Innate immune lectins kill bacteria expressing blood group antigen

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Supplementary Information

Supplementary Methods

Preparation of recombinant human galectins- We prepared Gal-1, Gal-3, Gal-4, Gal-4 domains, Gal-8, Gal-8 domains, and Gal-8 mutants as outlined previously[1]. To generate Gal-8R69H we used forward primer 5'-GTGGCCTTTCATTTCAATCCTCATTTCAAAAGGGCCGGCTGCATG-3' and reverse primer 5'-CAATGCAGCCGGCCCTTTTGAAATGAGGATTGAATGAAAGG CCAC-3'. To generate Gal-8R233H we used forward primer 5'-GCTCTACACTTGAACCCACACCTGAATATTAAAGCATTTG-3' and reverse primer 5'CAAATGCTTTAATATTCAGGTGTGGGTTCAAGTGTAGAGC-3'. We purified recombinant galectins by affinity chromatography on lactosyl-sepharose and eluted with 100 mM lactose in PBS plus 2-mercaptoethanol (2-ME). We purified galectins to apparent homogeneity as observed by SDS-PAGE (**Supplementary Figure 1**). Prior to derivatization, we removed 2-ME from galectin samples using a PD-10 gel filtration column (GE Healthcare), followed by addition of lactose (100 mM final concentration) to help maintain galectin stability and reduce the likelihood of adduct formation at or near the carbohydrate recognition domain (CRD). We biotinylated all galectins by incubating 3-5 mg mL^{-1} of galectin with 2 mM EZ-link^{TM} Sulfo-NHS-LC-Biotin (Sulfosuccinimidyl-6-(biotinamido) hexanoate) (Pierce) for 2 h at 4 ºC. We separated unconjugated EZ-link^{TM} Sulfo-NHS-LC-Biotin and free lactose from derivatized protein using a PD-10 gel filtration column.

Glycan array preparation and analysis- We obtained from the Consortium for Functional Glycomics (http://www.functionalglycomics.org/) glycan microarrays prepared as described previously[2]. For galectin recognition of glycans on the printed glycan microarray, we incubated 0.2 μM Gal-1, 0.2 μM Gal-3, 0.5 μM Gal-4, or 0.02 μM Gal-8 in Tris buffer/Salts/Metal ions (TSM) Binding Buffer (20 mM Tris-HCl, 150 mM sodium chloride, 2 mM calcium chloride, 2 mM magnesium chloride, pH 7.4, 1% BSA, and 0.05% Tween 20, with 14 mM 2-ME) for 1 h at room temperature in a dark humid chamber. We washed the slide by successive immersion in TSM containing 0.05% Tween 20 (4x) and TSM (4x). We incubated the slide with Alexa Fluor-488-streptavidin. After 1 h at room temperature in a dark humid chamber, we washed the slide by successive immersion in TSM containing 0.05% Tween 20 (4x), TSM (4x), and water (4x). We dried the slide by microcentrifugation and obtained an image of bound fluorescence using a microarray scanner (Scan Array Express, PerkinElmer Lifer Sciences). We determined the integrated spot intensities using Imagene software (BioDiscovery).

Generating GFP expressing P. aeruginosa- We obtained *P. aeruginosa* strain 8830 from Dr. Ananda Chakrabaty (University of Illinois College of Medicine). To generate a GFP expressing *P. aeruginosa*, we grew bacteria in trypicase soy broth at 37 °C until the OD 600 nm was

between 0.8 and 0.9. We pelleted bacteria by centrifugation at 5,000 rpm for 15 min at 4 °C and washed them first in PBS at 4 °C, then water at 4 °C and finally resuspended them in 10% glycerol. We added approximately 1 μg of plasmid pSMC21 encoding GFP, provided by Dr. O'Toole (Dartmouth Medical School), to 50 μL of the bacteria, then electroporated the bacteria using a 2-mm-gap electroporation cuvette (Bio-Rad Laboratories) at 18 kV with a Transporator^{TM} plus (BTX). We diluted the electroporated cells into 1 ml LB medium and grew them for 1 h followed by plating on LB agar supplemented with 500 μg mL^{-1} ampicillin. We identified positive colonies by fluorescence microscopy.

Preparation of samples for SEM- We incubated blood group B positive *E. coli* O86 (BG B+ *E. coli*), grown to mid-log phase, for 30 min with PBS control or 5 μM Gal-8 at 37 °C then added 20 mM lactose to halt treatment and reduce agglutination. We washed bacteria 2x with PBS to remove debris. Droplets containing either untreated or Gal-8-treated bacteria were placed onto poly-L-Lysine treated silicon chips and allowed to settle, then fixed overnight in 2.5% glutaraldehyde in 0.1 M cacodylate buffer, pH 7.4. We washed samples with distilled water, post fixed them in 1% osmium tetroxide, then washed with distilled water and dehydrated them through an ascending ethanol series to three changes of 100% ethanol. The ethanol was exchanged with Hexamethyldisilizane (HMDS) via three changes of HMDS then allowed the HMDS level to drop and the samples allowed to dry completely overnight. We mounted samples onto SEM stubs and sputter coated with either gold or chromium and viewed them in the DS130 SEM (ISI-TOPCON) using in-lens imaging. We viewed the displayed images at 20,000x magnification.

Preparation of samples for TEM- We treated and washed BG B+ *E. coli* as described for SEM preparation then centrifuged bacteria in a table-top centrifuge and fixed them overnight with 2.5% glutaraldehyde in 0.1 M cacodylate buffer, pH 7.4. We washed the bacterial pellets 2x in distilled water and post fixed them in 1% osmium tetroxide, then washed them in distilled water and dehydrated them through an ascending ethanol series to two changes of 100% ethanol. At the 50% ethanol step we en bloc stained the cells with 2.5% Uranyl Acetate in 50% ethanol. We accomplished resin infiltration via two steps of ethanol and resin mixtures (1:1 and 1:2) and finally two exchanges of 100% fresh resin and then embedded cells in fresh resin and polymerized them for three days. We performed microtomy using glass knives and an MT-7000 (RMC) ultra-microtome, and cut thin sections to about 70 to 90 nm thickness and collected onto 200 mesh copper grids. We post stained thin sections with 5% Uranyl acetate and Reynold's Lead Citrate and documented results using a JEOL JEM 1210 TEM at 100KV. We viewed the displayed images at 8,000x magnification and also show a close up view of a single bacterium from the same field.

