

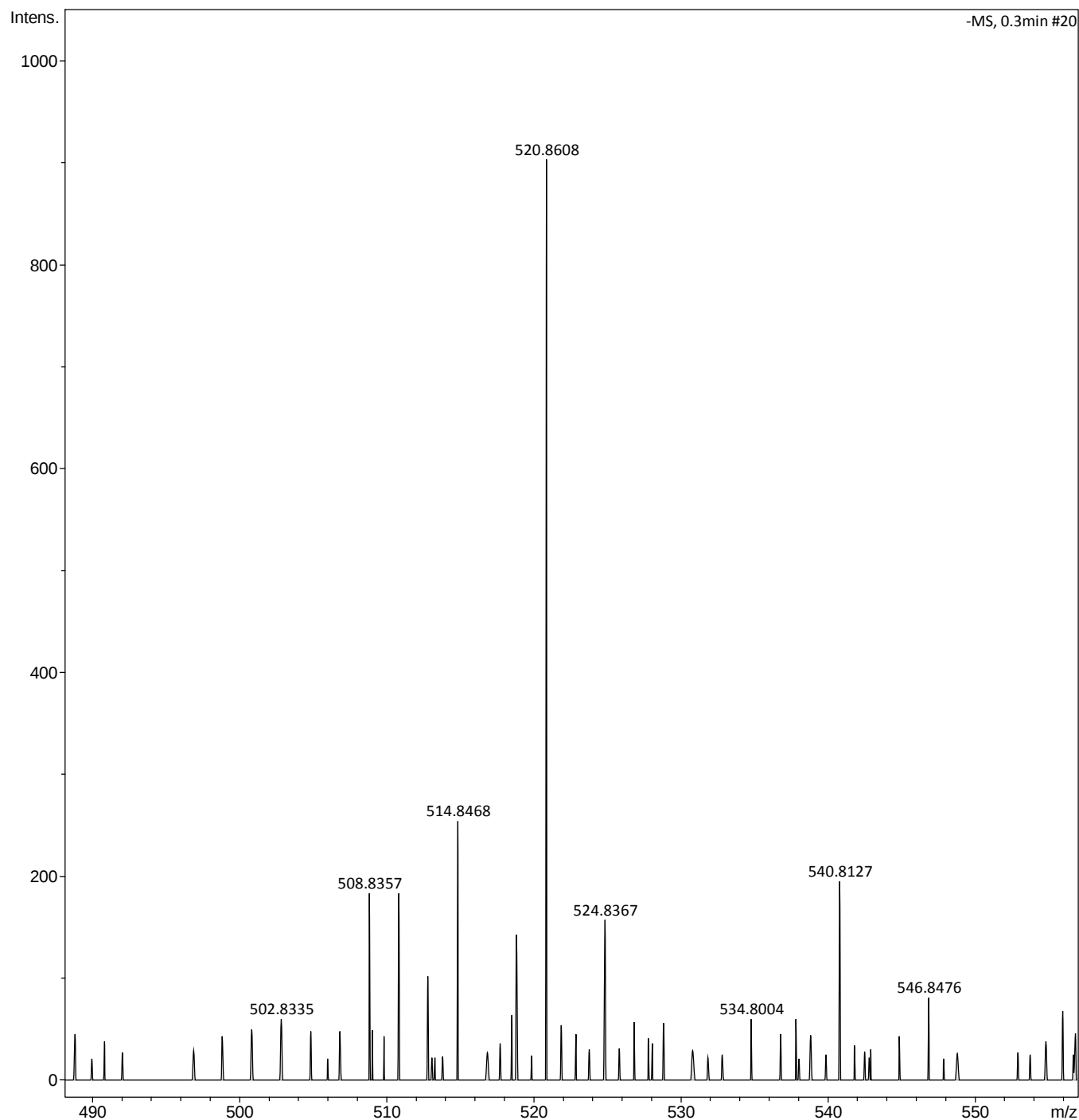
Generic Display Report

Analysis Info

Analysis Name D:\Data\ggc\24-100101_P1-B-1_01_9567.d
Method lc ms directos_241016neg.m
Sample Name 24-100101
Comment JM-01
Sv: DCM + MeOH + HCOOH
Argüello - UNC

Acquisition Date 10/16/2024 12:14:49 PM

Operator EB - MV
Instrument microTOF-Q



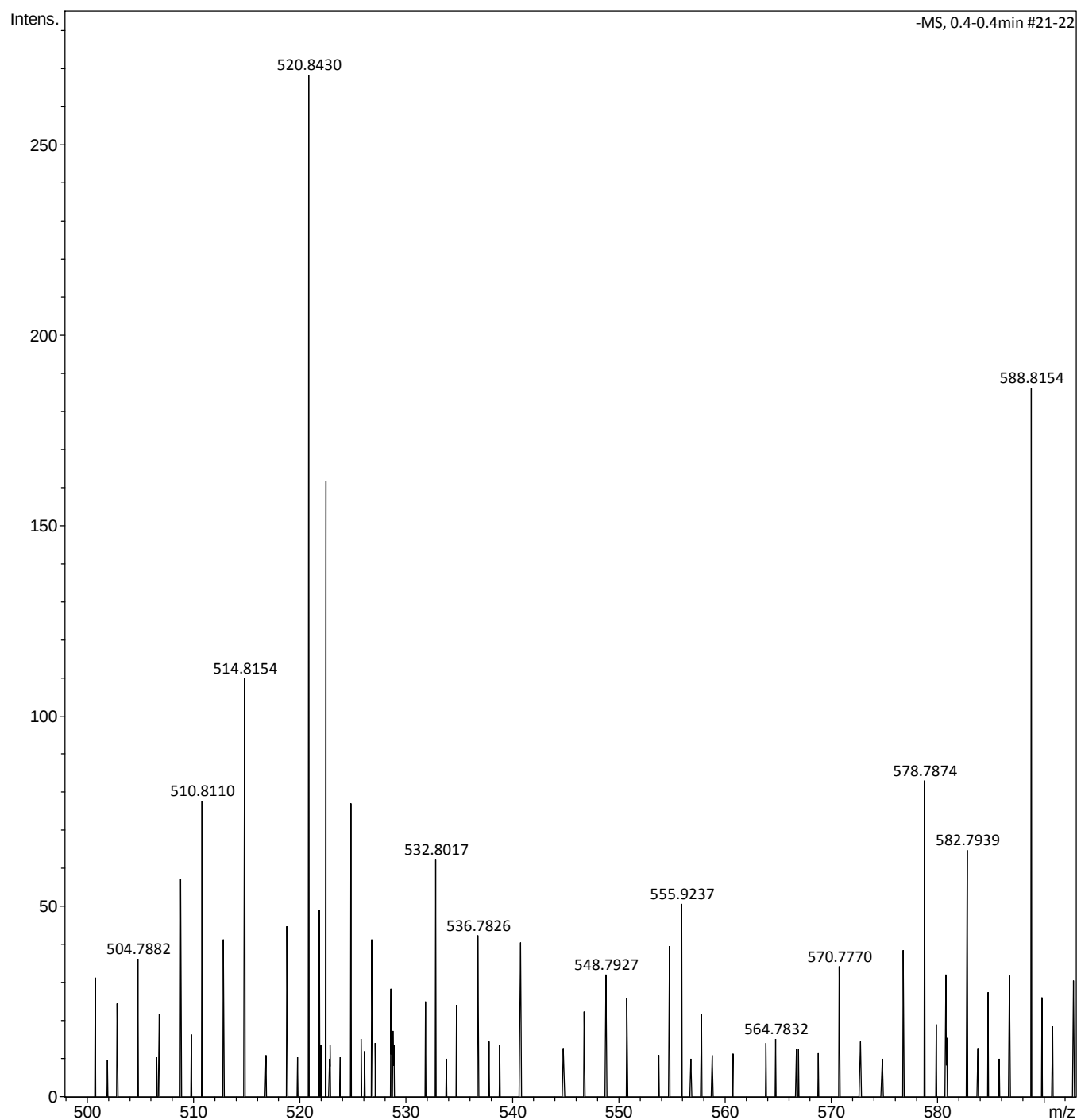
Generic Display Report

Analysis Info

Analysis Name D:\Data\ggc\24-100102_P1-B-2_01_9568.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100102
 Comment JM-02
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 12:19:57 PM

Operator EB - MV
 Instrument microTOF-Q



Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-100103_P1-B-3_01_9569.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100103
 Comment JM-03
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

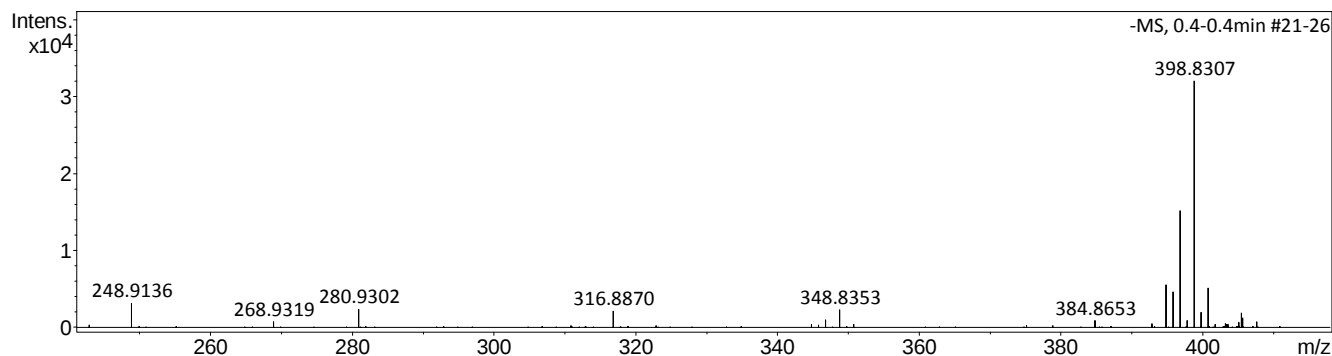
Acquisition Date 10/16/2024 12:25:03 PM

Operator EB - MV

Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.9432	490	1.5
2	242.9013	314	1.0
3	248.9136	3158	9.9
4	268.9319	772	2.4
5	280.9302	2417	7.6
6	316.8870	2127	6.7
7	344.8402	421	1.3
8	345.8388	309	1.0
9	346.8335	1012	3.2
10	348.8353	2328	7.3
11	350.8361	418	1.3
12	384.8653	876	2.7
13	392.8373	528	1.7
14	394.8311	5574	17.4
15	395.8335	4603	14.4
16	396.8311	15160	47.5
17	397.8345	880	2.8
18	398.8307	31942	100.0
19	399.8327	1961	6.1
20	400.8310	5136	16.1
21	401.8345	403	1.3
22	403.2390	510	1.6
23	403.4719	408	1.3
24	403.6070	442	1.4
25	405.1116	632	2.0
26	405.5261	1945	6.1
27	405.6445	1255	3.9
28	407.6955	769	2.4
29	452.8511	442	1.4
30	520.8489	287	0.9

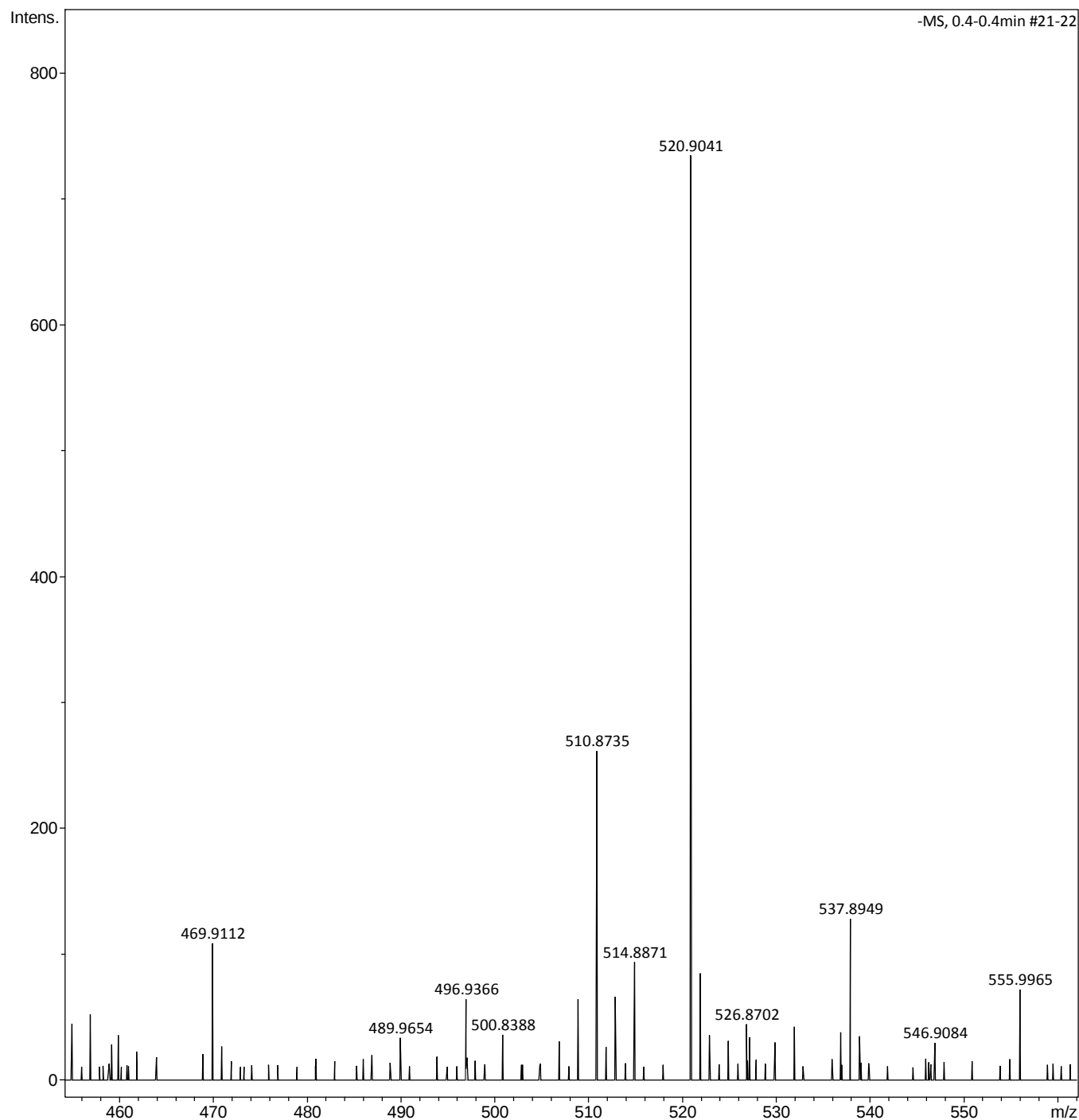
Generic Display Report

Analysis Info

Analysis Name D:\Data\ggc\24-100104_P1-B-4_01_9570.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100104
 Comment JM-04
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 12:31:35 PM

