Mass Spectrometry-Based Characterization of New Spirolides from *Alexandrium ostenfeldii* (Dinophyceae)

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Figure S1. HRMS/MS spectrum of compound **1** (670>164) from AON 24.



Figure S2. HRMS/MS spectrum of compound 2 (666>164) from NX-56-10.



Figure S3. HRMS/MS of compound 3 (696>164) from NX-56-10.



Figure S4. HRMS/MS spectrum of compound 4 (678>150) from MX-S-B11.



Figure S5. HRMS/MS spectrum of compound 5 (694>164) from MX-S-B11.



Figure S6. HRMS/MS spectrum of compound **6** (708>164) from MX-S-B11. The 708.4857 peak in the HRMS/MS spectrum displayed an uneven shape. The m/z 690 and 672 peaks are clearly two water losses that do not fit the 708.4857 value with a reasonable ppm error. They, however, do perfectly fit the 708.4836 ion observed in the full scan. Therefore, we argue that the m/z 708.4857 reading in the MSMS scan is created by two unresolved peaks and used the m/z value from the full scan for the calculation of the elemental formula of the pseudo-molecular ion.



Figure S8. HRMS/MS spectrum compound 8 (678>164) from MX-S-B11.



Figure S9. HRMS/MS spectrum compound 9 (738>180) from MX-S-B11.

Exact mass: 670.46773





Exact mass: 592.43604



		Fragments (<i>m</i> / <i>z</i>)						
Spirolide	Mass transition (m/z)	Group 1	Group 2	Group 3	Group 4	Reference		
А	692 > 150	692/674/624	444/390	190	150	[7]		
В	694 > 150	694/676/658/640	462/444/426		150	[3-4]		
С	706 > 164	706/688/638	458/404	204	164	[7]		
13-desMethyl C	692 > 164	692/674/656/638	462/444/426	230	164	[7]		
13,19-didesMethyl C	678 > 164	678/660/642/624	448/430/412/394		164	[9,15]		
20-Hydroxy-13,19-didesMethyl C	694 > 164	694/676/658/640	446/428/410/392	292/274/248/230	164	[11]		
27-Hydroxy-13-desMethyl C	708 > 180	708/690/672/654/636	478/460/442/424		180	[10]		
27-Hydroxy-13,19-didesMethyl C	694 > 180	694/676/658/640	464/446/428/410		180	[10]		
27-Oxo-13,19-didesMethyl C	692 > 178	692/674/624	444		178	[10]		
D	708 > 164	708/690/672/654	458/440	230/206/204/177	164	[3]		
13-desMethyl D	694 > 164	694/676/658/640	444/426	230/204/177	164	[8]		
20-Hydroxy-13,19-didesMethyl D	696 > 164	696/678/660/642	446/428/410/392	292/274/248/230	164	[11]		
G	692 > 164	692/674/656/638	378/360/332	258	164	[12]		
20-Methyl G	706 > 164	706/688/670/652	392/374/346	258	164	[12]		
Н	650 > 164	650/632/614	402/384	206	164	[13]		
Ι	652 > 164	652/634/616	402/384	206	164	[13]		

Table S1. Extended fragment list from known spirolides.

Compound 1 (670>164)							
m/z	Intensity	Relative	Theoretical Mass	Δ (ppm)	Elemental Composition		
670.4678	631	9.48	670.4677	0.04	C40H64NO7 ⁺		
652.4574	4794	72.00	652.4572	0.23	C40 H62N O6 ⁺		
634.4470	1451	21.80	634.4466	0.36	$C_{40}H_{60}NO_{5}^{+}$		
616.4365	890	13.36	616.436	0.49	C40H58NO4 ⁺		
592.4363	373	5.60	592.436	0.30	C38 H58 NO4+		
574.4258	344	5.16	574.4255	0.31	C38H56NO3 ⁺		
462.3219	175	2.62	462.3214	0.47	C27H44NO5+		
444.3111	1087	16.33	444.3108	0.29	C27H42NO4+		
426.3006	416	6.25	426.3003	0.30	C27H40NO3+		
230.1904	477	7.17	230.1903	0.07	$C_{16}H_{24}N^+$		
177.1513	804	12.07	177.1512	0.06	C12H19N+		
164.1435	6659	100.00	164.1434	0.13	$C_{11}H_{18}N^{+}$		

 Table S2. Extended HRMS/MS fragment list of compounds 1 from AON 24.

