

Qualitative Compound Report

Analysis Info

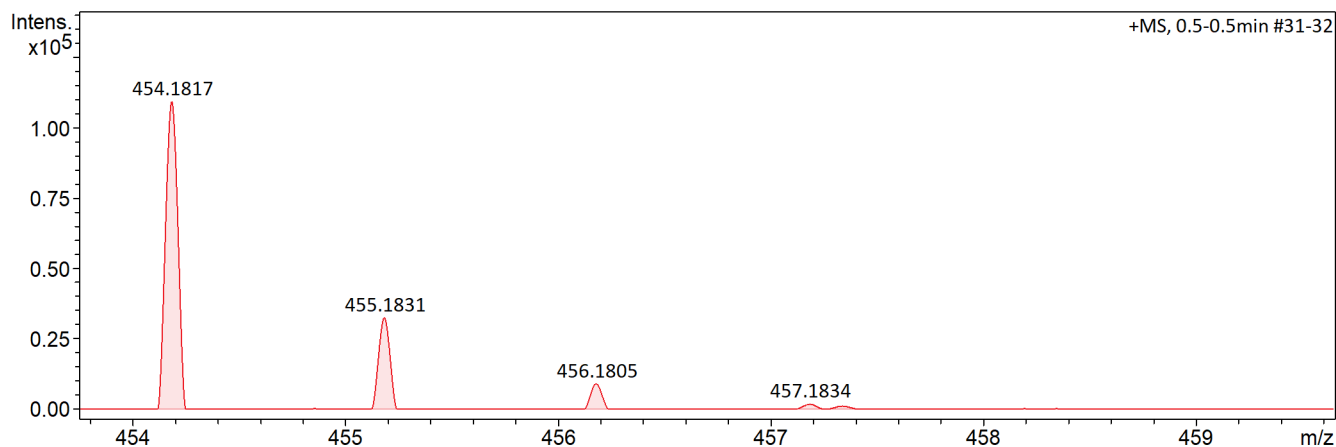
Analysis Name C:\Data\24-092021_P1-D-3_01_9470.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092021
 Comment NI-S-Ph
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 16:54:10

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
454.1817	1	C27H29NNaO2S	454.1811	-1.3	7.2	1	100.00	13.5	even	ok

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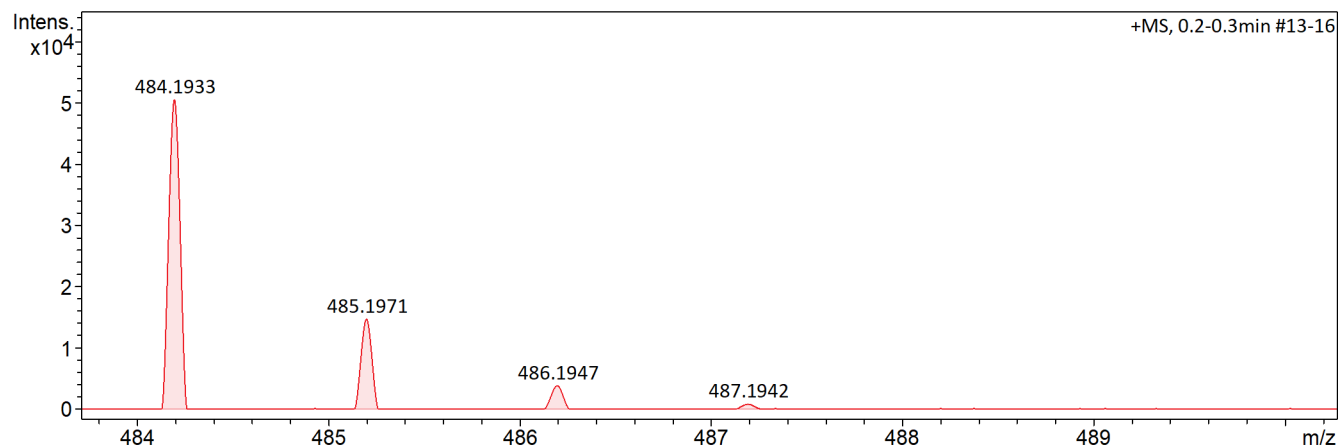
Analysis Name C:\Data\24-092022_P1-D-4_01_9471.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092022
 Comment NI-S-PhOMe
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 16:59:17

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
484.1933	1	C28H31NNaO3S	484.1917	-3.2	18.1	2	66.31	13.5	even	ok

