

Qualitative Compound Report

Analysis Info

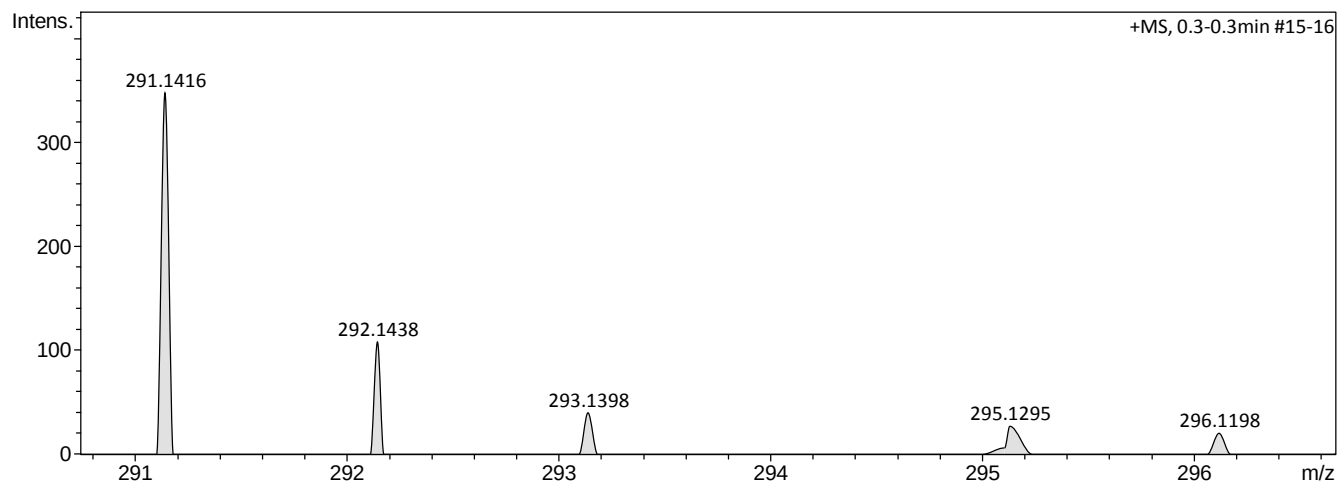
Analysis Name D:\Data\ggc\24-121821_P2-E-1_01_9876.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121821
 Comment XK-088
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/26/2024 2:23:30 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
291.1416	1	C16H23O3Si	291.1411	-1.7	48.8	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

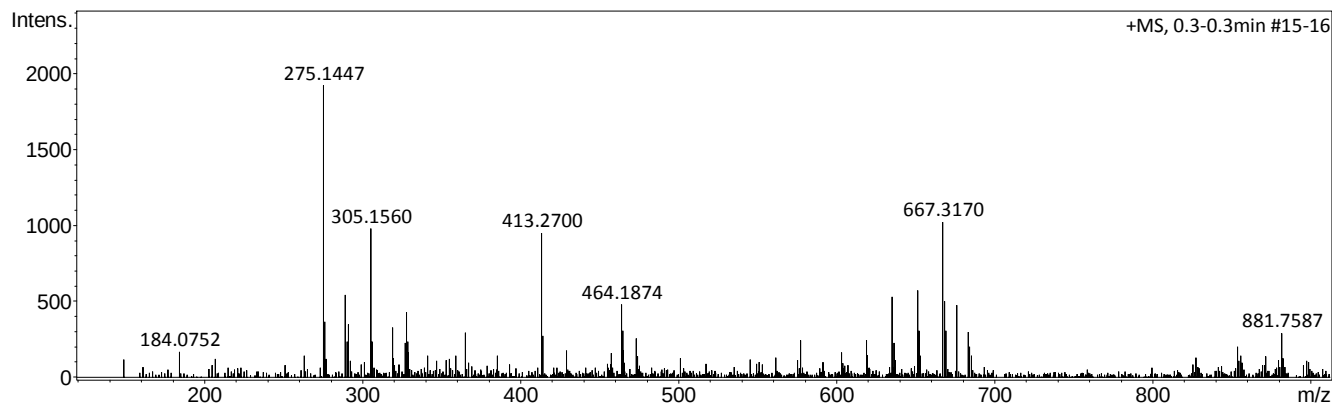
Analysis Name D:\Data\ggc\24-121821_P2-E-1_01_9876.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121821
 Comment XK-088
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/26/2024 2:23:30 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	275.1447	1920	100.0
2	276.1451	365	19.0
3	289.1228	541	28.1
4	290.1320	237	12.3
5	291.1416	347	18.1
6	305.1560	977	50.9
7	306.1542	234	12.2
8	319.1215	329	17.1
9	327.1021	228	11.9
10	328.1265	428	22.3
11	328.6257	238	12.4
12	365.1071	294	15.3
13	413.2700	951	49.5
14	414.2698	272	14.2
15	464.1874	480	25.0
16	464.6886	308	16.1
17	473.1965	257	13.4
18	577.5117	242	12.6
19	619.2311	244	12.7
20	635.2793	531	27.7
21	636.2879	228	11.9
22	651.2546	573	29.8
23	652.2601	307	16.0
24	667.3170	1022	53.2
25	668.3065	502	26.1
26	669.3128	305	15.9
27	676.1343	476	24.8
28	683.2816	299	15.6
29	684.2744	203	10.6
30	881.7587	289	15.0

