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## O-Linked glycosylation in *Acanthamoeba polyphaga mimivirus*

Hülsmeier, A J; Hennet, T

**Abstract:** *Acanthamoeba polyphaga mimivirus* is a member of the giant nucleocytoplasmic large DNA viruses, infecting various *Acanthamoeba* spp. The genomes of giant viruses encode components previously thought to be exclusive to cellular life, such as proteins involved in nucleic acid and protein synthesis. Recent work on enzymes involved in carbohydrate biosynthesis and metabolism show that instead of utilizing host cell resources, Mimivirus produces its own glycosylation machinery. To obtain a more detailed view of glycosylation in Mimivirus, we developed a periodate oxidation-based method to selectively enrich Mimivirus surface glycoproteins. O-Glycosylation in Mimivirus glycoproteins was identified by permethylation and matrix-assisted laser desorption/ionization-mass spectrometry analyses of beta-eliminated glycans. We sequenced 26 previously undescribed O-glycans, most of which contain glucose as their reducing end saccharide. These data will facilitate future studies on the functional significance of glycosylation in Mimivirus.

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## O 1.4 permethylated

m/z	intensity	relative intensity	annotation
262.1759	63.1	3.9	y1y1
282.1162	109.2	6.8	b1
415.2140	49.0	3.1	<sup>2,4</sup> X <sub>2</sub> (HexNAc)Z <sub>1</sub>
466.3075	63.1	3.9	y1y2
521.2516	175.5	10.9	y1
619.3081	56.7	3.5	<sup>2,4</sup> X <sub>2</sub> (HexNAc)Z <sub>2</sub> Z <sub>1</sub> <sup>2,4</sup> X <sub>3</sub> (HexNAc)
725.2722	1603.7	100.0	y2
753.3639	66.5	4.1	<sup>1,5</sup> X <sub>2</sub> (HexNAc) <sup>1,5</sup> X <sub>3</sub> (HexNAc)
984.4069	256.9	16.0	M+Na <sup>+</sup>

## O 1.6 perdeuteromethylated

m/z	intensity	relative intensity	annotation
254.2295	6.0	1.7	c2y2
274.2805	12.0	3.5	y1y1
277.2449	11.1	3.3	b2y2 c2z2
291.2484	10.4	3.0	b1
433.4450	4.5	1.3	<sup>2,4</sup> X <sub>2</sub> (HexNAc)Z <sub>1</sub>
487.3069	13.8	4.0	y1y2
528.4772	7.1	2.1	y1y2
585.4053	4.5	1.3	<sup>2,5</sup> X <sub>2</sub> (HexNAc)Z <sub>2</sub>
587.4867	3.8	1.1	y <sub>2</sub> <sup>0,2</sup> X <sub>2</sub> (Hex)
646.5425	7.1	2.1	z <sub>2</sub> <sup>1,3</sup> X <sub>2</sub> (Hex) Z <sub>2</sub> <sup>2,4</sup> X <sub>2</sub> (Hex) <sup>2,4</sup> X <sub>2</sub> (HexNAc)Z <sub>2</sub>
664.3674	4.4	1.3	y <sub>2</sub> <sup>1,3</sup> X <sub>2</sub> (Hex) Y <sub>2</sub> <sup>2,4</sup> X <sub>2</sub> (Hex) <sup>2,4</sup> X <sub>2</sub> (HexNAc)Y <sub>2</sub>
711.4971	30.7	9.0	y1
723.4536	8.5	2.5	y2z2 z2y2
737.6381	10.6	3.1	z1
739.6395	10.3	3.0	<sup>1,5</sup> X <sub>2</sub> (Hex)
755.5779	54.6	15.9	y1
783.6697	7.8	2.3	<sup>1,5</sup> X <sub>2</sub> (HexNAc)
906.6845	9.6	2.8	z2
924.6546	342.4	100.0	y2
1009.9621	17.6	5.2	y2
1192.8677	7.6	2.2	M+Na <sup>+</sup>

## O 1.6 permethylated

m/z	intensity	relative intensity	annotation
197.0851	27.5	4.4	b1
215.0924	32.5	5.2	c1
227.1197	26.1	4.2	b2y2 c2z2 (Hex)
250.1051	32.3	5.2	b2z2 (HexNAc)
262.1699	45.8	7.4	y1y1
268.1579	76.3	12.3	b2y2 c2z2 (HexNAc)
282.1361	48.4	7.8	b1
466.2913	70.3	11.3	y1y2
563.1174	21.3	3.4	<sup>0,2</sup> X <sub>2</sub> (HexNAc)Y Y <sub>2</sub> <sup>0,2</sup> X <sub>2</sub> (Hex)
593.4737	23.5	3.8	y <sub>2</sub> <sup>1,4</sup> X <sub>2</sub> (Hex)
619.2633	39.1	6.3	z <sub>2</sub> <sup>1,3</sup> X <sub>2</sub> (Hex) Z <sub>2</sub> <sup>2,4</sup> X <sub>2</sub> (Hex) <sup>2,4</sup> X <sub>2</sub> (HexNAc)Z <sub>2</sub>
681.3225	97.9	15.7	y1
725.2949	146.4	23.5	y1
885.3341	622.4	100.0	y2
1144.4947	141.2	22.7	M+Na <sup>+</sup>

## O 1.7 permethylated

m/z	intensity	relative intensity	annotation
197.0214	9.8	7.4	b1
215.0998	22.9	17.4	c1
262.1296	32.4	24.5	y1y1
268.1363	31.4	23.8	b2y2 c2z2
431.1867	32.9	25.0	b2y2 c2z2
535.3115	26.5	20.1	y <sub>2</sub> <sup>1,5</sup> X <sub>2</sub> (Hex)
558.1318	22.2	16.8	b <sub>2</sub> <sup>1,4</sup> X <sub>3</sub> (Hex)
681.2449	52.7	40.0	y1
837.4947	29.8	22.6	z <sub>1</sub> <sup>0,4</sup> X <sub>3</sub> (Hex)
915.2821	29.4	22.3	y2y2
929.4276	39.6	30.0	y1
939.3524	30.0	22.7	z <sub>2</sub> <sup>1,4</sup> X <sub>3</sub> (Hex)
1071.3984	42.7	32.4	z2
1089.4261	132.0	100.0	y2
1156.6014	36.9	27.9	z2
1348.6403	9.8	7.4	M+Na <sup>+</sup>

## O 1.7 perdeuteromethylated

m/z	intensity	relative intensity	annotation
224.2138	5.1	1.5	c1
271.2765	4.6	1.3	c1
274.3494	8.6	2.5	y1y1
277.2074	10.7	3.2	b2y2
291.2197	5.8	1.7	b1

344.3192	6.5	1.9	<sup>3.5</sup> a <sub>2</sub> (Hex)	<sup>2.5</sup> a <sub>2</sub> (HexNAC)
510.5138	11.1	3.3	y2z1	z2y1
528.4126	7.8	2.3	y1y2	
700.6541	24.7	7.3	y1y2	
711.5773	54.4	16.0	y1	
968.7223	48.9	14.4	y1	
1137.9046	339.9	100.0	y2	
1203.8774	20.1	5.9	<sup>1.5</sup> x <sub>3</sub> (Hex)	
1406.0099	4.8	1.4	M+Na <sup>+</sup>	

O 2.4 perdeuteromethylated

m/z	intensity	relative intensity	annotation	
236.2025	18.7	52.4	b <sub>2/3</sub> y <sub>3/2</sub>	C <sub>2/3</sub> Z <sub>3/2</sub> b1-Me
252.2048	8.6	24.2	y1	
271.1679	6.9	19.4	c1	
311.3026	14.5	40.7	b <sub>2/3</sub> <sup>2.5</sup> x <sub>4/3</sub> (Hex)	<sup>0.2</sup> x <sub>2</sub> (Hex)
313.1187	6.4	17.9	C <sub>2/3</sub> <sup>0.2</sup> x <sub>3/2</sub> (Hex)	<sup>2.4</sup> a <sub>3</sub> (Hex)y <sub>3</sub>
356.3453	5.5	15.4	<sup>2.5</sup> a <sub>3</sub> (Hex)z <sub>3</sub>	
465.2484	8.8	24.5	y2	
466.3282	16.7	46.9	b2	
467.4092	17.1	48.0	c3y3	
484.3637	35.7	100.0	C2	
660.5462	13.3	37.4	z3	
678.5051	16.5	46.2	y3	
679.5283	33.9	94.9	b3	
697.5825	23.7	66.3	c3	
706.4502	15.0	42.1	<sup>1.5</sup> x <sub>4</sub> (Hex)	
908.6193	4.4	12.2	M+Na <sup>+</sup>	