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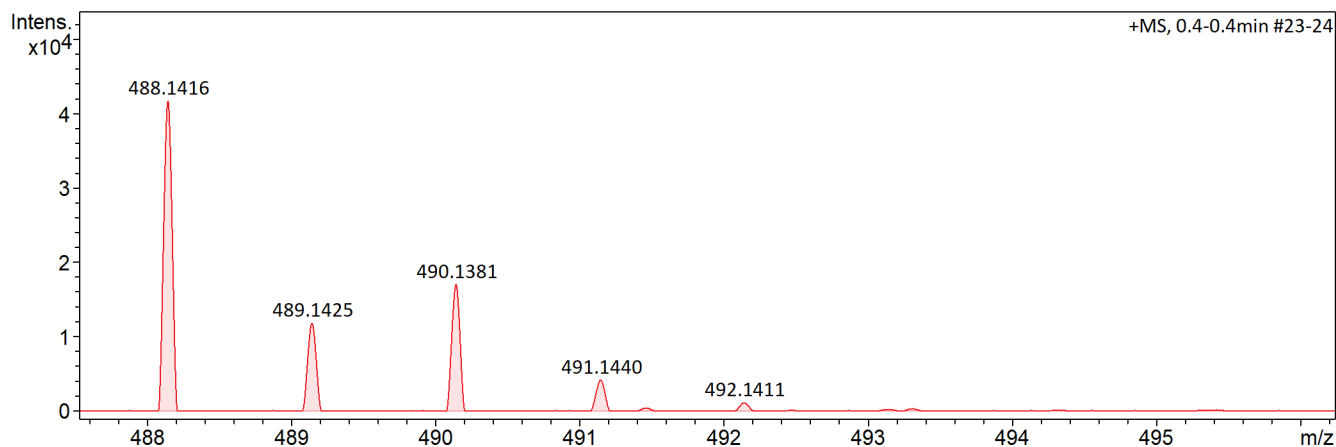
Analysis Name C:\Data\24-092023_P1-D-5_01_9472.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092023
 Comment NI-S-PhCl
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:04:26

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
488.1416	1	C27H28ClNNaO2S	488.1421	1.1	13.6	1	100.00	13.5	even	ok

Qualitative Compound Report

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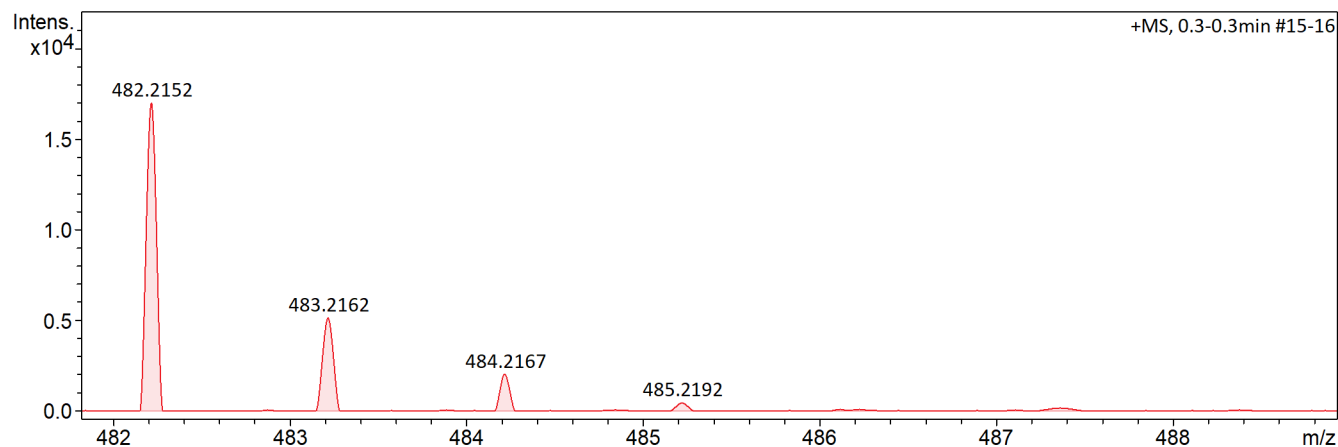
Analysis Name C:\Data\24-092024_P1-D-6_01_9473.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092024
 Comment NI-S-Naf
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:09:34

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
482.2152	1	C31H32NO2S	482.2148	-0.7	25.3	1	100.00	16.5	even	ok