		С	ompound 2 (666>164	4)	
m/z	Intensity	Relative	Theoretical Mass	Δ (ppm)	Elemental Composition
666.4365	4596	12.69	666.4364	0.09	C40H60NO7+
648.4259	17328	47.83	648.4259	0.04	$C_{40}H_{58}NO_{6^+}$
630.4154	20498	56.58	630.4153	0.10	C40H56NO5 ⁺
550.3898	25	/	550.3891	1.36	C35H52NO4 ⁺
532.3787	326	/	532.3785	0.38	C35H50NO3 ⁺
378.2640	966	2.67	378.2639	0.12	C22H36NO4 ⁺
360.2533	7620	21.03	360.2533	-0.02	C22H34NO3+
332.2584	21586	59.59	332.2584	-0.04	C21H34NO2 ⁺
246.2216	7500	20.70	246.2216	0.02	C17H28N ⁺
177.1513	4933	13.62	177.1512	0.07	$C_{12}H_{19}N^+$
164.1435	36225	100.00	164.1434	0.10	$C_{11}H_{18}N^{+}$
		С	ompound 3 (696>164	4)	
m/z	Intensity	Relative	Theoretical Mass	Δ (ppm)	Elemental Composition
696.4471	18674	90.33	696.4470	0.09	C41H62NO8+
678.4366	20673	100.00	678.4364	0.15	C41H60NO7 ⁺
660.426	10407	50.34	660.4259	0.16	C41H58NO6 ⁺
642.4156	3308	16.00	642.4153	0.29	$C_{41}H_{56}NO_{5^+}$
624.4048	514	2.49	624.4047	0.05	$C_{41}H_{54}NO_{4^+}$
608.4315	70.3	/	608.43146	0.83	C38H58NO5+
590.4208	491	2.37	590.4204	0.45	C38H56NO4 ⁺
572.4100	664	3.21	572.4098	0.21	$C_{38}H_{54}NO_{3^+}$
554.3998	127	0.62	554.3993	0.52	C38H52NO2+
500.1120	40	0.19	500.1129	-0.89	C31H18NO6+
448.3060	1961	9.49	448.3057	0.25	C26H42NO5 ⁺
432.3114	43	0.21	432.3108	0.60	C ₂₆ H ₄₂ NO ₄ +
430.2954	9046	43.76	430.2952	0.22	$C_{26}H_{40}NO_{4^+}$
412.2848	1342	6.49	412.2846	0.17	C26H38NO3+
394.2742	69	0.34	394.2741	0.18	C26H36NO2 ⁺
248.2009	63	0.31	248.2009	0.05	$C_{16}H_{26}NO^+$
246.2217	1776	8.59	246.2216	0.08	C17H28N ⁺
177.1513	1612	7.80	177.1512	0.10	C12H19N+
164.1435	15352	74.26	164.1434	0.15	$C_{11}H_{18}N^+$

Table S3. Extended HRMS/MS fragment list of compounds 2 and 3 from NX-56-10.