O 2.5 perdeuteromethylated

m/z	intensity	relative intensity	annotation	
236.2406	7.6	30.7	b <sub>2/3/4</sub> y <sub>4/3/2</sub>	C <sub>2/3/4</sub> Z <sub>4/3/2</sub> b1-Me
252.1937	6.1	24.9	y1	
253.2547	5.2	21.2	b1	
325.3567	5.8	23.3	b <sub>2/3/4</sub> <sup>1.4</sup> x <sub>5/4/3</sub> (Hex)	<sup>0.3</sup> a <sub>3/4</sub> (Hex)z <sub>4/3</sub>
330.2841	7.1	28.6	<sup>2.4</sup> a <sub>2</sub> (Hex)	
465.3692	9.3	37.6	y2	
484.3753	20.4	82.5	c2	
493.2435	8.8	35.4	<sup>1.5</sup> x <sub>3</sub> (Hex)	
495.4995	6.9	28.0	C <sub>3/4</sub> <sup>1.5</sup> x <sub>5/4</sub> (Hex)	
569.0486	11.6	47.1	<sup>2.5</sup> a <sub>4</sub> (Hex)z <sub>4</sub>	
678.5707	14.8	59.8	y3	
680.6533	11.8	47.6	c4y4	
697.5558	24.7	100.0	c3	
708.5667	10.5	42.3	c <sub>4</sub> <sup>1.5</sup> x <sub>5</sub> (Hex)	
751.6868	11.5	46.6	b <sub>4</sub> <sup>1.4</sup> x <sub>5</sub> (Hex)	
768.5957	17.3	69.8	b <sub>4</sub> <sup>0.3</sup> x <sub>5</sub> (Hex)	
873.8270	13.2	53.4	z4	
891.7580	17.5	70.9	y4	
892.9318	16.1	65.1	b4	
910.8249	12.2	49.2	c4	

O 3.2 perdeuteromethylated

m/z	intensity	relative intensity	annotation
236.2152	54.9	16.7	b1-Me
253.1781	26.1	7.9	b1
271.2316	275.2	83.6	c1 y1
299.2208	25.5	7.7	<sup>1.5</sup> x <sub>2</sub> (Hex)
330.2122	84.3	25.6	<sup>0.2</sup> x <sub>2</sub> (Hex)
501.3756	329.0	100.0	M+Na <sup>+</sup>

O 3.3 perdeuteromethylated

m/z	intensity	relative intensity	annotation
236.1710	212.5	27.7	b2y2 c2z2
253.2454	68.6	9.0	b1 z1
271.2091	194.5	25.4	c1 y1
299.2236	241.8	31.5	<sup>1.5</sup> x <sub>2</sub> (Hex)
330.2306	58.2	7.6	<sup>2.4</sup> a <sub>2</sub> (Hex) <sup>0.2</sup> x <sub>2</sub> (Hex)
344.3449	121.2	15.8	<sup>3.5</sup> a <sub>2</sub> (Hex)
449.3547	218.2	28.5	b2-Me z2-Me
466.3260	376.1	49.1	b2 z2
484.3101	766.7	100.0	c2 y2
512.4025	181.8	23.7	<sup>1.5</sup> x <sub>3</sub> (Hex)
543.3934	56.1	7.3	<sup>0.2</sup> x <sub>3</sub> (Hex)
714.4809	555.6	72.5	M+Na <sup>+</sup>

O 3.4 perdeuteromethylated

m/z	intensity	relative intensity	annotation
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218.1460	11.8	2.8	$b_{2/3}z_{3/2}$		
236.1651	89.8	21.1	$b_2y_2$	c2z2	b1-Me
253.2259	46.3	10.9	b1	z1	
254.1667	23.7	5.6	$c_{2/3}y_{3/2}$		
264.1264	12.0	2.8	$b_{2/3}^{1.5}x_{3/2(Hex)}$		
271.2242	62.7	14.7	c1	y1	
299.2521	57.6	13.5	$^{1.5}x_{2(Hex)}$		
330.3795	24.3	5.7	$^{2.4}a_{2(Hex)}$	$^{0.2}x_{2(Hex)}$	
344.2867	55.5	13.0	$^{3.5}a_{2(Hex)}$		
377.1763	17.3	4.1	$^{1.4}a_{2(Hex)}$	$^{0.3}x_{2(Hex)}$	
393.2505	14.7	3.5	$^{3.5}x_{2(Hex)}$		
407.1432	17.3	4.1	$^{0.2}a_{2(Hex)}$	$c_{3/4}^{0.4}x_{4/3}$	$^{2.4}x_{2(Hex)}$
438.3122	23.5	5.5	$^{1.5}a_{2(Hex)}$		
449.3380	88.2	20.7	$b_3y_3$	c3z3	b2-Me
466.3585	142.2	33.4	b2	z2	
467.2704	47.8	11.2	$c_3y_3$		
484.3217	425.9	100.0	c2	y2	
512.3954	109.6	25.7	$^{1.5}x_{3(Hex)}$		
542.3718	28.6	6.7	$c_3^{2.5}x_{4(Hex)}$		
543.5028	34.3	8.1	$^{2.4}a_{3(Hex)}$	$^{0.2}x_{3(Hex)}$	
557.4282	66.7	15.7	$^{3.5}a_{3(Hex)}$		
651.4857	23.3	5.5	$^{1.5}a_{3(Hex)}$		
679.4659	195.1	45.8	b3	z3	
697.5143	257.5	60.5	c3	y3	
725.6774	76.3	17.9	$^{1.5}x_{4(Hex)}$		
756.4878	32.4	7.6	$^{0.2}x_{4(Hex)}$		
927.7294	94.1	22.1		M+Na <sup>+</sup>	

#### O 4.4 perdeuteromethylated

m/z	intensity	relative intensity	annotation		
236.1860	24.2	25.8	$b_{2/3}y_{3/2}$	$c_{2/3}z_{3/2}$	b1-Me
271.2424	19.3	20.6	c1		
309.3678	13.9	14.8	$^{3.5}a_{3(Hex)}z_3$		
311.3424	16.5	17.5	$b_{2/3}^{2.5}x_{3/2(Hex)}$		
330.2783	12.2	13.0	$^{2.4}a_{2(Hex)}$		
344.3259	16.5	17.5	$^{3.5}a_{2(Hex)}$	$^{0.2}x_{2(Hex)}$	
449.3663	16.7	17.8	$b_3y_3$	c3z3	b2-Me
466.4184	28.2	30.1	b2		
467.4315	18.8	20.1	$c_3y_3$		
484.4141	93.9	100.0	c2		
498.3140	14.6	15.6	y2		
679.5785	45.5	48.5	b3		
697.5834	69.4	74.0	c3		
711.6750	41.6	44.3	y3		
941.7865	9.8	10.4		M+Na <sup>+</sup>	

#### O 4.5 perdeuteromethylated

m/z	intensity	relative intensity	annotation		
236.1940	15.9	28.6	$b_{2/3/4}y_{4/3/2}$	$c_{2/3/4}z_{4/3/2}$	b1-Me
271.2717	14.4	25.8	c1		
330.2632	12.4	22.2	$^{2.4}a_{2(Hex)}$		
344.3718	9.4	16.9	$^{3.5}a_{2(Hex)}$	$^{0.2}x_{2(Hex)}$	
360.0488	9.5	17.1	$c_{2/3/4}^{0.3}x_{5/4/3(Hex)}$	$^{1.4}a_{3/4(Hex)}y_{4/3}$	$^{0.3}a_{2(Hex)}$ $^{2.5}x_{2(Hex)}$
377.3498	8.2	14.8	$^{1.4}a_{2(Hex)}$		
449.3013	14.0	25.1	$b_{3/4}y_{4/3}$	$c_{3/4}z_{4/3}$	b2-Me
484.4431	48.8	87.4	c2		
557.5617	9.0	16.2	$^{3.5}a_{3(Hex)}$	$^{0.2}x_{3(Hex)}$	
585.4310	8.0	14.3	$b_{3/4}^{1.3}x_{5/4(Hex)}$	$b_{3/4}^{2.4}x_{5/4(Hex)}$	
634.5536	9.3	16.6	$^{1.5}a_{4(Hex)}y_4$	$^{2.4}x_{3(Hex)}$	
651.5373	10.8	19.4	$^{1.5}a_{3(Hex)}$		
662.5306	17.5	31.4	$c_4z_4$	b4y4	
679.6459	16.7	30.0	b3		
680.5035	14.1	25.3	$c_4y_4$		
690.5902	10.2	18.3	$b_4^{1.5}x_{5(Hex)}$		
697.6465	55.8	100.0	c3		
711.6185	45.5	81.5	y3		
739.6897	16.2	29.0	$c_4^{0.2}x_{5(Hex)}$	$^{1.5}x_{4(Hex)}$	
755.6354	13.2	23.7	$c_4^{2.5}x_{5(Hex)}$		
756.6701	13.7	24.6	$^{2.4}a_{4(Hex)}$		
847.8269	13.7	24.6	$^{2.4}x_{4(Hex)}$		
892.7233	18.0	32.3	b4		
910.8443	32.0	57.4	c4		
924.7490	19.7	35.4	y4		

