

Qualitative Compound Report

Analysis Info

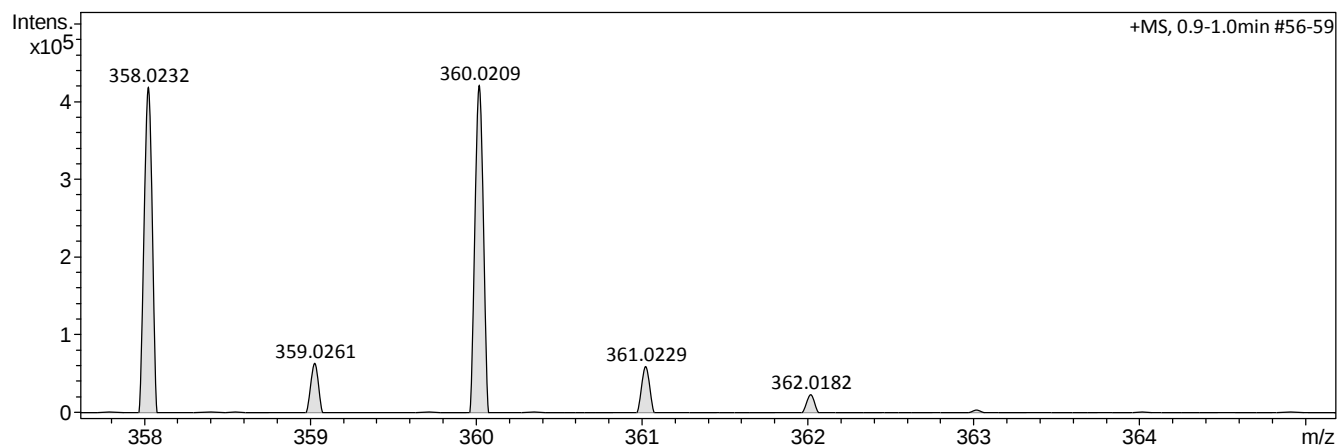
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 Method lc_qtof_directospos.m
 Sample Name 24-060536
 Comment EJG-II-76
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:32:40 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
358.0232	1	C13H17BrN3O2S	358.0219	-3.4	15.8	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

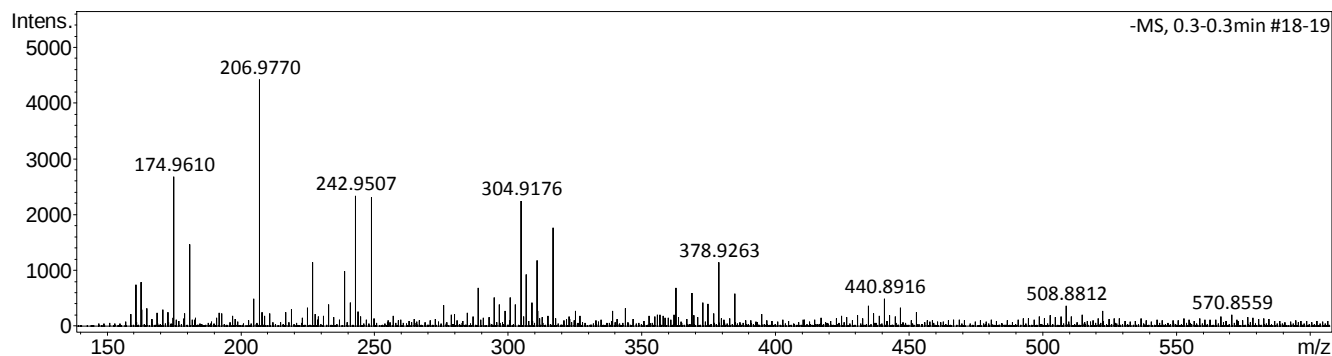
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 Method lc_qtof_directosneg.m
 Sample Name 24-060536
 Comment EJG-II-76
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:42:10 AM

Operator MV
 Instrument / Ser# 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



#	m/z	I	I %
1	160.8465	747	16.9
2	162.8447	795	18.0
3	174.9610	2677	60.7
4	180.9765	1470	33.3
5	204.9942	489	11.1
6	206.9770	4409	100.0
7	226.9708	1146	26.0
8	232.9156	389	8.8
9	238.9382	990	22.5
10	240.9359	431	9.8
11	242.9507	2331	52.9
12	248.9645	2313	52.5
13	276.0885	385	8.7
14	288.9415	694	15.7
15	294.9569	513	11.6
16	296.8997	395	8.9
17	300.9077	513	11.6
18	302.9120	392	8.9
19	304.9176	2244	50.9
20	306.9275	933	21.2
21	308.9181	430	9.8
22	310.9374	1176	26.7
23	316.9551	1756	39.8
24	362.9437	693	15.7
25	368.8955	595	13.5
26	372.9080	421	9.5
27	374.9142	401	9.1
28	378.9263	1149	26.1
29	384.9411	585	13.3
30	440.8916	489	11.1

Qualitative Compound Report

Analysis Info

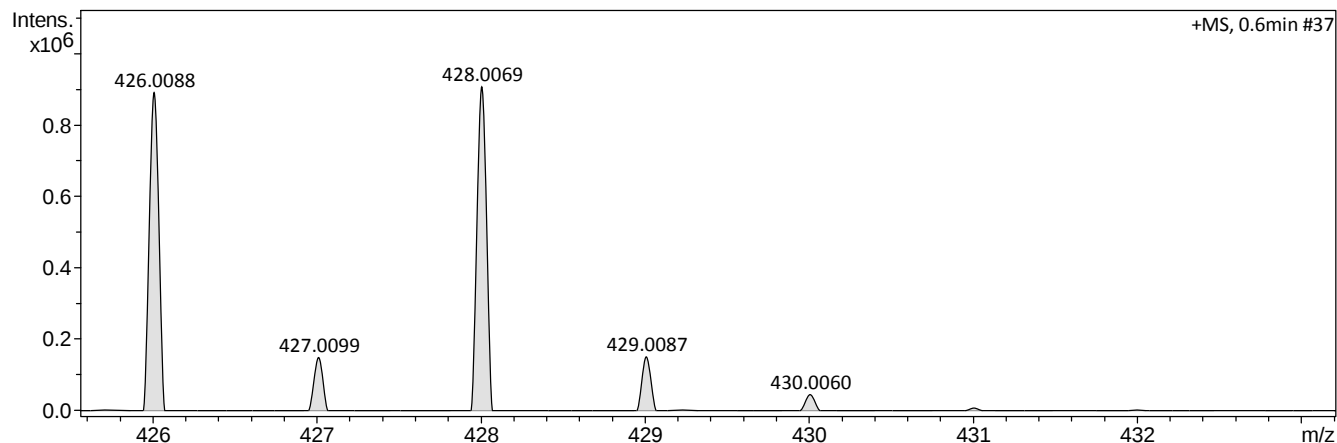
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 Sample Name 24-060537
 Comment EJG-II-77
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:37:47 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
426.0088	1	C ₁₄ H ₁₆ BrF ₃ N ₃ O ₂ S	426.0093	1.3	9.3	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

