

Qualitative Compound Report

Analysis Info

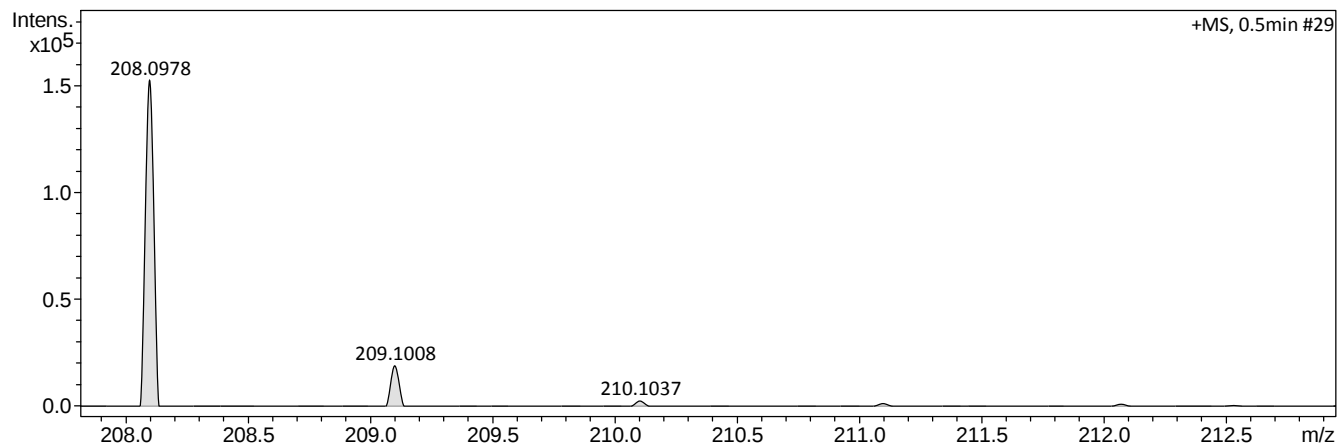
Analysis Name D:\Data\ggc\24-031512_P1-C-1_01_8809.d
 Method lc_qtof_directospos.m
 Sample Name 24-031512
 Comment DFV-620
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 1:45:03 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
208.0978	1	C11H14NO3	208.0968	-4.7	2.0	1	100.00	5.5	even	ok

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Analysis Info

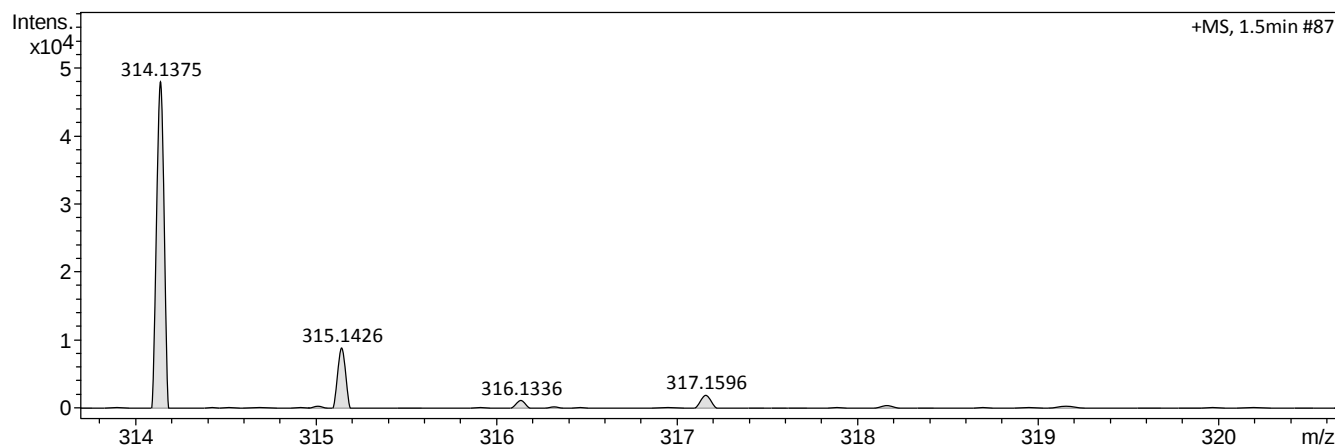
Analysis Name D:\Data\ggc\24-031513_P1-C-2_01_8810.d
 Method lc_qtof_directospos.m
 Sample Name 24-031513
 Comment DFV-623
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 1:50:11 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
314.1375	1	C16H21NNaO4	314.1363	-4.0	2.4	1	58.76	6.5	even	ok

