

Qualitative Compound Report

Analysis Info

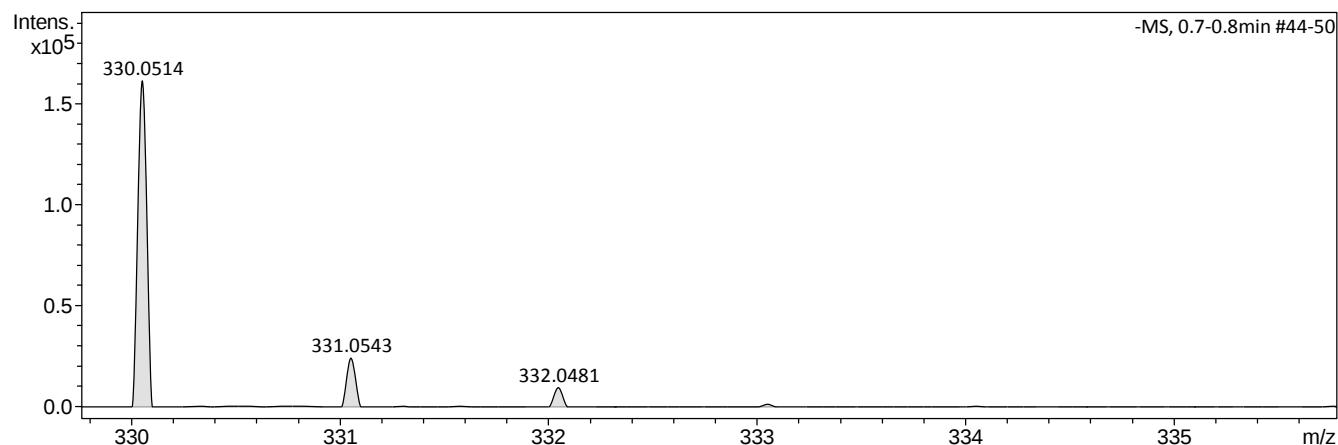
Analysis Name D:\Data\ggc\24-031201_P1-C-7_01_8757.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031201
 Comment MAC-III-27
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:32:42 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻ Conf	N-Rule
330.0514	1	C13H11F3N3O2S	330.0530	4.6	6.8	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

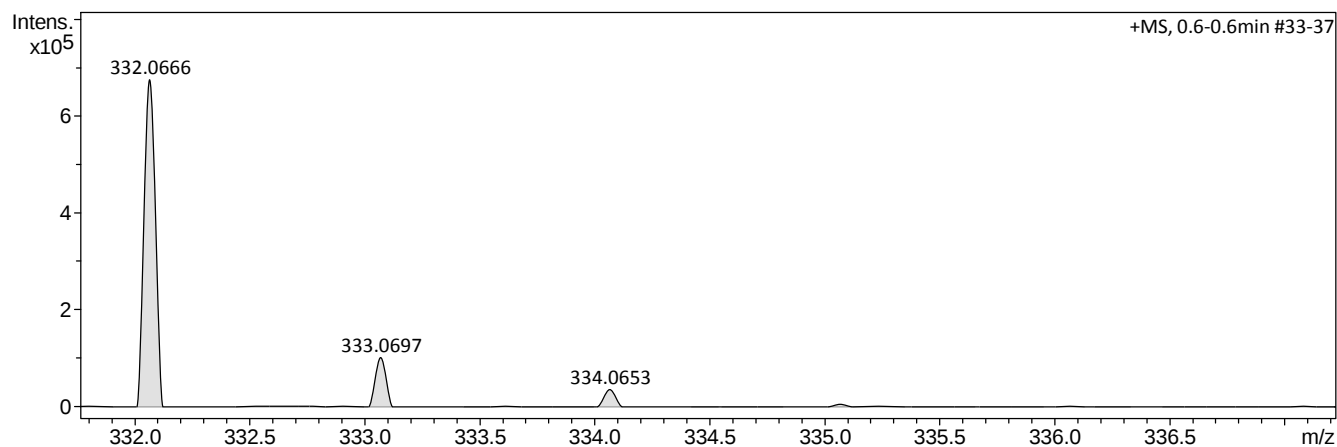
Analysis Name D:\Data\ggc\24-031201_P1-C-7_01_8727.d
 Method lc_qtof_directospos.m
 Sample Name 24-031201
 Comment MAC-III-27
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 3:58:47 PM