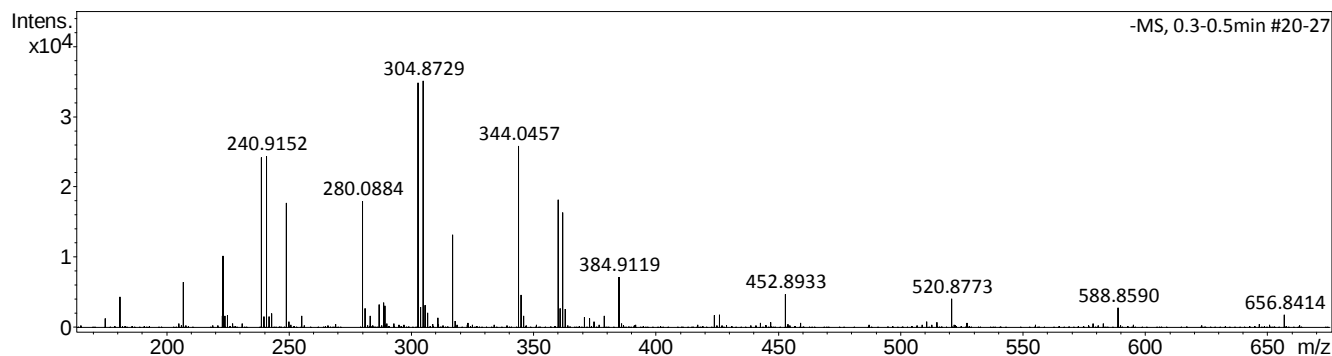
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 Method lc_qtof_directosneg.m
 Sample Name 24-060537
 Comment EJG-II-77
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:47:16 AM

Operator MV
 Instrument / Ser# 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



#	m/z	I	I %
1	180.9630	4342	12.4
2	206.9585	6483	18.5
3	223.0208	10183	29.1
4	238.9179	24099	68.8
5	240.9152	24321	69.4
6	242.9271	2015	5.7
7	248.9446	17715	50.5
8	280.0884	18003	51.4
9	281.0921	2744	7.8
10	286.8812	3256	9.3
11	288.8789	3582	10.2
12	289.1604	3058	8.7
13	302.8744	34744	99.1
14	303.8771	2927	8.4
15	304.8729	35046	100.0
16	305.8763	3160	9.0
17	306.8812	2135	6.1
18	316.9272	13201	37.7
19	344.0457	25799	73.6
20	345.0475	4598	13.1
21	360.0095	18153	51.8
22	361.0111	2749	7.8
23	362.0072	16375	46.7
24	363.0089	2591	7.4
25	384.9119	7180	20.5
26	425.9644	1781	5.1
27	452.8933	4726	13.5
28	520.8773	4044	11.5
29	588.8590	2788	8.0
30	656.8414	1782	5.1

Qualitative Compound Report

Analysis Info

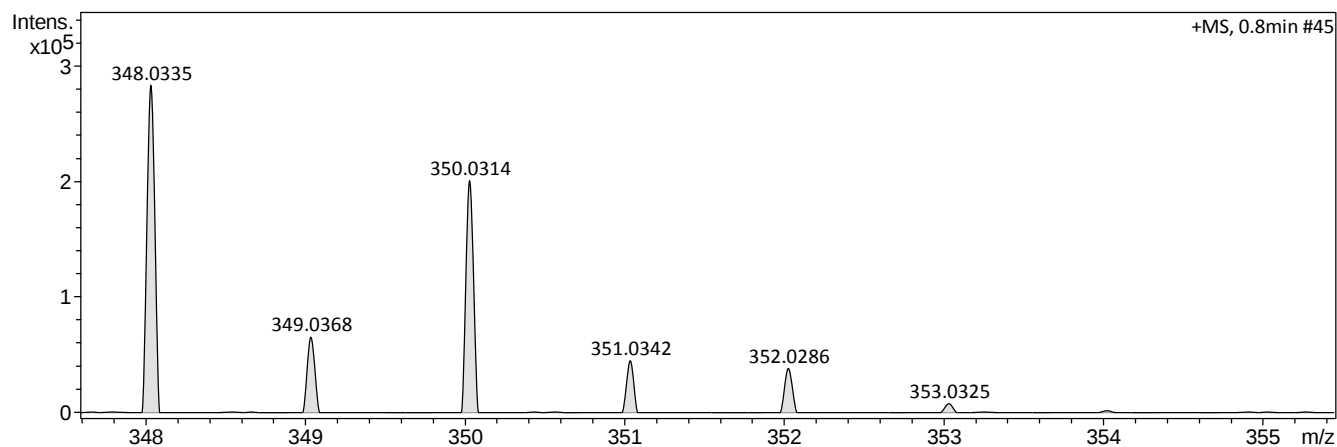
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 Method lc_qtof_directospos.m
 Sample Name 24-060538
 Comment EJG-II-78
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:42:56 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
348.0335	1	C ₁₃ H ₁₆ Cl ₂ N ₃ O ₂ S	348.0335	-0.0	34.3	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

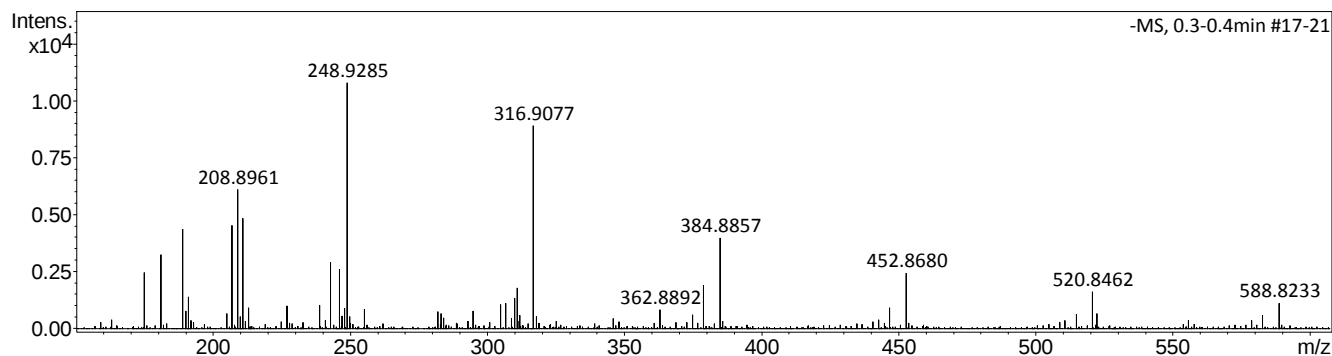
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 Method lc_qtof_directosneg.m
 Sample Name 24-060538
 Comment EJG-II-78
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:52:22 AM

Operator MV
 Instrument / Ser# 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