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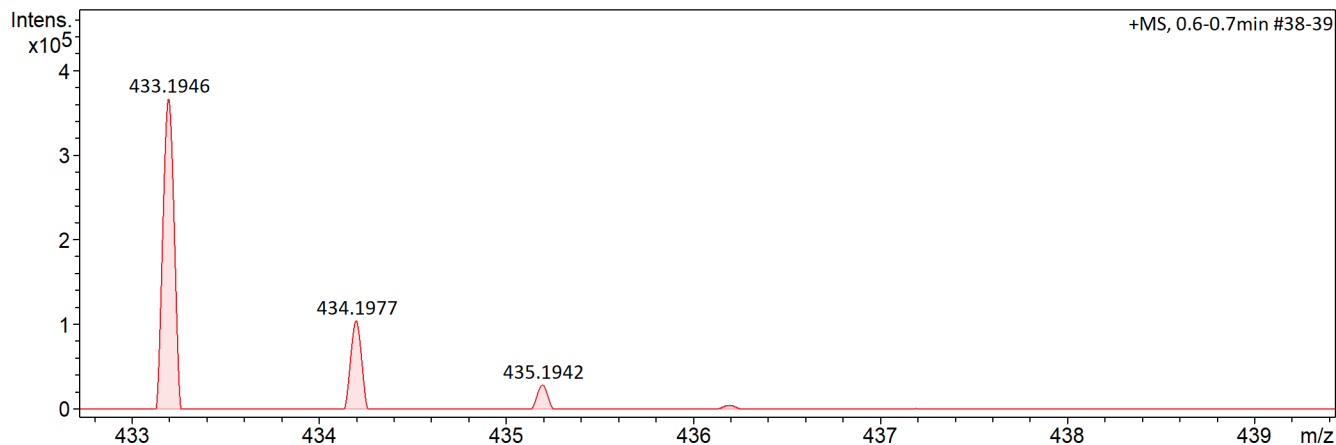
Analysis Name C:\Data\24-092025_P1-D-7_01_9474.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092025
 Comment NI-S-oPy
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:14:43

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
433.1946	1	C26H29N2O2S	433.1944	-0.5	11.1	1	100.00	13.5	even	ok

Qualitative Compound Report

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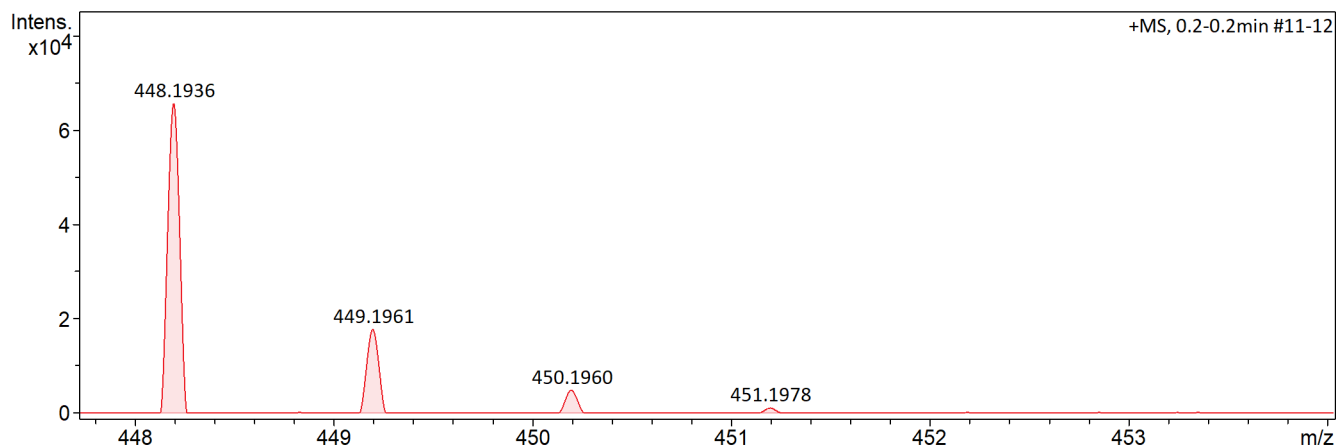
Analysis Name C:\Data\24-092026_P1-D-8_01_9475.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092026
 Comment NI-SO-Ph
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:19:50

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
448.1936	1	C27H30NO3S	448.1941	1.1	21.9	1	100.00	13.5	even	ok