#### O 5.3 perdeuteromethylated

m/z	intensity	relative intensity	annotation		
236.2101	11.4	36.9	b2y2	c2z2	b1-Me
271.2677	10.7	34.7	c1		
313.3942	5.6	18.2	C <sub>2</sub> <sup>0.2</sup> X <sub>3(Hex)</sub>		
319.3067	12.4	40.3	1.5 <sup>1.5</sup> X <sub>2(Hex)</sub>		
342.2481	4.6	14.8	b <sub>2</sub> <sup>0.3</sup> X <sub>3(Hex)</sub>		
344.3318	13.3	43.2	3.5 <sup>3.5</sup> a <sub>2(Hex)</sub>		
350.3291	5.6	18.2	0.2 <sup>0.2</sup> X <sub>2(Hex)</sub>		
358.0333	6.7	21.6	b <sub>2</sub> <sup>3.5</sup> X <sub>3(Hex)</sub>		
360.0765	5.6	18.2	C <sub>2</sub> <sup>0.3</sup> X <sub>3(Hex)</sub>	0.3 <sup>0.3</sup> a <sub>2(Hex)</sub>	
366.2118	6.7	21.6	2.5 <sup>2.5</sup> X <sub>2(Hex)</sub>		
376.2112	8.0	25.8	C <sub>2</sub> <sup>3.5</sup> X <sub>3(Hex)</sub>		
377.0608	19.5	63.1	1.4 <sup>1.4</sup> a <sub>2(Hex)</sub>		
391.3137	9.9	32.2	2.5 <sup>2.5</sup> a <sub>2(Hex)</sub>		
397.2153	6.7	21.6	0.3 <sup>0.3</sup> X <sub>2(Hex)</sub>		
407.0675	12.9	41.9	C <sub>2</sub> <sup>0.4</sup> X <sub>2(Hex)</sub>	0.2 <sup>0.2</sup> a <sub>2(Hex)</sub>	
427.2718	8.5	27.5	2.4 <sup>2.4</sup> X <sub>2(Hex)</sub>		
484.4873	12.9	41.9	c2		
504.4721	19.0	61.4	y2		
532.5600	30.8	100.0	1.5 <sup>1.5</sup> X <sub>3(Hex)</sub>		
610.3911	2.5	8.1	0.3 <sup>0.3</sup> X <sub>3(Hex)</sub>		
640.5718	2.9	9.3	1.3 <sup>1.3</sup> X <sub>3(Hex)</sub>	2.4 <sup>2.4</sup> X <sub>3(Hex)</sub>	
734.6345	10.5	33.9		M+Na <sup>+</sup>	

#### O 5.3 permethylated

m/z	intensity	relative intensity	annotation		
227.1210	79.8	14.5	b2y2	c2z2	b1-Me
255.1501	12.7	2.3	b <sub>2</sub> <sup>1.5</sup> X <sub>3(Hex)</sub>		
259.1215	18.9	3.4	c1		
276.1734	86.2	15.6	y1		
283.2385	10.9	2.0	b <sub>2</sub> <sup>0.3</sup> X <sub>3(Hex)</sub>		
299.2585	6.9	1.3	b <sub>2</sub> <sup>2.5</sup> X <sub>3(Hex)</sub>		
301.1775	16.9	3.1	C <sub>2</sub> <sup>0.3</sup> X <sub>3(Hex)</sub>		
304.1630	28.8	5.2	1.5 <sup>1.5</sup> X <sub>2(Hex)</sub>		
315.1461	21.5	3.9	2.4 <sup>2.4</sup> a <sub>2(Hex)</sub>		
329.2112	16.5	3.0	3.5 <sup>3.5</sup> a <sub>2(Hex)</sub>		
357.2186	17.2	3.1	b <sub>2</sub> <sup>1.3</sup> X <sub>3(Hex)</sub>	b <sub>2</sub> <sup>2.4</sup> X <sub>3(Hex)</sub>	
359.2300	19.1	3.5	1.4 <sup>1.4</sup> a <sub>2(Hex)</sub>		
373.1390	19.7	3.6	2.5 <sup>2.5</sup> a <sub>2(Hex)</sub>		
376.2261	10.6	1.9	0.3 <sup>0.3</sup> X <sub>2(Hex)</sub>		
389.2291	12.7	2.3	C <sub>2</sub> <sup>0.4</sup> X <sub>2(Hex)</sub>	0.2 <sup>0.2</sup> a <sub>2(Hex)</sub>	
417.2235	32.1	5.8	1.5 <sup>1.5</sup> a <sub>2(Hex)</sub>		
445.1884	79.1	14.4	b2		
463.2228	39.5	7.2	c2		
480.2487	266.9	48.4	y2		
508.2876	44.7	8.1	1.5 <sup>1.5</sup> X <sub>3(Hex)</sub>		
536.3064	35.8	6.5	0.2 <sup>0.2</sup> X <sub>3(Hex)</sub>		
566.3686	13.7	2.5	1.4 <sup>1.4</sup> X <sub>3(Hex)</sub>		
580.4839	18.2	3.3	0.3 <sup>0.3</sup> X <sub>3(Hex)</sub>		
596.1980	15.4	2.8	3.5 <sup>3.5</sup> X <sub>3(Hex)</sub>		
610.2998	39.3	7.1	1.3 <sup>1.3</sup> X <sub>3(Hex)</sub>	2.4 <sup>2.4</sup> X <sub>3(Hex)</sub>	
698.3535	551.0	100.0		M+Na <sup>+</sup>	

#### O 5.4 perdeuteromethylated

m/z	intensity	relative intensity	annotation		
236.2224	5.4	17.4	b <sub>2/3</sub> Y <sub>3/2</sub>	C <sub>2/3</sub> Z <sub>3/2</sub>	b1-Me
254.1735	3.5	11.5	C <sub>2/3</sub> Y <sub>3/2</sub>		
264.2075	5.1	16.6	b <sub>2/3</sub> <sup>1.5</sup> X <sub>4/3(Hex)</sub>		
271.2283	15.2	49.4	c1		
273.2037	3.0	9.8	z1		
282.2486	2.6	8.5	C <sub>2/3</sub> <sup>1.5</sup> X <sub>4/3(Hex)</sub>		
291.3104	5.9	19.1	y1		
295.3341	3.3	10.6	b <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	2.4 <sup>2.4</sup> a <sub>3(Hex)</sub> Z <sub>3</sub>	
309.1316	5.0	16.2	3.5 <sup>3.5</sup> a <sub>3(Hex)</sub> Z <sub>3</sub>		
311.2152	6.3	20.4	b <sub>2/3</sub> <sup>2.5</sup> X <sub>4/3(Hex)</sub>		
313.1956	4.8	15.7	2.4 <sup>2.4</sup> a <sub>3(Hex)</sub> Y <sub>3</sub>	C <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	
319.3145	13.9	45.1	1.5 <sup>1.5</sup> X <sub>2(Hex)</sub>		
325.3811	3.8	12.3	0.3 <sup>0.3</sup> a <sub>3(Hex)</sub> Z <sub>3</sub>	b <sub>2/3</sub> <sup>1.4</sup> X <sub>4/3(Hex)</sub>	
327.2378	4.3	14.0	3.5 <sup>3.5</sup> a <sub>3(Hex)</sub> Y <sub>3</sub>		
330.1178	4.7	15.3	2.4 <sup>2.4</sup> a <sub>2(Hex)</sub>		
342.4291	4.7	15.3	1.4 <sup>1.4</sup> a <sub>3(Hex)</sub> Z <sub>3</sub>	b <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	
344.4214	10.2	33.2	3.5 <sup>3.5</sup> a <sub>2(Hex)</sub>		