Operator EB - MV
 Instrument microTOF-Q



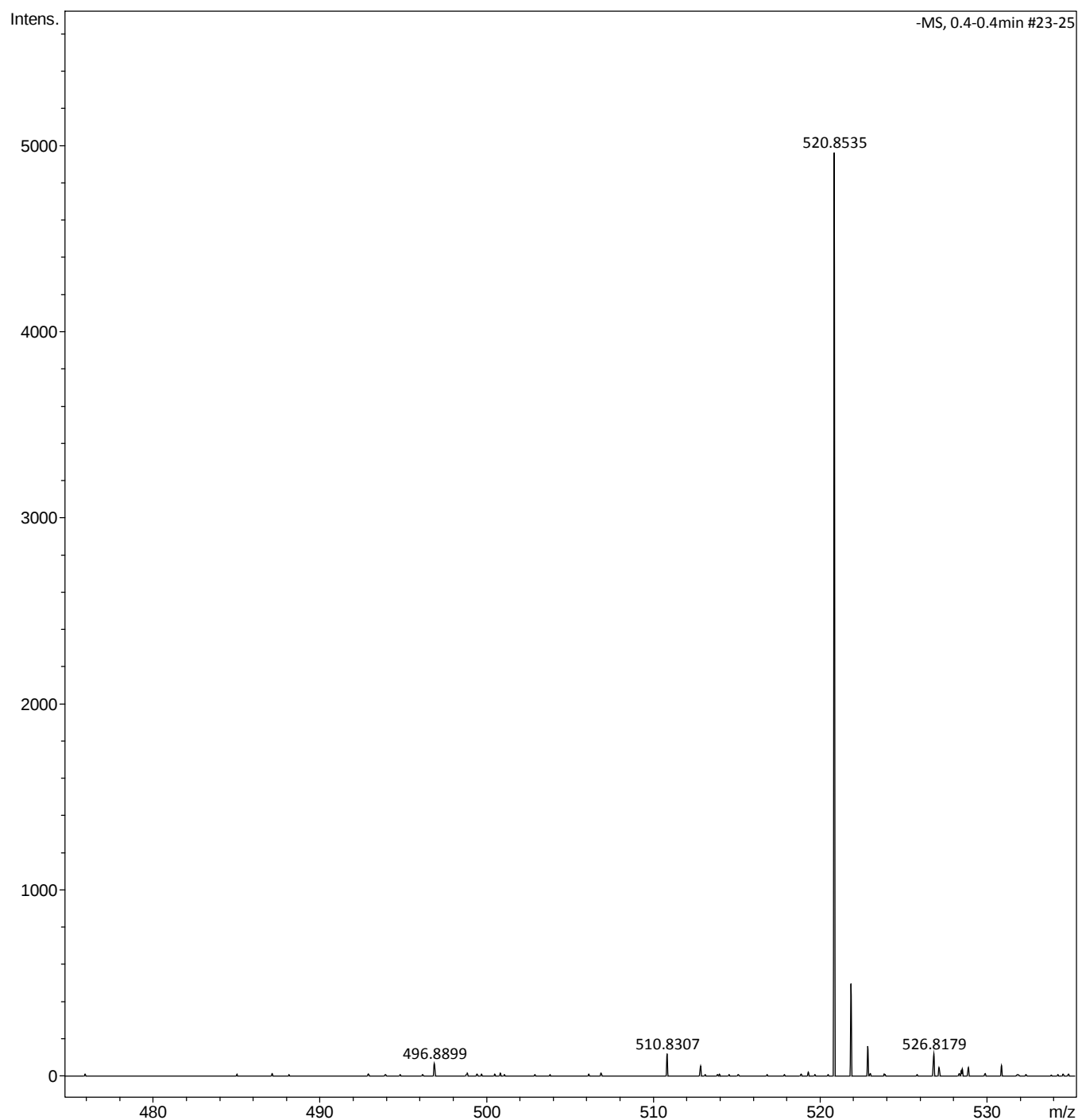
Generic Display Report

Analysis Info

Analysis Name D:\Data\ggc\24-100105_P1-B-5_01_9571.d
Method lc ms directos_241016neg.m
Sample Name 24-100105
Comment JM-05
Sv: DCM + MeOH + HCOOH
Argüello - UNC

Acquisition Date 10/16/2024 12:36:43 PM

Operator EB - MV
Instrument microTOF-Q



Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-100106_P1-B-6_01_9572.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100106
 Comment JM-06
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

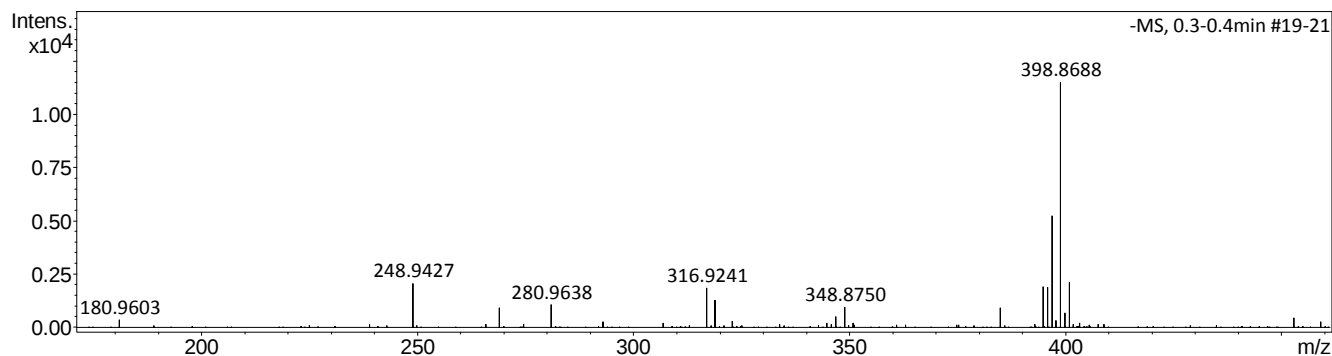
Acquisition Date 10/16/2024 12:41:49 PM

Operator EB - MV

Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.9603	350	3.0
2	248.9427	2056	17.9
3	268.9633	943	8.2
4	280.9638	1080	9.4
5	292.9658	275	2.4
6	306.8963	217	1.9
7	316.9241	1854	16.1
8	318.9547	1277	11.1
9	322.8835	292	2.5
10	344.8753	224	1.9
11	346.8771	507	4.4
12	348.8750	957	8.3
13	384.9072	941	8.2
14	394.8737	1918	16.7
15	395.8748	1873	16.3
16	396.8704	5227	45.5
17	397.8754	323	2.8
18	398.8688	11493	100.0
19	399.8747	679	5.9
20	400.8693	2133	18.6
21	452.8967	458	4.0
22	459.1746	281	2.4
23	520.8823	404	3.5
24	530.9354	341	3.0
25	588.8712	339	3.0
26	660.8593	263	2.3
27	678.9782	371	3.2
28	726.8682	270	2.4
29	784.8958	278	2.4
30	786.8984	549	4.8

Mass Spectrum List Report

Analysis Info

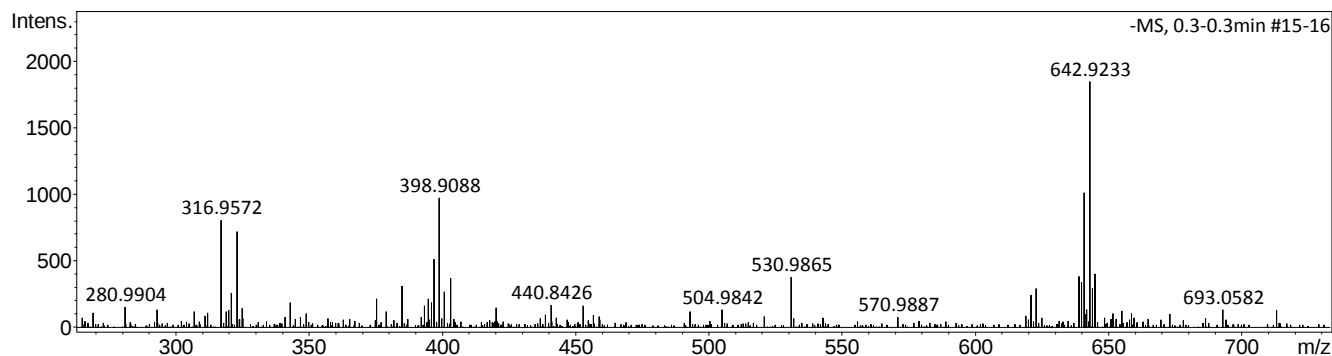
Analysis Name D:\Data\ggc\24-100107_P1-B-7_01_9573.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100107
 Comment JM-07
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 12:46:57 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.9758	199	10.8
2	192.9941	235	12.7
3	225.0640	330	17.9
4	238.9361	153	8.3
5	248.9681	1067	57.9
6	280.9904	153	8.3
7	316.9572	802	43.6
8	320.9129	261	14.2
9	322.9140	720	39.1
10	342.9186	185	10.0
11	375.2834	215	11.7
12	384.9463	313	17.0
13	393.2815	162	8.8
14	394.9118	216	11.7
15	395.9163	188	10.2
16	396.9108	511	27.7
17	398.9088	971	52.7
18	400.9080	270	14.7
19	403.3202	367	19.9
20	440.8426	170	9.2
21	452.9416	162	8.8
22	530.9865	378	20.5
23	620.9230	246	13.4
24	622.9125	292	15.8
25	638.9194	384	20.9
26	639.9277	338	18.3
27	640.9252	1008	54.8
28	642.9233	1842	100.0
29	643.9213	290	15.8
30	644.9247	401	21.8

Mass Spectrum List Report

Analysis Info

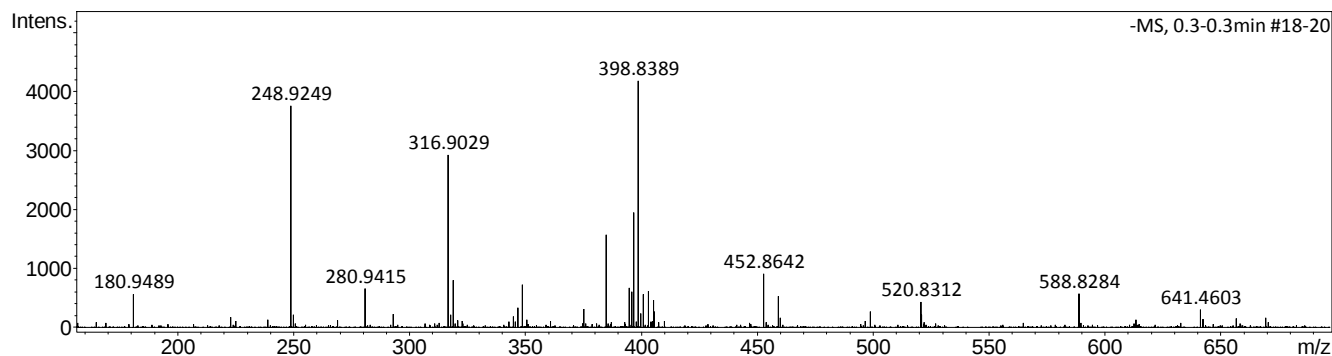
Analysis Name D:\Data\ggc\24-100108_P1-B-8_01_9574.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100108
 Comment JM-09
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 12:52:04 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.9489	561	13.4
2	248.9249	3752	89.9
3	249.9291	215	5.1
4	280.9415	659	15.8
5	292.9449	230	5.5
6	316.9029	2923	70.1
7	317.9067	217	5.2
8	318.9297	803	19.3
9	346.8508	341	8.2
10	348.8462	726	17.4
11	375.2215	311	7.4
12	384.8841	1567	37.6
13	394.8442	671	16.1
14	395.8477	609	14.6
15	396.8404	1943	46.6
16	398.8389	4172	100.0
17	399.8487	239	5.7
18	400.8344	558	13.4
19	400.8703	218	5.2
20	403.2516	618	14.8
21	405.4646	466	11.2
22	405.6118	274	6.6
23	452.8642	910	21.8
24	459.1398	525	12.6
25	498.8216	271	6.5
26	520.8312	438	10.5
27	520.8783	217	5.2
28	588.8284	573	13.7
29	641.4603	301	7.2
30	912.7421	345	8.3

Mass Spectrum List Report

Analysis Info

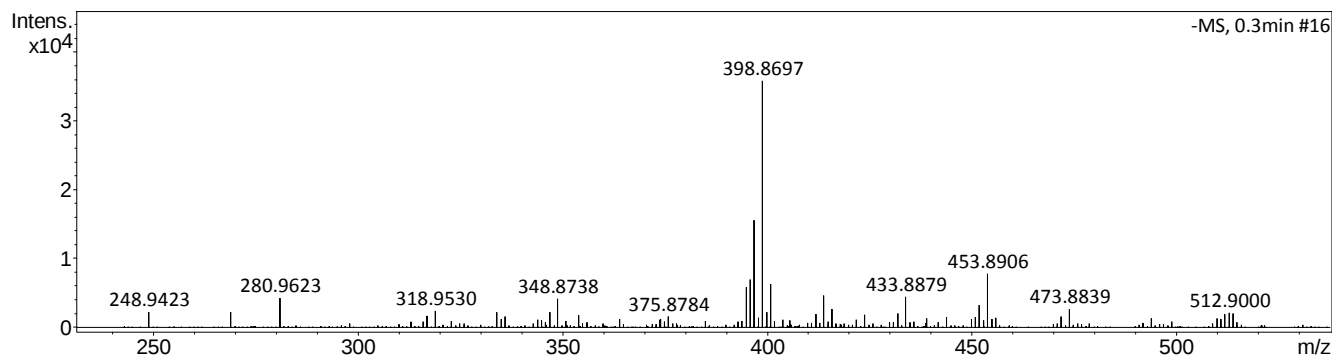
Analysis Name D:\Data\ggc\24-100109_P1-B-9_01_9575.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100109
 Comment JM-10
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 12:57:09 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	248.9423	2249	6.3
2	268.9643	2217	6.2
3	280.9623	4289	12.0
4	316.9238	1633	4.6
5	318.9530	2416	6.8
6	333.9644	2195	6.1
7	335.9803	1605	4.5
8	346.8786	2270	6.4
9	348.8738	4146	11.6
10	353.9709	1745	4.9
11	375.8784	1618	4.5
12	394.8722	5793	16.2
13	395.8779	6947	19.4
14	396.8703	15577	43.6
15	398.8697	35718	100.0
16	399.8725	2193	6.1
17	400.8709	6324	17.7
18	411.8842	1909	5.3
19	413.8817	4597	12.9
20	415.8891	2682	7.5
21	423.8746	1820	5.1
22	431.8925	2071	5.8
23	433.8879	4438	12.4
24	451.8907	3225	9.0
25	453.8906	7788	21.8
26	471.8848	1559	4.4
27	473.8839	2724	7.6
28	511.8981	1968	5.5
29	512.9000	2152	6.0
30	513.8942	2029	5.7

