

Supplementary Information

Plasticity of the β -trefoil protein fold in the recognition and control of invertebrate predators and parasites by a fungal defence system

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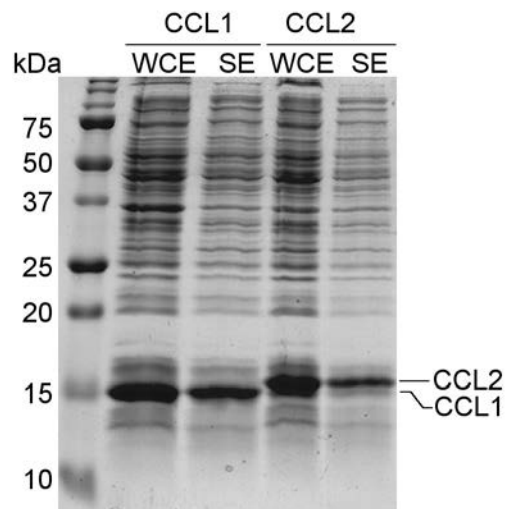


Figure S1. Coomassie-stained SDS-PAGE showing the expression and solubility of CCL1 and CCL2 recombinantly expressed in *E.coli*. WCE: whole cell extracts; SE: soluble fraction of WCE.

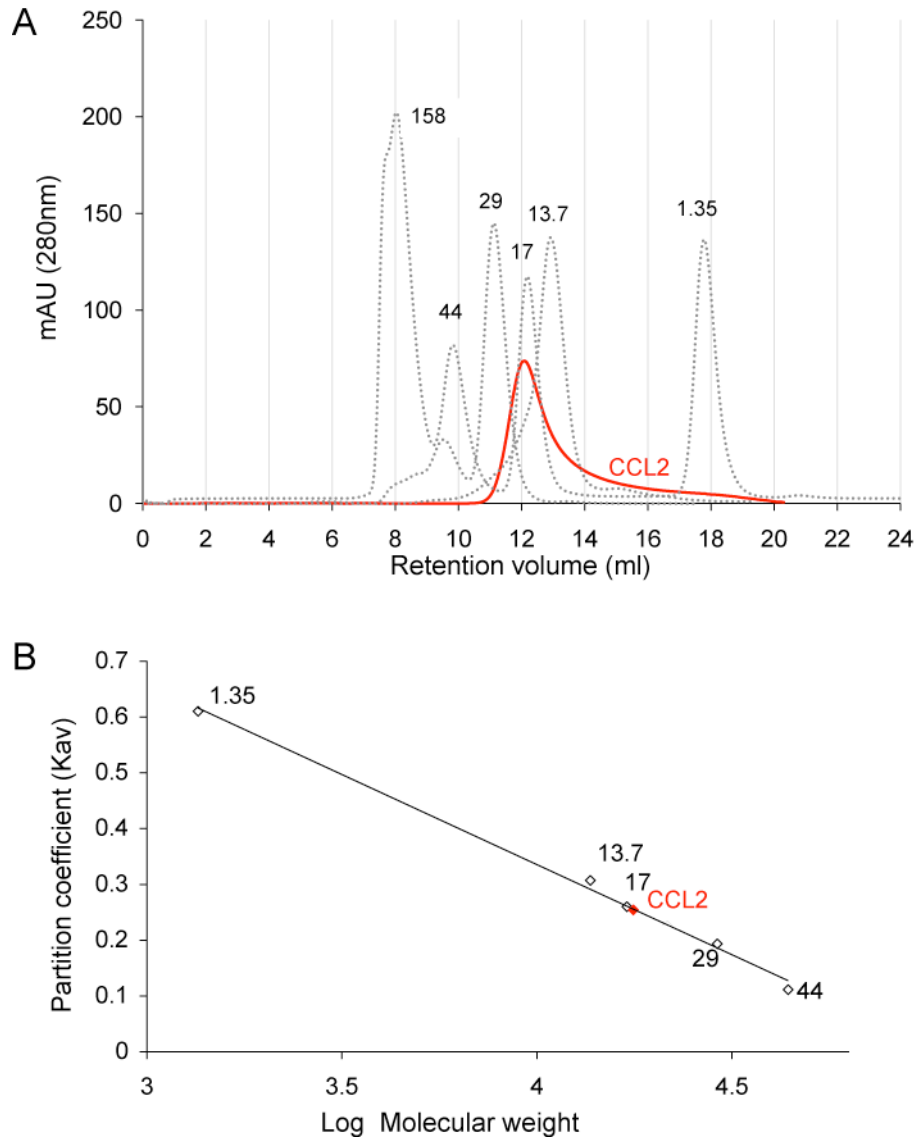


Figure S2. Size exclusion chromatography showing the monomeric state of CCL2 compared to standard proteins. (A) Elution profile of standard proteins (dotted lines, numbers indicate size in kDa) and CCL2 (red) which elutes at 12.1 ml from a Superdex 75 10/300 (GL) column. (B) Calibration curve done with the following standards: Ovalbumin 44 kDa, Carbonic anhydrase (29 kDa), Myoglobin (17 kDa), RNase A (13.7 kDa) and Vitamin B₁₂ (1.35 kDa). The void volume was determined by elution of bovine γ -globulin (8.04 ml). The calculated molecular weight for CCL2 (in red) is 17.6. Gel filtration was performed at a flow rate of 0.5 ml/min in 10 mM sodium phosphate, 150mM NaCl buffer pH 6.2. Samples of 2-5 mg/ml of protein in 0.1 ml were injected, and the eluate was monitored at 280 nm.

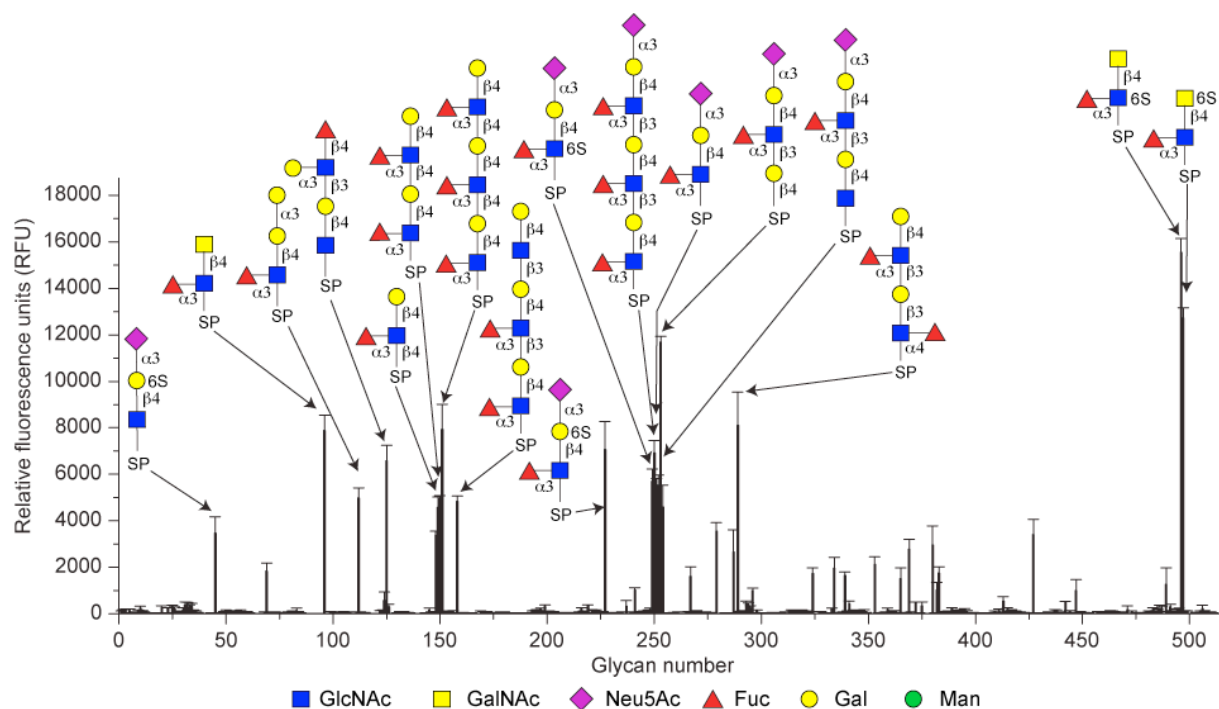


Figure S3. Glycan array analysis showing the carbohydrate-binding specificity of CCL1. Results shown are averages of triplicate measurements of fluorescence intensity at a lectin concentration of $200\mu\text{g/ml}$ probed on the Mammalian Glycan Array (V 4.2). Error bars indicate the standard deviations of the mean. Glycan structures are depicted for those epitopes with highest relative fluorescence. The raw data and the entire list of glycans with the respective spacers can be found on the CFG homepage [<http://functionalglycomics.org>] or in Table S3. Binding of 6'sulfo-sialyllactose (glycan #45) is likely to be an artifact since it is also bound by fucose-binding lectin AAL [<http://functionalglycomics.org>].

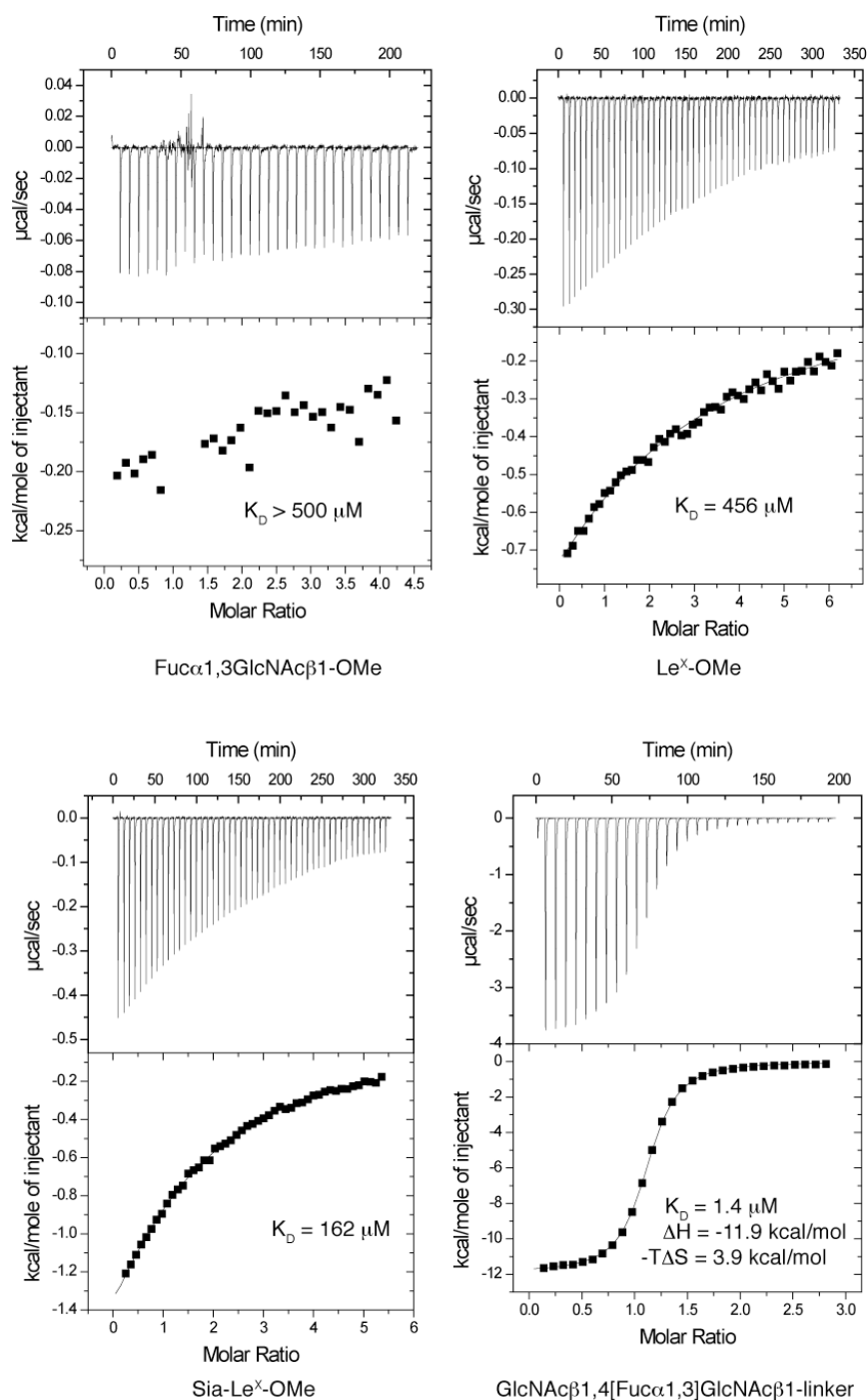


Figure S4. Isothermal titration calorimetry binding experiments between wild type CCL2 and different carbohydrate ligands. Raw calorimetric outputs are shown on the top and binding isotherms describing the complex formation are shown at the bottom. The protein concentration in the cell was 70 μM and the carbohydrate concentration was 3.0 mM.

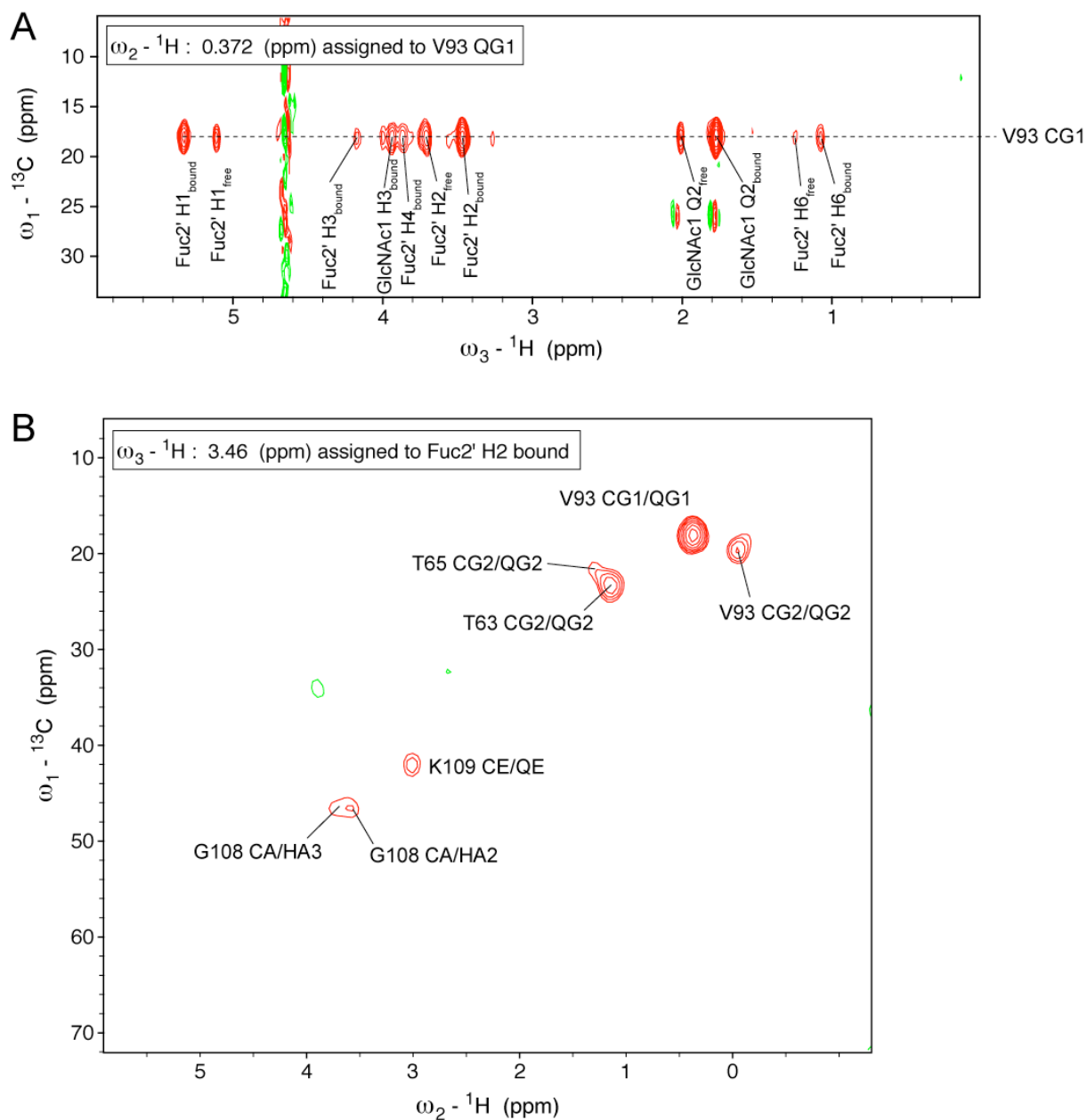


Figure S5. 3D F1-edited F3-filtered HSQC-NOESY spectrum. A) Carbohydrate resonances are well dispersed in the direct dimension ω_3 (^{13}C filtered/suppressed). Shown is a slice at the ω_2 (^{13}C edited/selected) resonance of V93 methyl group QG2 displaying intermolecular NOEs. B) Slice of the two indirect dimensions ω_1 and ω_2 at the ω_3 resonance of Fucose H2_{bound} showing intermolecular NOEs to Fucose H2. The ^1H - ^{13}C correlations of the ^{13}C labelled protein were directly compared to the ^{13}C HSQC spectrum of the protein to assign the intermolecular NOEs.

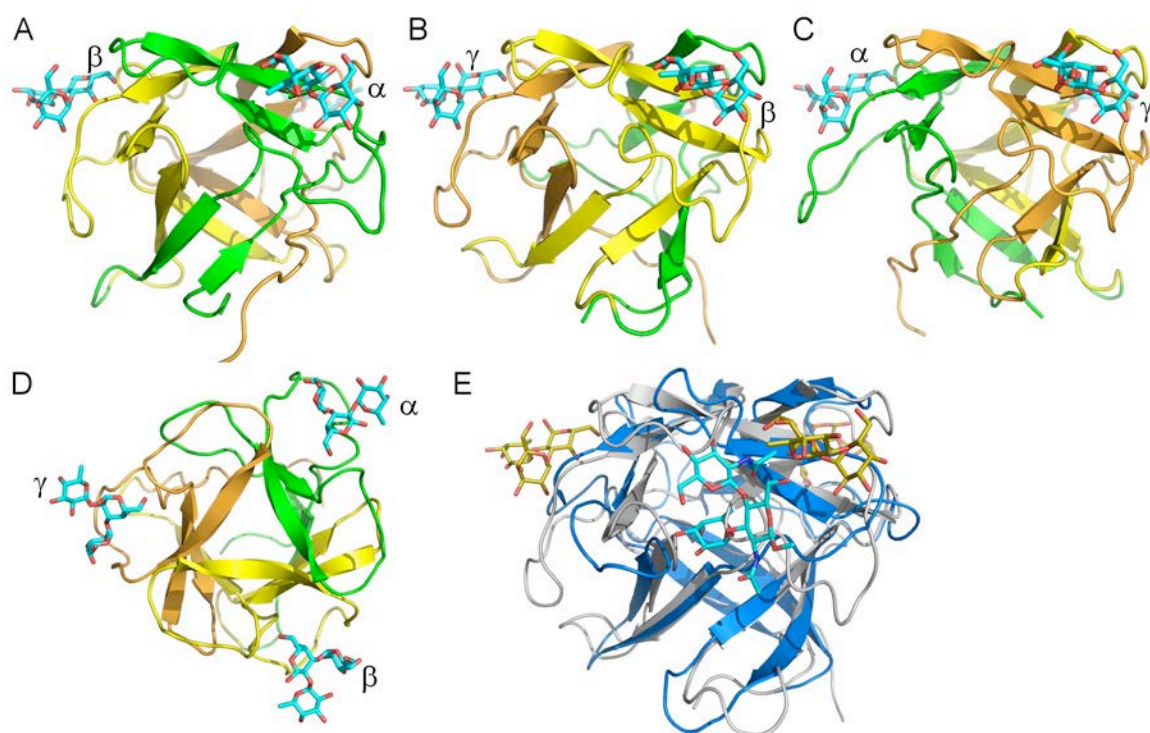


Figure S6. The three symmetry-related canonical binding sites of β -trefoil proteins illustrated by the lectin MOA. (A-C) Three different side views related to each other by rotation of 120° around the z axis of MOA in complex with Gal α 1,3(Fuc α 1,2)Gal (PDB: 3EF2). The binding sites are indicated by Greek letters. (D) Top view of the same complex. The same colors and similar orientations are used as for CCL2 in Figs. 4 and 5. (E) Superposition of the CCL2 complex structure (blue) with ligand (cyan) on the MOA complex structure 3EF2 (grey) with ligands (yellow). The β subunit is located in front.