	Сс	mpound	4 (678>150)			
	Talaasita	Dalation	Theoretical	Δ	Elemental	
<i>m/z</i>	Intensity	Relative	Mass	(ppm)	Composition	
678.4363	107716	100.00	678.4364	-0.15	$C_{41}H_{60}NO_{7}{}^{\scriptscriptstyle +}$	
660.4260	93076	86.41	660.4259	0.10	$C_{41}H_{58}NO_{6^+}$	
642.4155	39210	36.40	642.4153	0.17	$C_{41}H_{56}NO_{5^+}$	
624.4049	17080	15.86	624.4047	0.17	$C_{41}H_{54}NO_{4^+}$	
508.3426	1867	1.73	508.3421	0.45	C32H46NO4 ⁺	
490.3318	576	0.53	490.3316	0.25	C32H44NO3+	
448.3059	4390	4.08	448.3057	0.19	C26H42NO5 ⁺	
430.2953	35422	32.88	430.2952	0.16	$C_{26}H_{40}NO_{4^+}$	
412.2848	13180	12.24	412.2846	0.14	C26H38NO3+	
394.2742	1535	1.43	394.2741	0.14	C26H36NO2+	
380.2584	467	0.43	380.2584	-0.01	C25H34NO2+	
244.2061	1573	1.46	244.2060	0.08	C17H26N+	
230.1904	1180	1.10	230.1903	0.09	$C_{16}H_{24}N^+$	
216.1747	3648	3.39	216.1747	0.07	$C_{15}H_{22}N^+$	
206.1904	3209	2.98	206.1903	0.09	$C_{14}H_{24}N^+$	
192.1748	4859	4.51	192.1747	0.11	C13H22N+	
190.1591	6194	5.75	190.1590	0.06	$C_{13}H_{20}N^+$	
150.1278	77982	72.40	150.1277	0.10	$C_{10}H_{16}N^+$	
$150.1278 77982 72.40 150.1277 0.10 C_{10}H_{16}N^{+}$						
	Co	mpound	5 (694>164)			
	Co Intensity	mpound Relative	5 (694>164) Theoretical	Δ	Elemental	
m/z	Intensity	mpound Relative	5 (694>164) Theoretical Mass	Δ (ppm)	Elemental Composition	
m/z 694.4679	Intensity 439976	Relative 100.00	5 (694>164) Theoretical Mass 694.4677	Δ (ppm) 0.24	Elemental Composition C42H64NO7 ⁺	
m/z 694.4679 676.4574	Intensity 439976 215774	Relative 100.00 49.04	5 (694>164) Theoretical Mass 694.4677 676.4572	Δ (ppm) 0.24 0.34	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469	Intensity 439976 215774 113275	mpound Relative 100.00 49.04 25.75	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466	Δ (ppm) 0.24 0.34 0.45	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363	Intensity 439976 215774 113275 20366	mpound Relative 100.00 49.04 25.75 4.63	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436	Δ (ppm) 0.24 0.34 0.45 0.48	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258	Intensity 439976 215774 113275 20366 3963	mpound Relative 100.00 49.04 25.75 4.63 0.90	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255	Δ (ppm) 0.24 0.34 0.45 0.48 0.60	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571	Co Intensity 439976 215774 113275 20366 3963 1110	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102	Intensity 439976 215774 113275 20366 3963 1110 1784	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺ C37H54NO3 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺ C37H54NO3 ⁺ C29H48NO4 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺ C37H54NO3 ⁺ C29H48NO4 ⁺ C27H46NO5 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476	Control Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺ C37H54NO3 ⁺ C29H48NO4 ⁺ C29H46NO5 ⁺ C29H46NO3 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268	Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73	Elemental Composition C42H64NO7 ⁺ C42H62NO6 ⁺ C42H60NO5 ⁺ C42H58NO4 ⁺ C42H56NO3 ⁺ C42H56NO3 ⁺ C41H60NO3 ⁺ C37H54NO3 ⁺ C29H48NO4 ⁺ C29H46NO5 ⁺ C29H46NO3 ⁺ C27H44NO4 ⁺	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268 444.3476	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845 18160	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69 4.13	