Supplementary Data

GlycoCAP: A cell-free, bacterial glycosylation platform for building clickable azido-sialoglycoproteins

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Supplementary Figures 1-5

Supplementary Tables 1-5

Supplementary Figures
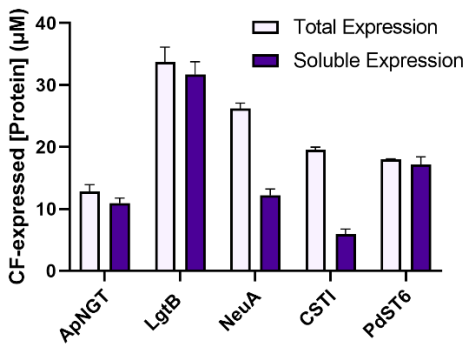
Figure S1. Total and soluble cell-free expression of pathway enzymes. Total and soluble expression of each enzyme is quantified by incorporation of radioactive [^{14}C]-leucine (n=3; error bars = standard deviation). ApNGT, LgtB, and PdST6 demonstrate a high degree of relative soluble expression to total expression, where NeuA and CSTI have a lesser degree of relative soluble expression. Only the soluble portion is assembled into *in vitro* glycosylation reactions and all pathway enzymes have sufficient solubility and activity for the GlycoCAP platform.
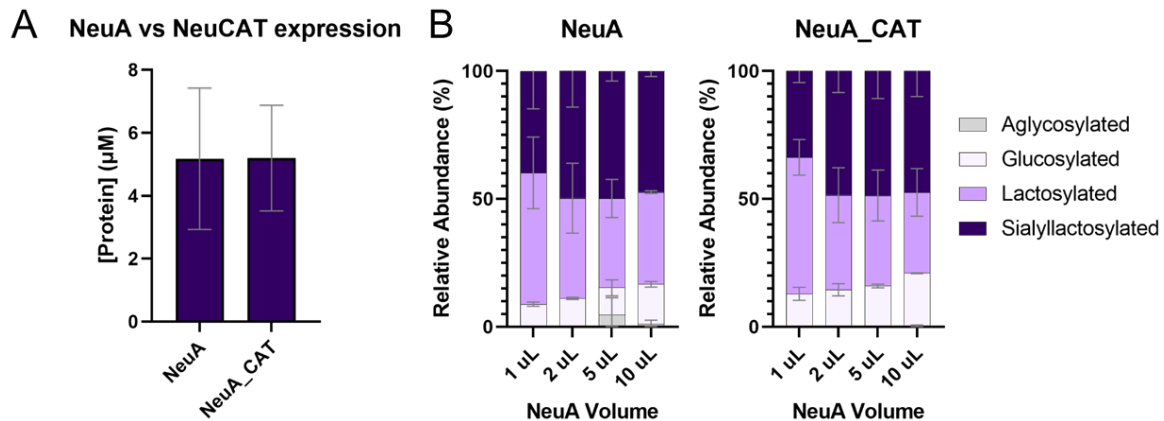
Figure S2. NeuA DNA expression and glycosylation with and without a CAT linker. NeuA was designed with and without a 5' CAT linker nucleotide sequence, which is often used to improve expression. **(A)** Both versions of NeuA expressed similarly as determined by incorporation of radioactive [^{14}C]-leucine (n=3; error bars = standard deviation). **(B)** Both versions of NeuA also led to similar glycosylation efficiencies at equivalent titration volumes (n=2; errors bars = average error). Therefore, the CAT linker is not necessary to optimize NeuA expression and function in the GlycoCAP platform.
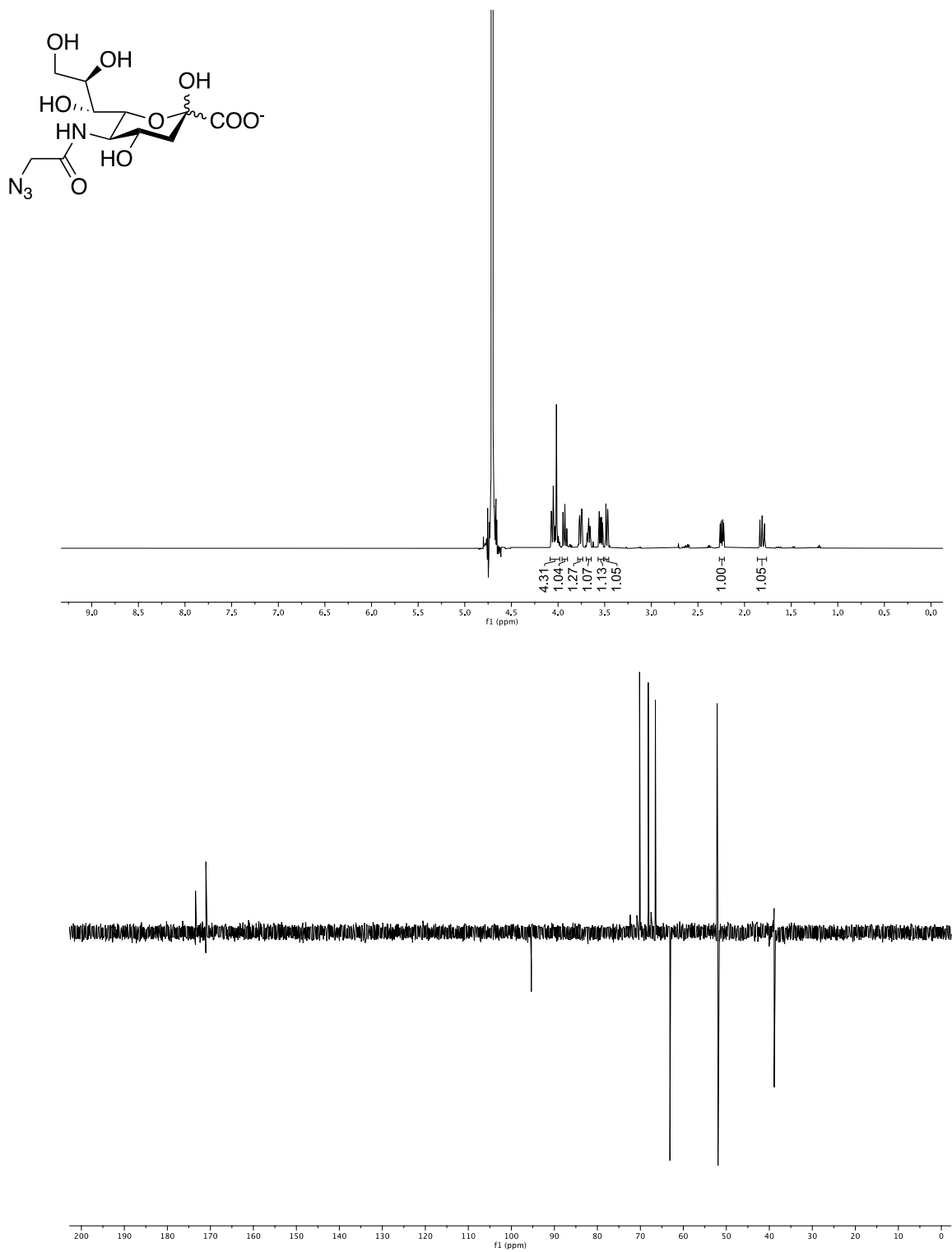
Figure S3. ^1H and ^{13}C NMR spectra of synthesized *N*-azidoacetylneuraminic acid (C5-azido sialic acid) in D_2O (500 MHz).
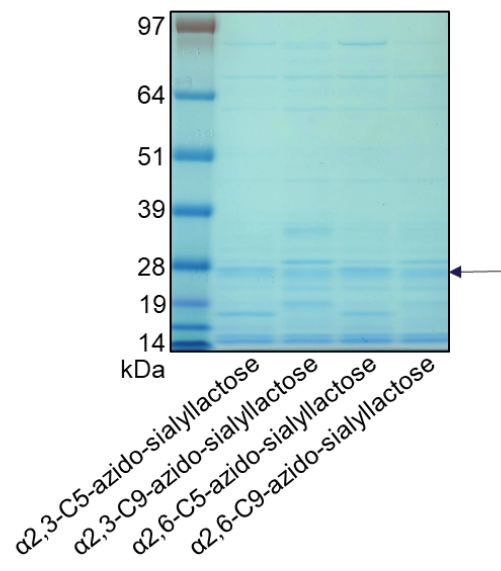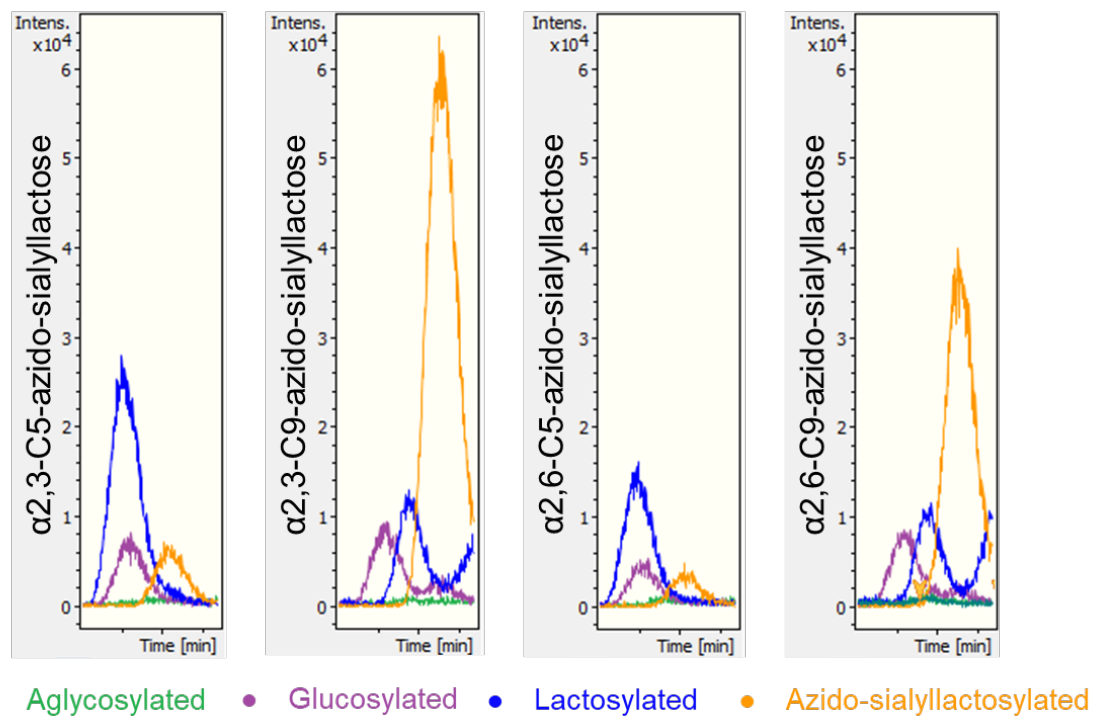
Figure S4. Coomassie-stained protein gel and extracted ion chromatograms (EICs) of 1 mL IVG azido-sialoglycoprotein products. Area under the curve of each EIC estimates relative abundance of each pathway intermediate and is used to calculate glycosylation efficiency.

Increasing [C9-azido sialic acid] ⟶

Figure S5. C9-azido sialic acid demonstrates *E. coli* cell toxicity. *E. coli* cells were supplemented with increasing [C9-azido sialic acid] from left to right (0.25, 0.5, 1, 1.5, 2, 2.5 mM) in otherwise equivalent culture conditions. Decreasing optical densities were observed for cultures incubated with increasing [C9-azido sialic acid], indicating some degree of cellular toxicity caused by the compound.

Supplementary Tables

Supplementary Table S1. DNA design of target glycoprotein. The target glycoprotein, dust mite allergen (Der p 2), was designed to have a 5' CAT linker sequence (orange) to standardize the ribosome binding site for improved translation. A BamHI restriction site (gray) separated the endogenous protein sequence from its encoded Glyctag (purple) and purification affinity His tag (brown). This sequence was cloned into the pJL1 backbone at the NdeI (5') and SalI (3') restriction sites.

DNA Sequence of target glycoprotein (in pJL1 backbone):

Der p 2 (His-tag)

Cat linker Protein BamHI linker Glyctag His tag <u>Stop codon</u>

ATGGAGAAAAAAATCGATCAGGTGGATGTTAAAGATTGCGCCAACCACGAAATCAAAAAAGTTCTGG
TTCCGGGTTGTCATGGTAGCGAACCGTGTATTATTCATCGTGGTAAACCGTTTCAGCTGGAAGCAGT
TTTTGAAGCAAATCAGAATACCAAAACCGCCAAGATTGAAATCAAAGCCAGCATTGATGGTCTGGAA
GTTGATGTTCCGGGTATTGATCCGAATGCATGCCACTATATGAAATGTCCGCTGGTTAAAGGTCAGC
AGTATGATATCAAATATACCTGGAACGTGCCGAAAATTGCACCGAAAAGCGAAATGTTGTTGTGACC
GTTAAAGTGATGGGTGATGATGGTGTTCTGGCATGTGCCATTGCAACCCATGCAAAAATTCGTGATG
GATCCGGTCGTGCAACCACAGGTGGTAATTGGACAACCCGTGCCGGTGGTCATCACCATCATCACC
AT<u>TAA</u>

Supplementary Table S2. NeuA DNA design with (top) and without (bottom) a CAT linker.
A CAT linker sequence (orange) was included at the 5' end of the NeuA sequence, which serves to standardize the ribosome binding site and can improve expression.

ATGGAGAAAAAATCCGCACCAAAATTATCGCAATTATTCCGGCACGTAGCGGTAGCAAAGGTCTGC
GTAACAAAAATGCACTGATGCTGATTGATAAACCGCTGCTGGCATATACCATTGAAGCAGCACTGCA
GAGCGAAATGTTTGAAAAAGTTATTGTTACCACCGACAGCGAACAGTATGGTGCAATTGCCGAAAGC
TATGGTGCAGATTTTCTGCTGCGTCCGGAAGAACTGGCAACCGATAAAGCAAGCAGCTTTGAATTTA
TCAAACATGCCCTGAGCATCTATACCGATTATGAAAATTTTGCACTGCTGCAGCCGACCAGTCCGTTT
CGTGATAGCACCCATATTATTGAAGCCGTGAAACTGTATCAGACCCTGGAAAAGTATCAGTGTGTTGT
TAGCGTTACCCGTAGCAATAAACCGAGCCAGATTATTCGTCCGCTGGATGATTATAGCACCCTGAGC
TTTTTTGATCTGGACTACAGCAAATATAACCGCAACAGCATTGTTGAATATCATCCGAATGGTGCCAT
TTTTATCGCCAACAAACAGCATTATCTGCATACCAAACATTTTTTCGGTCGTTATAGCCTGGCCTACAT
CATGGATAAAGAAAGCTCACTGGATATCGATGATCGCATGGATTTTGAACTGGCCATTACCATTCAGC
AGAAGAAAAATCGTCAGAAGATTCTGTACCAGAACATCCATAATCGCATCAACGAAAAACGCAACGA
ATTTGATAGCGTGAGCGATATTACCCTGATTGGTCATAGCCTGTTTGATTATTGGGACGTGAAAAAGA
TCAACGACATCGAAGTTAATAACCTGGGTATTGCCGGTATCAACAGCAAAGAATATTACGAGTACATC
ATCGAGAAAGAGCGCATTGTTAATTTTGGCGAATTCGTGTTTATCTTTTTCGGCACCAATGATATTGTT
GTGAGCGACTGGAAAAAAGAGGATACCCTTTGGTATCTGAAAAAGACCTGCCAGTACATCAAAAAAA
AGAATGCAGCCAGCAAAATCTACCTGCTGAGCGTTCCGCCTGTTTTTGGTCGTATTGATCGTGATAAT
CGTATCATCAATGACCTGAATAGCTATCTGCGTGAAAATGTGGATTTCGCCAAATTTATCAGCCTGGA
TCATGTTCTGAAAGATTCCTATGGCAACCTGAACAAAATGTATACCTATGATGGCCTGCACTTTAACA
GCAATGGTTATACCGTTCTGGAAAACGAAATTGCCGAGATCGTTAAATGGAGCCATCCGCAGTTCGA
AAAAGGTGGTGGTTCTGGTGGTGGTTCTGGTGGTTCTGCGTGGAGCCATCCGCAGTTCGAAAAATA
A

ATGCGCACCAAAATTATCGCAATTATTCCGGCACGTAGCGGTAGCAAAGGTCTGCGTAACAAAAATG
CACTGATGCTGATTGATAAACCGCTGCTGGCATATACCATTGAAGCAGCACTGCAGAGCGAAATGTT
TGAAAAAGTTATTGTTACCACCGACAGCGAACAGTATGGTGCAATTGCCGAAAGCTATGGTGCAGAT
TTTCTGCTGCGTCCGGAAGAACTGGCAACCGATAAAGCAAGCAGCTTTGAATTTATCAAACATGCCC
TGAGCATCTATACCGATTATGAAAATTTTGCACTGCTGCAGCCGACCAGTCCGTTTCGTGATAGCAC
CCATATTATTGAAGCCGTGAAACTGTATCAGACCCTGGAAAAGTATCAGTGTGTTGTTAGCGTTACCC
GTAGCAATAAACCGAGCCAGATTATTCGTCCGCTGGATGATTATAGCACCCTGAGCTTTTTTGATCTG
GACTACAGCAAATATAACCGCAACAGCATTGTTGAATATCATCCGAATGGTGCCATTTTTATCGCCAA
CAAACAGCATTATCTGCATACCAAACATTTTTTCGGTCGTTATAGCCTGGCCTACATCATGGATAAAG
AAAGCTCACTGGATATCGATGATCGCATGGATTTTGAACTGGCCATTACCATTCAGCAGAAGAAAAAT
CGTCAGAAGATTCTGTACCAGAACATCCATAATCGCATCAACGAAAAACGCAACGAATTTGATAGCGT
GAGCGATATTACCCTGATTGGTCATAGCCTGTTTGATTATTGGGACGTGAAAAAGATCAACGACATC
GAAGTTAATAACCTGGGTATTGCCGGTATCAACAGCAAAGAATATTACGAGTACATCATCGAGAAAGA
GCGCATTGTTAATTTTGGCGAATTCGTGTTTATCTTTTTCGGCACCAATGATATTGTTGTGAGCGACT
GGAAAAAAGAGGATACCCTTTGGTATCTGAAAAAGACCTGCCAGTACATCAAAAAAAAGAATGCAGC
CAGCAAAATCTACCTGCTGAGCGTTCCGCCTGTTTTTGGTCGTATTGATCGTGATAATCGTATCATCA
ATGACCTGAATAGCTATCTGCGTGAAAATGTGGATTTCGCCAAATTTATCAGCCTGGATCATGTTCTG
AAAGATTCCTATGGCAACCTGAACAAAATGTATACCTATGATGGCCTGCACTTTAACAGCAATGGTTA
TACCGTTCTGGAAAACGAAATTGCCGAGATCGTTAAATGGAGCCATCCGCAGTTCGAAAAAGGTGGT
GGTTCTGGTGGTGGTTCTGGTGGTTCTGCGTGGAGCCATCCGCAGTTCGAAAAATAA

Supplementary Table S3. Addgene ID's for plasmid accession. All plasmids used in this study have been made accessible on Addgene. Addgene ID and plasmid name are listed here for easy retrieval.