Mass Spectrum List Report

Analysis Info

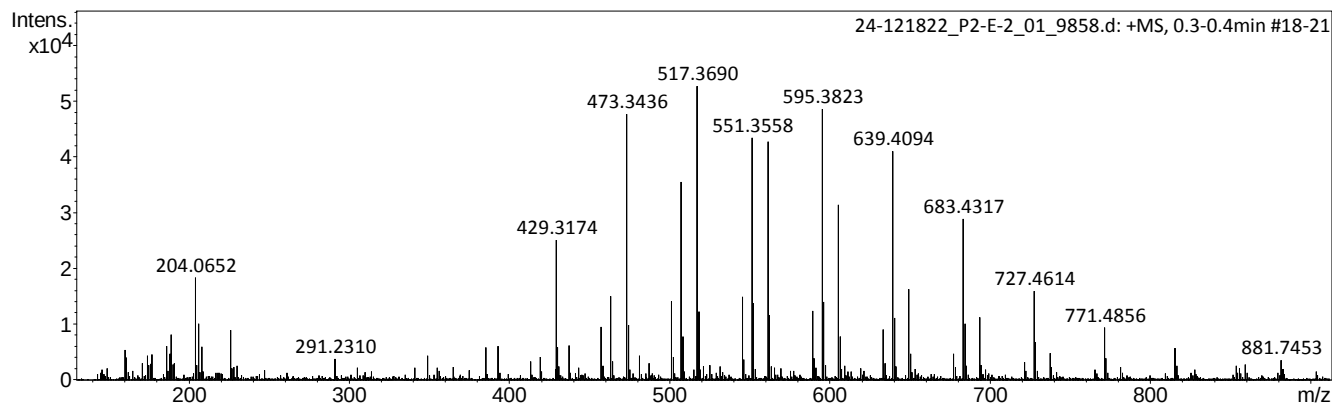
Analysis Name D:\Data\ggc\24-121822_P2-E-2_01_9858.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121822
 Comment XK-147
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:17:07 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	204.0652	18341	34.8
2	206.0806	10046	19.1
3	226.0502	8942	17.0
4	429.3174	25021	47.5
5	457.3487	9491	18.0
6	463.3045	14970	28.4
7	473.3436	47556	90.4
8	474.3444	9784	18.6
9	501.3743	14074	26.7
10	507.3295	35403	67.3
11	517.3690	52631	100.0
12	518.3746	12192	23.2
13	545.3982	14817	28.2
14	551.3558	43366	82.4
15	552.3567	13711	26.1
16	561.3975	42661	81.1
17	562.4025	11588	22.0
18	589.4331	12397	23.6
19	595.3823	48523	92.2
20	596.3839	13920	26.4
21	605.4228	31314	59.5
22	633.4522	9077	17.2
23	639.4094	40939	77.8
24	640.4133	11137	21.2
25	649.4529	16259	30.9
26	683.4317	28872	54.9
27	684.4381	10103	19.2
28	693.4778	11176	21.2
29	727.4614	15863	30.1
30	771.4856	9338	17.7