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265 444.3472	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73 0.77	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268 444.3476 436.3425	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845 18160 28540	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69 4.13 6.49	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265 436.3421	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73 0.77 0.76	$\begin{array}{c} \mbox{Elemental} \\ \mbox{Composition} \\ \mbox{C42H64NO7}^+ \\ \mbox{C42H62NO6}^+ \\ \mbox{C42H60NO5}^+ \\ \mbox{C42H58NO4}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C41H60NO3}^+ \\ \mbox{C37H54NO3}^+ \\ \mbox{C29H48NO4}^+ \\ \mbox{C227H46NO5}^+ \\ \mbox{C227H44NO4}^+ \\ \mbox{C22H46NO3}^+ \\ \mbox{C226H46NO4}^+ \\ \mb$	
m/z 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268 444.3476 436.3425 428.3163	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845 18160 28540 10930	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69 4.13 6.49 2.48	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265 444.3472 436.3421 428.3159	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73 0.77 0.76 0.85	$\begin{array}{r} \mbox{Elemental} \\ \mbox{Composition} \\ \mbox{C42H64NO7}^+ \\ \mbox{C42H62NO6}^+ \\ \mbox{C42H60NO5}^+ \\ \mbox{C42H58NO4}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C41H60NO3}^+ \\ \mbox{C37H54NO3}^+ \\ \mbox{C27H46NO5}^+ \\ \mbox{C227H46NO3}^+ \\ \mbox{C227H44NO4}^+ \\ \mbox{C228H46NO3}^+ \\ \mbox{C227H42NO3}^+ \\ \mbox{C227H42NO3}^+ \end{array}$	
m/z 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268 444.3476 436.3425 428.3163 420.3111	Co Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845 18160 28540 10930 22489	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69 4.13 6.49 2.48 5.11	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265 444.3472 436.3421 428.3159 420.3108	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73 0.77 0.76 0.85 0.55	$\begin{array}{r} \mbox{Elemental} \\ \mbox{Composition} \\ \mbox{C42H64NO7}^+ \\ \mbox{C42H62NO6}^+ \\ \mbox{C42H60NO5}^+ \\ \mbox{C42H58NO4}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C42H56NO3}^+ \\ \mbox{C37H54NO3}^+ \\ \mbox{C29H48NO4}^+ \\ \mbox{C27H46NO5}^+ \\ \mbox{C29H46NO3}^+ \\ \mbox{C28H46NO3}^+ \\ \mbox{C26H46NO4}^+ \\ \mbox{C25H42NO4}^+ \\ \mbox{C25H42NO4}^+ \end{array}$	
<i>m/z</i> 694.4679 676.4574 658.4469 640.4363 622.4258 614.4571 560.4102 474.3581 464.3374 456.3476 446.3268 444.3476 436.3425 428.3163 420.3111 418.3318	Intensity 439976 215774 113275 20366 3963 1110 1784 5138 107168 7674 33845 18160 28540 10930 22489 64135	mpound Relative 100.00 49.04 25.75 4.63 0.90 0.25 0.41 1.17 24.36 1.74 7.69 4.13 6.49 2.48 5.11 14.58	5 (694>164) Theoretical Mass 694.4677 676.4572 658.4466 640.436 622.4255 614.4568 560.4098 474.3578 464.337 456.3472 446.3265 444.3472 436.3421 428.3159 418.3316	Δ (ppm) 0.24 0.34 0.45 0.48 0.60 0.52 0.71 0.65 0.76 0.82 0.73 0.77 0.76 0.85 0.55 0.59	Elemental Composition $C_{42}H_{64}NO7^+$ $C_{42}H_{62}NO6^+$ $C_{42}H_{60}NO5^+$ $C_{42}H_{58}NO4^+$ $C_{42}H_{56}NO3^+$ $C_{41}H_{60}NO3^+$ $C_{37}H_{54}NO3^+$ $C_{29}H_{48}NO4^+$ $C_{29}H_{46}NO3^+$ $C_{29}H_{46}NO3^+$ $C_{28}H_{46}NO3^+$ $C_{28}H_{46}NO3^+$ $C_{27}H_{42}NO3^+$ $C_{27}H_{42}NO3^+$ $C_{25}H_{42}NO4^+$	