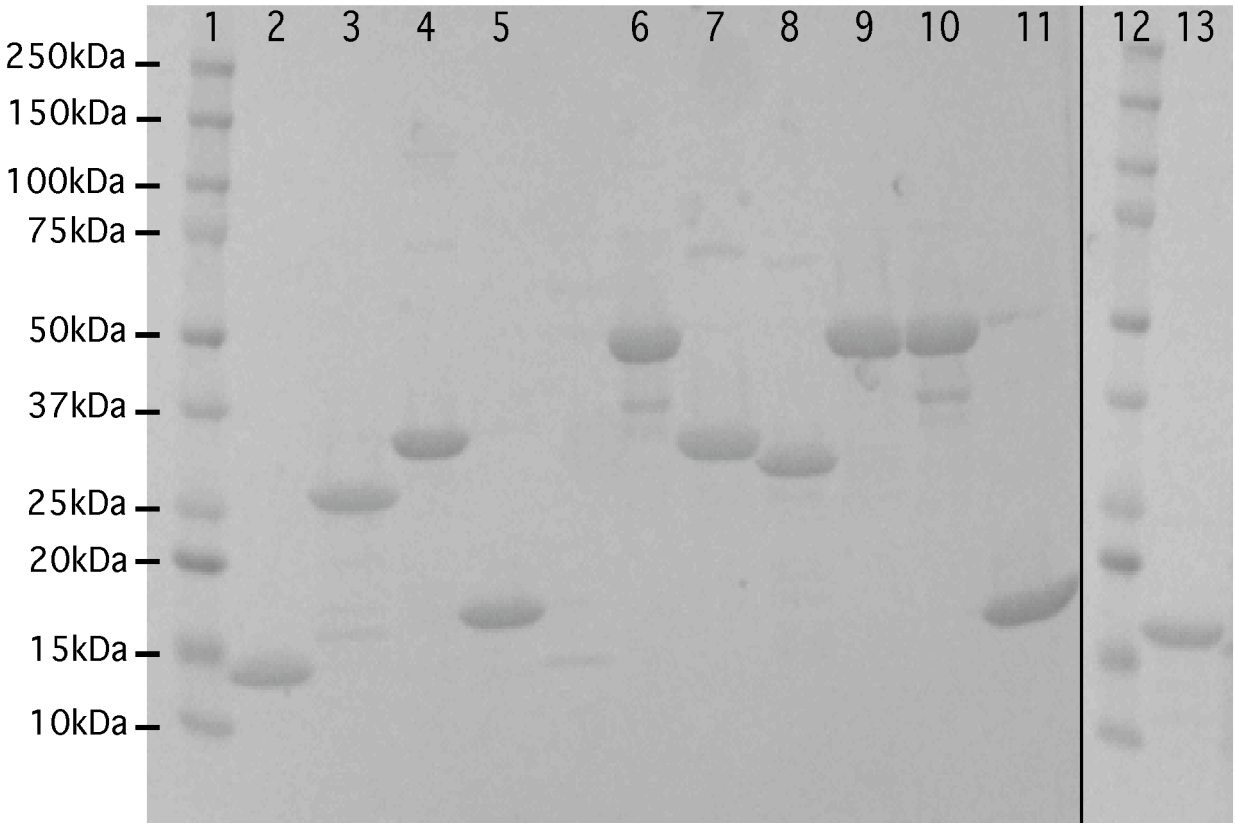
Animal studies- We obtained C57BL/6 Specific Pathogens Free (SPF) mice from the animal facilities of the Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Brazil and maintained them at 20 °C in an isolator rack (Alesco, Monte Mor-SP, Brazil) with an autoclaved water and chow diet *ad libitum*, on 12 h light cycles. We conducted all experiments in accordance with the guidelines of the Animal Care Committee from this University (process # 09.1.543.53.5)

In vivo bacterial killing assay- We plated *E. coli* strains (BG B^+ *E. coli* and *WaaL*$^-$ BG B^- *E. coli*) for isolation on LB agar (Difco Laboratories) and selected colonies to inoculate 50 mL of LB broth (Difco Laboratories), to grow overnight at 37 °C. To eliminate resident facultative bacteria and optimize intestinal colonization with *E. coli* strains, we treated 5 week old male mice for 48 h with streptomycin sulfate (5 g L^{-1}) (Sigma-Aldrich) in sterile drinking water followed by sterile water for 24 h prior to ingestion of bacterial suspension[3,4]. We inoculated mice (four per group) by oral gavage with 10^6 colony-forming units (CFU) per mL of BG B^+ *E. coli* or *WaaL*$^-$ *E. coli* in 100 µL (10^5 CFU) of sterile PBS using a 22-gauge stainless steel animal feeding needle. Mice also received by oral gavage 300 µL of TDG (50 mM – 5.38 mg per animal) or 300 µL of PBS divided into three injections of 100 µL administered immediately before, 6 h after and 12 h after inoculation. Control mice, treated with streptomycin, received PBS alone. To recover bacteria, we sacrificed mice 24 h after bacteria inoculation, using CO_2 inhalation. From each mouse we aseptically excised, weighed, and homogenized the entire intestine in 6 mL sterile PBS using a homogenizer T10 (IKA®-Works, Inc.). We determined the number of viable bacteria in each intestine homogenate by plating serial dilutions (1000-fold) onto lactose MacConkey agar plates. After incubation at 37 °C for 20 h, we enumerated CFU and expressed per intestine ± SEM. We applied student's t-test for statistical analysis of data. P-values were <0.05, which was considered statistically significant. Results represent two independent experiments.

Supplementary References

1. Stowell, S.R. et al. Galectin-1, -2, and -3 exhibit differential recognition of sialylated glycans and blood group antigens. *J Biol Chem* **283**, 10109-23 (2008).
2. Blixt, O. et al. Printed covalent glycan array for ligand profiling of diverse glycan binding proteins. *Proc Natl Acad Sci U S A* **101**, 17033-8 (2004).
3. Miller, C.P. & Bohnhoff, M. Changes in the Mouse's Enteric Microflora Associated with Enhanced Susceptibility to Salmonella Infection Following Streptomycin Treatment. *J Infect Dis* **113**, 59-66 (1963).
4. Posekany, K.J., Pittman, H.K., Bradfield, J.F., Haisch, C.E. & Verbanac, K.M. Induction of cytolytic anti-Gal antibodies in alpha-1,3-galactosyltransferase gene knockout mice by oral inoculation with Escherichia coli O86:B7 bacteria. *Infect Immun* **70**, 6215-22 (2002).