Plasmid Name	Addgene ID
ApNGT.pJL1	199111
LgtB.pJL1	199112
CSTI.pJL1	199113
PdST6.pJL1	199114
NeuA.pJL1	199115
Derp2.pJL1	199116

Supplementary Table S4. Theoretical m/z values. Calculated m/z values were used to make extracted ion chromatograms for each species to calculate area under the curve as an estimation of glycosylation efficiency. Sugars were installed onto the asparagine within the peptide sequence ATTGGNWTTR. Glycoprotein samples were trypsinized to yield this remaining glycopeptide sequence.

Species	Theoretical m/z in +2 charge state
Aglycosylated peptide	532.7596
Glucosylated peptide	613.78665
Lactosylated peptide	694.81165
Sialyllactosylated peptide	840.35935
C5-azido-sialyllactosylated peptide	860.94601
C9-azido-sialyllactosylated peptide	852.94651

Supplementary Table S5. Peak lists used to generate mass spectra. Yellow highlight = species of interest. Red = contaminating species carried over from purification. Intensity of species in red was manually reduced (I% deconvolute column) to eliminate noise and emphasize peaks of interest in final spectra.

Peak list for α2,3 C5-azido-sialyllactose species

1

m/z	I %	I % deconvolute	m/z	I %	I % deconvolute	m/z	I %	I % deconvolute
500.2512	0.3	0.3	511.2524	1	1	521.0177	1.6	1.6
500.286	0.9	0.9	511.7492	0.3	0.3	521.2734	1.4	1.4
500.7582	0.3	0.3	511.8988	0.2	0.2	521.3372	0.4	0.4
501.2483	0.8	0.8	512.0602	0.2	0.2	521.5176	0.3	0.3
501.3139	0.3	0.3	512.2611	3.2	1	521.6117	1.1	1.1
501.3414	0.5	0.5	512.5963	2.5	1	521.7625	0.2	0.2
501.5764	0.3	0.3	512.7519	0.2	0.2	521.9434	0.7	0.7
501.7557	0.2	0.2	512.9305	1.1	1.1	522.2876	2.1	1
501.7822	0.2	0.2	513.2326	2.7	1	522.3314	1.4	1.4
501.9105	0.2	0.2	513.2794	2.7	1	522.5576	1	1
502.3255	7.5	1	513.4827	2.7	1	522.6083	0.2	0.2
502.4919	0.3	0.3	513.5934	0.1	0.1	522.7007	1.8	1.8
502.7709	0.5	0.5	513.7337	2	2	522.7867	0.9	0.9
502.9968	0.2	0.2	513.9233	0.2	0.2	522.8439	1.9	1.9
503.1104	0.2	0.2	513.9835	1	1	522.9868	1.5	1.5
503.2606	1.2	1.2	514.0148	0.2	0.2	523.1301	1	1
503.3032	1.2	1.2	514.2774	0.9	0.9	523.2843	1	1
503.3284	2.1	1	514.484	0.2	0.2	523.3343	0.6	0.6
503.5052	0.1	0.1	514.5201	0.2	0.2	523.4161	0.3	0.3
503.6548	0.1	0.1	514.5625	4.5	1	523.5817	13.3	1
503.7724	2.3	1	514.7852	7.5	1	523.7852	0.4	0.4
503.8553	0.2	0.2	514.7926	1	1	523.9162	10.9	1
504.0553	0.1	0.1	514.8966	7.1	1	524.2514	9.8	1
504.2716	1.6	1.6	514.9904	0.2	0.2	524.4268	0.4	0.4
504.3302	0.4	0.4	515.0634	4.7	1	524.5113	0.2	0.2
504.4014	0.2	0.2	515.231	2.6	1	524.5836	2.5	1
504.4991	0.2	0.2	515.2916	0.6	0.6	524.6236	0.4	0.4
504.5451	0.2	0.2	515.3297	0.8	0.8	524.7635	0.2	0.2
504.581	0.2	0.2	515.3972	1.1	1.1	524.828	0.2	0.2
504.6882	0.1	0.1	515.5648	0.5	0.5	524.917	1	1
504.7734	0.4	0.4	515.7371	0.2	0.2	525.019	0.1	0.1
504.917	0.2	0.2	515.7907	0.2	0.2	525.2698	5	1
505.2554	2.2	1	515.9254	0.1	0.1	525.6308	0.2	0.2
505.5904	1.5	1.5	516.2578	1	1	525.7727	2.2	1
505.7435	0.2	0.2	516.3155	1.7	1.7	525.8287	0.1	0.1
505.9245	0.7	0.7	516.5904	0.7	0.7	525.9173	0.1	0.1
506.2667	3.6	1	516.7814	0.2	0.2	525.9633	0.2	0.2
506.5902	0.2	0.2	516.8613	0.2	0.2	526.202	0.2	0.2
506.7788	0.4	0.4	516.9236	0.4	0.4	526.2701	1.6	1.6
506.8916	0.3	0.3	517.0623	0.3	0.3	526.3087	0.5	0.5
507.2698	1	1	517.2625	0.7	0.7	526.5207	0.6	0.6
507.5729	0.2	0.2	517.3068	1.4	1.4	526.7713	0.7	0.7
507.7865	0.4	0.4	517.5239	0.3	0.3	526.942	0.3	0.3
508.2553	3.2	1	517.5783	2.3	1	527.0182	0.2	0.2
508.7662	0.3	0.3	517.7682	1.3	1.3	527.2838	100	1
508.936	0.4	0.4	517.9095	2.9	1	527.4217	0.1	0.1
509.2612	1.1	1.1	518.0259	0.2	0.2	527.459	0.3	0.3
509.602	0.2	0.2	518.2452	2.3	1	527.5117	0.2	0.2
509.6501	0.1	0.1	518.2987	0.8	0.8	527.6181	84.7	1
509.7383	0.2	0.2	518.5763	1	1	527.7465	0.2	0.2
509.7606	0.1	0.1	518.7703	0.6	0.6	527.7796	0.3	0.3
509.9849	0.2	0.2	518.9099	0.4	0.4	527.952	42.9	1
510.2617	0.7	0.7	519.141	0.2	0.2	528.2338	1.3	1.3
510.4139	0.3	0.3	519.2728	0.7	0.7	528.2841	22.8	1
510.5817	0.3	0.3	519.4912	0.6	0.6	528.6197	4.9	1
510.7454	0.6	0.6	519.7434	0.7	0.7	528.7322	0.7	0.7
510.7913	0.3	0.3	519.9933	0.4	0.4	528.7875	0.2	0.2
510.9103	0.2	0.2	520.2691	1	1	528.9157	0.5	0.5
			520.516	2.3	1	528.9534	1.4	1.4
			520.767	2.7	1	529.1763	0.1	0.1

529.2835	3	1	545.7609	0.1	0.1	561.3029	2.6	1
529.375	1.6	1.6	545.9312	0.1	0.1	561.5854	0.2	0.2
529.5078	0.1	0.1	546.0712	1	1	561.6266	0.3	0.3
529.5818	0.3	0.3	546.273	1.9	1.9	561.7876	0.5	0.5
529.7639	0.7	0.7	546.3166	2.7	1	561.8169	0.6	0.6
529.8104	0.1	0.1	546.3679	0.2	0.2	561.962	0.2	0.2
529.9199	0.1	0.1	546.472	1.3	1.3	562.0629	0.1	0.1
529.9509	0.3	0.3	546.6724	0.8	0.8	562.3049	0.8	0.8
530.2778	0.7	0.7	546.7772	0.3	0.3	562.9891	0.2	0.2
530.3322	1.1	1.1	546.8725	0.4	0.4	563.2385	0.5	0.5
530.3779	0.5	0.5	547.0705	0.2	0.2	563.2993	0.4	0.4
530.5862	0.2	0.2	547.3102	1	1	563.5948	0.2	0.2
530.7648	0.3	0.3	547.6269	0.2	0.2	563.7431	0.2	0.2
530.9176	0.1	0.1	548.2905	0.4	0.4	563.9298	0.2	0.2
531.2815	1.5	1.5	549.2695	3	1	564.2765	0.4	0.4
531.3234	0.6	0.6	549.589	0.3	0.3	564.5217	0.1	0.1
531.6017	0.2	0.2	549.77	1.6	1.6	564.7726	0.1	0.1
531.781	0.7	0.7	549.924	0.2	0.2	564.9789	0.3	0.3
531.9368	0.1	0.1	550.0325	0.2	0.2	565.2717	1.7	1.7
532.2788	0.6	0.6	550.2613	3.8	1	565.3148	2	2
532.6152	0.8	0.8	550.5326	0.1	0.1	565.538	0.3	0.3
==532.7657==	0.3	0.3	550.61	0.2	0.2	565.6461	0.2	0.2
532.9495	0.7	0.7	550.7626	2.2	1	565.7762	1	1
==533.2824==	1.1	1.1	550.9411	0.2	0.2	565.8167	0.6	0.6
533.3277	0.2	0.2	551.2658	0.9	0.9	566.0393	0.3	0.3
533.5321	0.5	0.5	551.7655	0.3	0.3	566.2816	0.6	0.6
533.6159	0.2	0.2	551.8255	1.1	1.1	566.7803	0.2	0.2
==533.7794==	0.3	0.3	552.2754	0.5	0.5	567.2918	0.5	0.5
534.0336	0.1	0.1	552.3088	0.9	0.9	567.3491	0.1	0.1
534.2795	2.1	2.1	552.6152	0.3	0.3	567.7833	0.2	0.2
534.6192	0.1	0.1	552.7708	0.2	0.2	568.2454	0.2	0.2
534.759	0.2	0.2	552.8278	0.2	0.2	568.3053	1.6	1.6
535.279	0.7	0.7	552.9493	0.2	0.2	568.6422	1.3	1.3
535.775	0.2	0.2	553.281	0.4	0.4	568.8575	0.5	0.5
536.1697	0.2	0.2	553.303	0.4	0.4	568.955	1	1
536.2053	0.2	0.2	553.6141	0.2	0.2	569.0579	0.4	0.4
536.272	1.1	1.1	553.7628	0.3	0.3	569.2872	1	1
536.5654	0.1	0.1	553.9461	0.1	0.1	569.4589	0.2	0.2
537.2758	0.5	0.5	554.2687	0.4	0.4	569.62	0.7	0.7
538.2898	5.3	1	554.7046	0.1	0.1	569.7846	0.1	0.1
539.0014	0.2	0.2	554.7705	0.1	0.1	569.9514	0.4	0.4
539.2915	1.7	1.7	554.8481	0.1	0.1	570.1478	0.2	0.2
539.5043	0.1	0.1	555.2846	0.3	0.3	570.29	1	1
539.7762	0.2	0.2	555.3635	0.2	0.2	570.4343	0.1	0.1
539.9352	0.8	0.8	555.6187	0.1	0.1	570.7911	0.5	0.5
540.2715	0.9	0.9	555.7876	0.2	0.2	571.3115	0.5	0.5
540.603	0.3	0.3	555.9138	0.2	0.2	571.7996	0.2	0.2
540.7671	0.2	0.2	556.0379	0.4	0.4	572.2959	0.7	0.7
540.9376	0.2	0.2	556.1639	0.4	0.4	572.3535	0.3	0.3
541.2833	22.7	1	556.2889	0.6	0.6	572.6267	0.5	0.5
541.3489	0.9	0.9	556.4152	0.3	0.3	572.8084	0.2	0.2
541.7394	2.9	1	556.5385	0.2	0.2	572.9602	0.3	0.3
541.7847	12.5	1	556.7524	0.1	0.1	573.2902	0.4	0.4
542.2414	1.6	1.6	556.9212	0.2	0.2	573.3383	2.6	1
542.286	4.7	1	557.2581	0.3	0.3	573.6116	0.2	0.2
542.3484	0.3	0.3	557.3313	0.3	0.3	573.9485	0.2	0.2
542.7431	0.5	0.5	557.3794	0.2	0.2	574.2877	0.4	0.4
542.7867	1.2	1.2	557.7654	0.3	0.3	574.3412	0.9	0.9
543.2495	0.2	0.2	558.2675	0.4	0.4	574.6174	0.2	0.2
543.2843	0.5	0.5	558.3623	0.1	0.1	574.785	0.3	0.3
543.3622	0.3	0.3	558.7991	0.5	0.5	574.8495	0.1	0.1
543.7653	0.5	0.5	559.3047	0.4	0.4	575.2173	0.3	0.3
544.0166	0.2	0.2	559.3466	0.7	0.7	575.3108	0.5	0.5
544.2883	1.7	1.7	559.8033	0.2	0.2	575.62	19.5	1
544.5173	0.2	0.2	560.2616	0.5	0.5	575.7819	0.5	0.5
544.7648	0.3	0.3	560.3135	0.5	0.5	575.9544	17.3	1
544.9301	0.4	0.4	560.6246	0.8	0.8	576.0307	0.4	0.4
545.3136	8.9	1	560.7606	0.3	0.3	576.2903	11.3	1
545.3679	0.5	0.5	560.8069	0.4	0.4	576.5329	0.2	0.2
545.5971	0.3	0.3	560.9575	0.9	0.9	576.6225	3.3	1

