

Qualitative Compound Report

Analysis Info

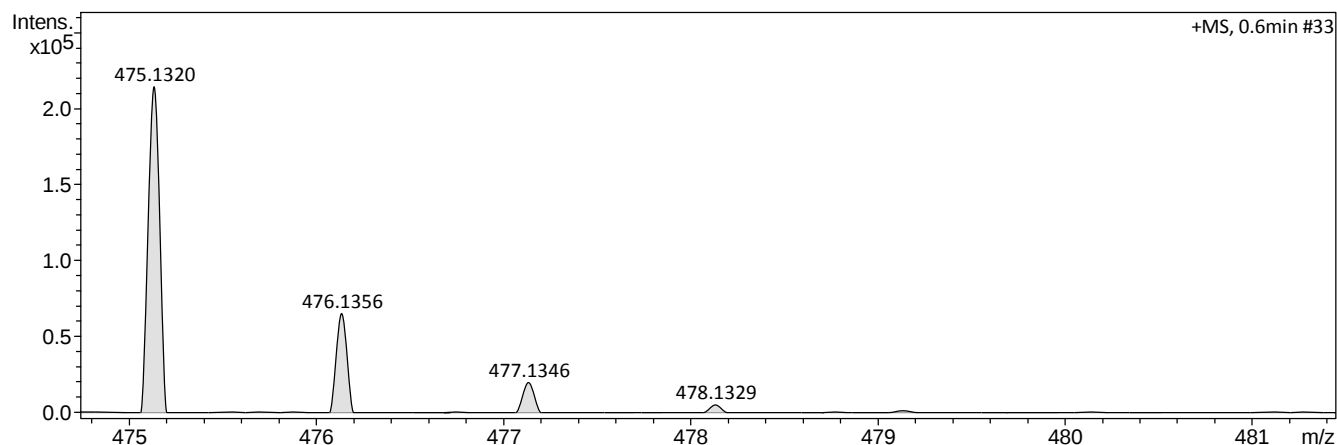
Analysis Name D:\Data\ggc\24-060517_P1-F-1_01_9276.d
 Method lc_qtof_directospos.m
 Sample Name 24-060517
 Comment CALI-34F1
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 11:55:48 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
475.1320	1	C26H23N2O5S	475.1322	0.4	4.4	1	100.00	16.5	even	ok

Qualitative Compound Report

Analysis Info

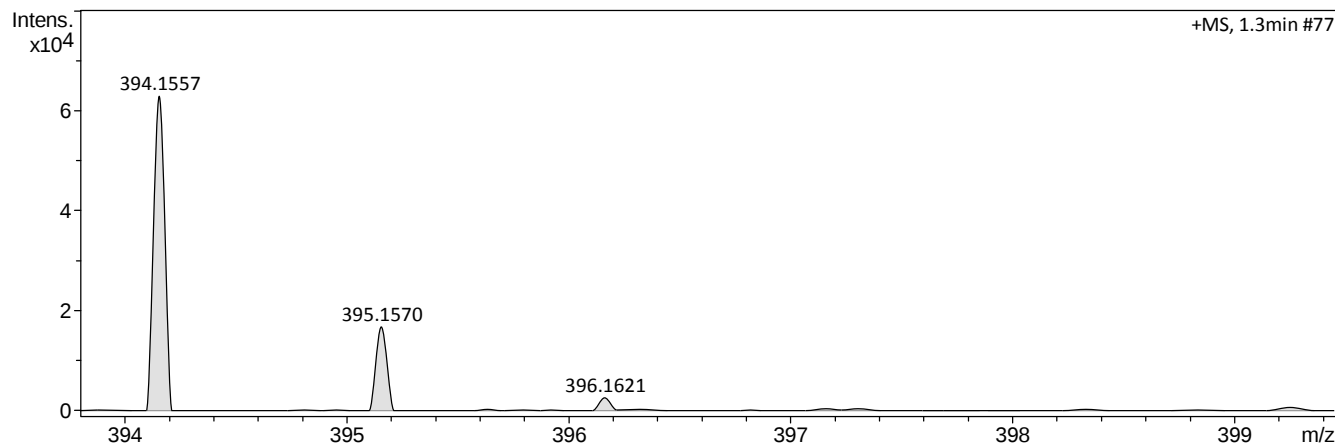
Analysis Name D:\Data\ggc\24-060518_P1-F-2_01_9277.d
 Method lc_qtof_directospos.m
 Sample Name 24-060518
 Comment CALI-28
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 12:00:53 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
394.1557	1	C25H20N3O2	394.1550	-1.9	10.8	1	100.00	17.5	even	ok