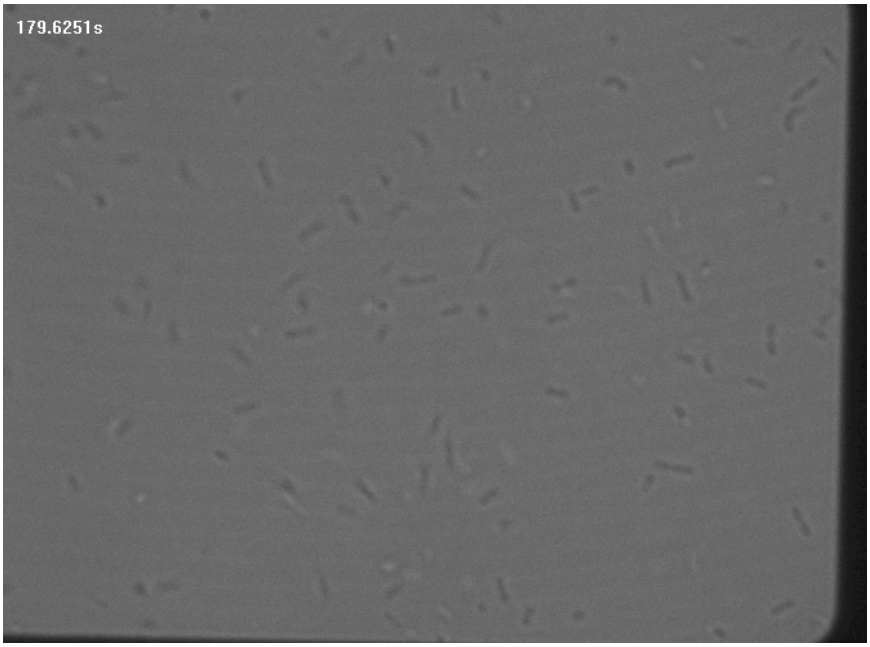
Stowell et al Supplemental Figure 1



Supplementary Figure 1. Purity of Galectins. Coomassie blue staining of human (h) and mouse (m) galectin preparations on SDS-PAGE, 10 ug per well. Lane 1- Molecular weight markers, lane 2- hGal-1, lane 3- hGal-3, lane 4- hGal-4, lane 5- hGal-4N, lane 6- hGal-8, lane 7- hGal-8N, lane 8- hGal-8C, lane 9- hGal-8R69H, lane 10- hGal-8R223H, lane 11- mGal-4, lane 12- molecular weight markers, lane 13- hGal-4C.

Supplementary video 1. Immobilization of BG B$^+$ *E. coli* after addition of Gal-8.

(Below is a still shot as a placeholder and readers should access the video to make observations).



Supplementary Table 1. **Complete list of glycans present on the CFG glycan microarray and raw data for galectin binding.** Binding of human Gal-1 (0.2 μM), -3 (0.2 μM), -4 (0.5 μM), and -8 (0.02 μM), and mouse Gal-4 (0.2 μM) to the array. Blue = blood group B type structures, Orange = blood group A type structures. RFU= relative fluorescence units, SEM= standard error of the mean of 4 replicates after removal of the high and low value for each glycan.

		Human Gal-1		Human Gal-3		Human Gal-4		Human Gal-8		Mouse Gal-4	
#	CFG Array Version 3.0 Structure	RFU	SEM	RFU	SEM	RFU	SEM	RFU	SEM	RFU	SEM
1	Neu5Acα2-8Neu5Acα-Sp8	-107	90	27	35	17	6	22	13	51	6
2	Neu5Acα2-8Neu5Acβ-Sp17	-41	25	120	56	19	14	87	37	77	6
3	Neu5Acα2-8Neu5Acα2-8Neu5Acβ-Sp8	5	23	68	71	10	5	50	10	71	8
4	Neu5Gcβ2-6Galβ1-4GlcNAc-Sp8	36	56	79	40	32	9	8	2	82	16
5	Galβ1-3GlcNAcβ1-2Manα1-3(Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	175	41	186	65	37	4	17	9	117	13
6	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	89	67	-6	25	18	14	28	14	61	3
7	α-D-Gal–Sp8	158	36	73	32	23	8	15	5	47	8
8	α-D-Glc–Sp8	-23	45	30	51	18	8	60	29	46	7
9	α-D-Man–Sp8	85	45	79	21	25	9	32	6	28	4
10	α-GalNAc–Sp8	9	120	60	92	29	13	23	7	87	9
11	α-L-Fuc–Sp8	36	69	66	41	21	6	42	20	23	7
12	α-L-Fuc–Sp9	116	153	9	32	18	6	14	23	93	12
13	α-L-Rhα–Sp8	-36	57	26	21	107	11	38	18	52	6
14	α-Neu5Ac–Sp8	32	33	48	17	57	17	85	42	83	12
15	α-Neu5Ac–Sp11	-36	27	-23	13	27	3	22	7	96	17
16	β-Neu5Ac-Sp8	-79	78	8	32	15	4	31	12	51	14
17	β-D-Gal–Sp8	66	19	101	59	17	8	45	23	64	11
18	β-D-Glc–Sp8	61	69	62	17	26	8	47	13	66	6
19	β-D-Man–Sp8	227	94	95	34	15	4	26	1	36	4
20	β-GalNAc–Sp8	-79	47	156	211	32	4	28	14	47	21
21	β-GlcNAc–Sp0	-2	22	47	12	13	9	39	15	63	23
22	β-GlcNAc–Sp8	-21	31	58	78	9	5	44	21	55	10
23	β-GlcN(Gc)-Sp8	90	44	48	49	17	7	68	32	58	6
24	Galb1-4GlcNAcb1-3(Galb1-4GlcNAcb1-6)GalNAca-Sp8	7138	3013	79	14	17	4	75	6	84	10
25	GlcNAcβ1-3(GlcNAcβ1-4)(GlcNAcβ1-6)GlcNAc-Sp8	17	51	105	89	71	8	15	7	72	5