576.803	0.4	0.4	596.6953	0.3	0.3	612.8026	0.2	0.2
576.9567	1	1	596.8976	0.1	0.1	612.8407	0.3	0.3
577.298	1.6	1.6	596.9659	0.3	0.3	612.8954	0.2	0.2
577.6375	0.4	0.4	597.2941	0.8	0.8	613.3096	0.4	0.4
577.9717	0.4	0.4	597.6392	0.2	0.2	613.7901	1.1	1.1
578.2982	0.6	0.6	597.701	0.2	0.2	614.2924	0.9	0.9
578.8193	0.1	0.1	597.9017	0.4	0.4	614.3271	0.4	0.4
578.9413	0.1	0.1	597.9728	0.1	0.1	614.4118	2.3	2.3
579.2807	0.7	0.7	598.102	0.4	0.4	614.7943	0.5	0.5
579.3226	0.4	0.4	598.3018	0.5	0.5	614.9902	0.2	0.2
579.8057	0.6	0.6	598.5015	0.1	0.1	615.3102	0.3	0.3
580.3126	3.2	1	599.3368	9.5	1	615.4141	0.7	0.7
580.82	0.5	0.5	599.6767	0.2	0.2	615.6432	0.9	0.9
581.3045	1.5	1.5	599.8381	5.6	1	615.8029	0.2	0.2
581.8049	0.5	0.5	600.3399	2.3	1	615.9767	0.8	0.8
582.3037	0.6	0.6	600.4107	1	1	616.2778	0.3	0.3
582.5478	0.3	0.3	600.8405	0.6	0.6	616.3114	0.7	0.7
582.801	0.5	0.5	601.3022	0.3	0.3	616.3434	1.2	1.2
582.9479	0.1	0.1	601.369	0.9	0.9	616.3789	0.8	0.8
583.0168	0.1	0.1	601.4133	0.3	0.3	616.6447	0.3	0.3
583.0491	0.3	0.3	601.7967	0.2	0.2	616.7883	0.1	0.1
583.3104	0.4	0.4	601.9713	0.9	0.9	617.0463	0.4	0.4
583.5191	0.1	0.1	602.3049	1.2	1.2	617.2737	5.4	1
583.7701	0.1	0.1	602.3643	0.5	0.5	617.3444	0.8	0.8
584.3214	0.7	0.7	602.6397	0.5	0.5	617.4736	8.4	1
584.3784	0.1	0.1	602.816	1.4	1.4	617.547	0.3	0.3
584.6155	1.5	1.5	602.993	41.2	1	617.674	8	1
584.7636	0.2	0.2	603.3272	40.5	1	617.7949	0.2	0.2
584.9509	1.9	1.9	603.6613	22.5	1	617.8744	5.2	1
585.3033	2.4	1	603.8201	0.4	0.4	618.0745	2.8	1
585.3749	3.6	1	603.9951	9.4	1	618.276	1.4	1.4
585.6208	0.5	0.5	604.2748	0.2	0.2	618.3386	1.5	1.5
585.8078	1.4	1.4	604.3289	3.5	1	618.475	0.6	0.6
585.9554	0.2	0.2	604.6665	0.9	0.9	618.6736	0.2	0.2
586.3063	1	1	604.7839	0.3	0.3	618.8099	0.3	0.3
586.3761	1.4	1.4	605.0088	0.4	0.4	618.877	0.1	0.1
586.8059	0.5	0.5	605.2771	0.3	0.3	619.3265	3.1	1
586.8948	0.2	0.2	605.3429	0.4	0.4	619.8001	0.2	0.2
587.2302	0.2	0.2	605.7833	0.1	0.1	619.9749	0.1	0.1
587.3084	0.3	0.3	606.3048	0.3	0.3	620.227	0.1	0.1
587.3547	1.6	1.6	606.813	1.4	1.4	620.2885	1	1
588.1327	0.3	0.3	607.0654	1.5	1.5	620.3286	1.4	1.4
588.3383	13.2	1	607.3192	1.4	1.4	620.476	0.1	0.1
588.4667	0.7	0.7	607.5659	0.6	0.6	620.6319	0.2	0.2
588.6049	0.3	0.3	607.8305	0.6	0.6	620.7887	0.6	0.6
588.6334	0.5	0.5	608.3264	0.7	0.7	620.9667	0.3	0.3
588.8016	0.5	0.5	608.659	0.4	0.4	621.3296	0.7	0.7
588.9658	0.2	0.2	608.7938	0.1	0.1	621.6343	0.2	0.2
589.0116	0.3	0.3	608.9927	0.2	0.2	621.9805	0.1	0.1
589.2702	0.3	0.3	609.3029	1.2	1.2	622.0331	0.2	0.2
589.3347	16.2	1	609.4818	2.8	1	622.3241	0.3	0.3
589.5112	0.2	0.2	609.6489	5.6	1	622.6501	0.2	0.2
589.7632	0.2	0.2	609.8159	6	1	622.8258	0.8	0.8
590.3369	4.6	1	609.9829	4.5	1	622.9795	0.1	0.1
590.7937	0.3	0.3	610.15	3	1	623.3043	4	1
591.2956	0.5	0.5	610.3176	2.3	1	623.349	0.8	0.8
591.3368	1	1	610.4839	0.7	0.7	623.8213	0.5	0.5
592.2468	0.1	0.1	610.6531	0.8	0.8	624.3102	1.3	1.3
592.3117	0.3	0.3	610.7905	0.4	0.4	624.8247	0.3	0.3
593.2987	0.2	0.2	610.8204	0.2	0.2	625.0617	0.2	0.2
593.8049	0.2	0.2	610.9869	0.4	0.4	625.303	0.6	0.6
594.2801	0.3	0.3	611.0386	0.4	0.4	625.8002	0.2	0.2
594.3348	0.2	0.2	611.2909	0.4	0.4	626.301	0.4	0.4
595.0548	0.1	0.1	611.5406	0.2	0.2	626.3496	0.1	0.1
595.2865	7.6	1	611.793	0.2	0.2	627.2997	0.2	0.2
595.6909	0.7	0.7	612.0942	0.3	0.3	627.3849	0.5	0.5
595.8912	1.1	1.1	612.2959	0.6	0.6	628.3097	0.2	0.2
596.0919	1	1	612.4929	0.5	0.5	628.3854	0.3	0.3
596.2902	3	1	612.6469	0.1	0.1	628.8519	0.2	0.2
596.4941	0.4	0.4	612.6958	0.3	0.3	629.3476	0.3	0.3

629.78	0.1	0.1	653.6999	0.2	0.2	682.3347	0.5	0.5
629.839	0.4	0.4	653.8367	0.2	0.2	682.4126	0.2	0.2
629.9345	0.1	0.1	653.9	0.2	0.2	682.5869	0.4	0.4
630.062	0.1	0.1	654.1014	0.1	0.1	682.8364	0.5	0.5
630.3493	0.3	0.3	654.3305	0.3	0.3	683.0879	0.3	0.3
630.3855	0.2	0.2	655.0303	0.2	0.2	683.3405	0.2	0.2
631.3426	0.4	0.4	655.2817	0.3	0.3	683.9725	0.8	0.8
632.2504	0.2	0.2	655.5307	0.2	0.2	684.3074	1	1
632.3454	0.9	0.9	655.8272	0.1	0.1	684.3511	0.1	0.1
632.4488	0.1	0.1	656.3253	0.2	0.2	684.6407	0.6	0.6
632.6451	0.1	0.1	656.3993	0.2	0.2	684.9745	0.3	0.3
632.8341	0.2	0.2	656.84	0.2	0.2	685.3088	0.2	0.2
633.3354	0.6	0.6	657.322	0.3	0.3	685.3615	0.2	0.2
633.8319	0.3	0.3	657.4039	0.2	0.2	685.4036	0.5	0.5
634.2902	0.1	0.1	657.8256	0.2	0.2	685.4375	1	1
634.3457	1	1	658.3448	0.2	0.2	686.2709	0.4	0.4
634.7963	0.2	0.2	658.3915	1.2	1.2	686.3688	0.8	0.8
634.8398	0.1	0.1	659.3408	0.8	0.8	686.4248	0.6	0.6
635.1851	0.2	0.2	659.3943	0.5	0.5	686.6049	0.4	0.4
635.3314	0.6	0.6	659.7005	0.3	0.3	686.8699	0.6	0.6
635.4713	0.6	0.6	659.8408	0.5	0.5	686.9405	0.2	0.2
635.6153	0.5	0.5	659.9011	0.5	0.5	687.2735	0.1	0.1
635.7579	0.3	0.3	660.1007	0.4	0.4	687.3814	2.8	1
635.9008	0.2	0.2	660.3022	0.5	0.5	688.3874	1.1	1.1
636.0439	0.1	0.1	660.3702	4.6	1	688.8242	1.2	1.2
636.302	0.2	0.2	660.5017	0.2	0.2	689.3264	0.9	0.9
636.3489	0.4	0.4	660.8552	0.2	0.2	689.3774	0.4	0.4
636.5617	0.1	0.1	661.3725	1.7	1.7	689.6952	0.1	0.1
636.81	0.2	0.2	662.2927	0.5	0.5	689.8267	0.3	0.3
637.3377	0.4	0.4	662.3529	0.8	0.8	690.0305	0.1	0.1
637.8189	5	1	663.3315	0.4	0.4	690.3265	0.4	0.4
638.32	3.4	1	663.845	0.1	0.1	690.3663	0.3	0.3
638.8209	1.3	1.3	664.3084	3	1	690.8256	0.3	0.3
639.3466	0.7	0.7	664.6597	0.2	0.2	691.3289	0.3	0.3
639.8236	0.1	0.1	664.8423	0.1	0.1	692.3602	2.4	1
640.3451	0.3	0.3	665.0005	0.3	0.3	692.6535	0.4	0.4
640.8329	0.1	0.1	665.1711	0.2	0.2	692.861	1.6	1.6
641.3238	0.2	0.2	665.3121	1.1	1.1	692.9873	0.2	0.2
641.36	0.2	0.2	666.3477	1.1	1.1	693.3632	0.8	0.8
642.3595	0.6	0.6	667.3496	0.4	0.4	693.685	0.7	0.7
642.834	0.3	0.3	668.3134	0.4	0.4	693.8616	0.3	0.3
643.3474	1.2	1.2	668.3468	0.2	0.2	694.0196	0.7	0.7
643.4133	0.2	0.2	668.5054	0.1	0.1	694.3549	3.6	3.6
644.3566	0.5	0.5	668.8144	0.2	0.2	694.6872	0.2	0.2
644.4317	0.2	0.2	669.3177	0.2	0.2	<mark>694.8161</mark>	3.2	3.2
644.8392	0.4	0.4	669.3534	0.3	0.3	<mark>695.3175</mark>	2.5	2.5
645.3513	0.3	0.3	669.8108	0.1	0.1	695.3565	1.2	1.2
645.8175	0.7	0.7	670.3138	3.7	1	<mark>695.8189</mark>	0.9	0.9
646.3549	2.2	1	670.3916	2.5	1	696.3701	2.7	2.7
646.8199	0.3	0.3	670.8149	2.4	1	697.3733	1	1
646.9881	0.1	0.1	671.3184	1.1	1.1	698.3756	0.3	0.3
647.1569	0.1	0.1	671.395	0.9	0.9	698.9185	0.1	0.1
647.3125	0.9	0.9	671.8217	0.3	0.3	699.2538	0.1	0.1
647.3566	0.8	0.8	672.3258	0.2	0.2	699.3534	0.1	0.1
647.7125	0.2	0.2	672.3965	0.2	0.2	699.4053	0.2	0.2
647.8126	0.5	0.5	672.8232	0.1	0.1	700.3502	0.2	0.2
648.3164	0.4	0.4	673.3657	1	1	701.3634	0.4	0.4
648.8523	1.5	1.5	674.297	0.1	0.1	701.4216	0.4	0.4
649.3494	1.3	1.3	674.3674	0.4	0.4	701.6856	0.1	0.1
649.5572	0.1	0.1	675.283	0.2	0.2	701.8754	0.2	0.2
649.8484	0.5	0.5	675.3634	1.2	1.2	702.3269	0.2	0.2
650.3582	0.7	0.7	675.8391	0.2	0.2	702.3759	0.5	0.5
650.8517	0.5	0.5	676.366	0.5	0.5	702.4226	0.2	0.2
651.3056	0.2	0.2	677.3642	0.7	0.7	703.3658	0.5	0.5
651.3541	0.4	0.4	678.3639	0.4	0.4	703.4312	0.1	0.1
651.7854	0.1	0.1	679.3793	0.9	0.9	704.3942	0.4	0.4
652.0342	0.2	0.2	680.3795	0.4	0.4	705.34	1.1	1.1
652.3269	1	1	680.4477	0.2	0.2	705.3914	0.2	0.2
652.8354	0.2	0.2	681.3507	0.2	0.2	705.5569	0.2	0.2
653.3291	0.4	0.4	681.826	0.3	0.3	705.7578	0.4	0.4

705.8418	0.7	0.7	732.3792	0.6	0.6	771.8397	2	2
705.9587	0.4	0.4	732.5768	0.1	0.1	772.0901	1.5	1.5
706.1586	0.3	0.3	733.3806	0.2	0.2	772.3021	0.3	0.3
706.3487	0.4	0.4	734.3772	0.2	0.2	772.3408	0.8	0.8
706.8231	0.4	0.4	735.3733	0.4	0.4	772.459	3.8	1
707.356	4.4	1	736.3294	0.5	0.5	772.5908	0.4	0.4
707.824	0.1	0.1	736.3711	0.2	0.2	772.6333	0.4	0.4
708.3584	1.8	1.8	737.335	0.3	0.3	772.8417	0.2	0.2
709.36	0.5	0.5	737.3937	0.3	0.3	772.9664	0.3	0.3
710.3851	0.8	0.8	738.342	1.2	1.2	773.4556	8.6	1
710.7064	0.1	0.1	738.415	0.4	0.4	773.8764	0.2	0.2
710.8215	0.1	0.1	739.3508	0.5	0.5	774.4581	3.2	1
710.8878	0.5	0.5	739.4108	0.2	0.2	775.4375	1.3	1.3
711.0431	0.1	0.1	740.355	0.2	0.2	776.4144	0.8	0.8
711.3262	0.2	0.2	740.8797	0.2	0.2	777.4113	0.3	0.3
711.3845	0.3	0.3	741.0482	0.5	0.5	777.4604	0.3	0.3
712.3367	1.1	1.1	741.2147	0.6	0.6	778.4071	0.1	0.1
712.3884	0.2	0.2	741.3839	0.7	0.7	779.408	0.2	0.2
712.8352	0.2	0.2	741.549	0.4	0.4	781.3272	0.1	0.1
712.9594	0.1	0.1	741.7164	0.2	0.2	781.3976	0.2	0.2
713.0403	0.2	0.2	741.8925	0.8	0.8	784.8664	1.8	1.8
713.087	0.2	0.2	742.2693	0.2	0.2	785.3671	1.6	1.6
713.2117	0.1	0.1	742.3348	3.4	1	785.8679	0.9	0.9
713.3396	0.5	0.5	742.3936	0.5	0.5	786.3676	0.4	0.4
713.3763	0.2	0.2	742.6018	0.1	0.1	786.4579	0.9	0.9
713.8425	0.4	0.4	742.8364	2.3	1	786.8681	0.1	0.1
714.342	0.5	0.5	742.8958	0.2	0.2	787.4563	0.7	0.7
714.8467	0.2	0.2	743.3377	1.1	1.1	788.4367	0.3	0.3
715.3457	0.2	0.2	743.3995	0.3	0.3	789.4227	0.1	0.1
715.416	0.1	0.1	743.8394	0.4	0.4	790.4202	3.4	1
716.3375	0.2	0.2	744.3599	0.3	0.3	790.9217	2.8	1
718.3418	0.1	0.1	744.4028	0.2	0.2	791.4225	1.5	1.5
718.6658	0.1	0.1	744.6112	0.4	0.4	791.9235	0.6	0.6
719.3479	0.3	0.3	744.8621	0.3	0.3	792.4237	0.2	0.2
719.4945	0.3	0.3	745.1134	0.2	0.2	793.3513	0.4	0.4
719.6388	0.3	0.3	745.3661	0.2	0.2	793.4119	0.8	0.8
719.7816	0.4	0.4	746.4071	0.3	0.3	794.3565	0.2	0.2
719.9245	0.3	0.3	747.332	0.5	0.5	794.4162	0.5	0.5
720.0686	0.2	0.2	747.3761	0.2	0.2	795.3915	1.5	1.5
720.2853	0.2	0.2	748.3419	0.3	0.3	795.4344	0.5	0.5
720.3134	0.1	0.1	749.3826	0.2	0.2	796.3941	0.6	0.6
720.3568	0.2	0.2	749.4399	0.2	0.2	796.4386	0.2	0.2
720.4207	0.1	0.1	750.3169	0.2	0.2	797.3999	0.2	0.2
721.3683	0.1	0.1	750.6485	0.2	0.2	798.0022	0.1	0.1
722.859	0.1	0.1	751.3998	0.2	0.2	798.4097	0.2	0.2
723.36	0.1	0.1	751.4851	0.2	0.2	799.3759	0.4	0.4
725.3496	2.2	1	757.3806	0.4	0.4	800.3848	0.2	0.2
725.8479	0.1	0.1	757.8803	0.3	0.3	800.8464	0.3	0.3
726.3529	0.9	0.9	758.3824	0.2	0.2	801.3479	0.2	0.2
726.8664	0.1	0.1	758.4799	0.6	0.6	801.4849	0.8	0.8
727.3571	0.3	0.3	759.4373	0.4	0.4	802.4853	0.5	0.5
727.448	0.1	0.1	759.4817	0.2	0.2	803.487	0.1	0.1
727.8306	0.1	0.1	760.4163	1.5	1.5	804.3915	0.2	0.2
728.3692	0.3	0.3	761.3175	0.2	0.2	804.4461	0.2	0.2
728.8714	0.2	0.2	761.4174	0.6	0.6	807.4391	0.8	0.8
729.2851	0.9	0.9	762.4162	0.2	0.2	808.4419	0.4	0.4
729.3591	0.2	0.2	762.8982	0.2	0.2	808.7487	0.2	0.2
729.427	0.2	0.2	763.3956	0.2	0.2	809.0834	0.2	0.2
729.6191	0.9	0.9	764.3809	0.2	0.2	809.4224	0.2	0.2
729.9535	0.5	0.5	765.1191	0.1	0.1	810.4127	0.2	0.2
730.2881	0.3	0.3	765.384	0.2	0.2	814.3821	0.2	0.2
730.3396	0.2	0.2	766.3995	0.1	0.1	814.4807	0.2	0.2
730.415	0.2	0.2	767.3761	0.1	0.1	814.5232	0.2	0.2
730.8421	0.1	0.1	767.888	0.4	0.4	814.6686	0.2	0.2
731.1762	1.5	1.5	768.3883	0.4	0.4	814.8109	0.2	0.2
731.377	2.7	1	768.8896	0.1	0.1	815.4628	0.2	0.2
731.577	3	1	769.3874	0.1	0.1	816.449	0.5	0.5
731.7775	2.4	1	771.3391	1.4	1.4	817.4454	0.7	0.7
731.9778	1.4	1.4	771.4747	0.5	0.5	818.4471	0.3	0.3
732.1782	0.7	0.7	771.5892	2.3	2.3	819.4393	0.4	0.4

