UMYMFOR

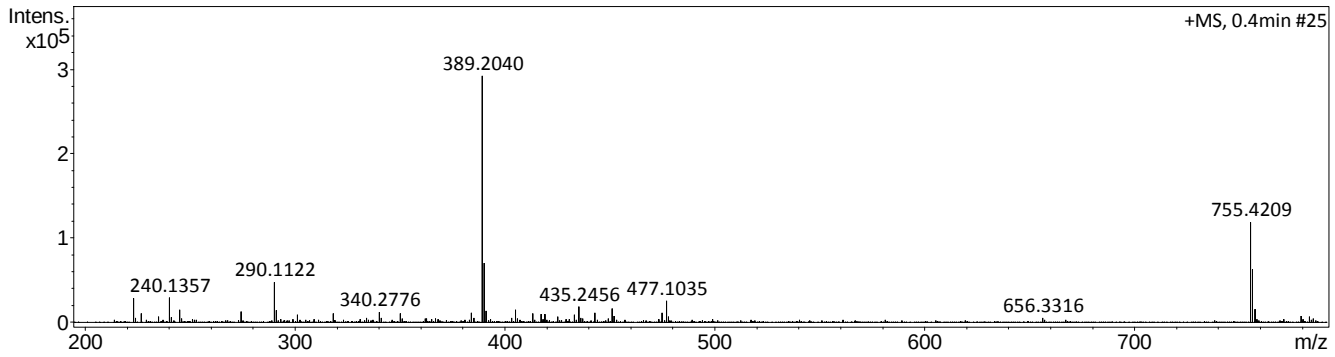
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\ggc\24-060525_P1-C-1_01_9285.d	Acquisition Date	6/12/2024 12:57:24 PM
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060525	Instrument / Ser#	micrOTOF-Q II
Comment	NLM224a Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	223.1101	28825	9.9
2	226.9494	10689	3.7
3	240.1357	29530	10.1
4	245.0922	15253	5.2
5	274.2701	12893	4.4
6	290.1122	47894	16.4
7	291.1224	14087	4.8
8	301.1410	8936	3.1
9	318.2972	10948	3.8
10	340.2776	12090	4.1
11	350.1644	10315	3.5
12	384.2502	11079	3.8
13	389.2040	291641	100.0
14	390.2074	69978	24.0
15	391.2078	13418	4.6
16	405.1873	15071	5.2
17	413.2664	10832	3.7
18	417.2341	10090	3.5
19	419.2164	9556	3.3
20	433.2279	8856	3.0
21	435.2456	18686	6.4
22	443.0987	11371	3.9
23	451.2381	16528	5.7
24	452.2293	7599	2.6
25	475.0870	11341	3.9
26	477.1035	25835	8.9
27	755.4209	118360	40.6
28	756.4226	63054	21.6
29	757.4235	16100	5.5
30	779.4721	7942	2.7

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U M Y M F O R

Qualitative Compound Report

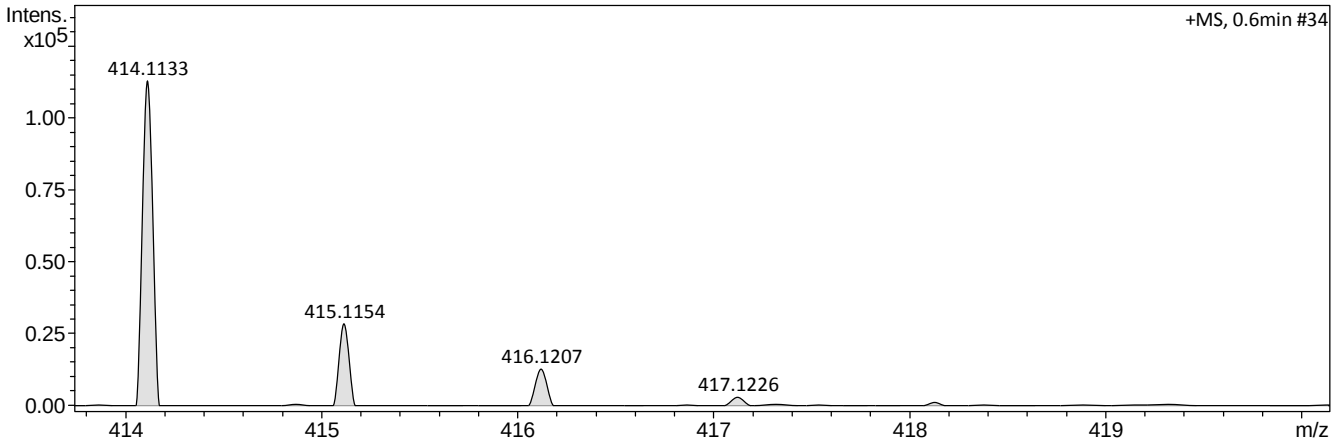
Analysis Info

Acquisition Date 6/12/2024 1:02:31 PM

Analysis Name	D:\Data\ggc\24-060526_P1-C-2_01_9286.d		
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060526	Instrument	micrOTOF-Q II
Comment	NLM226a Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
414.1133	1	C23H21NNaO3S	414.1134	0.2	15.5	1	100.00	13.5	even	ok