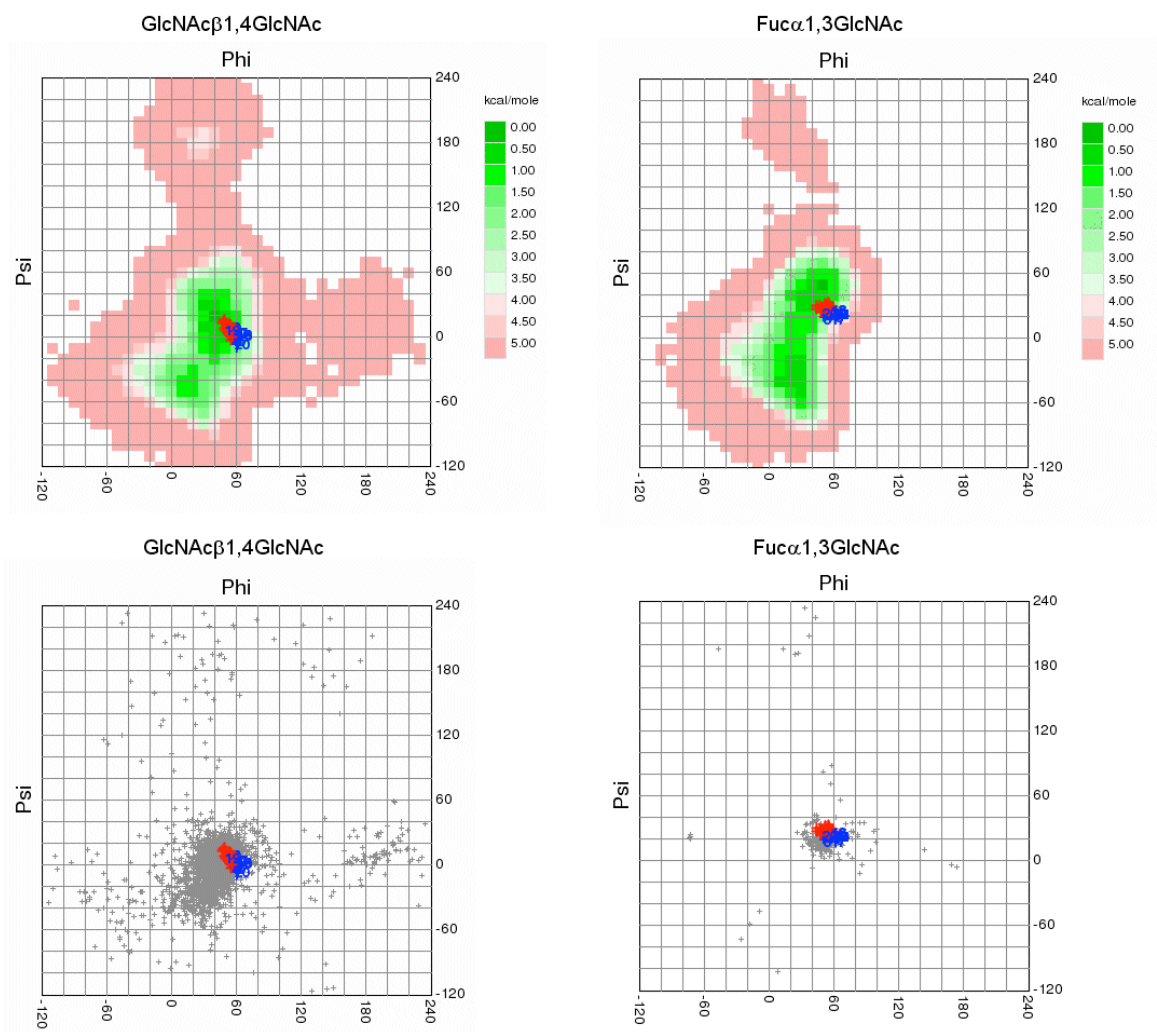


Figure S7: Angle plots of the glycosidic linkages of fucosylated chitobiose found in the 20 calculated complex structures. The plots, generated by CARP [1], display the observed angles (red with labels in blue) on top of an energy landscape calculated by modelling (top) or on top of angles of the same disaccharide linkage found in all structures deposited in the PDB database (bottom).

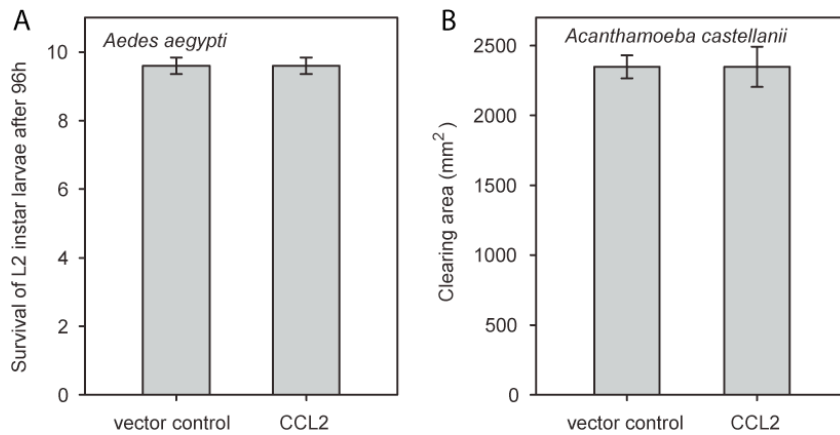


Figure S8. Toxicity of CCL2 towards *A. aegypti* and *A. castellanii*. Toxicity of CCL2-expressing *E. coli* towards larvae of the mosquito *A. aegypti* (A) and the amoebozoan *A. castellanii* (B) was assessed as described in Materials and Methods. Error bars indicate standard errors of the mean. No significant differences were observed between CCL2 and VC ($p > 0.05$).

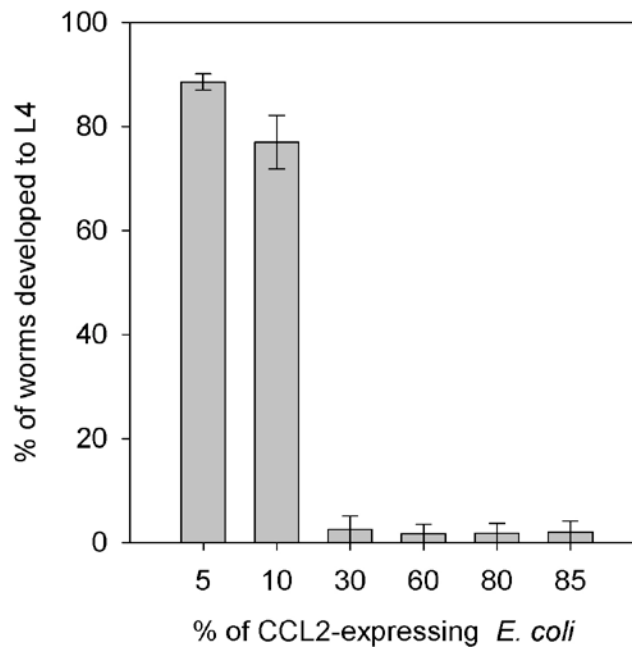


Figure S9. Dose-dependence of CCL2-mediated nematotoxicity. Wildtype *C. elegans* (N2) were fed with mixtures of CCL2-expressing *E. coli* expressing CCL2 and empty vector-containing *E. coli*. Error bars indicate standard errors of the mean.

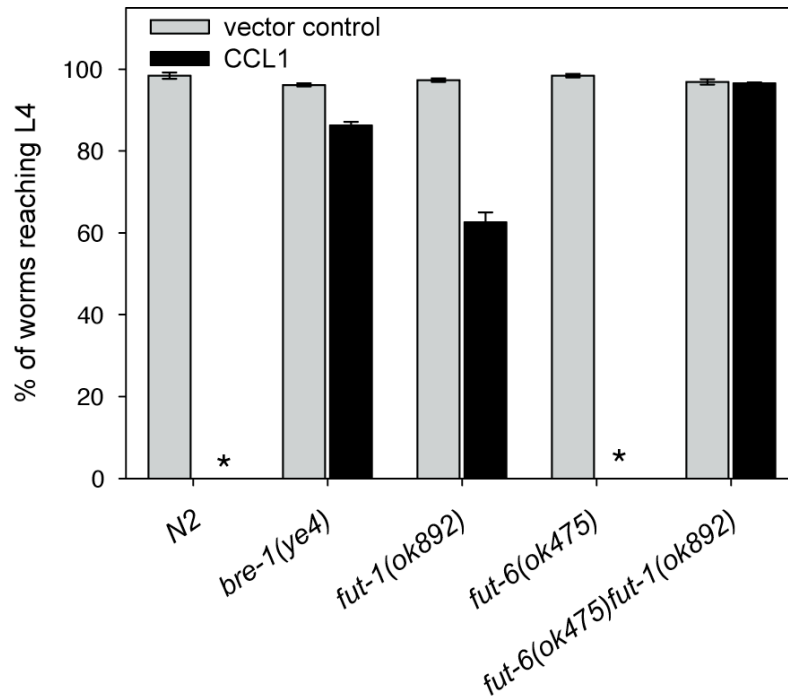


Figure S10. Carbohydrate-binding dependence of CCL1-mediated nematotoxicity. Toxicity of CCL1-expressing *E. coli* towards *C. elegans* wild type (N2) and various fucosylation mutants. Error bars indicate standard errors of the mean. Asterisks (*) show cases where all data were 0. Assays were done in solid media as described [2].

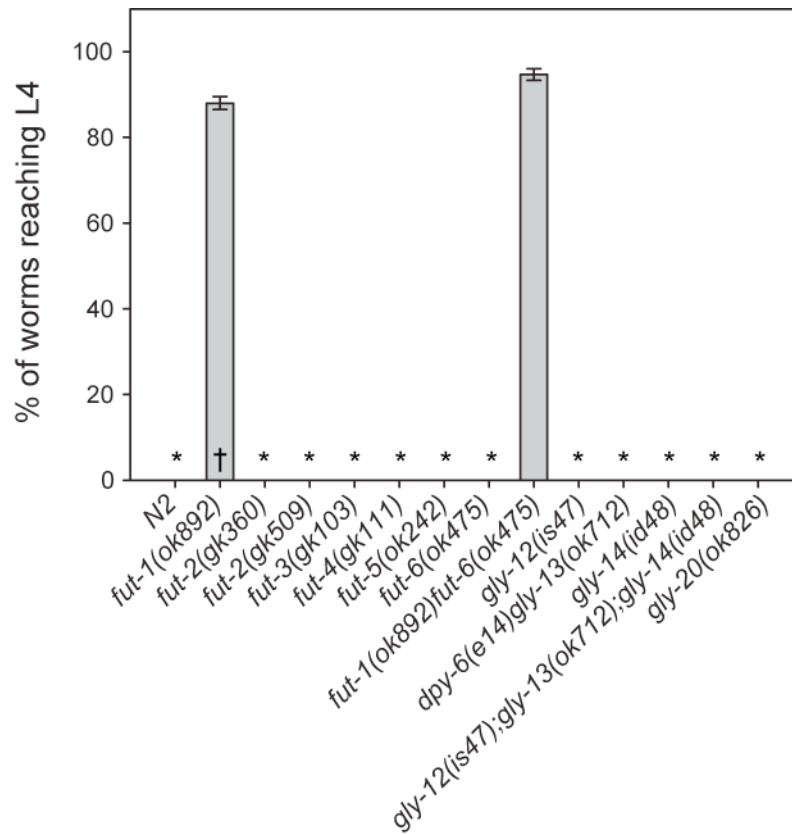


Figure S11. Toxicity of recombinant *E. coli* expressing CCL2 towards *C. elegans* wildtype (N2) and various mutants in predicted or characterized fucosyltransferases (fut) or GlcNAc-transferases (gly). Assays were done in solid media as described [2]. Error bars indicate standard errors of the mean. Asterisks (*) show cases where all data were 0. †: In the *fut-1(ok892)* mutants a partial resistance is observed. Although the larvae survive and develop, they require at least 24h more to reach L4 and look thinner and paler than the complete resistant double mutant *fut-6(ok475)fut-1(ok892)*.

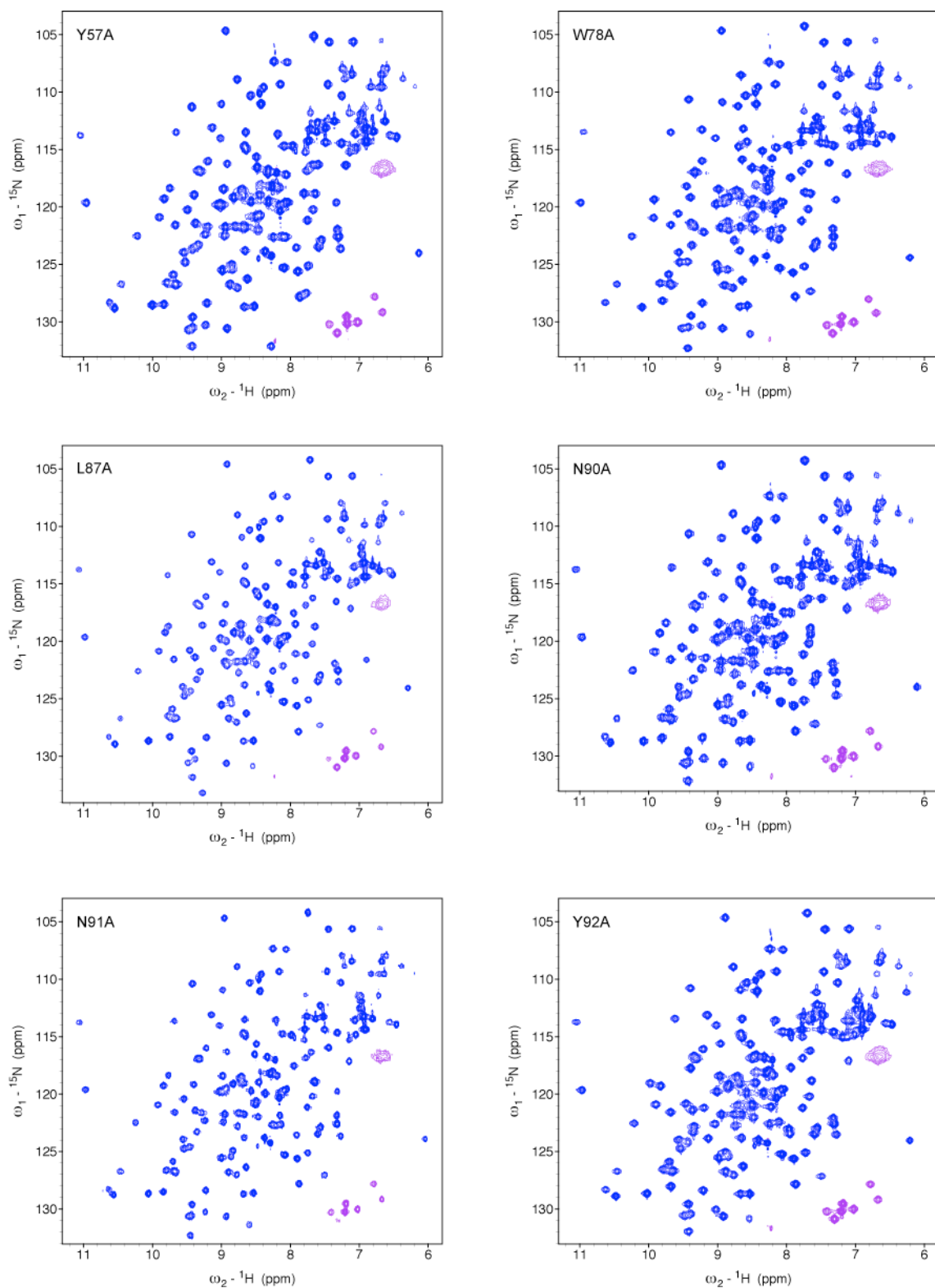


Figure S12. All CCL2 proteins containing a point mutant are folded. ^{15}N -HSQC spectra of ^{15}N labelled proteins.