m/z	I %	I %	m/z	I %	I %	m/z	I %	I %
820.4005	0.1	0.1	844.4871	0.1	0.1	876.4691	0.5	0.5
820.4463	0.3	0.3	846.4699	0.3	0.3	876.9192	0.4	0.4
820.5966	0.2	0.2	847.4526	0.2	0.2	877.4227	0.3	0.3
820.7387	0.2	0.2	851.4283	0.9	0.9	877.4717	0.2	0.2
820.8826	0.2	0.2	852.4303	0.4	0.4	878.4757	0.5	0.5
822.3636	0.3	0.3	852.9226	0.1	0.1	879.4235	0.7	0.7
822.4452	0.2	0.2	853.4285	0.2	0.2	879.4774	0.2	0.2
822.9703	0.1	0.1	855.4962	0.4	0.4	879.8388	0.2	0.2
823.1128	0.1	0.1	856.4991	0.2	0.2	880.3408	0.2	0.2
823.3966	2.1	2.1	857.4375	0.2	0.2	880.4259	0.3	0.3
823.8793	0.1	0.1	857.5205	0.2	0.2	881.8971	0.2	0.2
824.3986	0.9	0.9	858.4408	0.1	0.1	882.4055	0.2	0.2
824.6237	0.2	0.2	860.4304	0.2	0.2	883.4109	0.2	0.2
824.8745	0.2	0.2	860.5382	0.2	0.2	885.4312	0.2	0.2
825.1237	0.1	0.1	860.8645	4.9	4.9	887.497	3	3
825.3997	0.3	0.3	861.3658	3.9	3.9	888.5043	1.4	1.4
832.4322	0.2	0.2	861.8674	1.9	1.9	889.0557	0.2	0.2
835.3948	0.1	0.1	862.3681	0.7	0.7	889.256	0.2	0.2
835.5174	0.2	0.2	862.4785	0.1	0.1	889.4603	0.2	0.2
839.0766	0.2	0.2	862.9242	3.2	3.2	889.5089	0.4	0.4
839.2431	0.4	0.4	863.4261	3	3	889.6557	0.2	0.2
839.4096	0.6	0.6	863.9273	1.5	1.5	891.4612	0.2	0.2
839.5763	0.5	0.5	864.4289	0.6	0.6	892.431	0.1	0.1
839.7442	0.4	0.4	864.9288	0.2	0.2	895.413	0.1	0.1
839.9107	0.3	0.3	871.855	0.1	0.1	897.3962	0.1	0.1
840.0793	0.1	0.1	873.9161	0.2	0.2	898.4441	0.2	0.2
840.4279	0.1	0.1	874.4176	0.2	0.2	900.4488	0.2	0.2
843.4952	0.1	0.1	876.4184	0.5	0.5			

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3

4 **Peak list for α2,3 C9-azido-sialyllactose species**

m/z	I %	I % deconvolute	m/z	I %	I %	m/z	I %	I %
500.236	0.8	0.8	510.7623	0.7	0.7	520.2638	9.2	1
500.2775	1.8	1.8	510.7852	0.8	0.8	520.5976	6.6	1
500.351	0.9	0.9	511.2473	1.4	1.4	520.7365	1.1	1.1
500.753	1.5	1.5	511.3621	0.7	0.7	520.9318	3.4	3.4
501.2404	4.5	4.5	511.7458	0.7	0.7	521.2232	2.2	2.2
501.3085	1.5	1.5	512.2544	11.3	1	521.2658	2.3	2.3
501.7534	0.7	0.7	512.5888	8.4	1	521.3307	2.7	2.7
502.2343	1.8	1.8	512.9231	3.8	3.8	522.2256	0.8	0.8
502.2697	5.2	5.2	513.1917	0.7	0.7	522.2771	1.6	1.6
502.3192	17.4	1	513.2581	1.9	1.9	522.3267	1.7	1.7
502.4812	1.7	1.7	513.2944	0.9	0.9	522.7746	0.6	0.6
502.7494	4.6	4.6	514.2582	2.5	2.5	523.2489	1.8	1.8
503.2095	0.8	0.8	514.5552	4.4	4.4	523.3277	1.3	1.3
503.2527	4.2	4.2	514.5896	5.2	5.2	523.7544	1	1
503.3223	4.7	4.7	514.7224	7.6	7.6	524.2423	16	1
503.7614	1.7	1.7	514.7861	5.7	5.7	524.2983	1	1
504.2546	1.3	1.3	514.8894	6.5	6.5	524.4196	0.8	0.8
504.3243	1	1	514.9228	4.1	4.1	524.6195	0.7	0.7
504.5715	0.8	0.8	515.0558	4.5	4.5	524.7056	1.3	1.3
505.2451	1.8	1.8	515.2245	2.9	2.9	525.2544	3.1	3.1
505.9088	0.6	0.6	515.2544	2.3	2.3	525.5111	0.7	0.7
506.2638	3.3	3.3	515.287	3.2	3.2	525.764	3.4	3.4
506.7717	1.3	1.3	515.317	1	1	525.9092	1.4	1.4
507.2641	1.1	1.1	515.3899	1.1	1.1	526.2494	2.4	2.4
507.7694	1	1	515.5891	0.8	0.8	526.3003	1.4	1.4
507.8682	1	1	515.7877	1.2	1.2	526.7621	0.6	0.6
508.2039	1.1	1.1	516.2536	2	2	527.276	9.1	1
508.2507	1.9	1.9	516.3052	3.4	3.4	527.6106	7.5	1
508.2915	3.4	3.4	516.5821	0.6	0.6	527.734	1	1
508.585	1.1	1.1	516.7585	0.9	0.9	527.9443	4	4
508.7632	0.8	0.8	517.2545	2.1	2.1	528.224	3.6	1
508.7942	1.2	1.2	517.3027	8.3	8.3	528.2775	1.8	1.8
508.9168	1.1	1.1	517.7605	2.2	2.2	528.7249	1.9	1.9
509.248	1.6	1.6	518.2581	2.4	2.4	528.9065	1.2	1.2
510.2605	3.1	3.1	518.3032	2.1	2.1	529.2349	1	1
510.3606	2	2	518.7612	0.7	0.7	529.3718	3.9	1
510.73	0.9	0.9	519.1685	0.8	0.8	529.7604	7.8	1
			519.2605	1.1	1.1	530.2593	4.8	1
			519.7847	0.6	0.6	530.3256	5.7	1

530.3748	1.3	1.3	548.0653	1.6	1.6	574.2893	4.5	4.5
530.5558	0.7	0.7	548.2699	0.9	0.9	574.3502	1.2	1.2
530.6958	0.9	0.9	548.8511	0.7	0.7	574.6274	1.7	1.7
530.7603	2.1	2.1	548.9955	1	1	574.7833	3.8	3.8
530.8388	0.9	0.9	549.1382	0.8	0.8	574.9626	1.6	1.6
530.984	0.6	0.6	549.2609	9.2	1	575.2071	0.7	0.7
531.2744	3.2	1	549.7622	5	1	575.2898	3.8	3.8
531.307	3.1	3.1	550.2563	3.5	3.5	575.6119	80.4	1
531.7726	1.5	1.5	550.5018	1	1	575.7879	1.3	1.3
532.2699	1.5	1.5	550.602	1.4	1.4	575.9462	69.3	1
532.3091	1.1	1.1	550.7549	1.9	1.9	576.2373	0.6	0.6
532.607	0.9	0.9	550.9337	1.4	1.4	576.2821	42.4	1
532.756	2.6	2.6	551.2759	1.9	1.9	576.6147	13.3	1
532.9407	0.7	0.7	551.8177	3	3	576.7933	1.5	1.5
533.2508	2.3	2.3	552.2983	18.9	1	576.9487	3.8	3.8
533.321	0.9	0.9	552.6051	1.3	1.3	577.2816	3.7	3.7
533.7632	1.3	1.3	552.7633	0.6	0.6	577.6247	16.1	1
533.7994	8.1	8.1	552.82	0.6	0.6	577.9589	15.3	1
534.2994	8.7	8.7	552.9396	1	1	578.2923	8.7	1
534.7521	1	1	553.3009	5.8	1	578.6276	3	3
534.7999	1.4	1.4	554.2505	1.6	1.6	578.9608	0.8	0.8
534.9286	0.7	0.7	554.2995	1.3	1.3	579.2754	0.7	0.7
535.2561	1.5	1.5	554.5833	1.1	1.1	579.7914	0.7	0.7
535.3006	1.7	1.7	556.2995	0.8	0.8	580.3042	6	6
536.1944	1.8	1.8	557.2717	0.7	0.7	580.8047	1.1	1.1
536.2665	1.2	1.2	557.7575	1.3	1.3	581.295	2.8	2.8
536.3107	0.9	0.9	558.2598	1.6	1.6	581.5561	1.4	1.4
536.7341	0.9	0.9	558.3141	0.9	0.9	581.7973	0.9	0.9
537.1964	0.6	0.6	559.2714	1.3	1.3	581.8906	1.2	1.2
537.2633	1.3	1.3	559.3176	2.2	2.2	582.2265	0.7	0.7
537.7634	0.8	0.8	559.7771	0.7	0.7	582.2921	1.3	1.3
537.9178	0.7	0.7	560.2492	1	1	582.938	0.7	0.7
538.2585	7.8	1	560.3021	1.5	1.5	583.2696	0.9	0.9
539.2619	2.6	2.6	560.4367	0.6	0.6	583.3027	0.8	0.8
539.9289	0.9	0.9	560.9451	0.7	0.7	583.6008	0.6	0.6
540.264	1.6	1.6	561.3016	9.3	1	584.2726	0.8	0.8
541.2756	34.3	1	561.8112	1.8	1.8	584.3321	0.9	0.9
541.6049	0.6	0.6	562.3047	3	3	584.6068	3.2	3.2
541.7343	2.2	2.2	563.2289	1.3	1.3	584.9422	2.9	2.9
541.7771	18.9	1	563.3247	21.7	1	585.2983	43.6	1
541.9087	1.9	1.9	563.7457	0.7	0.7	585.3667	13	1
541.9554	1.5	1.5	564.275	1.1	1.1	585.6121	1	1
542.0755	1.8	1.8	564.3276	6.9	1	585.8	25.8	1
542.2381	2.1	2.1	565.2636	5.9	1	586.3012	11	1
542.2797	6.8	6.8	565.3095	3.5	3.5	586.3676	5	1
542.4094	0.8	0.8	565.7651	3.5	3.5	586.8004	4	4
542.627	0.7	0.7	565.8092	1.7	1.7	587.3027	1.2	1.2
542.7788	1.7	1.7	566.27	1.8	1.8	587.3473	4.8	4.8
543.2744	1	1	566.7738	0.8	0.8	588.2681	1.4	1.4
543.7553	5.2	1	567.2773	1.1	1.1	588.3306	27.8	1
543.9424	3	3	567.7768	1.1	1.1	588.5968	0.9	0.9
544.0594	0.9	0.9	568.2352	0.6	0.6	589.3309	9.4	1
544.2815	14.1	1	568.279	0.9	0.9	590.2829	4.6	4.6
544.61	1.2	1.2	568.7932	0.7	0.7	590.3303	2	2
544.7475	2.6	2.6	569.2728	1.1	1.1	590.7839	2.4	2.4
544.9117	4.7	4.7	569.6089	1	1	590.8125	1	1
545.0776	5	5	569.9413	1.3	1.3	591.2882	2	2
545.2474	3.8	3.8	570.2795	1.6	1.6	591.3167	3.6	3.6
545.2872	4.4	4.4	570.7323	1.1	1.1	592.2315	1.3	1.3
545.3595	0.6	0.6	570.7844	0.6	0.6	592.2842	0.7	0.7
545.4107	2.1	2.1	570.9335	0.8	0.8	592.3179	1	1
545.5814	1.1	1.1	571.2669	4.2	4.2	593.2474	1.2	1.2
545.7609	0.7	0.7	571.3057	1.8	1.8	593.3274	0.6	0.6
546.2702	4.4	4.4	571.596	0.8	0.8	593.5837	1.1	1.1
546.7705	2.3	2.3	572.2698	1.2	1.2	593.7955	0.8	0.8
547.2666	1.3	1.3	572.3029	0.9	0.9	593.9188	0.7	0.7
547.4627	2.2	2.2	572.3478	1.1	1.1	594.0222	0.7	0.7
547.5837	0.7	0.7	573.2888	1.4	1.4	594.2741	1.2	1.2
547.6639	2.6	2.6	573.3195	1.1	1.1	594.5247	0.7	0.7
547.8645	2.3	2.3	573.3538	1.2	1.2	595.2768	3	3

595.5968	0.8	0.8	623.3459	5.4	1	661.3869	1.1	1.1
596.2847	2.1	2.1	624.3137	1.6	1.6	662.2862	1	1
596.7902	0.8	0.8	624.3474	2	2	662.339	1.5	1.5
597.2886	1.3	1.3	624.8196	1.1	1.1	663.3207	2.9	2.9
597.4616	1	1	625.3026	0.8	0.8	664.2998	17.3	1
597.6285	1.2	1.2	625.7995	1.2	1.2	665.304	6.2	6.2
597.7935	1.1	1.1	626.2996	1	1	666.3398	10.5	1
598.3098	1.1	1.1	627.3771	5.6	1	667.343	4	4
599.3189	2.3	2.3	628.272	0.6	0.6	668.3447	1.2	1.2
599.6531	1.7	1.7	628.3788	1.8	1.8	670.305	6.4	1
599.9872	0.9	0.9	629.3847	0.8	0.8	670.8062	4.1	4.1
600.3389	1.3	1.3	629.8319	0.7	0.7	671.3082	2	2
601.2757	1.6	1.6	630.2414	0.9	0.9	671.8092	0.7	0.7
601.3619	11.2	1	630.3046	1.5	1.5	672.3982	1	1
601.791	0.7	0.7	630.3657	1.3	1.3	673.3563	1.4	1.4
602.2852	1.1	1.1	630.4913	0.9	0.9	674.3545	0.7	0.7
602.364	3.6	3.6	630.6159	0.6	0.6	675.9702	0.7	0.7
602.7912	0.9	0.9	631.3172	1.1	1.1	676.3073	1	1
602.9848	3.8	3.8	632.3393	6.2	1	677.3558	1.6	1.6
603.321	5.3	5.3	633.3436	2	2	678.3101	0.8	0.8
603.6528	2.1	2.1	634.3377	2.4	2.4	678.3555	1	1
603.9867	0.9	0.9	634.7881	0.9	0.9	679.3046	0.9	0.9
604.2726	0.7	0.7	635.2893	1.3	1.3	679.3716	3.5	3.5
604.3256	1.1	1.1	635.3434	0.8	0.8	680.3721	1.5	1.5
604.775	0.7	0.7	638.2947	0.8	0.8	680.4431	1.7	1.7
605.2714	0.6	0.6	638.3454	0.8	0.8	680.5897	2.8	2.8
605.7766	0.8	0.8	638.7958	0.7	0.7	680.7326	4.7	4.7
606.2792	0.6	0.6	639.3228	0.6	0.6	680.8732	4.8	4.8
607.2914	0.7	0.7	640.1603	0.8	0.8	681.0184	3.5	3.5
608.3111	3.3	3.3	640.3249	1.5	1.5	681.1616	2.3	2.3
608.9831	0.8	0.8	640.4939	0.8	0.8	681.305	1.5	1.5
609.2958	6.5	1	641.3	0.7	0.7	681.3415	4	4
609.3271	7.2	7.2	643.3394	13.1	1	681.4451	1	1
610.2976	2.1	2.1	643.4081	4.4	4.4	682.2989	1.2	1.2
610.3303	2.5	2.5	644.3444	4.9	4.9	682.3468	2.1	2.1
611.3018	0.8	0.8	644.3971	2	2	683.3511	0.7	0.7
611.3376	0.7	0.7	645.3506	1.8	1.8	684.0778	5.2	1
611.7547	0.7	0.7	645.8081	1.5	1.5	684.3283	8.8	1
613.2619	0.7	0.7	646.3113	1.3	1.3	684.5788	6.7	1
613.3044	10.8	10.8	646.3465	4.4	4.4	684.8289	4	4
613.7815	9.9	9.9	647.3482	1.9	1.9	685.0798	1.9	1.9
614.2863	6	6	648.3266	0.9	0.9	685.332	1	1
614.4029	3.7	3.7	648.8437	6.5	1	685.3935	3.8	3.8
614.7844	2.6	2.6	649.2761	0.8	0.8	685.4293	2.9	2.9
615.2965	1	1	649.3443	4.6	4.6	686.2622	0.6	0.6
615.4051	1.3	1.3	649.8459	1.8	1.8	686.358	0.7	0.7
615.8207	2.6	2.6	650.2881	0.7	0.7	686.4008	1.6	1.6
616.3289	2.1	2.1	650.3462	2.7	2.7	686.862	0.7	0.7
616.3724	4.5	4.5	650.844	2.1	2.1	687.3735	5.4	5.4
616.7975	0.8	0.8	651.3496	1.4	1.4	688.3842	2.2	2.2
617.2652	4.4	4.4	652.3183	2.7	2.7	689.3855	0.7	0.7
617.3345	2.2	2.2	652.8291	1	1	691.3247	2.4	2.4
617.3731	1.5	1.5	653.3238	1.3	1.3	692.3261	0.9	0.9
617.4654	6.7	1	653.4919	4.6	4.6	693.3521	0.7	0.7
617.6654	6.1	1	653.6914	9.3	1	694.3482	2	2
617.8662	4	4	653.7979	0.9	0.9	694.8071	15	15
618.0659	2.4	2.4	653.8205	0.9	0.9	695.3085	10.6	10.6
618.2667	1.4	1.4	653.8914	9.8	1	695.8097	4.5	4.5
618.3307	9.3	1	654.0914	7.8	1	696.3195	2.4	2.4
618.6436	0.8	0.8	654.2919	5.1	1	697.3258	0.9	0.9
618.8114	1.2	1.2	654.3683	0.9	0.9	700.3406	1.2	1.2
618.9781	1.6	1.6	654.4918	2	2	701.3499	0.6	0.6
619.1448	1	1	654.6924	1	1	701.4136	0.9	0.9
619.3196	11	1	655.2731	0.6	0.6	702.3709	1.1	1.1
620.2795	2.9	2.9	656.3919	0.8	0.8	703.3566	10.3	1
620.3243	3.8	3.8	658.3829	2	2	704.3609	4	4
620.7801	1.8	1.8	659.3274	1	1	705.3244	0.9	0.9
621.2868	1	1	659.3891	0.8	0.8	705.3601	1.2	1.2
621.3223	1.4	1.4	659.8298	0.9	0.9	705.7994	0.7	0.7
623.2957	3.8	3.8	660.3855	2.3	2.3	706.806	0.6	0.6