#	m/z	I	I %
1	174.9322	2444	22.7
2	180.9485	3238	30.1
3	188.9863	4362	40.5
4	189.9890	791	7.3
5	190.9824	1404	13.0
6	206.9447	4530	42.0
7	208.8961	6097	56.6
8	210.8944	4833	44.9
9	212.8897	926	8.6
10	226.9341	1000	9.3
11	238.9003	1019	9.5
12	242.9102	2896	26.9
13	246.0483	2599	24.1
14	248.0464	886	8.2
15	248.9285	10775	100.0
16	255.2005	871	8.1
17	282.0214	756	7.0
18	294.9141	787	7.3
19	304.8688	1045	9.7
20	306.8797	1109	10.3
21	310.0002	1345	12.5
22	310.8896	1788	16.6
23	316.9077	8899	82.6
24	362.8892	833	7.7
25	378.8674	1903	17.7
26	384.8857	3967	36.8
27	446.8475	913	8.5
28	452.8680	2415	22.4
29	520.8462	1626	15.1
30	588.8233	1112	10.3

Qualitative Compound Report

Analysis Info

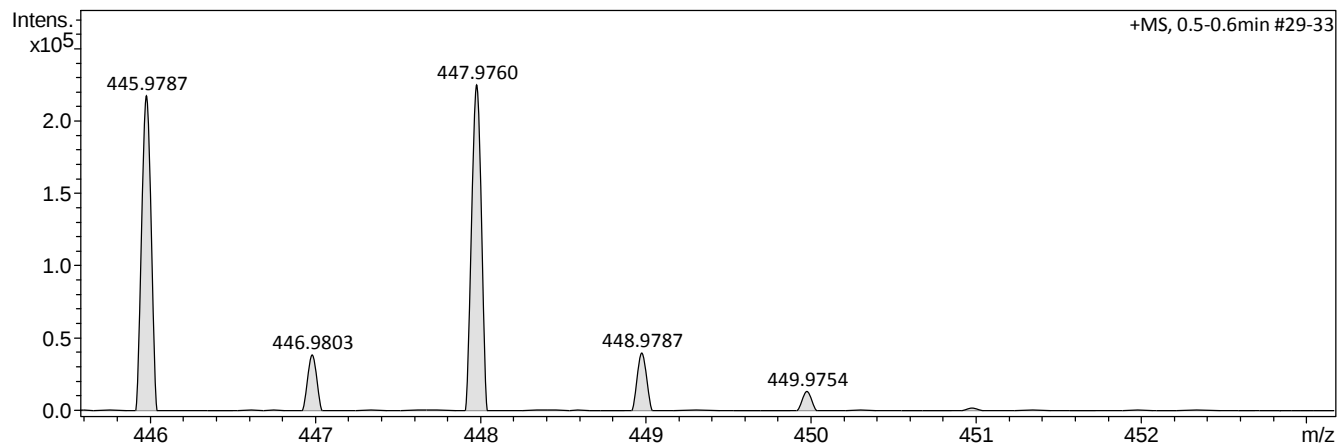
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 Comment EJG-I-78
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:48:05 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
445.9787	1	C16H12BrF3N3O2S	445.9780	-1.5	10.8	1	100.00	10.5	even	ok

Qualitative Compound Report

Analysis Info

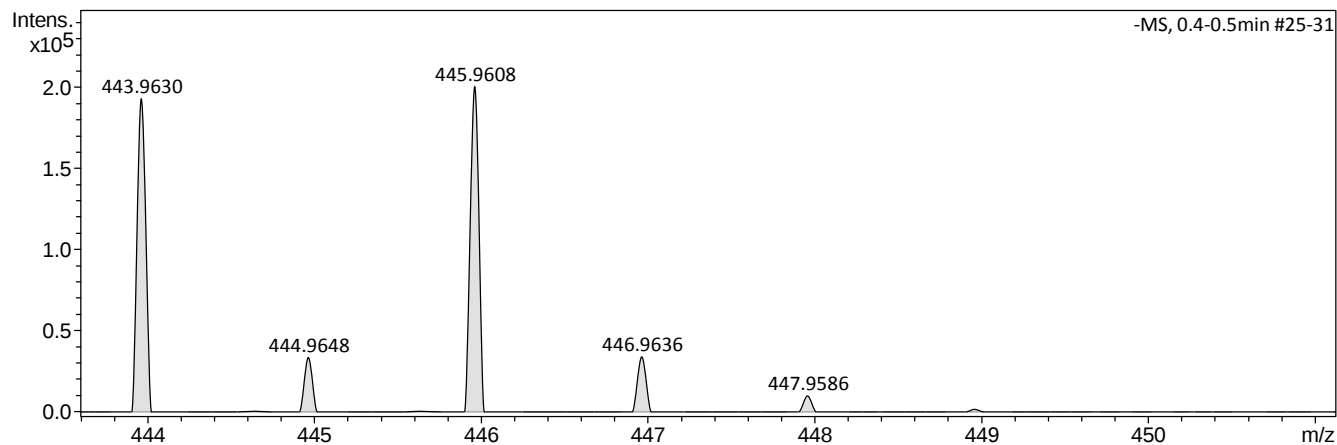
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 Sample Name 24-060539
 Comment EJG-I-78
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:57:30 AM

Operator MV
 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
443.9630	1	C16H10BrF3N3O2S	443.9635	1.1	14.7	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

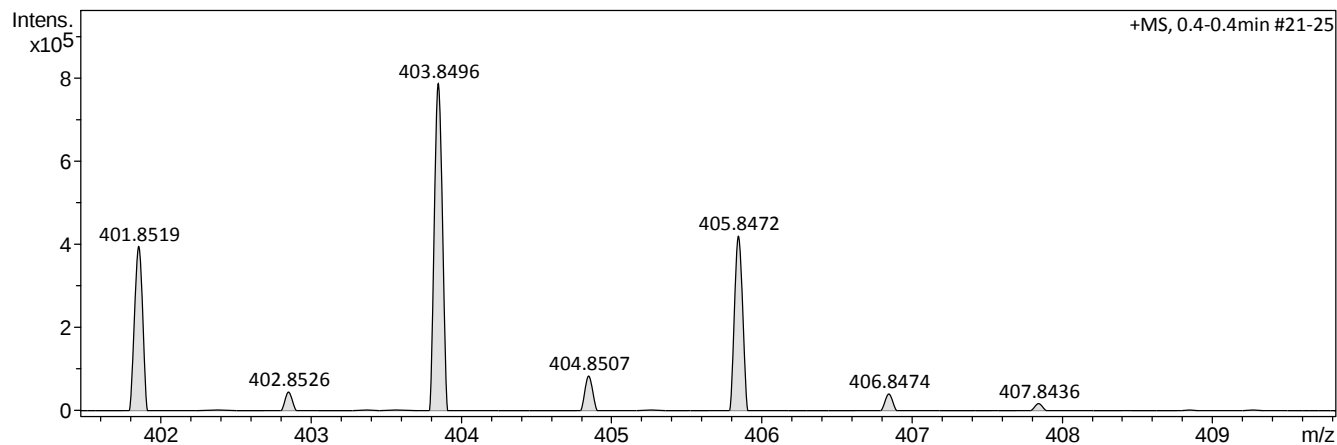
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 Method lc_qtof_directospos.m
 Sample Name 24-060540
 Comment EJG-II-79
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:53:13 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
401.8519	1	C9H7Br2N3NaO2S	401.8518	-0.3	7.0	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