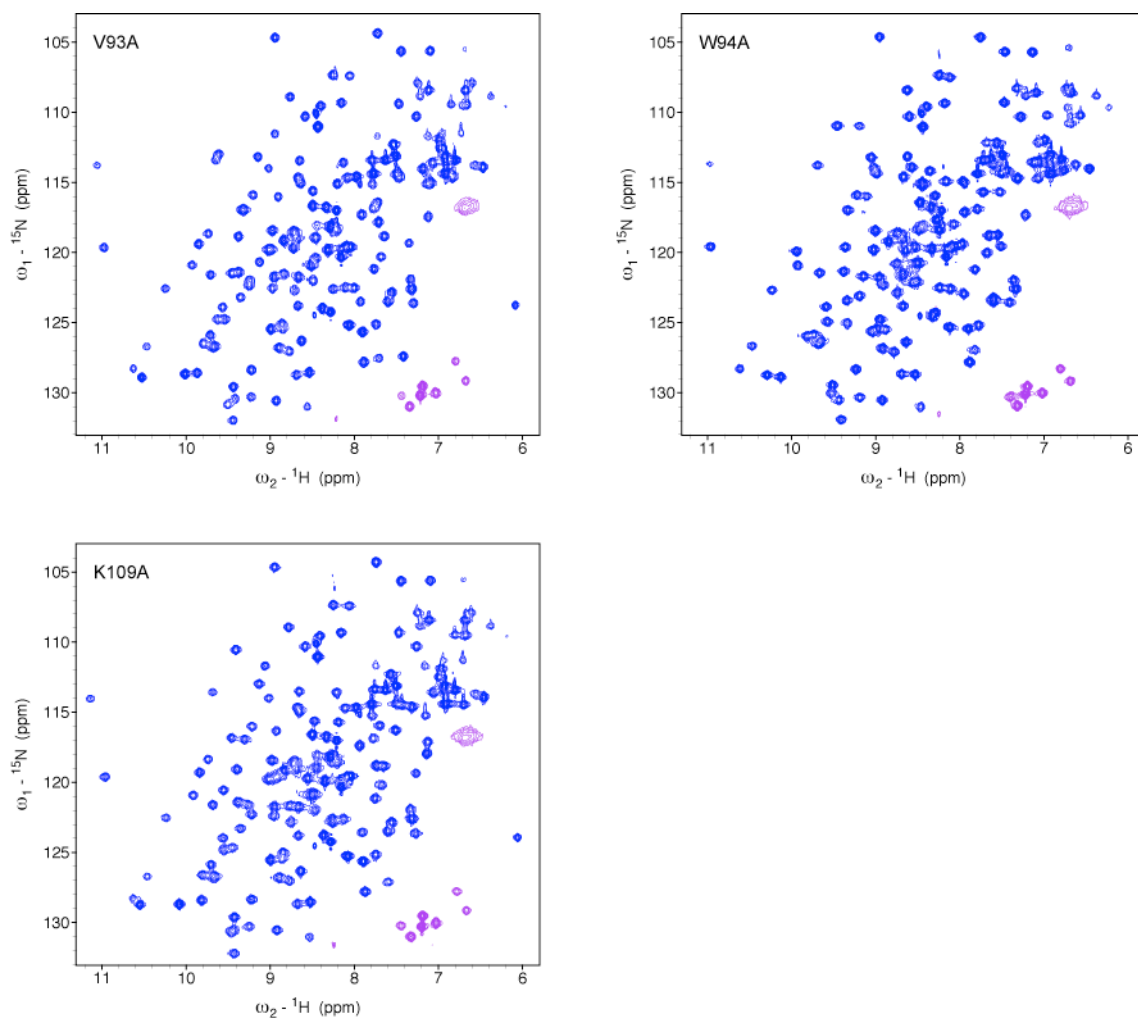


Figure S12. (continuation)

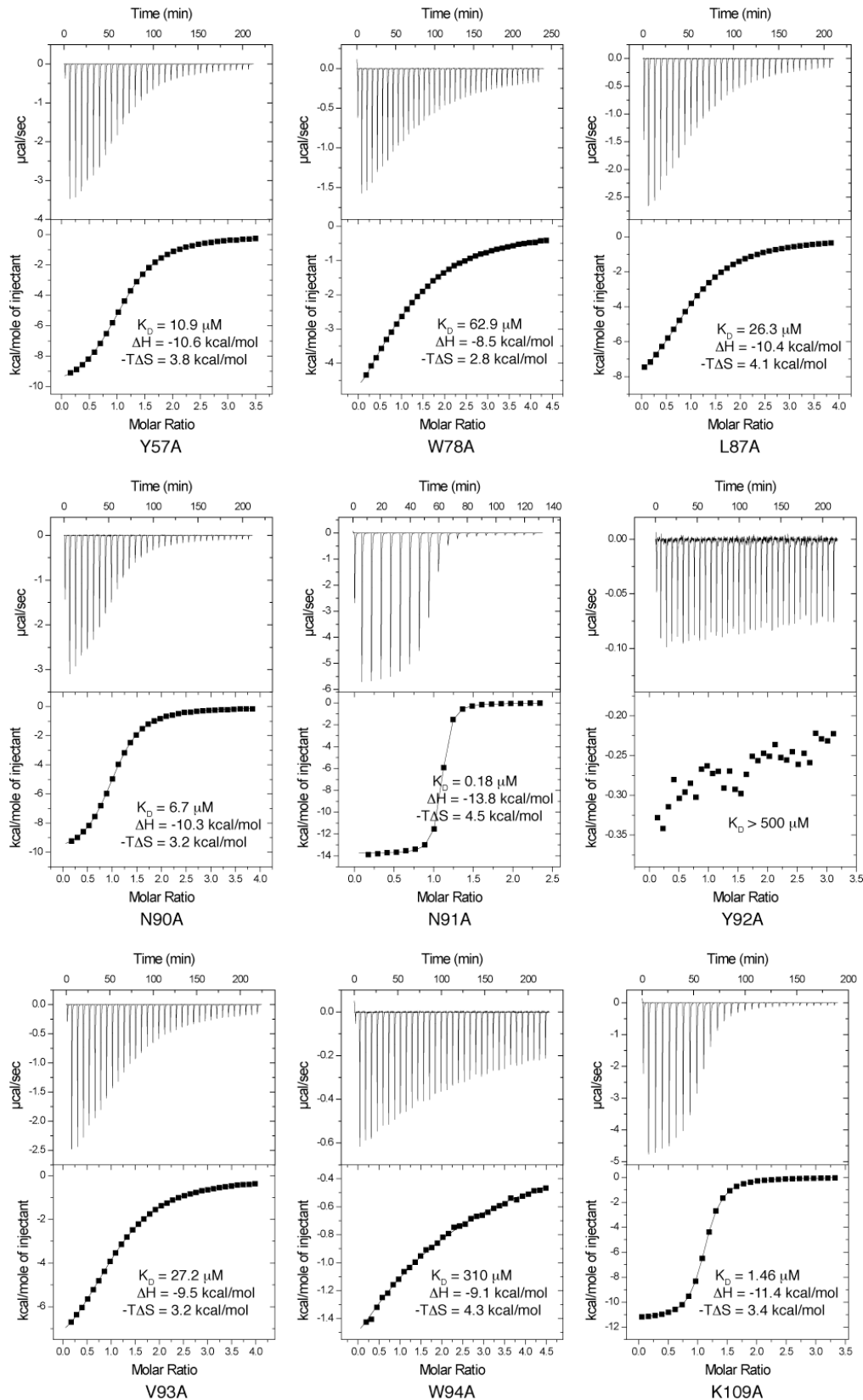


Figure S13. Isothermal titration calorimetry binding experiments between CCL2 mutants and fucosylated chitobiose (GlcNAc β 1,4[Fuc α 1,3]GlcNAc β 1-spacer). Raw calorimetric outputs are shown on the top and binding isotherms describing the complex formation K_D are shown at the bottom. The protein concentration in the cell was 70 μM and the carbohydrate concentration was 3.0 mM.

Table S1. Sequence identities among the CCL2 orthologues found in fungi and the lectin MOA and SNA-II. CCL2_A: CCL2 of *C. cinerea* strain AmutBmut; CCL2_O: CCL2 of *C. cinerea* strain Okayama7; CCL1_A: CCL1 of *C. cinerea* strain AmutBmut; CCL1_O: CCL1 of *C. cinerea* strain Okayama7; PP_L1: *Postia placenta* lectin 1 (Posp11_130016); PP_L2: *Postia placenta* lectin 2 (Posp11_121916); SL_L1: *Serpula lacrymans* lectin 1 (SerlaS7_144703); CP_L1: *Coniophora puteana* lectin 1 (Conpu1_119225); PO_L1: *Pleurotus ostreatus* lectin 1 (PleosPC9_89828); PO_L2: *Pleurotus ostreatus* lectin 2 (PleosPC15_1043947); PO_L3: *Pleurotus ostreatus* lectin 3 (PleosPC9_64199); PO_L4: *Pleurotus ostreatus* lectin 4 (PleosPC15_1065820); DS_L1: *Dicomitus squalis* lectin 1 (Dicsq1); AO_L1: *Arthrobotrys oligospora* lectin 1 (s00075g2); LB_L1: *Laccaria bicolor* lectin 1 (Lbic_330799); LB_L2: *Laccaria bicolor* lectin 2 (Lbic_327918); MOA: *Marasmius oreades* agglutinin; SNA-II: *Sambucus nigra* agglutinin/ribosome inactivating protein type II.

	CCL2_A	CCL2_O	CCL1_A	CCL1_O	PP_L1	PP_L2	SL_L1	CP_L1	PO_L1	PO_L2	PO_L3	PO_L4	DS_L1	AO_L2	LB_L1	LB_L2	MOA	SNA-II
CCL2_A	—	93%	54%	52%	44%	44%	39%	37%	42%	42%	40%	34%	33%	30%	34%	24%	14%	13%
CCL2_O		—	54%	52%	42%	42%	40%	39%	44%	44%	40%	35%	33%	30%	34%	25%	14%	12%
CCL1_A			—	97%	42%	42%	48%	44%	40%	40%	34%	34%	36%	32%	32%	20%	14%	11%
CCL1_O				—	42%	42%	48%	43%	39%	38%	34%	34%	35%	32%	32%	20%	13%	10%
PP_L1					—	95%	56%	54%	43%	44%	42%	42%	39%	34%	39%	29%	14%	15%
PP_L2						—	55%	54%	43%	44%	42%	43%	39%	36%	40%	28%	14%	15%
SL_L1							—	54%	47%	48%	43%	40%	45%	38%	37%	27%	16%	14%
CP_L1								—	46%	45%	40%	38%	40%	33%	37%	26%	14%	12%
PO_L1									—	88%	66%	50%	38%	37%	34%	24%	11%	12%
PO_L2										—	62%	47%	37%	35%	37%	26%	11%	12%
PO_L3											—	45%	34%	34%	36%	22%	13%	16%
PO_L4												—	31%	34%	29%	23%	13%	9%
DS_L1													—	31%	29%	24%	14%	12%
AO_L2														—	28%	20%	12%	10%
LB_L1															—	26%	15%	12%
LB_L2																—	15%	13%
MOA																	—	9%
SNA-II																		—

Table S2. Raw data of glycan array analysis performed with CCL2. RFU = Relative Fluorescence Units; SD = Standard deviation

No.	Glycan structure – spacer*	RFU	SD
1	Neu5Ac α 2-8Neu5Ac β -Sp17	155.0	88.2
2	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac β Sp8	66.6	38.8
3	Neu5Gc β 2-6Gal β 1-4GlcNAc-Sp8	182.6	74.3
4	Gal β 1-3GlcNAc β 1-2Man α 1-3(Gal β 1-3GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp19	453.7	150.8
5	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	183.9	43.5
6	α -D-Gal-Sp8	280.7	94.2
7	α -D-Glc-Sp8	594.5	365.1
8	α -D-Man-Sp8	152.9	88.5
9	α -GalNAc-Sp8	151.8	60.8
10	α -L-Fuc-Sp8	416.6	386.4
11	α -L-Fuc-Sp9	136.8	10.1
12	α -L-Rha-Sp8	112.5	57.6
13	α -Neu5Ac-Sp8	247.4	195.8
14	α -Neu5Ac-Sp11	119.3	140.3
15	β -Neu5Ac-Sp8	122.4	61.6
16	β -D-Gal-Sp8	194.7	83.6
17	β -D-Glc-Sp8	113.2	9.4
18	β -D-Man-Sp8	130.5	60.3
19	β -GalNAc-Sp8	273.6	160.5
20	β -GlcNAc-Sp0	172.7	36.2
21	β -GlcNAc-Sp8	160.7	63.6
22	β -GlcN(Gc)-Sp8	136.2	139.4
23	(Gal β 1-4GlcNAc β)2-3,6-GalNAc α -Sp8	397.4	201.5
24	GlcNAc β 1-3(GlcNAc β 1-4)(GlcNAc β 1-6)GlcNAc-Sp8	103.1	41.2
25	[3OSO3][6OSO3]Gal β 1-4[6OSO3]GlcNAc β -Sp0	367.7	238.4
26	[3OSO3][6OSO3]Gal β 1-4GlcNAc β -Sp0	193.4	34.3
27	[3OSO3]Gal β 1-4Glc β -Sp8	152.3	96.0
28	[3OSO3]Gal β 1-4(6OSO3)Glc β -Sp0	151.3	50.4
29	[3OSO3]Gal β 1-4(6OSO3)Glc β -Sp8	1039.1	720.1
30	[3OSO3]Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp8	628.7	695.7
31	[3OSO3]Gal β 1-3GalNAc α -Sp8	216.8	113.9
32	[3OSO3]Gal β 1-3GlcNAc β -Sp8	403.9	425.3
33	[3OSO3]Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	265.1	74.5
34	[3OSO3]Gal β 1-4[6OSO3]GlcNAc β -Sp8	101.0	90.0
35	[3OSO3]Gal β 1-4GlcNAc β -Sp0	115.6	12.2
36	[3OSO3]Gal β 1-4GlcNAc β -Sp8	110.8	72.3
37	[3OSO3]Gal β -Sp8	75.5	25.5
38	[4OSO3][6OSO3]Gal β 1-4GlcNAc β -Sp0	222.7	221.8
39	[4OSO3]Gal β 1-4GlcNAc β -Sp8	350.4	63.8
40	6-H2PO3Man α -Sp8	118.9	53.1
41	[6OSO3]Gal β 1-4Glc β -Sp0	307.4	46.8
42	[6OSO3]Gal β 1-4Glc β -Sp8	269.4	180.9
43	[6OSO3]Gal β 1-4GlcNAc β -Sp8	133.9	115.9
44	[6OSO3]Gal β 1-4[6OSO3]Glc β -Sp8	298.1	154.7
45	NeuAc α 2-3[6OSO3]Gal β 1-4GlcNAc β -Sp8	40316.6	1380.1
46	[6OSO3]GlcNAc β -Sp8	141.7	114.3
47	9NAcNeu5Ac α -Sp8	8595.4	918.0
48	9NAcNeu5Ac α 2-6Gal β 1-4GlcNAc β -Sp8	239.4	174.8
49	Man α 1-3(Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp13	525.3	166.5
50	GlcNAc β 1-2Man α 1-3(GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp13	674.3	270.7

51	Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	575.8	464.2
52	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	336.0	84.3
53	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp8	535.8	285.5
54	Fuca1-2Galβ1-3GalNAcβ1-3Gala-Sp9	854.8	233.8
55	Fuca1-2Galβ1-3GalNAcβ1-3Gala1-4Galβ1-4Glcβ-Sp9	146.7	31.0
56	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ-Sp8	101.3	43.1
57	Fuca1-2Galβ1-3GalNAcα-Sp8	83.3	18.4
58	Fuca1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp0	108.9	42.3
59	Fuca1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp9	190.1	16.2
60	Fuca1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ-Sp10	99.7	48.5
61	Fuca1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ-Sp8	261.3	84.7
62	Fuca1-2Galβ1-3GlcNAcβ-Sp0	154.5	95.8
63	Fuca1-2Galβ1-3GlcNAcβ-Sp8	197.8	44.3
64	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	495.0	369.3
65	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	1323.8	228.2
66	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	80.7	29.0
67	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ-Sp8	3466.0	907.7
68	Fuca1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAc-Sp0	57.3	54.0
69	Fuca1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	282.4	119.0
70	Fuca1-2Galβ1-4GlcNAcβ-Sp0	246.8	94.3
71	Fuca1-2Galβ1-4GlcNAcβ-Sp8	288.4	84.2
72	Fuca1-2Galβ1-4Glcβ-Sp0	250.1	152.4
73	Fuca1-2Galβ-Sp8	200.0	100.4
74	Fuca1-3GlcNAcβ-Sp8	211.4	160.5
75	Fuca1-4GlcNAcβ-Sp8	183.1	9.3
76	Fucβ1-3GlcNAcβ-Sp8	297.6	398.7
77	GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ-Sp0	107.7	46.0
78	GalNAcα1-3(Fuca1-2)Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	192.0	73.9
79	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ-Sp0	193.0	98.0
80	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ-Sp8	104.3	38.4
81	GalNAcα1-3(Fuca1-2)Galβ1-4Glcβ-Sp0	94.5	79.5
82	GalNAcα1-3(Fuca1-2)Galβ-Sp8	90.7	10.7
83	GalNAcα1-3GalNAcβ-Sp8	162.6	41.6
84	GalNAcα1-3Galβ-Sp8	176.6	38.9
85	GalNAcα1-4(Fuca1-2)Galβ1-4GlcNAcβ-Sp8	248.7	68.9
86	GalNAcβ1-3GalNAcα-Sp8	123.7	70.5
87	GalNAcβ1-3(Fuca1-2)Galβ-Sp8	304.1	176.9
88	GalNAcβ1-3Gala1-4Galβ1-4GlcNAcβ-Sp0	204.6	208.7
89	GalNAcβ1-4(Fuca1-3)GlcNAcβ-Sp0	40042.3	1963.4
90	GalNAcβ1-4GlcNAcβ-Sp0	285.8	388.3
91	GalNAcβ1-4GlcNAcβ-Sp8	117.5	83.8
92	Gala1-2Galβ-Sp8	119.5	55.8
93	Gala1-3(Fuca1-2)Galβ1-3GlcNAcβ-Sp0	91.2	21.8
94	Gala1-3(Fuca1-2)Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	236.8	52.3
95	Gala1-3(Fuca1-2)Galβ1-4GlcNAc-Sp0	113.8	39.2
96	Gala1-3(Fuca1-2)Galβ1-4Glcβ-Sp0	64.7	27.1
97	Gala1-3(Fuca1-2)Galβ-Sp8	300.8	78.4
98	Gala1-3(Gala1-4)Galβ1-4GlcNAcβ-Sp8	298.6	276.1
99	Gala1-3GalNAcα-Sp8	445.6	175.2
100	Gala1-3GalNAcβ-Sp8	856.8	310.3
101	Gala1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp8	10567.5	1155.2
102	Gala1-3Galβ1-3GlcNAcβ-Sp0	95.8	24.3
103	Gala1-3Galβ1-4GlcNAcβ-Sp8	165.9	121.6
104	Gala1-3Galβ1-4Glcβ-Sp0	52.1	21.0
105	Gala1-3Galβ-Sp8	31.4	22.3