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Analysis Info

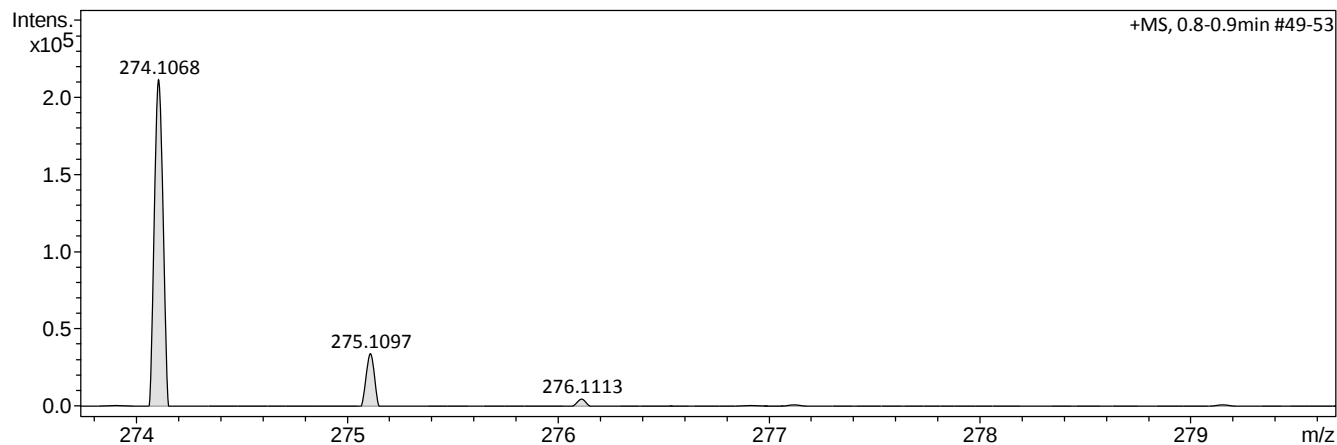
Analysis Name D:\Data\ggc\24-031514_P1-C-3_01_8811.d
 Method lc_qtof_directospos.m
 Sample Name 24-031514
 Comment DFV-640
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 1:55:20 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
274.1068	1	C15H16NO4	274.1074	2.2	4.7	2	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

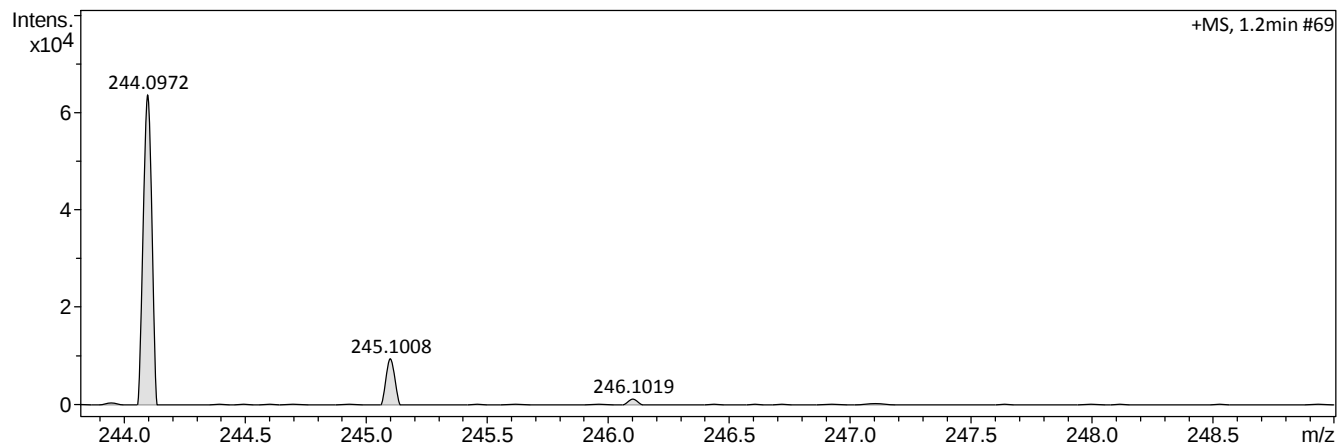
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 Sample Name 24-031515
 Comment DFV-673A
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:00:27 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
244.0972	1	C14H14NO3	244.0968	-1.6	6.0	1	100.00	8.5	even	ok