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
332.0666	1	C13H13F3N3O2S	332.0675	2.9	7.7	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

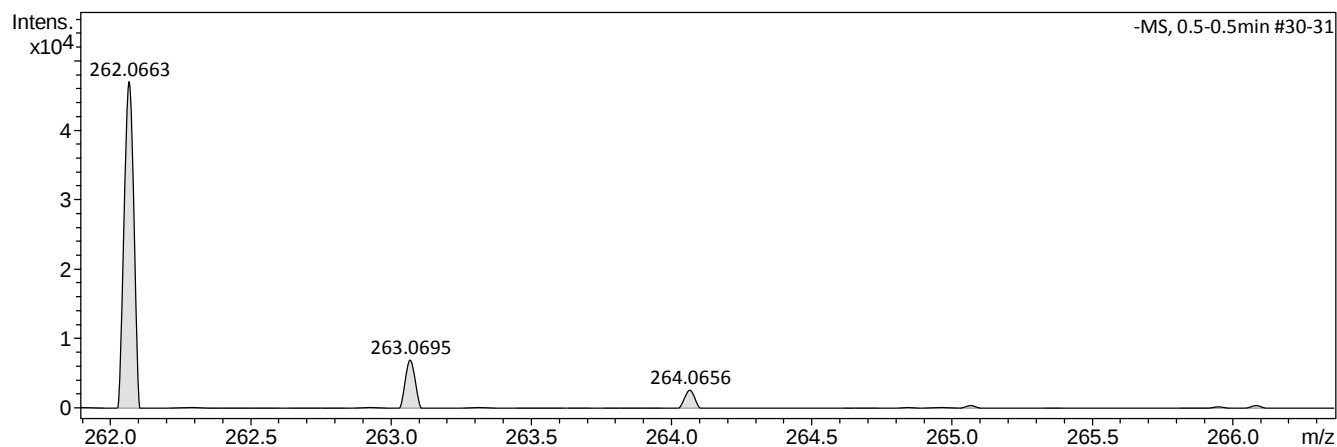
Analysis Name D:\Data\ggc\24-031202_P1-C-8_01_8758.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031202
 Comment MAC-III-33
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:37:49 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
262.0663	1	C12H12N3O2S	262.0656	-2.7	3.1	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

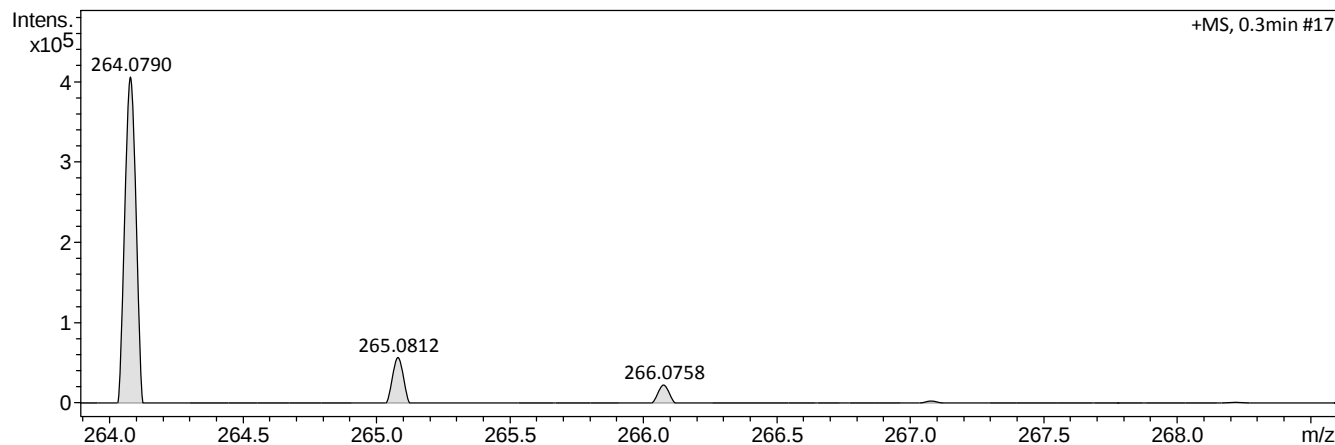
Analysis Name D:\Data\ggc\24-031202_P1-C-8_01_8728.d
 Method lc_qtof_directospos.m
 Sample Name 24-031202
 Comment MAC-III-33
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:03:55 PM