402.3006	12085	2.75	402.3003	0.74	$C_{25}H_{40}NO_{3^+}$		
400.3213	19423	4.41	400.321	0.63	C26H42NO2+		
382.3107	3077	0.70	382.3104	0.75	$C_{26}H_{40}NO^+$		
236.2010	44657	10.15	236.2009	0.35	C15H26NO+		
204.1748	16971	3.86	204.1747	0.78	$C_{14}H_{22}N^+$		
177.1513	4197	0.95	177.1512	0.76	C12H19N+		
164.1435	269143	61.17	164.1434	0.90	$C_{11}H_{18}N^+$		
Compound 6 (708>164)							
m/7	Intensity	Relative	Theoretical	Δ	Elemental		
1111 2	interisity	iciuive	Mass	(ppm)	Composition		
708.4857	119695	100.00	708.4834	1.06	C43H66NO7 ⁺		
690.4710	82644	69.05	690.4728	-2.62	C43H64NO6+		
672.4593	18347	15.33	672.4623	-2.96	C43H63NO5 ⁺		
392.2798	49950	41.73	392.2795	0.56	C23H38NO4+		
346.2744	18766	15.68	346.2741	0.86	C22H36NO2 ⁺		
164.1439	47095	39.35	164.1434	3.30	$C_{11}H_{18}N^+$		
	Co	ompound	7 (720>164)	Γ			
m/z	Intensity	Relative	Theoretical		Elemental		
500 100	00001(10.04	Mass	(ppm)	Composition		
720.4836	838216	18.34	720.4834	0.36	C44H66NO7 ⁺		
702.4730	1006502	22.02	702.4728	0.30	C44H64NO6+		
684.4625	524711	11.48	684.4623	0.31	C44H62NO5+		
666.4520	219421	4.80	666.4517	0.42	C44H60NO4+		
586.4254	16660	0.36	586.4255	-0.20	C39H56NO3+		
490.3530	43167	0.94	490.3527	0.61	C29H48NO5+		
472.3425	809589	17.71	472.3421	0.70	C29H46NO4+		
454.3318	778851	17.04	454.3316	0.61	C29H44NO3+		
436.3214	91264	2.00	436.3210	0.86	C29H42NO2+		
376.2849	14601	0.32	376.2846	0.77	C23H38NO3 ⁺		
358.2741	181103	3.96	358.2741	0.15	C23H36NO2+		
346.2743	14120	0.31	346.2741	0.59	C22H36NO2+		
340.2637	47557	1.04	340.2635	0.71	C23H34NO+		
302.2480	17381	0.38	302.2478	0.58	C20H32NO+		
246.2217	115447	2.53	246.2216	0.22	$C_{17}H_{28}N^+$		
230.1905	76776	1.68	230.1903	0.58	$C_{16}H_{24}N^+$		
177.1513	623947	13.65	177.1512	0.59	$C_{12}H_{19}N^+$		
164.1435	4570111	100.00	164.1434	0.72	$C_{11}H_{18}N^+$		
	Co	mpound	8 (722>164)				
m/z	Intensity	Relative	Theoretical	Δ	Elemental		
			Mass	(ppm)	Composition		
722.4994	3498	2.98	722.4990	0.50	C44H68NO7 ⁺		
704.4886	24066	20.48	704.4885	0.26	$C_{44}H_{66}NO_{6^+}$		
686.4780	20248	17.23	686.4779	0.18	$C_{44}H_{64}NO_{5^+}$		