707.3455	22.1	1	768.8805	0.7	0.7	839.4011	1.9	1.9
708.3485	9.1	1	769.2836	0.9	0.9	839.5665	1.9	1.9
708.3952	1.1	1.1	769.3311	1.7	1.7	839.7327	1.4	1.4
709.3507	2.3	2.3	770.3329	0.8	0.8	839.8994	0.9	0.9
710.3772	3	3	771.3303	1.4	1.4	839.9852	0.7	0.7
710.8792	2.2	2.2	771.4663	2.5	2.5	840.153	0.7	0.7
711.3801	1	1	771.5796	2	2	840.3203	0.7	0.7
712.3273	2.5	2.5	771.8309	1.9	1.9	846.4594	1.7	1.7
713.3305	1	1	772.081	1.3	1.3	847.4629	0.9	0.9
714.3316	0.7	0.7	772.3318	0.8	0.8	851.4187	14.7	14.7
717.4177	0.7	0.7	772.4509	7.2	1	852.4218	6.6	6.6
718.1377	0.8	0.8	773.4507	4.1	4.1	852.8567	74.5	74.5
718.2648	0.7	0.7	774.4514	1.3	1.3	853.3582	61.1	61.1
719.3353	0.6	0.6	775.3682	1.5	1.5	853.4233	2	2
719.4863	1	1	775.4231	2.7	2.7	853.8595	30.8	30.8
719.629	1.6	1.6	776.4017	4.4	4.4	854.3609	10.9	10.9
719.7722	1.6	1.6	777.4039	1.8	1.8	854.8619	3.1	3.1
719.9145	1.1	1.1	778.3981	0.7	0.7	855.364	1	1
720.0574	0.7	0.7	786.4413	1.6	1.6	855.4866	3.3	3.3
720.1312	1.1	1.1	787.4399	1.2	1.2	856.4887	1.4	1.4
720.2734	1.6	1.6	793.3419	2.2	2.2	857.5126	6.6	6.6
720.4169	1.3	1.3	793.6872	3.2	3.2	858.4601	1	1
720.5594	1	1	793.8535	10.1	1	858.5158	3	3
720.7036	0.7	0.7	794.0201	16.8	1	859.5186	0.9	0.9
721.2644	0.9	0.9	794.1867	17.4	1	862.9138	15.5	1
721.7656	1	1	794.3534	14.7	1	863.4156	13.6	1
722.401	0.7	0.7	794.5205	9.3	1	863.8475	2.9	2.9
724.3475	1.4	1.4	794.6876	5	5	863.917	7.2	7.2
726.8516	2	2	794.8545	2.5	2.5	864.349	2.3	2.3
727.3524	1.5	1.5	795.0206	1.1	1.1	864.4182	2.6	2.6
727.8208	0.7	0.7	795.3819	35.1	1	864.8459	1.4	1.4
727.8519	0.6	0.6	796.385	14.4	1	864.919	0.8	0.8
729.2759	1.1	1.1	797.3873	3.8	3.8	865.3423	0.7	0.7
729.3263	1.3	1.3	798.3919	1	1	865.9338	4.4	4.4
729.6095	1.1	1.1	800.3846	0.7	0.7	866.4346	4.5	4.5
729.9443	0.6	0.6	800.4559	1.5	1.5	866.9366	2.4	2.4
730.3296	1.2	1.2	801.4759	7.5	1	867.438	0.9	0.9
737.3874	1.5	1.5	802.4789	3.1	3.1	869.3514	0.9	0.9
738.3351	5.5	5.5	802.839	0.7	0.7	871.8309	1.6	1.6
738.8451	0.7	0.7	803.0062	0.9	0.9	872.3323	1.4	1.4
739.3454	4.6	4.6	803.1729	0.7	0.7	872.8329	0.7	0.7
739.3929	0.8	0.8	803.4853	0.7	0.7	873.4006	1.3	1.3
740.3501	1.6	1.6	804.3817	1.7	1.7	873.9047	1.2	1.2
742.3254	35.5	1	805.3841	0.8	0.8	874.4062	1.4	1.4
742.3683	0.8	0.8	816.4399	13.6	1	874.8375	0.6	0.6
742.4504	0.7	0.7	816.612	1.5	1.5	875.4094	0.7	0.7
742.8268	26.3	1	816.8625	3	3	876.4085	1	1
743.3281	11.2	1	817.1124	3	3	876.4591	0.8	0.8
743.8295	3.8	3.8	817.3632	4.6	4.6	876.9166	1	1
743.9039	1.2	1.2	817.4418	7	7	877.4213	0.8	0.8
744.331	1.1	1.1	817.6122	1.3	1.3	878.4659	2.8	2.8
744.4269	1.9	1.9	817.8659	1	1	879.3127	1.8	1.8
745.4299	0.8	0.8	818.366	1	1	879.4139	1.9	1.9
746.3729	1.9	1.9	818.4437	2.2	2.2	879.4697	1.4	1.4
746.874	1.6	1.6	819.4383	0.7	0.7	879.8149	2	2
747.3755	1	1	820.3002	0.7	0.7	880.317	1.2	1.2
748.353	1.2	1.2	820.381	0.8	0.8	880.4191	0.7	0.7
749.357	0.7	0.7	820.4417	1.1	1.1	880.8176	0.8	0.8
751.3931	1.3	1.3	820.586	1.1	1.1	882.3899	0.6	0.6
753.316	1.2	1.2	820.7305	0.9	0.9	885.4201	2.9	2.9
753.8174	0.9	0.9	820.872	0.9	0.9	886.4237	1.4	1.4
760.4067	3.5	3.5	821.0152	0.7	0.7	887.487	5.6	5.6
761.3016	0.8	0.8	823.3876	3	3	888.4967	3	3
761.3977	1.3	1.3	824.3902	1.3	1.3	889.3688	1	1
762.4064	2.1	2.1	825.3921	0.8	0.8	889.503	1.2	1.2
763.4098	1.2	1.2	835.5087	0.7	0.7	889.8717	0.8	0.8
765.3808	0.7	0.7	838.4221	1	1	890.372	0.6	0.6
767.8782	1.8	1.8	839.0649	0.7	0.7	893.4317	1.4	1.4
768.3813	1.6	1.6	839.2321	1.4	1.4	894.4357	0.8	0.8
768.7829	0.8	0.8	839.345	0.6	0.6	903.973	0.9	0.9

Peak list for α2,6 C5-azido-sialyllactose species

m/z	I %	I % deconvolute
500.2871	1.7	1.7
500.7772	0.5	0.5
501.2495	1.1	1.1
501.2799	0.7	0.7
501.3401	0.6	0.6
501.5755	0.9	0.9
501.7542	0.4	0.4
501.7826	0.4	0.4
501.9098	0.6	0.6
502.3023	6.2	1
502.5095	0.4	0.4
502.5767	0.2	0.2
502.6026	0.2	0.2
502.7637	0.6	0.6
503.0053	0.2	0.2
503.1105	0.2	0.2
503.2606	1.3	1.3
503.3018	1.9	1.9
503.7718	2	1
504.2682	1.8	1.8
504.4006	0.2	0.2
504.4998	0.9	0.9
504.5454	0.2	0.2
504.5991	0.7	0.7
504.6888	0.2	0.2
504.7522	1.2	1.2
504.9307	0.4	0.4
505.0007	0.5	0.5
505.2565	3.5	1
505.5909	2.1	1
505.7486	0.2	0.2
505.9246	1.1	1.1
506.266	4.4	1
506.4587	0.2	0.2
506.5914	0.2	0.2
506.659	0.2	0.2
506.7783	2.5	1
506.8603	0.2	0.2
506.8909	0.7	0.7
507.226	0.8	0.8
507.2741	1.9	1.9
507.5612	0.3	0.3
507.783	0.9	0.9
508.256	4.6	1
508.281	2.6	1
508.7583	0.4	0.4
508.9358	0.9	0.9
508.9824	0.3	0.3
509.2676	1.7	1.7
509.6026	0.6	0.6
509.7565	0.2	0.2
509.9356	0.4	0.4
510.2643	1.2	1.2
510.2901	1.1	1.1
510.4137	0.2	0.2
510.5823	0.2	0.2
510.7439	0.5	0.5
510.7902	0.7	0.7
511.2618	1.1	1.1
511.4552	0.2	0.2
511.6073	0.7	0.7
511.7505	0.3	0.3
511.8999	0.3	0.3
511.9398	0.4	0.4
512.0605	0.2	0.2
512.2589	1.7	1.7
512.5964	0.9	0.9

m/z	I %	I % deconvolute
512.7523	0.3	0.3
512.7787	0.3	0.3
512.931	0.5	0.5
513.2324	9.9	1
513.2783	1.3	1.3
513.4828	10.8	1
513.7333	7.6	1
513.9247	0.2	0.2
513.9834	3.6	1
514.2358	1.7	1.7
514.28	1.5	1.5
514.484	0.6	0.6
514.5178	0.2	0.2
514.5629	5.1	1
514.7301	8.6	1
514.7894	1	1
514.897	7.7	1
515.0638	5.2	1
515.2317	2.9	1
515.2856	0.8	0.8
515.3318	1.4	1.4
515.3975	1.2	1.2
515.5654	0.6	0.6
515.7389	0.2	0.2
515.7847	0.4	0.4
516.2602	1.1	1.1
516.3139	1.7	1.7
516.5079	0.2	0.2
516.5906	0.5	0.5
516.7705	0.3	0.3
516.863	0.2	0.2
516.9232	0.3	0.3
517.0618	0.2	0.2
517.2602	1.6	1.6
517.3079	1.9	1.9
517.5243	1.5	1.5
517.5783	3.1	1
517.7713	2.1	1
517.9098	4	1
518.0257	0.9	0.9
518.2458	3.5	1
518.2988	0.8	0.8
518.5765	1.4	1.4
518.7694	0.5	0.5
518.91	0.6	0.6
519.2755	1.2	1.2
519.4918	0.3	0.3
519.7629	0.4	0.4
519.995	0.2	0.2
520.2556	3.2	1
520.5161	5.5	1
520.6064	0.3	0.3
520.7669	6.2	1
520.9393	0.2	0.2
521.0174	3.7	1
521.2672	2.9	1
521.3374	0.5	0.5
521.5183	0.7	0.7
521.6116	0.8	0.8
521.7672	0.4	0.4
521.9417	0.7	0.7
522.2852	1.3	1.3
522.3315	3.3	1
522.558	0.6	0.6
522.6043	0.2	0.2
522.7013	1.1	1.1
522.7841	0.6	0.6
522.8437	1.2	1.2
522.9403	0.2	0.2

m/z	I %	I % deconvolute
522.986	0.9	0.9
523.1305	0.6	0.6
523.2856	1.7	1.7
523.3345	1.1	1.1
523.417	0.2	0.2
523.5819	17.8	1
523.7768	0.7	0.7
523.9162	14.9	1
524.2527	15.3	1
524.4274	0.3	0.3
524.5837	3.4	1
524.7647	0.4	0.4
524.8287	0.2	0.2
524.9174	1.2	1.2
525.2678	4.7	1
525.6335	0.2	0.2
525.6545	0.2	0.2
525.7719	1.6	1.6
525.9174	0.7	0.7
526.201	0.3	0.3
526.2635	1.5	1.5
526.3	0.9	0.9
526.5185	0.3	0.3
526.5864	0.3	0.3
526.7704	0.7	0.7
526.9409	0.3	0.3
527.0153	0.3	0.3
527.2842	59.8	1
527.4585	0.2	0.2
527.5112	0.2	0.2
527.6185	49.6	1
527.7483	0.3	0.3
527.7797	0.8	0.8
527.9524	25.5	1
528.2316	3	1
528.283	22.4	1
528.6199	3.1	1
528.7325	1.6	1.6
528.7886	0.5	0.5
528.916	0.5	0.5
528.9531	0.9	0.9
529.175	0.5	0.5
529.2835	4.4	1
529.3431	1.6	1.6
529.3743	1.1	1.1
529.5084	0.4	0.4
529.582	0.3	0.3
529.7628	1.5	1.5
529.842	0.2	0.2
529.952	0.7	0.7
530.2699	1.2	1.2
530.3333	3.6	1
530.3769	0.4	0.4
530.6201	0.3	0.3
530.7638	0.7	0.7
531.2847	1.6	1.6
531.3286	1.7	1.7
531.6031	0.5	0.5
531.7803	0.7	0.7
531.9362	0.3	0.3
532.2745	1	1
532.3268	0.6	0.6
532.6154	0.9	0.9
532.7643	0.4	0.4
532.9497	0.8	0.8
533.2816	1.5	1.5
533.3298	0.6	0.6
533.5325	0.4	0.4
533.6159	0.2	0.2