Mass Spectrum List Report

Analysis Info

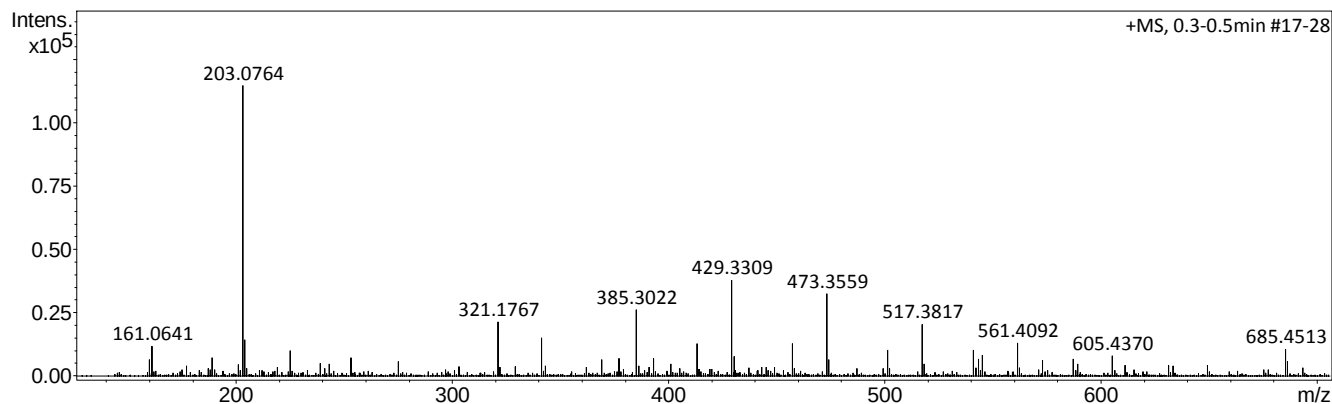
Analysis Name D:\Data\ggc\24-121823_P2-E-3_01_9859.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121823
 Comment XK-174
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:22:14 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	160.0609	6511	5.7
2	161.0641	11818	10.3
3	189.0828	7477	6.5
4	203.0764	114669	100.0
5	204.0819	14428	12.6
6	225.0571	10049	8.8
7	253.0575	7286	6.4
8	321.1767	21359	18.6
9	341.2734	15176	13.2
10	369.2950	6683	5.8
11	377.1557	7025	6.1
12	385.3022	26179	22.8
13	393.1485	7166	6.2
14	413.3019	12925	11.3
15	429.3309	37934	33.1
16	430.3350	7843	6.8
17	457.3547	12824	11.2
18	473.3559	32426	28.3
19	474.3568	6721	5.9
20	501.3762	10443	9.1
21	517.3817	20474	17.9
22	541.1982	10505	9.2
23	543.3470	6807	5.9
24	545.4055	8475	7.4
25	561.4092	13168	11.5
26	573.2254	6404	5.6
27	587.3736	6746	5.9
28	605.4370	8213	7.2
29	685.4513	10717	9.3
30	686.4582	5856	5.1

Qualitative Compound Report

Analysis Info

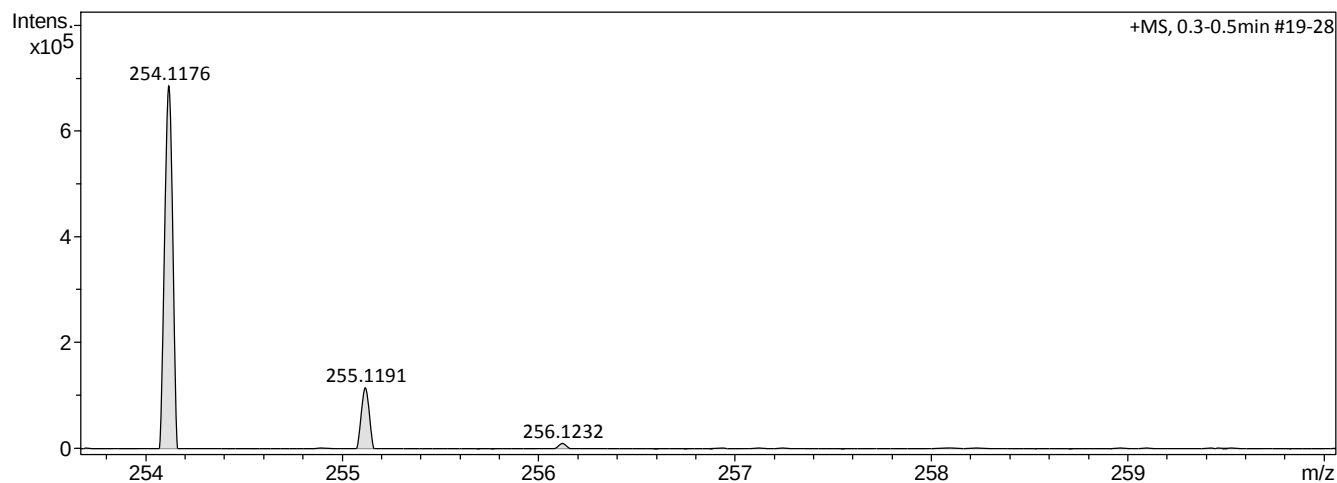
Analysis Name D:\Data\ggc\24-121824_P2-E-4_01_9860.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121824
 Comment XK-191
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:27:22 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
254.1176	1	C16H16NO2	254.1176	-0.2	8.0	1	100.00	9.5	even	ok