686.4420	1734	1.48	686.4415	0.73	$C_{43}H_{60}NO_{6^+}$
668.4677	4385	3.73	668.4673	0.56	$C_{44}H_{62}NO_{4^+}$
668.4315	1014	0.86	668.4310	0.76	C43H58NO5+
650.4568	371	0.32	650.4568	0.12	C44H60NO3 ⁺
392.2796	31295	26.63	392.2795	0.17	C23H38NO4+
374.2691	16917	14.39	374.2690	0.28	C23H36NO3+
372.2897	660	0.56	372.2897	-0.09	C24H38NO2+
364.2846	1170	1.00	364.2846	-0.12	C22H38NO3 ⁺
356.2585	2172	1.85	356.2584	0.22	C23H34NO2+
354.2794	701	0.60	354.2791	0.87	C24H36NO+
348.2534	5914	5.03	348.2533	0.37	C21H34NO3+
346.2741	47722	40.60	346.2741	0.24	C22H36NO2+
302.2480	2632	2.24	302.2478	0.48	C20H32NO ⁺
258.2217	6122	5.21	258.2216	0.32	$C_{18}H_{28}N^+$
230.1904	2108	1.79	230.1903	0.45	$C_{16}H_{24}N^{+}$
177.1513	22196	18.89	177.1512	0.51	$C_{12}H_{19}N^+$
164.1435	117532	100.00	164.1434	0.72	$C_{11}H_{18}N^+$
	Co	mpound	9 (738>180)		
m/z	Intensity	Relative	Theoretical	Δ	Elemental
<i>m/z</i>	Intensity	Relative	Theoretical Mass	Δ (ppm)	Elemental Composition
m/z 738.4579	Intensity 5015	Relative 2.43	Theoretical Mass 738.4576	Δ (ppm) 0.44	Elemental Composition C43H64NO9+
<i>m/z</i> 738.4579 720.4478	Intensity 5015 10345	Relative 2.43 5.01	Theoretical Mass 738.4576 720.4470	Δ (ppm) 0.44 1.14	Elemental Composition C43H64NO9 ⁺ C43H62NO8 ⁺
<i>m/z</i> 738.4579 720.4478 702.4365	Intensity 5015 10345 12580	Relative 2.43 5.01 6.09	Theoretical Mass 738.4576 720.4470 702.4364	Δ (ppm) 0.44 1.14 0.13	Elemental Composition C43H64NO9+ C43H62NO8+ C43H60NO7+
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267	Intensity 5015 10345 12580 10002	Relative 2.43 5.01 6.09 4.85	Theoretical Mass 738.4576 720.4470 702.4364 684.4259	Δ (ppm) 0.44 1.14 0.13 1.22	Elemental Composition C43H64NO9 ⁺ C43H62NO8 ⁺ C43H60NO7 ⁺ C43H58NO6 ⁺
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155	Intensity 5015 10345 12580 10002 2887	Relative 2.43 5.01 6.09 4.85 1.40	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153	Δ (ppm) 0.44 1.14 0.13 1.22 0.34	Elemental Composition C43H64NO9* C43H62NO8* C43H60NO7* C43H58NO6* C43H56NO5*
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697	Intensity 5015 10345 12580 10002 2887 10171	Relative 2.43 5.01 6.09 4.85 1.40 4.93	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694	$\begin{array}{c} \Delta \\ (\text{ppm}) \\ \hline 0.44 \\ \hline 1.14 \\ \hline 0.13 \\ \hline 1.22 \\ \hline 0.34 \\ \hline 0.68 \end{array}$	Elemental Composition C43H64NO9+ C43H62NO8+ C43H60NO7+ C43H58NO6+ C43H56NO5+ C23H38NO6+
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591	Intensity 5015 10345 12580 10002 2887 10171 21182	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588	$\begin{array}{c} \Delta \\ (\text{ppm}) \\ \hline 0.44 \\ \hline 1.14 \\ \hline 0.13 \\ \hline 1.22 \\ \hline 0.34 \\ \hline 0.68 \\ \hline 0.80 \\ \end{array}$	Elemental Composition C43H64NO9 ⁺ C43H62NO8 ⁺ C43H60NO7 ⁺ C43H58NO6 ⁺ C43H56NO5 ⁺ C23H38NO6 ⁺ C23H36NO5 ⁺
