

Qualitative Compound Report

Analysis Info

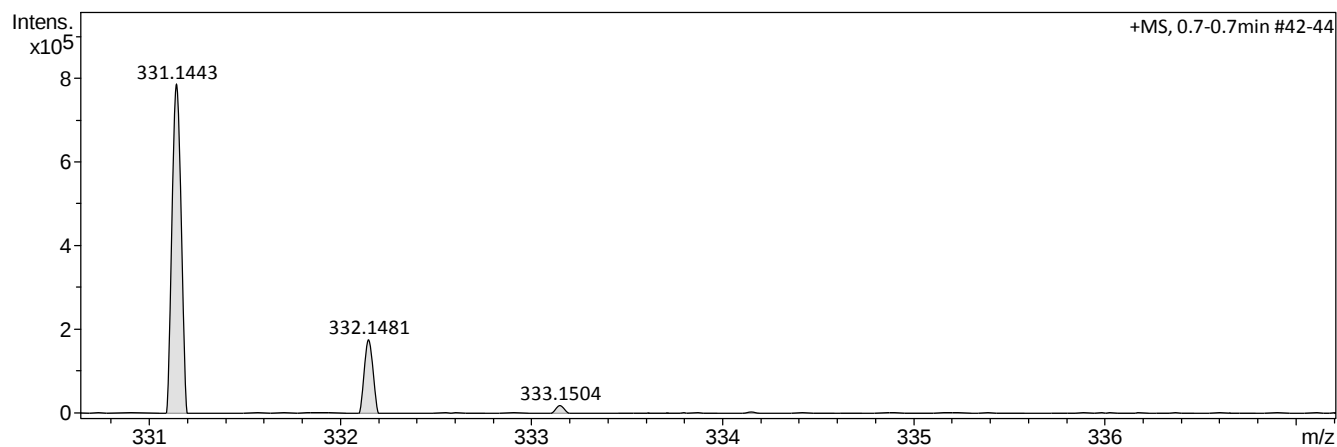
Analysis Name D:\Data\ggc\24-092001_P1-B-1_01_9450.d
Method lc_ms directos tunelow300924.m
Sample Name 24-092001
Comment BCD57
Sv: DCM + MeOH + HCOOH
Eugenia Buden

Acquisition Date 10/1/2024 3:11:33 PM

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
331.1443	1	C21H19N2O2	331.1441	-0.6	9.4	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

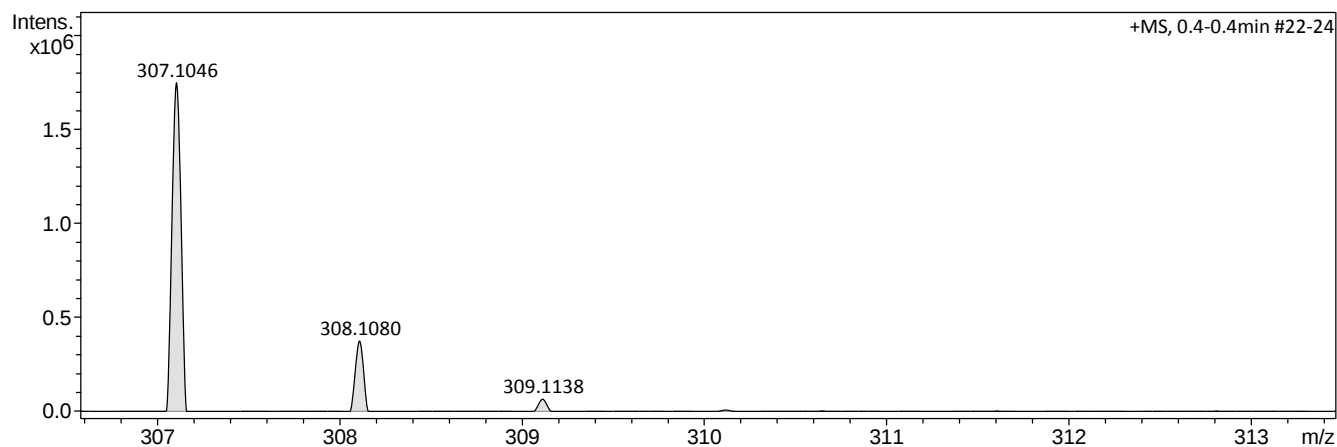
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 Method lc_ms directos tunelow300924.m
 Sample Name 24-092002
 Comment BCD63
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 10/1/2024 3:16:43 PM

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
307.1046	1	C19H13F2N2	307.1041	-1.6	9.5	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