Qualitative Compound Report

Analysis Info

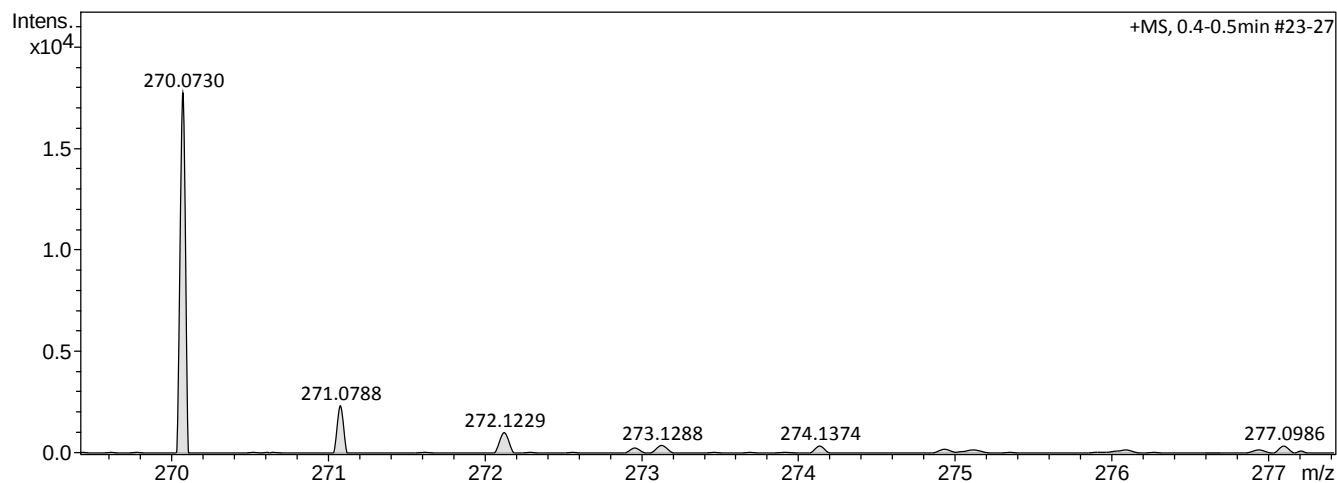
Analysis Name D:\Data\ggc\24-121825_P2-E-5_01_9861.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121825
 Comment XK-150
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:32:32 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
270.0730	1	C13H13NNaO4	270.0737	2.6	14.5	2	87.51	7.5	even	ok

Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-121825_P2-E-5_01_9861.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121825
 Comment XK-150
 Sv: MeOH + HCOOH
 Bracca Andrea

