

Mass Spectrum List Report

Analysis Info

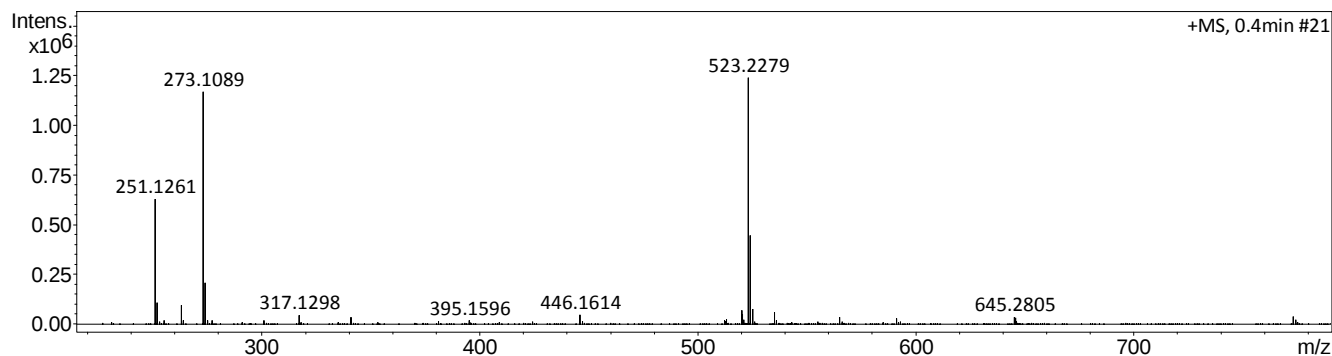
Analysis Name D:\Data\ggc\24-020804_P1-D-1_01_8603.d
 Method lc_qtof_directospos.m
 Sample Name 24-020804
 Comment 24-1
 Sv: MeOH + HCOOH
 Di Salvo

Acquisition Date 2/21/2024 9:41:29 AM

Operator ELB
 Instrument / Ser# microTOF-Q II

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	251.1261	626570	50.7
2	252.1327	109878	8.9
3	255.1565	17824	1.4
4	263.1259	95906	7.8
5	264.1287	19122	1.5
6	273.1089	1167170	94.4
7	274.1114	209170	16.9
8	275.1138	18983	1.5
9	301.1063	17912	1.4
10	317.1298	43665	3.5
11	341.0984	33465	2.7
12	395.1596	17677	1.4
13	446.1614	46549	3.8
14	512.2300	17466	1.4
15	513.2395	24077	1.9
16	520.2195	69220	5.6
17	520.7220	51129	4.1
18	521.2202	21253	1.7
19	523.2279	1236348	100.0
20	524.2309	446508	36.1
21	525.2340	75311	6.1
22	535.2266	59576	4.8
23	536.2276	18961	1.5
24	565.2345	33306	2.7
25	591.2157	27632	2.2
26	645.2805	36330	2.9
27	645.7819	31610	2.6
28	773.3448	37997	3.1
29	774.3474	22297	1.8
30	835.3176	20008	1.6

Qualitative Compound Report

Analysis Info

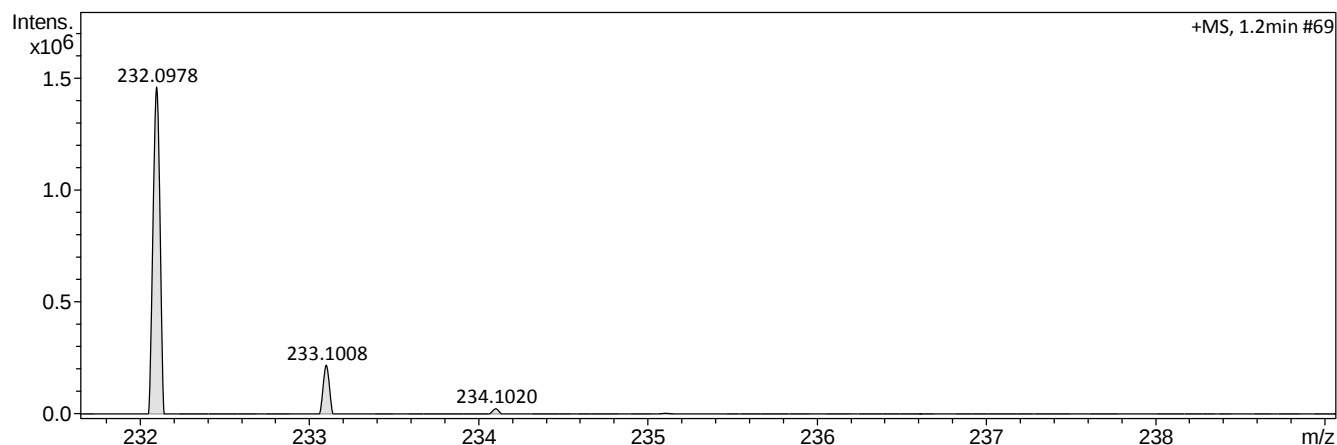
Analysis Name D:\Data\ggc\24-020805_P1-D-2_01_8604.d
 Method lc_qtof_directospos.m
 Sample Name 24-020805
 Comment 24-2
 Sv: MeOH + HCOOH
 Di Salvo