Mass Spectrum List Report

Analysis Info

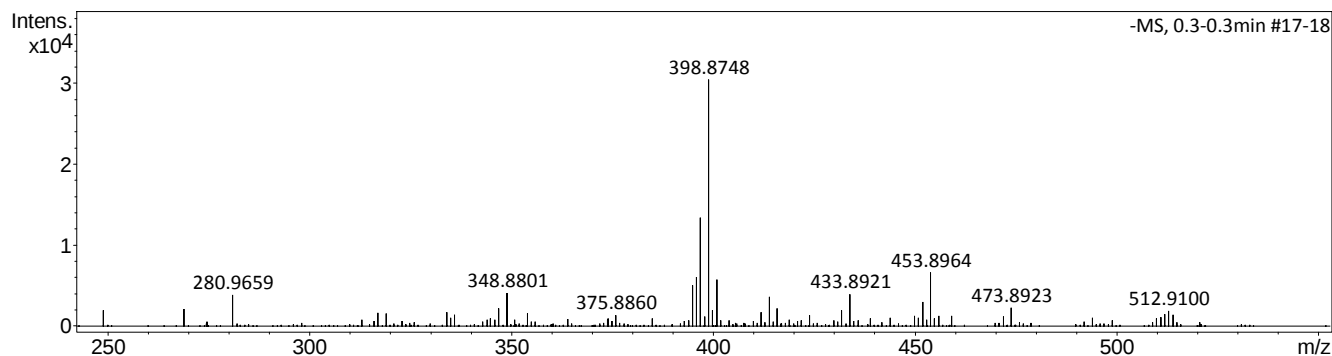
Analysis Name D:\Data\ggc\24-100110_P1-C-1_01_9576.d
 Method lc ms directos_241016neg.m
 Sample Name 24-100110
 Comment JM-11
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/16/2024 1:02:15 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	248.9466	2005	6.6
2	268.9664	2157	7.1
3	280.9659	3870	12.7
4	316.9291	1714	5.6
5	318.9589	1575	5.2
6	333.9685	1768	5.8
7	335.9871	1426	4.7
8	346.8820	2214	7.3
9	348.8801	4146	13.6
10	353.9741	1613	5.3
11	375.8860	1351	4.4
12	394.8797	5057	16.6
13	395.8827	6059	19.9
14	396.8762	13365	44.0
15	398.8748	30382	100.0
16	399.8767	1955	6.4
17	400.8755	5766	19.0
18	411.8917	1767	5.8
19	413.8872	3668	12.1
20	415.8942	2232	7.3
21	423.8848	1339	4.4
22	431.8948	1965	6.5
23	433.8921	3928	12.9
24	451.8995	3014	9.9
25	453.8964	6627	21.8
26	455.8974	1319	4.3
27	473.8923	2300	7.6
28	511.9041	1492	4.9
29	512.9100	1945	6.4
30	513.9009	1473	4.8

Qualitative Compound Report

Analysis Info

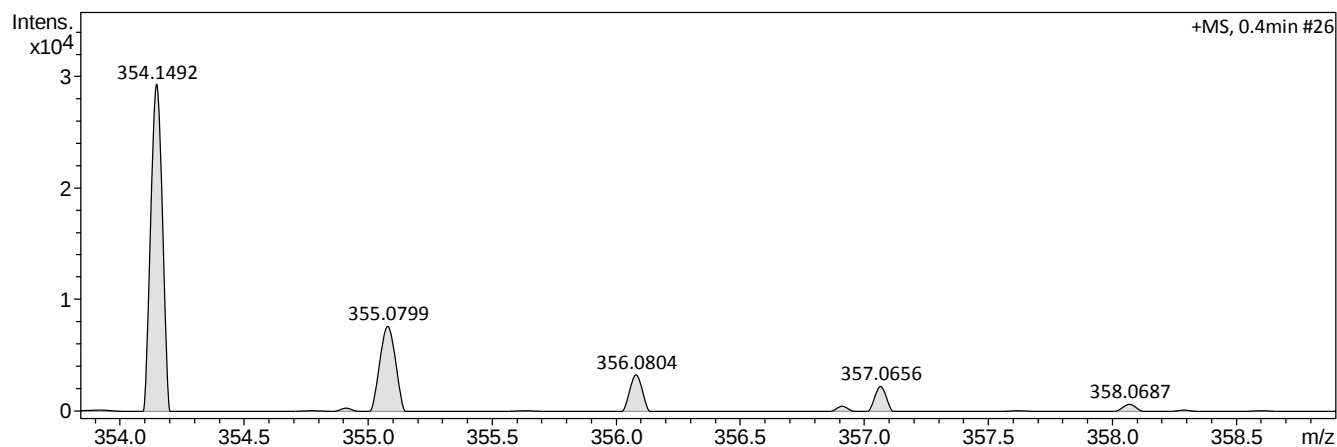
Analysis Name D:\Data\ggc\24-100111_P1-C-2_01_9509.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100111
 Comment HG1
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:03:51 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
354.1492	1	C19H25NNaO2S	354.1498	1.7	n.a.	2	87.69	7.5	even	ok

Mass Spectrum List Report

Analysis Info

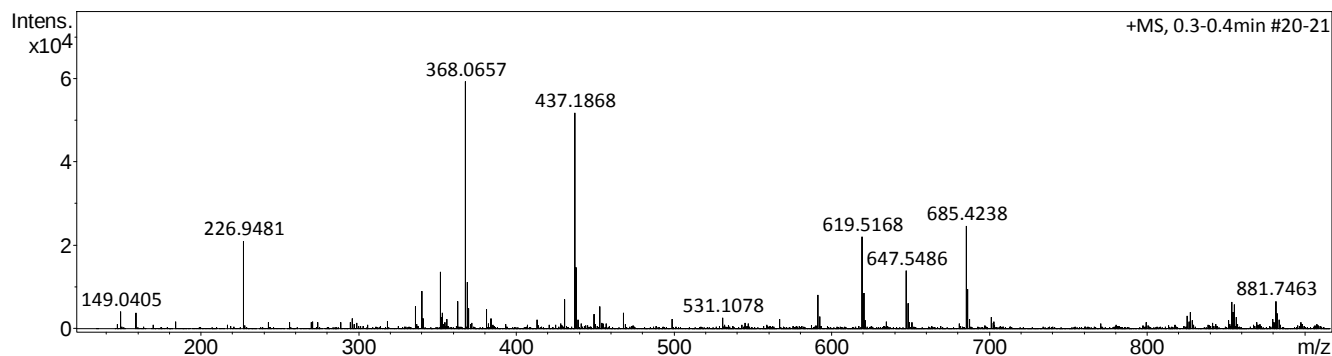
Analysis Name D:\Data\ggc\24-100112_P1-C-3_01_9510.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100112
 Comment HG2
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:09:03 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	149.0405	4101	6.9
2	158.9629	3718	6.3
3	226.9481	20865	35.2
4	336.0396	5258	8.9
5	340.2744	8964	15.1
6	352.0358	13519	22.8
7	353.2609	3793	6.4
8	362.9202	6524	11.0
9	368.0657	59209	100.0
10	369.0671	11120	18.8
11	370.0646	4816	8.1
12	381.2914	4687	7.9
13	430.9063	6998	11.8
14	437.1868	51607	87.2
15	438.1908	14665	24.8
16	453.1614	5283	8.9
17	468.1172	3773	6.4
18	591.4861	8013	13.5
19	619.5168	22018	37.2
20	620.5193	8598	14.5
21	647.5486	13928	23.5
22	648.5499	6051	10.2
23	685.4238	24563	41.5
24	686.4298	9474	16.0
25	827.6923	3931	6.6
26	853.7127	6454	10.9
27	854.7161	3929	6.6
28	855.7270	5730	9.7
29	881.7463	6527	11.0
30	882.7547	3563	6.0

Qualitative Compound Report

Analysis Info

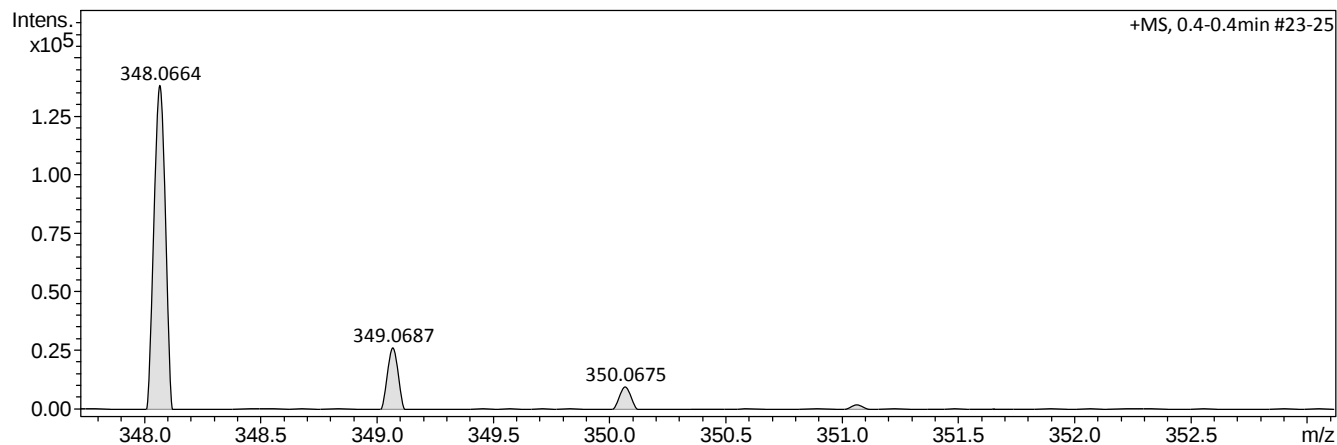
Analysis Name D:\Data\ggc\24-100113_P1-C-4_01_9511.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100113
 Comment HG3
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:14:12 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
348.0664	1	C18H15NNaO3S	348.0665	0.3	10.1	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

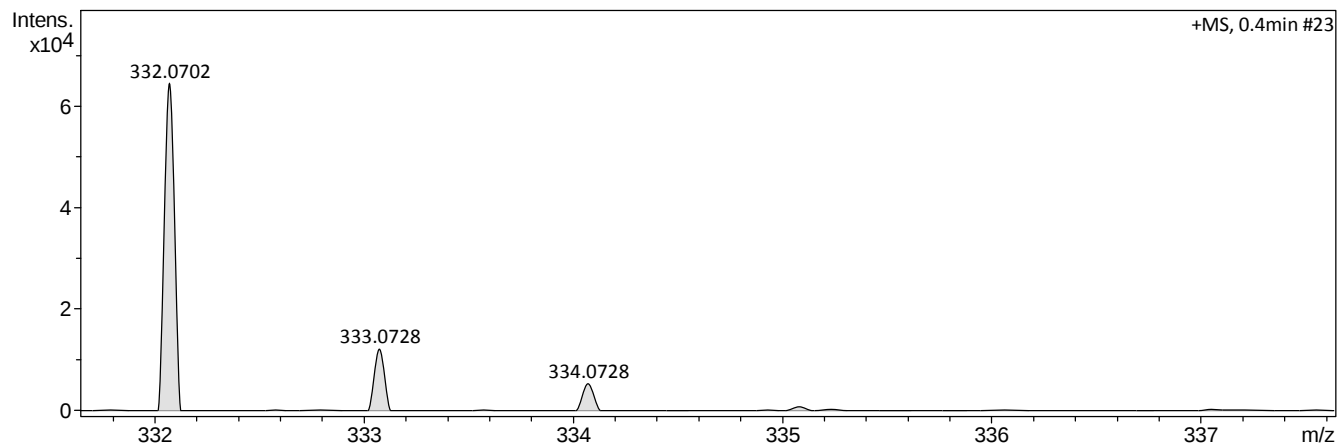
Analysis Name D:\Data\ggc\24-100114_P1-C-5_01_9512.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100114
 Comment HG4
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:19:22 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
332.0702	1	C18H15NNaO2S	332.0716	4.2	11.8	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

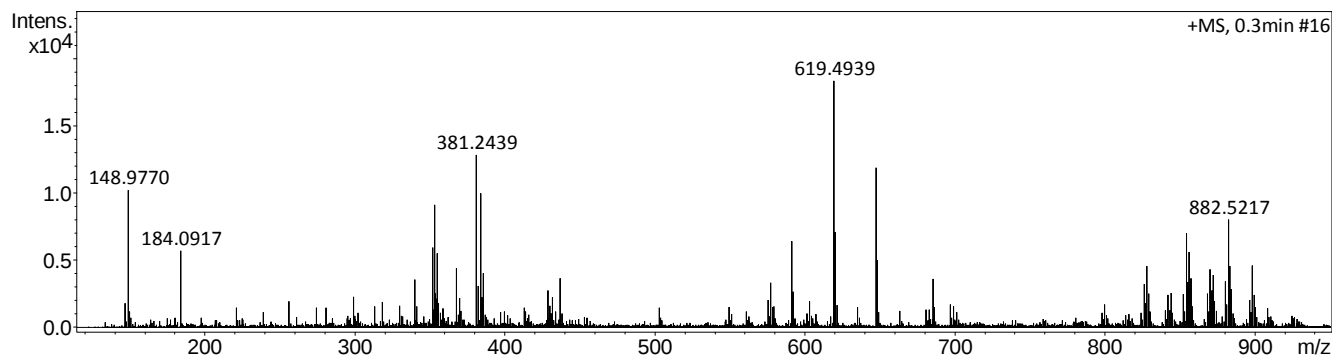
Analysis Name D:\Data\ggc\24-100115_P1-C-6_01_9513.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100115
 Comment HG5
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:24:30 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	148.9770	10231	55.9
2	184.0917	5715	31.2
3	340.2663	3573	19.5
4	351.9873	5929	32.4
5	353.2368	9112	49.8
6	355.0360	5504	30.1
7	367.9622	4410	24.1
8	381.2439	12800	69.9
9	383.9835	9971	54.5
10	385.9782	4035	22.0
11	437.1012	3679	20.1
12	577.4422	3313	18.1
13	591.4339	6399	35.0
14	619.4939	18309	100.0
15	620.4965	7070	38.6
16	647.5684	11855	64.7
17	648.5761	4976	27.2
18	685.5198	3634	19.8
19	826.2097	3212	17.5
20	828.2353	4540	24.8
21	854.3635	7004	38.3
22	855.3762	3391	18.5
23	856.3848	5595	30.6
24	857.3936	3674	20.1
25	870.4125	4330	23.6
26	872.4268	3898	21.3
27	880.4928	3411	18.6
28	882.5217	8025	43.8
29	883.5274	4548	24.8
30	898.5809	4592	25.1

Mass Spectrum List Report

Analysis Info

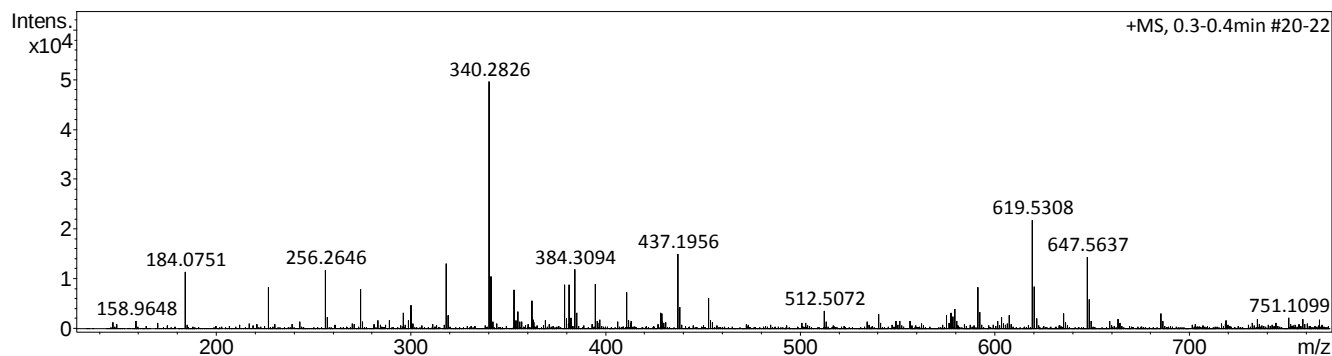
Analysis Name D:\Data\ggc\24-100116_P1-C-7_01_9514.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100116
 Comment HG6
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:29:37 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0751	11359	22.9
2	226.9518	8267	16.7
3	256.2646	11772	23.8
4	274.2744	7932	16.0
5	300.2900	4665	9.4
6	318.3009	12987	26.2
7	340.2826	49502	100.0
8	341.2857	10510	21.2
9	353.2685	7773	15.7
10	362.3264	5560	11.2
11	379.0308	8807	17.8
12	381.2995	8846	17.9
13	384.3094	11901	24.0
14	395.0413	8998	18.2
15	411.0486	7305	14.8
16	437.1956	14953	30.2
17	438.2007	4299	8.7
18	453.1714	6171	12.5
19	579.5367	3942	8.0
20	591.5002	8293	16.8
21	619.5308	21681	43.8
22	620.5339	8366	16.9
23	647.5637	14248	28.8
24	648.5639	5837	11.8
25	853.7319	7234	14.6
26	854.7314	4161	8.4
27	855.7431	6165	12.5
28	881.7678	7316	14.8
29	882.7692	4354	8.8
30	897.7438	3828	7.7