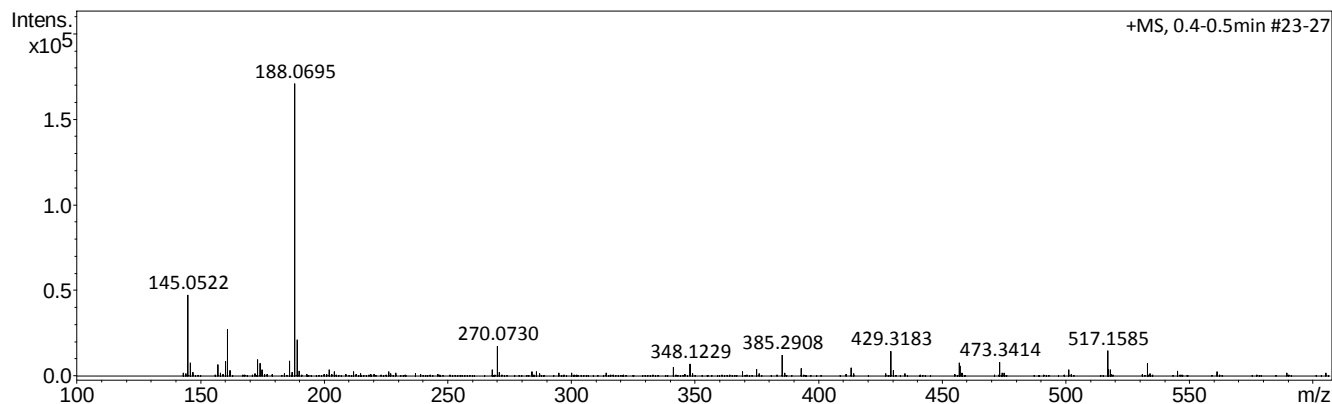
Acquisition Date 12/23/2024 4:32:32 PM

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	145.0522	47432	27.8
2	146.0473	7942	4.7
3	157.0511	6670	3.9
4	160.0727	8723	5.1
5	161.0597	27274	16.0
6	162.0607	3540	2.1
7	173.0475	9782	5.7
8	174.0564	7495	4.4
9	175.0678	3801	2.2
10	186.0535	9038	5.3
11	188.0695	170660	100.0
12	189.0716	21345	12.5
13	202.0827	3980	2.3
14	268.0580	3679	2.2
15	270.0730	17719	10.4
16	341.2621	5432	3.2
17	348.1229	7136	4.2
18	375.1318	4302	2.5
19	385.2908	12561	7.4
20	393.1443	4643	2.7
21	413.3116	5066	3.0
22	429.3183	14579	8.5
23	457.1351	7899	4.6
24	457.3481	6203	3.6
25	473.3414	8134	4.8
26	501.3730	3970	2.3
27	517.1585	14979	8.8
28	517.3596	4308	2.5
29	518.1564	3842	2.3
30	533.1339	7474	4.4

Mass Spectrum List Report

Analysis Info

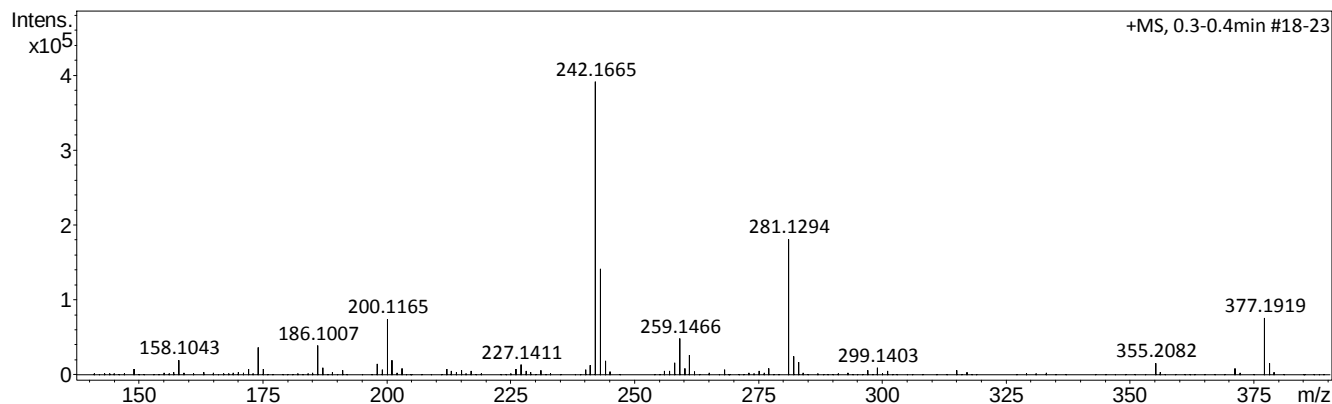
Analysis Name D:\Data\ggc\24-121826_P2-E-6_01_9862.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121826
 Comment XK-050
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:37:43 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	149.0681	8021	2.1
2	158.1043	19619	5.0
3	174.0991	36526	9.4
4	175.0921	8040	2.1
5	186.1007	39136	10.0
6	187.1049	9977	2.6
7	198.1021	14998	3.8
8	200.1165	74451	19.1
9	201.1101	19649	5.0
10	203.0842	8675	2.2
11	212.1211	8284	2.1
12	226.1348	8202	2.1
13	227.1411	14040	3.6
14	241.1346	13120	3.4
15	242.1665	390209	100.0
16	243.1581	141125	36.2
17	244.1582	18995	4.9
18	258.1587	16404	4.2
19	259.1466	48372	12.4
20	260.1534	8586	2.2
21	261.1612	27058	6.9
22	277.1570	8717	2.2
23	281.1294	180843	46.3
24	282.1313	24997	6.4
25	283.1411	16968	4.3
26	299.1403	9580	2.5
27	355.2082	15429	4.0
28	371.2607	8466	2.2
29	377.1919	76164	19.5
30	378.1923	15881	4.1