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
264.0790	1	C ₁₂ H ₁₄ N ₃ O ₂ S	264.0801	4.4	6.1	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

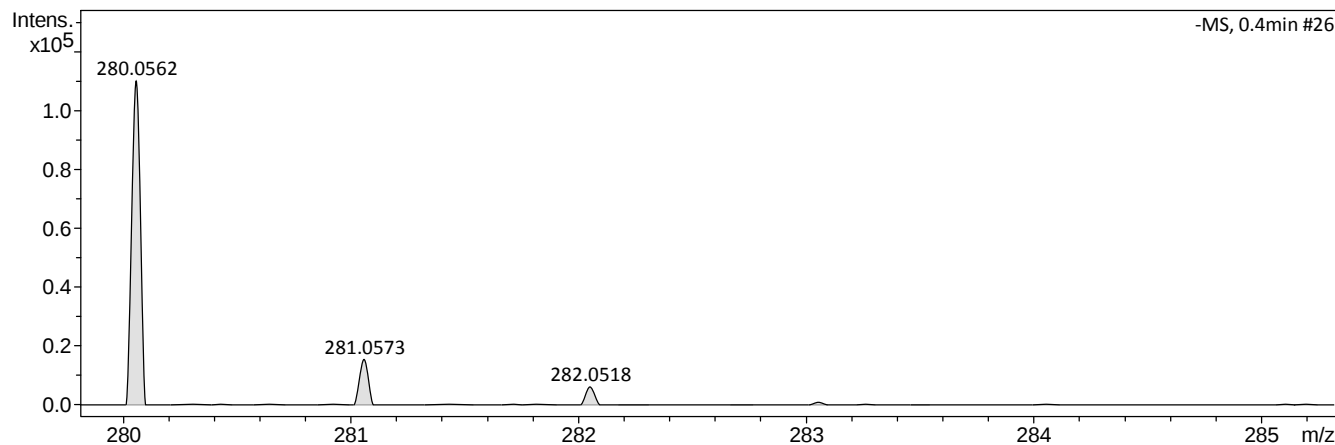
Analysis Name D:\Data\ggc\24-031203_P1-C-9_01_8759.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031203
 Comment MAC-III-35
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:42:59 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
280.0562	1	C12H11FN3O2S	280.0561	-0.2	5.7	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

