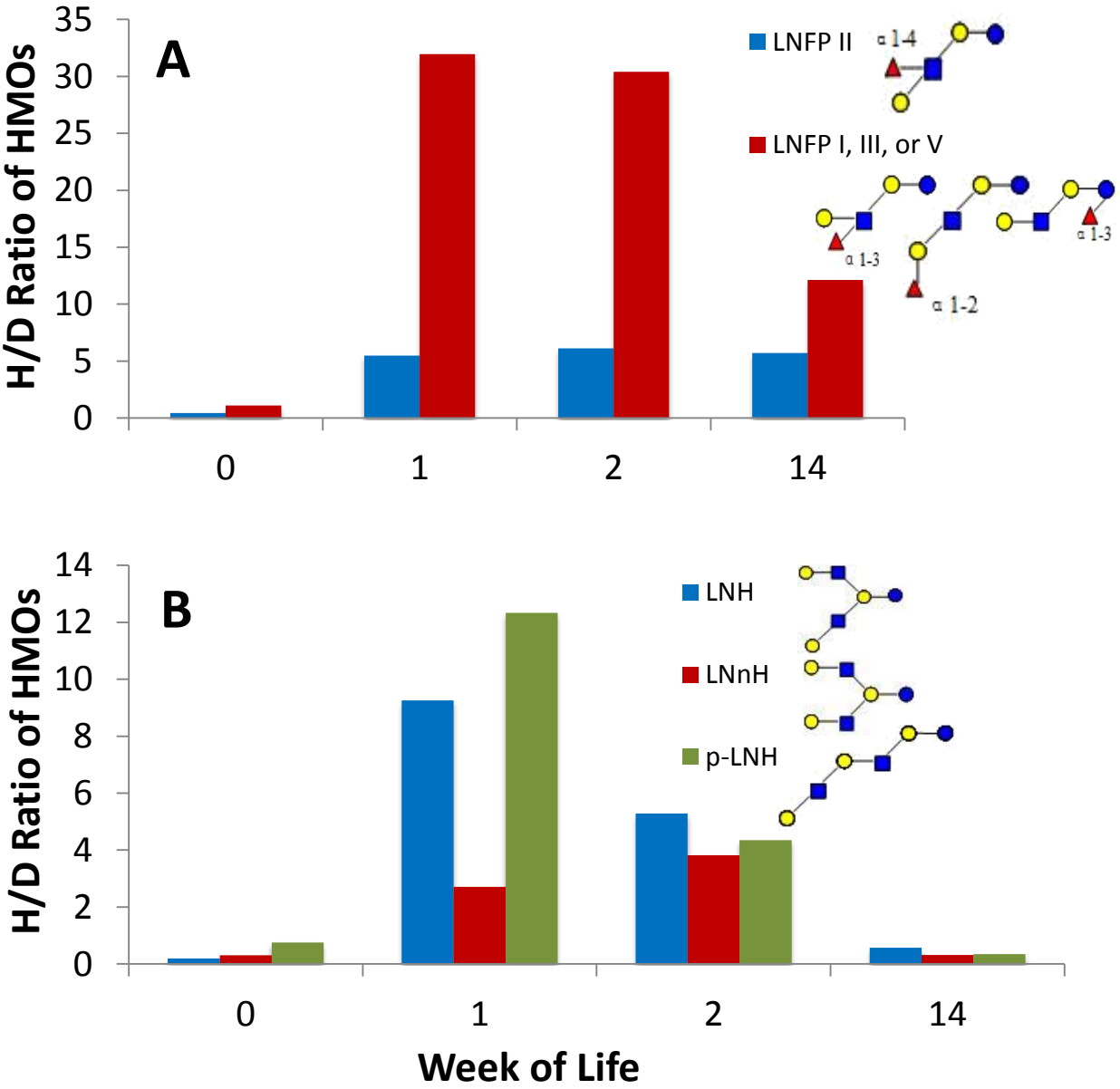
Supporting Information for Publication

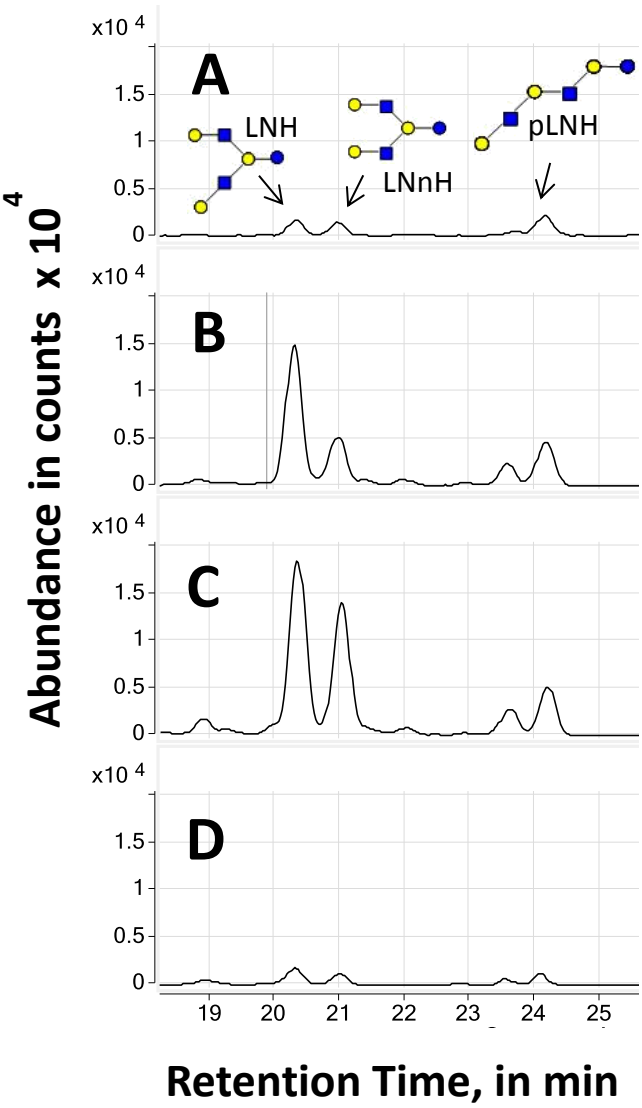
Supplementary Table 1. qPCR Primers and Probes.

Primer/Probe	Taxonomy	Assay	Sequence (5' to 3')	Concentration	Tm (C°)	Reference
Uni334F	universal Bacteria	SYBR Green	ACTCCTACGGGAGGCAGCAGT	400 nM	65.5	Hartman *et al.*, 2009
Uni514R	universal Bacteria	SYBR Green	ATTACCGCGGCTGCTGGC	400 nM	65.5	Hartman *et al.*, 2009
Bdes1038F	*Bacteroidales*	SYBR Green	GGTGTCGGCTTAAGTGCCAT	400 nM	61	Hartman *et al.*, 2009
Bdes1189R	*Bacteroidales*	SYBR Green	CGGAYGTAAGGGCCGTGC	400 nM	61	Hartman *et al.*, 2009
Bif F	*Bifidobacteria*	TaqMan	GCGTGCTTAACACATGCAAGTC	300 nM	60	Penders *et al.*, 2005