26	[3OSO3][6OSO3]Galβ1-4[6OSO3]GlcNAcβ-Sp0	30	35	182	148	20	5	29	9	112	10
27	[3OSO3][6OSO3]Galβ1-4GlcNAcβ-Sp0	-29	113	248	346	19	6	37	10	74	10
28	[3OSO3]Galβ1-4Glcβ-Sp8	749	396	68	38	117	15	62	16	106	12
29	[3OSO3]Galβ1-4(6OSO3)Glcβ–Sp0	2227	3008	674	70	607	181	361	69	134	14
30	[3OSO3]Galβ1-4(6OSO3)Glcβ–Sp8	4809	1006	444	191	967	37	117	65	67	6
31	[3OSO3]Galβ1-3(Fucα1-4)GlcNAcβ–Sp8	-48	38	16	64	20	9	21	6	78	12
32	[3OSO3]Galβ1-3GalNAcα–Sp8	37	88	75	39	385	83	65	15	77	16
33	[3OSO3]Galβ1-3GlcNAcβ–Sp8	19099	3018	301	69	84	19	41	3	54	2
34	[3OSO3]Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	56	32	18	35	39	14	60	18	62	2
35	[3OSO3]Galβ1-4[6OSO3]GlcNAcβ-Sp8	39931	4579	944	45	-9	5	7	10	81	11
36	[3OSO3]Galβ1-4GlcNAcβ–Sp0	13488	11547	354	40	25	10	40	9	78	11
37	[3OSO3]Galβ1-4GlcNAcβ-Sp8	29310	5953	242	156	55	16	53	27	76	5
38	[3OSO3]Galβ–Sp8	-123	58	7	41	20	7	20	10	76	11
39	[4OSO3][6OSO3]Galβ1-4GlcNAcβ-Sp0	50	159	38	55	26	2	11	3	79	13
40	[4OSO3]Galβ1-4GlcNAcβ-Sp8	-53	43	36	21	3	5	28	13	33	22
41	6-H_2PO_3Manα–Sp8	1135	120	139	41	11	4	31	14	65	19
42	[6OSO3]Galβ1-4Glcβ–Sp0	600	291	87	40	11	9	48	31	38	6
43	[6OSO3]Galβ1-4Glcβ–Sp8	193	77	682	114	-12	4	21	8	133	26
44	[6OSO3]Galβ1-4GlcNAcβ–Sp8	104	46	53	31	18	6	47	17	51	4
45	[6OSO3]Galβ1-4[6OSO3]Glcβ-Sp8	267	76	209	26	15	9	70	26	138	14
46	Neu5Acα2-3[6OSO3]Galβ1-4GlcNAcβ–Sp8	127	73	120	25	17	9	30	2	78	11
47	[6OSO3]GlcNAcβ–Sp8	-8	31	20	18	28	3	20	13	71	4
48	9NAcNeu5Acα-Sp8	63	66	59	57	21	7	13	18	70	9
49	9NAcNeu5Acα2-6Galβ1-4GlcNAcβ-Sp8	27	31	35	28	38	5	28	15	97	12
50	Manα1-3(Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	142	61	59	38	43	10	25	13	46	4
51	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	97	35	42	67	21	2	93	27	50	15
52	Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	47992	4892	1	43	0	0	0	23	0	0
53	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	-143	142	0	92	22	3	10	3	139	7
54	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp8	-52	30	-18	87	10	8	-3	4	116	11

55	Fucα1-2Galβ1-3GalNAcβ1-3Galα-Sp9	282	50	336	120	19	7	36	14	59	6
56	Fucα1-2Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Sp9	95	113	53	78	38	17	41	5	50	12
57	Fucα1-2Galβ1-3(Fucα1-4)GlcNAcβ–Sp8	129	100	143	63	19	10	20	12	43	2
58	Fucα1-2Galβ1-3GalNAcα–Sp8	-21	25	74	41	47	16	41	9	78	15
59	Fucα1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp0	22	18	70	75	23	6	157	29	62	13
60	Fucα1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp9	101	165	106	129	5	4	60	34	18	8
61	Fucα1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ–Sp10	1268	627	165	117	28	8	64	15	75	7
62	Fucα1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ–Sp8	796	495	230	136	373	17	27	5	76	7
63	Fucα1-2Galβ1-3GlcNAcβ–Sp0	197	79	198	109	16	24	10	6	68	11
64	Fucα1-2Galβ1-3GlcNAcβ–Sp8	154	91	128	100	5	1	30	19	74	15
65	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	26	14	23	36	22	13	44	21	99	12
66	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	-31	47	-12	39	6	1	65	34	54	9
67	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ–Sp0	56	42	58	58	30	13	63	22	52	10
68	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	35	150	74	22	11	6	74	13	71	18
69	Fucα1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAc–Sp0	2656	285	1762	142	79	13	45	11	99	15
70	Fucα1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	2616	1228	2488	495	18	5	19	8	85	13
71	Fucα1-2Galβ1-4GlcNAcβ–Sp0	93	143	71	71	10	1	17	9	42	7
72	Fucα1-2Galβ1-4GlcNAcβ–Sp8	357	178	48	22	6	4	22	12	37	17
73	Fucα1-2Galβ1-4Glcβ–Sp0	91	80	35	32	83	12	95	24	51	13
74	Fucα1-2Galβ–Sp8	9	11	59	24	28	16	46	12	65	13
75	Fucα1-3GlcNAcβ-Sp8	62	79	59	59	26	3	-3	10	35	12
76	Fucα1-3GlcNAcβ-Sp8	-36	73	38	49	26	3	38	32	35	12
77	Fucα1-4GlcNAcβ–Sp8	92	53	75	32	35	16	27	9	56	3
78	Fucβ1-3GlcNAcβ-Sp8	12	40	42	13	48	9	29	5	38	5
79	GalNAcα1-3(Fucα1-2)Galβ1-3GlcNAcβ-Sp0	163	40	396	237	4664	523	254	81	13390	871
80	GalNAcα1-3(Fucα1-2)Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	658	121	163	124	40	14	104	23	115	16
81	GalNAcα1-3(Fucα1-2)Galβ1-4GlcNAcβ-Sp0	21	40	1133	129	443	35	7069	496	3798	175