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Analysis Info

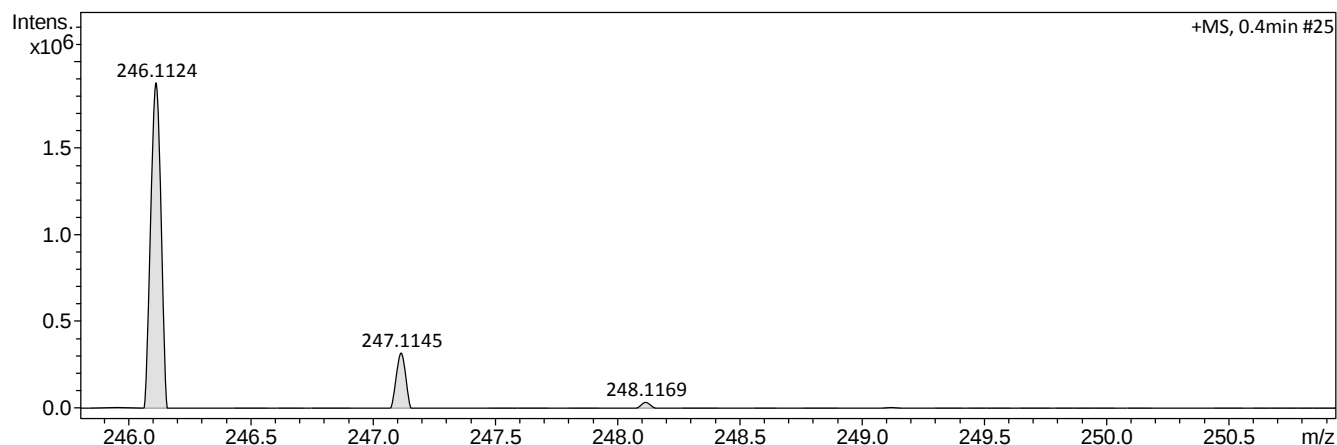
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 Method lc_qtof_directospos.m
 Sample Name 24-031516
 Comment DFV-678
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:05:34 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
246.1124	1	C14H16NO3	246.1125	0.5	6.0	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