533.7772	0.5	0.5	550.2616	4.5	1	565.7743	1.7	1.7
534.2795	1.8	1.8	550.5337	0.2	0.2	565.8181	1.2	1.2
534.7656	0.2	0.2	550.6102	0.9	0.9	566.026	0.4	0.4
535.2765	1	1	550.7622	2.6	1	566.2804	1.1	1.1
535.7765	0.4	0.4	550.9426	1	1	566.3139	0.8	0.8
536.1703	0.2	0.2	551.2694	1.3	1.3	566.7828	0.5	0.5
536.2625	1.9	1.9	551.609	0.3	0.3	567.2885	0.5	0.5
536.3185	0.4	0.4	551.7657	0.4	0.4	567.7848	0.3	0.3
536.6086	0.3	0.3	551.8259	0.3	0.3	568.3044	1.1	1.1
536.776	0.2	0.2	552.3043	0.8	0.8	568.6446	0.8	0.8
536.9426	0.2	0.2	552.6125	0.4	0.4	568.7956	0.2	0.2
537.2709	0.7	0.7	552.7576	0.3	0.3	568.8587	0.5	0.5
537.6292	0.2	0.2	552.9479	0.3	0.3	568.955	0.7	0.7
537.7923	0.3	0.3	553.2783	0.6	0.6	569.0578	0.4	0.4
537.9394	0.3	0.3	553.7643	0.6	0.6	569.2876	0.9	0.9
538.2902	7	1	554.273	0.5	0.5	569.3218	0.9	0.9
538.773	0.2	0.2	554.7044	0.2	0.2	569.4588	0.2	0.2
539.2921	2.4	1	554.772	0.3	0.3	569.6204	0.6	0.6
539.6018	0.2	0.2	555.2866	1.9	1.9	569.8239	0.2	0.2
539.7771	0.3	0.3	555.7882	1.1	1.1	569.9518	0.4	0.4
539.9364	0.8	0.8	555.9139	0.6	0.6	570.1474	0.2	0.2
540.2715	0.9	0.9	556.0389	1.4	1.4	570.2905	1.1	1.1
540.6044	0.3	0.3	556.1643	1.8	1.8	570.3232	0.4	0.4
540.768	0.3	0.3	556.2892	2.3	1	570.4347	0.2	0.2
541.2837	10.1	1	556.4156	1.1	1.1	570.7901	0.4	0.4
541.3429	0.3	0.3	556.54	0.6	0.6	571.2741	0.7	0.7
541.3702	0.2	0.2	556.6664	0.3	0.3	571.3157	1.1	1.1
541.5163	0.2	0.2	556.7496	0.4	0.4	571.6033	0.4	0.4
541.7397	2.6	1	556.7903	0.3	0.3	571.8046	0.3	0.3
541.7851	5.7	1	556.9222	0.2	0.2	571.9381	0.3	0.3
542.2426	1.5	1.5	557.2585	0.5	0.5	572.2933	1.9	1.9
542.2863	2.5	1	557.2961	0.6	0.6	572.3581	0.5	0.5
542.7452	0.5	0.5	557.3791	0.2	0.2	572.3746	0.5	0.5
542.785	0.9	0.9	557.8123	0.4	0.4	572.6271	1.6	1.6
542.8412	0.3	0.3	557.8123	0.2	0.2	572.8019	0.3	0.3
543.2434	0.5	0.5	558.2678	0.5	0.5	572.9604	1	1
543.2813	0.5	0.5	558.2978	0.5	0.5	573.2963	1.1	1.1
543.3222	0.3	0.3	558.3639	0.3	0.3	573.3386	4.5	1
543.3633	0.9	0.9	558.7934	0.4	0.4	573.6276	0.3	0.3
543.7665	0.6	0.6	559.2954	0.4	0.4	573.7918	0.2	0.2
544.0162	0.5	0.5	559.3483	2.6	1	573.9533	0.2	0.2
544.2872	1.8	1.8	560.3072	1.6	1.6	574.2967	0.9	0.9
544.3633	0.3	0.3	560.3492	0.9	0.9	574.3425	1.5	1.5
544.5169	0.5	0.5	560.6248	0.6	0.6	574.6201	0.3	0.3
544.7673	0.5	0.5	560.7739	0.2	0.2	574.7821	0.3	0.3
544.9329	0.6	0.6	560.9576	0.6	0.6	575.2174	0.3	0.3
545.3129	11	1	561.0309	0.2	0.2	575.2962	0.6	0.6
545.3676	0.8	0.8	561.252	1.3	1.3	575.6205	15.4	1
545.6005	0.5	0.5	561.3101	3.2	1	575.7827	0.5	0.5
545.6269	0.3	0.3	561.5322	0.2	0.2	575.9547	13.6	1
545.7646	0.2	0.2	561.5848	1	1	576.0314	0.3	0.3
545.9333	0.2	0.2	561.6261	0.3	0.3	576.2906	9.1	1
546.071	1	1	561.7882	0.4	0.4	576.6231	2.6	1
546.2754	2.2	1	561.8185	1.2	1.2	576.8032	0.6	0.6
546.3158	3.3	1	561.9186	0.5	0.5	576.9561	0.9	0.9
546.3684	0.3	0.3	561.9604	0.2	0.2	577.2859	1.7	1.7
546.472	1.2	1.2	562.3145	1.2	1.2	577.335	0.8	0.8
546.6723	0.8	0.8	562.6259	0.2	0.2	577.6314	0.5	0.5
546.7774	0.5	0.5	562.7915	0.2	0.2	577.798	0.2	0.2
546.8719	0.4	0.4	563.2431	0.3	0.3	577.9669	0.4	0.4
547.0717	0.2	0.2	563.3054	1.2	1.2	578.2913	0.7	0.7
547.3093	1.4	1.4	563.7565	0.2	0.2	578.7639	0.3	0.3
547.6156	0.3	0.3	564.1478	0.2	0.2	578.823	0.3	0.3
547.7783	0.2	0.2	564.2807	0.9	0.9	579.0165	0.2	0.2
547.9513	0.2	0.2	564.5226	0.3	0.3	579.2803	0.9	0.9
548.2872	1.2	1.2	564.7748	0.3	0.3	579.325	0.5	0.5
548.81	0.2	0.2	564.9789	0.2	0.2	579.6939	0.6	0.6
549.2722	1.9	1.9	565.2721	2.5	1	579.7768	0.5	0.5
549.7713	1	1	565.3159	3	1	579.8026	0.6	0.6
550.0329	0.3	0.3	565.5266	0.4	0.4	579.8938	0.9	0.9

580.0941	0.8	0.8	597.0961	0.4	0.4	612.4941	0.3	0.3
580.3092	1.7	1.7	597.2927	2.3	1	612.6961	0.2	0.2
580.4943	0.3	0.3	597.4943	0.2	0.2	612.802	0.2	0.2
580.8144	0.3	0.3	597.6956	0.2	0.2	612.84	0.2	0.2
581.303	1.4	1.4	597.7982	0.2	0.2	613.3115	0.5	0.5
581.8045	0.4	0.4	597.9012	0.4	0.4	613.7905	1.6	1.6
582.298	0.6	0.6	598.1013	0.4	0.4	614.2927	1.2	1.2
582.5478	3.3	1	598.2989	1.3	1.3	614.4117	1	1
582.6145	0.2	0.2	598.3627	0.2	0.2	614.7957	0.7	0.7
582.7988	4.2	1	598.5004	0.2	0.2	615.2987	0.7	0.7
582.9503	0.2	0.2	599.3368	17.9	1	615.3871	0.5	0.5
583.0493	2.7	1	599.3778	1.7	1.7	615.643	0.5	0.5
583.2996	1.7	1.7	599.6643	0.5	0.5	615.8032	0.3	0.3
583.5497	0.5	0.5	599.8383	10.5	1	615.9766	0.5	0.5
583.7723	0.2	0.2	599.9986	0.3	0.3	616.2749	0.8	0.8
583.801	0.3	0.3	600.2623	0.3	0.3	616.3058	0.6	0.6
584.2932	0.4	0.4	600.3396	4.3	1	616.3444	0.8	0.8
584.3214	0.7	0.7	600.382	0.6	0.6	616.3802	1	1
584.6164	1.7	1.7	600.8404	1.1	1.1	616.648	0.2	0.2
584.7644	0.5	0.5	600.9566	0.2	0.2	617.0467	0.3	0.3
584.796	0.2	0.2	601.2965	0.7	0.7	617.2739	6.3	1
584.9514	1.8	1.8	601.3695	1.3	1.3	617.3416	0.9	0.9
585.3049	3.8	1	601.801	0.4	0.4	617.474	9.6	1
585.375	6	1	601.9715	5.5	1	617.5488	0.3	0.3
585.6221	0.5	0.5	602.3058	5.6	1	617.6744	8.8	1
585.808	2.3	1	602.3638	1.4	1.4	617.7966	0.3	0.3
585.9568	0.2	0.2	602.6403	2.8	1	617.8749	6.1	1
586.305	2.3	1	602.8172	3.8	1	618.0751	3.1	1
586.3766	2.3	1	602.9933	25.8	1	618.2782	1.7	1.7
586.8051	1.1	1.1	603.3271	26.4	1	618.3389	3.9	1
587.3091	0.6	0.6	603.6617	14.3	1	618.4756	0.6	0.6
587.3555	1.5	1.5	603.8197	1	1	618.6352	0.5	0.5
587.8062	0.3	0.3	603.9955	6	1	618.6682	0.2	0.2
588.1331	0.5	0.5	604.3288	2.5	1	618.811	0.5	0.5
588.3052	1.3	1.3	604.671	0.6	0.6	618.9723	0.2	0.2
588.3389	7.3	1	604.7847	0.2	0.2	619.3307	2.8	1
588.4671	0.9	0.9	605.012	0.6	0.6	619.7959	0.2	0.2
588.6332	0.7	0.7	605.2798	0.5	0.5	620.2887	2.2	1
588.8005	0.6	0.6	605.3427	0.7	0.7	620.3293	2.5	1
588.966	0.3	0.3	605.7854	0.2	0.2	620.7889	1.2	1.2
589.3348	10.9	1	606.3061	1.1	1.1	620.967	0.2	0.2
590.2933	1.1	1.1	606.8135	2.9	1	621.2943	0.7	0.7
590.3367	3.2	1	607.0654	3.1	1	621.3314	1	1
590.5539	0.4	0.4	607.3158	2.7	1	621.7923	0.3	0.3
590.6292	0.2	0.2	607.5663	1.1	1.1	621.9819	0.4	0.4
590.7998	0.7	0.7	607.8126	1	1	622.0323	0.2	0.2
590.964	0.2	0.2	608.0678	0.2	0.2	622.3196	0.6	0.6
591.0557	0.4	0.4	608.3188	1.7	1.7	622.6503	0.3	0.3
591.2992	0.7	0.7	608.6587	0.5	0.5	622.8262	5.4	1
591.3297	0.8	0.8	608.8061	0.3	0.3	622.9813	0.2	0.2
591.7705	0.2	0.2	608.9925	0.3	0.3	623.3518	5.6	1
592.2937	0.4	0.4	609.3012	2	2	623.8243	1.8	1.8
593.3057	0.5	0.5	609.4822	1.6	1.6	624.1661	0.2	0.2
593.8071	0.3	0.3	609.6487	3.1	1	624.3226	1.6	1.6
594.2967	0.4	0.4	609.8157	3.4	1	624.3558	1.9	1.9
594.3374	1.1	1.1	609.9828	2.6	1	624.824	0.6	0.6
594.841	0.6	0.6	610.1502	1.6	1.6	625.0641	0.2	0.2
595.0563	0.2	0.2	610.3167	1.7	1.7	625.3075	0.4	0.4
595.2866	25.8	1	610.4844	0.4	0.4	625.3584	0.5	0.5
595.6911	0.8	0.8	610.6536	0.4	0.4	625.794	0.3	0.3
595.8005	0.2	0.2	610.7898	1	1	626.2962	0.4	0.4
595.8916	1.3	1.3	610.8225	0.4	0.4	626.8014	0.2	0.2
595.9675	0.3	0.3	610.9868	0.2	0.2	627.301	0.3	0.3
596.092	1	1	611.0391	1.1	1.1	627.3852	0.6	0.6
596.2904	9.1	1	611.2509	0.2	0.2	628.3219	0.3	0.3
596.4955	1.1	1.1	611.2909	1	1	628.4038	0.7	0.7
596.636	0.2	0.2	611.54	0.4	0.4	629.3495	0.4	0.4
596.6959	0.9	0.9	611.792	0.3	0.3	629.402	0.3	0.3
596.8961	0.6	0.6	612.0947	0.2	0.2	629.777	0.7	0.7
596.9879	0.2	0.2	612.296	0.5	0.5	629.8404	0.4	0.4

629.9897	0.3	0.3	652.3272	2.5	1	674.3589	0.3	0.3
630.2801	0.5	0.5	652.836	0.3	0.3	674.4182	0.2	0.2
630.3298	0.6	0.6	653.3262	1	1	675.2853	0.2	0.2
630.6569	0.2	0.2	653.8167	0.2	0.2	675.3469	0.5	0.5
630.7798	0.2	0.2	653.8367	0.2	0.2	675.406	0.3	0.3
631.3006	0.4	0.4	654.3192	0.4	0.4	675.8423	0.3	0.3
631.3409	0.6	0.6	655.2839	0.3	0.3	676.3522	0.4	0.4
631.6275	0.3	0.3	655.3207	0.2	0.2	677.3638	0.4	0.4
631.9632	0.2	0.2	655.577	0.2	0.2	678.3584	0.4	0.4
632.344	1.1	1.1	655.8277	0.4	0.4	679.3745	0.3	0.3
632.8271	0.3	0.3	656.0786	0.3	0.3	680.3423	0.5	0.5
633.0718	0.2	0.2	656.3265	0.3	0.3	680.4494	0.2	0.2
633.3317	3.1	1	656.4012	0.3	0.3	681.35	0.3	0.3
633.8328	1.9	1.9	656.8437	0.6	0.6	681.8274	0.2	0.2
634.3404	1.6	1.6	657.3435	0.6	0.6	682.3371	0.5	0.5
634.7982	0.2	0.2	657.4052	0.3	0.3	682.5872	0.5	0.5
634.8369	0.3	0.3	657.8387	0.4	0.4	682.8369	0.4	0.4
635.1854	0.8	0.8	658.0006	0.2	0.2	683.0882	0.2	0.2
635.3294	2.1	1	658.3915	5.5	1	683.3327	0.3	0.3
635.4717	2.4	1	659.3432	0.7	0.7	683.9727	3.7	1
635.6153	2	1	659.3942	1.9	1.9	684.3071	4.1	1
635.7583	1.4	1.4	659.7007	0.2	0.2	684.6407	2.8	1
635.9017	0.8	0.8	659.8436	0.4	0.4	684.9747	1.3	1.3
636.0443	0.4	0.4	659.9009	0.4	0.4	685.3087	0.7	0.7
636.1887	0.2	0.2	660.1011	0.4	0.4	685.403	1.8	1.8
636.3018	0.3	0.3	660.3686	4.1	1	685.4355	0.9	0.9
636.3481	0.6	0.6	660.8572	1	1	685.6423	0.2	0.2
636.8098	0.2	0.2	661.2998	0.3	0.3	686.2721	0.3	0.3
637.3396	0.4	0.4	661.3703	1.5	1.5	686.3691	1.3	1.3
637.6473	0.2	0.2	661.8223	0.2	0.2	686.413	0.8	0.8
637.8237	1.1	1.1	661.8547	0.2	0.2	686.6045	0.2	0.2
637.9813	0.2	0.2	662.2942	0.8	0.8	686.87	0.8	0.8
638.2863	0.4	0.4	662.3551	0.9	0.9	687.3809	1.6	1.6
638.3232	1	1	662.6879	0.3	0.3	688.3973	0.9	0.9
638.8203	0.5	0.5	662.7972	0.2	0.2	688.8243	5.1	1
639.0669	0.2	0.2	662.8491	0.5	0.5	689.326	3.8	1
639.3247	0.4	0.4	663.0243	0.2	0.2	689.3891	0.6	0.6
639.345	0.5	0.5	663.3313	0.8	0.8	689.6961	0.6	0.6
639.6447	0.2	0.2	663.8494	0.2	0.2	689.8272	1.5	1.5
639.981	0.2	0.2	664.309	4.1	1	690.0304	0.7	0.7
640.323	0.4	0.4	664.3452	2.1	1	690.3296	0.7	0.7
641.3239	0.2	0.2	664.6609	0.3	0.3	690.3613	0.7	0.7
641.3622	0.3	0.3	664.8439	0.2	0.2	690.4027	0.4	0.4
642.3196	0.3	0.3	665.0004	0.3	0.3	690.6968	0.2	0.2
642.359	0.5	0.5	665.1713	0.3	0.3	690.8277	0.3	0.3
642.8324	0.3	0.3	665.3126	1.4	1.4	691.329	0.4	0.4
643.2202	0.2	0.2	666.3484	1.7	1.7	692.3611	1.7	1.7
643.347	1.5	1.5	667.3105	0.3	0.3	692.6542	0.3	0.3
643.4153	0.3	0.3	667.3497	0.6	0.6	692.8616	1	1
644.3563	0.6	0.6	668.3132	0.5	0.5	692.9892	0.2	0.2
644.4329	0.3	0.3	668.3509	0.3	0.3	693.3643	0.6	0.6
644.8397	1.9	1.9	668.8146	0.3	0.3	693.6853	1.8	1.8
645.3425	1.5	1.5	669.3505	0.4	0.4	693.8614	0.2	0.2
645.8247	0.5	0.5	669.6804	0.4	0.4	694.0194	1.9	1.9
646.3543	1.4	1.4	670.0132	0.2	0.2	694.3551	7.6	1
646.6136	0.2	0.2	670.3147	2	1	694.6869	0.6	0.6
646.8205	0.3	0.3	670.3956	3.7	1	==694.8168==	5.1	5.1
647.3116	2.3	1	670.816	1.3	1.3	695.0213	0.2	0.2
647.3535	1	1	671.3297	0.6	0.6	==695.3184==	3.6	3.6
647.7126	0.2	0.2	671.3998	1.2	1.2	695.3575	2.4	2.4
647.8129	1.4	1.4	671.8333	0.3	0.3	==695.8199==	1.5	1.5
648.3165	0.8	0.8	672.331	0.5	0.5	696.3698	4.4	4.4
648.8528	1.4	1.4	672.4038	0.4	0.4	696.8236	0.2	0.2
649.3401	1.3	1.3	672.6646	0.3	0.3	697.3185	0.3	0.3
649.8387	0.8	0.8	672.8207	0.2	0.2	697.3727	1.5	1.5
650.0521	0.2	0.2	672.999	0.2	0.2	697.8155	0.2	0.2
650.3605	1	1	673.3328	0.3	0.3	698.3756	0.5	0.5
650.8483	0.3	0.3	673.3663	0.6	0.6	698.8449	0.2	0.2
651.3519	1.2	1.2	673.3966	0.3	0.3	699.354	0.2	0.2
651.9954	0.2	0.2	674.3028	0.2	0.2	699.4052	0.3	0.3