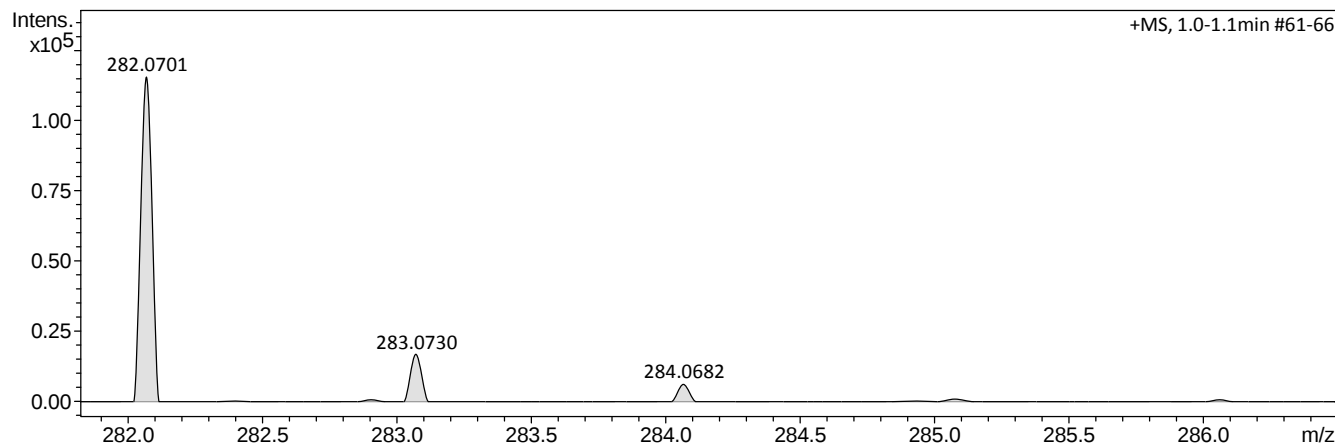
Analysis Name D:\Data\ggc\24-031203_P1-C-9_01_8729.d
 Method lc_qtof_directospos.m
 Sample Name 24-031203
 Comment MAC-III-35
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:09:02 PM

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
282.0701	1	C12H13FN3O2S	282.0707	2.1	4.2	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

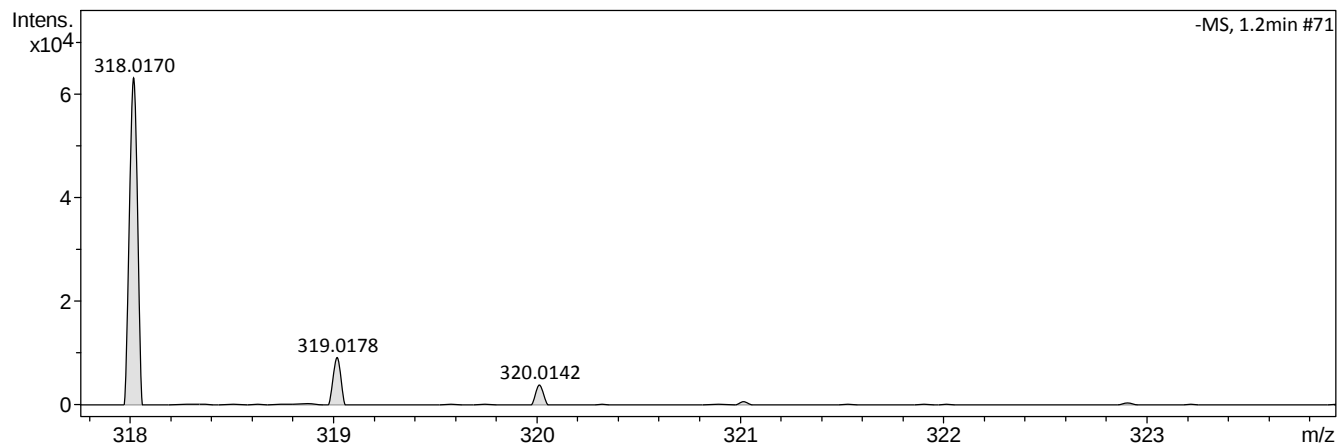
Analysis Name D:\Data\ggc\24-031204_P1-D-1_01_8760.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031204
 Comment MAC-III-61
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:48:05 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
318.0170	1	C11H7F3N3O3S	318.0166	-1.3	2.5	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