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Qualitative Compound Report

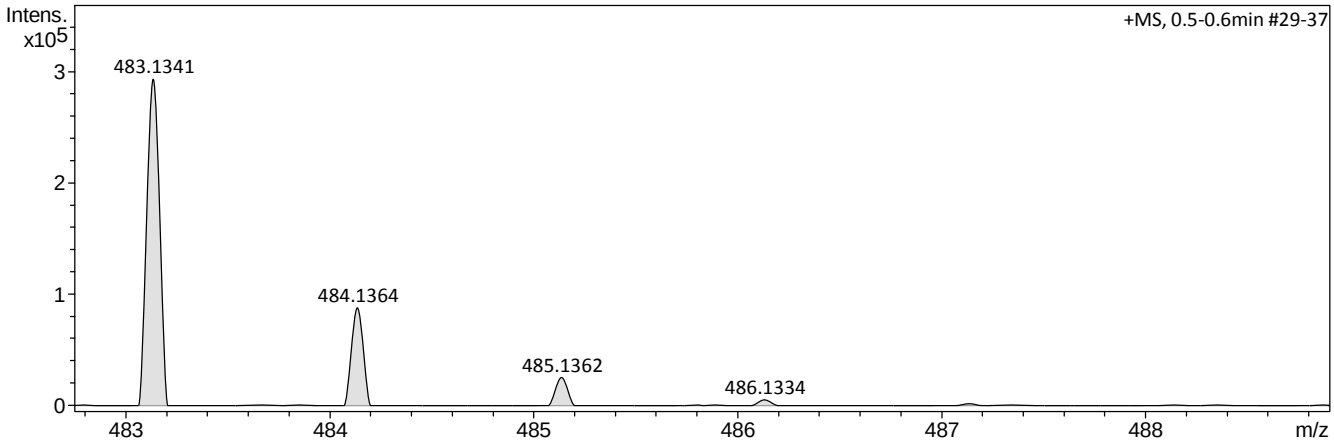
Analysis Info

Acquisition Date 6/12/2024 1:07:42 PM

Analysis Name	D:\Data\ggc\24-060527_P1-C-3_01_9287.d		
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060527	Instrument	micrOTOF-Q II
Comment	NLM245b1 Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
483.1341	1	C26H24N2NaO4S	483.1349	1.7	5.3	1	100.00	15.5	even	ok

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Qualitative Compound Report

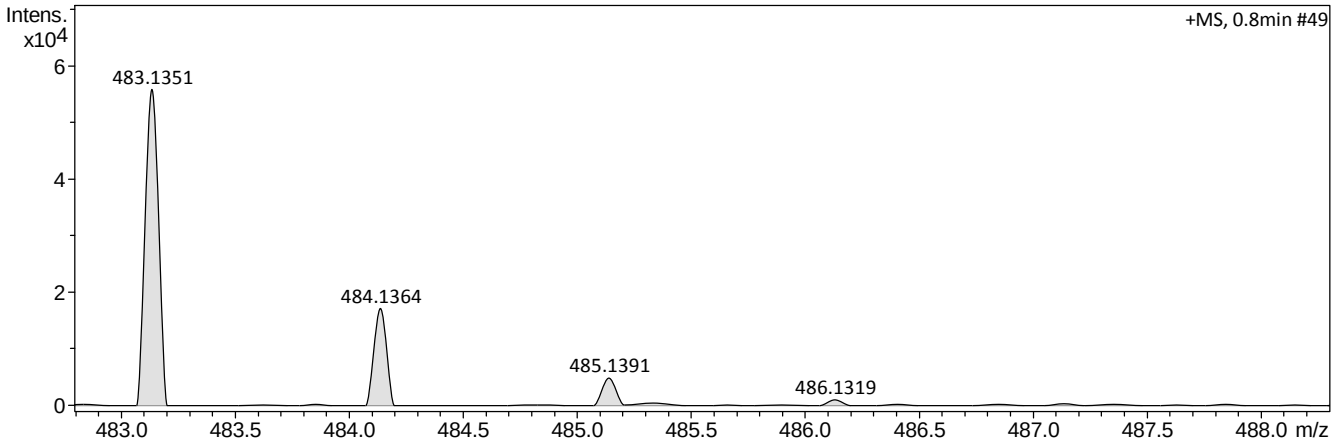
Analysis Info

Acquisition Date 6/12/2024 1:12:50 PM

Analysis Name	D:\Data\ggc\24-060528_P1-C-4_01_9288.d		
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060528	Instrument	micrOTOF-Q II
Comment	NLM245b2 Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
483.1351	1	C26H24N2NaO4S	483.1349	-0.5	5.7	1	100.00	15.5	even	ok