700.3516	0.3	0.3	722.8575	0.3	0.3	747.3342	0.7	0.7
701.0048	0.6	0.6	723.3601	0.3	0.3	747.3686	0.3	0.3
701.3563	1	1	724.3636	0.5	0.5	747.7059	0.2	0.2
701.4226	0.4	0.4	724.6141	0.5	0.5	747.8422	0.5	0.5
701.6741	0.5	0.5	724.8646	0.5	0.5	748.3624	0.6	0.6
701.8377	0.2	0.2	725.0179	0.2	0.2	748.8536	0.2	0.2
701.8753	0.6	0.6	725.1162	0.3	0.3	749.3847	0.4	0.4
702.0098	0.2	0.2	725.3502	3.6	1	749.4259	0.3	0.3
702.3264	0.6	0.6	725.6856	0.2	0.2	750.3878	0.2	0.2
702.3729	0.7	0.7	725.8496	0.2	0.2	750.7383	0.2	0.2
702.4204	0.2	0.2	726.3526	1.4	1.4	750.9393	0.2	0.2
702.8266	0.3	0.3	727.3582	0.4	0.4	751.1422	0.2	0.2
703.3647	0.5	0.5	728.3707	2.2	1	751.344	0.2	0.2
703.4327	0.3	0.3	728.8718	1.6	1.6	751.4014	0.5	0.5
703.843	0.2	0.2	729.2862	0.5	0.5	752.3927	0.4	0.4
704.3837	0.3	0.3	729.3719	0.9	0.9	752.7257	0.3	0.3
705.3396	0.8	0.8	729.4266	0.3	0.3	753.3928	0.2	0.2
705.5575	0.4	0.4	729.6191	0.4	0.4	754.3585	0.3	0.3
705.7583	0.6	0.6	729.8722	0.3	0.3	755.3566	0.2	0.2
705.842	0.5	0.5	729.9535	0.3	0.3	756.3988	0.3	0.3
705.9588	0.7	0.7	730.3462	0.2	0.2	757.3807	0.6	0.6
706.1593	0.5	0.5	730.3801	0.2	0.2	757.8806	0.4	0.4
706.3526	0.5	0.5	730.418	0.3	0.3	758.3824	0.3	0.3
706.5588	0.2	0.2	731.1764	0.8	0.8	758.4802	1.2	1.2
706.8237	0.3	0.3	731.3776	1.7	1.7	759.4388	1.5	1.5
707.3591	15	1	731.5773	1.8	1.8	759.4817	0.5	0.5
708.3617	5.5	1	731.7778	1.4	1.4	759.8315	0.2	0.2
709.3639	1.4	1.4	731.9767	0.9	0.9	760.331	0.2	0.2
710.3852	1.7	1.7	732.1785	0.4	0.4	760.4206	1	1
710.8227	0.2	0.2	732.3814	0.4	0.4	761.3248	0.4	0.4
710.8886	1.2	1.2	733.3812	0.3	0.3	761.4117	0.4	0.4
711.3251	0.3	0.3	734.3767	0.2	0.2	762.4124	0.2	0.2
711.3853	0.7	0.7	735.3742	0.7	0.7	762.8991	0.4	0.4
711.8901	0.2	0.2	736.3298	0.7	0.7	763.3978	0.5	0.5
712.3364	0.9	0.9	736.3774	0.3	0.3	763.8983	0.3	0.3
712.3847	0.2	0.2	737.338	0.3	0.3	764.379	0.7	0.7
713.0405	0.3	0.3	737.3965	1.1	1.1	765.13	0.2	0.2
713.3402	0.5	0.5	738.3442	2.5	1	765.387	0.8	0.8
713.3768	0.4	0.4	738.3982	0.4	0.4	766.3997	0.4	0.4
713.7098	0.2	0.2	739.3544	1.8	1.8	767.3899	0.2	0.2
713.7903	0.2	0.2	740.3591	0.6	0.6	767.8872	0.2	0.2
713.8424	0.3	0.3	740.8809	0.9	0.9	768.3899	0.3	0.3
713.8839	0.4	0.4	741.0483	2.1	1	769.3419	0.2	0.2
714.3437	0.4	0.4	741.2153	2.7	1	771.3394	1.8	1.8
714.3828	0.5	0.5	741.3836	2.8	1	771.4742	0.2	0.2
714.8155	0.3	0.3	741.5495	1.6	1.6	771.5899	3	1
714.8825	0.2	0.2	741.7165	1	1	771.8405	2.7	1
715.3121	0.2	0.2	741.8897	1.1	1.1	772.0907	1.8	1.8
715.3485	0.2	0.2	742.0512	0.2	0.2	772.3411	1	1
715.3884	0.2	0.2	742.3354	4.9	1	772.4595	2.1	1
716.3354	0.8	0.8	742.3924	0.6	0.6	772.5918	0.4	0.4
716.4322	0.7	0.7	742.4591	0.3	0.3	772.6326	0.2	0.2
716.8368	0.5	0.5	742.8367	3.6	1	772.843	0.2	0.2
717.3404	0.3	0.3	742.8943	0.2	0.2	773.4555	6.4	1
717.4302	0.5	0.5	743.3388	1.6	1.6	773.8772	0.2	0.2
718.277	0.2	0.2	743.3999	0.6	0.6	774.4064	0.3	0.3
718.3484	0.2	0.2	743.4629	0.2	0.2	774.4587	2.6	1
718.397	0.2	0.2	743.8362	0.6	0.6	775.3763	0.4	0.4
719.3473	0.4	0.4	744.3623	0.4	0.4	775.4384	1.1	1.1
719.4956	0.2	0.2	744.4018	0.4	0.4	776.407	1.8	1.8
719.6396	0.3	0.3	744.4366	0.5	0.5	776.7277	1	1
719.7832	0.3	0.3	744.6118	0.5	0.5	777.0623	0.7	0.7
719.9252	0.2	0.2	744.8621	0.4	0.4	777.4113	1	1
720.1402	0.2	0.2	745.115	0.4	0.4	778.414	0.4	0.4
720.2848	0.3	0.3	745.3669	0.5	0.5	779.4103	0.2	0.2
720.3605	0.3	0.3	745.4121	0.2	0.2	781.3964	0.2	0.2
720.4198	0.3	0.3	745.6171	0.3	0.3	782.3976	0.2	0.2
720.571	0.2	0.2	745.863	0.2	0.2	783.3786	0.5	0.5
721.3717	0.3	0.3	746.3757	0.2	0.2	783.8806	0.3	0.3
722.3923	0.2	0.2	746.4059	0.3	0.3	784.3804	0.2	0.2

m/z	I %	I % deconvolute	m/z	I %	I %	m/z	I %	I %
784.867	3.1	1	809.7515	0.2	0.2	849.4512	0.2	0.2
785.3685	2.5	1	810.4435	0.3	0.3	850.4452	0.2	0.2
785.8696	1.3	1.3	814.0448	0.2	0.2	851.429	1.5	1.5
786.3691	0.6	0.6	814.3811	0.4	0.4	852.4292	0.7	0.7
786.46	0.6	0.6	814.5251	0.2	0.2	853.4276	0.3	0.3
786.869	0.2	0.2	814.7141	0.2	0.2	855.496	0.5	0.5
787.45	0.7	0.7	815.393	0.2	0.2	856.498	0.2	0.2
788.3719	0.3	0.3	816.4031	0.2	0.2	857.5213	0.4	0.4
788.4247	0.5	0.5	816.4495	0.4	0.4	857.9333	0.3	0.3
788.8715	0.2	0.2	817.7454	1.1	1.1	858.4367	0.3	0.3
789.4154	0.3	0.3	817.8937	0.2	0.2	858.5249	0.2	0.2
790.3529	0.2	0.2	817.9413	0.5	0.5	858.936	0.2	0.2
790.4205	2.4	1	818.4475	0.6	0.6	860.4246	0.3	0.3
790.9222	1.9	1.9	819.4404	0.4	0.4	860.8651	1.5	1.5
791.4227	1	1	820.3115	0.2	0.2	861.3663	1.3	1.3
791.9231	0.4	0.4	820.4478	0.4	0.4	861.8683	0.6	0.6
792.3636	0.2	0.2	820.5973	0.3	0.3	862.3695	0.3	0.3
792.4209	0.2	0.2	820.7397	0.3	0.3	862.4769	0.2	0.2
793.2573	0.3	0.3	820.9191	0.5	0.5	862.9247	3.1	3.1
793.3523	0.5	0.5	821.4217	0.5	0.5	863.4267	3.2	3.2
793.4123	1.7	1.7	821.9221	0.2	0.2	863.9278	1.4	1.4
793.7583	0.2	0.2	822.3652	0.4	0.4	864.4296	0.8	0.8
793.8649	0.2	0.2	822.409	0.3	0.3	864.9283	0.2	0.2
794.0307	0.3	0.3	823.1145	0.2	0.2	865.4477	0.2	0.2
794.1984	0.2	0.2	823.3974	1.1	1.1	866.4498	0.2	0.2
794.361	0.4	0.4	824.3993	0.5	0.5	874.422	0.2	0.2
794.4156	0.9	0.9	824.8759	0.2	0.2	876.4192	0.6	0.6
795.3933	1	1	825.4039	0.4	0.4	876.469	0.6	0.6
795.4346	0.8	0.8	825.9071	0.2	0.2	876.9203	0.6	0.6
796.3958	0.5	0.5	826.4077	0.2	0.2	877.4235	0.4	0.4
796.4378	0.3	0.3	828.4344	0.2	0.2	877.4707	0.3	0.3
797.4016	0.2	0.2	829.4271	0.2	0.2	878.476	1.4	1.4
797.804	0.2	0.2	831.4228	0.2	0.2	879.4251	0.3	0.3
798.0032	0.2	0.2	832.4335	0.7	0.7	879.4788	0.6	0.6
798.3685	0.4	0.4	833.4367	0.4	0.4	880.482	0.2	0.2
798.403	0.2	0.2	834.4452	0.3	0.3	881.9003	0.2	0.2
798.8692	0.3	0.3	835.3971	0.2	0.2	882.1954	0.2	0.2
799.3752	0.4	0.4	836.4635	0.2	0.2	882.4441	0.2	0.2
800.3814	0.2	0.2	837.4947	0.3	0.3	885.4325	0.3	0.3
800.4646	0.2	0.2	839.2432	0.4	0.4	886.4331	0.2	0.2
800.8465	0.5	0.5	839.4112	0.5	0.5	887.4975	1.7	1.7
801.3476	0.4	0.4	839.5772	0.5	0.5	888.5041	0.9	0.9
801.4849	1	1	839.7441	0.4	0.4	888.855	0.4	0.4
801.8484	0.2	0.2	839.9097	0.2	0.2	889.056	0.8	0.8
802.482	1.9	1.9	840.1623	0.2	0.2	889.2563	1	1
803.4841	0.7	0.7	840.3264	0.2	0.2	889.4573	1	1
804.3516	0.2	0.2	840.4142	0.3	0.3	889.5076	0.3	0.3
804.3932	0.5	0.5	840.4898	0.2	0.2	889.6566	0.6	0.6
804.4496	0.8	0.8	841.3714	0.3	0.3	889.8586	0.4	0.4
805.3965	0.3	0.3	841.4183	0.2	0.2	890.0578	0.2	0.2
805.4523	0.4	0.4	841.8718	0.2	0.2	891.4636	0.3	0.3
806.3812	0.2	0.2	843.4957	0.2	0.2	892.4295	0.3	0.3
807.439	6.8	1	844.4808	1.1	1.1	893.4358	0.2	0.2
808.4421	3	1	845.4834	0.6	0.6	895.4166	0.2	0.2
808.7488	0.5	0.5	846.4731	0.5	0.5	898.439	0.2	0.2
809.0835	0.5	0.5	847.4479	1	1	898.4879	0.2	0.2
809.4408	1	1	848.4499	0.5	0.5	900.4486	0.4	0.4

7

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9 **Peak list for α2,6 C9-azido-sialyllactose**

m/z	I %	I % deconvolute	m/z	I %	I %	m/z	I %	I %
500.2349	0.7	0.7	501.3061	0.9	0.9	503.2519	2.2	2.2
500.2762	1.8	1.8	501.3338	0.9	0.9	503.3223	3.4	3.4
500.35	0.5	0.5	501.7543	0.7	0.7	503.7634	1	1
500.7527	1.9	1.9	502.2674	2.6	2.6	504.2491	1.2	1.2
501.2405	4	4	502.319	12.4	5	504.3238	0.7	0.7
			502.7471	1	1	504.5714	0.8	0.8
			502.7661	1	1	504.7458	0.5	0.5

504.905	0.7	0.7	523.3273	0.8	0.8	542.4085	0.5	0.5
505.2444	1.4	1.4	523.7571	1	1	542.626	0.6	0.6
505.7355	0.6	0.6	524.243	7.2	1	542.7776	1.1	1.1
505.9067	0.5	0.5	524.297	0.8	0.8	543.2734	0.6	0.6
506.2686	2.4	2.4	524.4187	0.5	0.5	543.7555	1.9	1.9
506.7747	1.2	1.2	524.6192	0.5	0.5	543.9415	3.6	3.6
507.2082	1.1	1.1	524.7052	1	1	544.0586	0.5	0.5
507.268	0.9	0.9	525.2528	1.6	1.6	544.2802	9.4	1
507.7742	1.1	1.1	525.5106	0.8	0.8	544.6101	1.6	1.6
507.8677	0.5	0.5	525.762	1.6	1.6	544.745	1.9	1.9
508.2054	0.7	0.7	525.9089	1.6	1.6	544.7745	0.7	0.7
508.2479	3	3	526.0126	0.5	0.5	544.9106	3.3	3.3
508.2896	2.2	2.2	526.2458	2.1	2.1	545.077	3.6	3.6
508.5848	1.2	1.2	526.2988	0.9	0.9	545.2466	2.8	2.8
508.7661	0.5	0.5	526.5779	0.7	0.7	545.2881	2.9	2.9
508.7931	0.9	0.9	527.2756	11.7	1	545.36	0.5	0.5
508.9163	1.3	1.3	527.6101	9.6	1	545.4104	1.4	1.4
509.2485	1.9	1.9	527.7342	0.6	0.6	545.5794	0.8	0.8
510.2583	1.8	1.8	527.9439	4.8	4.8	545.7635	0.6	0.6
510.3597	1.4	1.4	528.2227	2.8	2.8	546.2703	2.2	2.2
510.7851	1.4	1.4	528.277	2.2	2.2	546.7699	1.1	1.1
511.2483	0.8	0.8	528.6117	0.6	0.6	547.2635	0.7	0.7
511.283	1.1	1.1	528.7245	1.5	1.5	547.4632	1.2	1.2
511.7472	0.5	0.5	529.2383	0.6	0.6	547.6635	1.6	1.6
512.254	4.7	4.7	529.3691	3.9	3.9	547.8635	1.3	1.3
512.5879	3.4	3.4	529.7599	4	4	548.0652	0.7	0.7
512.7435	0.5	0.5	530.2587	2.6	2.6	548.2698	0.7	0.7
512.7797	0.6	0.6	530.3245	3.6	3.6	548.8521	0.6	0.6
512.9223	1.6	1.6	530.3728	1.1	1.1	548.9947	0.7	0.7
513.2537	0.9	0.9	530.6954	0.6	0.6	549.2604	7.1	1
513.2829	0.9	0.9	530.7605	1.1	1.1	549.7619	4	4
513.743	0.6	0.6	531.2796	2.1	2.1	550.2577	2.2	2.2
514.2587	3.4	3.4	531.306	2.2	2.2	550.5016	0.7	0.7
514.555	2.2	2.2	531.7724	1	1	550.6016	1.2	1.2
514.5886	6.7	1	532.2682	1.1	1.1	550.7553	1.1	1.1
514.7222	3.7	3.7	532.306	0.9	0.9	550.9351	1.1	1.1
514.7854	2	2	532.6058	0.7	0.7	551.281	1.2	1.2
514.8888	3.4	3.4	532.7552	3.6	3.6	551.8171	1.6	1.6
514.9223	5.2	1	532.9393	0.5	0.5	552.2976	8.8	1
515.0557	2.5	2.5	533.2548	2.4	2.4	552.604	0.8	0.8
515.2261	1.4	1.4	533.287	2	2	552.7496	0.7	0.7
515.2549	2.6	2.6	533.7641	1.2	1.2	552.9386	0.7	0.7
515.2859	1.2	1.2	533.7978	4	4	553.2995	2.5	2.5
515.3157	1.1	1.1	534.2987	4.9	4.9	554.2497	1.2	1.2
515.3899	0.5	0.5	534.7986	0.9	0.9	554.2935	0.7	0.7
515.5893	1	1	534.9267	0.6	0.6	554.5825	0.8	0.8
515.7836	0.5	0.5	535.2572	1.5	1.5	554.9161	0.6	0.6
516.2508	1.8	1.8	535.3005	1.1	1.1	555.2511	0.6	0.6
516.3014	2	2	535.5941	0.5	0.5	557.2546	0.7	0.7
516.5821	0.9	0.9	536.1938	0.9	0.9	557.7565	0.6	0.6
516.916	0.5	0.5	536.2741	1	1	557.7915	1.2	1.2
517.2508	2	2	537.2643	1	1	558.2582	0.7	0.7
517.3012	5.1	1	537.51	0.7	0.7	558.2939	0.9	0.9
517.7598	1.6	1.6	537.7622	0.8	0.8	558.7876	0.7	0.7
518.2565	1.7	1.7	537.9211	0.6	0.6	559.2763	0.9	0.9
518.301	1.3	1.3	538.2578	5.2	1	559.3162	1.5	1.5
518.7607	0.6	0.6	538.7591	0.5	0.5	559.7783	0.5	0.5
519.2581	0.8	0.8	539.2625	2	2	560.2504	0.6	0.6
520.2632	11.7	1	539.7717	0.6	0.6	560.2954	1.3	1.3
520.597	9.3	1	539.9282	0.8	0.8	560.4377	0.5	0.5
520.7367	0.6	0.6	540.2603	1.5	1.5	560.5488	0.5	0.5
520.9311	4.2	4.2	540.7556	0.9	0.9	560.7803	0.5	0.5
521.2213	2.2	2.2	541.2751	18.7	1	561.3031	8.6	1
521.2652	2.4	2.4	541.7377	0.8	0.8	561.81	3	3
521.3302	1.9	1.9	541.7764	10.9	1	562.3075	2.7	2.7
522.225	0.7	0.7	541.9085	1.2	1.2	563.2266	0.7	0.7
522.2785	1.6	1.6	541.9568	1.2	1.2	563.3241	7.7	1
522.3279	0.8	0.8	542.0749	1.4	1.4	564.274	0.7	0.7
522.7775	0.9	0.9	542.2404	1.4	1.4	564.327	2.4	2.4
523.2508	1.8	1.8	542.2797	3.8	3.8	565.2633	3.5	3.5