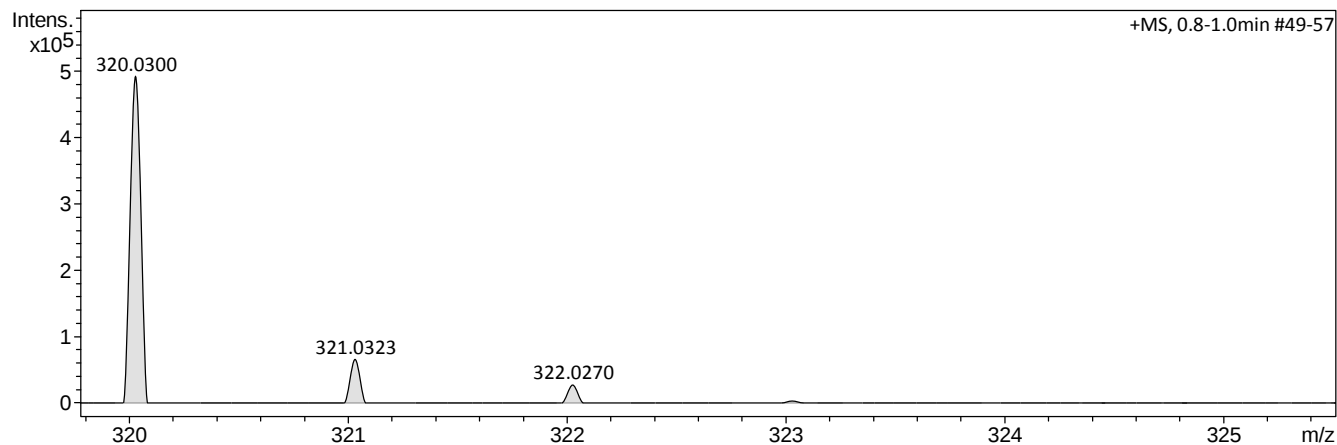
Analysis Name D:\Data\ggc\24-031204_P1-D-1_01_8730.d
 Method lc_qtof_directospos.m
 Sample Name 24-031204
 Comment MAC-III-61
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:14:09 PM

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
320.0300	1	C11H9F3N3O3S	320.0311	3.7	4.0	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

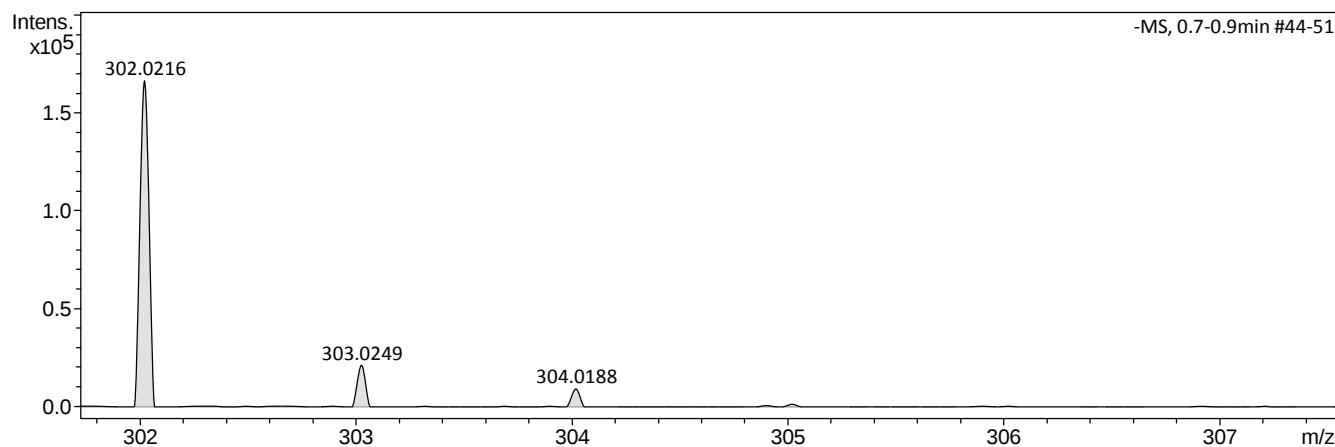
Analysis Name D:\Data\ggc\24-031205_P1-D-2_01_8761.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031205
 Comment EJG-I-85
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:53:12 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
302.0216	1	C11H7F3N3O2S	302.0217	0.2	6.9	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