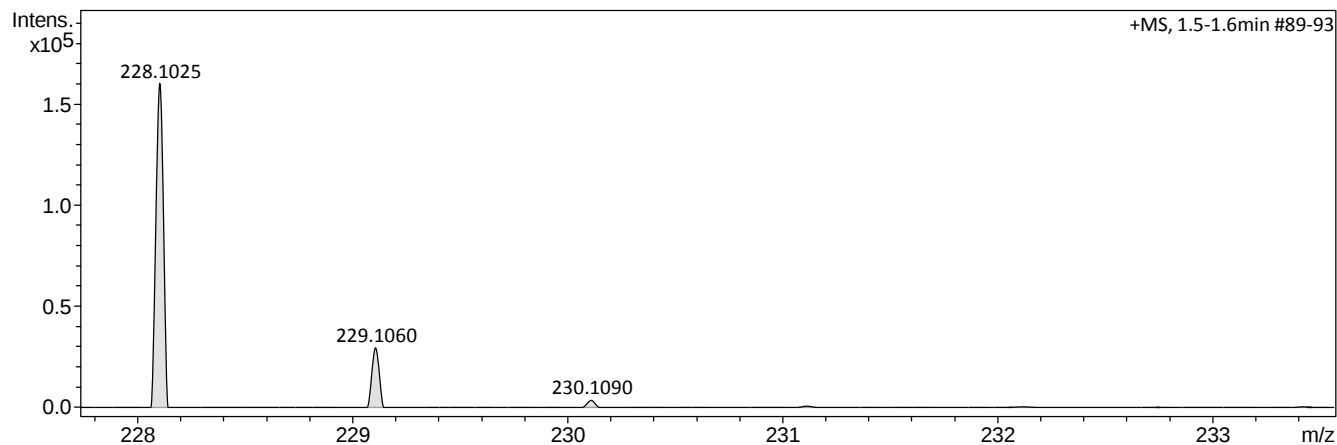
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 Sample Name 24-031517
 Comment DFV-711B
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:10:42 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
228.1025	1	C14H14NO2	228.1019	-2.8	16.3	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

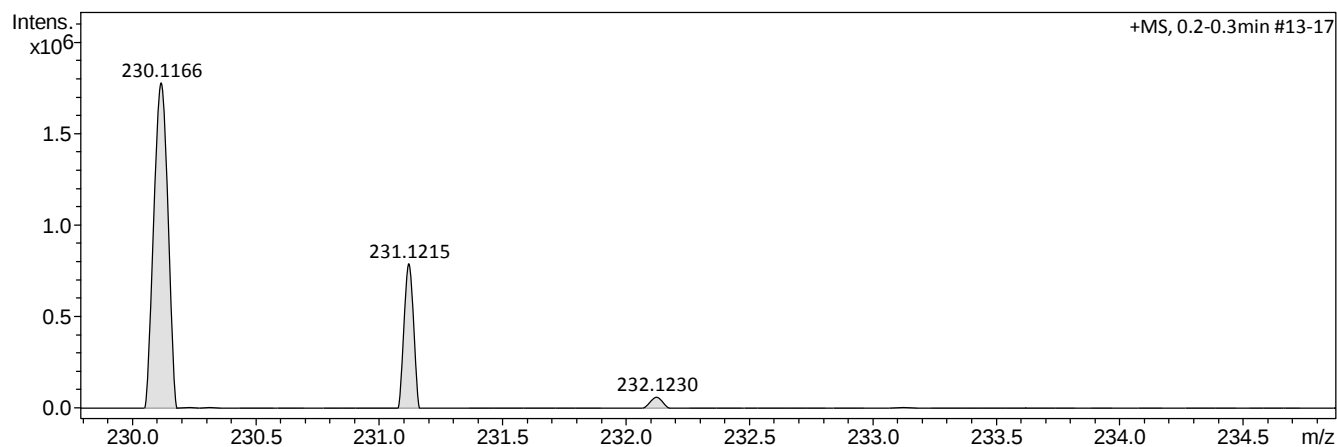
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 Sample Name 24-031518
 Comment DFV-722
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:15:49 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
230.1166	1	C14H16NO2	230.1176	4.2	165.8	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