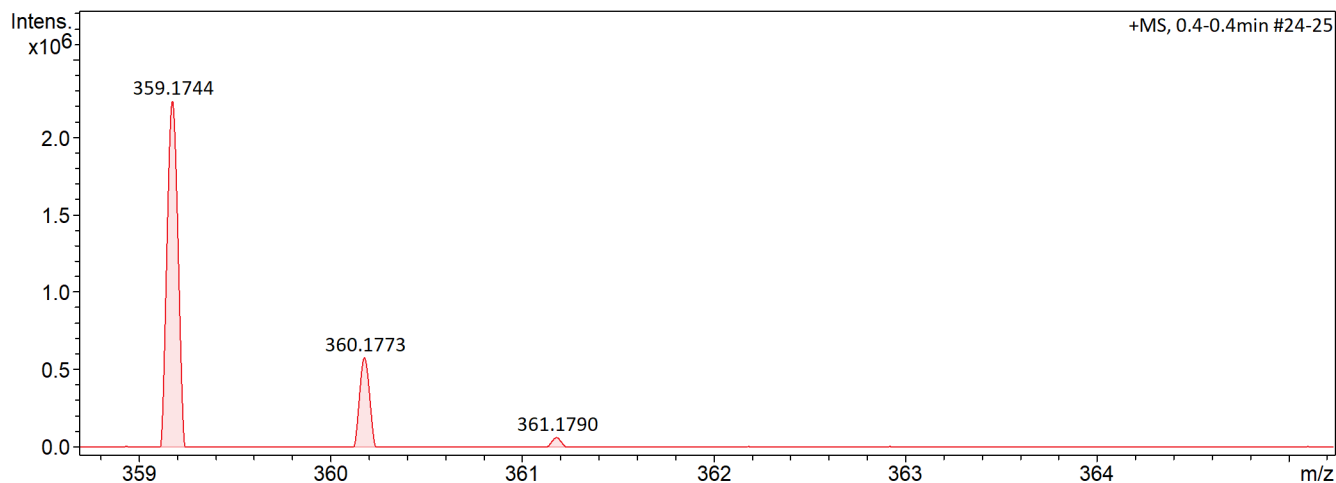
Analysis Name C:\Data\24-092003_P1-B-3_01_9452.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092003
 Comment BCD79
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:21:51

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
359.1744	1	C23H23N2O2	359.1754	2.8	5.2	1	100.00	13.5	even	ok

Qualitative Compound Report

Analysis Info

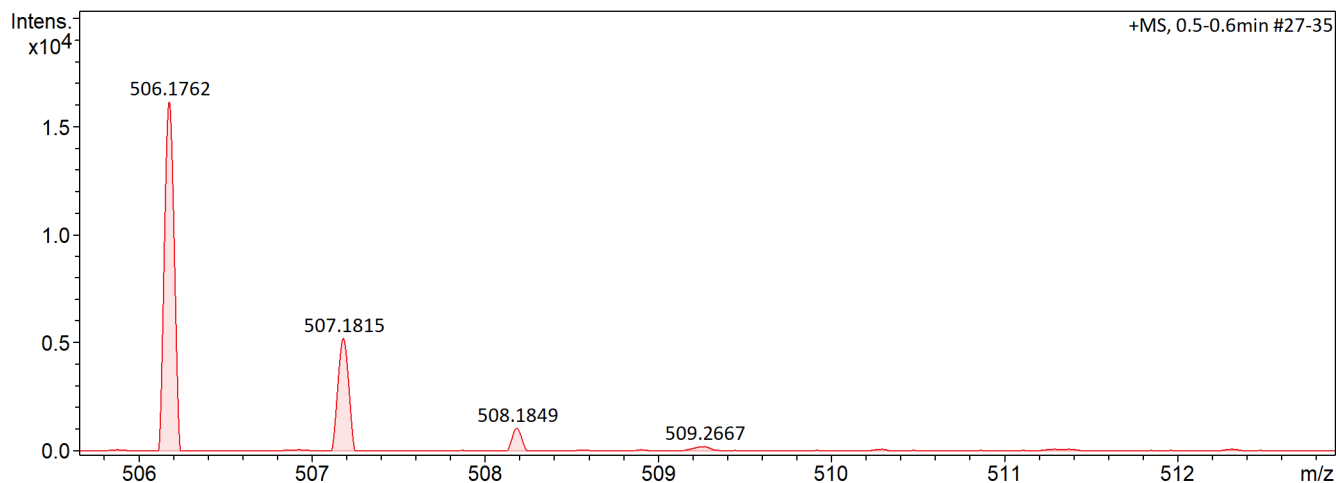
Analysis Name C:\Data\24-092004_P1-B-4_01_9453.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092004
 Comment AE1
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:26:59