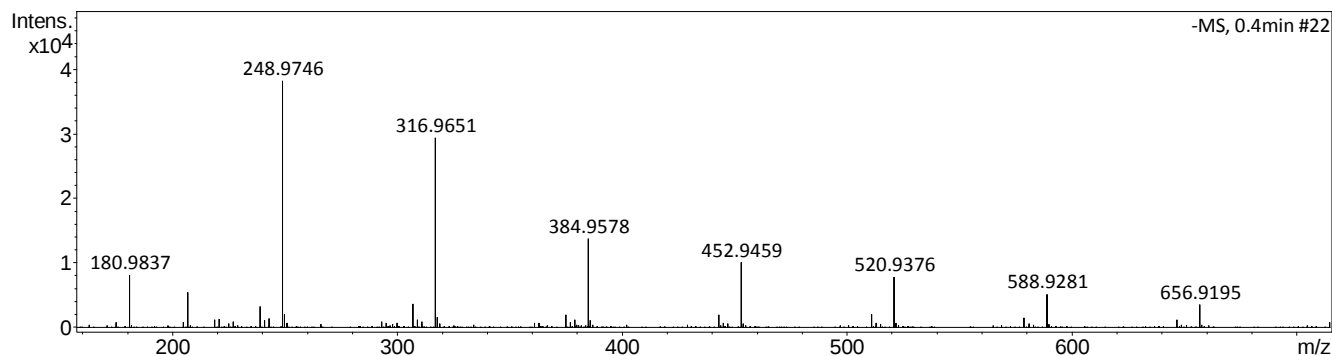
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 Method lc_qtof_directosneg.m
 Sample Name 24-060540
 Comment EJG-II-79
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:02:38 PM

Operator MV
 Instrument / Ser# 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



#	m/z	I	I %
1	180.9837	8062	21.1
2	206.9842	5441	14.3
3	218.9271	1148	3.0
4	220.9209	1336	3.5
5	238.9455	3300	8.6
6	240.9438	1091	2.9
7	242.9587	1362	3.6
8	248.9746	38165	100.0
9	249.9792	2076	5.4
10	306.9358	3639	9.5
11	308.9328	1212	3.2
12	316.9651	29353	76.9
13	317.9707	1590	4.2
14	374.9289	1944	5.1
15	378.9340	1152	3.0
16	384.9578	13739	36.0
17	385.9591	1057	2.8
18	442.9180	1985	5.2
19	452.9459	10092	26.4
20	510.9091	2064	5.4
21	520.9376	7798	20.4
22	578.9045	1484	3.9
23	588.9281	5109	13.4
24	646.8872	1174	3.1
25	656.9195	3561	9.3
26	724.9136	2821	7.4
27	792.9058	1836	4.8
28	860.8964	1534	4.0
29	928.8891	1089	2.9
30	939.3103	1462	3.8

Qualitative Compound Report

Analysis Info

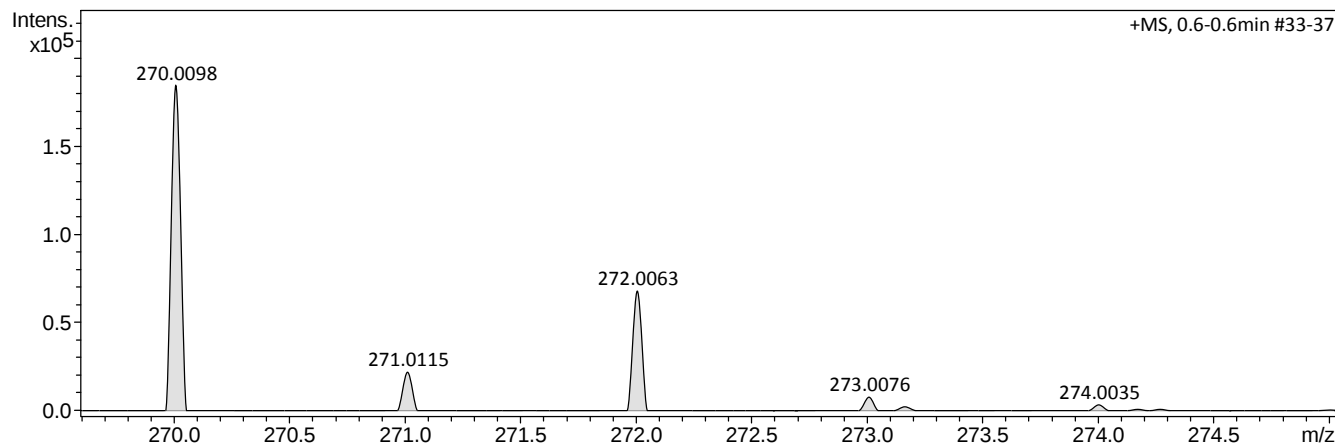
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 Sample Name 24-060541
 Comment MAC-III-98
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 10:58:22 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
270.0098	1	C10H9CIN3O2S	270.0099	0.1	7.0	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

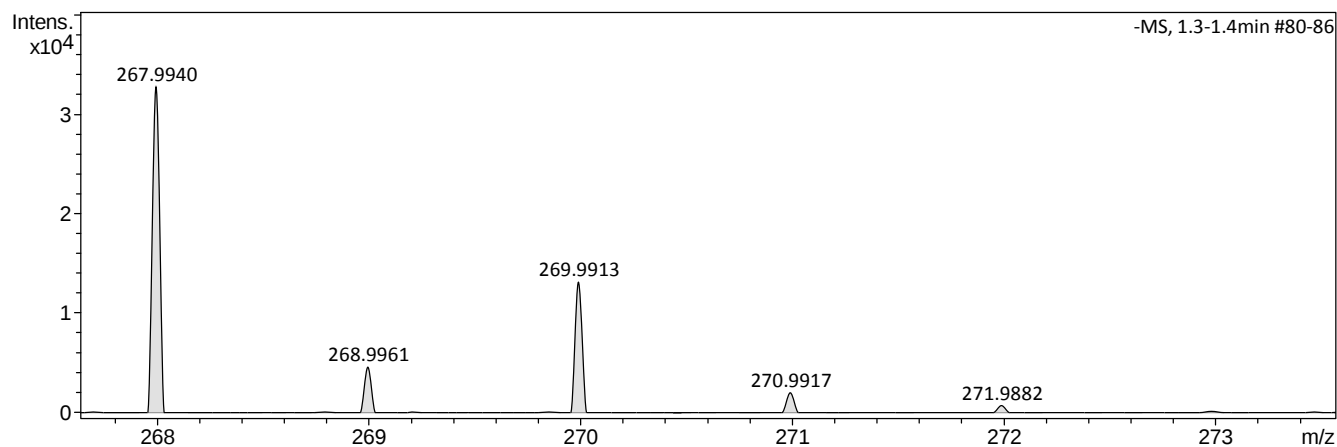
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 Sample Name 24-060541
 Comment MAC-III-98
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:07:45 PM