Qualitative Compound Report

Analysis Info

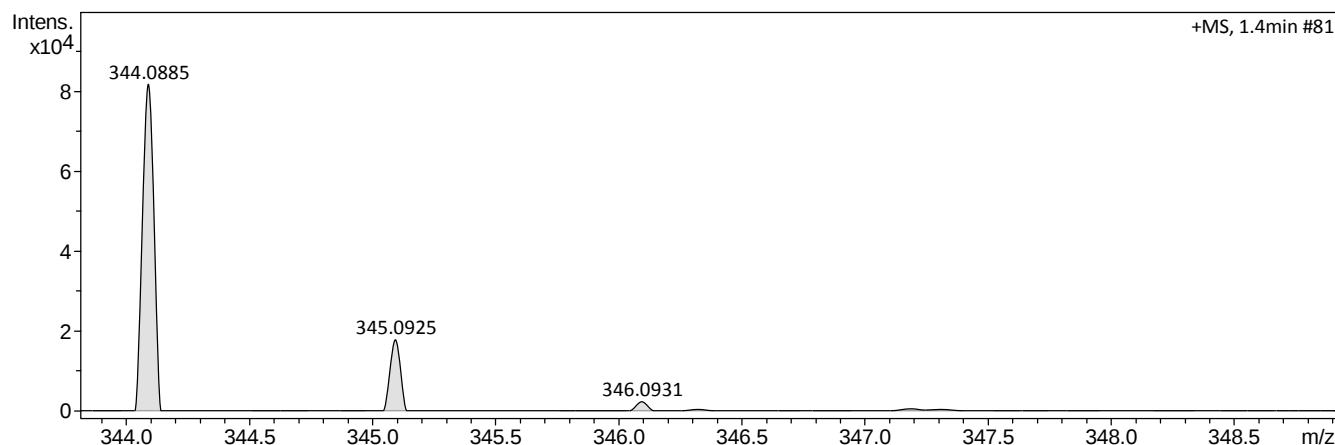
Analysis Name D:\Data\ggc\24-060519_P1-F-3_01_9278.d
 Method lc_qtof_directospos.m
 Sample Name 24-060519
 Comment CALI-26
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 12:06:00 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
344.0885	1	C19H15NNaO4	344.0893	2.3	3.7	1	100.00	12.5	even	ok

Qualitative Compound Report

Analysis Info

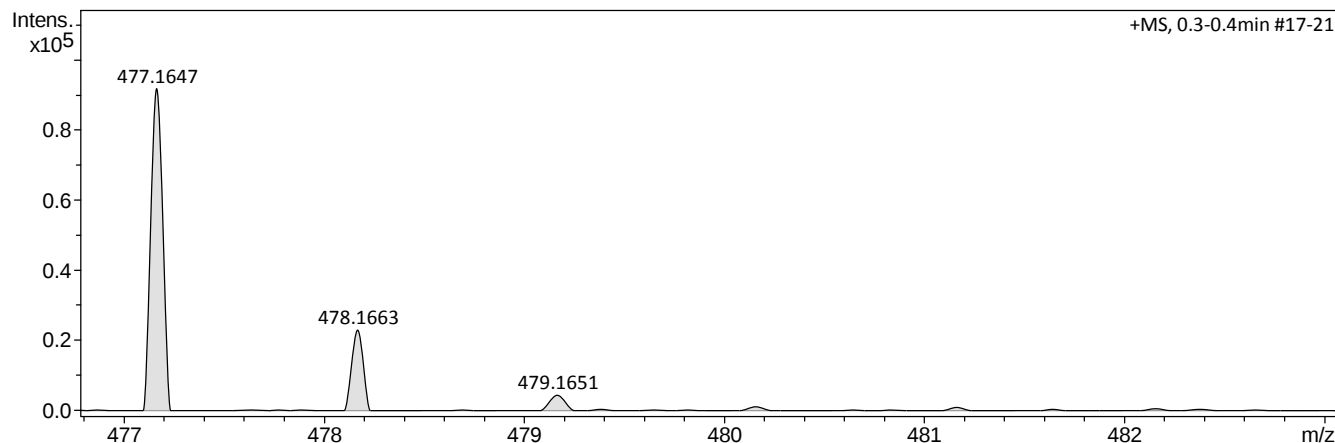
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 Method lc_qtof_directospos.m
 Sample Name 24-060520
 Comment FF-145F3
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 12:11:06 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
477.1647	1	C24H26N2NaO7	477.1632	-3.1	11.9	1	100.00	12.5	even	ok