Qualitative Compound Report

Analysis Info

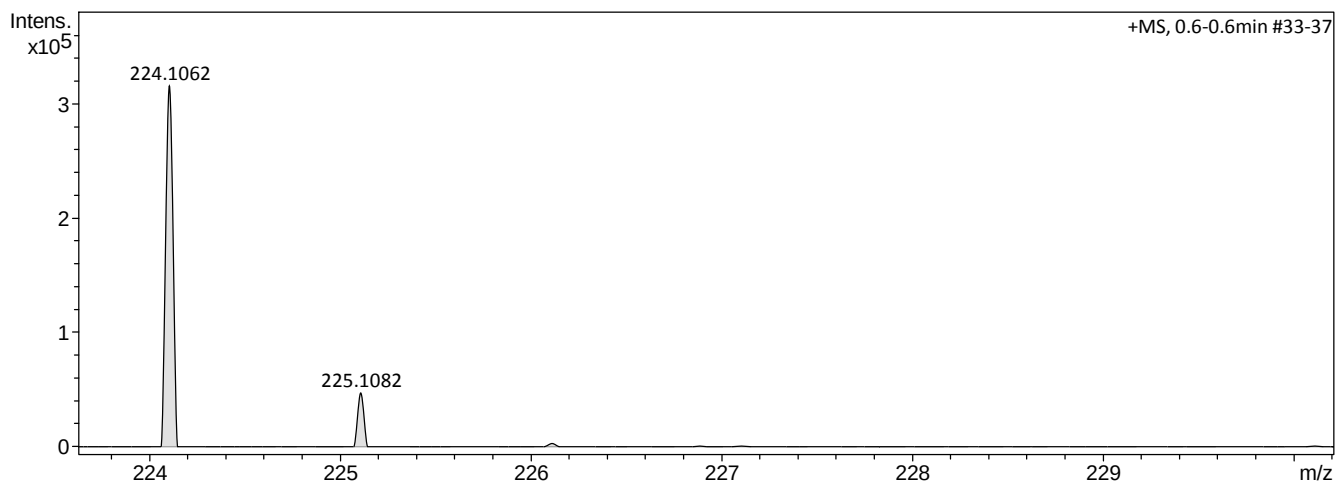
Analysis Name D:\Data\ggc\24-121827_P2-E-7_01_9863.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121827
 Comment XK-183
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:42:50 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
224.1062	1	C15H14NO	224.1070	3.3	11.3	2	82.19	9.5	even	ok

Qualitative Compound Report

Analysis Info

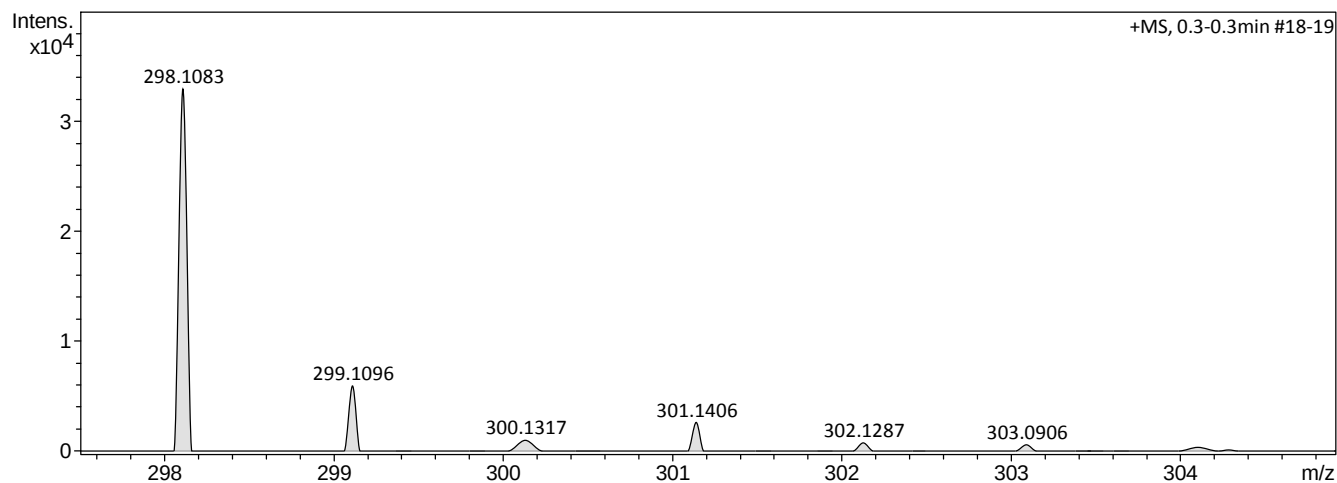
Analysis Name D:\Data\ggc\24-121828_P2-E-8_01_9864.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121828
 Comment XK-203
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:48:00 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
298.1083	1	C17H16NO4	298.1074	-3.1	16.1	1	90.78	10.5	even	ok

Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\ggc\24-121829_P2-E-9_01_9865.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121829
 Comment XK-153
 Sv: MeOH + HCOOH
 Bracca Andrea

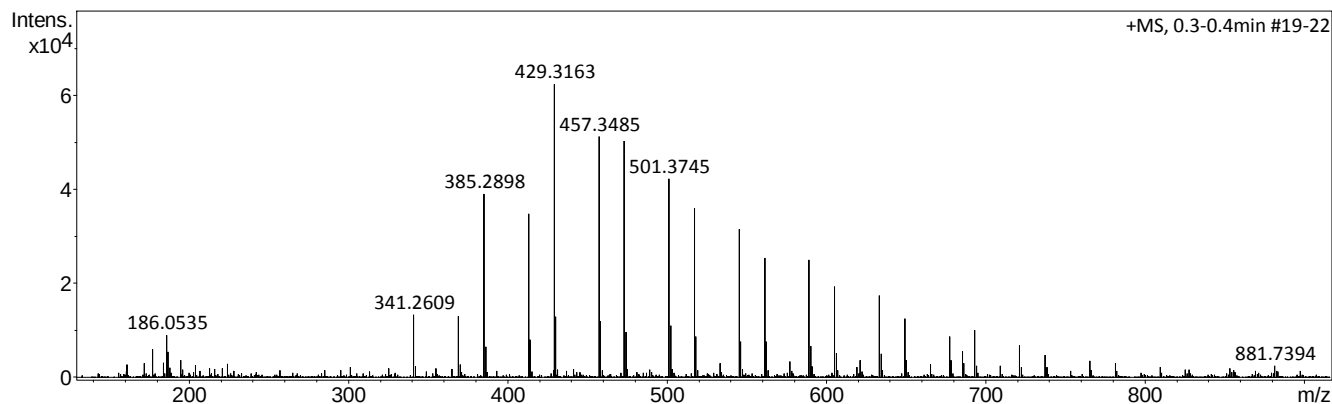
Acquisition Date 12/23/2024 4:53:15 PM

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	177.1093	5955	9.6
2	186.0535	8978	14.4
3	341.2609	13375	21.5
4	369.2942	12993	20.8
5	385.2898	38944	62.5
6	386.2967	6496	10.4
7	413.3146	34719	55.7
8	414.3162	7985	12.8
9	429.3163	62334	100.0
10	430.3189	12968	20.8
11	457.3485	51130	82.0
12	458.3502	11949	19.2
13	473.3434	50206	80.5
14	474.3433	9677	15.5
15	501.3745	42158	67.6
16	502.3734	10987	17.6
17	517.3667	35993	57.7
18	518.3716	8772	14.1
19	545.3983	31432	50.4
20	546.4066	7577	12.2
21	561.3934	25336	40.6
22	562.3976	7682	12.3
23	589.4302	24955	40.0
24	590.4321	6717	10.8
25	605.4179	19313	31.0
26	633.4509	17334	27.8
27	649.4443	12518	20.1
28	677.4789	8713	14.0
29	693.4675	10016	16.1
30	721.5089	6752	10.8

