

Qualitative Compound Report

Analysis Info

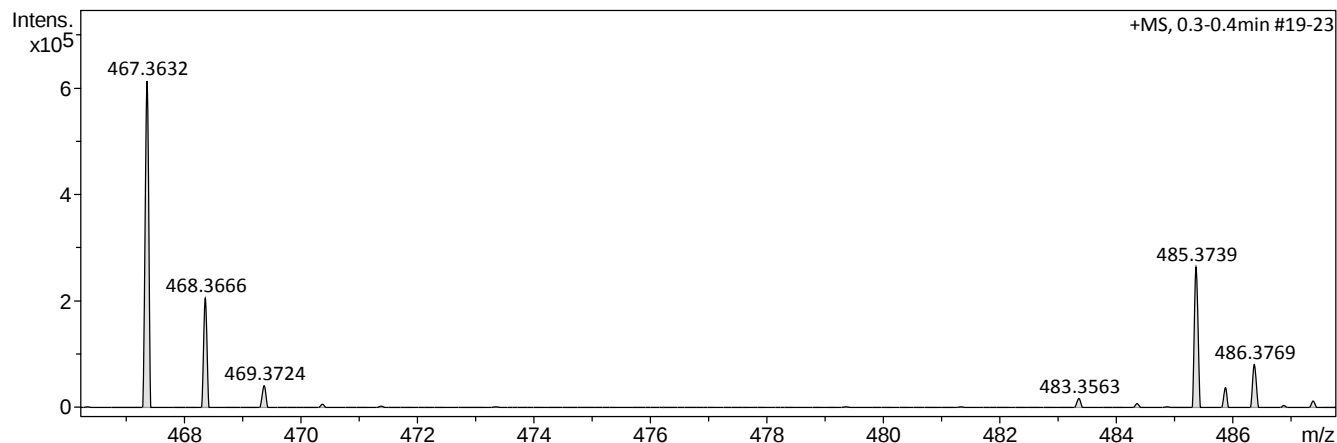
Analysis Name D:\Data\ggc\24-052412_P1-B-1_01_9216.d
 Method lc_qtof_directospos.m
 Sample Name 24-052412
 Comment Acrilico
 Sv: MeOH + HCOOH
 Manuela García - UNC

Acquisition Date 6/5/2024 11:49:52 AM

Operator MV
 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
467.3632	1	C30H47N2O2	467.3632	0.1	4.2	1	100.00	8.5	even	ok
485.3739	1	C30H49N2O3	485.3738	-0.2	18.7	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

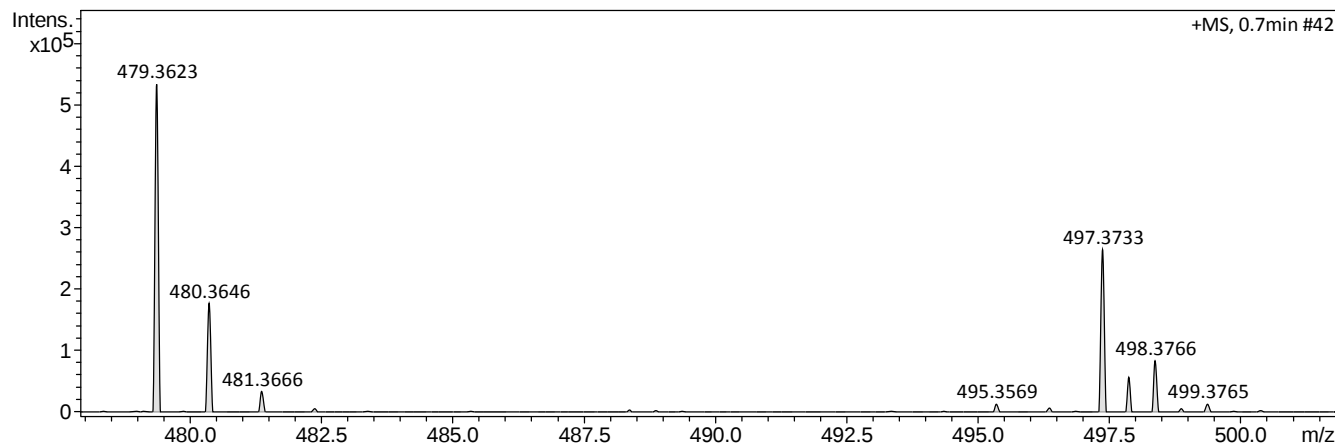
Analysis Name D:\Data\ggc\24-052413_P1-B-2_01_9217.d
 Method lc_qtof_directospos.m
 Sample Name 24-052413
 Comment Butanoico
 Sv: MeOH + HCOOH
 Manuela García - UNC

Acquisition Date 6/5/2024 11:55:02 AM

Operator MV
 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
479.3623	1	C31H47N2O2	479.3632	1.9	8.3	1	100.00	9.5	even	ok
497.3733	1	C31H49N2O3	497.3738	0.9	19.6	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