106	Gal α 1-4(Fuca1-2)Gal β 1-4GlcNAc β -Sp8	133.8	72.7
107	Gal α 1-4Gal β 1-4GlcNAc β -Sp0	86.7	20.3
108	Gal α 1-4Gal β 1-4GlcNAc β -Sp8	257.8	45.7
109	Gal α 1-4Gal β 1-4Glc β -Sp0	123.3	43.5
110	Gal α 1-4GlcNAc β -Sp8	610.1	876.5
111	Gal α 1-6Glc β -Sp8	236.9	167.1
112	Gal β 1-2Gal β -Sp8	109.0	41.8
113	Gal β 1-3(Fuca1-4)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	457.2	336.6
114	Gal β 1-3(Fuca1-4)GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	24347.1	2789.4
115	Gal β 1-3(Fuca1-4)GlcNAc-Sp0	115.3	16.2
116	Gal β 1-3(Fuca1-4)GlcNAc-Sp8	97.0	69.6
117	Gal β 1-3(Fuca1-4)GlcNAc β -Sp8	98.4	53.2
118	Gal β 1-3(Gal β 1-4GlcNAc β 1-6)GalNAc α -Sp8	105.8	31.3
119	Gal β 1-3(GlcNAc β 1-6)GalNAc α -Sp8	103.1	40.4
120	Gal β 1-3(Neu5Ac α 2-6)GalNAc α -Sp8	183.1	117.7
121	Gal β 1-3(Neu5Ac β 2-6)GalNAc α -Sp8	154.0	33.0
122	Gal β 1-3(Neu5Ac α 2-6)GlcNAc β 1-4Gal β 1-4Glc β -Sp10	154.4	92.3
123	Gal β 1-3GalNAc α -Sp8	244.6	147.8
124	Gal β 1-3GalNAc β -Sp8	159.6	127.1
125	Gal β 1-3GalNAc β 1-3Gal α 1-4Gal β 1-4Glc β -Sp0	154.2	53.9
126	Gal β 1-3GalNAc β 1-4(Neu5Ac α 2-3)Gal β 1-4Glc β -Sp0	64.6	19.7
127	Gal β 1-3GalNAc β 1-4Gal β 1-4Glc β -Sp8	95.5	93.4
128	Gal β 1-3Gal β -Sp8	106.4	21.5
129	Gal β 1-3GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	119.3	29.1
130	Gal β 1-3GlcNAc β 1-3Gal β 1-4Glc β -Sp10	188.3	32.2
131	Gal β 1-3GlcNAc β -Sp0	117.3	33.5
132	Gal β 1-3GlcNAc β -Sp8	138.7	45.6
133	Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	7830.5	6655.6
134	Gal β 1-4(Fuca1-3)GlcNAc β -Sp8	8611.1	3385.6
135	Gal β 1-4(Fuca1-3)GlcNAc β 1-4Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	35683.2	863.8
136	Gal β 1-4(Fuca1-3)GlcNAc β 1-4Gal β 1-4(Fuca1-3)GlcNAc β 1-4Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	30025.6	536.4
137	Gal β 1-4[6OSO3]Glc β -Sp0	160.0	132.5
138	Gal β 1-4[6OSO3]Glc β -Sp8	96.1	25.5
139	Gal β 1-4GalNAc α 1-3(Fuca1-2)Gal β 1-4GlcNAc β -Sp8	235.3	81.3
140	Gal β 1-4GalNAc β 1-3(Fuca1-2)Gal β 1-4GlcNAc β -Sp8	319.4	225.3
141	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1 β 1-4GlcNAc β -Sp12	316.8	240.3
142	Gal β 1 β 1-4GlcNAc β 1 β 1-3GalNAc α -Sp8	188.0	82.4
143	Gal β 1 β 1-4GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	33357.1	1008.9
144	Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	145.9	37.9
145	Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	87.6	118.0
146	Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp0	263.9	75.0
147	Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp8	37.1	85.8
148	Gal β 1-4GlcNAc β 1-6(Gal β 1-3)GalNAc α -Sp8	137.2	71.5
149	Gal β 1-4GlcNAc β 1-6GalNAc α -Sp8	139.4	7.6
150	Gal β 1-4GlcNAc β -Sp0	165.4	72.6
151	Gal β 1-4GlcNAc β -Sp8	84.7	33.1
152	Gal β 1-4Glc β -Sp0	76.3	70.4
153	Gal β 1-4Glc β -Sp8	119.7	27.0
154	GlcNAc α 1-3Gal β 1-4GlcNAc β -Sp8	113.3	43.4
155	GlcNAc α 1-6Gal β 1-4GlcNAc β -Sp8	158.8	60.0
156	GlcNAc β 1-2Gal β 1-3GalNAc α -Sp8	219.7	122.7
157	GlcNAc β 1-3(GlcNAc β 1-6)GalNAc α -Sp8	219.8	150.8
158	GlcNAc β 1-3(GlcNAc β 1-6)Gal β 1-4GlcNAc β -Sp8	74.0	19.0
159	GlcNAc β 1-3GalNAc α -Sp8	45.0	56.9
160	GlcNAc β 1-3Gal β -Sp8	70.4	30.7
161	GlcNAc β 1-3Gal β 1-3GalNAc α -Sp8	325.8	92.3

162	GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	62.3	43.3
163	GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp8	161.9	75.3
164	GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	165.9	83.8
165	GlcNAc β 1-3Gal β 1-4Glc β -Sp0	91.8	39.9
166	GlcNAc β 1-4MDPLys	182.7	81.5
167	GlcNAc β 1-4(GlcNAc β 1-6)GalNAc α -Sp8	159.7	28.4
168	GlcNAc β 1-4Gal β 1-4GlcNAc β -Sp8	59.3	54.8
169	(GlcNAc β 1-4)6 β -Sp8	465.2	132.9
170	(GlcNAc β 1-4)5 β -Sp8	388.9	141.3
171	GlcNAc β 1-4GlcNAc β 1-4GlcNAc β -Sp8	457.8	146.9
172	GlcNAc β 1-6(Gal β 1-3)GalNAc α -Sp8	190.8	64.7
173	GlcNAc β 1-6GalNAc α -Sp8	35.9	67.7
174	GlcNAc β 1-6Gal β 1-4GlcNAc β -Sp8	157.0	51.4
175	Glc α 1-4Glc β -Sp8	44.7	81.9
176	Glc α 1-4Glc α -Sp8	59.7	14.7
177	Glc α 1-6Glc α 1-6Glc β -Sp8	42.3	50.3
178	Glc β 1-4Glc β -Sp8	38.6	13.0
179	Glc β 1-6Glc β -Sp8	101.4	32.3
180	G-ol-Sp8	103.1	14.8
181	GlcA α -Sp8	348.3	225.8
182	GlcA β -Sp8	285.1	226.5
183	GlcA β 1-3Gal β -Sp8	246.0	98.7
184	GlcA β 1-6Gal β -Sp8	160.2	71.1
185	KDNa2-3Gal β 1-3GlcNAc β -Sp0	375.8	360.0
186	KDNa2-3Gal β 1-4GlcNAc β -Sp0	147.2	45.4
187	Man α 1-2Man α 1-2Man α 1-3Man α -Sp9	1134.1	254.5
188	Man α 1-2Man α 1-3(Man α 1-2Man α 1-6)Man α -Sp9	208.0	130.8
189	Man α 1-2Man α 1-3Man α -Sp9	142.4	69.9
190	Man α 1-6(Man α 1-2Man α 1-3)Man α 1-6(Man α 2Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	130.1	26.3
191	Man α 1-2Man α 1-6(Man α 1-3)Man α 1-6(Man α 2Man α 2Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	62.3	25.9
192	Man α 1-2Man α 1-2Man α 1-3(Man α 1-2Man α 1-3(Man α 1-2Man α 1-6)Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	104.4	82.1
193	Man α 1-3(Man α 1-6)Ma α -Sp9	312.6	113.9
194	Man α 1-3(Man α 1-2Man α 1-2Man α 1-6)Man α -Sp9	365.1	219.3
195	Man α 1-6(Man α 1-3)Man α 1-6(Man α 2Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	219.0	43.3
196	Man α 1-6(Man α 1-3)Man α 1-6(Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	573.5	117.5
197	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	302.8	115.7
198	Man β 1-4GlcNAc β -Sp0	36.3	20.1
199	Fuc α 1-3(Gal β 1-4)GlcNAc β 1-2Man α 1-3(Fuc α 1-3(Gal β 1-4)GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	29817.8	1325.1
200	Neu5Ac α 2-3Gal β 1-3GalNAc α -Sp8	276.0	115.2
201	NeuAc α 2-8NeuAc α 2-8NeuAc α 2-8NeuAc α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	145.1	100.3
202	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	413.8	307.5
203	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α 2-3Gal β 1-4Glc β -Sp0	211.6	53.8
204	Neu5Ac α 2-8Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	271.9	51.3
205	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α -Sp8	389.8	131.9
206	Neu5Ac α 2-3(6-O-Su)Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	34863.4	1455.7
207	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4GlcNAc β -Sp0	301.6	116.7
208	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4GlcNAc β -Sp8	117.1	61.9
209	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	276.8	138.6
210	NeuAc α 2-3(NeuAc α 2-3Gal β 1-3GalNAc β 1-4)Gal β 1-4Glc β -Sp0	434.6	50.8
211	Neu5Ac α 2-3(Neu5Ac α 2-6)GalNAc α -Sp8	326.1	208.1
212	Neu5Ac α 2-3GalNAc α -Sp8	114.4	22.2
213	Neu5Ac α 2-3GalNAc β 1-4GlcNAc β -Sp0	82.6	67.6
214	Neu5Ac α 2-3Gal β 1-3(6OSO3)GlcNAc-Sp8	177.0	114.8
215	Neu5Ac α 2-3Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp8	171.7	45.0

216	NeuAca2-3Galβ1-3(Fuca1-4)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ Sp0	1565.8	249.1
217	Neu5Aca2-3Galβ1-3(Neu5Aca2-3Galβ1-4)GlcNAcβ-Sp8	357.4	127.0
218	Neu5Aca2-3Galβ1-3[6OSO3]GalNAca-Sp8	560.4	101.5
219	Neu5Aca2-3Galβ1-3(Neu5Aca2-6)GalNAca-Sp8	285.6	74.0
220	Neu5Aca2-3Galβ-Sp8	629.4	483.7
221	NeuAca2-3Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-β-Sp0	207.0	41.4
222	NeuAca2-3Galβ1-3GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	70.9	35.5
223	Neu5Aca2-3Galβ1-3GlcNAcβ-Sp0	197.3	108.0
224	Neu5Aca2-3Galβ1-3GlcNAcβ-Sp8	154.9	86.6
225	Neu5Aca2-3Galβ1-4[6OSO3]GlcNAcβ-Sp8	309.3	158.8
226	Neu5Aca2-3Galβ1-4(Fuca1-3)(6OSO3)GlcNAcb-Sp8	36947.0	2195.1
227	Neu5Aca2-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcb-Sp0	34978.0	2173.3
228	Neu5Aca2-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	30564.6	2432.0
229	Neu5Aca2-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp8	32433.2	1831.5
230	Neu5Aca2-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ-Sp8	44306.4	3354.3
231	Neu5Aca2-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp8	40692.5	2620.9
232	Neu5Aca2-3Galβ1-4GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAc-Sp0	258.4	57.3
233	Neu5Aca2-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	283.7	128.1
234	Neu5Aca2-3Galβ1-4GlcNAcβ-Sp0	28.4	106.5
235	Neu5Aca2-3Galβ1-4GlcNAcβ-Sp8	383.4	521.5
236	Neu5Aca2-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	163.9	62.0
237	Neu5Aca2-3Galβ1-4Glcβ-Sp0	161.7	34.0
238	Neu5Aca2-3Galβ1-4Glcβ-Sp8	232.4	241.6
239	Galβ1-4GlcNAcβ1-2Manα1-3(Fuca1-3(Galβ1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	45.2	24.4
240	Neu5Aca2-6GalNAca-Sp8	220.3	68.6
241	Neu5Aca2-6GalNAcβ1-4GlcNAcβ-Sp0	218.5	106.9
242	Neu5Aca2-6Galβ1-4[6OSO3]GlcNAcβ-Sp8	775.4	202.0
243	Neu5Aca2-6Galβ1-4GlcNAcβ-Sp0	200.0	117.0
244	Neu5Aca2-6Galβ1-4GlcNAcβ-Sp8	127.0	38.3
245	Neu5Aca2-6Galβ1-4GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	17423.1	1436.2
246	Neu5Aca2-6Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	82.4	44.5
247	Neu5Aca2-6Galβ1-4Glcβ-Sp0	101.5	51.7
248	Neu5Aca2-6Galβ1-4Glcβ-Sp8	132.3	60.9
249	Neu5ca2-Aca2-6Galβ-Sp8	121.8	14.0
250	Neu5Aca2-8Neu5Aca-Sp8	134.5	55.2
251	Neu5Aca2-8Neu5ca2-Aca2-3Galβ1-4Glcβ-Sp0	236.7	115.3
252	Neu5Acβ2-6GalNAca-Sp8	129.7	83.9
253	Neu5Acβ2-6Galβ1-4GlcNAcβ-Sp8	558.5	305.7
254	Galβ1-4GlcNAcβ1-2Manα1-3(Neu5ca2-Aca2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp21	174.0	40.1
255	Neu5Gca2-3Galβ1-3(Fuca1-4)GlcNAcβ-Sp0	206.0	31.5
256	Neu5Gca2-3Galβ1-3GlcNAcβ-Sp0	175.6	32.7
257	Neu5Gca2-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	23519.8	570.8
258	Neu5Gca2-3Galβ1-4GlcNAcβ-Sp0	51.7	24.7
259	Neu5Gca2-3Galβ1-4Glcβ-Sp0	154.7	38.3
260	Neu5Gca2-6GalNAca-Sp0	178.0	35.7
261	Neu5Gca2-6Galβ1-4GlcNAcβ-Sp0	204.2	260.3
262	Neu5Gca-Sp8	269.8	99.7
263	[3OSO3]Galβ1-4(Fuca1-3)(6OSO3)Glc-Sp0	959.8	115.2
264	[3OSO3]Galβ1-4(Fuca1-3)Glc-Sp0	291.6	142.0
265	[3OSO3]Galβ1-4[Fuca1-3][6OSO3]GlcNAc-Sp8	613.8	110.9
266	[3OSO3]Galβ1-4[Fuca1-3]GlcNAc-Sp0	145.7	84.6
267	Fuca1-2[6OSO3]Galβ1-4GlcNAc-Sp0	126.3	81.1
268	Fuca1-2Galβ1-4[6OSO3]GlcNAc-Sp8	178.0	113.8
269	Fuca1-2[6OSO3]Galβ1-4[6OSO3]Glc-Sp0	135.7	49.3
270	Fuca1-2-(6OSO3)-Galβ1-4Glc-Sp0	192.5	138.5

271	Fuca1-2-Galβ1-4[6OSO3]Glc-Sp0	117.4	41.4
272	Galβ1-3(Fuca1-4)GlcNAcβ1-3Galβ1-3(Fuca1-4)GlcNAcβ-Sp0	319.9	113.3
273	Galβ1-3-(Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	76.5	16.5
274	Galβ1-3(GlcNAcβ1-6)GalNAc-Sp14	274.1	85.9
275	Galβ1-3-(Neu5Ac2-3Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	190.1	10.6
276	Galβ1-3GalNAc-Sp14	159.7	97.2
277	Galβ1-3GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	173.3	82.0
278	Galβ1-4[Fuca1-3][6OSO3]GlcNAc-Sp0	22650.6	1308.3
279	Galβ1-4[Fuca1-3][6OSO3]Glc-Sp0	115.8	34.4
280	Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-3(Fuca1-4)GlcNAcβ-Sp0	18517.7	2530.1
281	Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	298.9	191.5
282	Neu5Ac2-3Galβ1-3GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	808.2	772.3
283	Neu5Ac2-3Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	382.7	193.3
284	[3OSO3]Galβ1-4[6OSO3]GlcNAcβ-Sp0	345.4	367.1
285	[3OSO3][4OSO3]Galβ1-4GlcNAcβ-SpSp0	309.4	125.7
286	[6OSO3]Galβ1-4[6OSO3]GlcNAcβ-Sp0	814.5	432.7
287	6-H2PO3Glcβ-Sp10	122.8	15.9
288	Galα1-3(Fuca1-2)Galα-Sp18	144.9	55.3
289	Galα1-3GalNAcα-Sp16	186.0	98.6
290	Galβ1-3GalNAcα-Sp16	80.4	51.8
291	Galβ1-3(Neu5Ac2-3Galβ1-4(Fuca1-3)GlcNAcβ1-6)GalNAc-Sp14	33773.1	1891.6
292	Galβ1-3Galβ1-4GlcNAcβ-Sp8	118.8	47.1
293	Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	244.1	114.7
294	Galβ1-4GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)Galβ1-4GlcNAc-Sp0	337.4	323.3
295	Galβ1-4GlcNAcβ1-3(GlcNAcβ1-6)Galβ1-4GlcNAc-Sp0	95.9	57.6
296	Galβ1-4GlcNAcα1-6Galβ1-4GlcNAcβ-Sp0	304.3	96.3
297	Galβ1-4GlcNAcβ1-6Galβ1-4GlcNAcβ-Sp0	134.4	56.2
298	GalNAcα-Sp15	377.3	413.0
299	GalNAcα1-3(Fuca1-2)Galβ-Sp18	126.3	54.6
300	GalNAcβ1-3Galβ-Sp8	288.1	123.9
301	GlcAβ1-3GlcNAcβ-Sp8	150.6	84.2
302	GlcNAcβ1-2Manα1-3(Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	217.3	114.6
303	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	78.9	47.4
304	GlcNAcβ1-3Man-Sp10	22.9	32.2
305	GlcNAcβ1-4GlcNAcβ-Sp10	50.8	29.5
306	GlcNAcβ1-4GlcNAcβ-Sp12	84.1	14.3
307	HOOC(CH3)CH-3-O-GlcNAcβ1-4GlcNAcβ-Sp10	252.8	143.8
308	Manα1-3(Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	494.0	213.4
309	Manα1-6Manβ-Sp10	66.6	59.5
310	Manα1-6(Manα1-3)Manα1-6(Manα1-3)Manβ-Sp10	467.6	210.1
311	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-6(Manα1-3)Manα1-6)Manα-Sp9	236.2	69.0
312	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-6(Manα1-2Manα1-3)Manα1-6)Manα-Sp9	186.4	79.4
313	Neu5Ac2-3Galβ1-3(Neu5Ac2-3Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	270.5	79.9
314	Neu5Ac2-3Galβ1-3(Neu5Ac2-6)GalNAc-Sp14	17670.9	3980.3
315	Neu5Ac2-3Galβ1-3GalNAc-Sp14	1893.9	192.9
316	Neu5Ac2-3Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	189.8	63.7
317	Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	227.7	110.5
318	Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	202.1	79.0
319	Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Ac2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-N(LT)AVL	720.7	102.5
320	Fuca1-2Galβ1-3GalNAcα-Sp14	169.4	35.8
321	Galβ1-3(Neu5Ac2-6)GalNAcα-Sp14	1132.5	238.3
322	Galβ1-4GlcNAcβ1-3GalNAc-Sp14	95.5	27.3
323	NeuAc(9Ac) α2-3Galβ1-4GlcNAcβ-Sp0	66.2	41.8
324	NeuAc(9Ac) α2-3Galβ1-3GlcNAcβ-Sp0	87.7	31.3

325	NeuAcα2-6Galβ1-4GlcNAcβ1-3Galβ1-3GlcNAcβ-Sp0	174.3	83.6
326	NeuAcα2-3Galβ1-3(Fuca1-4)GlcNAcβ1-3Galβ1-3(Fuca1-4)GlcNAcβ-Sp0	2901.9	454.3
327	NeuAcα2-6Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	334.1	115.7
328	Galα1-4Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp0	262.5	233.3
329	GalNAcβ1-3Galα1-4Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp0	37.4	36.2
330	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	249.0	40.8
331	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	579.5	199.8
332	(Neu5Acα2-3-Galβ1-3)((Neu5Acα2-3-Galβ1-4(Fuca1-3))GlcNAcβ1-6)GalNAc-Sp14	34815.0	2170.5
333	GlcNAcα1-4Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	255.5	90.3
334	GlcNAcα1-4Galβ1-4GlcNAcβ-Sp0	184.3	75.1
335	GlcNAcα1-4Galβ1-3GlcNAcβ-Sp0	321.8	51.0
336	GlcNAcα1-4Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp0	265.3	145.1
337	GlcNAcα1-4Galβ1-4GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	20406.5	1020.1
338	GlcNAcα1-4Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	1060.7	214.8
339	GlcNAcα1-4Galβ1-3GalNAc-Sp14	286.7	136.6
340	Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	87.1	37.1
341	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	131.2	57.2
342	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	92.0	58.1
343	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	244.8	166.6
344	Galβ1-4GlcNAcβ1-2Manα1-3Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	268.8	101.8
345	Galβ1-4GlcNAcβ1-2Manα1-6Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	212.6	66.7
346	Galβ1-4GlcNAcβ1-2Manα1-3(Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	127.1	46.6
347	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	353.0	68.3
348	Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	264.4	94.3
349	Galβ1-3GlcNAcβ1-2Manα1-3(Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	170.4	104.0
350	Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3[Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	3266.8	264.2
351	(6SO3)GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	144.4	155.9
352	KDNa2-3Galβ1-4(Fuca1-3)GlcNAc-Sp0	455.8	164.3
353	KDNa2-6Galβ1-4GlcNAc-Sp0	172.2	109.6
354	KDNa2-3Galβ1-4Glc-Sp0	155.2	161.9
355	KDNa2-3Galβ1-3GalNAcα-Sp14	1067.3	198.9
356	Fuca1-2Galβ1-3GlcNAcβ1-2Manα1-3(Fuca1-2Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	356.3	167.9
357	Fuca1-2Galβ1-4GlcNAcβ1-2Manα1-3(Fuca1-2Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	56.3	92.5
358	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-3[Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	2082.7	93.4
359	Galα1-3Galβ1-4GlcNAcβ1-2Manα1-3(Galα1-3Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	207.4	25.6
360	Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	94.4	84.2
361	Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3[Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	893.6	341.1
362	Neu5Acα2-6GlcNAcβ1-4GlcNAc-Sp21	131.6	61.5
363	Neu5Acα2-6GlcNAcβ1-4GlcNAcβ1-4GlcNAc-Sp21	94.7	33.5
364	Fuca1-2Galβ1-3GlcNAcβ1-3[Galβ1-4(Fuca1-3)GlcNAcβ1-6]Galβ1-4Glc-Sp21	10810.2	673.9
365	Galβ1-4GlcNAcβ1-2(Galβ1-4GlcNAcβ1-4)Manα1-3[Galβ1-4GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	288.6	118.4
366	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3[GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	280.8	59.3
367	Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3[Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	291.4	147.3
368	Galα1-3Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-3[Galα1-3Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	36390.2	567.2
369	GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3[GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	421.1	129.6
370	Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3[Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	423.2	87.9
371	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3[Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6]Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	1853.6	480.9
372	NeuAcα2-3Galβ1-4GlcNAcβ1-3GalNAc-Sp14	604.0	284.8
373	NeuAcα2-6Galβ1-4GlcNAcβ1-3GalNAc-Sp14	5153.4	733.3