Bif R	*Bifidobacteria*	TaqMan	CACCCGTTTCCAGGAGCTATT	300 nM	60	Penders *et al.*, 2005
Bif P	*Bifidobacteria*	TaqMan	[6-FAM]TCACGCATTACTCACCCGTTCGCC[BHQ1]	150 nM	60	Penders *et al.*, 2005
BiLONF	*B. longum* group	TaqMan	CAGTTGATCGCATGGTCTT	500 nM	58	Malinen *et al.*, 2005
BiLONR	*B. longum* group	TaqMan	TACCCGTCGAAGCCAC	500 nM	58	Malinen *et al.*, 2005
BifSpP	*B. longum* group	TaqMan	[6-FAM]TGGGATGGGGTCGCGTCCTATCAG[TAMRA]	80 nM	58	Malinen *et al.*, 2005
BiADOg-1a	*B. adolescentis* group	SYBR Green	CTCCAGTTGGATGCATGTC	250 nM	55	Matsuki *et al,* 2004
BiADOg-1b	*B. adolescentis* group	SYBR Green	TCCAGTTGACCGCATGGT	250 nM	55	Matsuki *et al,* 2004
BiADO-2	*B. adolescentis* group	SYBR Green	CGAAGGCTTGCTCCCAGT	250 nM	55	Matsuki *et al,* 2004