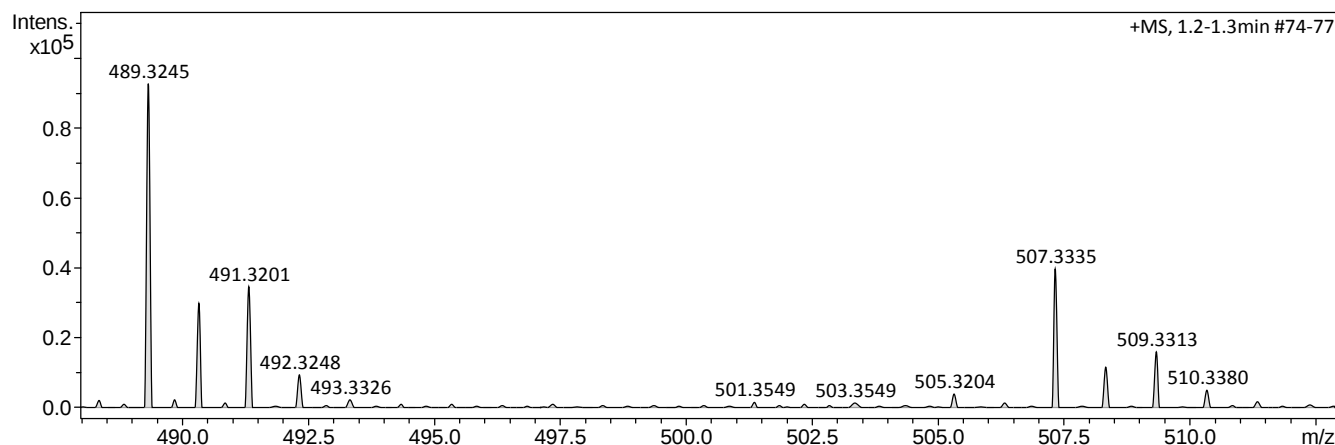
Analysis Name D:\Data\ggc\24-052414_P1-B-3_01_9218.d
 Method lc_qtof_directospos.m
 Sample Name 24-052414
 Comment a-cloro
 Sv: MeOH + HCOOH
 Manuela García - UNC

Acquisition Date 6/5/2024 12:00:08 PM

Operator MV
 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
489.3245	1	C29H46ClN2O2	489.3242	-0.5	6.0	1	100.00	7.5	even	ok
507.3335	1	C29H48ClN2O3	507.3348	2.5	22.5	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

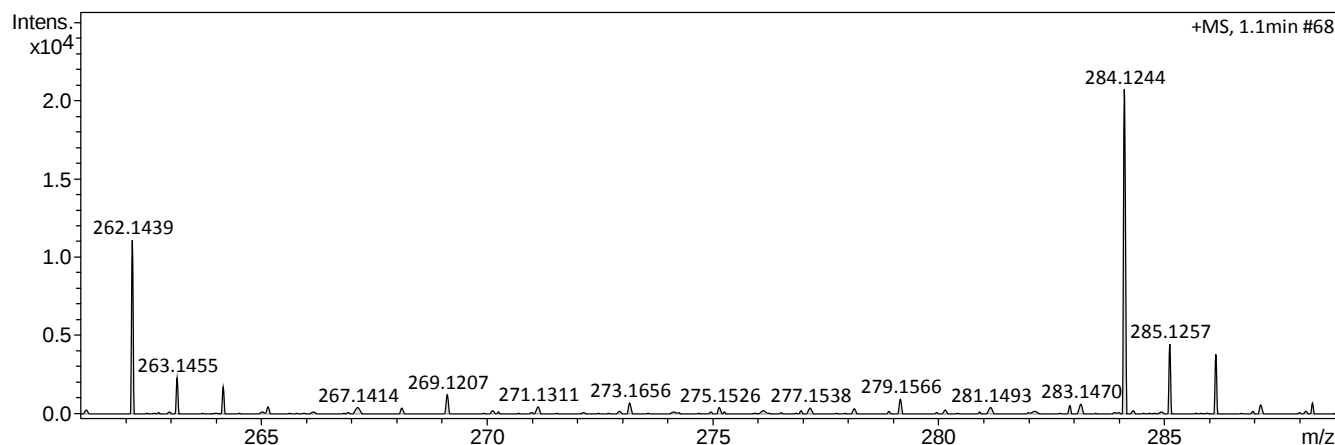
Analysis Name D:\Data\ggc\24-052415_P1-B-4_01_9219.d
 Method lc_qtof_directospos.m
 Sample Name 24-052415
 Comment AR-35F6
 Sv: MeOH + HCOOH
 Manuela García - UNC

Acquisition Date 6/5/2024 12:05:20 PM

Operator MV
 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
262.1439	1	C15H20NO3	262.1438	-0.5	79.5	1	100.00	6.5	even	ok
284.1244	1	C15H19NNaO3	284.1257	4.6	97.6	1	100.00	6.5	even	ok