Qualitative Compound Report

Analysis Info

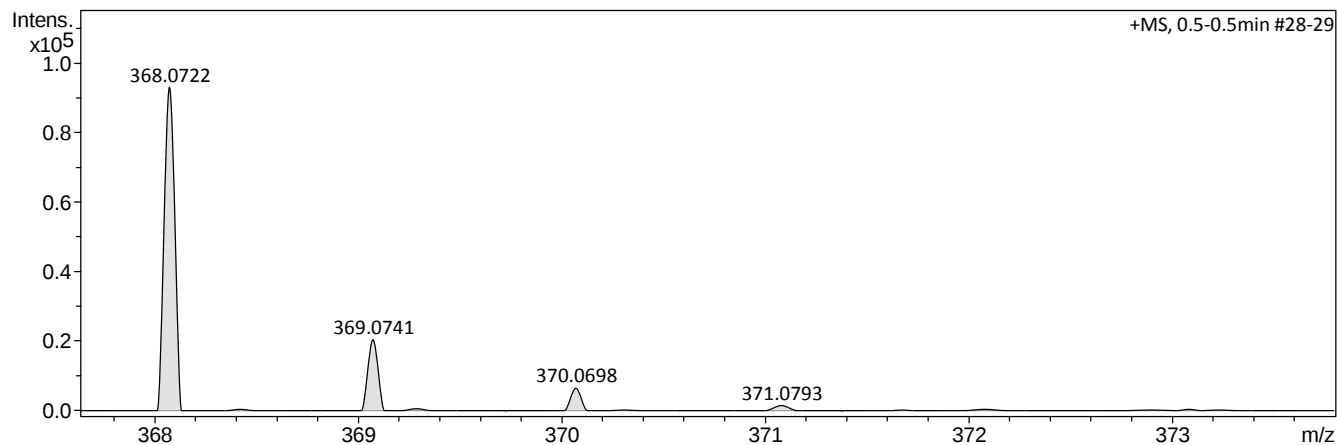
Analysis Name D:\Data\ggc\24-100117_P1-C-8_01_9515.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100117
 Comment HG7
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:34:47 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
368.0722	1	C21H15NNaO2S	368.0716	-1.8	11.8	1	100.00	14.5	even	ok

Qualitative Compound Report

Analysis Info

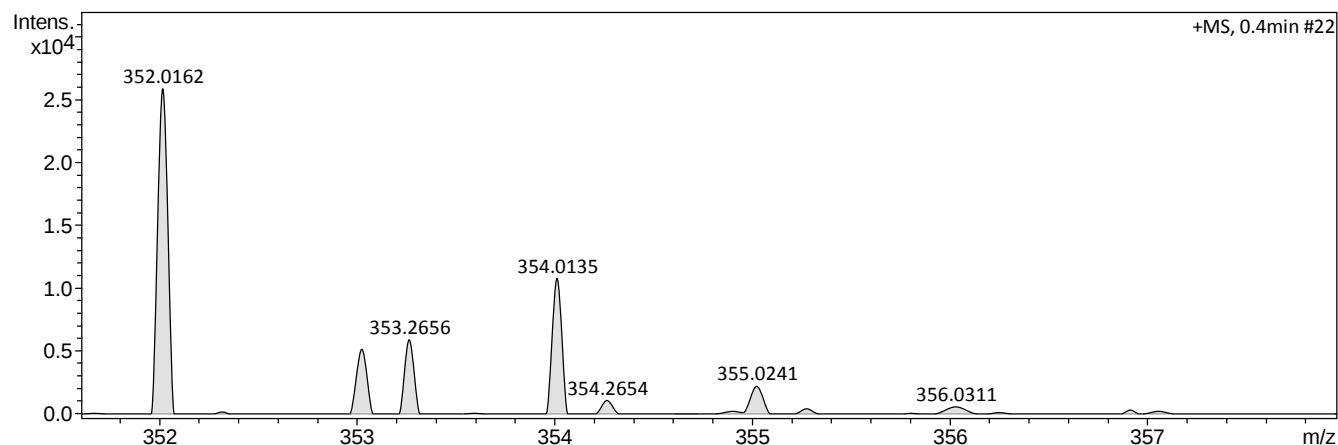
Analysis Name D:\Data\ggc\24-100118_P1-C-9_01_9516.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100118
 Comment HG8
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:39:57 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
352.0162	1	C17H12CINNaO2S	352.0169	2.0	17.5	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

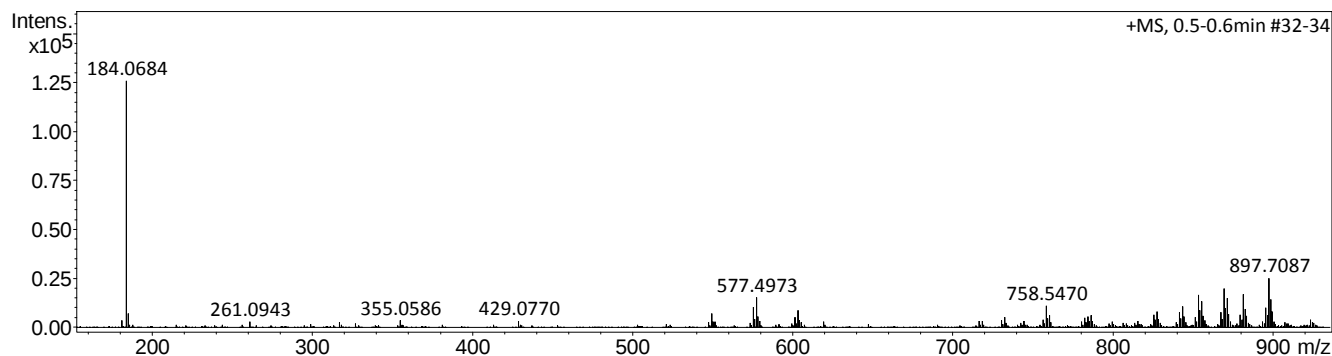
Analysis Name D:\Data\ggc\24-100119_P1-D-1_01_9517.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100119
 Comment HG9
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:45:05 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0684	125487	100.0
2	185.0702	7184	5.7
3	549.4705	7063	5.6
4	575.4875	10410	8.3
5	577.4973	15183	12.1
6	603.5156	8767	7.0
7	758.5470	11106	8.9
8	760.5654	6155	4.9
9	786.5772	6249	5.0
10	825.6704	6634	5.3
11	827.6760	8306	6.6
12	841.6584	7853	6.3
13	843.6591	10634	8.5
14	853.7005	16725	13.3
15	854.7025	8924	7.1
16	855.7105	13365	10.7
17	867.6595	7892	6.3
18	869.6732	19914	15.9
19	870.6772	9782	7.8
20	871.6864	14941	11.9
21	872.6931	6990	5.6
22	879.7196	6619	5.3
23	881.7322	16786	13.4
24	882.7359	9497	7.6
25	883.7229	5889	4.7
26	895.6883	10155	8.1
27	896.6948	6069	4.8
28	897.7087	25084	20.0
29	898.7090	14371	11.5
30	899.7134	8144	6.5

Mass Spectrum List Report

Analysis Info

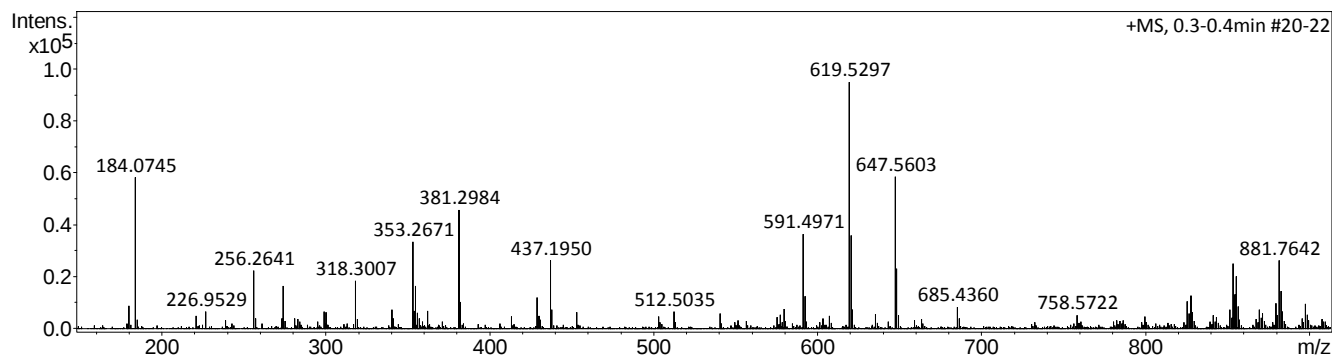
Analysis Name D:\Data\ggc\24-100120_P1-D-2_01_9518.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100120
 Comment HG11
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:50:13 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.0806	8884	9.4
2	184.0745	58085	61.3
3	256.2641	22406	23.6
4	274.2740	16355	17.3
5	318.3007	18462	19.5
6	340.2819	7410	7.8
7	353.2671	33258	35.1
8	355.0706	16286	17.2
9	381.2984	45624	48.1
10	382.3002	10351	10.9
11	429.0898	11973	12.6
12	437.1950	26146	27.6
13	579.5343	7556	8.0
14	591.4971	36254	38.3
15	592.4999	12523	13.2
16	619.5297	94755	100.0
17	620.5327	35826	37.8
18	647.5603	58479	61.7
19	648.5620	22941	24.2
20	685.4360	8250	8.7
21	825.6996	10391	11.0
22	827.7070	12605	13.3
23	853.7275	25097	26.5
24	854.7302	13304	14.0
25	855.7410	20003	21.1
26	856.7391	8440	8.9
27	879.7483	9764	10.3
28	881.7642	26179	27.6
29	882.7674	14453	15.3
30	897.7401	9403	9.9

Mass Spectrum List Report

Analysis Info

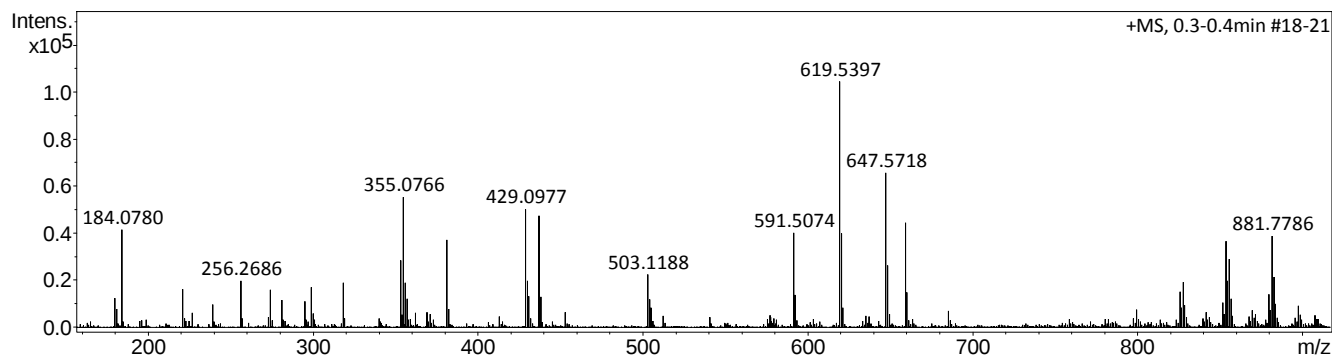
Analysis Name D:\Data\ggc\24-100121_P1-D-3_01_9519.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100121
 Comment HG13
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 3:55:21 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0780	41311	39.7
2	221.0902	16126	15.5
3	256.2686	19687	18.9
4	274.2787	16070	15.4
5	299.0681	17081	16.4
6	318.3053	18926	18.2
7	353.2726	28449	27.3
8	355.0766	55207	53.0
9	356.0756	19029	18.3
10	381.3052	37094	35.6
11	429.0977	50006	48.0
12	430.0958	19680	18.9
13	437.2028	47340	45.4
14	503.1188	22584	21.7
15	591.5074	40020	38.4
16	592.5093	13843	13.3
17	619.5397	104173	100.0
18	620.5431	39794	38.2
19	647.5718	65642	63.0
20	648.5731	26223	25.2
21	659.2995	44481	42.7
22	660.3058	14930	14.3
23	825.7120	15244	14.6
24	827.7205	19111	18.3
25	853.7430	36549	35.1
26	854.7445	19660	18.9
27	855.7565	29018	27.9
28	879.7619	13970	13.4
29	881.7786	38791	37.2
30	882.7821	21353	20.5

Mass Spectrum List Report

Analysis Info

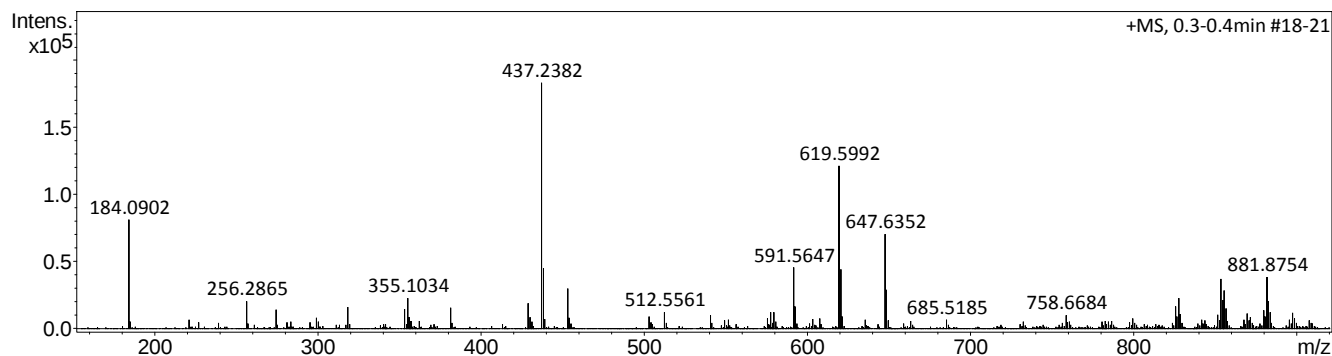
Analysis Name D:\Data\ggc\24-100122_P1-D-4_01_9520.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100122
 Comment HG15
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:00:31 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0902	81010	44.3
2	256.2865	20254	11.1
3	274.2979	13985	7.6
4	318.3302	15990	8.7
5	353.3001	14589	8.0
6	355.1034	22585	12.3
7	381.3347	15577	8.5
8	429.1335	18893	10.3
9	437.2382	182899	100.0
10	438.2431	44970	24.6
11	453.2153	30052	16.4
12	512.5561	12397	6.8
13	577.5786	12109	6.6
14	579.6004	12419	6.8
15	591.5647	45572	24.9
16	592.5669	16764	9.2
17	619.5992	121011	66.2
18	620.6009	44157	24.1
19	647.6352	70053	38.3
20	648.6380	28808	15.8
21	825.8035	16301	8.9
22	827.8131	22511	12.3
23	853.8402	37002	20.2
24	854.8444	21262	11.6
25	855.8523	28260	15.5
26	856.8512	15072	8.2
27	879.8548	13646	7.5
28	881.8754	38281	20.9
29	882.8779	20245	11.1
30	883.8756	12018	6.6