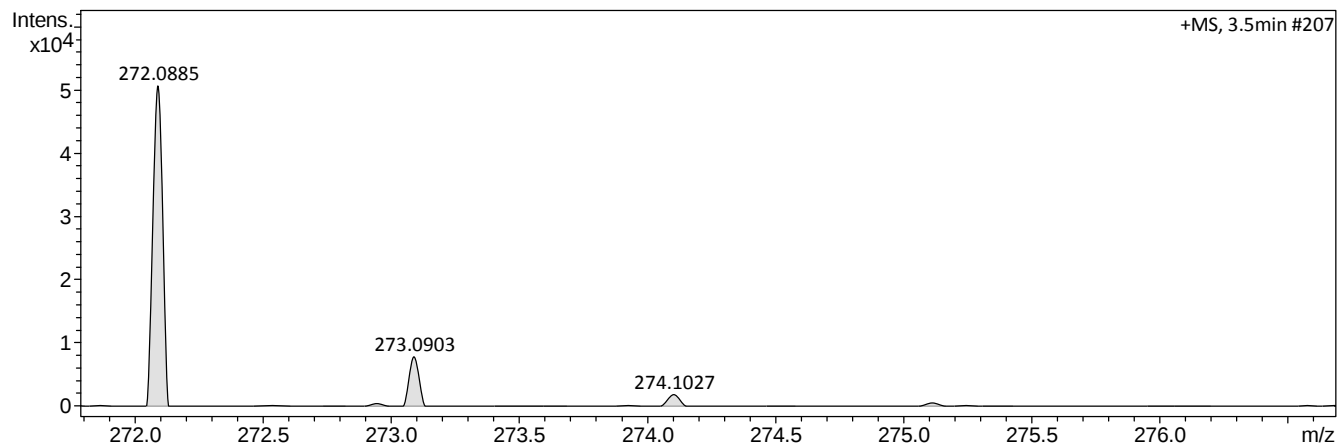
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 Method lc_qtof_directospos.m
 Sample Name 24-031519
 Comment DFV-754
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:20:56 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
272.0885	1	C13H15NNaO4	272.0893	3.0	11.1	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

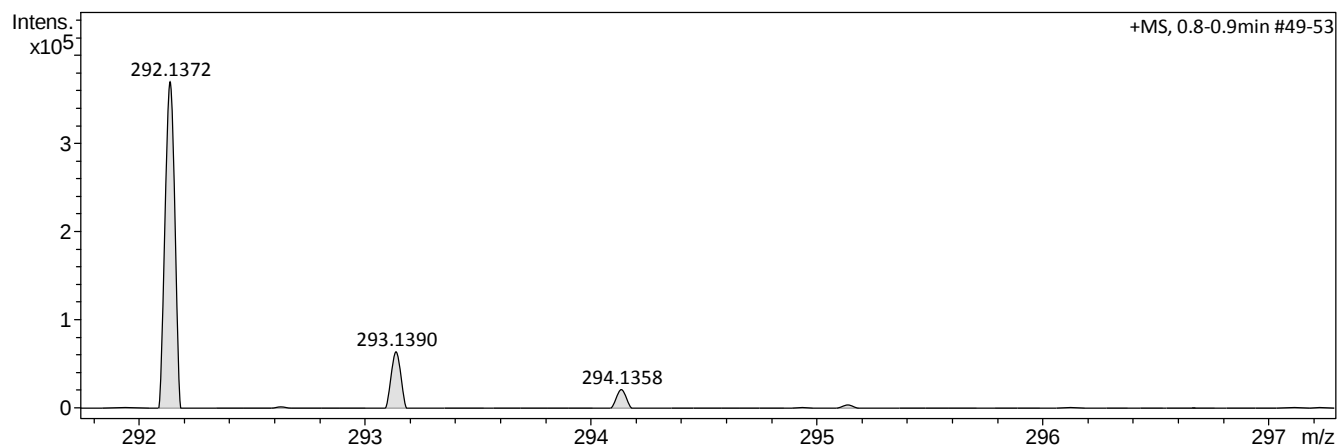
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 Method lc_qtof_directospos.m
 Sample Name 24-031520
 Comment DFV-759A
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:26:03 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
292.1372	1	C16H22NO2S	292.1366	-2.2	9.0	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