82	GalNAcα1-3(Fucα1-2)Galβ1-4GlcNAcβ–Sp8	78	56	1081	174	103	49	497	69	3495	50
83	GalNAcα1-3(Fucα1-2)Galβ1-4Glcβ-Sp0	58	2	231	117	6841	1381	2223	170	4798	149
84	GalNAcα1-3(Fucα1-2)Galβ–Sp8	152	79	178	22	20	3	47	6	49	8
85	GalNAcα1-3GalNAcβ–Sp8	-157	23	72	22	-2	15	75	12	33	9
86	GalNAcα1-3Galβ–Sp8	-4	56	107	21	12	6	48	20	34	10
87	GalNAcα1-4(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	45	70	92	39	28	9	9	6	53	4
88	GalNAcβ1-3GalNAcα–Sp8	73	47	103	62	68	14	22	11	44	7
89	GalNAcβ1-3(Fucα1-2)Galβ-Sp8	54	53	42	29	38	9	25	2	42	5
90	GalNAcβ1-3Galα1-4Galβ1-4GlcNAcβ-Sp0	115	37	59	35	14	6	12	10	38	7
91	GalNAcβ1-4(Fucα1-3)GlcNAcβ-Sp0	24	141	132	94	28	8	61	18	42	10
92	GalNAcβ1-4GlcNAcβ–Sp0	120	127	109	33	22	4	63	20	26	7
93	GalNAcβ1-4GlcNAcβ–Sp8	-14	13	-12	39	47	18	19	4	21	6
94	Galα1-2Galβ–Sp8	89	26	66	18	18	11	33	10	89	26
95	Galα1-3(Fucα1-2)Galβ1-3GlcNAcβ-Sp0	524	138	649	391	4807	168	8769	538	3847	165
96	Galα1-3(Fucα1-2)Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	276	46	140	56	70	12	48	8	98	5
97	Galα1-3(Fucα1-2)Galβ1-4GlcNAc-Sp0	-17	86	18681	9226	913	133	412	303	843	8
98	Galα1-3(Fucα1-2)Galβ1-4Glcβ-Sp0	47	16	161	27	4581	171	1058	54	798	32
99	Galα1-3(Fucα1-2)Galβ–Sp8	93	60	70	71	37	13	67	6	76	7
100	Galα1-3(Galα1-4)Galβ1-4GlcNAcβ-Sp8	129	67	107	72	14	9	36	8	106	11
101	Galα1-3GalNAcα-Sp8	73	60	53	51	7	6	6	5	71	14
102	Galα1-3GalNAcβ–Sp8	108	65	109	47	24	5	43	8	45	13
103	Galα1-3Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	-168	72	204	124	0	2	4	39	49	12
104	Galα1-3Galβ1-3GlcNAcβ-Sp0	1014	58	22	27	54	10	35	19	89	10
105	Galα1-3Galβ1-4GlcNAcβ–Sp8	952	578	-18	76	20	9	26	5	72	11
106	Galα1-3Galβ1-4Glcβ–Sp0	172	90	69	29	142	46	26	8	91	15
107	Galα1-3Galβ–Sp8	66	78	75	29	9	2	40	12	79	1
108	Galα1-4(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	-15	42	35	45	50	8	234	137	55	5
109	Galα1-4Galβ1-4GlcNAcβ–Sp0	-20	41	52	38	39	11	27	16	75	19
110	Galα1-4Galβ1-4GlcNAcβ–Sp8	21	68	87	18	32	5	32	20	51	8
111	Galα1-4Galβ1-4Glcβ–Sp0	559	626	51	4	59	19	17	9	33	7
112	Galα1-4GlcNAcβ–Sp8	95	109	42	24	14	5	82	26	52	6
113	Galα1-6Glcβ-Sp8	63	87	54	30	8	3	8	5	44	13
114	Galβ1-2Galβ–Sp8	138	122	57	27	9	8	78	40	49	5
115	Galβ1-3(Fucα1-4)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	-57	106	26	29	29	8	45	20	59	13
116	Galβ1-3(Fucα1-4)GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	967	325	59	62	43	8	27	8	48	4

117	Galβ1-3(Fucα1-4)GlcNAc–Sp0	0	28	47	39	51	16	39	8	60	11
118	Galβ1-3(Fucα1-4)GlcNAc–Sp8	30	26	43	10	50	10	48	16	59	13
119	Galβ1-3(Fucα1-4)GlcNAcβ–Sp8	55	61	127	193	49	14	8	9	69	24
120	Galβ1-3(Galβ1-4GlcNAcβ1-6)GalNAcα-Sp8	184	161	35	42	17	7	8	5	44	11
121	Galβ1-3(GlcNAcβ1-6)GalNAcα-Sp8	-11	148	30	64	26	8	6	14	60	16
122	Galβ1-3(Neu5Acα2-6)GalNAcα-Sp8	21	32	74	34	10	10	3	4	103	4
123	Galβ1-3(Neu5Acβ2-6)GalNAcα-Sp8	4	19	46	25	8	5	26	15	48	10
124	Galβ1-3(Neu5Acα2-6)GlcNAcβ1-4Galβ1-4Glcβ-Sp10	122	116	50	92	46	5	68	32	79	11
125	Galβ1-3GalNAcα-Sp8	126	93	50	47	2	3	9	10	32	7
126	Galβ1-3GalNAcβ–Sp8	52	77	105	46	57	16	30	18	51	11
127	Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Sp0	31	161	-26	31	37	12	-10	5	89	12
128	Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp0	46	65	97	82	16	8	26	9	80	12
129	Galβ1-3GalNAcβ1-4Galβ1-4Glcβ–Sp8	8	38	60	80	18	13	50	11	1256	84
130	Galβ1-3Galβ–Sp8	75	60	47	35	439	55	28	6	36	7
131	Galβ1-3GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	692	74	192	36	45	18	74	19	52	12
132	Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ–Sp10	1117	82	204	44	1012	25	34	18	60	12
133	Galβ1-3GlcNAcβ–Sp0	545	264	58	23	33	12	33	15	65	6
134	Galβ1-3GlcNAcβ–Sp8	480	220	63	19	16	3	7	12	48	3
135	Galβ1-4(Fucα1-3)GlcNAcβ–Sp0	125	29	133	49	13	9	45	25	47	13
136	Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	5504	1179	103	80	42	14	44	17	70	12
137	Galβ1-4(Fucα1-3)GlcNAcβ1-4Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	74	166	25	36	22	5	39	6	50	6
138	Galβ1-4(Fucα1-3)GlcNAcβ1-4Galβ1-4(Fucα1-3)GlcNAcβ1-4Galβ1-4(Fucα1-3)GlcNAcβ–Sp0	-59	30	66	50	23	8	23	15	78	5
139	Galβ1-4[6OSO3]Glcβ–Sp0	72	44	176	114	108	10	57	14	70	6
140	Galβ1-4[6OSO3]Glcβ–Sp8	91	78	35	13	80	25	39	13	110	8
141	Galβ1-4GalNAcα1-3(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	51	75	1548	155	1840	64	114	36	5993	279
142	Galβ1-4GalNAcβ1-3(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	168	161	34	41	3	2	23	2	155	41
143	Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	13707	1281	12	49	35	7	397	390	100	17
144	Galβ1-4GlcNAcβ1-3GalNAcα–Sp8	1813	350	33	48	10	13	2	5	117	10

