

Single-pot enzymatic synthesis of cancer-associated MUC16 O-glycopeptides libraries and multivalent protein glycoconjugates: a step towards cancer glycovaccines

-Supporting Information-

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Keywords: enzymatic synthesis; glycopeptides; protein glycoconjugates; cancer glycovaccines

Table S1. Products from the single-pot enzymatic synthesis of MUC16-Tn glycopeptides and corresponding mass for double and triple charged MUC16 and peptide derivatives.

<i>O</i> -glycans	Glycopeptides Monoisotopic mass [M+2H] ²⁺ / [M+3H] ³⁺
MUC16 20-mer peptide (VDVGTSGTPSSSPSTTAGP)	
Unglycosylated	901.43 / 601.29
MUC16-Tn glycopeptides	
1 Tn	1002.97 / 668.98
2 Tn	1104.51 / 736.67
3 Tn	1206.05 / 804.37
4 Tn	1307.59 / 872.06
5 Tn	1409.13 / 939.75

Tables S2-13. Product ion tables for assigned glycopeptides identified in Figure 3, highlighting the Tn-glycosylated sites and corresponding chromatographic retention times (RT)

S2.

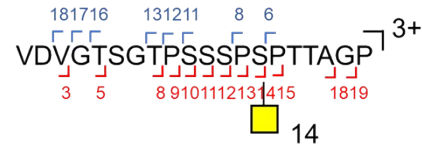
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1	100.07569	50.54148	34.03008	V				20
2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	559.27222	280.13975	187.09559	S	1533.69149	767.34938	511.90201	15
7	616.29368	308.65048	206.10274	G	1446.65946	723.83337	482.89134	14
8	717.34136	359.17432	239.78530	T	1389.63800	695.32264	463.88418	13
9	814.39412	407.70070	272.13623	P	1288.59032	644.79880	430.20162	12
10	901.42615	451.21671	301.14690	S	1191.53755	596.27242	397.85070	11
11	988.45818	494.73273	330.15758	S	1104.50553	552.75640	368.84003	10
12	1075.49021	538.24874	359.16825	S	1017.47350	509.24039	339.82935	9
13	1172.54297	586.77512	391.51918	P	930.44147	465.72437	310.81867	8
14	1259.57500	630.29114	420.52985	S	833.38870	417.19799	278.46775	7
15	1356.62776	678.81752	452.88077	P	746.35668	373.68198	249.45708	6
16	1660.75482	830.88105	554.25646	T-HexNAc	649.30391	325.15559	217.10616	5
17	1761.80249	881.40489	587.93902	T	345.17686	173.09207	115.73047	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



RT=15.5 min

S3.

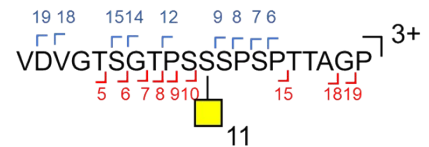
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1	100.07569	50.54148	34.03008	V				20
2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	559.27222	280.13975	187.09559	S	1533.69149	767.34938	511.90201	15
7	616.29368	308.65048	206.10274	G	1446.65946	723.83337	482.89134	14
8	717.34136	359.17432	239.78530	T	1389.63800	695.32264	463.88418	13
9	814.39412	407.70070	272.13623	P	1288.59032	644.79880	430.20162	12
10	901.42615	451.21671	301.14690	S	1191.53755	596.27242	397.85070	11
11	988.45818	494.73273	330.15758	S	1104.50553	552.75640	368.84003	10
12	1075.49021	538.24874	359.16825	S	1017.47350	509.24039	339.82935	9
13	1172.54297	586.77512	391.51918	P	930.44147	465.72437	310.81867	8
14	1462.65437	731.83083	488.22298	S-HexNAc	833.38870	417.19799	278.46775	7
15	1559.70714	780.35721	520.57390	P	543.27730	272.14229	181.76395	6
16	1660.75482	830.88105	554.25646	T	446.22454	223.61591	149.41303	5
17	1761.80249	881.40489	587.93902	T	345.17686	173.09207	115.73047	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
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RT=21.63 min