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 6666.4155 424.2697 406.2591 362.2693	Intensity 5015 10345 12580 10002 2887 10171 21182 11554	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690	$\begin{array}{c} \Delta \\ (\text{ppm}) \\ \hline 0.44 \\ \hline 1.14 \\ \hline 0.13 \\ \hline 1.22 \\ \hline 0.34 \\ \hline 0.68 \\ \hline 0.80 \\ \hline 0.79 \end{array}$	Elemental Composition C43H64NO9* C43H62NO8* C43H60NO7* C43H56NO5* C43H56NO5* C23H38NO6* C23H38NO6* C23H36NO5*
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533	$\begin{array}{c} \Delta \\ (\text{ppm}) \\ \hline 0.44 \\ \hline 1.14 \\ 0.13 \\ \hline 1.22 \\ 0.34 \\ \hline 0.68 \\ 0.80 \\ \hline 0.79 \\ \hline 1.11 \end{array}$	Elemental Composition C43H64NO9+ C43H62NO8+ C43H60NO7+ C43H58NO6+ C43H56NO5+ C23H38NO6+ C23H38NO6+ C23H36NO5+ C22H36NO3+ C20H34NO3+
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428	$\begin{array}{c} \Delta \\ (\text{ppm}) \\ \hline 0.44 \\ \hline 1.14 \\ 0.13 \\ \hline 1.22 \\ 0.34 \\ \hline 0.68 \\ 0.80 \\ \hline 0.79 \\ \hline 1.11 \\ \hline 0.42 \end{array}$	Elemental Composition C43H64NO9* C43H62NO8* C43H60NO7* C43H56NO5* C43H56NO5* C23H36NO5* C23H36NO5* C22H36NO3* C20H32NO2*
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 6666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852	$\begin{array}{c} \Delta \\ (ppm) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \end{array}$	Elemental Composition C43H64NO9+ C43H62NO8+ C43H60NO7+ C43H56NO5+ C43H56NO5+ C23H38NO6+ C23H38NO6+ C22H36NO3+ C22H36NO3+ C20H34NO3+ C20H32NO2+ C17H24NO+
<i>m/z</i> 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852 242.1904	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081 16377	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01 7.93	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852 242.1903	$\begin{array}{c} \Delta \\ (ppm) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \\ 0.43 \end{array}$	Elemental Composition $C_{43}H_{64}NO_{9^+}$ $C_{43}H_{62}NO_{8^+}$ $C_{43}H_{60}NO_{7^+}$ $C_{43}H_{58}NO_{6^+}$ $C_{43}H_{56}NO_{5^+}$ $C_{23}H_{36}NO_{5^+}$ $C_{22}H_{36}NO_{5^+}$ $C_{22}H_{36}NO_{3^+}$ $C_{20}H_{32}NO_{2^+}$ $C_{17}H_{24}NO_{+}$ $C_{17}H_{24}N^+$
m/z 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852 242.1904 236.2010	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081 16377 9959	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01 7.93 4.82	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852 242.1903 236.2009	$\begin{array}{c} \Delta \\ (ppm) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \\ 0.43 \\ 0.67 \end{array}$	Elemental Composition C43H64NO9+ C43H62NO8+ C43H60NO7+ C43H56NO5+ C43H56NO5+ C23H36NO5+ C22H36NO5+ C22H36NO3+ C20H32NO2+ C17H24NO+ C17H24N+ C15H26NO+