Acquisition Date 2/21/2024 9:46:36 AM

Operator ELB
 Instrument micrOTOF-Q II

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
232.0978	1	C13H14NO3	232.0968	-4.0	1.3	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

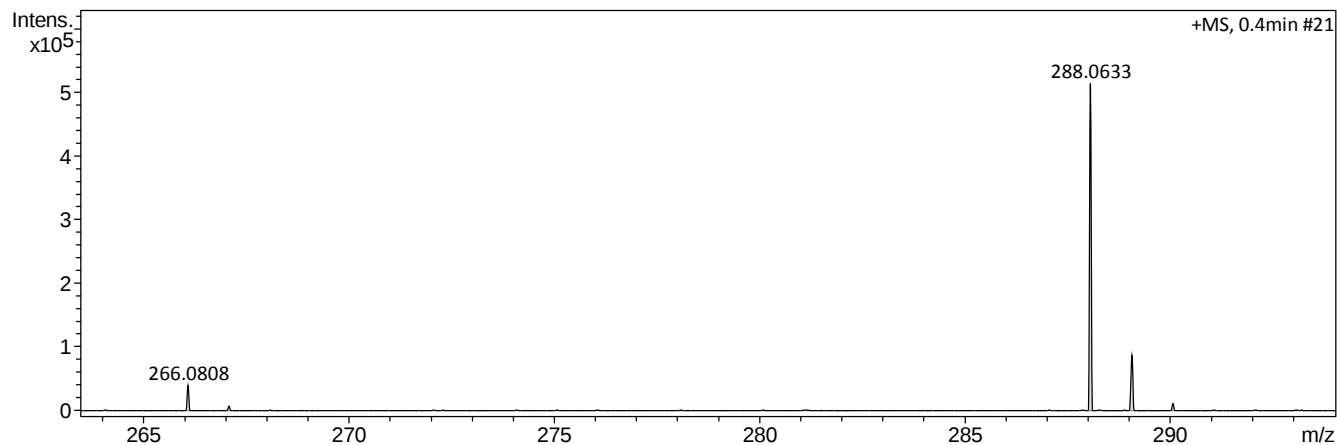
Analysis Name D:\Data\ggc\24-020806_P1-D-3_01_8605.d
 Method lc_qtof_directospos.m
 Sample Name 24-020806
 Comment 24-3
 Sv: MeOH + HCOOH
 Di Salvo

Acquisition Date 2/21/2024 9:51:44 AM

Operator ELB
 Instrument micrOTOF-Q II

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
266.0808	1	C16H12NO3	266.0812	1.4	2.2	1	100.00	11.5	even	ok
288.0633	1	C16H11NNaO3	288.0631	-0.7	6.6	3	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