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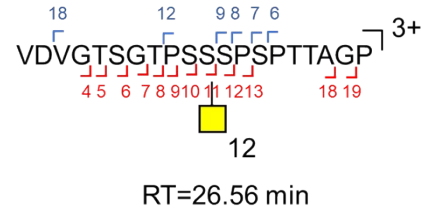
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3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	559.27222	280.13975	187.09559	S	1533.69149	767.34938	511.90201	15
7	616.29368	308.65048	206.10274	G	1446.65946	723.83337	482.89134	14
8	717.34136	359.17432	239.78530	T	1389.63800	695.32264	463.88418	13
9	814.39412	407.70070	272.13623	P	1288.59032	644.79880	430.20162	12
10	901.42615	451.21671	301.14690	S	1191.53755	596.27242	397.85070	11
11	988.45818	494.73273	330.15758	S	1104.50553	552.75640	368.84003	10
12	1075.49021	538.24874	359.16825	S	1017.47350	509.24039	339.82935	9
13	1172.54297	586.77512	391.51918	P	930.44147	465.72437	310.81867	8
14	1462.65437	731.83083	488.22298	S	814.39412	407.70070	272.13623	7
15	1559.70714	780.35721	520.57390	P	727.36210	364.18469	243.12555	6
16	1660.75482	830.88105	554.25646	T	630.30933	315.65830	210.77463	5
17	1761.80249	881.40489	587.93902	T	543.27730	272.14229	181.76395	4
18	1832.83961	916.92344	611.61805	A	446.22454	223.61591	149.41303	3
19	1889.86107	945.43417	630.62521	G	345.17686	173.09207	115.73047	2
20				P	244.12918	122.56823	82.04791	1



RT=23.29 min

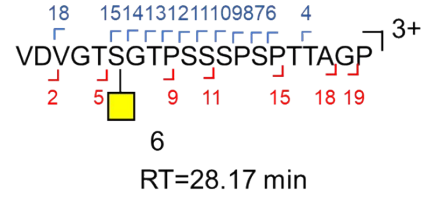
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2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	559.27222	280.13975	187.09559	S	1533.69149	767.34938	511.90201	15
7	616.29368	308.65048	206.10274	G	1446.65946	723.83337	482.89134	14
8	717.34136	359.17432	239.78530	T	1389.63800	695.32264	463.88418	13
9	814.39412	407.70070	272.13623	P	1288.59032	644.79880	430.20162	12
10	901.42615	451.21671	301.14690	S	1191.53755	596.27242	397.85070	11
11	988.45818	494.73273	330.15758	S	1104.50553	552.75640	368.84003	10
12	1278.56958	639.78843	426.86138	S-HexNAc	1017.47350	509.24039	339.82935	9
13	1375.62235	688.31481	459.21230	P	727.36210	364.18469	243.12555	8
14	1462.65437	731.83083	488.22298	S	630.30933	315.65830	210.74633	7
15	1559.70714	780.35721	520.57390	P	543.27730	272.14229	181.76395	6
16	1660.75482	830.88105	554.25646	T	446.22454	223.61591	149.41303	5
17	1761.80249	881.40489	587.93902	T	345.17686	173.09207	115.73047	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



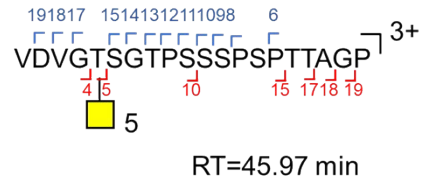
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2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	762.35159	381.67943	254.78871	S-HexNAc	1533.69149	767.34938	511.90201	15
7	819.37305	410.19017	273.79587	G	1243.58009	622.29368	415.19821	14
8	920.42073	460.71400	307.47843	T	1186.55862	593.78295	396.19106	13
9	1017.47350	509.24039	339.82935	P	1085.51094	543.25911	362.50850	12
10	1104.50553	552.75640	368.84003	S	988.45818	494.73273	330.15758	11
11	1191.53755	596.27242	397.85070	S	901.42615	451.21671	301.14690	10
12	1278.56958	639.78843	426.86138	S	814.39412	407.70070	272.13623	9
13	1375.62235	688.31481	459.21230	P	727.36210	364.18469	243.12555	8
14	1462.65437	731.83083	488.22298	S	630.30933	315.65830	210.74633	7
15	1559.70714	780.35721	520.57390	P	543.27730	272.14229	181.76395	6
16	1660.75482	830.88105	554.25646	T	446.22454	223.61591	149.41303	5
17	1761.80249	881.40489	587.93902	T	345.17686	173.09207	115.73047	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