Qualitative Compound Report

Analysis Info

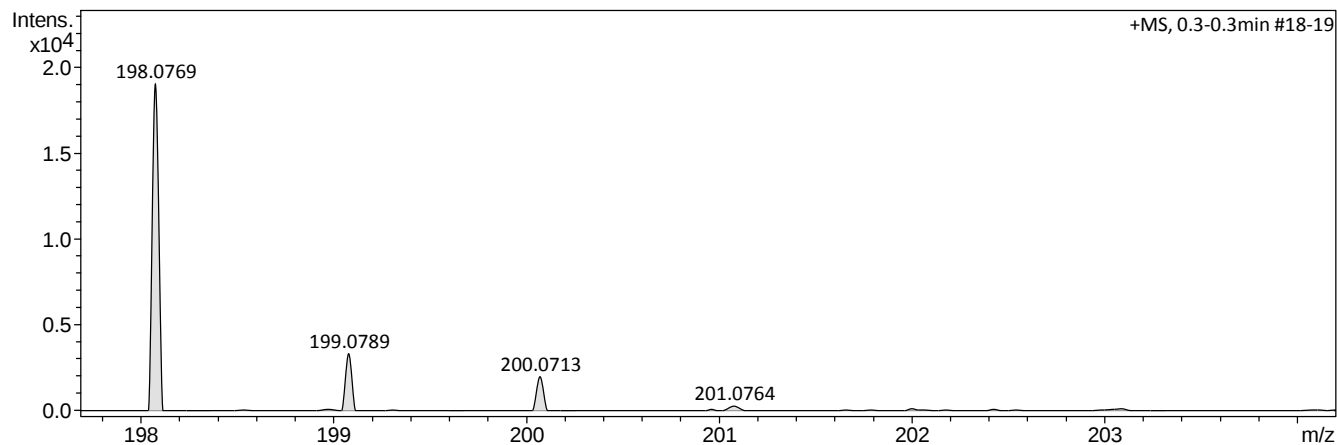
Analysis Name D:\Data\ggc\24-100123_P1-D-5_01_9521.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100123
 Comment HG17
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:05:37 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
198.0769	1	C9H16NSSi	198.0767	-0.9	9.4	1	100.00	3.5	even	ok

Qualitative Compound Report

Analysis Info

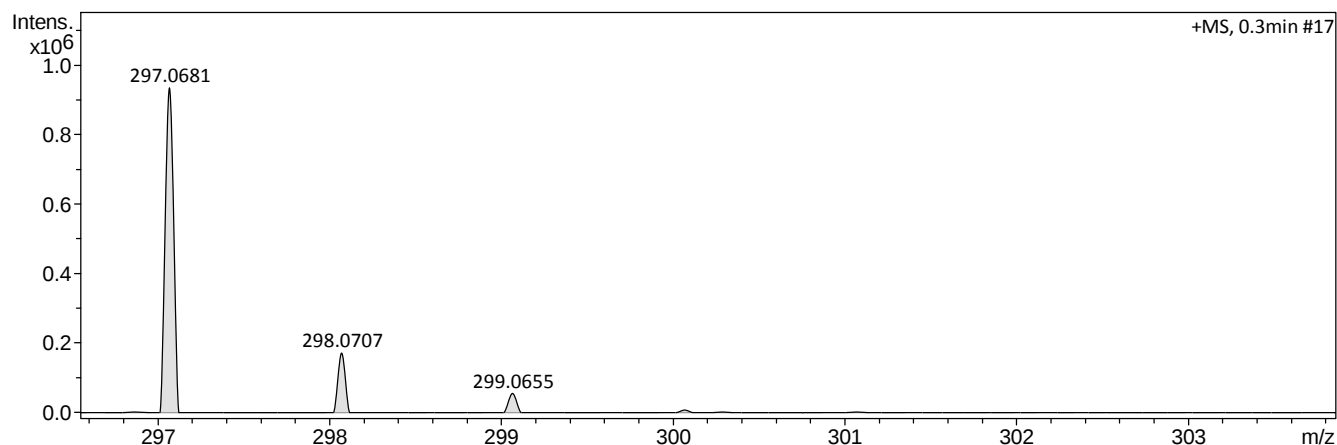
Analysis Name D:\Data\ggc\24-100124_P1-D-6_01_9522.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100124
 Comment HG18
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:10:48 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
297.0681	1	C16H13N2O2S	297.0692	3.7	5.0	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

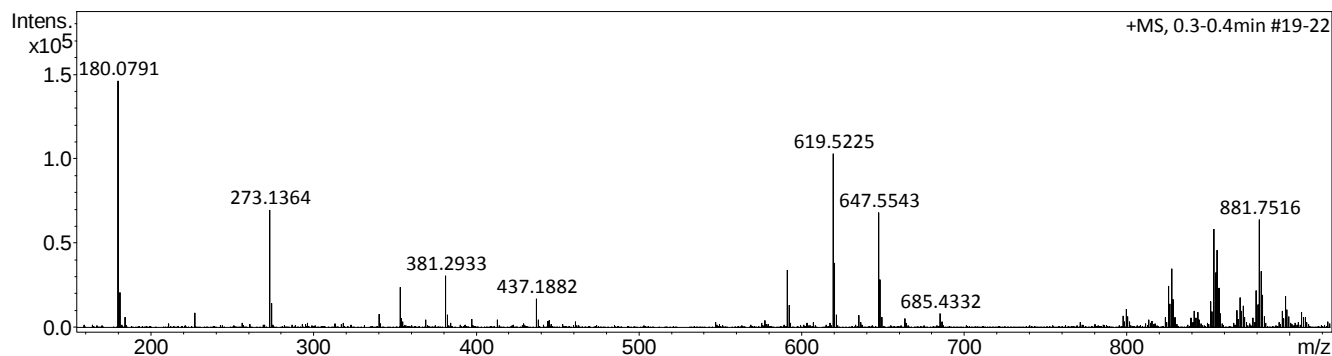
Analysis Name D:\Data\ggc\24-100125_P1-D-7_01_9523.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100125
 Comment HG19
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:15:56 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	180.0791	145681	100.0
2	181.0818	20871	14.3
3	273.1364	69572	47.8
4	274.1394	14250	9.8
5	353.2625	23754	16.3
6	381.2933	30773	21.1
7	437.1882	16981	11.7
8	591.4923	34031	23.4
9	592.4951	13081	9.0
10	619.5225	102897	70.6
11	620.5244	38203	26.2
12	647.5543	67925	46.6
13	648.5567	28369	19.5
14	825.6901	24735	17.0
15	826.6928	13966	9.6
16	827.7020	34821	23.9
17	828.7043	16816	11.5
18	851.7008	15632	10.7
19	853.7220	58059	39.9
20	854.7267	32426	22.3
21	855.7343	45553	31.3
22	856.7348	23512	16.1
23	869.7002	17772	12.2
24	871.7047	12889	8.8
25	879.7309	21882	15.0
26	880.7365	13483	9.3
27	881.7516	63931	43.9
28	882.7532	33217	22.8
29	883.7548	19267	13.2
30	897.7257	18679	12.8

Qualitative Compound Report

Analysis Info

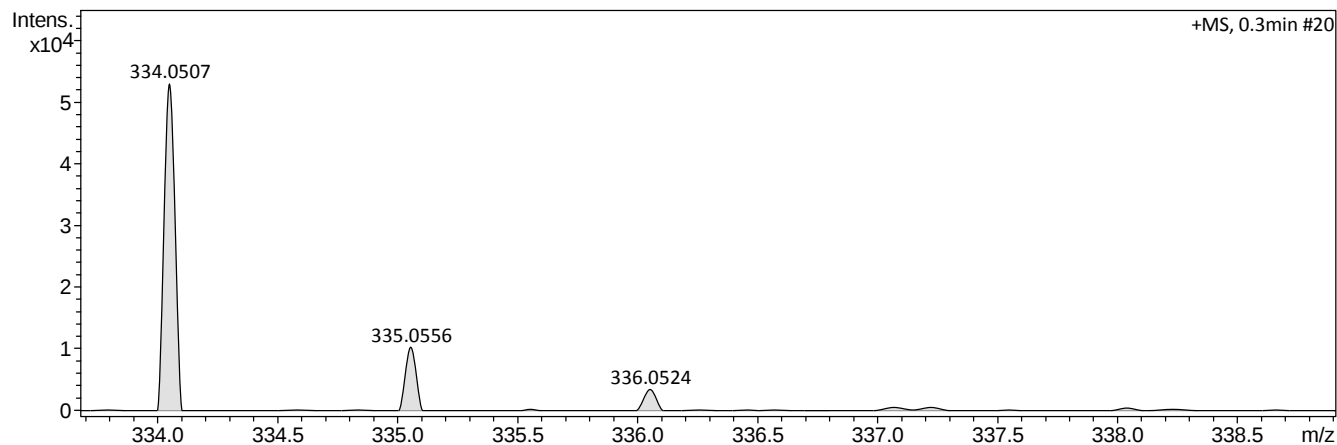
Analysis Name D:\Data\ggc\24-100126_P1-D-8_01_9524.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100126
 Comment HG20
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:21:05 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
334.0507	1	C17H13NNaO3S	334.0508	0.3	6.5	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-100127_P1-D-9_01_9525.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100127
 Comment HG21
 Sv: MeOH + HCOOH
 Argüello - UNC

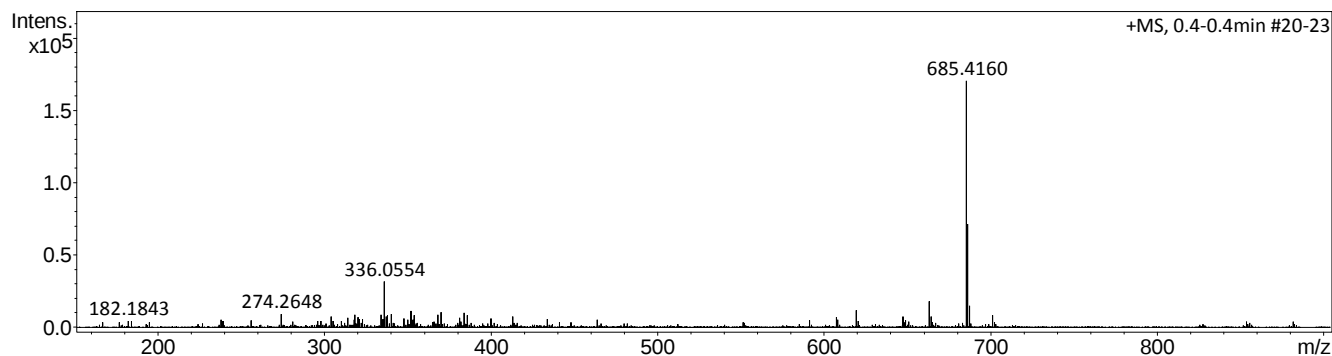
Acquisition Date 10/7/2024 4:26:16 PM

Operator EB - MV

Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	274.2648	9399	5.5
2	304.0853	7701	4.5
3	314.0736	6431	3.8
4	318.2903	8793	5.2
5	320.0616	7056	4.2
6	321.0742	5929	3.5
7	334.0426	9034	5.3
8	336.0554	31882	18.8
9	337.0596	7431	4.4
10	338.0691	8467	5.0
11	340.2711	9202	5.4
12	348.0219	6051	3.6
13	352.0508	11365	6.7
14	354.0630	8215	4.8
15	368.0671	8984	5.3
16	370.0682	10679	6.3
17	381.2854	6727	4.0
18	384.0691	10065	5.9
19	386.0783	8337	4.9
20	400.0581	6308	3.7
21	413.2551	7375	4.3
22	607.3722	7238	4.3
23	619.5069	11837	7.0
24	647.5387	7480	4.4
25	663.4334	18263	10.7
26	664.4385	7614	4.5
27	685.4160	169948	100.0
28	686.4198	71448	42.0
29	687.4216	14849	8.7
30	701.3923	8271	4.9

Mass Spectrum List Report

Analysis Info

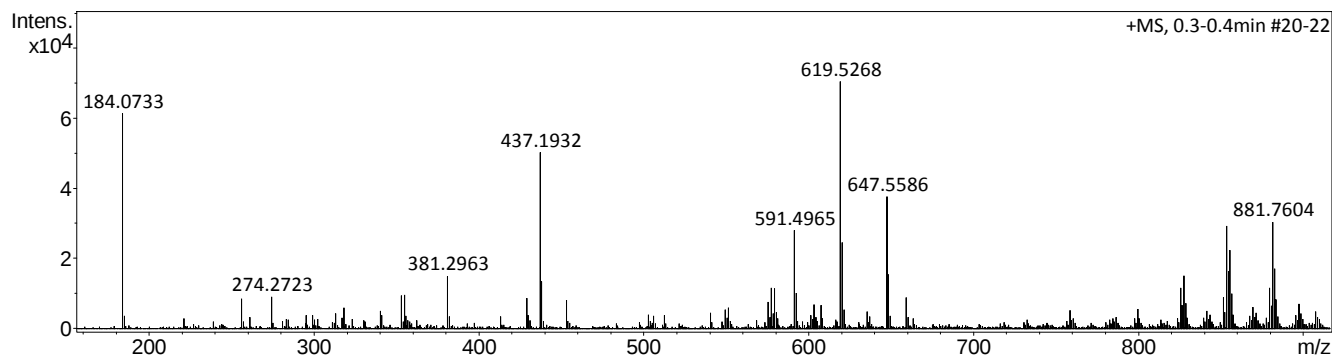
Analysis Name D:\Data\ggc\24-100128_P1-E-1_01_9526.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100128
 Comment HG22
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:31:24 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0733	61297	87.2
2	256.2625	8590	12.2
3	274.2723	9129	13.0
4	353.2648	9498	13.5
5	355.0691	9574	13.6
6	381.2963	14805	21.1
7	429.0884	8708	12.4
8	437.1932	50041	71.2
9	438.1976	13388	19.0
10	453.1689	8206	11.7
11	577.5147	11608	16.5
12	579.5334	11365	16.2
13	591.4965	27988	39.8
14	592.4974	10099	14.4
15	619.5268	70290	100.0
16	620.5307	24438	34.8
17	647.5586	37541	53.4
18	648.5609	15480	22.0
19	659.2859	8899	12.7
20	825.6955	11624	16.5
21	827.7041	14967	21.3
22	851.7162	8844	12.6
23	853.7258	29136	41.5
24	854.7283	16383	23.3
25	855.7390	22304	31.7
26	856.7367	9989	14.2
27	879.7442	11521	16.4
28	881.7604	30336	43.2
29	882.7642	17055	24.3
30	883.7645	8388	11.9