Operator MV
 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
267.9940	1	C10H7CIN3O2S	267.9953	4.7	12.8	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

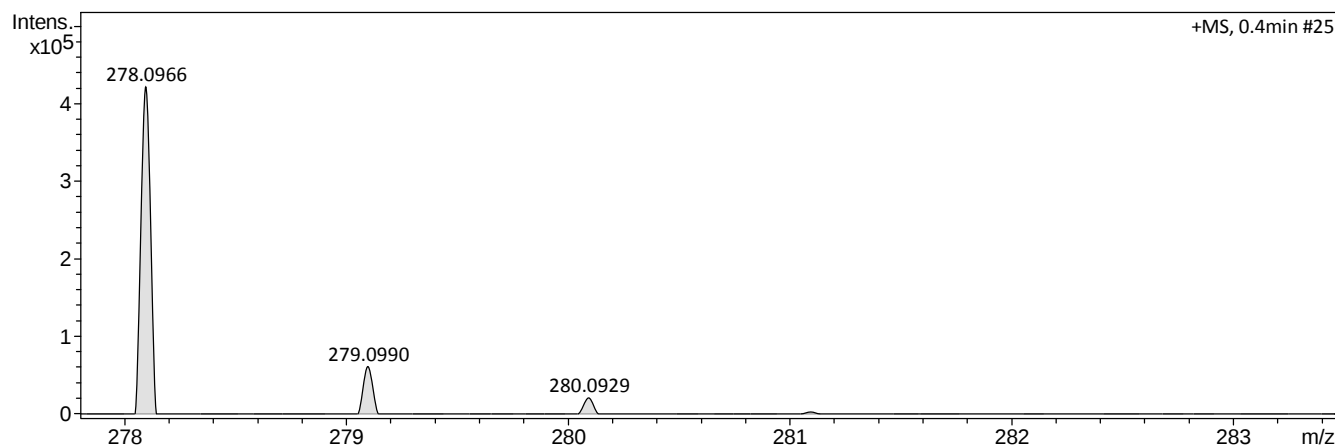
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 Method lc_qtof_directospos.m
 Sample Name 24-060542
 Comment MAC-III-102
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:03:30 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
278.0966	1	C13H16N3O2S	278.0958	-2.8	10.0	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

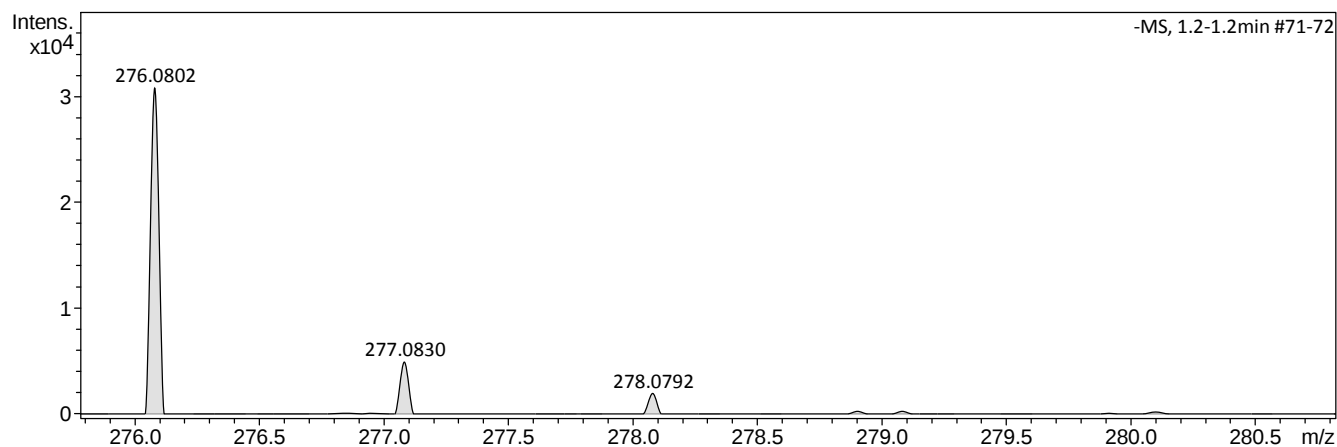
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 Sample Name 24-060542
 Comment MAC-III-102
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:12:54 PM

Operator MV
 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
276.0802	1	C13H14N3O2S	276.0812	3.7	2.3	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

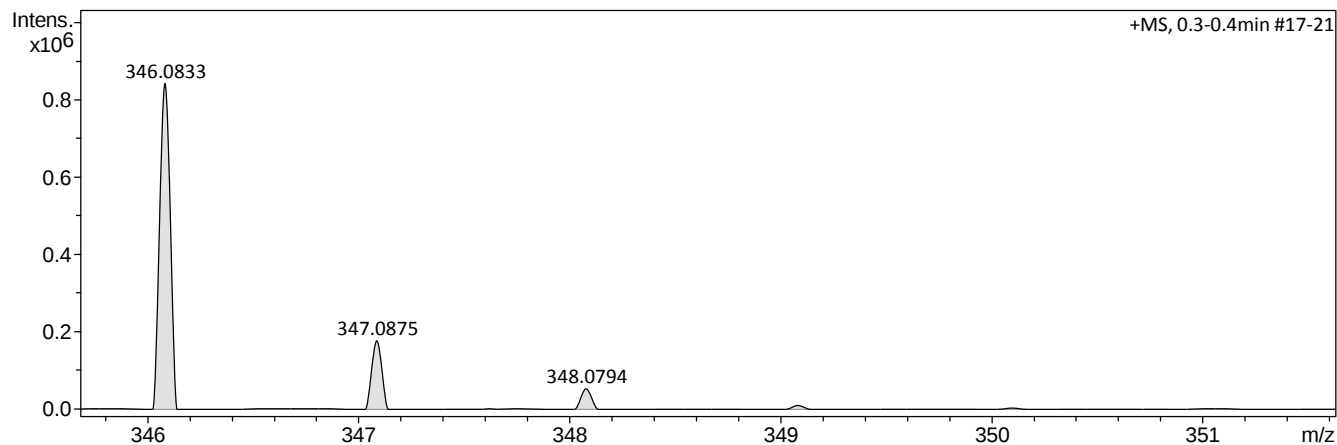
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 Method lc_qtof_directospos.m
 Sample Name 24-060543
 Comment MAC-III-101
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:08:40 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
346.0833	1	C14H15F3N3O2S	346.0832	-0.4	17.9	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