350.4335	5.9	19.1	$^{0.2}X_{2(\text{Hex})}$		
356.3809	5.6	18.3	$^{2.5}a_{3(\text{Hex})}Z_3$		
358.0305	4.3	14.0	$b_{2/3}^{3.5}X_{4/3(\text{Hex})}$		
366.2772	6.3	20.4	$^{2.5}X_{2(\text{Hex})}$		
372.2994	4.7	15.3	$^{0.2}a_{3(\text{Hex})}Z_3$	$b_{2/3}^{2.4}X_{4/3(\text{Hex})}$	$b_2^{1.3}X_{4(\text{Hex})}$
374.3782	9.5	31.1	$^{2.5}a_{3(\text{Hex})}Y_3$		
377.0986	24.4	79.6	$^{1.4}a_{2(\text{Hex})}$		
380.3459	5.9	19.1	$^{1.4}X_{2(\text{Hex})}$		
389.1261	4.6	14.9	$b_{2/3}^{0.4}X_{4/3(\text{Hex})}$		
391.4374	5.1	16.6	$^{2.5}a_{2(\text{Hex})}$		
397.1685	4.7	15.3	$^{0.3}X_{2(\text{Hex})}$		
403.3180	4.2	13.6	$^{1.5}a_{3(\text{Hex})}Z_3$		
413.3145	3.9	12.8	$^{3.5}X_{2(\text{Hex})}$		
449.4024	11.6	37.9	b3y3	c3z3	
484.4491	17.4	56.6	c2		
504.4422	23.8	77.4	y2		
526.3913	12.2	39.6	$c_3^{0.2}X_{4(\text{Hex})}$		
532.4769	30.7	100.0	$^{1.5}X_{3(\text{Hex})}$		
556.4380	7.3	23.8	$c_3^{1.4}X_{4(\text{Hex})}$		
557.5097	19.0	61.7	$^{3.5}a_{3(\text{Hex})}$		
563.5903	11.8	38.3	$^{0.2}X_{3(\text{Hex})}$		
679.5629	9.7	31.5	b3		
697.6075	15.2	49.4	c3		
717.6611	27.3	88.9	y3		
947.8015	26.1	85.1		M+Na <sup>+</sup>	

O 5.4 permethylated

m/z	intensity	relative intensity	annotation
227.0971	49.5	9.5	$b_{2/3}Y_{3/2}$ $C_{2/3}Z_{3/2}$
241.0482	13.9	2.7	b1
245.0944	11.2	2.2	$C_{2/3}Y_{3/2}$
255.0245	6.5	1.3	$b_{2/3}^{1.5}X_{4/3(\text{Hex})}$
258.1375	5.0	1.0	z1
259.1377	60.0	11.5	c1
273.1158	8.4	1.6	$C_{2/3}^{1.5}X_{4/3(\text{Hex})}$
276.1320	30.1	5.8	y1
283.2615	12.2	2.3	$^{2.4}a_{3(\text{Hex})}Z_3$ $b_{2/3}^{0.2}X_{4/3(\text{Hex})}$
297.1266	14.5	2.8	$^{3.5}a_{3(\text{Hex})}Z_3$
301.1114	23.1	4.4	$^{2.4}a_{3(\text{Hex})}Y_3$ $C_{2/3}^{0.2}X_{4/3(\text{Hex})}$
304.1449	85.1	16.3	$^{1.5}X_{2(\text{Hex})}$
313.0901	11.1	2.1	$b_{2/3}^{1.4}X_{4/3(\text{Hex})}$ $^{0.3}a_{3(\text{Hex})}Z_3$
315.1604	38.0	7.3	$^{3.5}a_{3(\text{Hex})}Y_3$ $^{2.4}a_{2(\text{Hex})}$
317.0989	9.9	1.9	$C_{2/3}^{2.5}X_{4/3(\text{Hex})}$
327.1640	6.4	1.2	$^{1.4}a_{3(\text{Hex})}Z_3$ $b_{2/3}^{0.2}X_{4/3(\text{Hex})}$
329.2245	67.1	12.9	$^{3.5}a_2$
331.1498	18.7	3.6	$C_{2/3}^{1.4}X_{4/3(\text{Hex})}$ $^{0.3}a_{3(\text{Hex})}Y_3$
332.1714	39.6	7.6	$^{0.2}X_{2(\text{Hex})}$
343.2259	13.9	2.7	$b_{2/3}^{3.5}X_{4/3(\text{Hex})}$
345.1635	8.6	1.7	$^{1.4}a_{3(\text{Hex})}Y_3$ $C_{2/3}^{0.2}X_{4/3(\text{Hex})}$ $^{0.3}a_{2(\text{Hex})}$
348.2403	9.2	1.8	$^{2.5}X_{2(\text{Hex})}$
357.2298	21.0	4.0	$b_{2/3}^{2.4}X_{4/3(\text{Hex})}$ $b_{2/3}^{1.3}X_{4/3(\text{Hex})}$ $^{0.2}a_{3(\text{Hex})}Z_3$
359.1776	30.3	5.8	$^{2.5}a_{3(\text{Hex})}Y_3$ $^{1.4}a_{2(\text{Hex})}$
361.1901	12.5	2.4	$C_{2/3}^{3.5}X_{4/3(\text{Hex})}$
362.1689	9.5	1.8	$^{1.4}X_{2(\text{Hex})}$
371.2185	18.3	3.5	$b_{2/3}^{0.4}X_{4/3(\text{Hex})}$
373.1747	16.1	3.1	$^{2.5}a_{2(\text{Hex})}$
375.1361	9.2	1.8	$^{0.3}a_{3(\text{Hex})}Y_3$ $C_{2/3}^{2.4}X_{4/3(\text{Hex})}$ $C_{2/3}^{1.3}X_{4/3(\text{Hex})}$
376.2549	8.2	1.6	$^{0.3}X_{2(\text{Hex})}$
385.2362	22.1	4.2	$^{1.5}a_{3(\text{Hex})}Z_3$
403.2095	24.2	4.6	$^{1.5}a_{3(\text{Hex})}Y_3$
406.3191	7.3	1.4	$^{2.4}X_{2(\text{Hex})}$
413.1461	20.1	3.9	b3z3
417.1553	24.8	4.8	$^{1.5}a_{2(\text{Hex})}$
431.1811	75.7	14.5	b3y3 c3z3
445.2459	45.2	8.7	b2
449.2121	37.9	7.3	c3y3
459.2733	22.5	4.3	$b_3^{1.5}X_{4(\text{Hex})}$
462.1928	34.4	6.6	z2
463.2017	244.4	46.9	c2
477.1715	33.3	6.4	$c_3^{1.5}X_{4(\text{Hex})}$
480.2171	406.3	77.9	y2
487.1318	13.3	2.6	$b_3^{0.2}X_{4(\text{Hex})}$

505.2202	156.5	30.0	$c_3^{0.2}x_4(\text{Hex})$		
508.2500	212.5	40.8	$^{1.5}x_3(\text{Hex})$		
517.2173	15.2	2.9	$b_3^{1.4}x_4(\text{Hex})$		
519.1773	47.5	9.1	$a_3^{2.4}(\text{Hex})$		
521.2483	15.6	3.0	$c_3^{2.5}x_4(\text{Hex})$		
531.2336	12.8	2.5	$b_3^{0.3}x_4(\text{Hex})$		
533.1844	131.6	25.2	$a_3^{3.5}(\text{Hex})$		
535.2838	77.0	14.8	$c_3^{1.4}x_4(\text{Hex})$		
536.2626	96.2	18.4	$x_3^{0.2}(\text{Hex})$		
547.2725	30.2	5.8	$b_3^{3.5}x_4(\text{Hex})$		
549.2532	31.8	6.1	$a_3^{0.3}(\text{Hex})$	$c_3^{0.3}x_4(\text{Hex})$	
561.2888	33.6	6.4	$b_3^{1.3}x_4(\text{Hex})$	$b_3^{2.4}x_4(\text{Hex})$	
563.2953	41.8	8.0	$a_3^{1.4}(\text{Hex})$		
565.2310	28.0	5.4	$c_3^{3.5}x_4(\text{Hex})$		
566.3120	16.3	3.1	$x_3^{1.4}(\text{Hex})$		
575.2612	21.4	4.1	$b_3^{0.4}x_4(\text{Hex})$		
577.3308	20.9	4.0	$a_3^{2.5}(\text{Hex})$		
579.3287	14.8	2.8	$c_3^{1.3}x_4(\text{Hex})$	$c_3^{2.4}x_4(\text{Hex})$	
580.3101	15.2	2.9	$x_3^{0.3}(\text{Hex})$		
593.2606	21.4	4.1	$a_3^{0.2}(\text{Hex})$	$c_3^{0.4}x_4(\text{Hex})$	
610.1487	12.2	2.3	$x_3^{2.4}(\text{Hex})$		
621.2425	36.7	7.0	$a_3^{1.5}(\text{Hex})$		
649.2460	52.4	10.1	b3		
666.2387	45.5	8.7	z3		
667.2525	187.1	35.9	c3		
684.3196	521.6	100.0	y3		
712.3476	206.7	39.6	$^{1.5}x_4(\text{Hex})$		
740.4403	76.6	14.7	$x_4^{0.2}(\text{Hex})$		
814.5787	17.6	3.4	$x_4^{1.3}(\text{Hex})$	$x_4^{2.4}(\text{Hex})$	
828.3466	30.7	5.9	$x_4^{0.4}(\text{Hex})$		
902.5205	124.2	23.8		M+Na <sup>+</sup>	