374	Fuc α 1-3[NeuAc α 2-3Gal β 1-4]GlcNAc β 1-3GalNAc-Sp14	2469.4	472.5
375	GalNAc β 1-4GlcNAc β 1-2Man α 1-6(GalNAc β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	221.0	87.4
376	Gal β 1-3GalNAc α 1-3(Fuc α 1-2)Gal β 1-4Glc-Sp14	328.6	244.0
377	Gal β 1-3GalNAc α 1-3(Fuc α 1-2)Gal β 1-4GlcNAc-Sp14	346.2	66.3

* Spacers:

Sp0	CH ₂ CH ₂ NH ₂
Sp8	CH ₂ CH ₂ CH ₂ NH ₂
Sp9	CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ NH ₂
Sp10	NHCOCH ₂ NH
Sp11	OCH ₂ C ₆ H ₄ -p-NHCOCH ₂ NH
Sp12	Asparagine (N)
Sp13	Glycine (G)
Sp14	Threonine (T)
Sp15	Serine (S)
Sp16	PNP (OC ₆ H ₄ NH ₂)
Sp17	OCH ₂ C ₆ H ₄ NH ₂
Sp18	O(CH ₂) ₃ NHCO(CH ₂) ₅ NH ₂
Sp19	GluAsn (EN) or AsnLys (NK)
Sp20	GlyGluAsnTrp (GENR)
Sp21	N(CH ₃)-O-(CH ₂) ₂ -NH ₂
Sp22	AsnSerThr (NST)
Sp23	(OCH ₂ CH ₂) ₆ NH ₂
MDPLys	Mur-L-Ala-D-iGln β -(CH ₂) ₄ NH ₂

Table S3. Raw data of glycan array analysis performed with CCL1. RFU = Relative Fluorescence Units; SD = Standard deviation

No.	Glycan structure – spacer*	RFU	SD
1	Gal α -Sp8	99	19
2	Glc α -Sp8	138	49
3	Man α -Sp8	136	68
4	GalNAc α -Sp8	41	11
5	GalNAc α -Sp15	148	57
6	Fuc α -Sp8	26	22
7	Fuc α -Sp9	-10	20
8	Rha α -Sp8	46	35
9	Neu5Ac α -Sp8	113	60
10	Neu5Ac α -Sp11	247	80
11	Neu5Ac β -Sp8	98	35
12	Gal β -Sp8	68	20
13	Glc β -Sp8	25	8
14	Man β -Sp8	7	6
15	GalNAc β -Sp8	15	17
16	GlcNAc β -Sp0	6	5
17	GlcNAc β -Sp8	4	14
18	GlcN(Gc) β -Sp8	32	10
19	Gal β 1-4GlcNAc β 1-3(Gal β 1-4GlcNAc β 1-6)GalNAc α -Sp8	24	17
20	GlcNAc β 1-3(GlcNAc β 1-4)(GlcNAc β 1-6)GlcNAc-Sp8	264	91
21	[3OSO3][6OSO3]Gal β 1-4[6OSO3]GlcNAc β -Sp0	3	7
22	[3OSO3][6OSO3]Gal β 1-4GlcNAc β -Sp0	25	2
23	[3OSO3]Gal β 1-4(Fuc α 1-3)[6OSO3]Glc-Sp0	250	14
24	[3OSO3]Gal β 1-4Glc β -Sp8	29	10
25	[3OSO3]Gal β 1-4[6OSO3]Glc β -Sp0	329	38
26	[3OSO3]Gal β 1-4[6OSO3]Glc β -Sp8	228	73
27	[3OSO3]Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp8	89	14
28	[3OSO3]Gal β 1-3GalNAc α -Sp8	118	11
29	[3OSO3]Gal β 1-3GlcNAc β -Sp0	93	12
30	[3OSO3]Gal β 1-3GlcNAc β -Sp8	173	83
31	[3OSO3]Gal β 1-4(Fuc α 1-3)GlcNAc-Sp0	383	119
32	[3OSO3]Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	407	76
33	[3OSO3]Gal β 1-4[6OSO3]GlcNAc β -Sp0	293	85
34	[3OSO3]Gal β 1-4[6OSO3]GlcNAc β -Sp8	333	120
35	[3OSO3]Gal β 1-4GlcNAc β -Sp0	141	21
36	[3OSO3]Gal β 1-4GlcNAc β -Sp8	110	21
37	[3OSO3]Gal β -Sp8	42	10
38	[4OSO3][6OSO3]Gal β 1-4GlcNAc β -Sp0	5	4
39	[4OSO3]Gal β 1-4GlcNAc β -Sp8	17	9
40	6-H2PO3Man α -Sp8	3	2
41	[6OSO3]Gal β 1-4Glc β -Sp0	23	6
42	[6OSO3]Gal β 1-4Glc β -Sp8	9	3
43	[6OSO3]Gal β 1-4GlcNAc β -Sp8	27	8
44	[6OSO3]Gal β 1-4[6OSO3]Glc β -Sp8	20	8
45	Neu5Ac α 2-3[6OSO3]Gal β 1-4GlcNAc β -Sp8	3479	693
46	[6OSO3]GlcNAc β -Sp8	14	10
47	[9NAc]Neu5Ac α -Sp8	27	4
48	[9NAc]Neu5Ac α 2-6Gal β 1-4GlcNAc β -Sp8	6	2
49	Man α 1-3(Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	84	18
50	Man α 1-3(Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp13	116	57

51	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	90	9
52	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	68	14
53	Galβ1-4GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	121	19
54	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-N(LT)AVL	78	21
55	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	122	23
56	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp13	86	19
57	Fucα1-2Galβ1-3GalNAcβ1-3Galα-Sp9	129	29
58	Fucα1-2Galβ1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Sp9	76	16
59	Fucα1-2Galβ1-3(Fucα1-4)GlcNAcβ-Sp8	80	32
60	Fucα1-2Galβ1-3GalNAcα-Sp8	70	35
61	Fucα1-2Galβ1-3GalNAcα-Sp14	25	10
62	Fucα1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp0	5	4
63	Fucα1-2Galβ1-3GalNAcβ1-4(Neu5Acα2-3)Galβ1-4Glcβ-Sp9	20	10
64	Fucα1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ-Sp8	1	5
65	Fucα1-2Galβ1-3GlcNAcβ1-3Galβ1-4Glcβ-Sp10	20	6
66	Fucα1-2Galβ1-3GlcNAcβ-Sp0	3	1
67	Fucα1-2Galβ1-3GlcNAcβ-Sp8	18	5
68	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	54	21
69	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ1-3Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	1835	352
70	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	10	6
71	Fucα1-2Galβ1-4(Fucα1-3)GlcNAcβ-Sp8	29	16
72	Fucα1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	15	13
73	Fucα1-2Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	61	16
74	Fucα1-2Galβ1-4GlcNAcβ-Sp0	52	8
75	Fucα1-2Galβ1-4GlcNAcβ-Sp8	45	16
76	Fucα1-2Galβ1-4Glcβ-Sp0	47	21
77	Fucα1-2Galβ-Sp8	12	37
78	Fucα1-3GlcNAcβ-Sp8	30	13
79	Fucα1-4GlcNAcβ-Sp8	62	19
80	Fucβ1-3GlcNAcβ-Sp8	54	17
81	GalNAcα1-3(Fucα1-2)Galβ1-3GlcNAcβ-Sp0	100	28
82	GalNAcα1-3(Fucα1-2)Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	75	16
83	[3OSO3]Galβ1-4(Fucα1-3)Glc-Sp0	140	99
84	GalNAcα1-3(Fucα1-2)Galβ1-4GlcNAcβ-Sp0	82	17
85	GalNAcα1-3(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	25	8
86	GalNAcα1-3(Fucα1-2)Galβ1-4Glcβ-Sp0	2	3
87	GlcNAcβ1-3Galβ1-3GalNAcα-Sp8	11	10
88	GalNAcα1-3(Fucα1-2)Galβ-Sp8	7	6
89	GalNAcα1-3(Fucα1-2)Galβ-Sp18	19	9
90	GalNAcα1-3GalNAcβ-Sp8	7	7
91	GalNAcα1-3Galβ-Sp8	8	5
92	GalNAcα1-4(Fucα1-2)Galβ1-4GlcNAcβ-Sp8	13	5
93	GalNAcβ1-3GalNAcα-Sp8	14	10
94	GalNAcβ1-3(Fucα1-2)Galβ-Sp8	8	7
95	GalNAcβ1-3Galα1-4Galβ1-4GlcNAcβ-Sp0	18	8
96	GalNAcβ1-4(Fucα1-3)GlcNAcβ-Sp0	7887	646
97	GalNAcβ1-4GlcNAcβ-Sp0	-11	43
98	GalNAcβ1-4GlcNAcβ-Sp8	3	27
99	Galα1-2Galβ-Sp8	71	24
100	Galα1-3(Fucα1-2)Galβ1-3GlcNAcβ-Sp0	61	20
101	Galα1-3(Fucα1-2)Galβ1-3GlcNAcβ-Sp8	31	14
102	Galα1-3(Fucα1-2)Galβ1-4(Fucα1-3)GlcNAcβ-Sp0	46	11

103	Gal α 1-3(Fuc α 1-2)Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	35	22
104	Gal α 1-3(Fuc α 1-2)Gal β 1-4GlcNAc-Sp0	41	13
105	Gal α 1-3(Fuc α 1-2)Gal β 1-4Glc β -Sp0	79	22
106	Gal α 1-3(Fuc α 1-2)Gal β -Sp8	63	9
107	Gal α 1-3(Fuc α 1-2)Gal β -Sp18	40	46
108	Gal α 1-3(Gal α 1-4)Gal β 1-4GlcNAc β -Sp8	57	17
109	Gal α 1-3GalNAc α -Sp8	-7	14
110	Gal α 1-3GalNAc α -Sp16	9	6
111	Gal α 1-3GalNAc β -Sp8	55	17
112	Gal α 1-3Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	4988	428
113	Gal α 1-3Gal β 1-3GlcNAc β -Sp0	63	15
114	Gal α 1-3Gal β 1-4GlcNAc β -Sp8	8	2
115	Gal α 1-3Gal β 1-4Glc β -Sp0	42	17
116	Gal α 1-3Gal β -Sp8	2	2
117	Gal α 1-4(Fuc α 1-2)Gal β 1-4GlcNAc β -Sp8	4	6
118	Gal α 1-4Gal β 1-4GlcNAc β -Sp0	5	7
119	Gal α 1-4Gal β 1-4GlcNAc β -Sp8	1	5
120	Gal α 1-4Gal β 1-4Glc β -Sp0	15	4
121	Gal α 1-4GlcNAc β -Sp8	15	10
122	Gal α 1-6Glc β -Sp8	104	34
123	Gal β 1-2Gal β -Sp8	117	54
124	Gal β 1-3(Fuc α 1-4)GlcNAc β 1-3Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp0	562	385
125	Gal β 1-3(Fuc α 1-4)GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	6589	666
126	Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp0	311	95
127	Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp8	-2	6
128	Gal β 1-3(Fuc α 1-4)GlcNAc-Sp8	8	2
129	Gal β 1-4GlcNAc β 1-6GalNAc α -Sp8	20	7
130	Gal β 1-3(GlcNAc β 1-6)GalNAc α -Sp8	31	11
131	Gal β 1-3(GlcNAc β 1-6)GalNAc-Sp14	87	15
132	Gal β 1-3(Neu5Ac α 2-6)GalNAc α -Sp8	55	11
133	Gal β 1-3(Neu5Ac α 2-6)GalNAc α -Sp14	81	21
134	Gal β 1-3(Neu5Ac β 2-6)GalNAc α -Sp8	11	3
135	Gal β 1-3(Neu5Ac α 2-6)GlcNAc β 1-4Gal β 1-4Glc β -Sp10	43	14
136	Gal β 1-3GalNAc α -Sp8	28	18
137	Gal β 1-3GalNAc α -Sp14	17	13
138	Gal β 1-3GalNAc α -Sp16	3	3
139	Gal β 1-3GalNAc β -Sp8	6	3
140	Gal β 1-3GalNAc β 1-3Gal α 1-4Gal β 1-4Glc β -Sp0	6	5
141	Gal β 1-3GalNAc β 1-4(Neu5Ac α 2-3)Gal β 1-4Glc β -Sp0	26	3
142	Gal β 1-3GalNAc β 1-4Gal β 1-4Glc β -Sp8	6	9
143	Gal β 1-3Gal β -Sp8	22	26
144	Gal β 1-3GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	6	5
145	Gal β 1-3GlcNAc β 1-3Gal β 1-4Glc β -Sp10	171	75
146	Gal β 1-3GlcNAc β -Sp0	58	18
147	Gal β 1-3GlcNAc β -Sp8	46	54
148	Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp0	3376	175
149	Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp8	4569	467
150	Gal β 1-4(Fuc α 1-3)GlcNAc β 1-4Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp0	4957	140
151	Gal β 1-4(Fuc α 1-3)GlcNAc β 1-4Gal β 1-4(Fuc α 1-3)GlcNAc β 1-4Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp0	7933	1082
152	Gal β 1-4[6OSO3]Glc β -Sp0	81	6
153	Gal β 1-4[6OSO3]Glc β -Sp8	90	28
154	Gal β 1-4GalNAc α 1-3(Fuc α 1-2)Gal β 1-4GlcNAc β -Sp8	51	23
155	Gal β 1-4GalNAc β 1-3(Fuc α 1-2)Gal β 1-4GlcNAc β -Sp8	39	3
156	Gal β 1-4GlcNAc β 1-3GalNAc α -Sp8	89	46
157	Gal β 1-4GlcNAc β 1-3GalNAc α -Sp14	22	11

158	Galβ1-4GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ-Sp0	4838	221
159	Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	21	10
160	Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	9	7
161	Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp0	33	22
162	Galβ1-4GlcNAcβ1-3Galβ1-4Glcβ-Sp8	1	2
163	Galβ1-4GlcNAcβ1-6(Galβ1-3)GalNAcα-Sp8	19	6
164	Galβ1-3(Galβ1-4GlcNAcβ1-6)GalNAcα-Sp8	18	12
165	Galβ1-3(Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	26	10
166	Galβ1-4GlcNAcβ-Sp0	5	5
167	Galβ1-4GlcNAcβ-Sp8	7	3
168	Galβ1-4Glcβ-Sp0	2	2
169	Galβ1-4Glcβ-Sp8	101	18
170	GlcNAcα1-3Galβ1-4GlcNAcβ-Sp8	55	37
171	GlcNAcα1-6Galβ1-4GlcNAcβ-Sp8	58	24
172	GlcNAcβ1-2Galβ1-3GalNAcα-Sp8	77	34
173	GlcNAcβ1-3(GlcNAcβ1-6)GalNAcα-Sp8	30	13
174	GlcNAcβ1-3(GlcNAcβ1-6)Galβ1-4GlcNAcβ-Sp8	17	4
175	GlcNAcβ1-3GalNAcα-Sp8	7	7
176	GlcNAcβ1-3GalNAcα-Sp14	31	16
177	GlcNAcβ1-3Galβ-Sp8	25	14
178	GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	57	20
179	GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp8	47	17
180	GlcNAcβ1-3Galβ1-4GlcNAcβ1-3Galβ1-4GlcNAcβ-Sp0	55	30
181	GlcNAcβ1-3Galβ1-4Glcβ-Sp0	6	5
182	GlcNAcβ1-4-MDPLys	18	23
183	GlcNAcβ1-4(GlcNAcβ1-6)GalNAcα-Sp8	13	9
184	GlcNAcβ1-4Galβ1-4GlcNAcβ-Sp8	15	4
185	GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4β-Sp8	17	12
186	GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ-Sp8	8	5
187	GlcNAcβ1-4GlcNAcβ1-4GlcNAcβ-Sp8	25	25
188	GlcNAcβ1-6(Galβ1-3)GalNAcα-Sp8	8	6
189	GlcNAcβ1-6GalNAcα-Sp8	7	4
190	GlcNAcβ1-6GalNAcα-Sp14	12	10
191	GlcNAcβ1-6Galβ1-4GlcNAcβ-Sp8	23	11
192	Glcα1-4Glcβ-Sp8	15	5
193	Glcα1-4Glcα-Sp8	111	18
194	Glcα1-6Glcα1-6Glcβ-Sp8	113	32
195	Glcβ1-4Glcβ-Sp8	145	48
196	Glcβ1-6Glcβ-Sp8	89	52
197	G-ol-Sp8	209	43
198	GlcAα-Sp8	101	15
199	GlcAβ-Sp8	317	62
200	GlcAβ1-3Galβ-Sp8	105	23
201	GlcAβ1-6Galβ-Sp8	104	28
202	KDNα2-3Galβ1-3GlcNAcβ-Sp0	53	21
203	KDNα2-3Galβ1-4GlcNAcβ-Sp0	69	32
204	Manα1-2Manα1-2Manα1-3Manα-Sp9	42	9
205	Manα1-2Manα1-3(Manα1-2Manα1-6)Manα-Sp9	36	6
206	Manα1-2Manα1-3Manα-Sp9	18	3
207	Manα1-6(Manα1-2Manα1-3)Manα1-6(Manα1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	64	7
208	Manα1-2Manα1-6(Manα1-3)Manα1-6(Manα1-2Manα1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	23	10
209	Manα1-2Manα1-2Manα1-3(Manα1-2Manα1-3(Manα1-2Manα1-6)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	41	12
210	Manα1-3(Manα1-6)Manα-Sp9	8	1
211	Manα1-3(Manα1-2Manα1-2Manα1-6)Manα-Sp9	39	15