Qualitative Compound Report

Analysis Info

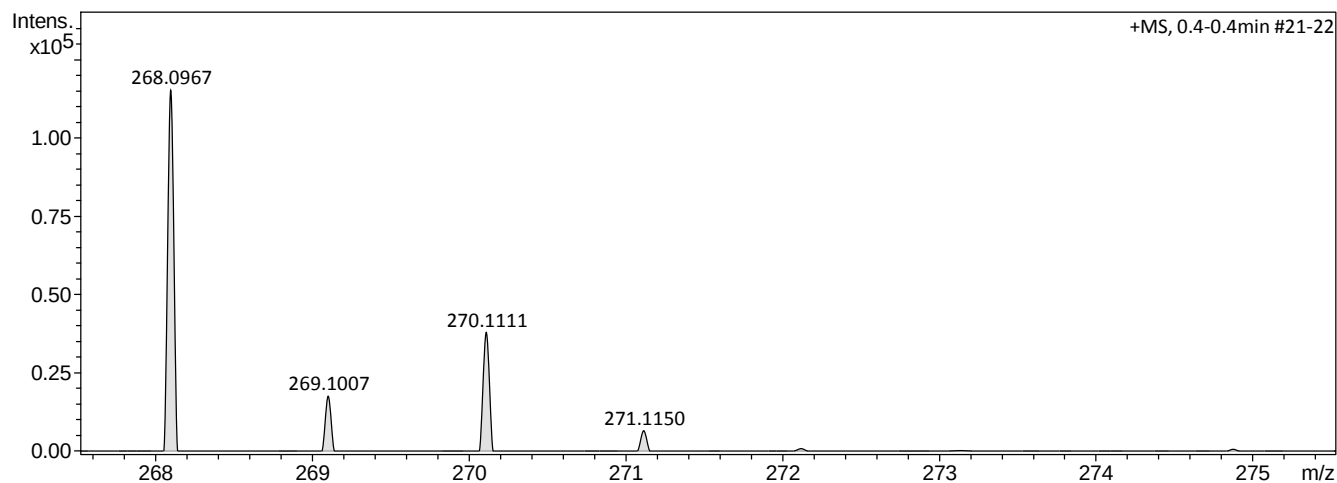
Analysis Name D:\Data\ggc\24-121830_P2-F-1_01_9866.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121830
 Comment XK-133
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 4:58:20 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
268.0967	1	C16H14NO3	268.0968	0.3	178.7	1	100.00	10.5	even	ok

Qualitative Compound Report

Analysis Info

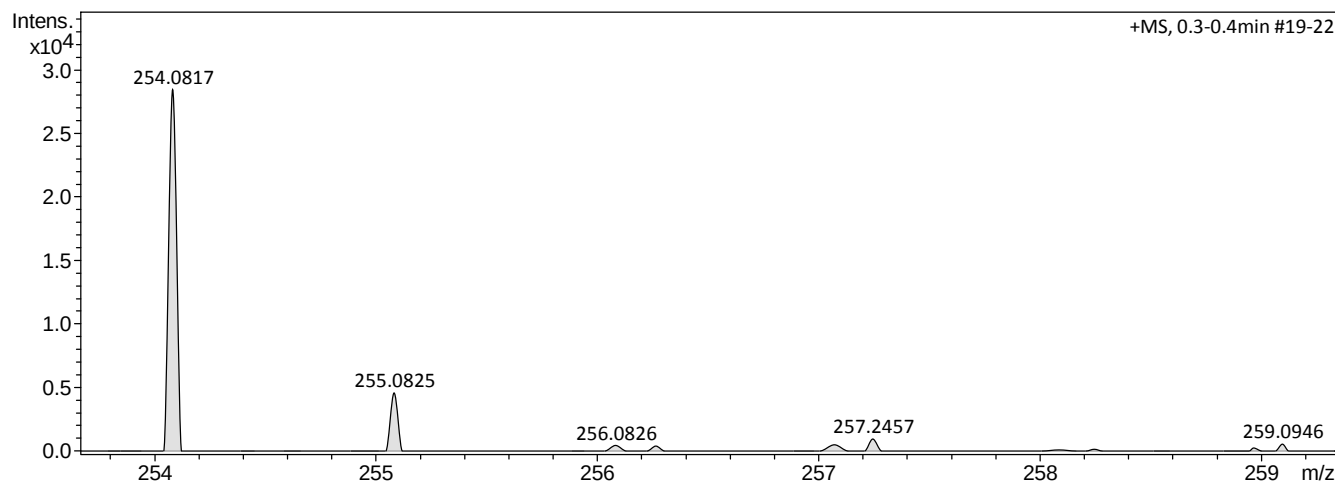
Analysis Name D:\Data\ggc\24-121831_P2-F-2_01_9867.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-121831
 Comment XK-187
 Sv: MeOH + HCOOH
 Bracca Andrea

Acquisition Date 12/23/2024 5:03:27 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
254.0817	1	C15H12NO3	254.0812	-2.0	4.4	1	100.00	10.5	even	ok