O 6.3 permethylated

m/z	intensity	relative intensity	annotation		
209.1087	16.9	14.9	b2z2		
227.0715	45.9	40.5	b2y2	c2z2	b1-Me
241.0983	21.0	18.6	b1		
245.1532	16.5	14.5	c2y2		
255.1051	18.4	16.3	$b_2^{1.5}x_3(\text{Hex})$		
259.1022	21.3	18.8	c1		
271.1551	16.6	14.6	z1		
273.1867	15.2	13.4	$c_2^{1.5}x_3(\text{Hex})$		
283.1198	11.8	10.4	$b_2^{0.2}x_3(\text{Hex})$		
289.1346	86.5	76.4	y1		
299.1136	15.8	14.0	$b_2^{2.5}x_3(\text{Hex})$		
301.0868	22.5	19.8	$c_2^{0.2}x_3(\text{Hex})$		
313.1479	13.5	11.9	$b_2^{1.4}x_3(\text{Hex})$		
315.1123	24.4	21.6	$a_2^{2.4}(\text{Hex})$		
317.1386	55.6	49.0	$x_2^{1.5}(\text{Hex})$	$c_2^{2.5}x_3(\text{Hex})$	
327.0869	17.6	15.6	$b_2^{0.3}x_3(\text{Hex})$		
329.1237	24.8	21.9	$a_2^{3.5}(\text{Hex})$		
331.1101	14.5	12.8	$c_2^{1.4}x_3(\text{Hex})$		
345.1570	22.1	19.5	$c_2^{0.3}x_3(\text{Hex})$	$a_2^{0.3}(\text{Hex})$	$x_2^{0.2}(\text{Hex})$
357.1348	23.9	21.1	$b_2^{1.3}x_3(\text{Hex})$	$b_2^{2.4}x_3(\text{Hex})$	
359.1464	19.9	17.5	$a_2^{1.4}(\text{Hex})$		
361.1341	15.8	14.0	$c_2^{3.5}x_3(\text{Hex})$		
361.2233	13.6	12.0	$x_2^{2.5}(\text{Hex})$		
371.1267	25.0	22.0	$b_2^{0.4}x_3(\text{Hex})$		
373.2084	14.4	12.7	$a_2^{2.5}(\text{Hex})$		
375.1446	19.9	17.5	$c_2^{1.3}x_3(\text{Hex})$	$c_2^{2.4}x_3(\text{Hex})$	
375.2961	12.8	11.3	$x_2^{1.4}(\text{Hex})$		
389.1808	12.3	10.8	$c_2^{0.4}x_3(\text{Hex})$	$c_2^{0.2}x_3(\text{Hex})$	
389.3660	11.1	9.8	$x_2^{0.3}(\text{Hex})$		
405.1805	20.5	18.1	$x_2^{3.5}(\text{Hex})$		
417.1488	23.4	20.6	$a_2^{1.5}(\text{Hex})$		
419.3265	20.0	17.6	$x_2^{2.4}(\text{Hex})$		
445.1845	69.8	61.6	b2		
463.1898	84.8	74.9	c2		
475.1801	20.8	18.3	z2		
493.1639	113.3	100.0	y2		
521.3022	38.2	33.7	$^{1.5}x_3(\text{Hex})$		

549.2107	29.7	26.2	$^{0.2}X_3(\text{Hex})$	
579.2288	23.1	20.4	$^{1.4}X_3(\text{Hex})$	
593.2808	22.5	19.8	$^{0.3}X_3(\text{Hex})$	
609.3303	13.7	12.1	$^{3.5}X_3(\text{Hex})$	
623.2399	14.9	13.1	$^{1.3}X_3(\text{Hex})$	$^{2.4}X_3(\text{Hex})$
637.2317	24.7	21.8	$^{0.4}X_3(\text{Hex})$	
711.3162	39.2	34.6		M+Na <sup>+</sup>

O 6.4 perdeuteromethylated

m/z	intensity	relative intensity	annotation	
236.1951	12.8	23.1	$b_{2/3}V_{3/2}$	$C_{2/3}Z_{3/2}$ b1-Me
253.1779	7.5	13.4	b1	
254.1926	6.1	11.0	$C_{2/3}V_{3/2}$	
264.2005	11.2	20.1	$b_{2/3}^{1.5}X_{4/3}(\text{Hex})$	
271.1948	11.9	21.4	c1	
282.2391	7.3	13.1	$C_{2/3}^{1.5}X_{4/3}(\text{Hex})$	
304.2397	27.7	50.0	y1	
309.2550	8.8	15.9	$a_{3(\text{Hex})}Z_3$	
311.2838	29.4	53.0	$b_{2/3}^{2.5}X_{4/3}(\text{Hex})$	
313.1815	9.8	17.7	$C_{2/3}^{0.2}X_{4/3}(\text{Hex})$	$^{2.4}a_{3(\text{Hex})}Y_3$
325.2808	6.4	11.5	$b_{2/3}^{1.4}X_{4/3}(\text{Hex})$	$^{0.3}a_{3(\text{Hex})}Z_3$
327.2497	7.6	13.8	$a_{3(\text{Hex})}Y_3$	
330.1859	9.4	17.0	$a_{2(\text{Hex})}^{2.4}$	
332.2265	18.2	32.9	$^{1.5}X_{2(\text{Hex})}$	
343.1891	6.3	11.3	$C_{2/3}^{1.4}X_{4/3}(\text{Hex})$	$^{0.3}a_{3(\text{Hex})}Y_3$
344.2577	6.2	11.1	$a_{2(\text{Hex})}^{3.5}$	
356.1832	5.8	10.4	$a_{3(\text{Hex})}Z_3$	
358.3040	7.0	12.5	$b_{2/3}^{3.5}X_{4/3}(\text{Hex})$	
360.2537	6.6	11.8	$C_{2/3}^{0.3}X_{4/3}(\text{Hex})$	$^{0.3}a_{3(\text{Hex})}$ $^{1.4}a_{3(\text{Hex})}Y_3$
363.2477	8.3	15.0	$^{0.2}X_{2(\text{Hex})}$	
372.2754	5.9	10.6	$a_{3(\text{Hex})}Z_3$	$b_{2/3}^{2.4}X_{4/3}(\text{Hex})$ $b_2^{1.3}X_{4(\text{Hex})}$
374.2031	9.0	16.3	$a_{3(\text{Hex})}Y_3$	
376.2870	9.2	16.6	$C_{2/3}^{3.5}X_{4/3}(\text{Hex})$	
377.3161	10.6	19.1	$a_{2(\text{Hex})}^{1.4}$	
389.3453	6.9	12.4	$b_2^{0.4}X_{4(\text{Hex})}$	
390.2383	6.8	12.2	$C_{2/3}^{2.4}X_{4/3}(\text{Hex})$	$^{0.2}a_{3(\text{Hex})}Y_3$ $C_2^{1.3}X_{4(\text{Hex})}$
393.3565	6.5	11.7	$^{1.4}X_{2(\text{Hex})}$	
403.1317	6.9	12.4	$a_{3(\text{Hex})}Z_3$	
407.2146	8.5	15.4	$a_{2(\text{Hex})}^{0.2}$	$C_2^{0.4}X_{4(\text{Hex})}$
431.3416	8.4	15.2	b3z3	
438.2764	8.2	14.8	$a_{2(\text{Hex})}^{1.5}$	
449.2975	14.3	25.8	b3y3	c3z3 b2-Me
466.3443	28.4	51.2	b2	
467.4247	12.4	22.3	c3y3	
484.3344	39.9	71.9	c2	
499.3473	10.0	18.0	z2	
508.3334	11.1	20.0	$b_3^{0.2}X_{4(\text{Hex})}$	
517.3304	55.5	100.0	y2	
526.3362	10.5	18.9	$C_3^{0.2}X_{4(\text{Hex})}$	
538.2498	10.0	18.0	$b_3^{1.4}X_{4(\text{Hex})}$	
543.3817	13.0	23.5	$a_{3(\text{Hex})}^{2.4}$	
545.3903	18.2	32.9	$^{1.5}X_{3(\text{Hex})}$	
555.3055	8.9	16.1	$b_3^{0.3}X_{4(\text{Hex})}$	
556.4498	12.5	22.6	$C_3^{1.4}X_{4(\text{Hex})}$	
557.4474	19.4	35.0	$a_{3(\text{Hex})}^{3.5}$	
571.4350	8.9	16.1	$b_3^{3.5}X_{4(\text{Hex})}$	
576.4252	7.9	14.3	$^{0.2}X_{3(\text{Hex})}$	
651.4227	13.7	24.7	$a_{3(\text{Hex})}^{1.5}$	
679.4700	43.5	78.4	b3	
697.4683	27.5	49.5	c3	
712.4766	15.6	28.1	z3	
730.5333	21.6	38.9	y3	
758.5730	17.5	31.4	$^{1.5}X_{4(\text{Hex})}$	
960.8300	10.5	18.8		M+Na <sup>+</sup>