145	Galβ1-4GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	1456	94	84	58	18	6	10	5	33	10
146	Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ–Sp0	1313	619	6295	2113	20	4	1662	152	38	9
147	Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ–Sp0	3025	531	1386	25	44	8	33	11	38	7
148	Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ–Sp0	365	309	464	73	18	7	477	137	35	5
149	Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ–Sp8	426	195	413	276	151	23	229	59	81	6
150	Galβ1-4GlcNAcβ1-6(Galβ1-3)GalNAcα–Sp8	76	54	10	21	5	2	54	29	38	5
151	Galβ1-4GlcNAcβ1-6GalNAcα–Sp8	446	57	37	35	22	7	32	11	75	3
152	Galβ1-4GlcNAcβ–Sp0	62	26	48	17	20	9	47	5	46	5
153	Galβ1-4GlcNAcβ–Sp8	297	207	54	22	21	6	46	22	66	9
154	Galβ1-4Glcβ–Sp0	42	35	103	30	13	17	30	11	50	12
155	Galβ1-4Glcβ–Sp8	111	21	43	55	26	9	32	7	112	61
156	GlcNAcα1-3Galβ1-4GlcNAcβ-Sp8	-33	49	565	1012	19	9	37	31	53	8
157	GlcNAcα1-6Galβ1-4GlcNAcβ-Sp8	-9	32	66	53	23	8	21	12	50	3
158	GlcNAcβ1-2Galβ1-3GalNAcα–Sp8	-16	9	48	82	43	15	37	19	35	6
159	GlcNAcβ1-3(GlcNAcβ1-6)GalNAcα–Sp8	18	114	65	63	54	18	42	24	64	7
160	GlcNAcβ1-3(GlcNAcβ1-6)Galβ1-4GlcNAcβ–Sp8	39	85	81	64	1	5	37	7	33	8
161	GlcNAcβ1-3GalNAcα–Sp8	40	90	79	49	9	5	25	7	41	2
162	GlcNAcβ1-3Galβ-Sp8	-92	28	30	56	37	9	18	9	39	6
163	GlcNAcβ1-3Galβ1-3GalNAcα-Sp8	-3	60	152	165	51	13	38	9	74	5
164	GlcNAcβ1-3Galβ1-4GlcNAcβ–Sp0	232	22	324	140	31	10	74	25	58	14
165	GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp8	43	115	122	90	26	8	24	14	50	15
166	GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	-2	55	2135	1550	36	15	147	41	75	11
167	GlcNAcβ1-3Galβ1-4Glcβ–Sp0	47	61	40	29	36	8	48	31	40	11
168	GlcNAcβ1-4MDPLys	-16	108	17	67	20	12	28	15	64	2
169	GlcNAcβ1-4(GlcNAcβ1-6)GalNAcα-Sp8	320	244	25	25	9	7	19	11	115	16
170	GlcNAcβ1-4Galβ1-4GlcNAcβ-Sp8	50	29	-21	18	6	5	3	7	70	17
171	(GlcNAcβ1-4)6β-Sp8	124	54	93	32	12	6	21	11	58	7
172	(GlcNAcβ1-4)5β-Sp8	62	63	69	64	7	5	14	6	32	6
173	GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ–Sp8	34	41	33	43	4	5	23	13	63	13
174	GlcNAcβ1-6(Galβ1-3)GalNAcα–Sp8	-158	56	43	17	30	7	78	26	50	15
175	GlcNAcβ1-6GalNAcα–Sp8	10	64	135	36	20	5	32	11	11	3
176	GlcNAcβ1-6Galβ1-4GlcNAcβ-Sp8	127	88	76	114	17	5	37	7	104	14
177	Glcα1-4Glcβ–Sp8	104	171	62	65	6	9	41	17	49	13

178	Glcα1-4Glca–Sp8	91	70	83	24	25	16	21	14	72	16
179	Glcα1-6Glcα1-6Glcβ-Sp8	174	50	42	40	-5	8	27	8	24	4
180	Glcβ1-4Glcβ-Sp8	-209	159	646	779	3	2	40	53	87	6
181	Glcβ1-6Glcβ-Sp8	84	39	-19	76	30	14	18	3	15	5
182	G-ol-Sp8	52	129	40	24	38	21	23	22	64	11
183	GlcAa-Sp8	92	44	114	45	17	10	52	2	45	7
184	GlcAβ-Sp8	4460	580	1153	295	37	15	207	97	123	21
185	GlcAβ1-3Galβ-Sp8	238	143	50	46	33	11	36	8	46	6
186	GlcAβ1-6Galβ-Sp8	60	38	-15	14	31	14	37	16	30	5
187	KDNα2-3Galβ1-3GlcNAcβ–Sp0	316	91	129	45	28	10	39	11	74	6
188	KDNα2-3Galβ1-4GlcNAcβ–Sp0	191	108	78	25	24	6	29	12	85	12
189	Manα1-2Manα1-2Manα1-3Manα-Sp9	-38	40	-26	25	42	8	15	12	140	20
190	Manα1-2Manα1-3(Manα1-2Manα1-6)Manα-Sp9	8	76	36	34	23	4	35	11	85	13
191	Manα1-2Manα1-3Manα-Sp9	-32	32	63	55	50	9	17	11	88	19
192	Manα1-6(Manα1-2Manα1-3)Manα1-6(Manα1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	80	108	53	75	12	8	18	7	149	9
193	Manα1-2Manα1-6(Manα1-3)Manα1-6(Manα1-2Manα1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	-30	80	77	20	9	2	27	11	100	6
194	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-3(Manα1-2Manα1-6)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	478	645	368	242	54	14	247	21	157	9
195	Manα1-3(Manα1-6)Manα–Sp9	4	57	72	31	19	5	26	2	35	5
196	Manα1-3(Manα1-2Manα1-2Manα1-6)Manα-Sp9	73	190	53	47	19	4	37	13	78	27
197	Manα1-6(Manα1-3)Manα1-6(Manα1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	2977	539	1966	40	239	20	110	24	277	26
198	Manα1-6(Manα1-3)Manα1-6(Manα1-3)Manβ1-4GlcNAcβ1-4 GlcNAcβ-Sp12	17	64	82	68	16	8	27	10	95	15
199	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	1100	92	124	60	81	12	34	35	36	22
200	Manβ1-4GlcNAcβ-Sp0	-49	46	26	34	12	7	12	10	51	11
201	Fucα1-3(Galβ1-4)GlcNAcβ1-2Manα1-3(Fucα1-3(Galβ1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	55	66	85	108	22	8	20	14	90	6