Mass Spectrum List Report

Analysis Info

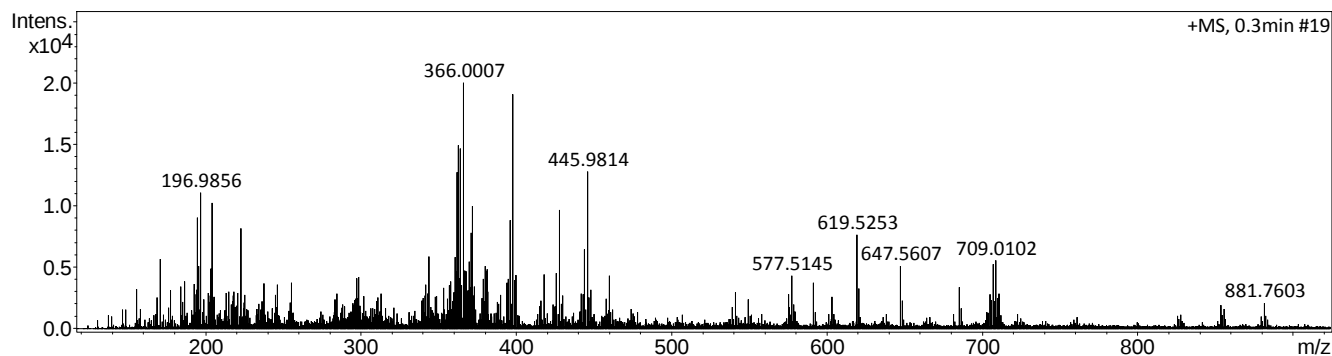
Analysis Name D:\Data\ggc\24-100129_P1-E-2_01_9527.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100129
 Comment HG23
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:36:30 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	170.9708	5639	28.2
2	194.9805	9046	45.2
3	195.5007	5103	25.5
4	196.9856	11034	55.1
5	203.5066	4874	24.4
6	204.5067	10233	51.1
7	222.9675	8119	40.6
8	344.0134	5852	29.2
9	360.9975	5810	29.0
10	361.4968	4657	23.3
11	361.9972	12702	63.5
12	362.9960	14903	74.5
13	363.9974	14643	73.2
14	366.0007	20009	100.0
15	367.0042	4713	23.6
16	369.9952	5450	27.2
17	370.9987	7778	38.9
18	371.9989	9984	49.9
19	380.0029	5078	25.4
20	381.0080	4668	23.3
21	381.2980	4797	24.0
22	396.0252	8793	43.9
23	398.0240	19023	95.1
24	427.9702	9666	48.3
25	443.9812	6439	32.2
26	445.9814	12771	63.8
27	619.5253	7629	38.1
28	647.5607	5097	25.5
29	707.0099	5235	26.2
30	709.0102	5529	27.6

Qualitative Compound Report

Analysis Info

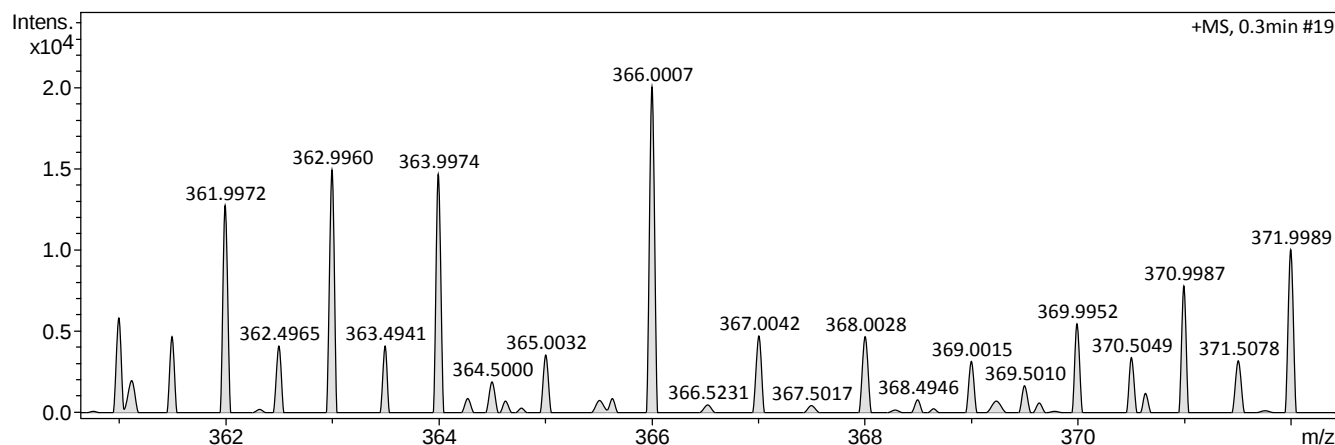
Analysis Name D:\Data\ggc\24-100129_P1-E-2_01_9527.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100129
 Comment HG23
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:36:30 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
366.0007	1	C17H13NNaO2Se	366.0004	-0.8	258.9	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

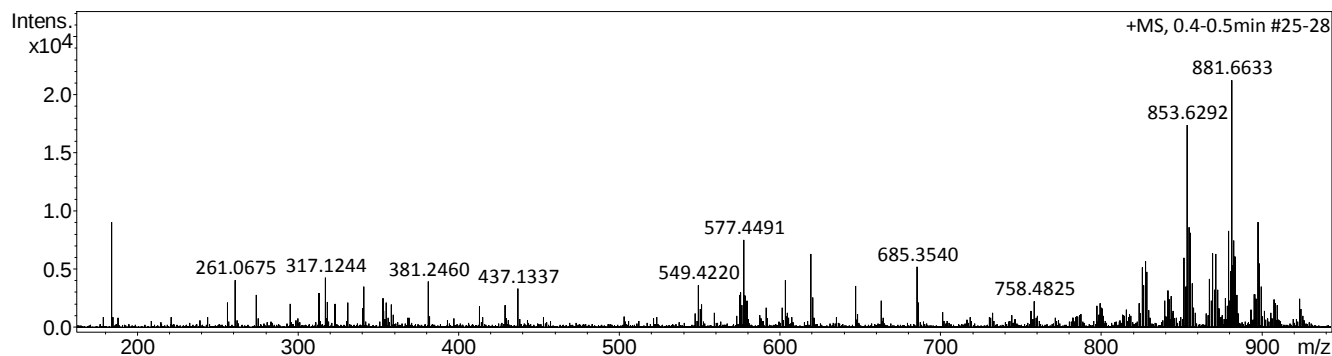
Analysis Name D:\Data\ggc\24-100130_P1-E-3_01_9528.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100130
 Comment HG24
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:41:37 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0448	8016	37.8
2	184.0620	9038	42.7
3	317.1244	4251	20.1
4	577.4491	7504	35.4
5	619.4476	6296	29.7
6	685.3540	5197	24.5
7	825.5786	5123	24.2
8	825.6674	4354	20.6
9	827.6001	5716	27.0
10	827.6771	5284	24.9
11	828.6239	4774	22.5
12	851.6154	5989	28.3
13	853.6292	17381	82.1
14	853.7254	5180	24.5
15	854.6367	8581	40.5
16	855.6239	8037	37.9
17	855.7115	8105	38.3
18	867.6216	4188	19.8
19	869.5943	4517	21.3
20	869.6743	6376	30.1
21	871.6223	6286	29.7
22	879.6434	8282	39.1
23	880.6506	4832	22.8
24	881.6633	21180	100.0
25	881.7489	5296	25.0
26	882.6443	7473	35.3
27	882.7274	6744	31.8
28	883.6665	6071	28.7
29	897.6364	9054	42.7
30	898.6374	5472	25.8

Qualitative Compound Report

Analysis Info

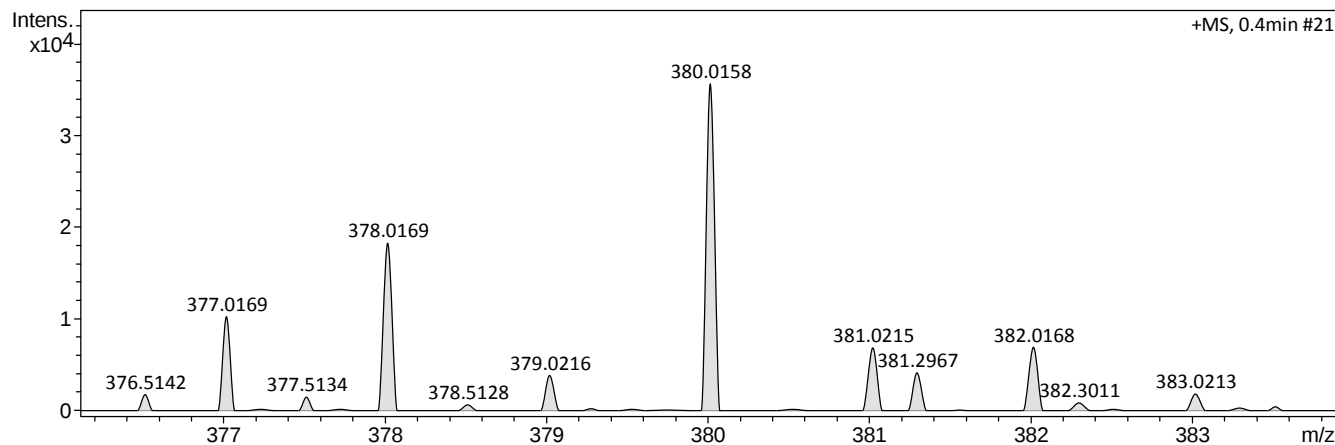
Analysis Name D:\Data\ggc\24-100131_P1-E-4_01_9529.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100131
 Comment HG25
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:46:48 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
380.0158	1	C18H15NNaO2Se	380.0160	0.9	43.5	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

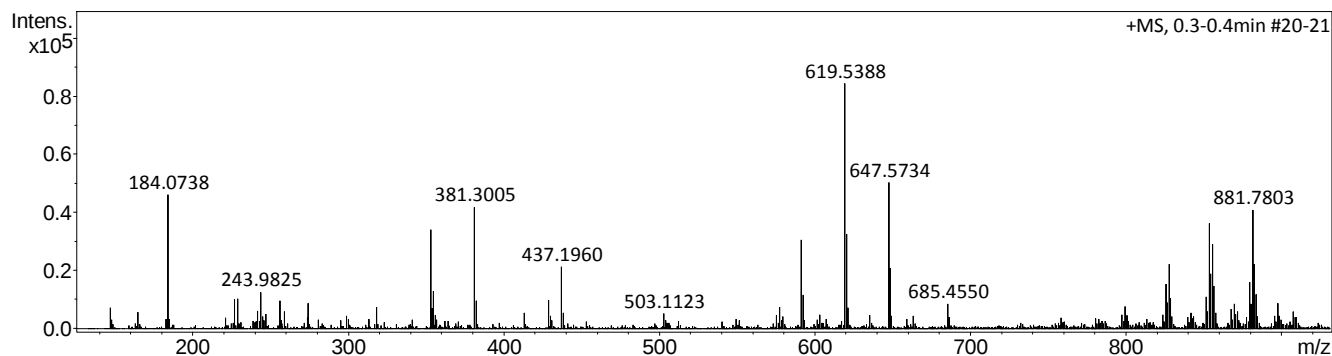
Analysis Name D:\Data\ggc\24-100132_P1-E-5_01_9530.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100132
 Comment HG26
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:51:56 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0738	46058	54.7
2	226.9544	10024	11.9
3	228.9581	10166	12.1
4	243.9825	12396	14.7
5	256.2653	9629	11.4
6	353.2689	33978	40.3
7	355.0714	12841	15.2
8	381.3005	41705	49.5
9	382.3027	9581	11.4
10	429.0940	9758	11.6
11	437.1960	21331	25.3
12	591.5094	30433	36.1
13	592.5115	11524	13.7
14	619.5388	84233	100.0
15	620.5415	32537	38.6
16	647.5734	50152	59.5
17	648.5784	20825	24.7
18	825.7168	15373	18.3
19	826.7236	8935	10.6
20	827.7351	22017	26.1
21	828.7366	10585	12.6
22	851.7294	11008	13.1
23	853.7517	36086	42.8
24	854.7585	18915	22.5
25	855.7641	28984	34.4
26	856.7693	14754	17.5
27	879.7624	15923	18.9
28	881.7803	40720	48.3
29	882.7800	22170	26.3
30	883.7899	11876	14.1

Qualitative Compound Report

Analysis Info

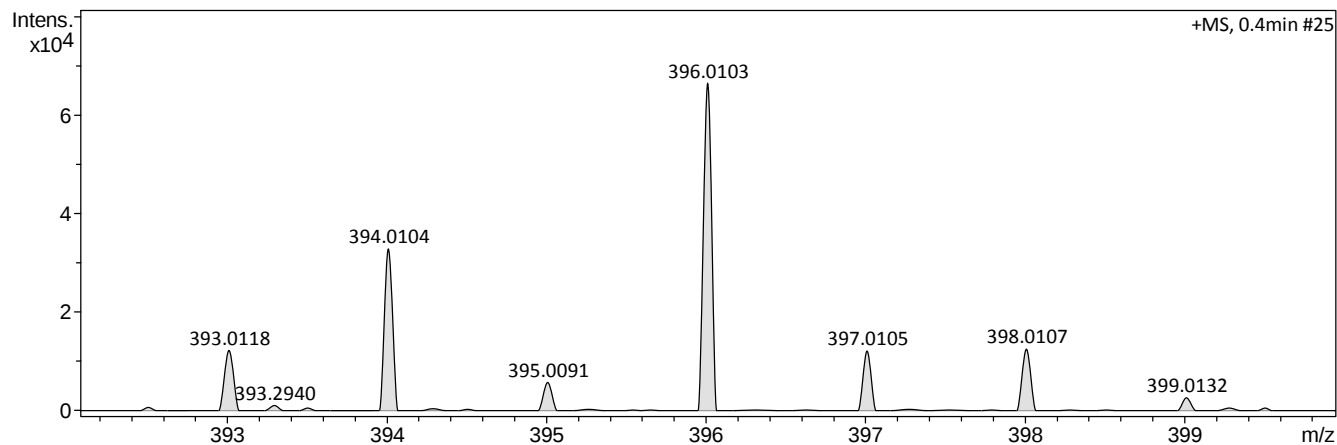
Analysis Name D:\Data\ggc\24-100133_P1-E-6_01_9531.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100133
 Comment HG27
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 4:57:03 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻ Conf	N-Rule
396.0103	1	C18H15NNaO3Se	396.0109	1.8	11.4	1	100.00	11.5	even	ok