212	Man α 1-6(Man α 1-3)Man α 1-6(Man α 1-2Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	18	8
213	Man α 1-6(Man α 1-3)Man α 1-6(Man α 1-3)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	35	14
214	Man β 1-4GlcNAc β -Sp0	3	1
215	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc-Sp0	60	17
216	[3OSO3]Gal β 1-4(Fuca1-3)[6OSO3]GlcNAc-Sp8	209	55
217	Fuca1-2[6OSO3]Gal β 1-4GlcNAc-Sp0	93	35
218	Fuca1-2Gal β 1-4[6OSO3]GlcNAc-Sp8	106	22
219	Fuca1-2[6OSO3]Gal β 1-4[6OSO3]Glc-Sp0	371	26
220	Neu5Ac α 2-3Gal β 1-3GalNAc α -Sp8	48	3
221	Neu5Ac α 2-3Gal β 1-3GalNAc α -Sp14	155	22
222	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	116	7
223	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	141	31
224	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α 2-3Gal β 1-4Glc β -Sp0	60	19
225	Neu5Ac α 2-8Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	94	11
226	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac α -Sp8	80	17
227	Neu5Ac α 2-3(6-O-Su)Gal β 1-4(Fuca1-3)GlcNAc β -Sp8	7065	1203
228	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4GlcNAc β -Sp0	52	7
229	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4GlcNAc β -Sp8	35	7
230	Neu5Ac α 2-3(GalNAc β 1-4)Gal β 1-4Glc β -Sp0	10	2
231	Neu5Ac α 2-3(Neu5Ac α 2-3Gal β 1-3GalNAc β 1-4)Gal β 1-4Glc β -Sp0	43	10
232	Neu5Ac α 2-3(Neu5Ac α 2-6)GalNAc α -Sp8	13	6
233	Neu5Ac α 2-3GalNAc α -Sp8	15	21
234	Neu5Ac α 2-3GalNAc β 1-4GlcNAc β -Sp0	11	11
235	Neu5Ac α 2-3Gal β 1-3[6OSO3]GlcNAc-Sp8	62	18
236	Neu5Ac α 2-3Gal β 1-3(Fuca1-4)GlcNAc β -Sp8	14	4
237	Neu5Ac α 2-3Gal β 1-3(Fuca1-4)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	321	259
238	Neu5Ac α 2-3Gal β 1-3(Neu5Ac α 2-3Gal β 1-4)GlcNAc β -Sp8	16	9
239	Neu5Ac α 2-3Gal β 1-3[6OSO3]GalNAc α -Sp8	60	12
240	Neu5Ac α 2-3Gal β 1-3(Neu5Ac α 2-6)GalNAc α -Sp8	3	2
241	Neu5Ac α 2-3Gal β 1-3(Neu5Ac α 2-6)GalNAc α -Sp14	1025	90
242	Neu5Ac α 2-3Gal β -Sp8	30	10
243	Neu5Ac α 2-3Gal β 1-3GalNAc β 1-3Gal α 1-4Gal β 1-4Glc β -Sp0	56	23
244	Neu5Ac α 2-3Gal β 1-3GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	75	22
245	Fuca1-2[6OSO3]Gal β 1-4Glc-Sp0	105	15
246	Neu5Ac α 2-3Gal β 1-3GlcNAc β -Sp0	79	17
247	Neu5Ac α 2-3Gal β 1-3GlcNAc β -Sp8	104	56
248	Neu5Ac α 2-3Gal β 1-4[6OSO3]GlcNAc β -Sp8	176	64
249	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)[6OSO3]GlcNAc β -Sp8	5708	520
250	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	6928	521
251	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	5563	253
252	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp8	5530	426
253	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β -Sp8	11685	250
254	Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp8	4596	943
255	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	23	8
256	Neu5Ac α 2-3Gal β 1-4GlcNAc β -Sp0	9	5
257	Neu5Ac α 2-3Gal β 1-4GlcNAc β -Sp8	17	12
258	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	8	6
259	Fuca1-2Gal β 1-4[6OSO3]Glc-Sp0	34	20
260	Neu5Ac α 2-3Gal β 1-4Glc β -Sp0	8	8
261	Neu5Ac α 2-3Gal β 1-4Glc β -Sp8	50	22
262	Neu5Ac α 2-6GalNAc α -Sp8	-1	5
263	Neu5Ac α 2-6GalNAc β 1-4GlcNAc β -Sp0	17	8
264	Neu5Ac α 2-6Gal β 1-4[6OSO3]GlcNAc β -Sp8	2	5
265	Neu5Ac α 2-6Gal β 1-4GlcNAc β -Sp0	65	11

266	Neu5Ac α 2-6Gal β 1-4GlcNAc β -Sp8	89	9
267	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	1606	409
268	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	50	20
269	Neu5Ac α 2-6Gal β 1-4Glc β -Sp0	61	15
270	Neu5Ac α 2-6Gal β 1-4Glc β -Sp8	111	23
271	Neu5Ac α 2-6Gal β -Sp8	73	8
272	Neu5Ac α 2-8Neu5Ac α -Sp8	86	5
273	Neu5Ac α 2-8Neu5Ac α 2-3Gal β 1-4Glc β -Sp0	65	11
274	Gal β 1-3(Fuca1-4)GlcNAc β 1-3Gal β 1-3(Fuca1-4)GlcNAc β -Sp0	71	18
275	Neu5Ac β 2-6GalNAc α -Sp8	57	12
276	Neu5Ac β 2-6Gal β 1-4GlcNAc β -Sp8	55	9
277	Neu5Gc α 2-3Gal β 1-3(Fuca1-4)GlcNAc β -Sp0	30	6
278	Neu5Gc α 2-3Gal β 1-3GlcNAc β -Sp0	6	5
279	Neu5Gc α 2-3Gal β 1-4(Fuca1-3)GlcNAc β -Sp0	3557	364
280	Neu5Gc α 2-3Gal β 1-4GlcNAc β -Sp0	12	12
281	Neu5Gc α 2-3Gal β 1-4Glc β -Sp0	26	3
282	Neu5Gc α 2-6GalNAc α -Sp0	2	6
283	Neu5Gc α 2-6Gal β 1-4GlcNAc β -Sp0	30	18
284	Neu5Gc α -Sp8	15	22
285	Gal β 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-6)GalNAc α -Sp14	25	7
286	Gal β 1-3GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp0	-1	2
287	Gal β 1-4(Fuca1-3)[6OSO ₃]GlcNAc-Sp0	2665	956
288	Gal β 1-4(Fuca1-3)[6OSO ₃]Glc-Sp0	20	13
289	Gal β 1-4(Fuca1-3)GlcNAc β 1-3Gal β 1-3(Fuca1-4)GlcNAc β -Sp0	8120	1426
290	Gal β 1-4GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp0	83	19
291	Neu5Ac α 2-3Gal β 1-3GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp0	104	31
292	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp0	114	12
293	[3OSO ₃][4OSO ₃]Gal β 1-4GlcNAc β -Sp0	469	83
294	[6OSO ₃]Gal β 1-4[6OSO ₃]GlcNAc β -Sp0	381	90
295	6-H ₂ PO ₃ Glc β -Sp10	244	110
296	Gal β 1-3(Neu5Ac α 2-3Gal β 1-4(Fuca1-3)GlcNAc β 1-6)GalNAc α -Sp14	994	119
297	Gal β 1-3Gal β 1-4GlcNAc β -Sp8	37	17
298	Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	131	36
299	Gal β 1-4GlcNAc β 1-3(Gal β 1-4GlcNAc β 1-6)Gal β 1-4GlcNAc-Sp0	5	29
300	Gal β 1-4GlcNAc β 1-3(GlcNAc β 1-6)Gal β 1-4GlcNAc-Sp0	13	24
301	Gal β 1-4GlcNAc α 1-6Gal β 1-4GlcNAc β -Sp0	9	13
302	Gal β 1-4GlcNAc β 1-6Gal β 1-4GlcNAc β -Sp0	11	7
303	GalNAc β 1-3Gal β -Sp8	8	9
304	GlcA β 1-3GlcNAc β -Sp8	16	7
305	GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	42	10
306	GlcNAc β 1-3Man-Sp10	22	3
307	GlcNAc β 1-4GlcNAc β -Sp10	29	28
308	GlcNAc β 1-4GlcNAc β -Sp12	15	12
309	HOOC(CH ₃)CH-3-O-GlcNAc β 1-4GlcNAc β -Sp10	42	10
310	Man α 1-6Man β -Sp10	21	4
311	Man α 1-6(Man α 1-3)Man α 1-6(Man α 1-3)Man β -Sp10	62	22
312	Man α 1-2Man α 1-2Man α 1-3(Man α 1-2Man α 1-6(Man α 1-3)Man α 1-6)Man α -Sp9	3	4
313	Man α 1-2Man α 1-2Man α 1-3(Man α 1-2Man α 1-6(Man α 1-2Man α 1-3)Man α 1-6)Man α -Sp9	66	11
314	Neu5Ac α 2-3Gal β 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-6)GalNAc α -Sp14	137	27
315	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	115	17
316	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	80	20
317	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	131	33

318	Neu5Ac α 2-8Neu5Ac β -Sp17	96	18
319	Neu5Ac α 2-8Neu5Ac α 2-8Neu5Ac β -Sp8	141	28
320	Neu5Gc β 2-6Gal β 1-4GlcNAc-Sp8	31	12
321	Gal β 1-3GlcNAc β 1-2Man α 1-3(Gal β 1-3GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp19	98	34
322	Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	82	6
323	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(Neu5Ac α 2-3Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	81	11
324	Fuc α 1-3(Gal β 1-4)GlcNAc β 1-2Man α 1-3(Fuc α 1-3(Gal β 1-4)GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	1733	246
325	Neu5Ac(9Ac) α 2-3Gal β 1-4GlcNAc β -Sp0	19	10
326	Neu5Ac(9Ac) α 2-3Gal β 1-3GlcNAc β -Sp0	8	4
327	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-3Gal β 1-3GlcNAc β -Sp0	9	11
328	Neu5Ac α 2-3Gal β 1-3(Fuc α 1-4)GlcNAc β 1-3Gal β 1-3(Fuc α 1-4)GlcNAc β -Sp0	94	18
329	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	38	9
330	Gal α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp0	6	7
331	GalNAc β 1-3Gal α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp0	21	10
332	GalNAc α 1-3(Fuc α 1-2)Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	6	4
333	GalNAc α 1-3(Fuc α 1-2)Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	200	48
334	Neu5Ac α 2-3-Gal β 1-3(Gal β 1-4(Fuc α 1-3)GlcNAc β 1-6)GalNAc-Sp14	1957	473
335	GlcNAc α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	12	4
336	GlcNAc α 1-4Gal β 1-4GlcNAc β -Sp0	45	20
337	GlcNAc α 1-4Gal β 1-3GlcNAc β -Sp0	39	15
338	GlcNAc α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4Glc β -Sp0	67	16
339	GlcNAc α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4(Fuc α 1-3)GlcNAc β 1-3Gal β 1-4(Fuc α 1-3)GlcNAc β -Sp0	1655	140
340	GlcNAc α 1-4Gal β 1-4GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	96	28
341	GlcNAc α 1-4Gal β 1-3GalNAc-Sp14	432	124
342	Man α 1-3(Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	93	13
343	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3(Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	106	48
344	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-6Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	78	6
345	Neu5Ac α 2-6Gal β 1-4GlcNAc β 1-2Man α 1-3Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	105	18
346	Gal β 1-4GlcNAc β 1-2Man α 1-3Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	59	9
347	Gal β 1-4GlcNAc β 1-2Man α 1-6Man β 1-4GlcNAc β 1-4GlcNAc-Sp12	90	20
348	Gal β 1-4GlcNAc β 1-2Man α 1-3(Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	135	40
349	GlcNAc β 1-2Man α 1-3(GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4(Fuc α 1-6)GlcNAc β -Sp22	35	19
350	Gal β 1-4GlcNAc β 1-2Man α 1-3(Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4(Fuc α 1-6)GlcNAc β -Sp22	8	3
351	Gal β 1-3GlcNAc β 1-2Man α 1-3(Gal β 1-3GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4(Fuc α 1-6)GlcNAc β -Sp22	8	17
352	[6OSO3]GlcNAc β 1-3Gal β 1-4GlcNAc β -Sp0	0	5
353	KDN α 2-3Gal β 1-4(Fuc α 1-3)GlcNAc-Sp0	2132	316
354	KDN α 2-6Gal β 1-4GlcNAc-Sp0	7	4
355	KDN α 2-3Gal β 1-4Glc-Sp0	19	16
356	KDN α 2-3Gal β 1-3GalNAc-Sp14	14	6
357	Fuc α 1-2Gal β 1-3GlcNAc β 1-2Man α 1-3(Fuc α 1-2Gal β 1-3GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	52	16
358	Fuc α 1-2Gal β 1-4GlcNAc β 1-2Man α 1-3(Fuc α 1-2Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	53	23
359	Fuc α 1-2Gal β 1-4(Fuc α 1-3)GlcNAc β 1-2Man α 1-3(Fuc α 1-2Gal β 1-4(Fuc α 1-3)GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	175	68
360	Gal α 1-3Gal β 1-4GlcNAc β 1-2Man α 1-3(Gal α 1-3Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp20	51	29
361	Man α 1-3(Gal β 1-4GlcNAc β 1-2Man α 1-6)Man β 1-4GlcNAc β 1-4GlcNAc β -Sp12	72	6

362	Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3(Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	116	19
363	Neu5Acα2-6GlcNAcβ1-4GlcNAc-Sp21	42	22
364	Neu5Acα2-6GlcNAcβ1-4GlcNAcβ1-4GlcNAc-Sp21	43	13
365	Fuca1-2Galβ1-3GlcNAcβ1-3(Galβ1-4(Fuca1-3)GlcNAcβ1-6)Galβ1-4Glc-Sp21	1510	465
366	Galβ1-4GlcNAcβ1-2(Galβ1-4GlcNAcβ1-4)Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	28	9
367	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3(GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	8	14
368	Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3(Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	50	13
369	Galα1-3Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-3(Galα1-3Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	2769	438
370	GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3(GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	60	25
371	Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3(Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp20	14	11
372	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3(Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	482	30
373	Neu5Acα2-3Galβ1-4GlcNAcβ1-3GalNAc-Sp14	28	2
374	Neu5Acα2-6Galβ1-4GlcNAcβ1-3GalNAc-Sp14	27	14
375	Neu5Acα2-3Galβ1-4(Fuca1-3)GlcNAcβ1-3GalNAcα-Sp14	339	162
376	(GalNAcβ1-4GlcNAcβ1-2Manα1-6)GalNAcβ1-4GlcNAcβ1-2Manα1-3Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	12	9
377	Galβ1-3GalNAcα1-3(Fuca1-2)Galβ1-4Glc-Sp0	21	6
378	Galβ1-3GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAc-Sp0	4	10
379	Galβ1-3GlcNAcβ1-3(Galβ1-3GlcNAcβ1-3Galβ1-4GlcNAcβ1-6)Galβ1-4Glcβ-Sp0	7	7
380	Galβ1-3GlcNAcβ1-3(Galβ1-4(Fuca1-3)GlcNAcβ1-6)Galβ1-4Glc-Sp21	2968	817
381	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)Galβ1-4Glc-Sp21	30	8
382	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-3(Galβ1-4(Fuca1-3)GlcNAcβ1-6)Galβ1-4Glc-Sp21	1012	333
383	Galβ1-3GlcNAcβ1-3(Galβ1-3GlcNAcβ1-3Galβ1-4(Fuca1-3)GlcNAcβ1-6)Galβ1-4Glc-Sp21	1750	276
384	Galβ1-4GlcNAcβ1-2(Galβ1-4GlcNAcβ1-4)Manα1-3(Galβ1-4GlcNAcβ1-2(Galβ1-4GlcNAcβ1-6)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp21	11	11
385	GlcNAcβ1-2(GlcNAcβ1-4)Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	29	28
386	Fuca1-2Galβ1-3GalNAcα1-3(Fuca1-2)Galβ1-4Glcβ-Sp0	81	24
387	Fuca1-2Galβ1-3GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ-Sp0	88	30
388	Galβ1-3GlcNAcβ1-3GalNAcα-Sp14	75	11
389	Neu5Acα2-3(GalNAcβ1-4)Galβ1-4GlcNAcβ1-3GalNAcα-Sp14	196	65
390	GalNAcα1-3(Fuca1-2)Galβ1-3GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ-Sp0	81	24
391	Galα1-3Galβ1-3GlcNAcβ1-2Manα1-3(Galα1-3Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp19	115	17
392	Galα1-3Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3(Galα1-3Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp19	145	14
393	Galβ1-4GlcNAcβ1-2Manα1-3(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	154	30
394	GlcNAcβ1-2Manα1-3(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp12	106	39
395	Neu5Acα2-3Galβ1-3GlcNAcβ1-3GalNAcα-Sp14	165	58
396	Fuca1-2Galβ1-4GlcNAcβ1-3GalNAcα-Sp14	106	40
397	Galβ1-4(Fuca1-3)GlcNAcβ1-3GalNAcα-Sp14	58	8
398	GalNAcα1-3GalNAcβ1-3Galα1-4Galβ1-4GlcNAcβ-Sp0	2	3
399	Galα1-4Galβ1-3GlcNAcβ1-2Manα1-3(Galα1-4Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	41	27
400	Galα1-4Galβ1-4GlcNAcβ1-2Manα1-3(Galα1-4Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-LVANKT	10	6
401	Galα1-3Galβ1-4GlcNAcβ1-3GalNAcα-Sp14	22	15
402	Galβ1-3GlcNAcβ1-6Galβ1-4GlcNAcβ-Sp0	8	7
403	Galβ1-3GlcNAcα1-6Galβ1-4GlcNAcβ-Sp0	22	10
404	GalNAcβ1-3Galα1-6Galβ1-4Glcβ-Sp8	12	10