202	Neu5Acα2-3Galβ1-3GalNAcα-Sp8	45	61	73	48	60	13	50	16	33	3
203	Neu5Acα2-8Neu5Acα2-8Neu5Acα2-8Neu5Acα2-3(GalNAcβ1-4)Galβ1-4Glcβ-Sp0	78	54	225	25	25	9	38	11	111	8
204	Neu5Acα2-8Neu5Acα2-8Neu5Acα2-3(GalNAcβ1-4)Galβ1-4Glcβ-Sp0	996	665	435	310	65	13	236	12	57	18
205	Neu5Acα2-8Neu5Acα2-8Neu5Acα2-3Galβ1-4Glcβ–Sp0	76	89	284	241	13	5	22	4	35	12
206	Neu5Acα2-8Neu5Acα2-3(GalNAcβ1-4)Galβ1-4Glcβ–Sp0	44	33	-3	26	11	11	5	6	34	8
207	Neu5Acα2-8Neu5Acα2-8Neu5Acα-Sp8	64	48	95	48	25	8	9	3	68	13
208	Neu5Acα2-3(6-O-Su)Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	91	56	-35	39	18	17	7	6	85	12
209	Neu5Acα2-3(GalNAcβ1-4)Galβ1-4GlcNAcβ-Sp0	26	42	103	43	24	10	47	8	92	17
210	Neu5Acα2-3(GalNAcβ1-4)Galβ1-4GlcNAcβ-Sp8	89	48	58	27	20	7	73	22	109	7
211	Neu5Acα2-3(GalNAcβ1-4)Galβ1-4Glcβ–Sp0	98	90	61	56	21	15	21	6	79	14
212	Neu5Acα2-3(NeuAcα2-3Galβ1-3GalNAcβ1-4)Galβ1-4Glcβ-Sp0	536	127	548	272	37	8	62	13	178	58
213	Neu5Acα2-3(Neu5Acα2-6)GalNAcα–Sp8	-95	66	118	94	12	6	14	3	108	12
214	Neu5Acα2-3GalNAcα–Sp8	-28	30	18	32	10	11	13	4	60	9
215	Neu5Acα2-3GalNAcβ1-4GlcNAcβ-Sp0	186	43	188	46	15	5	61	7	88	4
216	Neu5Acα2-3Galβ1-3(6OSO3)GlcNAc-Sp8	977	655	992	658	62	22	427	182	103	12
217	Neu5Acα2-3Galβ1-3(Fucα1-4)GlcNAcβ–Sp8	39	36	74	89	0	3	35	14	40	17
218	Neu5Acα2-3Galβ1-3(Fucα1-4)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ Sp0	204	37	55	82	21	5	36	12	82	7
219	Neu5Acα2-3Galβ1-3(Neu5Acα2-3Galβ1-4)GlcNAcβ-Sp8	-44	112	762	1495	22	4	70	25	63	14
220	Neu5Acα2-3Galβ1-3[6OSO3]GalNAcα-Sp8	33	68	42	42	32	17	36	7	68	10
221	Neu5Acα2-3Galβ1-3(Neu5Acα2-6)GalNAcα–Sp8	-96	70	78	47	12	3	47	16	103	10
222	Neu5Acα2-3Galβ-Sp8	133	87	82	103	46	22	89	14	53	11
223	Neu5Acα2-3Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Sp0	231	57	153	46	76	18	82	8	85	14
224	Neu5Acα2-3Galβ1-3GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	166	149	240	140	21	6	28	3	53	5
225	Neu5Acα2-3Galβ1-3GlcNAcβ–Sp0	150	114	67	34	47	10	19	6	52	5
226	Neu5Acα2-3Galβ1-3GlcNAcβ–Sp8	158	98	55	52	23	3	39	12	75	12
227	Neu5Acα2-3Galβ1-4[6OSO3]GlcNAcβ-Sp8	900	273	213	73	37	15	43	21	43	7

228	Neu5Acα2-3Galβ1-4(Fucα1-3)(6OSO3)GlcNAcβ–Sp8	119	91	-2	34	27	8	39	15	75	5
229	Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ–Sp0	-47	186	475	322	-8	3	301	44	31	13
230	Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ–Sp0	77	75	-6	34	16	1	5	7	45	3
231	Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ–Sp8	-92	23	-138	95	19	3	38	16	81	10
232	Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ-Sp8	16	88	5	7	8	3	28	8	57	7
233	Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp8	50	21	165	124	90	11	97	47	157	21
234	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAc-Sp0	4	83	56	89	39	15	36	11	91	27
235	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ–Sp0	2105	616	1730	47	17	3	35	11	92	15
236	Neu5Acα2-3Galβ1-4GlcNAcβ–Sp0	367	112	62	20	11	10	23	5	83	14
237	Neu5Acα2-3Galβ1-4GlcNAcβ–Sp8	119	40	43	16	33	9	12	4	0	0
238	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	738	631	147	53	27	6	42	8	46	6
239	Neu5Acα2-3Galβ1-4Glcβ–Sp0	29	26	82	53	33	8	38	6	67	13
240	Neu5Acα2-3Galβ1-4Glcβ–Sp8	-14	24	21	55	19	6	61	22	19	7
241	Galβ1-4GlcNAcβ1-2Manα1-3(Fucα1-3(Galβ1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	774	105	25	39	0	0	30	7	0	0
242	Neu5Acα2-6GalNAcα–Sp8	-10	33	12	38	25	6	15	4	63	14
243	Neu5Acα2-6GalNAcβ1-4GlcNAcβ-Sp0	226	125	78	43	11	7	81	43	66	16
244	Neu5Acα2-6Galβ1-4[6OSO3]GlcNAcβ-Sp8	120	159	39	120	13	4	67	19	118	16
245	Neu5Acα2-6Galβ1-4GlcNAcβ–Sp0	63	91	-1	26	20	7	67	29	121	53
246	Neu5Acα2-6Galβ1-4GlcNAcβ–Sp8	-38	41	56	35	21	4	34	8	61	12
247	Neu5Acα2-6Galβ1-4GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	72	40	142	67	29	8	47	14	90	21
248	Neu5Acα2-6Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	21	140	346	99	37	14	63	9	50	12
249	Neu5Acα2-6Galβ1-4Glcβ–Sp0	71	71	64	31	21	6	17	18	81	11
250	Neu5Acα2-6Galβ1-4Glcβ–Sp8	128	39	114	84	17	8	44	12	59	14
251	Neu5Acα2-6Galβ–Sp8	-1	47	42	29	26	2	13	8	72	8