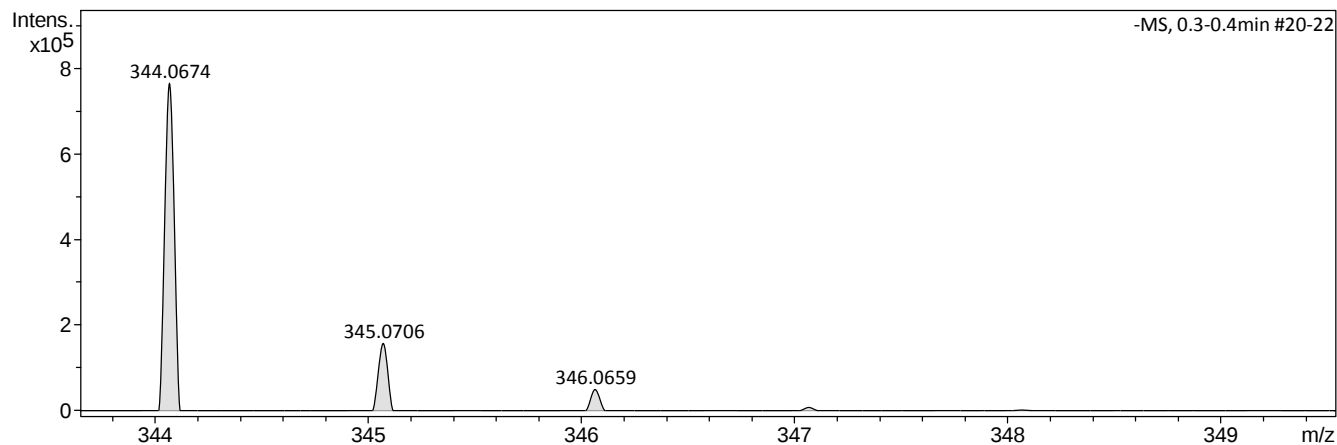
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 Sample Name 24-060543
 Comment MAC-III-101
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:18:04 PM

Operator MV
 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
344.0674	1	C14H13F3N3O2S	344.0686	3.5	15.9	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

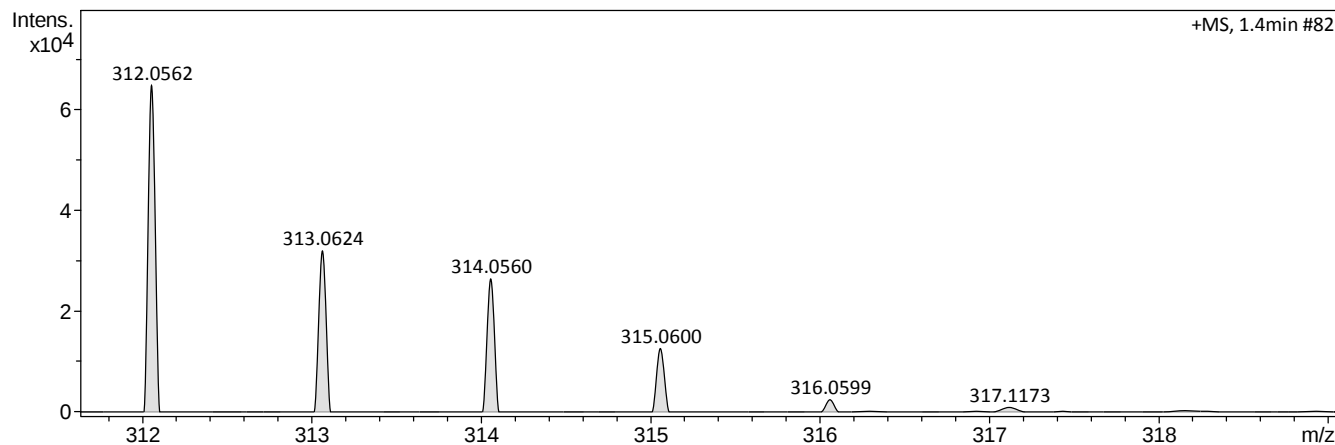
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 Method lc_qtof_directospos.m
 Sample Name 24-060544
 Comment MAC-III-97
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:13:48 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
312.0562	1	C13H15ClN3O2S	312.0568	2.0	160.3	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

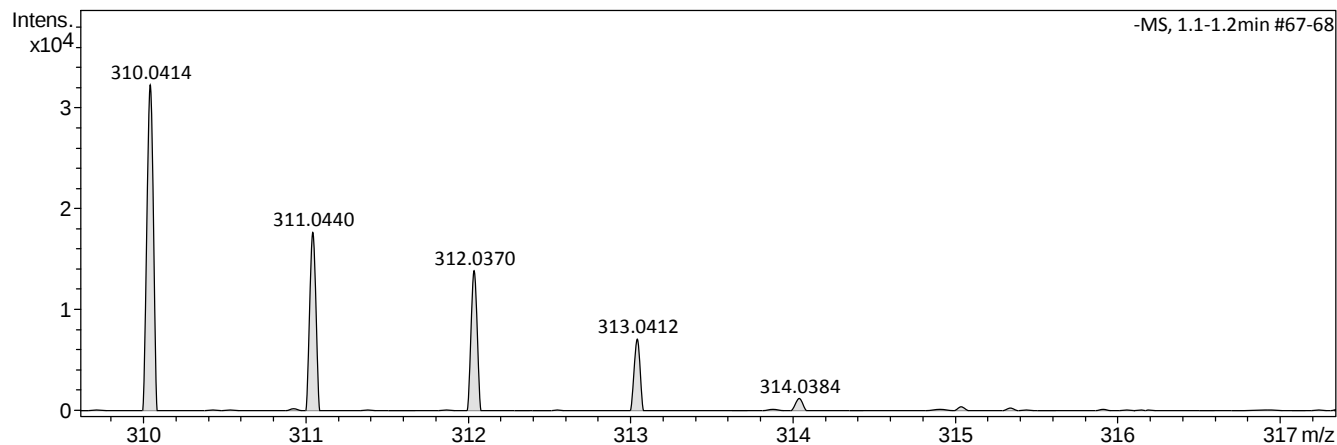
Analysis Name D:\Data\ggc\24-060544_P1-D-9_01_9314.d
 Method lc_qtof_directosneg.m
 Sample Name 24-060544
 Comment MAC-III-97
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:23:11 PM

Operator MV
 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
310.0414	1	C13H13ClN3O2S	310.0422	2.7	187.9	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