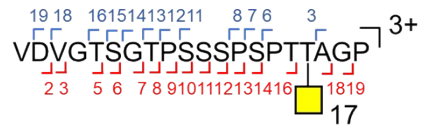
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2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	675.31956	338.16342	225.77804	T-HexNAc	1634.73917	817.87322	545.58457	16
6	762.35159	381.67943	254.78871	S	1330.61211	665.80970	444.20889	15
7	819.37305	410.19017	273.79587	G	1243.58009	622.29368	415.19821	14
8	920.42073	460.71400	307.47843	T	1186.55862	593.78295	396.19106	13
9	1017.47350	509.24039	339.82935	P	1085.51094	543.25911	362.50850	12
10	1104.50553	552.75640	368.84003	S	988.45818	494.73273	330.15758	11
11	1191.53755	596.27242	397.85070	S	901.42615	451.21671	301.14690	10
12	1278.56958	639.78843	426.86138	S	814.39412	407.70070	272.13623	9
13	1375.62235	688.31481	459.21230	P	727.36210	364.18469	243.12555	8
14	1462.65437	731.83083	488.22298	S	630.30933	315.65830	210.74633	7
15	1559.70714	780.35721	520.57390	P	543.27730	272.14229	181.76395	6
16	1660.75482	830.88105	554.25646	T	446.22454	223.61591	149.41303	5
17	1761.80249	881.40489	587.93902	T	345.17686	173.09207	115.73047	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



S8.

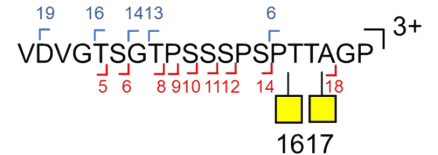
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2	215.10263	108.05496	72.37240	D	1905.85599	953.43163	635.95685	19
3	314.17105	157.58916	105.39520	V	1790.82904	895.91816	597.61453	18
4	371.19251	186.09989	124.40235	G	1691.76063	846.38395	564.59173	17
5	472.24019	236.62373	158.08491	T	1634.73917	817.87322	545.58457	16
6	559.27222	280.13975	187.09559	S	1533.69149	767.34938	511.90201	15
7	616.29368	308.65048	206.10274	G	1446.65946	723.83337	482.89134	14
8	717.34136	359.17432	239.78530	T	1389.63800	695.32264	463.88418	13
9	814.39412	407.70070	272.13623	P	1288.59032	644.79880	430.20162	12
10	901.42615	451.21671	301.14690	S	1191.53755	596.27242	397.85070	11
11	988.45818	494.73273	330.15758	S	1104.50553	552.75640	368.84003	10
12	1075.49021	538.24874	359.16825	S	1017.47350	509.24039	339.82935	9
13	1172.54297	586.77512	391.51918	P	930.44147	465.72437	310.81867	8
14	1259.57500	630.29114	420.52985	S	833.38870	417.19799	278.46775	7
15	1356.62776	678.81752	452.88077	P	746.35668	373.68198	249.45708	6
16	1457.67544	729.34136	486.56333	T	649.30991	325.15559	217.10616	5
17	1761.80249	881.40489	587.93902	T-HexNAc	548.25623	274.63176	183.42360	4
18	1832.83961	916.92344	611.61805	A	244.12918	122.56823	82.04791	3
19	1889.86107	945.43417	630.62521	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



RT=29.83 min

S9.

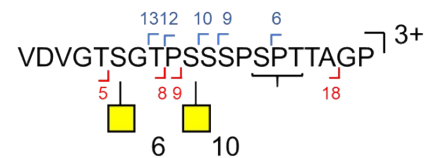
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2	215.10263	108.05496	72.37240	D	2108.93536	1054.97132	703.64997	19
3	314.17105	157.58916	105.39520	V	1993.90842	997.45785	665.30766	18
4	371.19251	186.09989	124.40235	G	1894.84000	947.92364	632.28485	17
5	472.24019	236.62373	158.08491	T	1837.81854	919.41291	613.27770	16
6	559.27222	280.13975	187.09559	S	1736.77086	868.88907	579.59514	15
7	616.29368	308.65048	206.10274	G	1649.73883	825.37305	550.58446	14
8	717.34136	359.17432	239.78530	T	1592.71737	796.86232	531.57731	13
9	814.39412	407.70070	272.13623	P	1491.66969	746.33848	497.89475	12
10	901.42615	451.21671	301.14690	S	1394.61693	697.81210	465.54383	11
11	988.45818	494.73273	330.15758	S	1307.58490	654.29609	436.53315	10
12	1075.49021	538.24874	359.16825	S	1220.55287	610.78007	407.52247	9
13	1172.54297	586.77512	391.51918	P	1133.52084	567.26406	378.51180	8
14	1259.57500	630.29114	420.52985	S	1036.46808	518.73768	346.16088	7
15	1356.62776	678.81752	452.88077	P	949.43055	475.22166	317.15020	6
16	1660.75482	830.88105	554.25646	T-HexNAc	852.38329	426.69528	284.79928	5
17	1964.88187	982.94457	655.63214	T-HexNAc	548.25623	274.63176	183.42360	4
18	2035.91898	1018.46313	679.31118	A	244.12918	122.56823	82.04791	3
19	2092.94044	1046.97386	698.31833	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