BiBIF-1	*B. bifidum*	SYBR Green	CCACATGATCGCATGTGATTG	250 nM	55	Matsuki *et al,* 2004
BiBIF-2	*B. bifidum*	SYBR Green	CCGAAGGCTTGCTCCCAAA	250 nM	55	Matsuki *et al,* 2004
BiBRE-1	*B. breve*	SYBR Green	CCGGATGCTCCATCACAC	250 nM	55	Matsuki *et al,* 2004
BiBRE-2	*B. breve*	SYBR Green	ACAAAGTGCCTTGCTCCCT	250 nM	55	Matsuki *et al,* 2004
BiCATg-1	*B. catenulatum* group	SYBR Green	CGGATGCTCCGACTCCT	250 nM	55	Matsuki *et al,* 2004
BiCATg-2	*B. catenulatum* group	SYBR Green	CGAAGGCTTGCTCCCGAT	250 nM	55	Matsuki *et al,* 2004

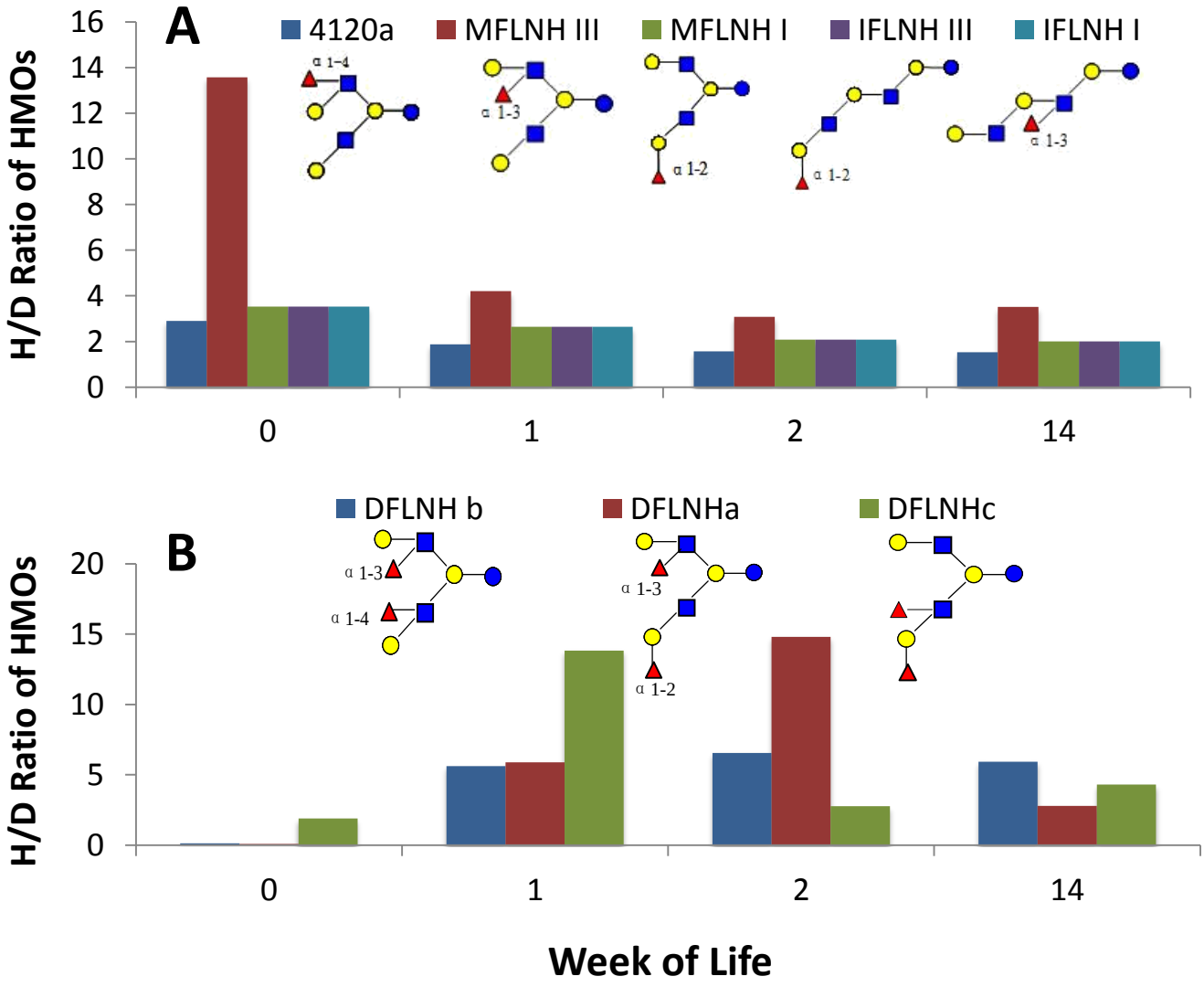
Supplementary Figure 1. H/D ratios of two isomeric groups of oligosaccharides in the fecal HMO profile of Infant B . H/D ratios were calculated using nano-HLPC chip/TOF MS data. (A) Four isomers of *m/z* 856 ($[M+H]^+$, z=1, M=855.3220, second bar from the left in each week in Figure 4A). (B) Three isomers of *m/z* 538 ($[M+2H]^{2+}$, z=2, M=1074.3963, fourth bar from the left in Figure 4A). M=monoisotopic (neutral) mass.

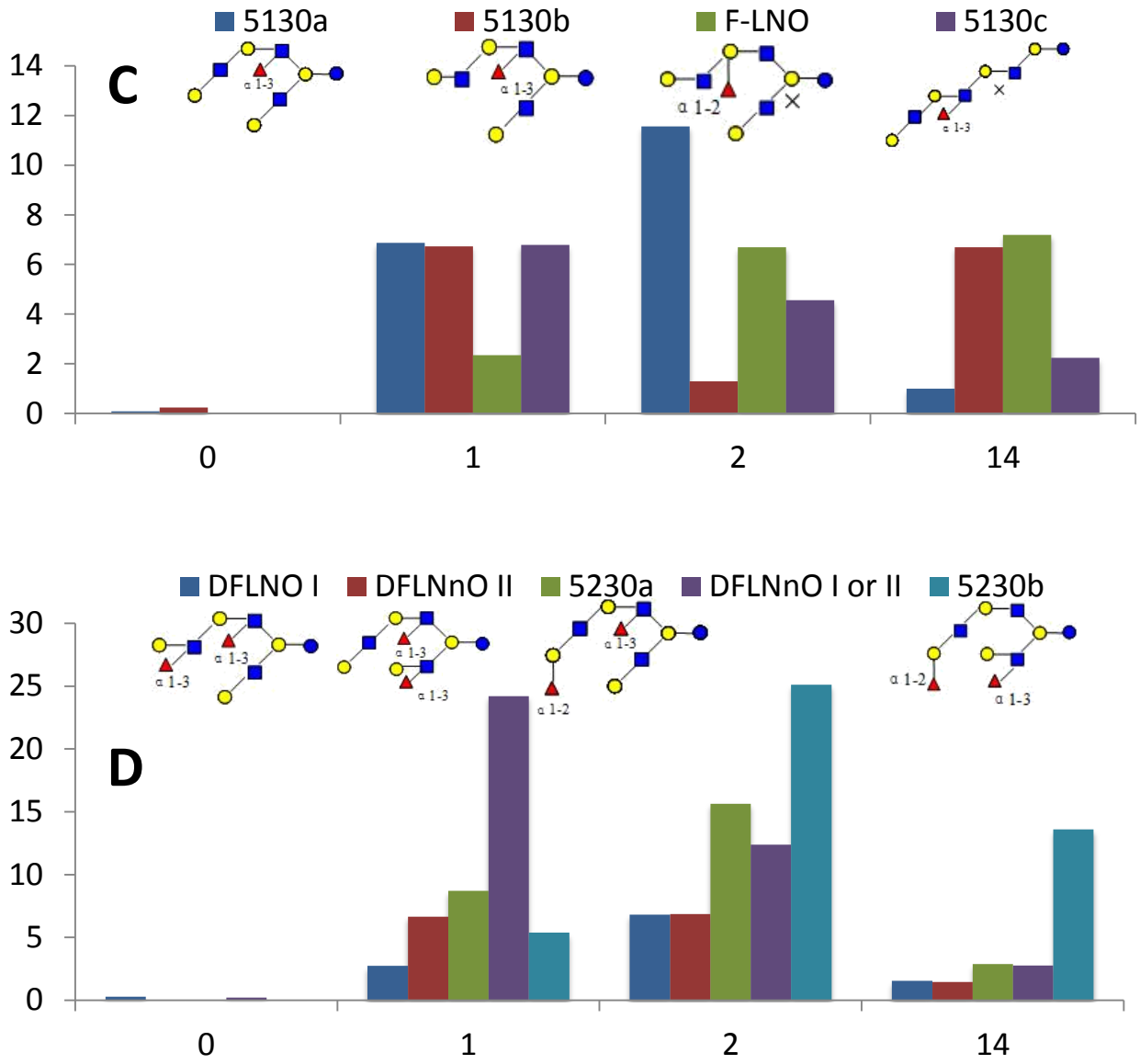


Supplementary Figure 2. LC/MS extracted ion chromatograms of *m/z* 538 ($[M+2H]^{2+}$, *z*=2, M=1074.3963) in the fecal HMO profile of Infant B using nano-HLPC chip/TOF MS. Chromatograms at (A) week 0, (B) week 1, (C) week 2, and (D) week 13. M=monoisotopic (neutral) mass.



Supplementary Figure 3. H/D ratios of four isomeric groups of oligosaccharides in the fecal HMO profile of Infant B. H/D ratios were calculated using nano-HLPC chip/TOF MS data. (A) Five isomers of *m/z* 611 ($[M+2H]^{2+}$, *z*=2, M=1220.4542, fifth bar from the left in each week in Figure 4A). (B) Three isomers of *m/z* 684 ($[M+2H]^{2+}$, *z*=2, M=1366.5121, sixth bar from the left in Figure 4A). (C) Four isomers of *m/z* 794 ($[M+2H]^{2+}$, *z*=2, M=1585.5864, ninth bar in Figure 4A). (D) Five isomers of *m/z* 867 ($[M+2H]^{2+}$, *z*=2, M=1731.6443, tenth bar from the left in Figure 4A). M=monoisotopic (neutral) mass.




C
5130a
5130b
F-LNO
5130c
14
12
10
8
6
4
2
0
0
1
2
14
α 1-3
α 1-2
D
DFLNO I
DFLNnO II
5230a
DFLNnO I or II
5230b
30
25
20
15
10
5
0
0
1
2
14
α 1-3
α 1-2