O 6.4 permethylated

m/z	intensity	relative intensity	annotation	
209.0107	10.7	13.9	$b_{2/3}Z_{3/2}$	
227.0726	21.8	28.2	$b_{2/3}V_{3/2}$	$C_{2/3}Z_{3/2}$ b1-Me
241.0214	11.6	15.0	b1	
245.1399	8.6	11.1	$C_{2/3}V_{3/2}$	
255.1442	6.0	7.8	$b_{2/3}^{1.5}X_{4/3}(\text{Hex})$	



259.1078	9.5	12.3 c1		
271.1592	14.4	18.6 z1		
273.0577	8.0	10.3 C <sub>2/3</sub> <sup>1.5</sup> X <sub>4/3(Hex)</sub>		
283.1749	13.7	17.7 b <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	<sup>2.4</sup> a <sub>3(Hex)Z3</sub>	
289.0704	30.3	39.2 y1		
297.1703	5.6	7.3 <sup>3.5</sup> a <sub>3(Hex)Z3</sub>		
299.1592	6.5	8.4 b <sub>2/3</sub> <sup>2.5</sup> X <sub>4/3(Hex)</sub>		
301.1009	9.2	11.8 C <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	<sup>2.4</sup> a <sub>3(Hex)Y3</sub>	
317.1138	14.1	18.2 C <sub>2/3</sub> <sup>2.5</sup> X <sub>4/3(Hex)</sub>	<sup>1.5</sup> X <sub>2(Hex)</sub>	
327.1496	8.5	11.0 b <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	<sup>1.4</sup> a <sub>3(Hex)Z3</sub>	
329.1816	11.5	14.9 <sup>3.5</sup> a <sub>2</sub>		
331.1916	9.0	11.7 C <sub>2/3</sub> <sup>1.4</sup> X <sub>4/3(Hex)</sub>	<sup>0.3</sup> a <sub>3(Hex)Y3</sub>	
341.1622	5.6	7.3 <sup>2.5</sup> a <sub>2Z3</sub>		
343.0936	5.9	7.6 b <sub>2/3</sub> <sup>3.5</sup> X <sub>4/3(Hex)</sub>		
345.1174	8.5	11.0 C <sub>2/3</sub> <sup>0.2</sup> X <sub>4/3(Hex)</sub>	<sup>0.3</sup> a <sub>2(Hex)</sub>	<sup>1.4</sup> a <sub>3(Hex)Y3</sub>
345.2043	7.1	9.1 <sup>0.2</sup> X <sub>2(Hex)</sub>		
357.1223	4.6	5.9 b <sub>2/3</sub> <sup>1.3</sup> X <sub>4/3(Hex)</sub>	b <sub>2/3</sub> <sup>2.4</sup> X <sub>4/3(Hex)</sub>	<sup>0.2</sup> a <sub>3(Hex)Z3</sub>
359.0991	6.3	8.1 <sup>1.4</sup> a <sub>2(Hex)</sub>	<sup>2.5</sup> a <sub>3(Hex)Y3</sub>	
361.0815	5.2	6.8 C <sub>2/3</sub> <sup>3.5</sup> X <sub>4/3(Hex)</sub>		
361.1704	4.3	5.6 <sup>2.5</sup> X <sub>2(Hex)</sub>		
371.2572	11.1	14.4 b <sub>2/3</sub> <sup>0.4</sup> X <sub>4/3(Hex)</sub>		
373.0023	8.8	11.3 <sup>2.5</sup> a <sub>2(Hex)</sub>		
389.2038	8.0	10.3 <sup>0.2</sup> a <sub>3(Hex)</sub>	C <sub>2/3</sub> <sup>0.4</sup> X <sub>4/3(Hex)</sub>	<sup>0.3</sup> X <sub>2(Hex)</sub>
403.1511	13.1	16.9 <sup>1.5</sup> a <sub>3(Hex)Y3</sub>		
417.2853	14.1	18.2 <sup>1.5</sup> a <sub>2(Hex)</sub>		
419.2014	11.2	14.5 <sup>2.4</sup> X <sub>2(Hex)</sub>		
431.1489	20.5	26.5 b3y3	c3z3	b2-Me
445.2110	28.1	36.3 b2		
449.3090	12.8	16.6 c3y3		
459.2022	12.4	16.0 b <sub>3</sub> <sup>1.5</sup> X <sub>4(Hex)</sub>		
463.1634	35.3	45.6 c2		
475.1854	8.6	11.1 z2		
477.1987	7.3	9.5 C <sub>3</sub> <sup>1.5</sup> X <sub>4(Hex)</sub>		
493.1489	77.4	100.0 y2		
503.2408	6.4	8.3 b <sub>3</sub> <sup>2.5</sup> X <sub>4(Hex)</sub>		
505.2084	5.5	7.1 C <sub>3</sub> <sup>0.2</sup> X <sub>4(Hex)</sub>		
521.1622	25.2	32.6 C <sub>3</sub> <sup>2.5</sup> X <sub>4(Hex)</sub>	<sup>1.5</sup> X <sub>3(Hex)</sub>	
531.1450	8.0	10.3 b <sub>3</sub> <sup>0.3</sup> X <sub>4(Hex)</sub>		
533.1676	24.4	31.6 <sup>3.5</sup> a <sub>3(Hex)</sub>		
547.2531	9.9	12.8 b <sub>3</sub> <sup>3.5</sup> X <sub>4(Hex)</sub>		
549.3068	13.5	17.4 <sup>0.3</sup> a <sub>3(Hex)</sub>	C <sub>3</sub> <sup>0.3</sup> X <sub>4(Hex)</sub>	<sup>0.2</sup> X <sub>3(Hex)</sub>
561.2668	8.0	10.3 b <sub>3</sub> <sup>1.3</sup> X <sub>4(Hex)</sub>	b <sub>3</sub> <sup>2.4</sup> X <sub>4(Hex)</sub>	
563.2729	11.5	14.9 <sup>1.4</sup> a <sub>3(Hex)</sub>		
593.2322	12.0	15.5 <sup>0.2</sup> a <sub>3(Hex)</sub>	C <sub>3</sub> <sup>0.4</sup> X <sub>4(Hex)</sub>	<sup>0.3</sup> X <sub>3(Hex)</sub>
649.3259	42.6	55.1 b3		
667.3301	25.1	32.4 c3		
697.2766	26.4	34.1 y3		
725.3984	26.3	34.0 <sup>1.5</sup> X <sub>4(Hex)</sub>		
783.3575	10.7	13.9 <sup>1.4</sup> X <sub>4(Hex)</sub>		
915.3971	10.9	14.1	M+Na <sup>+</sup>	

O 6.5 perdeuteromethylated

m/z	intensity	relative intensity	annotation	
218.1755	7.8	15.9	b <sub>2/3/4</sub> <sup>z4/3/2</sup>	
236.1886	13.3	27.0	b <sub>2/3/4</sub> <sup>Y4/3/2</sup>	C <sub>2/3/4</sub> <sup>z4/3/2</sup> b1-Me
253.1951	8.8	17.7	b1	
254.1588	6.1	12.4	C <sub>2/3/4</sub> <sup>Y4/3/2</sup>	
264.1759	4.8	9.8	b <sub>2/3/4</sub> <sup>1.5</sup> X <sub>5/4/3(Hex)</sub>	
271.2357	6.5	13.2	c1	
282.2373	5.1	10.3	C <sub>2/3/4</sub> <sup>1.5</sup> X <sub>5/4/3(Hex)</sub>	
304.2288	17.3	34.9	y1	
309.2356	8.4	16.9	<sup>3.5</sup> a <sub>3/4(Hex)Z4/3</sub>	
311.1787	6.5	13.2	b <sub>2/3/4</sub> <sup>2.5</sup> X <sub>5/4/3(Hex)</sub>	
313.2655	5.0	10.1	C <sub>2/3/4</sub> <sup>0.2</sup> X <sub>5/4/3(Hex)</sub>	<sup>2.4</sup> a <sub>3/4(Hex)Y4/3</sub>
325.2617	9.2	18.5	b <sub>2/3/4</sub> <sup>1.4</sup> X <sub>5/4/3(Hex)</sub>	<sup>0.3</sup> a <sub>3/4(Hex)Z4/3</sub>
327.2834	7.1	14.3	<sup>3.5</sup> a <sub>3/4(Hex)Y4/3</sub>	
329.1703	4.3	8.7	C <sub>2/3/4</sub> <sup>2.5</sup> X <sub>5/4/3(Hex)</sub>	
330.2430	14.6	29.6	<sup>2.4</sup> a <sub>2(Hex)</sub>	
332.2519	11.8	23.8	<sup>1.5</sup> X <sub>2(Hex)</sub>	
342.2169	5.9	11.9	b <sub>2/3/4</sub> <sup>0.3</sup> X <sub>5/4/3(Hex)</sub>	<sup>1.4</sup> a <sub>3/4(Hex)Z4/3</sub>
343.3398	6.4	13.0	C <sub>2/3/4</sub> <sup>1.4</sup> X <sub>5/4/3(Hex)</sub>	<sup>0.3</sup> a <sub>3/4(Hex)Y4/3</sub>