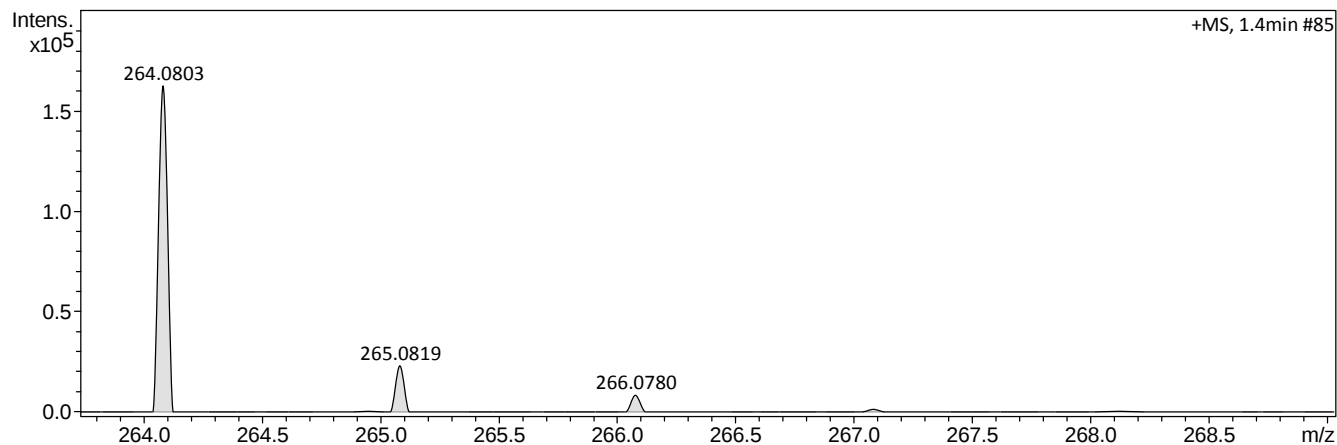
Analysis Name D:\Data\ggc\24-060545_P1-E-1_01_9303.d
 Method lc_qtof_directospos.m
 Sample Name 24-060545
 Comment MAC-III-33
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:18:57 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
264.0803	1	C ₁₂ H ₁₄ N ₃ O ₂ S	264.0801	-0.7	6.5	1	100.00	7.5	even	ok

Qualitative Compound Report

Analysis Info

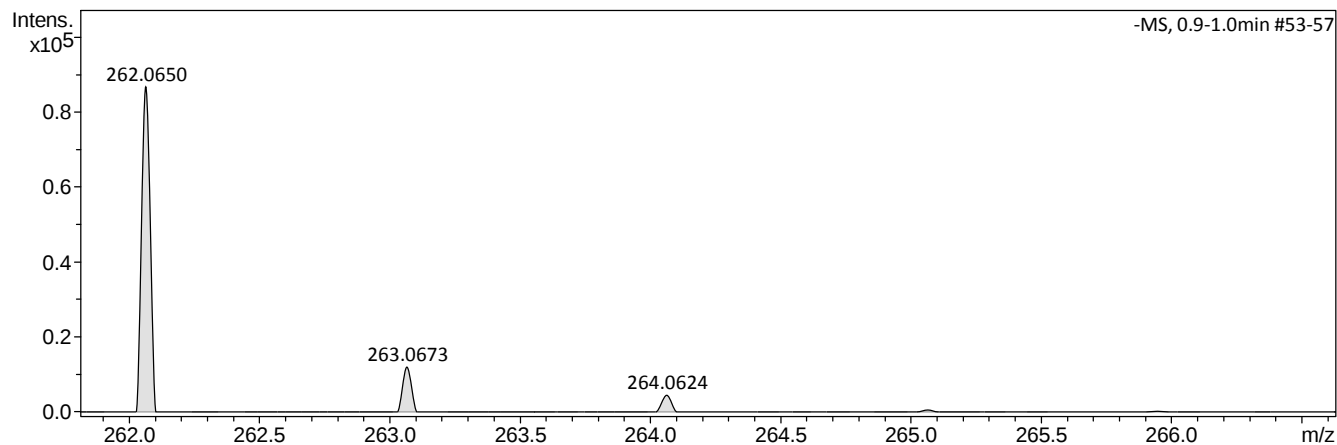
Analysis Name D:\Data\ggc\24-060545_P1-E-1_01_9315.d
 Method lc_qtof_directosneg.m
 Sample Name 24-060545
 Comment MAC-III-33
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:28:18 PM

Operator MV
 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
262.0650	1	C12H12N3O2S	262.0656	2.0	8.3	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

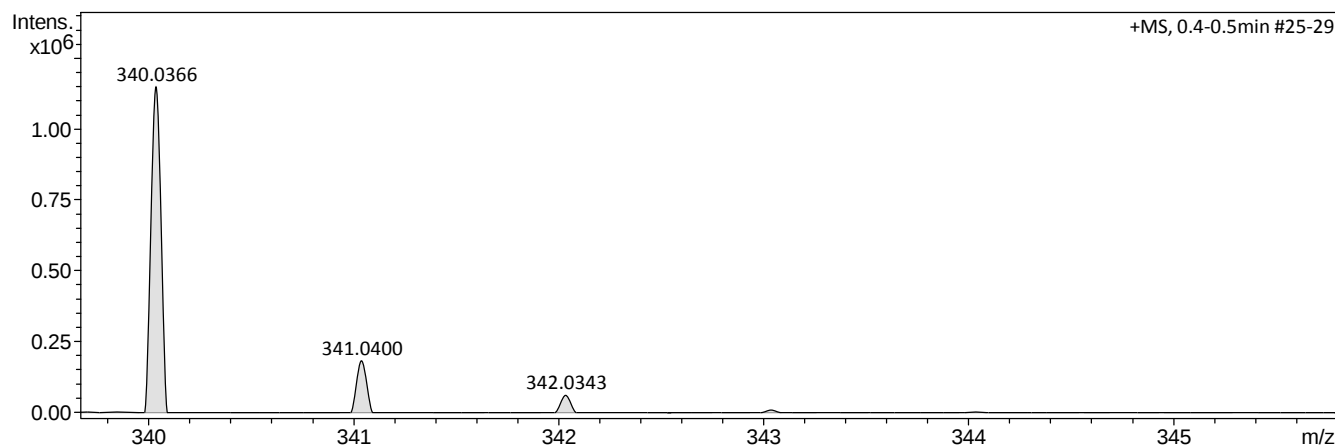
Analysis Name D:\Data\ggc\24-060546_P1-E-2_01_9304.d
 Method lc_qtof_directospos.m
 Sample Name 24-060546
 Comment MAC-III-60
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:24:04 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
340.0366	1	C14H9F3N3O2S	340.0362	-1.2	8.6	1	100.00	10.5	even	ok