Qualitative Compound Report

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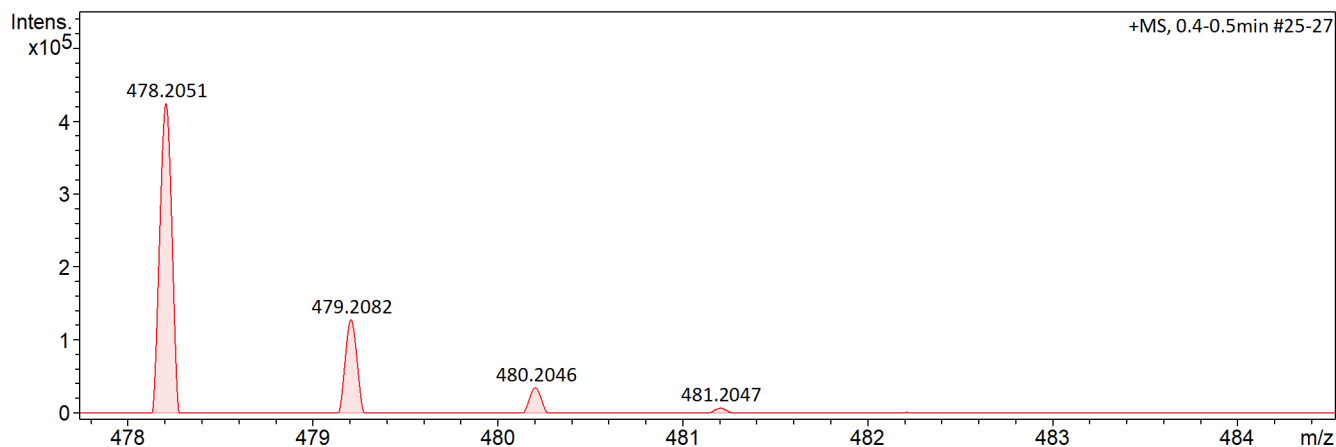
Analysis Name C:\Data\24-092027_P1-D-9_01_9476.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092027
 Comment NI-SO-PhOMe
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:24:57

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
478.2051	1	C28H32NO4S	478.2047	-0.9	13.8	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

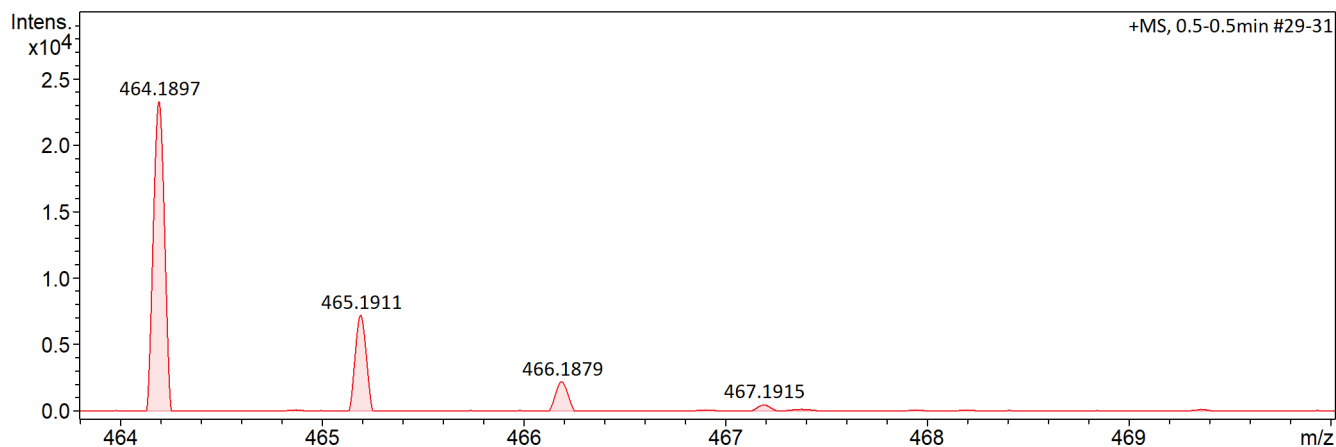
Analysis Name C:\Data\24-092028_P1-E-1_01_9477.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092028
 Comment NI-SO2-PhOMe
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:30:02

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
464.1897	1	C27H30NO4S	464.1890	-1.4	1.9	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