565.3067	2.8	2.8	588.3298	17.6	1	616.7968	0.5	0.5
565.765	2	2	588.5959	0.6	0.6	617.2648	2.4	2.4
565.807	1.4	1.4	589.3304	6.3	1	617.3346	1.7	1.7
566.2692	1.1	1.1	590.2817	3	3	617.3711	0.9	0.9
566.7725	0.5	0.5	590.3289	1.4	1.4	617.4647	3.3	3.3
567.2773	0.7	0.7	590.7832	1.7	1.7	617.665	3.1	3.1
568.283	0.5	0.5	591.2842	1.4	1.4	617.8653	2	2
568.794	0.7	0.7	591.3159	2	2	618.0659	1.2	1.2
569.269	0.6	0.6	592.2311	0.8	0.8	618.2654	0.9	0.9
569.6083	0.7	0.7	592.2758	0.7	0.7	618.3305	6.9	1
569.9402	0.7	0.7	592.3111	0.5	0.5	618.644	0.5	0.5
570.2814	1.4	1.4	593.2487	0.7	0.7	618.8088	0.7	0.7
570.7316	0.7	0.7	593.5836	0.7	0.7	618.9772	0.8	0.8
570.7843	0.7	0.7	593.795	1.1	1.1	619.1445	0.6	0.6
571.2654	3	3	594.2742	0.7	0.7	619.3197	7.2	1
571.3033	1.1	1.1	594.291	0.7	0.7	619.7899	0.5	0.5
571.5954	0.9	0.9	595.2769	5.8	1	620.2793	1.5	1.5
572.2687	1.2	1.2	595.5962	1	1	620.3235	2.7	2.7
572.3023	0.8	0.8	595.9319	0.8	0.8	620.7799	1	1
572.3468	0.7	0.7	596.2813	2.4	2.4	621.2925	0.6	0.6
572.8026	0.5	0.5	596.7872	0.5	0.5	621.3215	1.1	1.1
573.287	1.2	1.2	597.2843	1.1	1.1	623.2958	2	2
573.3192	1	1	597.4619	0.6	0.6	623.3453	4	4
573.621	0.7	0.7	597.6274	0.7	0.7	624.3097	0.7	0.7
574.2889	3.2	3.2	597.7961	0.7	0.7	624.3473	1.4	1.4
574.349	1	1	598.2612	0.5	0.5	624.8201	0.5	0.5
574.6245	0.7	0.7	598.3115	0.9	0.9	625.7993	0.6	0.6
574.7829	2.2	2.2	599.3188	2	2	626.2983	0.5	0.5
574.9606	0.5	0.5	599.6526	1.4	1.4	627.377	4.3	4.3
575.2894	2.4	2.4	599.9864	0.8	0.8	628.379	1.6	1.6
575.6114	43	1	600.3383	0.9	0.9	629.3777	0.6	0.6
575.7865	0.7	0.7	601.2804	0.9	0.9	629.8297	1	1
575.9456	38.2	1	601.3615	12.9	1	630.2397	0.7	0.7
576.2819	25.3	1	601.7917	0.7	0.7	630.3331	1	1
576.6143	7.4	1	602.2884	1.1	1.1	630.3714	1	1
576.7912	0.9	0.9	602.3632	3.9	3.9	630.4906	0.6	0.6
576.9477	2.2	2.2	602.7904	0.9	0.9	630.6157	0.6	0.6
577.2823	2.7	2.7	602.9842	5	5	631.3183	1.5	1.5
577.6241	21.6	1	603.3191	5.9	1	632.3374	4	4
577.9585	19.6	1	603.6524	2.7	2.7	633.3395	1.5	1.5
578.2921	10.9	1	603.9862	1.1	1.1	634.3358	1.9	1.9
578.6266	3.9	3.9	604.2697	0.7	0.7	634.788	0.6	0.6
578.9598	1.1	1.1	604.3226	1	1	634.83	0.5	0.5
579.2896	0.5	0.5	604.772	0.5	0.5	635.2885	0.9	0.9
579.3171	0.6	0.6	605.2701	0.6	0.6	635.3401	0.7	0.7
579.7923	0.9	0.9	605.3319	0.5	0.5	636.3423	0.7	0.7
580.3038	2.9	2.9	605.7768	1	1	638.2369	0.5	0.5
580.8063	0.5	0.5	606.2796	0.8	0.8	638.3082	0.6	0.6
581.2942	2.8	2.8	607.2923	0.6	0.6	638.346	0.7	0.7
581.5561	0.7	0.7	608.3102	2.1	2.1	638.4569	0.7	0.7
581.7966	1.2	1.2	608.7945	0.5	0.5	638.5681	0.7	0.7
581.8915	0.6	0.6	608.9826	0.6	0.6	638.6793	0.6	0.6
582.2935	1	1	609.2951	4.3	4.3	638.7949	0.5	0.5
583.2714	0.6	0.6	609.3261	4.1	4.1	640.1594	0.7	0.7
583.3003	0.6	0.6	610.2985	1.4	1.4	640.3248	1	1
584.2761	0.7	0.7	610.3281	1.4	1.4	640.4926	0.6	0.6
584.3304	0.5	0.5	611.2977	0.5	0.5	642.8229	0.5	0.5
584.6065	1.2	1.2	611.3383	0.5	0.5	643.3382	4.8	4.8
584.944	1.9	1.9	612.2598	0.5	0.5	643.4071	2.3	2.3
585.2977	25.7	1	613.2599	0.8	0.8	644.3446	1.8	1.8
585.3665	9.2	1	613.3035	7.8	7.8	644.3943	1.2	1.2
585.6127	1	1	613.7812	6.3	6.3	645.3517	0.9	0.9
585.7992	15.7	1	614.2862	4.3	4.3	645.8086	1.7	1.7
585.9453	0.5	0.5	614.4027	4.3	4.3	646.3102	1.3	1.3
586.3003	6.6	1	614.7848	1.8	1.8	646.3462	2.5	2.5
586.3675	3.4	3.4	615.3054	1.1	1.1	647.3484	1.2	1.2
586.7995	2.3	2.3	615.4056	1.3	1.3	648.3267	0.5	0.5
587.3049	0.8	0.8	615.6526	0.5	0.5	648.8434	5	5
587.3471	1.9	1.9	616.3322	1.4	1.4	649.2781	0.5	0.5
588.2657	0.9	0.9	616.3715	2.7	2.7	649.3441	3.5	3.5

649.8453	1.4	1.4	686.3994	1.1	1.1	743.829	2.3	2.3
650.3487	1.9	1.9	686.8606	0.5	0.5	743.9022	0.6	0.6
650.8435	1.1	1.1	687.3737	3.4	3.4	744.3301	0.7	0.7
651.3495	0.8	0.8	688.3816	1.2	1.2	744.4253	0.9	0.9
652.3193	1.8	1.8	689.3759	0.5	0.5	746.3723	1.4	1.4
652.8265	0.9	0.9	690.35	0.5	0.5	746.8719	0.9	0.9
653.3204	0.8	0.8	691.3243	1	1	747.3743	0.5	0.5
653.4913	3.3	3.3	692.3285	0.5	0.5	751.3924	0.8	0.8
653.6909	6.8	1	694.3461	3.6	3.6	753.3152	0.6	0.6
653.7891	0.5	0.5	<mark>694.8068</mark>	14.1	14.1	753.8166	0.5	0.5
653.8907	7.4	1	<mark>695.3082</mark>	10.2	10.2	759.424	0.5	0.5
654.091	5.5	5.5	695.3455	1.3	1.3	760.4076	2	2
654.2916	3.7	3.7	<mark>695.8097</mark>	4.1	4.1	761.4003	0.8	0.8
654.3689	0.6	0.6	696.3162	1.7	1.7	762.405	1.3	1.3
654.4915	1.5	1.5	697.3243	0.6	0.6	763.408	0.8	0.8
654.6913	0.7	0.7	700.3406	0.8	0.8	767.8772	0.7	0.7
655.2735	0.5	0.5	701.3504	0.6	0.6	768.3836	0.8	0.8
657.3064	0.7	0.7	701.4131	0.8	0.8	768.7823	0.5	0.5
658.3826	0.9	0.9	702.3701	1	1	769.283	0.6	0.6
659.3283	1.6	1.6	703.356	8.1	1	769.3301	1	1
659.83	1.3	1.3	704.3614	2.9	2.9	770.3335	0.5	0.5
660.333	0.6	0.6	705.3304	2.1	2.1	771.3296	0.8	0.8
660.3745	0.6	0.6	705.832	1.4	1.4	771.465	0.9	0.9
661.358	0.5	0.5	706.3346	0.9	0.9	771.5789	1	1
662.2856	0.5	0.5	707.3447	12.4	1	771.8294	1	1
662.3402	1.2	1.2	708.348	5	5	772.0801	0.7	0.7
662.7841	0.6	0.6	708.3933	0.7	0.7	772.4494	4.3	4.3
663.3196	2.4	2.4	709.3508	1.3	1.3	773.4491	2.6	2.6
664.2992	18.2	1	710.377	1.7	1.7	774.3945	0.5	0.5
665.3027	6.1	1	710.8781	1.2	1.2	774.4494	0.8	0.8
666.3392	5.3	1	711.3783	0.6	0.6	775.3695	0.6	0.6
667.3422	2.1	2.1	712.3273	1.6	1.6	775.4233	2.3	2.3
668.3429	0.6	0.6	713.3312	0.7	0.7	776.4025	3.9	3.9
670.3046	1.5	1.5	716.011	0.5	0.5	777.4048	1.5	1.5
670.8058	0.9	0.9	716.3493	0.6	0.6	778.4029	0.6	0.6
671.311	0.6	0.6	717.4172	0.5	0.5	781.4012	0.6	0.6
672.3352	0.6	0.6	718.0127	0.6	0.6	786.4415	0.9	0.9
672.3968	0.6	0.6	718.138	0.9	0.9	787.4383	0.6	0.6
673.356	1	1	718.2637	0.7	0.7	788.3593	0.7	0.7
673.392	0.5	0.5	718.3877	0.6	0.6	788.861	0.6	0.6
675.3352	0.9	0.9	719.6281	0.6	0.6	790.4114	0.5	0.5
675.3958	0.5	0.5	719.7709	0.6	0.6	793.3405	2.4	2.4
675.832	0.7	0.7	719.9859	0.5	0.5	793.6862	1.3	1.3
676.3048	0.7	0.7	720.1299	0.9	0.9	793.8527	4.4	4.4
677.3557	1.2	1.2	720.273	1.1	1.1	794.0192	7.7	1
678.3095	0.5	0.5	720.4158	0.9	0.9	794.1859	8.2	1
678.3559	0.6	0.6	720.5598	0.7	0.7	794.3518	7.5	1
679.3711	3.4	3.4	721.2636	0.5	0.5	794.4062	0.5	0.5
680.371	1.4	1.4	721.7642	0.5	0.5	794.5196	4.5	4.5
680.4431	0.7	0.7	724.3476	0.8	0.8	794.6861	2.5	2.5
680.5884	1.2	1.2	726.3432	0.5	0.5	794.8535	1.3	1.3
680.7321	2	2	726.85	0.5	0.5	795.0205	0.5	0.5
680.8719	2.4	2.4	727.3501	0.5	0.5	795.381	14.9	1
681.0174	1.8	1.8	727.8187	0.7	0.7	796.3839	6.3	1
681.1609	1.2	1.2	728.3201	0.5	0.5	797.3882	1.8	1.8
681.3068	0.8	0.8	729.2759	0.5	0.5	798.3899	0.6	0.6
681.3422	1.9	1.9	729.3258	0.8	0.8	800.4557	1	1
681.4461	0.5	0.5	729.6095	0.5	0.5	801.4749	7.4	7.4
681.8169	0.6	0.6	730.3298	0.5	0.5	802.4785	2.9	2.9
682.3052	0.7	0.7	731.4194	0.5	0.5	803.4825	0.9	0.9
682.343	0.8	0.8	737.3865	1.1	1.1	804.3811	0.9	0.9
684.0774	3.2	3.2	738.3344	2.6	2.6	816.4386	10.7	1
684.3279	5.1	1	739.345	2.5	2.5	816.6122	1.1	1.1
684.578	4.1	4.1	740.3493	0.9	0.9	816.8619	2.2	2.2
684.8285	2.3	2.3	742.3247	19.5	1	817.1116	2.3	2.3
685.0792	1.1	1.1	742.3707	0.5	0.5	817.3622	2.6	2.6
685.3331	0.6	0.6	742.4502	0.7	0.7	817.4404	5.1	1
685.3932	2.3	2.3	742.8262	15.2	1	817.6125	1	1
685.4278	1.7	1.7	743.3278	6.8	1	817.8652	0.8	0.8
686.3568	0.7	0.7	743.3675	0.5	0.5	818.0112	0.5	0.5

818.3642	0.5	0.5	880.4179	0.7	0.7
818.4423	1.9	1.9	885.4192	2.2	2.2
820.1561	0.5	0.5	886.4229	1	1
820.2984	1	1	887.4864	2.8	2.8
820.4406	1.3	1.3	888.4172	0.5	0.5
820.5861	1	1	888.5015	2.7	2.7
820.7284	1	1	889.3685	0.6	0.6
820.87	0.9	0.9	889.5054	1.1	1.1
821.014	0.7	0.7	889.8714	0.6	0.6
823.387	1.7	1.7	892.8868	0.6	0.6
823.455	0.6	0.6	893.4316	0.6	0.6
824.3895	0.7	0.7	903.9727	1.2	1.2
825.3926	0.7	0.7			
835.5074	0.5	0.5			
838.4209	0.8	0.8			
839.2318	0.6	0.6			
839.4038	0.7	0.7			
839.5655	0.7	0.7			
839.7321	0.5	0.5			
840.151	0.6	0.6			
840.3201	0.6	0.6			
840.4026	0.6	0.6			
846.46	1.1	1.1			
847.4603	0.5	0.5			
851.4182	7.3	7.3			
852.4212	3.3	3.3			
852.8564	29.6	29.6			
853.3578	24.3	24.3			
853.4235	1	1			
853.8593	11.8	11.8			
854.3609	4.4	4.4			
854.8614	1.3	1.3			
855.4859	2.5	2.5			
856.4894	1	1			
857.4288	0.6	0.6			
857.5114	3.3	3.3			
858.4571	0.7	0.7			
858.5143	1.5	1.5			
859.4614	0.5	0.5			
862.9134	9	9			
863.4148	8.2	1			
863.8467	1.2	1.2			
863.9164	4	4			
864.3485	1.1	1.1			
864.4179	1.6	1.6			
864.8462	0.6	0.6			
864.9173	0.5	0.5			
865.9323	6.5	1			
866.4338	6.1	1			
866.9345	3.2	3.2			
67.4358	1.2	1.2			
869.3523	0.6	0.6			
871.8298	0.8	0.8			
872.3318	0.7	0.7			
873.4003	0.6	0.6			
873.9039	0.7	0.7			
874.4047	0.8	0.8			
875.4107	0.6	0.6			
875.7476	0.6	0.6			
876.4103	0.5	0.5			
876.458	0.7	0.7			
876.9203	1.2	1.2			
877.4226	1.2	1.2			
877.9231	0.5	0.5			
878.4646	1.5	1.5			
879.3121	0.9	0.9			
879.4132	1.3	1.3			
879.4679	0.8	0.8			
879.8141	0.9	0.9			
880.315	0.6	0.6			

10