405	GlcNAcβ1-6(GlcNAcβ1-3)GalNAcα-Sp14	21	18
406	Galα1-3(Fuca1-2)Galβ1-4(Fuca1-3)Glcβ-Sp21	10	4
407	Neu5Acα2-6Galβ1-3GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)Galβ1-4Glc-Sp21	34	12
408	Galβ1-3GalNAcβ1-4(Neu5Acα2-8Neu5Acα2-3)Galβ1-4Glcβ-Sp0	21	9
409	Neu5Acα2-3Galβ1-3GalNAcβ1-4(Neu5Acα2-8Neu5Acα2-3)Galβ1-4Glcβ-Sp0	108	18
410	Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-3GalNAcα-Sp14	55	13
411	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-3GalNAcα-Sp14	147	50
412	GalNAcα1-3GalNAcβ1-3Galα1-4Galβ1-4Glcβ-Sp0	43	6
413	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-3GalNAcα-Sp14	543	194
414	Galα1-3(Fuca1-2)Galβ1-4(Fuca1-3)GlcNAcβ1-3GalNAc-Sp14	104	24
415	GalNAcα1-3(Fuca1-2)Galβ1-4(Fuca1-3)GlcNAcβ1-3GalNAc-Sp14	197	77
416	Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-3(Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	80	25
417	Fuca1-2Galβ1-4GlcNAcβ1-2Manα1-3(Fuca1-2Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	143	38
418	GlcNAcβ1-2Manα1-3(GlcNAcβ1-2(GlcNAcβ1-6)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	67	26
419	Fuca1-2Galβ1-3GlcNAcβ1-3GalNAc-Sp14	111	19
420	Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-3GalNAc-Sp14	77	10
421	GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-3GalNAc-Sp14	54	30
422	Galα1-3Galβ1-3GlcNAcβ1-3GalNAc-Sp14	10	4
423	Fuca1-2Galβ1-3GlcNAcβ1-2Manα1-3(Fuca1-2Galβ1-3GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	49	11
424	Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3(Galα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	8	8
425	Galβ1-3GlcNAcβ1-2Manα1-3(Galβ1-3GlcNAcβ1-2(Galβ1-3GlcNAcβ1-6)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	25	6
426	Fuca1-2Galβ1-3GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)Galβ1-4Glc-Sp21	7	2
427	Galβ1-4GlcNAcβ1-3Galβ1-4(Fuca1-3GlcNAcβ1-6)Galβ1-4Glc-Sp21	3417	656
428	GlcNAcβ1-2Manα1-3(GlcNAcβ1-4)(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	8	9
429	GlcNAcβ1-4(GlcNAcβ1-2)Manα1-3(GlcNAcβ1-4)(GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	20	12
430	GlcNAcβ1-2Manα1-3(GlcNAcβ1-4)(GlcNAcβ1-6(GlcNAcβ1-2)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	15	5
431	GlcNAcβ1-4(GlcNAcβ1-2)Manα1-3(GlcNAcβ1-4)(GlcNAcβ1-6(GlcNAcβ1-2)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	25	1
432	Galβ1-4GlcNAcβ1-2Manα1-3(GlcNAcβ1-4)(Galβ1-4GlcNAcβ1-2)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	22	9
433	Galβ1-4GlcNAcβ1-4(Galβ1-4GlcNAcβ1-2)Manα1-3(GlcNAcβ1-4)(Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	28	13
434	Galβ1-4GlcNAcβ1-2Manα1-3(GlcNAcβ1-4)(Galβ1-4GlcNAcβ1-6(Galβ1-4GlcNAcβ1-2)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	61	22
435	Galβ1-4GlcNAcβ1-4(Galβ1-4GlcNAcβ1-2)Manα1-3(GlcNAcβ1-4)(Galβ1-4GlcNAcβ1-6(Galβ1-4GlcNAcβ1-2)Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	63	5
436	Galα1-3Galβ1-4Glc-Sp10	52	15
437	Galβ1-4Galβ-Sp10	127	53
438	Galβ1-6Galβ-Sp10	117	41
439	Neu5Acα2-3Galβ1-4GlcNAcβ1-3Galβ-Sp8	71	19
440	GalNAcβ1-6GalNAcβ-Sp8	10	6
441	[6OSO3]Galβ1-3GlcNAcβ-Sp0	50	20
442	[6OSO3]Galβ1-3[6OSO3]GlcNAc-Sp0	482	51
443	Fuca1-2Galβ1-4GlcNAcβ1-2(Fuca1-2Galβ1-4GlcNAcβ1-4)Manα1-3(Fuca1-2Galβ1-4GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	18	32
444	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2(Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-4)Manα1-3(Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp12	106	31
445	Galβ1-4GlcNAcβ1-3(Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	45	14
446	Galβ1-4GlcNAcβ1-6GalNAc-Sp14	30	9
447	Galβ1-4(Fuca1-3)GlcNAcβ1-6GalNAc-Sp14	992	482
448	Galβ1-4GlcNAcβ1-2Manα-Sp0	4	2

449	Fuca1-2Galβ1-4GlcNAcβ1-3(Fuca1-2Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	71	28
450	Galα1-3Fuca1-2Galβ1-4GlcNAcβ1-3(Galα1-3Fuca1-2Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	30	17
451	GalNAcα1-3Fuca1-2Galβ1-4GlcNAcβ1-3(GalNAcα1-3Fuca1-2Galβ1-4GlcNAcβ1-6)GalNAc-Sp14	37	25
452	Neu5Acα2-8Neu5Acα2-3Galβ1-3GalNAcβ1-4(Neu5Acα2-8Neu5Acα2-3)Galβ1-4Glcβ-Sp0	7	4
453	GalNAcβ1-4Galβ1-4Glcβ-Sp0	33	13
454	GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-6(GalNAcα1-3(Fuca1-2)Galβ1-4GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	2	4
455	Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6(Galα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	17	10
456	Neu5Acα2-6Galβ1-4GlcNAcβ1-6(Fuca1-2Galβ1-3GlcNAcβ1-3)Galβ-4Glc-Sp21	5	2
457	GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-6(GalNAcα1-3(Fuca1-2)Galβ1-3GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp22	80	13
458	Galβ1-4GlcNAcβ1-6(Galβ1-4GlcNAcβ1-2)Manα1-6(Galβ1-4GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	87	16
459	Galβ1-4GlcNAcβ-(OCH ₂ CH ₂) ₆ NH ₂	7	5
460	Galα1-3(Fuca1-2)Galβ1-3GalNAcα-Sp8	21	15
461	Galα1-3(Fuca1-2)Galβ1-3GalNAcβ-Sp8	43	8
462	Glcα1-6Glcα1-6Glcα1-6Glcβ-Sp10	76	23
463	Glcα1-4Glcα1-4Glcα1-4Glcβ-Sp10	110	29
464	Neu5Acα2-3Galβ1-4GlcNAcβ1-6(Neu5Acα2-3Galβ1-4GlcNAcβ1-3)GalNAcα-Sp14	87	33
465	Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-6(Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-6AA	62	40
466	Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-6(Fuca1-2Galβ1-3(Fuca1-4)GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp19	61	27
467	Neu5Acα2-3Galβ1-3GlcNAcβ1-6(Neu5Acα2-3Galβ1-4GlcNAcβ1-2)Manα1-6(Neu5Acα2-3Galβ1-3GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp19	74	15
468	GlcNAcβ1-6(GlcNAcβ1-2)Manα1-6(GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-6AA	26	18
469	Galβ1-3GlcNAcβ1-2Manα1-6(GlcNAcβ1-4)(Galβ1-3GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAcβ-Sp21	53	23
470	Neu5Acα2-6Galβ1-4GlcNAcβ1-6(Galβ1-3GlcNAcβ1-3)Galβ1-4Glcβ-Sp21	6	7
471	Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα-Sp0	192	163
472	Neu5Acα2-3Galβ1-4GlcNAcβ1-6GalNAcα-Sp14	8	3
473	Neu5Acα2-6Galβ1-4GlcNAcβ1-6GalNAcα-Sp14	84	29
474	Neu5Acα2-6Galβ1-4GlcNAcβ1-6(Neu5Acα2-6Galβ1-4GlcNAcβ1-3)GalNAcα-Sp14	15	6
475	Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-6(Neu5Acα2-6Galβ1-4GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-6AA	39	11
476	Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-6(Neu5Acα2-3Galβ1-4GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-6AA	36	10
477	Manα1-6(Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-Sp19	39	20
478	Galβ1-4GlcNAcβ1-6(Galβ1-4GlcNAcβ1-2)Manα1-6(Galβ1-4GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4(Fuca1-6)GlcNAcβ-6AA	18	10
479	Neu5Acα2-3Galβ1-3GlcNAcβ1-2Manα1-6(GlcNAcβ1-4)(Neu5Acα2-3Galβ1-3GlcNAcβ1-2Manα1-3)Manβ1-4GlcNAcβ1-4GlcNAc-Sp21	21	20
480	Neu5Acα2-6Galβ1-4GlcNAcβ1-6(Fuca1-2Galβ1-4(Fuca1-3)GlcNAcβ1-3)Galβ1-4Glc-Sp21	6	11
481	Galβ1-3GlcNAcβ1-6GalNAcα-Sp14	113	11
482	Galα1-3Galβ1-3GlcNAcβ1-6GalNAcα-Sp14	86	18
483	Galβ1-3(Fuca1-4)GlcNAcβ1-6GalNAcα-Sp14	195	79
484	Neu5Acα2-3Galβ1-3GlcNAcβ1-6GalNAcα-Sp14	105	29
485	[3OSO ₃]Galβ1-3(Fuca1-4)GlcNAcα-Sp0	125	72
486	Neu5Acα2-3Galβ1-3(Neu5Acα2-6)GlcNAcβ1-3(Fuca1-3(Galβ1-4)GlcNAcβ1-6)Galβ1-4Glc-Sp21	187	177
487	Fuca1-2Galβ1-4GlcNAcβ1-6GalNAcα-Sp14	239	94
488	Galα1-3Galβ1-4GlcNAcβ1-6GalNAcα-Sp14	8	6
489	Galβ1-4(Fuca1-3)GlcNAcβ1-2Manα-Sp0	1261	714
490	[6OSO ₃](Fuca1-2)Galβ1-3GlcNAcβ-Sp0	82	17

491	Gal α 1-3(Fuca α 1-2)Gal β 1-4GlcNAc β 1-6GalNAc α -Sp14	300	110
492	Fuca1-2Gal β 1-4GlcNAc β 1-2Man α -Sp0	111	42
493	(Fuca1-2)Gal β 1-3[6OSO3]GlcNAc β -Sp0	77	15
494	[6OSO3](Fuca1-2)Gal β 1-3[6OSO3]GlcNAc β -Sp0	148	60
495	Neu5Ac α 2-6GalNAc β 1-4[6OSO3]GlcNAc β -Sp8	221	28
496	GalNAc β 1-4[6OSO3](Fuca1-3)GlcNAc β -Sp8	15553	584
497	[3OSO3]GalNAc β 1-4(Fuca1-3)GlcNAc β -Sp8	12725	438
498	(Fuca1-2)Gal β 1-3GlcNAc β 1-6(Fuca1-2Gal β 1-3GlcNAc β 1-3)GalNAc α -Sp14	99	41
499	GalNAc α 1-3(Fuca1-2)Gal β 1-3GlcNAc β 1-6GalNAc α -Sp14	93	37
500	GlcNAc β 1-2(GlcNAc β 1-4)Man α 1-3(GlcNAc β 1-4)[GlcNAc β 1-2(GlcNAc β 1-6)Man α 1-6]Man β 1-4GlcNAc β 1-4(Fuca1-6)GlcNAc-Sp21	15	14
501	Gal β 1-4GlcNAc β 1-2(Gal β 1-4GlcNAc β 1-4)Man α 1-3(GlcNAc β 1-4)[Gal β 1-4GlcNAc β 1-2(Gal β 1-4GlcNAc β 1-6)Man α 1-6]Man β 1-4GlcNAc β 1-4(Fuca1-6)GlcNAc-Sp21	10	6
502	Gal β 1-3GlcNAc α 1-3Gal β 1-4GlcNAc β -Sp8	8	2
503	Gal β 1-3[6OSO3]GlcNAc β -Sp8	45	13
504	[4OSO3][6OSO3]GalNAc β 1-4GlcNAc-Sp8	37	6
505	[6OSO3]GalNAc β 1-4GlcNAc-Sp8	78	41
506	[3OSO3]GalNAc β 1-4[3OSO3]GlcNAc-Sp8	234	128
507	GalNAc β 1-4[6OSO3]GlcNAc-Sp8	120	22
508	[3OSO3]GalNAc β 1-4GlcNAc-Sp8	65	13
509	[4OSO3]GalNAc β -Sp10	38	7
510	Gal β 1-4[6PO3]GlcNAc β -Sp0	54	27
511	[6PO3]Gal β 1-4GlcNAc β -Sp0	31	16

* for a detailed description of the spacers see Table S2

Table S4. Most prominent proteins structurally closest to CCL2 (free) obtained by a DALI search[3].

Protein	DALI score	Rmsd	Identity	Reference
Bacteria				
mosquitocidal toxin of <i>Bacillus sphaericus</i>	17.7	2.4 Å	16% (142 residues)	[4]
Fungi				
<i>Marasmius oreades</i> agglutinin (MOA)	15.5	1.9 Å	18% (128 residues)	[5]
<i>Sclerotinia sclerotiorum</i> agglutinin (SSA)	16.2	2.0 Å	14% (130 residues)	[6]
Plants				
<i>Sambucus nigra</i> agglutinin II (SNA-II)	14.4	3.8 Å	14% (122 residues)	[7]

Table S5. Carbohydrate ¹H and ¹³C chemical shifts [ppm] at 293 K referenced to DSS according to [8]. Bound chemical shifts were assigned via exchange peaks between the free and the bound form and by NOEs. Bound signals were not visible in a natural abundance ¹³C HSQC.

Chemical shifts [ppm]	GlcNAcβ1,4[Fucα1,3]GlcNAcβ1-sp free	GlcNAcβ1,4[Fucα1,3]GlcNAcβ1-sp bound
GlcNAc 1		
H1/C1	4.47 / 103.6	4.69
H2/C2	3.85 / 58.4	3.72
H3/C3	3.82 / 77.6	3.92
H4/C4	3.85 / 76.4	3.86
H5/C5	3.47 / 78.1	3.54
H6&H6'/C6	3.91 & 3.72 / 62.7	3.92 & 3.71
HN2	8.25	8.54
Q2/C8	2.00 / 25.0	1.76
GlcNAc 2		
H1/C1	4.50 / 103.1	4.68
H2/C2	3.70 / 58.6	3.99
H3/C3	3.53 / 76.4	3.25
H4/C4	3.23 / 73.5	2.84
H5/C5	3.41 / 78.7	3.36
H6&H6'/C6	3.95 & 3.59 / 64.3	3.93 & 3.59
HN2	8.24	7.88
Q2/C8	2.02 / 24.9	1.78
Fuc 2'		
H1/C1	5.09 / 101.2	5.31
H2/C2	3.69 / 70.5	3.46
H3/C3	3.93 / 71.9	4.16
H4/C4	3.78 / 74.8	3.88
H5/C5	4.71 / 69.4	5.05
H6/C6	1.24 / 18.2	1.06

Table S6. Thermodynamic data of selected lectin–carbohydrate interactions that are used in Fig 7B.

Lectin	ligand	K_D [μmol]	$-\Delta H$ [kJ/mol]	$-\Delta S$ [kJ/mol]	Source or reference
CCL2 WT	GlcNac β 1,4[Fuc α 1,3]GlcNAc-O-spacer	1.4	49.8	16.3	This study
CCL2 (N91A)	GlcNac β 1,4[Fuc α 1,3]GlcNAc-O-spacer	0.18	57.7	18.8	This study
Fab fragment of Anti-LeX Monoclonal antibody 291-2G3-A	Le ^X -OMe	10.8	20.9	-7.1	[9]
Calreticulin	Glc α 1,3Man α 1,2Man α 1,2Man	0.77	50.0	15.7	[10]
Calreticulin	Glc α 1,3Man α 1,2Man α OMe	1.8	29.9	-3.4	[11]
ConA	Man α 1,6[Man α 1,3]Man β OMe	2.0	60.2	27.6	[12]
Cholera toxin B subunit (CTB)	GM1os	0.043	72.4	30.8	[13]
Grifonia simplicifolia lectin 4	Fuc α 1,2Gal β 1,3[Fuc α 1,4]GlcNAc- β OMe (Le ^b)	17.0	49.8	22.6	[14]
Jacalin	Gal α OMe	58.0	45.3	21.2	[15]
MOA	Gal α 1,3Gal β 1,4GlcNAc	42.3	86.2	63.6	[16]
MOA	Gal α 1,3[Fuc α 1,2]Gal	36.0	86.2	61.1	[16]
PSL	Neu5Ac α 2,6Gal β 1,4Glc	1.28	36.1	2.1	[17]
RSL	Fuc α OMe	0.73	42.1	7.1	[18]
RSL	2-Fucosyllactose	0.25	39.3	1.6	[18]
TeNT	GD1b	0.045	31.8	-10.0	[19]
TeNT	GT1b	0.055	52.7	11.3	[19]
WBA II	Fuc α 1,2Gal β 1,4GlcNAc β OMe	3.2	57.3	27.7	[20]

Table S7. Strains used in this study.

Strain	Relevant characteristics or genotype	Source or reference
<i>E. coli</i>		
BL21(DE3)	F ⁻ ompT hsdSB(rB- mB-) gal dcm (λDE3)	Novagen
BL21(DE3)/pLysS	F ⁻ ompT hsdSB(rB- mB-) gal dcm (λDE3), pLysS Cmr	Novagen
OP50	Ura ^r	[21]
<i>C. cinerea</i>		
AmutBmut (<i>A43mut B43mut pab1.2</i>)	Mutations at the A and B mating type loci, mimics a dikaryon	[22]
<i>C. elegans</i>		
Bristol type (N2)	Wild type	CGC (U. of Minnesota, USA)
<i>bre-1(ye4)</i>	Mutant in GDP-mannose- 4,6-dehydratase	CGC (U. of Minnesota, USA)
<i>fut-1(ok892)</i>	Mutant in fucosyltransferase 1	CGC (U. of Minnesota, USA)
<i>fut-6(ok475)</i>	Mutant in fucosyltransferase 6	CGC (U. of Minnesota, USA)
<i>fut-6(ok475)fut-1(ok892)</i>	Double mutant in fucosyltransferases 1 and 6	This study
<i>fut-2(gk360)</i>	Mutant in alpha 1,2-fucosyltransferase	CGC (U. of Minnesota, USA)
<i>fut-2(gk509)</i>	Mutant in alpha 1,2-fucosyltransferase	CGC (U. of Minnesota, USA)
<i>fut-4(gk111)</i>	Mutant in fucosyltransferase 4	CGC (U. of Minnesota, USA)
<i>gly-12(is47)</i>	β 1,2 GnT I	CGC (U. of Minnesota, USA)
<i>dpy-6(e14)gly-13(ok712)</i>	β 1,2 GnT I (<i>dpy-6</i> for mapping purposes)	CGC (U. of Minnesota, USA)
<i>gly-14(id48)</i>	β 1,2 GnT I	CGC (U. of Minnesota, USA)
<i>gly-12(is47)gly-13(ok712);gly-14(id48)</i>	Triple mutant for all three β 1,2 GnT I genes	Prof. Harry Schachter (U. of Toronto, Canada)
<i>gly-20(ok826)</i>	β 1,2 GnT II	CGC (U. of Minnesota, USA)
<i>D. melanogaster</i>		
Canton-S	Wild type	Prof. E. Hafen (ETH Zürich)
<i>A. aegypti</i>		
Rockefeller	Laboratory strain, susceptible to insecticidals	Swiss Tropical and Public Health Institute (Basel, Switzerland)
<i>A. castellanii</i>		
ATCC 30234		Prof. H. Hilbi (Ludwig-Maximilians-Universität München, Germany)

Table S8. Oligonucleotides used in this study. Restriction sites in the oligonucleotides are underlined, and codon changes for site directed mutagenesis are in bold.