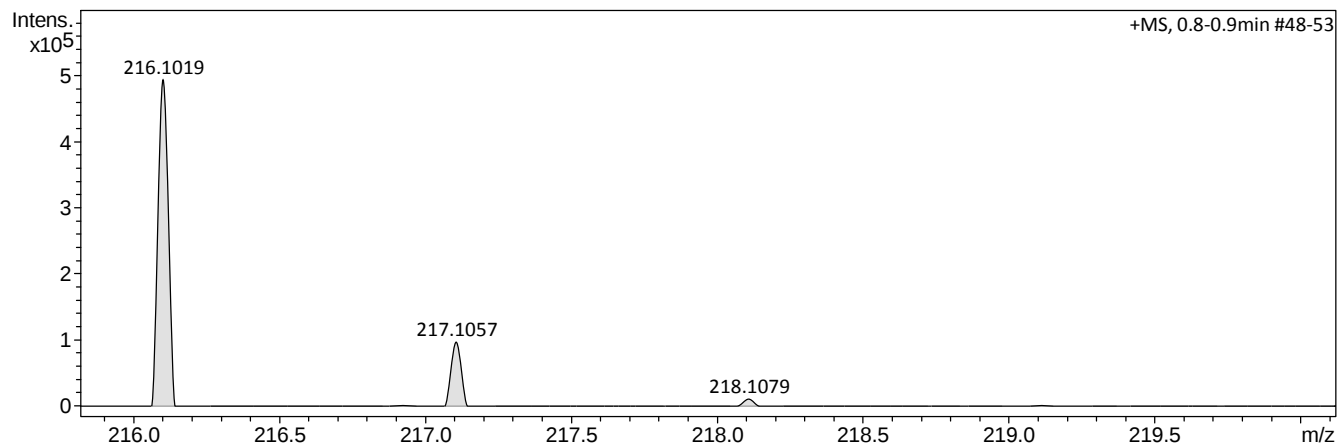
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 Method lc_qtof_directospos.m
 Sample Name 24-031521
 Comment DFV-759B
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:31:09 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
216.1019	1	C13H14NO2	216.1019	-0.1	28.4	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

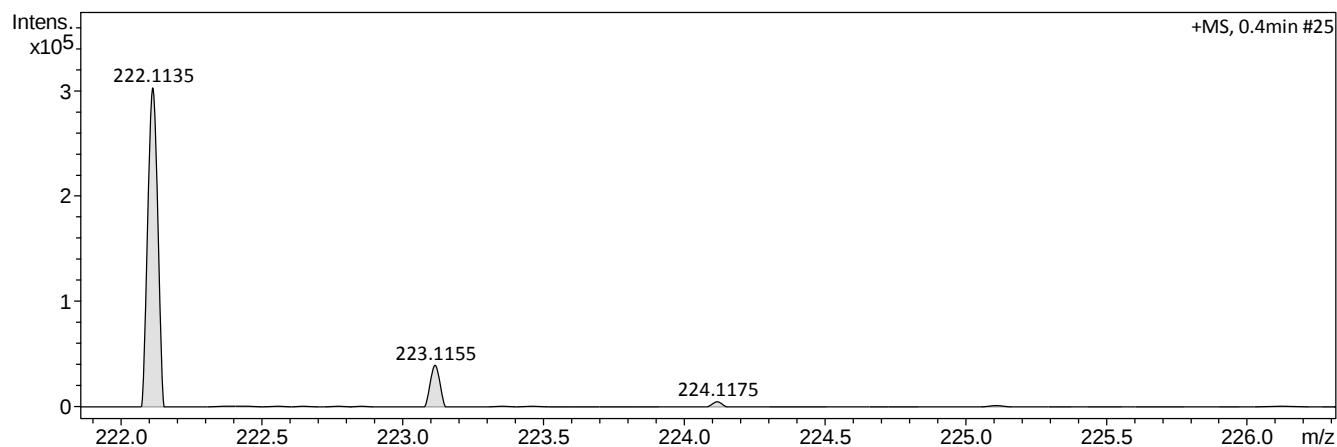
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 Method lc_qtof_directospos.m
 Sample Name 24-031522
 Comment SF-016
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 4/3/2024 2:36:15 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
222.1135	1	C12H16NO3	222.1125	-4.7	3.5	1	100.00	5.5	even	ok