m/z 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852 242.1904 236.2010 234.1854	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081 16377 9959 13794	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01 7.93 4.82 6.68	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852 242.1903 236.2009 234.1852	$\begin{array}{c} \Delta \\ (\mathrm{ppm}) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \\ 0.43 \\ 0.67 \\ 0.72 \\ \end{array}$	Elemental Composition $C_{43}H_{64}NO_{9}^{+}$ $C_{43}H_{62}NO_{8}^{+}$ $C_{43}H_{60}NO_{7}^{+}$ $C_{43}H_{58}NO_{6}^{+}$ $C_{43}H_{56}NO_{5}^{+}$ $C_{23}H_{36}NO_{5}^{+}$ $C_{23}H_{36}NO_{5}^{+}$ $C_{22}H_{36}NO_{3}^{+}$ $C_{20}H_{34}NO_{3}^{+}$ $C_{20}H_{32}NO_{2}^{+}$ $C_{17}H_{24}NO_{+}$ $C_{15}H_{26}NO_{+}$ $C_{15}H_{24}NO_{+}$
m/z 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852 242.1904 236.2010 234.1854 230.1905	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081 16377 9959 13794 2085	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01 7.93 4.82 6.68 1.01	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852 242.1903 236.2009 234.1852 230.1903	$\begin{array}{c} \Delta \\ (\mathrm{ppm}) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \\ 0.43 \\ 0.67 \\ 0.72 \\ 0.91 \\ \end{array}$	Elemental Composition $C_{43}H_{64}NO_{9^+}$ $C_{43}H_{62}NO_{8^+}$ $C_{43}H_{60}NO_{7^+}$ $C_{43}H_{56}NO_{5^+}$ $C_{43}H_{56}NO_{5^+}$ $C_{23}H_{36}NO_{5^+}$ $C_{23}H_{36}NO_{5^+}$ $C_{22}H_{36}NO_{3^+}$ $C_{20}H_{32}NO_{2^+}$ $C_{17}H_{24}NO_{4^-}$ $C_{17}H_{24}N^+$ $C_{15}H_{26}NO_{7^+}$ $C_{15}H_{24}N^+$
m/z 738.4579 720.4478 702.4365 684.4267 666.4155 424.2697 406.2591 362.2693 336.2537 318.2429 258.1852 242.1904 236.2010 234.1854 230.1905 230.1540	Intensity 5015 10345 12580 10002 2887 10171 21182 11554 3168 147628 2081 16377 9959 13794 2085 2970	Relative 2.43 5.01 6.09 4.85 1.40 4.93 10.26 5.60 1.53 71.51 1.01 7.93 4.82 6.68 1.01 1.44	Theoretical Mass 738.4576 720.4470 702.4364 684.4259 666.4153 424.2694 406.2588 362.2690 336.2533 318.2428 258.1852 242.1903 236.2009 234.1852 230.1903 230.1539	$\begin{array}{c} \Delta \\ (\mathrm{ppm}) \\ 0.44 \\ 1.14 \\ 0.13 \\ 1.22 \\ 0.34 \\ 0.68 \\ 0.80 \\ 0.79 \\ 1.11 \\ 0.42 \\ 0.00 \\ 0.43 \\ 0.67 \\ 0.72 \\ 0.91 \\ 0.42 \end{array}$	Elemental Composition $C_{43}H_{64}NO_{9}^{+}$ $C_{43}H_{62}NO_{8}^{+}$ $C_{43}H_{60}NO_{7}^{+}$ $C_{43}H_{56}NO_{5}^{+}$ $C_{23}H_{38}NO_{6}^{+}$ $C_{23}H_{38}NO_{6}^{+}$ $C_{23}H_{36}NO_{5}^{+}$ $C_{22}H_{36}NO_{3}^{+}$ $C_{20}H_{34}NO_{3}^{+}$ $C_{20}H_{34}NO_{3}^{+}$ $C_{20}H_{32}NO_{2}^{+}$ $C_{17}H_{24}NO_{+}$ $C_{15}H_{26}NO_{+}$ $C_{15}H_{24}NC_{+}$ $C_{15}H_{24}NC_{+}$