RT=14.8 min

S10.

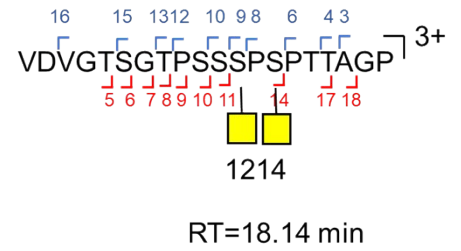
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2	215.10263	108.05496	72.37240	D	2108.93536	1054.97132	703.64997	19
3	314.17105	157.58916	105.39520	V	1993.90842	997.45785	665.30766	18
4	371.19251	186.09989	124.40235	G	1894.84000	947.92364	632.28485	17
5	472.24019	236.62373	158.08491	T	1837.81854	919.41291	613.27770	16
6	762.35159	381.67943	254.78871	S-HexNAc	1736.77086	868.88907	579.59514	15
7	819.37305	410.19017	273.79587	G	1446.65946	723.83337	482.89134	14
8	920.42073	460.71400	307.47843	T	1389.63800	695.32264	463.88418	13
9	1017.47350	509.24039	339.82935	P	1288.59032	644.79880	430.20162	12
10	1307.58490	654.29609	436.53315	S-HexNAc	1191.53755	596.27242	397.85070	11
11	1394.61693	697.81210	465.54383	S	901.42615	451.21671	301.14690	10
12	1481.64895	741.32812	494.55450	S	814.39412	407.70070	272.13623	9
13	1578.70172	789.85450	526.90542	P	727.36210	364.18469	243.12555	8
14	1665.73375	833.37051	555.91610	S	630.30933	315.65830	210.77463	7
15	1762.78651	881.89689	588.26702	P	543.27730	272.14229	181.76395	6
16	1863.83419	932.42073	621.94958	T	446.22454	223.61591	149.41303	5
17	1964.88187	982.94457	655.63214	T	345.17686	173.09207	115.73047	4
18	2035.91898	1018.46313	679.31118	A	244.12918	122.56823	82.04791	3
19	2092.94044	1046.97386	698.31833	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



RT=17.28 min

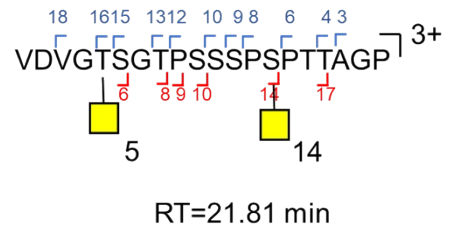
S11.

1	100.07569	50.54148	34.03008	V					20
2	215.10263	108.05496	72.37240	D	2108.93536	1054.97132	703.64997		19
3	314.17105	157.58916	105.39520	V	1993.90842	997.45785	665.30766		18
4	371.19251	186.09989	124.40235	G	1894.84000	947.92364	632.28485		17
5	472.24019	236.62373	158.08491	T	1837.81854	919.41291	613.27770		16
6	559.27222	280.13975	187.09559	S	1736.77086	868.88907	579.59514		15
7	616.29368	308.65048	206.10274	G	1649.73883	825.37305	550.58446		14
8	717.34136	359.17432	239.78530	T	1592.71737	796.86232	531.57731		13
9	814.39412	407.70070	272.13623	P	1491.66969	746.33848	497.89475		12
10	901.42615	451.21671	301.14690	S	1394.61693	697.81210	465.54383		11
11	988.45818	494.73273	330.15758	S	1307.58490	654.29609	436.53315		10
12	1278.56958	639.78843	426.86138	S-HexNAc	1220.55287	610.78007	407.52247		9
13	1375.62235	688.31481	459.21230	P	930.44147	465.72437	310.81867		8
14	1665.73375	833.37051	555.91610	S-HexNAc	833.38870	417.19799	278.46775		7
15	1762.78651	881.89689	588.26702	P	543.27730	272.14229	181.76395		6
16	1863.83419	932.42073	621.94958	T	446.22454	223.61591	149.41303		5
17	1964.88187	982.94457	655.63214	T	345.17686	173.09207	115.73047		4
18	2035.91898	1018.46313	679.31118	A	244.12918	122.56823	82.04791		3
19	2092.94044	1046.97386	698.31833	G	173.09207	87.04967	58.36887		2
20				P	116.07061	58.53894	39.36172		1



S12.