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U M Y M F O R

Qualitative Compound Report

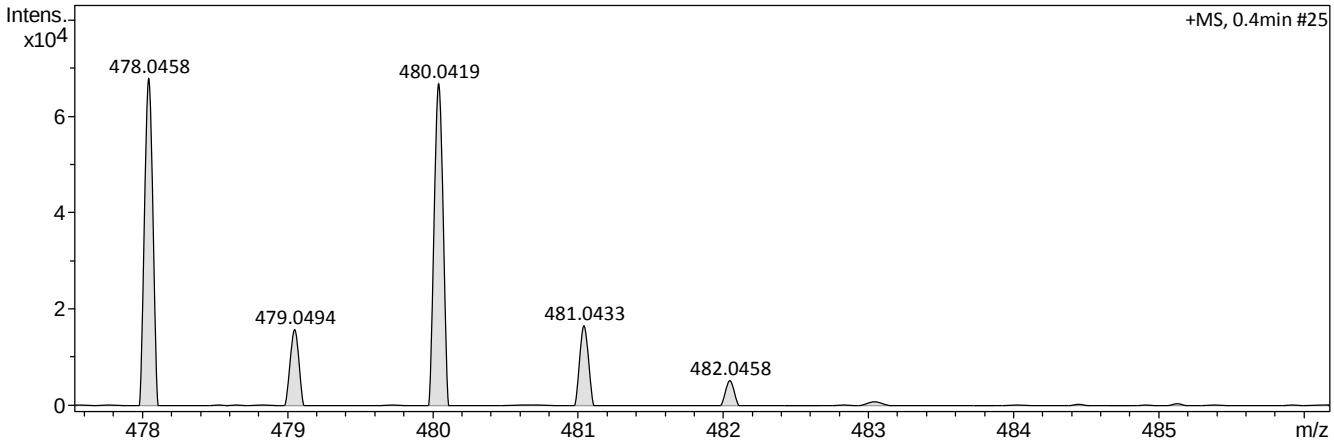
Analysis Info

Acquisition Date 6/12/2024 1:17:57 PM

Analysis Name	D:\Data\ggc\24-060529_P1-C-5_01_9289.d		
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060529	Instrument	micrOTOF-Q II
Comment	MAB1 Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
478.0458	1	C23H22BrNNaO2S	478.0447	-2.4	24.0	1	62.56	12.5	even	ok

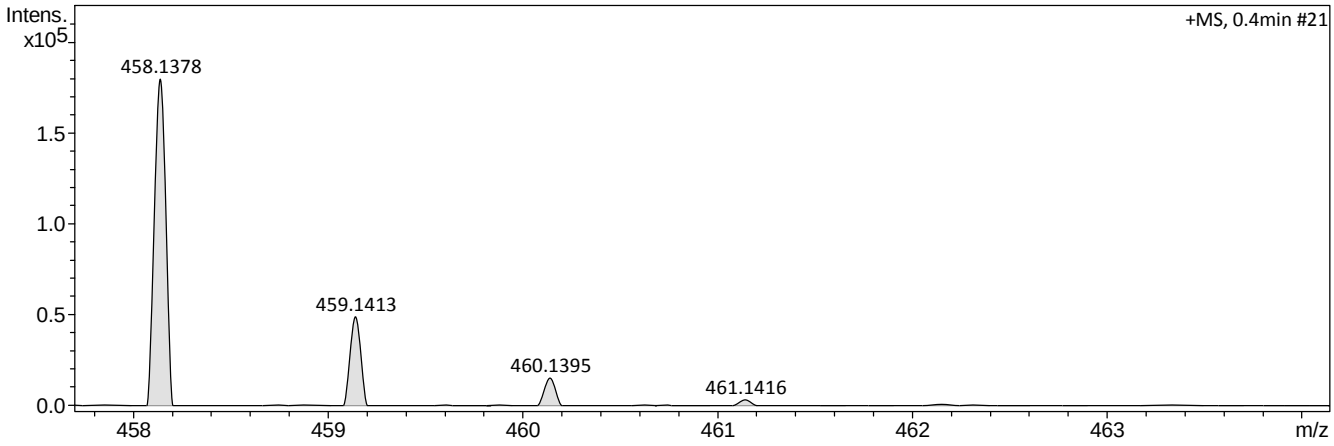
Qualitative Compound Report

Analysis Info

Analysis Name	D:\Data\ggc\24-060530_P1-C-6_01_9290.d	Acquisition Date	6/12/2024 1:23:06 PM
Method	lc_qtof_directospos.m	Operator	ELB
Sample Name	24-060530	Instrument	micrOTOF-Q II
Comment	MAB2 Sv: MeOH + HCOOH Nadia L. Martiren		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
458.1378	1	C25H25NNaO4S	458.1396	4.0	8.6	1	100.00	13.5	even	ok