Mass Spectrum List Report

Analysis Info

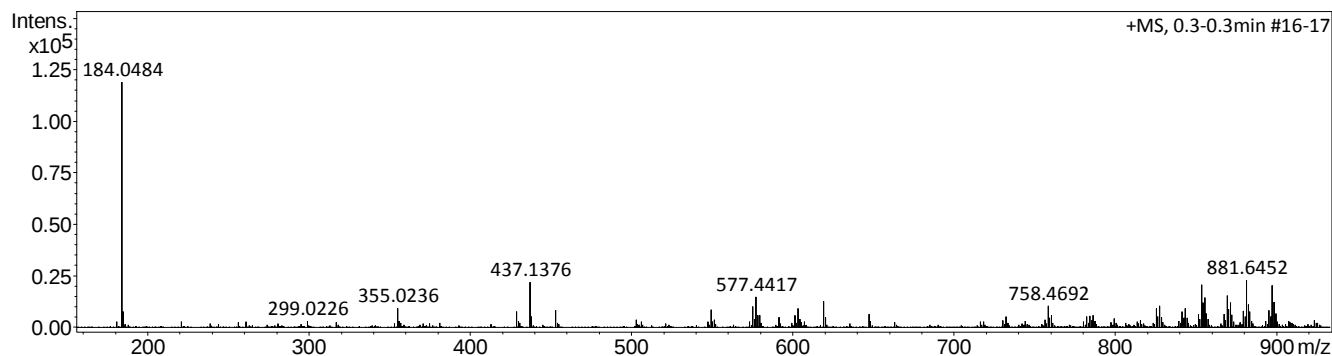
Analysis Name D:\Data\ggc\24-100134_P1-E-7_01_9532.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100134
 Comment HG28
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:02:10 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0484	118828	100.0
2	185.0512	7835	6.6
3	355.0236	9215	7.8
4	429.0317	7622	6.4
5	437.1376	21860	18.4
6	453.1075	8370	7.0
7	549.4132	8553	7.2
8	575.4269	10175	8.6
9	577.4417	14972	12.6
10	603.4541	9164	7.7
11	619.4497	12634	10.6
12	758.4692	10634	8.9
13	825.5863	9438	7.9
14	827.5970	10444	8.8
15	841.5752	7717	6.5
16	843.5726	9403	7.9
17	853.6151	20759	17.5
18	854.6186	12180	10.3
19	855.6196	14644	12.3
20	856.6264	6934	5.8
21	869.5887	15333	12.9
22	870.5896	8833	7.4
23	871.6032	12019	10.1
24	879.6272	8141	6.9
25	881.6452	22931	19.3
26	882.6488	11186	9.4
27	883.6485	7638	6.4
28	895.6016	8317	7.0
29	897.6138	20541	17.3
30	898.6167	12440	10.5

Qualitative Compound Report

Analysis Info

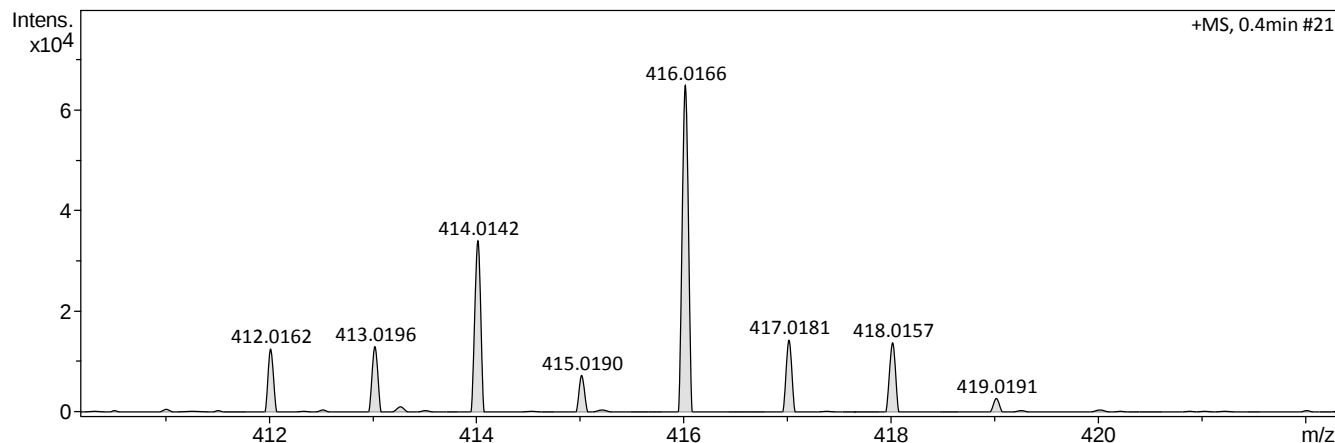
Analysis Name D:\Data\ggc\24-100135_P1-E-8_01_9533.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100135
 Comment HG29
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:07:18 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
416.0166	1	C21H15NNaO2Se	416.0160	-1.2	6.6	2	100.00	14.5	even	ok

Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-100136_P1-E-9_01_9534.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100136
 Comment HG30
 Sv: MeOH + HCOOH
 Argüello - UNC

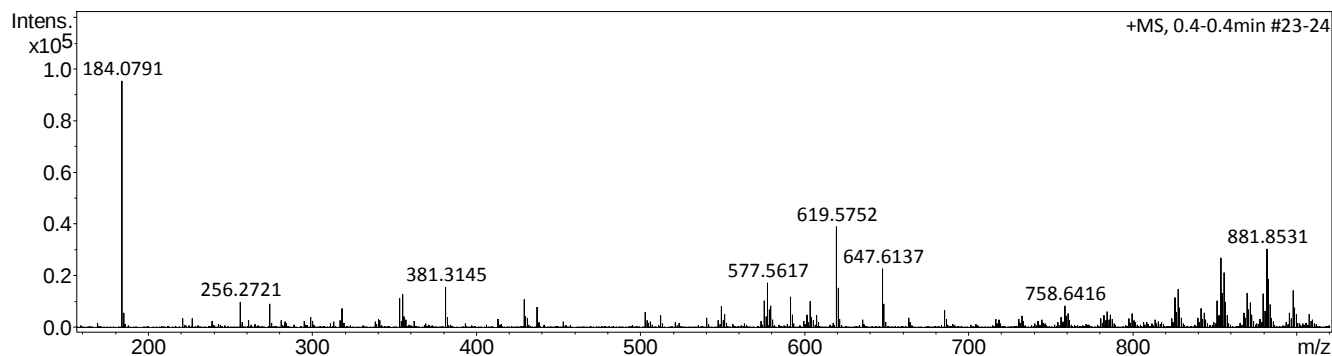
Acquisition Date 10/7/2024 5:12:24 PM

Operator EB - MV

Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0791	95037	100.0
2	256.2721	9802	10.3
3	274.2837	9090	9.6
4	353.2805	11419	12.0
5	355.0842	12772	13.4
6	381.3145	15585	16.4
7	429.1103	10747	11.3
8	575.5428	10277	10.8
9	577.5617	17329	18.2
10	591.5412	11855	12.5
11	603.5792	10058	10.6
12	619.5752	38956	41.0
13	620.5788	15356	16.2
14	647.6137	22795	24.0
15	648.6161	9043	9.5
16	758.6416	8437	8.9
17	825.7791	11659	12.3
18	827.7996	14896	15.7
19	851.8007	10285	10.8
20	853.8177	26961	28.4
21	854.8203	13368	14.1
22	855.8335	21302	22.4
23	856.8394	9786	10.3
24	869.8016	13311	14.0
25	871.8076	9594	10.1
26	879.8400	13195	13.9
27	881.8531	30386	32.0
28	882.8567	18846	19.8
29	883.8563	8770	9.2
30	897.8325	14288	15.0

Qualitative Compound Report

Analysis Info

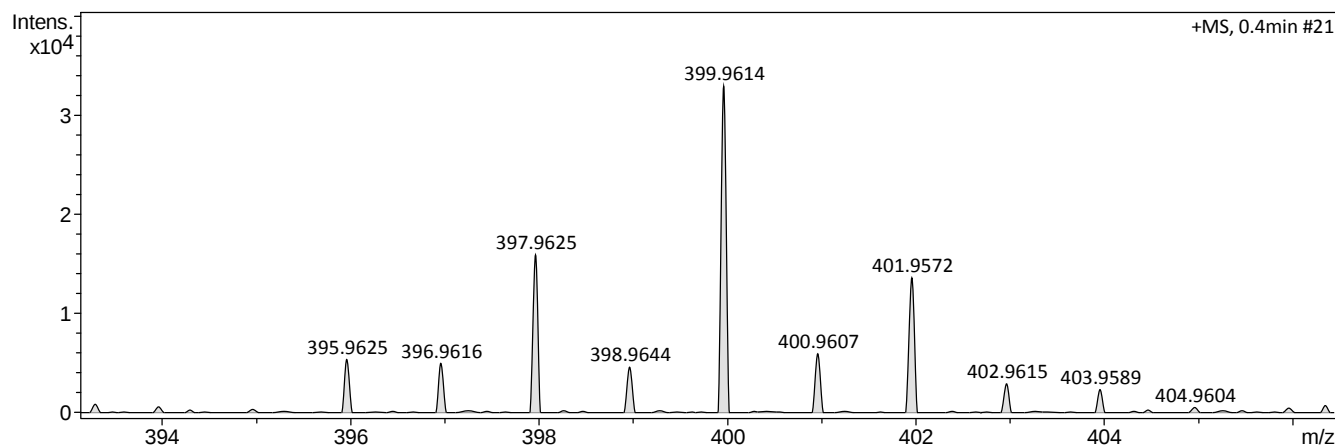
Analysis Name D:\Data\ggc\24-100137_P1-F-1_01_9535.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100137
 Comment HG31
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:17:30 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
399.9614	1	C17H12ClNNaO2Se	399.9614	-0.6	11.2	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

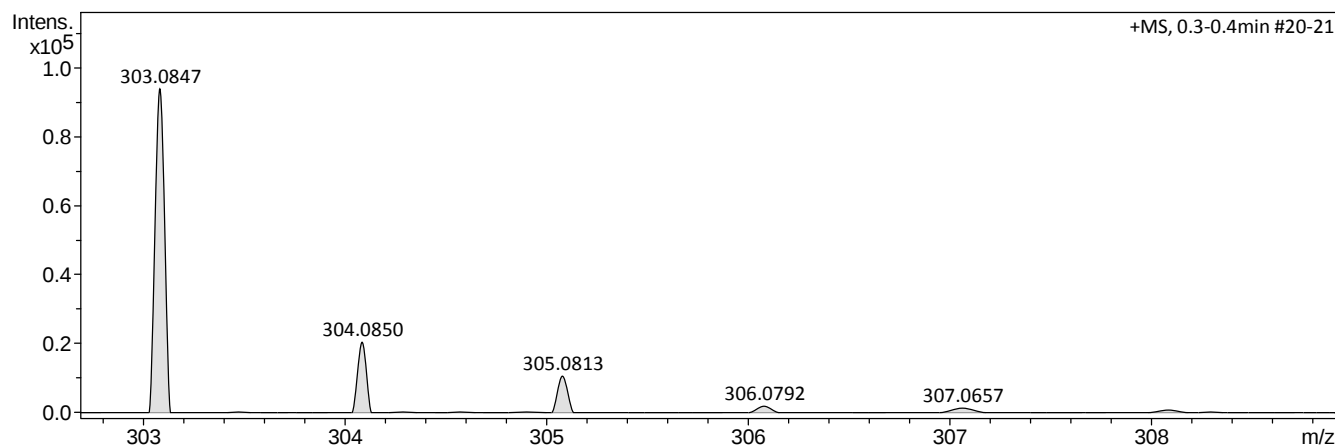
Analysis Name D:\Data\ggc\24-100138_P1-F-2_01_9536.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100138
 Comment HG32
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:22:36 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
303.0847	1	C14H20NaO2SSi	303.0845	-0.6	5.2	1	100.00	5.5	even	ok

Mass Spectrum List Report

Analysis Info

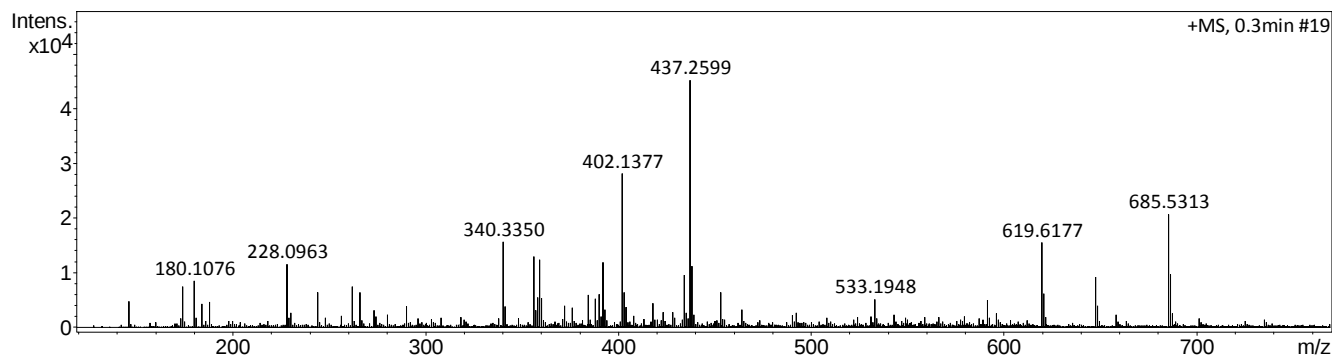
Analysis Name D:\Data\ggc\24-100139_P1-F-3_01_9537.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100139
 Comment HG33
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:27:44 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	146.0838	4787	10.6
2	174.0791	7510	16.7
3	180.1076	8484	18.8
4	188.0969	4721	10.5
5	228.0963	11551	25.6
6	244.0647	6386	14.2
7	262.0779	7420	16.5
8	266.1037	6451	14.3
9	340.3350	15629	34.7
10	356.0893	12983	28.8
11	358.1026	5510	12.2
12	359.1114	12323	27.3
13	360.1173	5387	12.0
14	384.3660	5964	13.2
15	388.1159	5303	11.8
16	390.1348	6071	13.5
17	392.1490	11845	26.3
18	402.1377	28057	62.2
19	403.1414	6423	14.2
20	434.1634	9603	21.3
21	437.2599	45079	100.0
22	438.2613	11242	24.9
23	453.2343	6386	14.2
24	533.1948	5144	11.4
25	591.5804	5021	11.1
26	619.6177	15510	34.4
27	620.6222	6176	13.7
28	647.6533	9247	20.5
29	685.5313	20654	45.8
30	686.5336	9698	21.5

Qualitative Compound Report

Analysis Info

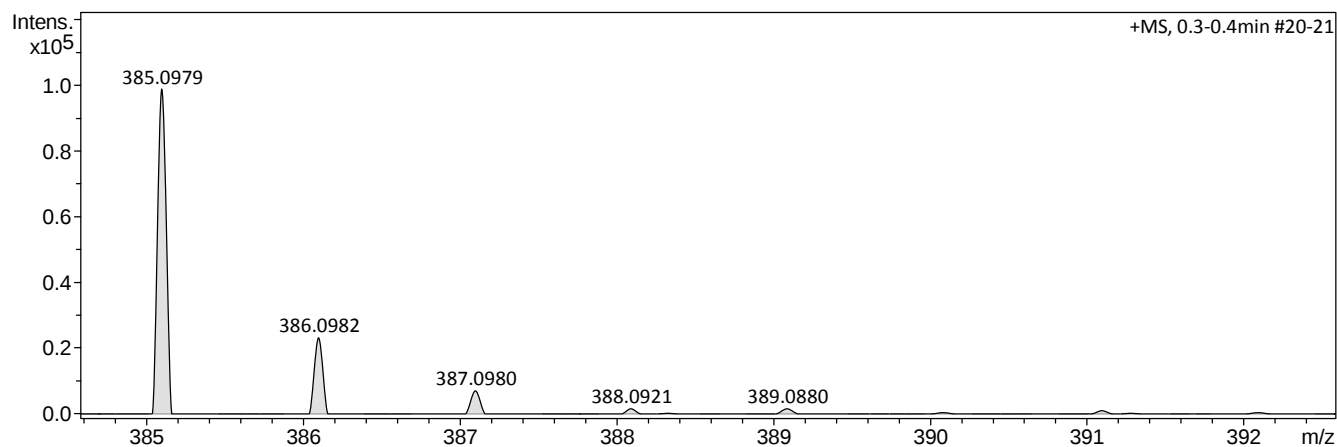
Analysis Name D:\Data\ggc\24-100140_P1-F-4_01_9538.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100140
 Comment HG34
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:32:49 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
385.0979	1	C21H18N2NaO2S	385.0981	0.6	6.1	1	100.00	13.5	even	ok