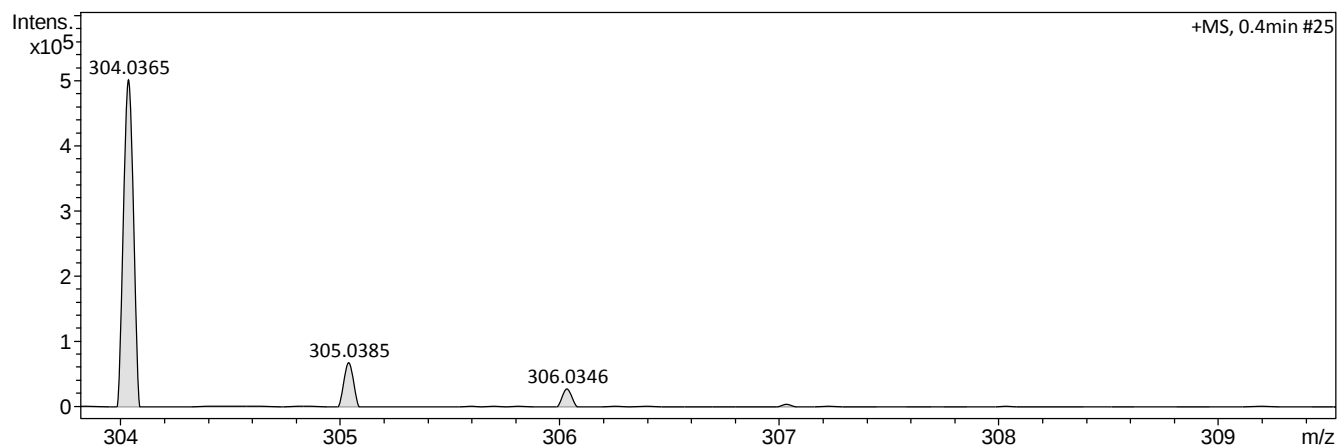
Analysis Name D:\Data\ggc\24-031205_P1-D-2_01_8731.d
 Method lc_qtof_directospos.m
 Sample Name 24-031205
 Comment EJG-I-85
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:19:17 PM

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
304.0365	1	C11H9F3N3O2S	304.0362	-1.0	3.7	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

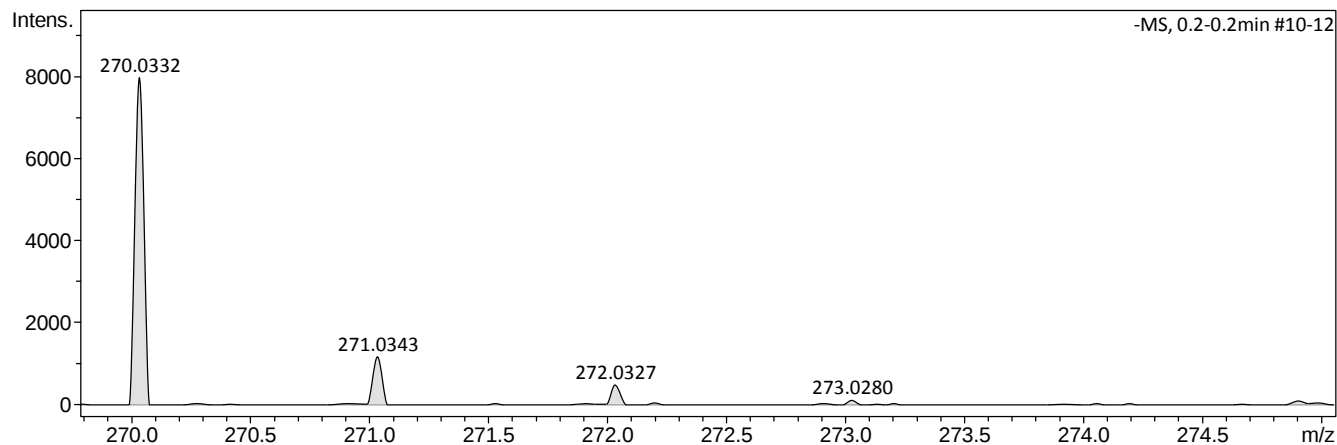
Analysis Name D:\Data\ggc\24-031206_P1-D-3_01_8762.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031206
 Comment EJG-II-26
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 6:58:21 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
270.0332	1	C13H8N3O2S	270.0343	3.9	7.8	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