#1	b ⁺	b ²⁺	b ³⁺	Seq.	y ⁻	y ²⁺	y ³⁺	#2
1	100.07569	50.54148	34.03008	V				20
2	215.10263	108.05496	72.37240	D	2108.93536	1054.97132	703.64997	19
3	314.17105	157.58916	105.39520	V	1993.90842	997.45785	665.30766	18
4	371.19251	186.09989	124.40235	G	1894.84000	947.92364	632.28485	17
5	675.31956	338.16342	225.77804	T-HexNAc	1837.81854	919.41291	613.27770	16
6	762.35159	381.67943	254.78871	S	1533.69149	767.34938	511.90201	15
7	819.37305	410.19017	273.79587	G	1446.65946	723.83337	482.89134	14
8	920.42073	460.71400	307.47843	T	1389.63800	695.32264	463.88418	13
9	1017.47350	509.24039	339.82935	P	1288.59032	644.79880	430.20162	12
10	1104.50553	552.75640	368.84003	S	1191.53755	596.27242	397.85070	11
11	1191.53755	596.27242	397.85070	S	1104.50553	552.75640	368.84003	10
12	1278.56958	639.78843	426.86138	S	1017.47350	509.24039	339.82935	9
13	1375.62235	688.31481	459.21230	P	930.44147	465.72437	310.81867	8
14	1665.73375	833.37051	555.91610	S-HexNAc	833.38870	417.19799	278.46775	7
15	1762.78651	881.89689	588.26702	P	543.27730	272.14229	181.76395	6
16	1863.83419	932.42073	621.94958	T	446.22454	223.61591	149.41303	5
17	1964.88187	982.94457	655.63214	T	345.17686	173.09207	115.73047	4
18	2035.91898	1018.46313	679.31118	A	244.12918	122.56823	82.04791	3
19	2092.94044	1046.97386	698.31833	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1



S13.

#1	b ⁺	b ²⁺	b ³⁺	Seq.	y ⁻	y ²⁺	y ³⁺	#2
1	100.07569	50.54148	34.03008	V				20
2	215.10263	108.05496	72.37240	D	2108.93536	1054.97132	703.64997	19
3	314.17105	157.58916	105.39520	V	1993.90842	997.45785	665.30766	18
4	371.19251	186.09989	124.40235	G	1894.84000	947.92364	632.28485	17
5	472.24019	236.62373	158.08491	T	1837.81854	919.41291	613.27770	16
6	559.27222	280.13975	187.09559	S	1736.77086	868.88907	579.59514	15
7	616.29368	308.65048	206.10274	G	1649.73883	825.37305	550.58446	14
8	920.42073	460.71400	307.47843	T-HexNAc	1592.71737	796.86232	531.57731	13
9	1017.47350	509.24039	339.82935	P	1288.59032	644.79880	430.20162	12
10	1104.50553	552.75640	368.84003	S	1191.53755	596.27242	397.85070	11
11	1191.53755	596.27242	397.85070	S	1104.50553	552.75640	368.84003	10
12	1278.56958	639.78843	426.86138	S	1017.47350	509.24039	339.82935	9
13	1375.62235	688.31481	459.21230	P	930.44147	465.72437	310.81867	8
14	1462.65437	731.83083	488.22298	S	833.38870	417.19799	278.46775	7
15	1559.70714	780.35721	520.57390	P	746.33668	373.68198	249.45708	6
16	1863.83419	932.42073	621.94958	T-HexNAc	649.30391	325.15559	217.10616	5
17	1964.88187	982.94457	655.63214	T	345.17686	173.09207	115.73047	4
18	2035.91898	1018.46313	679.31118	A	244.12918	122.56823	82.04791	3
19	2092.94044	1046.97386	698.31833	G	173.09207	87.04967	58.36887	2
20				P	116.07061	58.53894	39.36172	1