Qualitative Compound Report

Analysis Info

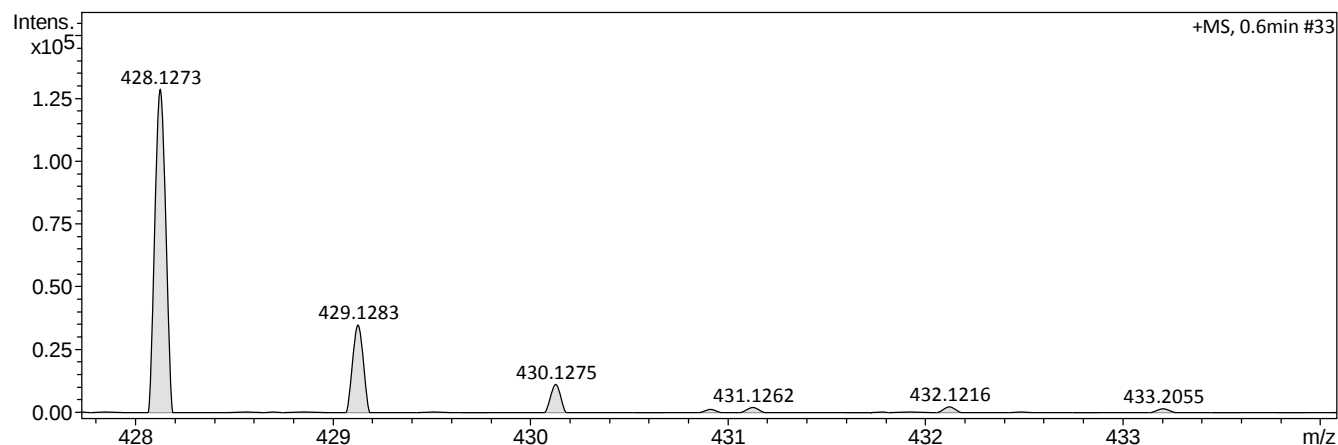
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 Method lc_qtof_directospos.m
 Sample Name 24-060521
 Comment CPS-5130bF1
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 12:16:12 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
428.1273	1	C24H23NNaO3S	428.1291	4.2	2.2	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

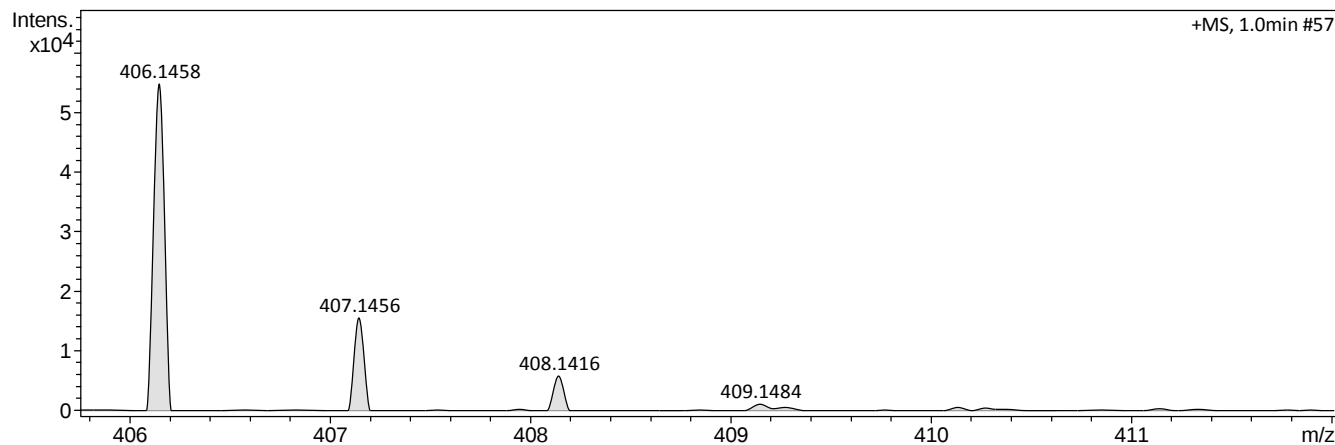
Analysis Name D:\Data\ggc\24-060522_P1-F-6_01_9281.d
 Method lc_qtof_directospos.m
 Sample Name 24-060522
 Comment CPS-5136F1
 Sv: MeOH + HCOOH
 Caterina Permingeat

Acquisition Date 6/12/2024 12:21:22 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
406.1458	1	C24H24NO3S	406.1471	3.4	10.3	1	100.00	13.5	even	ok