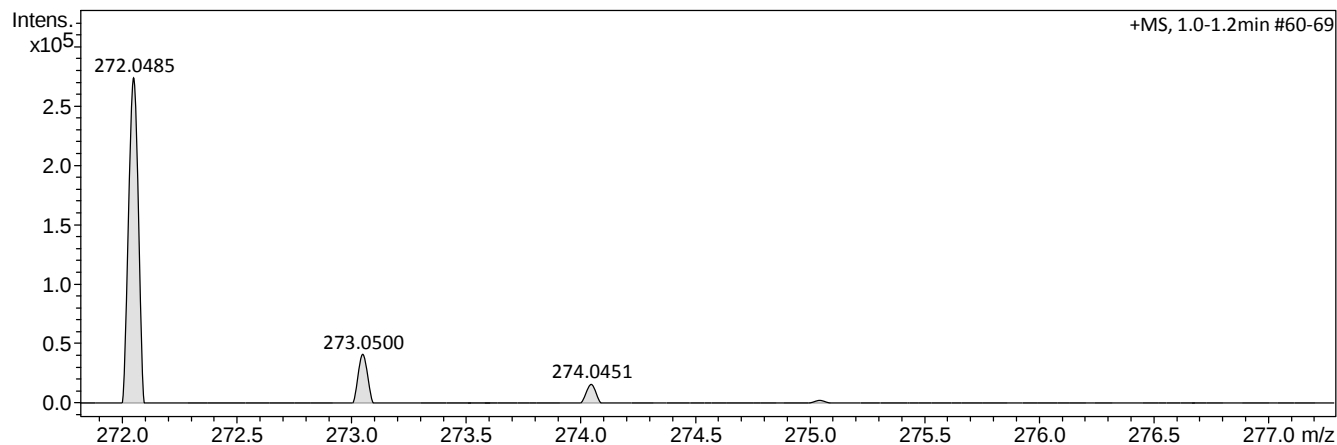
Analysis Name D:\Data\ggc\24-031206_P1-D-3_01_8732.d
 Method lc_qtof_directospos.m
 Sample Name 24-031206
 Comment EJG-II-26
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:24:24 PM

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
272.0485	1	C13H10N3O2S	272.0488	1.1	5.7	1	100.00	10.5	even	ok