252	Neu5Acα2-8Neu5Acα-Sp8	107	78	13	6	17	6	20	10	51	6
253	Neu5Acα2-8Neu5Acα2-3Galβ1-4Glcβ–Sp0	-72	55	245	556	13	9	11	27	99	8
254	Neu5Acβ2-6GalNAcα–Sp8	69	120	311	179	56	11	20	4	36	3
255	Neu5Acβ2-6Galβ1-4GlcNAcβ-Sp8	16	40	31	64	-14	6	32	8	50	16
256	Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp21	475	239	42	68	0	0	48	13	0	0
257	Neu5Gca2-3Galβ1-3(Fucα1-4)GlcNAcβ-Sp0	112	65	77	109	4	1	28	3	51	6
258	Neu5Gca2-3Galβ1-3GlcNAcβ-Sp0	302	106	91	60	36	7	40	12	62	8
259	Neu5Gca2-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	253	33	121	87	17	12	61	49	67	13
260	Neu5Gcα2-3Galβ1-4GlcNAcβ–Sp0	441	72	109	51	33	8	25	6	88	21
261	Neu5Gcα2-3Galβ1-4Glcβ–Sp0	170	81	48	20	15	7	34	22	102	11
262	Neu5Gcα2-6GalNAcα–Sp0	36	27	24	27	40	14	34	9	121	20
263	Neu5Gcα2-6Galβ1-4GlcNAcβ–Sp0	83	47	45	16	33	9	63	26	96	25
264	Neu5Gcα–Sp8	76	77	89	44	10	16	41	4	111	24
265	[3OSO3]Galβ1-4(Fucα1-3)(6OSO3)Glc-Sp0	118	118	3431	4148	31	21	52	8	165	39
266	[3OSO3]Galβ1-4(Fucα1-3)Glc-Sp0	32	32	65	38	24	5	44	16	95	11
267	[3OSO3]Galβ1-4[Fucα1-3][6OSO3]GlcNAc-Sp8	305	483	81	20	39	21	63	35	97	11
268	[3OSO3]Galβ1-4[Fucα1-3]GlcNAc-Sp0	240	70	377	105	10	6	111	32	93	15
269	Fucα1-2[6OSO3]Galβ1-4GlcNAc-Sp0	-23	68	48	39	23	10	46	10	71	7
270	Fucα1-2Galβ1-4[6OSO3]GlcNAc-Sp8	1194	646	176	78	15	3	72	23	61	19
271	Fucα1-2[6OSO3]Galβ1-4[6OSO3]Glc-Sp0	-44	85	38	42	2	11	24	14	115	4
272	Fucα1-2-(6OSO3)-Galβ1-4Glc-Sp0	56	71	70	44	0	0	0	4		
273	Fucα1-2-Galβ1-4[6OSO3]Glc-Sp0	49	69	121	17	469	82	53	17	79	25
274	Galβ1-3(Fucα1-4)GlcNAcβ1-3Galβ1-3(Fucα1-4)GlcNAcβ-Sp0	145	78	118	129	39	6	31	11	42	6
275	Galβ1-3-(Galβ1-4GlcNacβ1-6)GalNAc-Sp14	-40	39	155	147	37	16	10	22	47	19
276	Galβ1-3(GlcNacβ1-6)GalNAc-Sp14	74	49	30	28	35	11	21	5	55	7
277	Galβ1-3-(Neu5Aca2-3Galβ1-4GlcNacβ1-6)GalNAc-Sp14	460	132	378	208	18	8	66	13	87	7
278	Galβ1-3GalNAc-Sp14	55	89	58	10	38	18	88	38	99	16
279	Galβ1-3GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	426	217	132	24	148	36	62	16	85	13
280	Galβ1-4[Fucα1-3][6OSO3]GlcNAc-Sp0	115	42	281	207	41	7	38	11	85	21
281	Galβ1-4[Fucα1-3][6OSO3]Glc-Sp0	48	88	57	18	33	8	36	10	81	15

282	Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-3(Fucα1-4)GlcNAcβ-Sp0	127	46	31	11	89	14	87	24	56	6
283	Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	495	586	640	97	64	21	103	15	83	2
284	Neu5Acα2-3Galβ1-3GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	348	37	385	258	110	27	43	3	71	15
285	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	124	140	115	20	42	18	59	20	71	5
286	[3OSO3]Galβ1-4[6OSO3]GlcNAcβ-Sp0	27082	14870	687	402	38	8	68	41	85	6
287	[3OSO3][4OSO3]Galβ1-4GlcNacβ-Sp0	14	53	81	79	-14	14	53	26	47	5
288	[6OSO3]Galβ1-4[6OSO3]GlcNacβ-Sp0	20	51	51	33	42	9	29	13	126	12
289	6-H2PO3Glcβ-Sp10	67	59	344	493	3	2	34	3	26	5
290	Galα1-3(Fucα1-2)Galβ–Sp18	71	22	-1	13	24	11	17	6	71	7
291	Galα1-3GalNAcα-Sp16	170	161	290	177	11	7	50	19	70	23
292	Galβ1-3GalNAcα-Sp16	214	49	118	101	16	1	59	11	94	12
293	Galβ1-3(Neu5Acα2-3Galβ1-4(Fucα1-3)GlcNAcβ1-6)GalNAc–Sp14	141	84	31	437	86	16	32	5	86	10
294	Galβ1-3Galβ1-4GlcNAcβ-Sp8	652	262	47	29	256	24	18	9	66	10
295	Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	1140	16	13	20	24	16	55	19	116	19
296	Galβ1-4GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)Galβ1-4GlcNAc-Sp0	17520	7379	179	71	6	5	2	5	124	16
297	Galβ1-4GlcNAcβ1-3(GlcNAcβ1-6)Galβ1-4GlcNAc-Sp0	3521	158	5	59	15	10	23	22	63	7
298	Galβ1-4GlcNAcα1-6Galβ1-4GlcNAcβ-Sp0	28251	1882	117	106	18	6	21	8	86	17
299	Galβ1-4GlcNAcβ1-6Galβ1-4GlcNAcβ-Sp0	973	294	446	812	22	21	35	23	118	17
300	GalNAcα-Sp15	112	213	20	9	14	1	5	9	69	8
301	GalNAcα1-3(Fucα1-2)Galβ–Sp18	43	137	41	61	10	8	5	9	55	14
302	GalNAcβ1-3Galβ-Sp8	194	76	-1	35	190	53	27	8	69	11
303	GlcAβ1-3GlcNAcβ-Sp8	123	116	-17	24	174	37	45	15	477	13
304	GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	-47	30	36	71	21	12	31	13	109	23
305	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	-92	39	34	36	9	9	13	3	88	11
306	GlcNAcβ1-3Man-Sp10	61	73	71	54	15	2	160	37	68	12
307	GlcNAcβ1-4GlcNAcβ-Sp10	-6	28	-8	22	23	11	47	24	65	4
308	GlcNAcβ1-4GlcNAcβ-Sp12	35	49	19	14	49	10	40	18	39	7

309	HOOC(CH3)CH-3-O-GlcNAcβ1-4GlcNAcβ-Sp10	-114	76	17	22	26	2	61	35	77	2
310	Manα1-3(Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	43	86	73	56	25	9	5	4	97	7
311	Manα1-6Manβ-Sp10	-2	30	49	92	56	13	19	8	44	10
312	Manα1-6(Manα1-3)Manα1-6(Manα1-3)Manβ-Sp10	107	86	81	46	12	4	57	24	68	14
313	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-6(Manα1-3)Manα1-6)Manα-Sp9	66	48	37	57	13	2	27	16	42	13
314	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-6(Manα1-2Manα1-3)Manα1-6)Manα-Sp9	77	30	67	27	20	6	22	6	64	9
315	Neu5Acα2-3Galβ1-3(Neu5Acα2-3Galβ1-4GlcNAcβ1-6)GalNAc–Sp14	66	187	530	533	-17	7	145	54	54	7
316	Neu5Acα2-3Galβ1-3(Neu5Acα2-6)GalNAc-Sp14	166	109	30	15	75	32	76	21	118	2
317	Neu5Acα2-3Galβ1-3GalNAc–Sp14	521	316	48	55	-23	4	65	35	23	6
318	Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	883	375	41	17	34	11	21	10	84	4
319	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	1556	47	46	28	47	15	40	16	102	28
320	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	-68	106	12	21	24	8	20	15	61	7