344.3202	7.5	15.1	$^{3.5}a_{2(\text{Hex})}$		
356.2843	7.7	15.6	$^{2.5}a_{3/4(\text{Hex})Z_{4/3}}$		
358.3132	6.5	13.2	$b_{2/3/4}^{3.5}X_{5/4/3(\text{Hex})}$		
360.2003	12.3	24.9	$C_{2/3/4}^{0.3}X_{5/4/3(\text{Hex})}$	$^{0.3}a_{2(\text{Hex})}$	$^{1.4}a_{3/4(\text{Hex})Y_{4/3}}$
363.3667	8.1	16.4	$^{0.2}x_{2(\text{Hex})}$		
372.1692	8.5	17.2	$^{0.2}a_{3/4(\text{Hex})Z_{4/3}}$	$b_{2/3/4}^{2.4}X_{5/4/3(\text{Hex})}$	$b_{2/3/4}^{1.3}X_{5/4/3(\text{Hex})}$
374.2737	10.2	20.6	$^{2.5}a_{3/4(\text{Hex})Y_{4/3}}$		
390.0345	5.4	10.8	$^{2.5}x_{2(\text{Hex})}$		
391.2653	6.9	14.0	$^{2.5}a_{2(\text{Hex})}$		
393.3004	5.9	11.9	$^{1.4}x_{2(\text{Hex})}$		
403.2127	6.7	13.5	$^{1.5}a_{3/4(\text{Hex})Z_{4/3}}$		
407.2253	6.7	13.5	$^{0.2}a_{2(\text{Hex})}$	$C_{2/3/4}^{0.4}X_{5/4/3(\text{Hex})}$	
431.3375	7.5	15.1	$b_{3/4}Z_{4/3}$		
438.4543	7.5	15.1	$^{1.5}a_{2(\text{Hex})}$		
440.2183	6.8	13.8	$^{2.4}x_{2(\text{Hex})}$		
449.3895	11.2	22.8	$b_{3/4}Y_{4/3}$	$C_{3/4}Z_{4/3}$	b2-Me
466.4368	16.2	32.8	b2		
467.4814	20.1	40.7	$C_{3/4}Y_{4/3}$		
484.4942	22.9	46.3	c2		
495.3367	12.9	26.2	$C_{2/3}^{1.5}X_{5/4(\text{Hex})}$		
499.4778	10.2	20.6	z2		
508.3755	11.6	23.5	$C_{3/4}^{0.2}X_{5/4(\text{Hex})}$	$^{2.4}a_{4(\text{Hex})Z_4}$	
517.4599	49.4	100.0	y2		
522.3004	12.3	24.9	$a_{4(\text{Hex})Z_4}$		
524.4075	10.2	20.6	$b_{3/4}^{2.5}X_{5/4(\text{Hex})}$		
538.4808	9.8	19.8	$b_{3/4}^{1.4}X_{5/4(\text{Hex})}$	$^{0.3}a_{4(\text{Hex})Z_4}$	
542.3653	9.4	19.0	$C_{3/4}^{2.5}X_{5/4(\text{Hex})}$		
543.3841	7.8	15.9	$^{2.4}a_{3(\text{Hex})}$		
545.4612	16.7	33.9	$^{1.5}x_{3(\text{Hex})}$		
569.4332	8.2	16.7	$^{2.5}a_{4(\text{Hex})Z_4}$		
571.5605	8.4	16.9	$b_{3/4}^{3.5}X_{5/4(\text{Hex})}$		
585.3919	9.8	19.8	$b_{3/4}^{2.4}X_{5/4(\text{Hex})}$	$^{0.2}a_{4(\text{Hex})Z_4}$	$b_{3/4}^{1.3}X_{5/4(\text{Hex})}$
587.4736	7.8	15.9	$^{2.5}a_{4(\text{Hex})Y_4}$		
590.5843	8.1	16.4	$a_{3(\text{Hex})}$		
606.3790	11.4	23.0	$^{1.4}x_{3(\text{Hex})}$		
644.5518	13.6	27.5	b4z4		
651.4824	10.1	20.4	$^{1.5}a_{3(\text{Hex})}$		
679.5431	18.7	37.8	b3		
680.5229	12.0	24.3	c4y4		
697.6625	35.7	72.2	c3		
712.5094	27.3	55.3	z3		
721.5280	18.4	37.3	$b_4^{0.2}X_{5(\text{Hex})}$		
730.6471	29.7	60.1	y3		
737.5674	15.3	31.0	$b_4^{2.5}X_{5(\text{Hex})}$		
739.5691	18.6	37.6	$C_4^{0.2}X_{5(\text{Hex})}$		
755.6391	20.5	41.5	$C_4^{2.5}X_{5(\text{Hex})}$		
758.7017	21.3	43.1	$^{1.5}x_{4(\text{Hex})}$		
769.5792	12.5	25.4	$C_4^{1.4}X_{5(\text{Hex})}$		
770.7105	12.2	24.6	$^{3.5}a_{4(\text{Hex})}$		
786.6380	12.5	25.4	$^{0.3}a_{4(\text{Hex})}$	$C_4^{0.3}X_{5(\text{Hex})}$	
816.7058	13.2	26.7	$C_4^{1.3}X_{5(\text{Hex})}$	$C_4^{2.4}X_{5(\text{Hex})}$	
864.7153	12.7	25.7	$^{1.5}a_{4(\text{Hex})}$		
943.7362	19.0	38.4	y4		

#### O 6.5 permethylated

m/z	intensity	relative intensity	annotation
209.1211	4.3	3.9	$b_{2/3/4}Z_{4/3/2}$
227.0677	15.4	14.1	$b_{2/3/4}Y_{4/3/2}$ $C_{2/3/4}Z_{4/3/2}$ b1-Me
241.0915	8.2	7.5	b1
245.0829	7.6	6.9	$C_{2/3/4}Y_{4/3/2}$
255.0952	4.2	3.8	$b_{2/3/4}^{1.5}X_{5/4/3(\text{Hex})}$
259.0772	6.4	5.8	c1
271.0829	6.7	6.1	z1
273.0294	11.6	10.6	$C_{2/3/4}^{1.5}X_{5/4/3(\text{Hex})}$
283.0772	16.5	15.0	$b_{2/3/4}^{0.2}X_{5/4/3(\text{Hex})}$ $^{2.4}a_{3/4(\text{Hex})Z_{4/3}}$
289.1203	28.1	25.6	y1
297.1269	6.8	6.2	$^{3.5}a_{3/4(\text{Hex})Z_{4/3}}$
299.0855	8.0	7.3	$b_{2/3/4}^{2.5}X_{5/4/3(\text{Hex})}$
301.0775	6.9	6.3	$C_{2/3/4}^{0.2}X_{5/4/3(\text{Hex})}$ $^{2.4}a_{3/4(\text{Hex})Y_{4/3}}$
313.1433	8.5	7.7	$b_{2/3/4}^{1.4}X_{5/4/3(\text{Hex})}$ $^{0.3}a_{3/4(\text{Hex})Z_{4/3}}$
315.1823	6.4	5.8	$^{2.4}a_{2(\text{Hex})}$ $^{3.5}a_{3/4(\text{Hex})Y_{4/3}}$