Qualitative Compound Report

Analysis Info

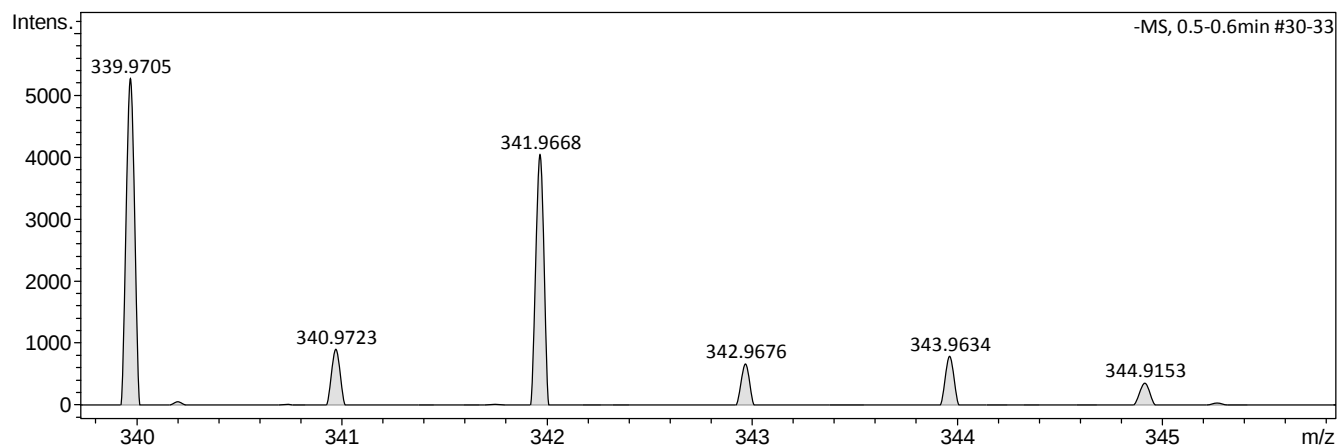
Analysis Name D:\Data\ggc\24-031207_P1-D-4_01_8763.d
 Method lc_qtof_directosneg.m
 Sample Name 24-031207
 Comment EJG-II-28
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 7:03:28 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	3.5 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	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
339.9705	1	C13H8Cl2N3O2S	339.9720	4.2	29.8	1	100.00	10.5	even	ok

Qualitative Compound Report

Analysis Info

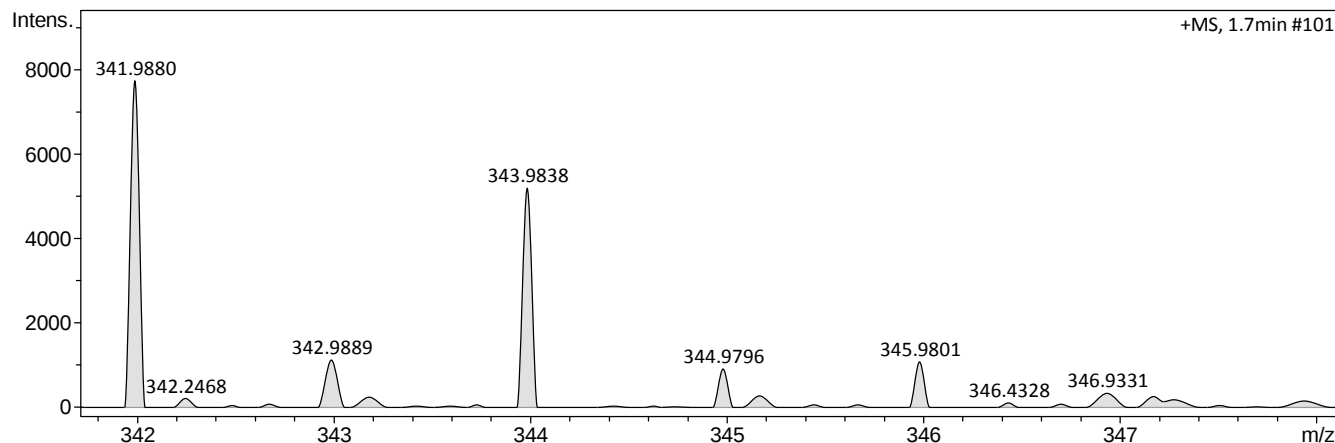
Analysis Name D:\Data\ggc\24-031207_P1-D-4_01_8733.d
 Method lc_qtof_directospos.m
 Sample Name 24-031207
 Comment EJG-II-28
 Sv: MeOH + HCOOH
 Eugenia Buden - INFIQC - UNC

Acquisition Date 3/18/2024 4:29:35 PM

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
341.9880	1	C13H10Cl2N3O2S	341.9865	-4.2	17.0	1	100.00	9.5	even	ok