Mass Spectrum List Report

Analysis Info

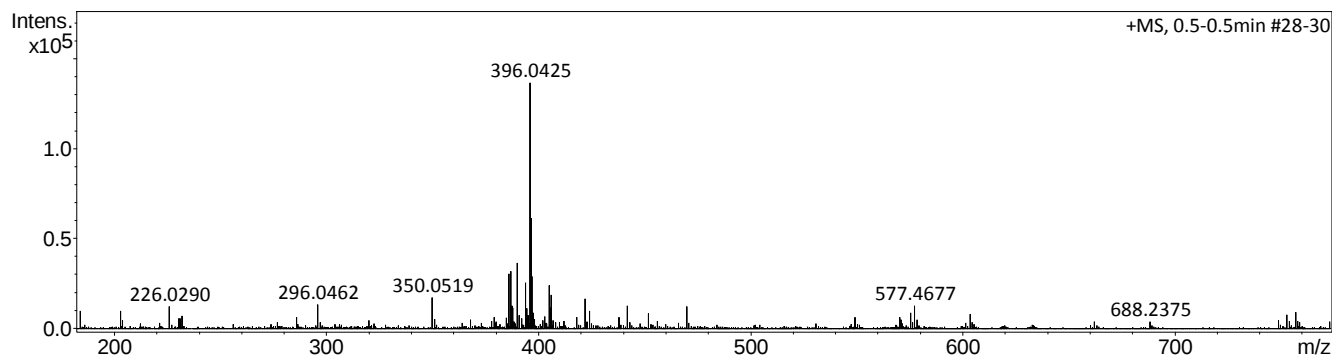
Analysis Name D:\Data\ggc\24-100141_P1-F-5_01_9539.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100141
 Comment HG35
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:37:56 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0558	9761	7.2
2	203.0333	9828	7.2
3	226.0290	12501	9.2
4	296.0462	13427	9.8
5	350.0519	17183	12.6
6	386.0146	30531	22.4
7	387.0321	31841	23.3
8	387.5372	12842	9.4
9	388.0374	11527	8.5
10	390.0413	36336	26.6
11	391.0442	7539	5.5
12	394.0274	25512	18.7
13	394.5274	11094	8.1
14	396.0425	136372	100.0
15	396.5430	61220	44.9
16	397.0419	28909	21.2
17	397.5434	8759	6.4
18	405.0455	23913	17.5
19	405.5480	11452	8.4
20	406.0190	18856	13.8
21	422.0644	16741	12.3
22	424.0178	9683	7.1
23	442.0244	12662	9.3
24	452.0071	8487	6.2
25	470.0172	12195	8.9
26	575.4539	8680	6.4
27	577.4677	12528	9.2
28	603.4841	8119	6.0
29	753.0726	7578	5.6
30	757.0990	8963	6.6

Qualitative Compound Report

Analysis Info

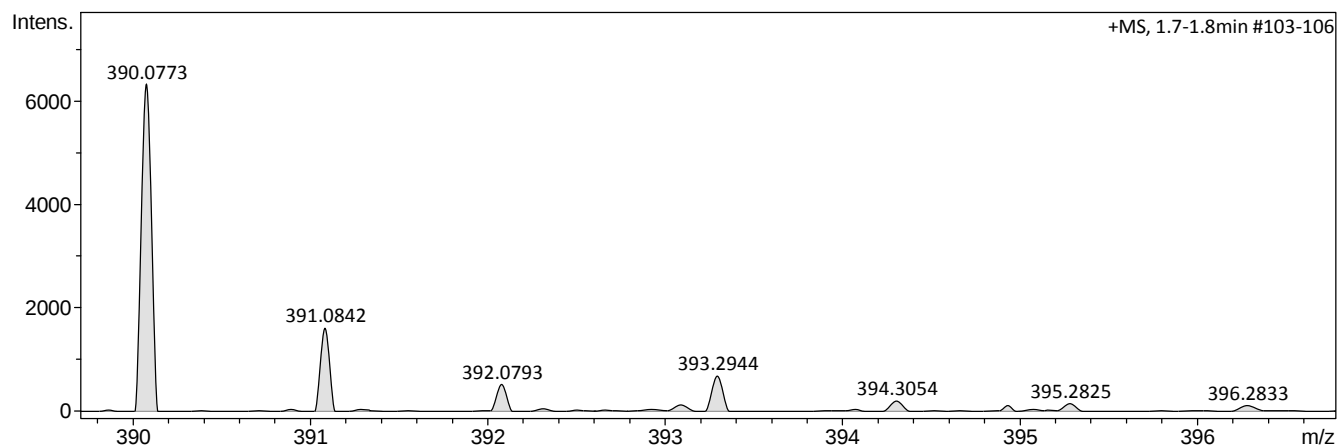
Analysis Name D:\Data\ggc\24-100141_P1-F-5_01_9539.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100141
 Comment HG35
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:37:56 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
390.0773	1	C20H17NNaO4S	390.0770	-0.7	13.4	1	100.00	12.5	even	ok

Qualitative Compound Report

Analysis Info

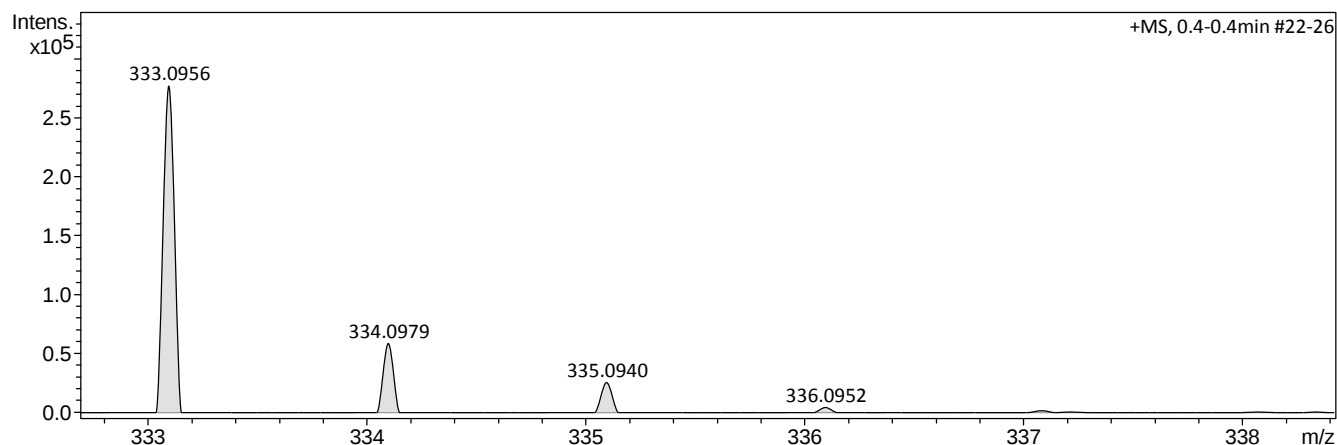
Analysis Name D:\Data\ggc\24-100142_P1-F-6_01_9540.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100142
 Comment HG36
 Sv: DCM + MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:43:04 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
333.0956	1	C15H22NaO3SSi	333.0951	-1.4	10.2	1	100.00	5.5	even	ok

Qualitative Compound Report

Analysis Info

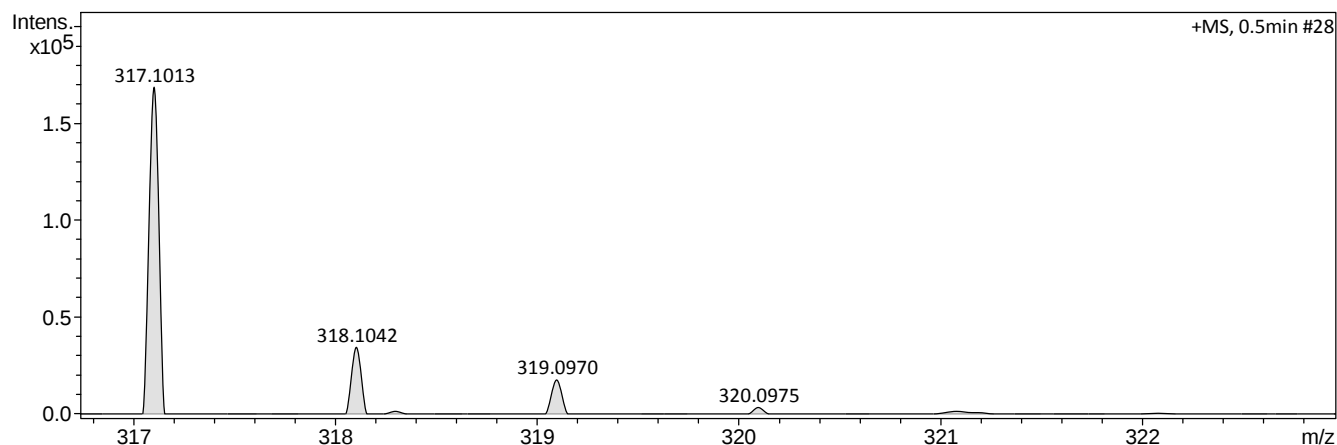
Analysis Name D:\Data\ggc\24-100143_P1-F-7_01_9541.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100143
 Comment HG37
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:48:10 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
317.1013	1	C15H22NaO2SSi	317.1002	-3.6	10.5	1	64.69	5.5	even	ok

Qualitative Compound Report

Analysis Info

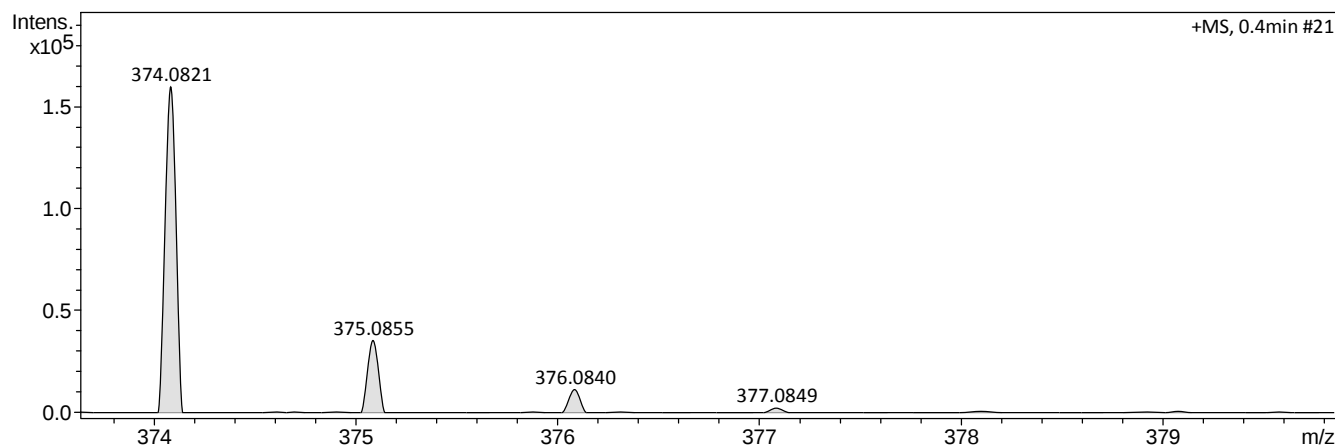
Analysis Name D:\Data\ggc\24-100144_P1-F-8_01_9542.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100144
 Comment HG38
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:53:16 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
374.0821	1	C20H17NNO3S	374.0821	0.2	5.4	1	100.00	12.5	even	ok

Mass Spectrum List Report

Analysis Info

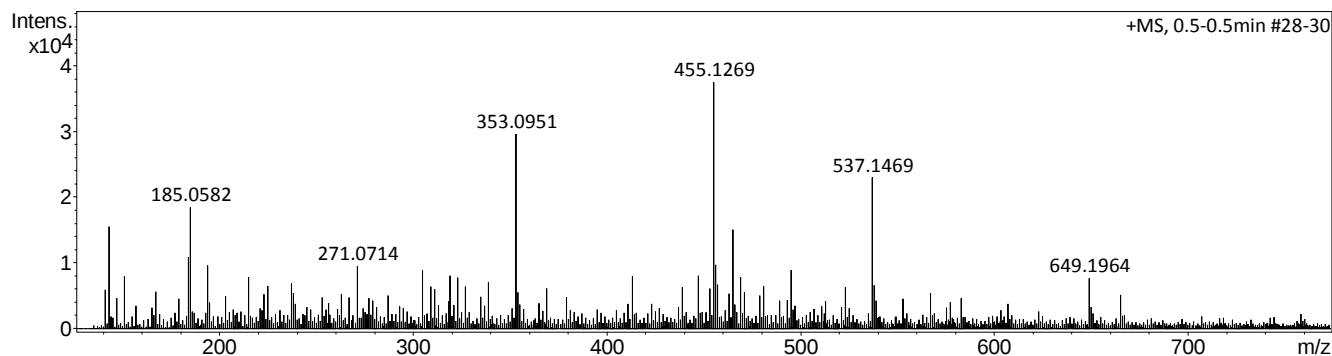
Analysis Name D:\Data\ggc\24-100145_P1-F-9_01_9543.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-100145
 Comment HG39
 Sv: MeOH + HCOOH
 Argüello - UNC

Acquisition Date 10/7/2024 5:58:22 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	143.0483	15487	41.4
2	151.0163	7981	21.3
3	184.0681	10856	29.0
4	185.0582	18375	49.1
5	194.0335	9601	25.6
6	215.0826	7832	20.9
7	225.0540	6436	17.2
8	237.0673	6837	18.3
9	271.0714	9442	25.2
10	305.0559	8827	23.6
11	309.0668	6361	17.0
12	319.0877	7984	21.3
13	323.0706	7739	20.7
14	327.0770	6379	17.0
15	339.0678	7087	18.9
16	353.0951	29581	79.0
17	413.1122	7897	21.1
18	439.1218	6243	16.7
19	447.1247	8043	21.5
20	455.1269	37435	100.0
21	456.1290	9680	25.9
22	457.1225	6688	17.9
23	465.1425	15065	40.2
24	469.0908	7829	20.9
25	481.1221	6518	17.4
26	495.1313	8880	23.7
27	523.1324	6285	16.8
28	537.1469	22992	61.4
29	538.1477	6559	17.5
30	649.1964	7617	20.3