Oligonucleotide	Sequence (5' → 3')	Source or reference
<i>Cloning</i>		
CCL2-seq fwd	AGGCCTCAGCACTCTCACTC	This study
CCL2-seq rev	GCTCTTCTGGGACTTGAGGA	This study
CCL2-fwd	GGGAATTCC <u>CATATG</u> GACTCCCCAGCTGTGAC	This study
CCL2-rev	GGGGGGG <u>GATCC</u> CTAGACCTTCTCGATGACCCAG	This study
CCL2-NHis fwd	GGGAATTCC <u>CATATG</u> GGCCATCATCATCATCATCACACAGCGGCGACTCCCCAGCTGTGACGCTC	This study
CCL1 fwd	CAAACCCAACCTTTACTTCTTCACCC	This study
CCL1 rev	CGAGTTGTGAAAAGGTTTACGTCCA	This study
CCL1 fwd	CCCC <u>CATATG</u> GATACTCAGGCCAAACCCC	This study
CCL1 rev	GGGGG <u>AATT</u> CTCAGACCCTCTCAAAGATCCAG	This study
CCL1-NHis fwd	GGG <u>CATATG</u> GATCATCATCATCATCATCATCACACTCAGGCCAAACCCCCCGCCGG	This study
dTomato fwd	GGGGGGGG <u>ATTA</u> TGGTGAGCAAGGGCGAGG	This study
dTomato rev	GGGGGGGGATCCCTAC <u>ATATG</u> CTTGTACAGCTCGTCCATGC	This study
fut1 A	CTAAATTGGCATCCACAACCT	This study
fut1 B	GCCATTTATTAACAGTTCTCAT	This study
fut1 C	CCGGAGTAATTAGACCTGC	This study
fut6 A	GAATGCCACCATGCAACAT	This study
fut6 B	GAATTACCCATGATACTAGAT	This study
fut6 C	GCCCCAAATATCAATCTGC	This study
<i>Site directed mutagenesis</i>		
CCL2 Y57A	TGGATCTTAAGGAG CG CCGACTCGAACTCGAACACC	This study
CCL2 W78A	CAGCCAGATCGGG GG CGGGCGCTGGTAAC	This study
CCL2 L87A	CGTCCCCGTCGTC G CCCCTCCCAACAAC	This study
CCL2 N90A	GTCGTCTCCCTCC CG CCAACTACGTCTGGACT	This study
CCL2 N91A	GTCCTCCCTCCCAAC GC CCTACGTCTGGACTCTG	This study
CCL2 Y92A	CTCCCTCCCAACAAC CG CGTCTGGACTCTGACT	This study
CCL2 V93A	CTCCCTCCCAACAAC AC CTGGACTCTGACTTTG	This study
CCL2 W94A	CCTCCCAACAAC AC CTCGCGACTCTGACTTTGACT	This study
CCL2 K109A	TACAACATTCAAGATGG CG CGAGGACCGTCTCTTGG	This study
CCL2 Y57A	TGGATCTTAAGGAG CG CCGACTCGAACTCGAACACC	This study
<i>qRT-PCR</i>		
Tubulin fwd	GTCATGTCCGGTATCACCAC	[23]
Tubulin rev	GGGAAAGGAACCATGTTGA	[23]
CCL2 fwd	CTGGTGGATAACAACATTCAAGATGGC	This study
CCL2 rev	AGACCTTCTCGATGACCCAGC	This study
CCL1 fwd	TGGCGGCTATATCATCCAAG	This study
CCL1 rev	CAGACCCTCTCAAAGATCCAG	This study

Supplementary Methods

Cultivation conditions. *E. coli* was cultivated on LB, M9 or NGM medium as described [24,25]. Cultivation of *C. elegans*, *A. aegypti* and *A. castellanii* for biotoxicity assays was done as described (Künzler et al., 2010). *Coprinopsis cinerea* was maintained on YMG solid medium (0.4% (w/v) yeast extract, 1% (w/v) malt extract, 0.4% (w/v) 1.5% agar) at 37°C. Cultivation conditions and techniques for harvesting *C. cinerea* vegetative mycelium and fruiting bodies have been described previously [23].

Isolation and purification of CCL2 from *C. cinerea*. Fruiting bodies or vegetative mycelium of *C. cinerea* were lyophilized and extracted as follows: the material was first homogenized using a mortar before the appropriate amount was weighed in, mixed with an equal volume of glass beads and ground using a FastPrep™ FP120 device (SAVANT). The powder was extracted by a second FastPrep round in the presence of extraction buffer (1 volume of phosphate buffered saline (PBS), 1 volume of water and 1 mM phenylmethanesulfonylfluoride) at a ratio of 1 ml/100 mg dry fungal tissue. Insoluble material was spun down at high speed (16100 g) at 4°C for 15 minutes, and the supernatant containing the soluble proteins was used as input for affinity chromatography.

Horseshoe peroxidase (Sigma) was coupled to CNBr-activated Sepharose 4B (GE Healthcare) according to the manufacturer's protocol. 150 µl of the HRP-sepharose beads were equilibrated with 1.5 ml PBS, and incubated with 500 µl soluble protein extract from fruiting bodies by rotation at 4°C. Flow through was collected by centrifugation, and beads were washed with 1.5 ml PBS, mixed with 100 µl SDS-PAGE sample buffer and boiled at 95°C for 10 minutes to release proteins bound to the matrix. Proteins from input, flow through and beads samples were separated by SDS-PAGE.

Identification of CCL2 by peptide mass fingerprinting. The excised gel piece was washed three times in 200mM ammonium bicarbonate pH 8.0 and dried in a Speed Vac. Protein contained in the sample was reduced with 10mM dithiothreitol in 100mM ammonium bicarbonate at 37 °C for 1h. After removal of dithiothreitol, cysteines were alkylated with 25mM iodoacetamide in 100mM ammonium bicarbonate at room temperature in the dark for 1h. The iodoacetamide was removed and the gel piece washed five times in 50% acetonitrile. After drying in a Speed Vac, the protein was digested overnight at 37 °C with 50 ng trypsin in a volume of 50mM ammonium bicarbonate enough to cover the gel piece. Supernatant was transferred to a fresh tube, dried in a Speed Vac and resuspended in 10µl 0.1% trifluoroacetic acid. Tryptic peptides were then desalted with a C18

ZipTip (Millipore, USA) and eluted in the MALDI-MS matrix solution (4 mg/ml α -cyano-4-hydroxy-cinnamic acid in 70% acetonitrile, 0.1% trifluoroacetic acid). Peptide masses and MS/MS results were used in MASCOT [26] to search a *C. cinerea* genome database.

Quantification of *ccl1* and *ccl2* expression by qRT-PCR. RNA was extracted from 30-50mg of lyophilized mycelium and fruiting bodies from *C. cinerea* using the RNeasy® Lipid Tissue Mini Kit (Qiagen). Isolated RNA was DNase-treated using the Qiagen RNase-Free DNase Set (Qiagen). For cDNA synthesis, 5 μ g RNA was combined with 2 μ l of oligo-dT primer (100 μ M) in a volume of 30 μ l, and incubated for 10 min at 70°C. The sample was cooled on ice for 10 min. Reverse transcription was carried out with M-MLV Reverse Transcriptase RNase H Minus (Promega), 1x reaction buffer provided with the enzyme, dNTPs (10mM each), 1 μ l of Ribolock™ (Fermentas), in a total final volume of 60 μ l. The reaction mixture was incubated at 25°C for 10 minutes, 40°C for 120 minutes and at 70°C for 10 minutes. RNA was hydrolyzed at 65°C for 15 min after the addition of 20 μ l of 1 M NaOH. For neutralization, 20 μ l of 1M HCl were added. cDNA was purified with the NucleoSpin Extract Kit II (Macherey-Nagel) following the manufacturer's recommendations. Real time PCR was performed in a thermocycler Rotorgene 3000 (Corbett Research) with SensiMix™Plus SYBR Kit (Quantace) in a volume of 20 μ l. β -tubulin was used as internal control template. Primers for amplification of CCL1, CCL2 and β -tubulin are given in Table S8. PCR conditions were: 95°C for 10 min, followed by 35 cycles of 95 °C for 15 s, 58°C for 30 s, and 72°C for 30 s. Amplicon size and specificity for each primer pair was verified by agarose gel electrophoresis and melting curve analysis. Relative expression ratio of each gene was calculated as described [27]. Standard errors of the mean are based on four technical replicates of each cDNA template and gene.

Cloning of CCL1- and CCL2-encoding genes. The CCL2 genomic locus of *C. cinerea* strain AmutBmut was PCR-amplified from chromosomal DNA using oligonucleotide primers CCL2-seq fwd and CCL2-seq rev (Table S8). CCL1- and CCL2-encoding cDNAs were synthesized and amplified using the OneStep RT-PCR Kit (Qiagen) using total RNA from lyophilized fruiting bodies and primers CCL1-seq fwd and CCL1-seq rev, and CCL2-seq fwd and CCL2-seq rev, respectively. RNA was isolated using the RNeasy® Lipid Tissue Mini Kit (Qiagen) according to the manufacturer's protocol. PCR products were ligated into pGEM-T easy vector (Promega), amplified in *E.coli* and sequenced. Plasmids for expression of CCL1 and CCL2 in *E. coli* were constructed by PCR-amplifying the coding regions of the respective cDNA clones using primers carrying suitable restriction sites (CCL1 fwd and CCL1 rev, as well as CCL2 fwd and CCL2 rev; Table S8) and ligating the purified and cut PCR-fragments into accordingly opened pET22b or pET24b (Novagen). Plasmids driving

the expression of N-terminally His8-tagged CCL1 and CCL2 were generated accordingly using the same reverse primers but the respective N-His containing forward primers (CCL1-NHis fwd and CCL2-NHis fwd; Table S8). For the cloning of dTomato-CCL2 fusion, the dTomato coding region was amplified by PCR from plasmid pRO020 [28] using the primers dTomato-fwd and dTomato-rev (Table S8). The PCR product was subcloned into pGEM-T easy and amplified in *E. coli*. The insert was released with *VspI* and *BamHI*, and ligated into a pET24b backbone previously linearized with *NdeI* and *BamHI*, resulting in plasmid pET24-dTomato. Finally, the CCL2 coding region was released from above expression plasmids as *NdeI-BamHI* fragment and inserted into pET24-dTomato that had previously been opened with the same restriction enzymes.

Expression of CCL1 and CCL2 in *E. coli* and purification of the His8-tagged CCL2. For expression, the various plasmids coding for wild type or mutant forms of the lectins were transformed into *E. coli* strains BL21(DE3). Transformants were cultivated at 37°C in either LB or M9 minimal medium containing 1 g/l ¹⁵NH₄Cl and 4 g/l glucose (for ¹⁵N-labeled proteins) or 1 g/l ¹⁵NH₄Cl and 2 g/l ¹³C-glucose (for ¹³C/¹⁵N labeled proteins) and 100 mg/l ampicillin or 25 mg/l carbenicillin (for pET22-based plasmids), 50 mg/l kanamycin (for pET24-based plasmids) and 17 mg/l chloramphenicol (for pLysS). CCL2(N91A) had to be expressed in BL21(DE3)/pLysS cells since BL21(DE3)-transformants did not grow on LB nor minimal medium, possibly due to toxicity of this variant for bacterial cells. Expression of CCL1 and CCL2 was induced at OD_{600nm} ~ 0.6-1 by adding 1mM isopropyl β-D-thiogalactoside and further incubation either at 37°C for 4h or at 23°C for 16h. Expression and solubility check of the recombinant proteins was done as previously described (Kunzler et al. 2010). For purification of His8-tagged CCL1 and CCL2, induced cells were collected by centrifugation, washed with water and stored at -20°C. Cells were resuspended in 50mM Na phosphate pH 8.0, 300mM NaCl, 10mM imidazole and disrupted by French Press (SLM Aminco; SLM instruments, Inc. UK) or M-110L Pneumatic Microfluidizer (Microfluidics). The lysate was cleared by centrifugation (30min, 18000 rpm, 4°C) and the supernatant was applied to metal-affinity chromatography using Ni-NTA resins (Qiagen Inc.), following the manufacturer's instructions, except that an additional washing step with a high salt buffer (1 M NaCl, 50 mM Na₂HPO₄, pH 8.0, 10 mM imidazole) was added. After elution, the buffer of the protein was exchanged (by dialysis or desalting) to either NMR buffer (50 mM KH₂PO₄ pH 5.7, 150 mM NaCl) or TOX buffer (50 mM Na₂HPO₄ pH 6.0, 150mM NaCl). Identity and purity were verified by SDS-PAGE.

CCL2-GlcNAcβ1,4[Fuca1,3]GlcNAc complex formation. The complexes were prepared by titrating the concentrated carbohydrate solution of typically 10 mM into a ~1 mM solution of CCL2 in NMR buffer (50 mM KH₂PO₄ pH 5.7, 150 mM NaCl) until a 1:1 stoichiometry was reached. Subsequently, the pH was lowered to 4.7

using 10% deuterated acetic acid to avoid precipitation. Protein concentrations were determined by UV spectroscopy ($\epsilon_{280} = 41940 \text{ M}^{-1} \text{ cm}^{-1}$). For measurements in D_2O samples were lyophilized and dissolved in D_2O containing the same amount of 10% deuterated acetic acid (in D_2O) as the sample originally contained in H_2O .

NMR spectroscopy. NMR spectra were acquired on Avance III 500, 600, 700 and Avance 900 Bruker spectrometers equipped with inverse triple resonance cryogenetic probes and pulse field gradient accessory. In addition an Avance III 750MHz with an inverse triple resonance room temperature probe and pulse field gradient accessory was used. Unless indicated otherwise, data were measured at 310 K. NMR data were processed using Topspin 2.1 (Bruker) and analyzed with Sparky [29]. The ^1H , ^{13}C , ^{15}N chemical shifts of the protein, free and in complex, were assigned using 2D ^1H - ^{15}N -HSQC, 2D ^1H - ^{13}C -HSQC, 3D HNCA, 3D CBCACONH, 3D HNCACB, 3D HNCO, 3D (H)CCH-TOCSY, 3D ^{15}N -edited NOESY-HSQC, 3D ^{13}C -edited NOESY-HSQC, 2D NOESY and 2D TOCSY experiments [30]. Assignment of carbohydrate resonances of the complex was achieved using NOE correlations and exchange peaks with signals of the free carbohydrate since neither TOCSY based spectra nor a natural abundance ^{13}C -HSQC did show signals of the bound carbohydrate. The following spectra were used for this purpose 2D ^1H - ^1H NOESY, 2D $^{13}\text{C}/^{15}\text{N}$ F1-filtered NOESY and 2D ^{13}C F1-filtered F2-filtered NOESY [31]. The assignments of intermolecular NOEs were derived from 3D ^{13}C F1-edited, F3-filtered NOESY-HSQC [32] spectra of the protein-carbohydrate complex. All NOESY spectra of the were recorded with a mixing time of either 100 ms (free protein) or 120 ms (complex). The 3D TOCSY spectrum was recorded with a mixing time of 23 ms and 2D TCOSY spectra with a mixing time of 15 or 60 ms.

Structure calculation and refinement. Initial CCL2 structures (free and bound) were generated using the AtnosCandid software package [33,34] using three 3D NOESY spectra ($^{13}\text{C}^{\text{ali}}$ -edited, $^{13}\text{C}^{\text{aro}}$ -edited and ^{15}N -edited) and a 2D NOESY spectrum. The automatically generated upper limit restraints file was used as a starting point for the first level of manually refining the protein structures by a simulated annealing protocol using the Cyana package [33]. Preliminary structures of the CCL2-carbohydrate complex were generated using the Cyana package with the above mentioned restraints and manually assigned intermolecular and intra-carbohydrate NOE distance constraints. To create the topology of the carbohydrate for the Cyana library file an initial model was generated by SWEET [35]. The carbohydrate spacer was truncated to a methyl group since we observed only few weak intermolecular NOEs between the spacer and N91 indicating that the spacer is projecting away from the protein and does not fold back. 300 structures were generated by CYANA starting from random carbohydrate and protein starting structures using 16,000 simulated annealing steps. Structures improved when backbone angle restraints derived from chemical shifts using TALOS+ [36] were

subsequently added to both AtnosCandid and Cyana. At later stages of the refinement, hydrogen-bond restraints (only within protein) were added. An ensemble of 30 structures, selected based on the lowest target function, served for the refinement in AMBER 9.0 [37]. Structures of CCL2 free and in complex were refined in implicit solvent using NOE-derived distances, torsion angles and hydrogen bond restraints as summarized in Table 2. In all AMBER calculations, the force-field 98 based on the Cornell et al. force-field [38] was used along with the generalized Born model [39] to mimic solvent. A 20-ps simulated annealing protocol consisting of 22,000 steps was used. NMR restraints were applied as square-well penalty functions with the force constants $50 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$ and $200 \text{ kcal mol}^{-1} \text{ rad}^{-2}$ for distance constraints and torsion angles, respectively. Relative weights of the valence-angle energy, torsion energy and 'improper' torsional terms were gradually increased during the simulated annealing to maintain the planarity of aromatic rings and proper local geometries. After the simulated annealing protocol a short energy minimization of 400 cycles was followed (a combination of steepest-descents minimization followed by conjugate gradient technique). 20 conformers with the lowest restraint violations were selected to obtain the final ensemble of structures. The quality of the complex was analyzed by PROCHECK-NMR [40] and CARP [1]. Figures of the complex structure were prepared using MOLMOL [41].

Preparation of the *C. elegans fut-1 fut-6* double mutant (F1F6) and PCR screening. All parent strains were obtained from the *C. elegans* gene knock-out consortium via the Caenorhabditis Genetics Centre (CGC). The experiment was designed based on the genetic crossing principle. Three L4 hermaphrodites of VC 585 *fut-1* (*ok892*) were transferred onto small NGM plates and mated with twelve N2 male adults; male adults of the F1 generation were mated with RB 706 *fut-6* (*ok475*) L4 hermaphrodites as above, in order to gain the F2 generation. Per plate, a previously singled hermaphrodite was isolated after egg laying and transferred into $7 \mu\text{l}$ of lysis buffer [50mM KCl, 10mM Tris-HCl (pH 8.3), 2.5mM MgCl₂, 0.45% NP40, 0.45% Tween 20, 60 $\mu\text{g/ml}$ Proteinase K], then incubated at 60°C for 1 hour to extract genomic DNA. Proteinase K was heat inactivated at 95°C for 15 mins. Primer set *fut1* (A,B,C) was designed for detecting *fut-1* genotypes; whereas Primer set *fut6* (A,B,C) was designed for detecting *fut-6* genotypes. Multiplex PCR reactions were carried out in a $20 \mu\text{l}$ standard reaction system with $1 \mu\text{l}$ gDNA, $1.2 \mu\text{l}$ of a primer sets mixture (*fut1* + *fut6*, $20 \mu\text{M}$ of each primer), $7.8 \mu\text{l}$ of H₂O, and $10 \mu\text{l}$ of GoTaq® Green Master Mix (Promega). In the case of performing triplex PCRs to detect a single gene in one PCR reaction, $0.6 \mu\text{l}$ of a primer set was added, therefore H₂O was increased to $8.4 \mu\text{l}$. The PCR program was: 95°C for 3 mins, followed by 30 cycles at 95°C for 30 s, 52°C for 30 s, 72°C for 30 s (1000 base pairs per minute). PCR screening was performed as follows: firstly, for screening of individuals carrying *fut-1/+; fut-6/+* genotype, 30 hermaphrodites of the F2 generation were transferred singly to small NGM plates

for laying eggs, prior to gDNA extraction and multiplex-PCR; secondly, 100 progeny from the *fut-1/+;fut-6/+* positive plates were then singled, and screened by multiplex-PCR after eggs were laid, in order to seek the *fut-1/fut-1;fut-6/+* and/or *fut-1/+;fut-6/fut-6* genotype; finally, 40 progeny from positive plates were singled; again, after eggs were laid, the genotypes were checked by triplex-PCR. The PCR products were loaded on to 3% agarose gels and analyzed by electrophoresis in TAE buffer at 100 volts for 75 mins. A product size of 270 nt indicated the wild type form of the *fut-1* gene, while 320 nt indicated the mutant form; a product size of 200 nt indicated the wild type form of the *fut-6* gene, while 158 nt indicated the mutant form.

Localization of CCL2-binding in *C. elegans*. A stationary culture of *E.coli* containing the dTomato-CCL2 expression plasmid was used to seed NGM plates containing 1mM IPTG and 50 mg/l kanamycin and incubated overnight at 23°C for protein expression before addition of nematodes. L4 staged *C. elegans* worms of indicated genotypes were transferred to the plates. After 36h the animals were transferred to standard *E. coli* OP50 to allow unbound lectin leave the intestinal tract. After 1 hr, 10 worms were placed on 3% agarose pads in M9, anaesthetized with 3–5 mM levamisole (Sigma) and mounted under a coverslip for observation using a Leica DM-RA or Zeiss Axiovert 200 microscope equipped with DIC (Nomarski) optics and standard epifluorescence with a DsRed filter set for detection of dTomato. Pictures were taken with a Hamamatsu ORCA-ER camera. Images were false-coloured using OpenLab software.

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