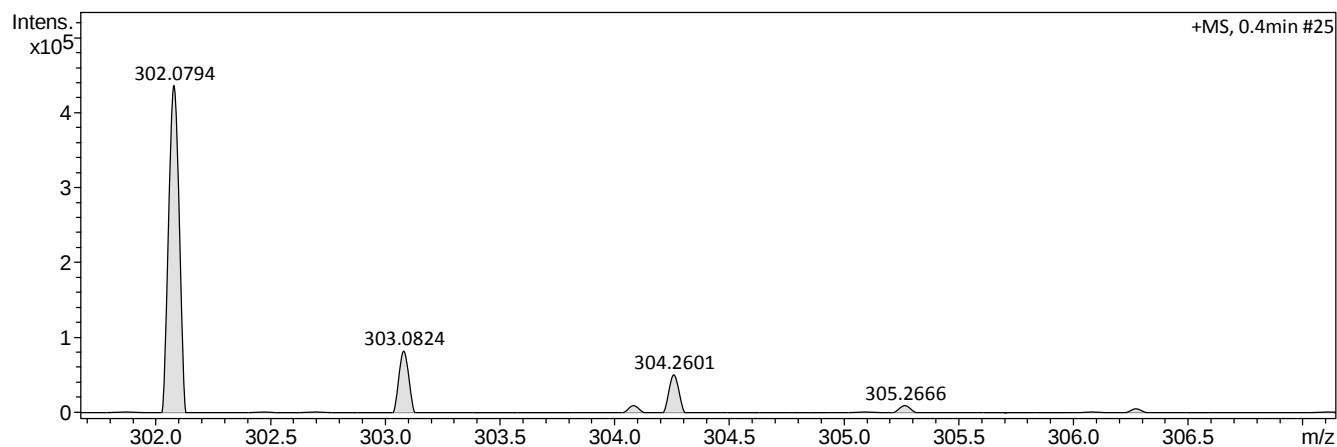
Analysis Name D:\Data\ggc\24-020807_P1-D-4_01_8606.d
 Method lc_qtof_directospos.m
 Sample Name 24-020807
 Comment 24-4
 Sv: MeOH + HCOOH
 Di Salvo

Acquisition Date 2/21/2024 9:56:51 AM

Operator ELB
 Instrument micrOTOF-Q II

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
302.0794	1	C17H13NNaO3	302.0788	-2.1	2.5	2	98.33	11.5	even	ok

Qualitative Compound Report

Analysis Info

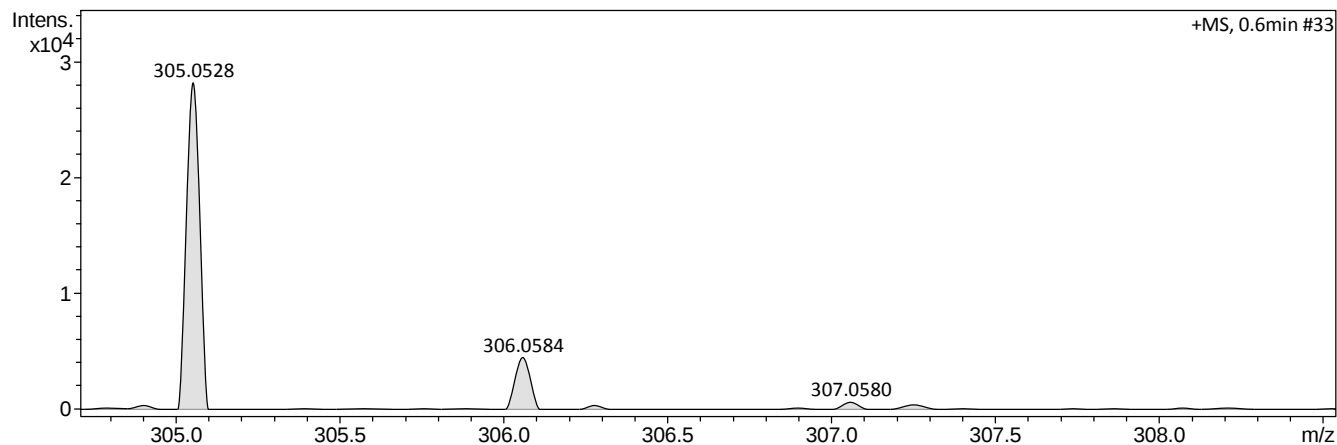
Analysis Name D:\Data\ggc\24-020808_P1-D-5_01_8607.d
 Method lc_qtof_directospos.m
 Sample Name 24-020808
 Comment 24-5
 Sv: MeOH + HCOOH
 Di Salvo

Acquisition Date 2/21/2024 10:01:59 AM

Operator ELB
 Instrument micrOTOF-Q II

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
305.0528	1	C15H10N2NaO4	305.0533	1.5	8.8	6	81.18	11.5	even	ok