Qualitative Compound Report

Analysis Info

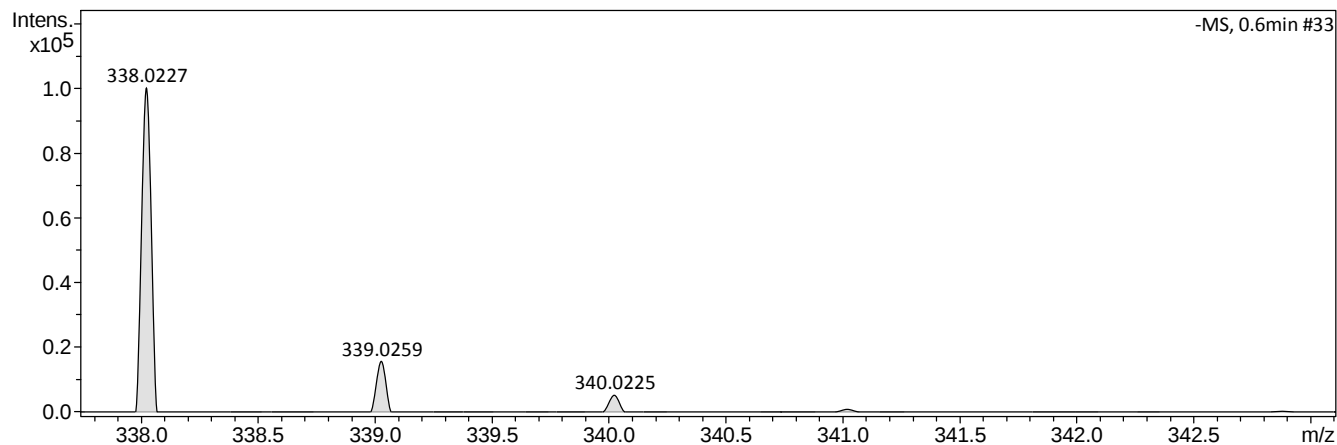
Analysis Name D:\Data\ggc\24-060546_P1-E-2_01_9316.d
 Method lc_qtof_directosneg.m
 Sample Name 24-060546
 Comment MAC-III-60
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:33:28 PM

Operator MV
 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
338.0227	1	C14H7F3N3O2S	338.0217	-3.0	10.1	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

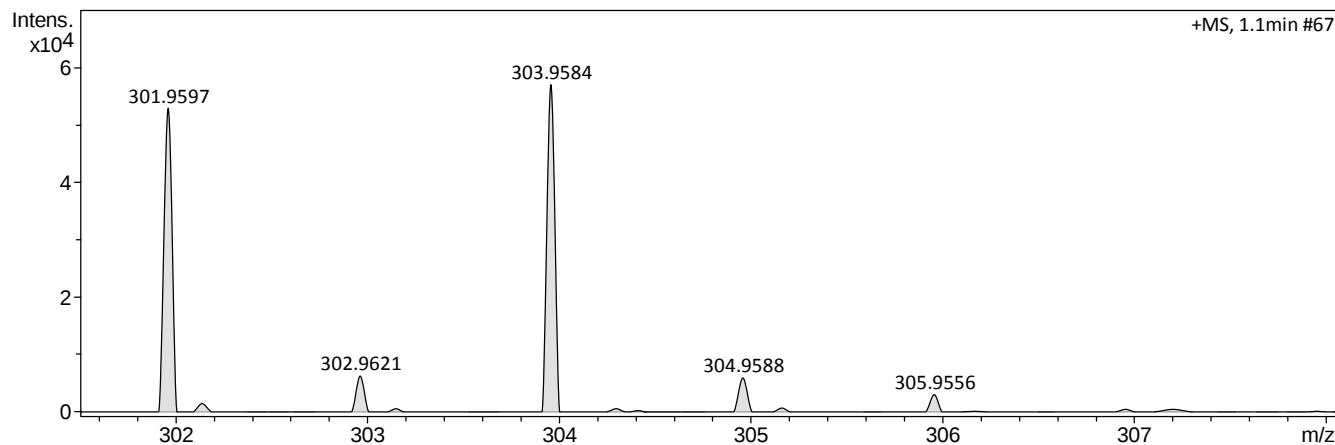
Analysis Name D:\Data\ggc\24-060547_P1-E-3_01_9305.d
 Method lc_qtof_directospos.m
 Sample Name 24-060547
 Comment EJG-II-17 f7-12
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 11:29:11 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
301.9597	1	C9H9BrN3O2S	301.9593	-1.3	21.1	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

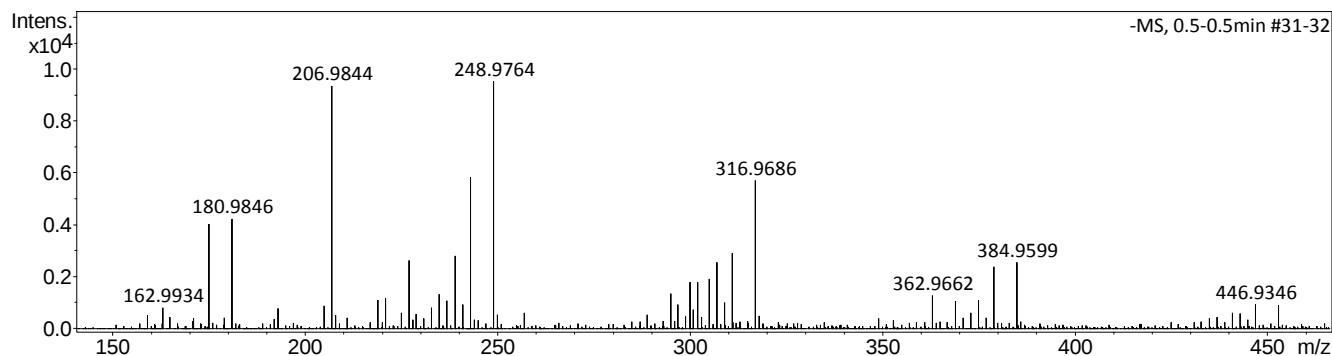
Analysis Name D:\Data\ggc\24-060547_P1-E-3_01_9317.d
 Method lc_qtof_directosneg.m
 Sample Name 24-060547
 Comment EJG-II-17 f7-12
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 6/13/2024 12:38:33 PM

Operator MV
 Instrument / Ser# 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



#	m/z	I	I %
1	174.9664	4012	42.2
2	180.9846	4211	44.3
3	205.0058	870	9.2
4	206.9844	9318	98.1
5	218.9271	1112	11.7
6	220.9227	1165	12.3
7	226.9803	2634	27.7
8	232.9298	816	8.6
9	234.9217	1315	13.8
10	236.9170	1068	11.2
11	238.9484	2796	29.4
12	240.9438	922	9.7
13	242.9608	5826	61.3
14	248.9764	9502	100.0
15	294.9686	1337	14.1
16	296.9099	921	9.7
17	299.9626	1785	18.8
18	301.9609	1783	18.8
19	304.9310	1922	20.2
20	306.9378	2550	26.8
21	308.9332	991	10.4
22	310.9489	2893	30.4
23	316.9686	5700	60.0
24	362.9662	1271	13.4
25	368.9120	1042	11.0
26	374.9319	1103	11.6
27	378.9412	2380	25.1
28	384.9599	2560	26.9
29	446.9346	927	9.8
30	452.9491	900	9.5