317.1726	14.6	13.3	$C_{2/3/4}^{2.5} X_{5/4/3}(\text{Hex})$	$^{1.5}X_2(\text{Hex})$		
327.1354	2.5	2.3	$b_{2/3/4}^{0.3} X_{5/4/3}(\text{Hex})$	$^{1.4}a_{3/4}(\text{Hex})Z_{4/3}$		
329.1355	5.9	5.4	$^{3.5}a_2(\text{Hex})$			
331.0569	5.4	4.9	$C_{2/3/4}^{1.4} X_{5/4/3}(\text{Hex})$	$^{0.3}a_{3/4}(\text{Hex})Y_{4/3}$		
341.1798	8.0	7.3	$^{2.5}a_{3/4}(\text{Hex})Z_{4/3}$			
343.1078	5.5	5.0	$b_{2/3/4}^{3.5} X_{5/4/3}(\text{Hex})$			
345.1279	3.7	3.3	$C_{2/3/4}^{0.3} X_{5/4/3}(\text{Hex})$	$^{0.3}a_2(\text{Hex})$	$^{1.4}a_{3/4}(\text{Hex})Y_{4/3}$	
357.1108	9.7	8.8	$b_{2/3/4}^{2.4} X_{5/4/3}(\text{Hex})$	$b_{2/3/4}^{1.3} X_{5/4/3}(\text{Hex})$	$^{0.2}a_{3/4}(\text{Hex})Z_{4/3}$	
359.1429	9.9	9.1	$^{2.5}a_{3/4}(\text{Hex})Y_{4/3}$	$^{1.4}a_2(\text{Hex})$		
361.1808	5.5	5.0	$C_{2/3/4}^{3.5} X_{5/4/3}(\text{Hex})$	$^{2.5}X_2(\text{Hex})$		
371.1288	10.2	9.3	$b_{2/3/4}^{0.4} X_{5/4/3}(\text{Hex})$			
373.2010	6.9	6.3	$^{2.5}a_2(\text{Hex})$			
375.1887	6.3	5.7	$C_{2/3/4}^{2.4} X_{5/4/3}(\text{Hex})$	$^{0.2}a_{3/4}(\text{Hex})Y_{4/3}$	$C_{2/3/4}^{1.3} X_{5/4/3}(\text{Hex})$	$^{1.4}X_2(\text{Hex})$
385.1464	5.1	4.6	$^{1.5}a_{3/4}(\text{Hex})Z_{4/3}$			
389.2220	5.1	4.6	$^{0.2}a_2(\text{Hex})$	$C_{2/3/4}^{0.4} X_{5/4/3}(\text{Hex})$	$^{0.3}X_2(\text{Hex})$	
403.1734	8.6	7.9	$^{1.5}a_{3/4}(\text{Hex})Y_{4/3}$			
405.2407	7.6	6.9	$^{3.5}X_2(\text{Hex})$			
413.1517	6.4	5.8	$b_{3/4}Z_{4/3}$			
417.1842	11.2	10.3	$^{1.5}a_2(\text{Hex})$			
419.1919	11.0	10.0	$^{2.4}X_2(\text{Hex})$			
431.1797	16.7	15.3	$b_{3/4}Y_{4/3}$	$C_{3/4}Z_{4/3}$	<b>b2-Me</b>	
445.1803	18.8	17.2	<b>b2</b>			
449.2696	9.0	8.2	$C_{3/4}Y_{4/3}$			
463.1948	19.3	17.6	<b>c2</b>			
475.2595	12.9	11.8	<b>z2</b>			
477.2686	6.8	6.2	$C_{2/3}^{1.5} X_{5/4}(\text{Hex})$			
493.1159	109.7	100.0	<b>y2</b>			
501.2959	6.1	5.6	$^{3.5}a_4(\text{Hex})Z_4$			
503.1502	8.0	7.3	$b_{3/4}^{2.5} X_{5/4}(\text{Hex})$			
505.2186	9.3	8.5	$C_{3/4}^{0.2} X_{5/4}(\text{Hex})$	$^{2.4}a_4(\text{Hex})Y_4$		
519.2132	6.7	6.1	$^{2.4}a_3(\text{Hex})$	$^{3.5}a_4(\text{Hex})Y_4$		
521.1724	19.1	17.4	$C_{3/4}^{2.5} X_{5/4}(\text{Hex})$			
521.2794	27.7	25.3	$^{1.5}X_3(\text{Hex})$			
531.2406	9.3	8.5	$a_4(\text{Hex})Z_4$	$b_{3/4}^{0.3} X_{5/4}(\text{Hex})$		
533.3310	10.5	9.5	$^{3.5}a_3(\text{Hex})$			
535.2448	6.4	5.8	$C_{3/4}^{1.5} X_{5/4}(\text{Hex})$	$^{0.3}a_4(\text{Hex})Y_4$		
545.1219	6.5	6.0	$^{2.5}a_4(\text{Hex})Z_4$			
547.3131	5.0	4.5	$b_{3/4}^{3.5} X_{5/4}(\text{Hex})$			
549.2524	4.6	4.2	$^{0.2}a_3(\text{Hex})$	$^{1.4}a_4(\text{Hex})Y_4$	$C_{3/4}^{0.3} X_{5/4}(\text{Hex})$	
549.3623	5.9	5.4	$^{0.2}X_3(\text{Hex})$			
561.2949	10.8	9.9	$^{0.2}a_4(\text{Hex})Z_4$	$b_{3/4}^{2.4} X_{5/4}(\text{Hex})$	$b_{3/4}^{1.3} X_{5/4}(\text{Hex})$	
563.1851	3.5	3.2	$^{1.4}a_3(\text{Hex})$	$^{2.5}a_4(\text{Hex})Y_4$		
565.2644	5.8	5.2	$C_{3/4}^{3.5} X_{5/4}(\text{Hex})$	$^{2.5}X_3(\text{Hex})$		
575.1569	6.0	5.5	$b_{3/4}^{0.4} X_{5/4}(\text{Hex})$			
577.1835	9.0	8.2	$^{2.5}a_3(\text{Hex})$			
579.3643	6.4	5.8	$C_{3/4}^{2.4} X_{5/4}(\text{Hex})$	$^{0.2}a_4(\text{Hex})Y_4$	$C_{3/4}^{1.3} X_{5/4}(\text{Hex})$	$^{1.4}X_3(\text{Hex})$
589.1918	10.5	9.5	$^{1.5}a_4(\text{Hex})Z_4$			
593.1845	6.8	6.2	$^{0.2}a_3(\text{Hex})$	$C_{3/4}^{0.4} X_{5/4}(\text{Hex})$	$^{0.3}X_3(\text{Hex})$	
607.3641	5.1	4.6	$^{1.5}a_4(\text{Hex})Y_4$			
609.2548	4.4	4.1	$^{3.5}X_3(\text{Hex})$			
617.3140	9.0	8.2	<b>b4z4</b>			
621.2079	15.7	14.3	$^{1.5}a_3(\text{Hex})$			
623.3158	3.5	3.2	$^{2.4}X_3(\text{Hex})$			
635.2113	19.1	17.4	<b>b4y4</b>	<b>c4z4</b>	<b>b3-Me</b>	
649.2547	34.5	31.5	<b>b3</b>			
653.2502	11.9	10.8	<b>c4y4</b>			
663.2133	8.4	7.6	$b_4^{1.5} X_{5}(\text{Hex})$			
667.2120	31.0	28.2	<b>c3</b>			
679.3638	11.6	10.6	<b>z3</b>			
681.2433	10.5	9.5	$C_4^{1.5} X_5(\text{Hex})$			
691.1335	6.7	6.1	$b_4^{0.2} X_5(\text{Hex})$			
697.2433	56.2	51.3	<b>y3</b>			
707.3348	8.5	7.7	$b_4^{2.5} X_5(\text{Hex})$			
709.2534	8.6	7.9	$C_4^{0.2} X_5(\text{Hex})$			
721.3686	13.3	12.2	$b_4^{1.4} X_5(\text{Hex})$			
723.3067	13.6	12.4	$^{2.4}a_4(\text{Hex})$			
725.3741	22.5	20.5	$C_4^{2.5} X_5(\text{Hex})$	$^{1.5}X_4(\text{Hex})$		
735.3312	6.1	5.6	$b_4^{0.3} X_5(\text{Hex})$			
737.2458	14.9	13.6	$^{3.5}a_4(\text{Hex})$			
739.4188	6.9	6.3	$C_4^{1.4} X_5(\text{Hex})$			

751.3643	12.5	11.4 $b_4^{3.5} X_{5(\text{Hex})}$	
753.3002	7.3	6.7 $c_4^{0.3} X_{5(\text{Hex})}$	$^{0.3} a_{4(\text{Hex})}$
753.3863	5.9	5.4 $x_4^{0.2} X_{4(\text{Hex})}$	
765.4031	6.7	6.1 $b_4^{1.3} X_{5(\text{Hex})}$	$b_4^{2.4} X_{5(\text{Hex})}$
769.3143	9.0	8.2 $x_4^{2.5} X_{4(\text{Hex})}$	
779.3123	10.1	9.2 $b_4^{0.4} X_{5(\text{Hex})}$	
781.2847	10.6	9.7 $a_4^{2.5} X_{4(\text{Hex})}$	
825.3261	14.5	13.2 $a_4^{1.5} X_{4(\text{Hex})}$	
853.4013	43.8	39.9 b4	
871.3034	17.6	16.1 c4	
883.3131	15.7	14.3 z4	
901.3916	25.0	22.8 y4	
929.4136	19.3	17.6 $x_4^{1.5} X_{5(\text{Hex})}$	
1001.5746	13.5	12.3 $x_4^{0.3} X_{5(\text{Hex})}$	