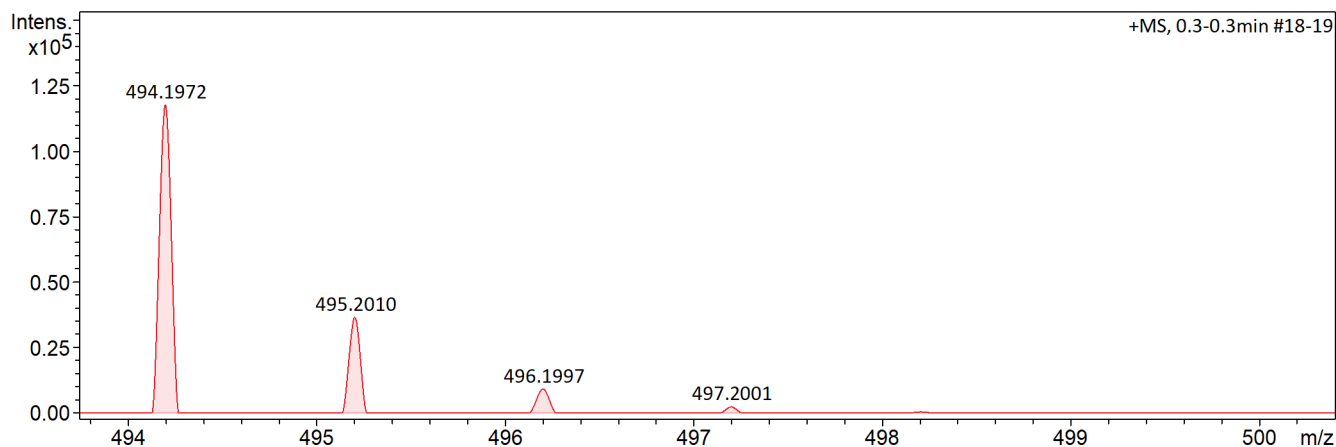
Analysis Name C:\Data\24-092029_P1-E-2_01_9478.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092029
 Comment NI-SO2-PhOMe
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:35:10

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
494.1972	1	C28H32NO5S	494.1996	4.7	13.9	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

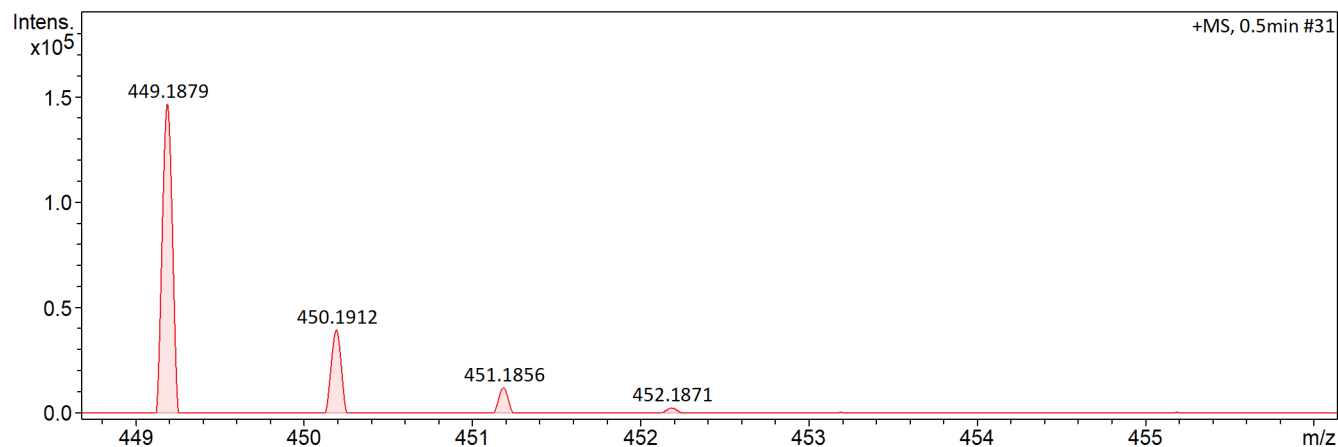
Analysis Name C:\Data\24-092030_P1-E-3_01_9479.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092030
 Comment NI-SO-oPy
 Sv: MeOH + HCOOH
 Liliana Jimenez

Acquisition Date 1/10/2024 17:40:17

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 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	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
449.1879	1	C26H29N2O3S	449.1893	3.3	16.9	1	100.00	13.5	even	ok