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
506.1762	1	C33H21FN5	506.1776	2.6	27.7	1	100.00	25.5	even	ok

Qualitative Compound Report

Analysis Info

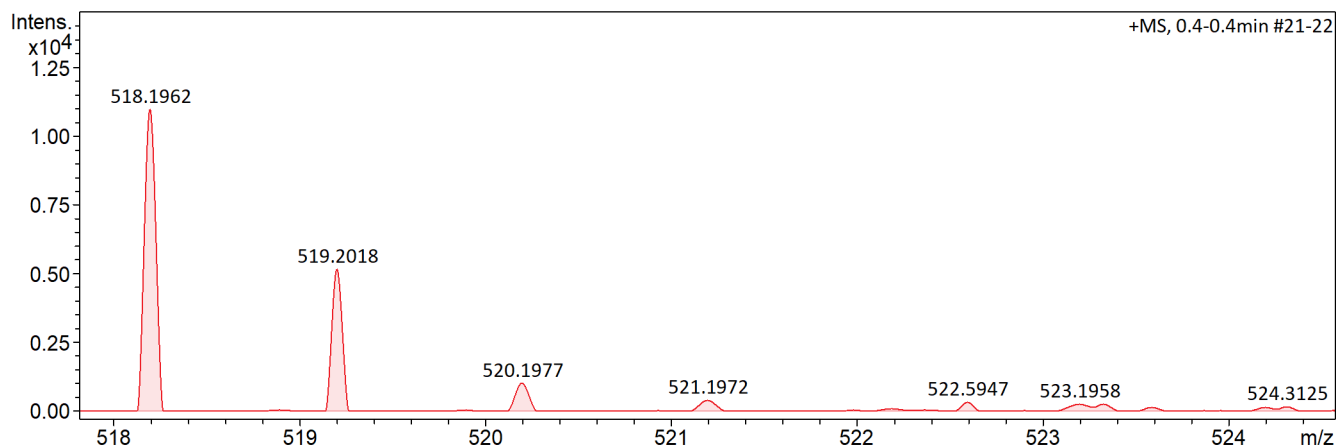
Analysis Name C:\Data\24-092005_P1-B-5_01_9454.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092005
 Comment AE6
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:32:08

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
518.1962	1	C34H24N5O	518.1975	2.7	43.7	1	100.00	25.5	even	ok

Mass Spectrum List Report

Analysis Info

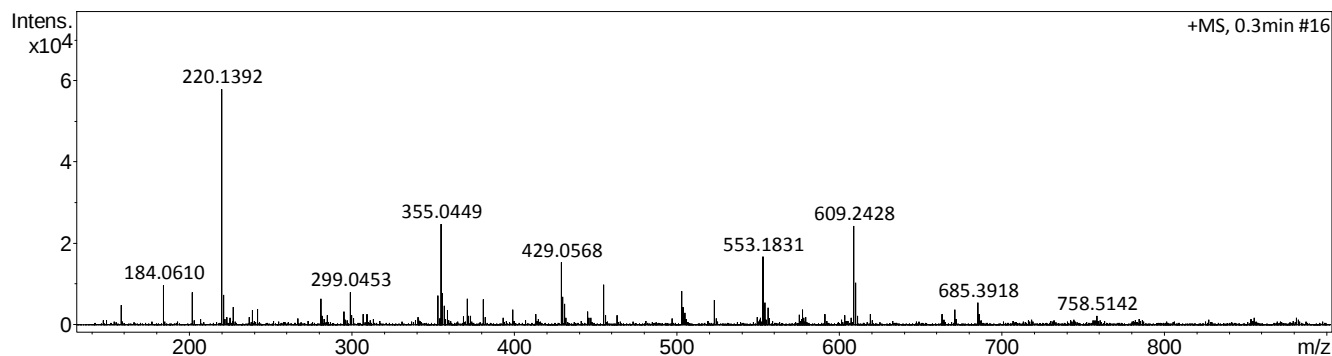
Analysis Name D:\Data\ggc\24-092006_P1-B-6_01_9481.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092006
 Comment AE17
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 10/2/2024 10:08:31 AM

Operator EB - MV
 Instrument / Ser# 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



#	m/z	I	I %
1	158.1064	4804	8.3
2	184.0610	9674	16.7
3	202.1307	7872	13.6
4	220.1392	57841	100.0
5	221.0729	5564	9.6
6	221.1389	7242	12.5
7	227.1860	4366	7.5
8	242.1192	3832	6.6
9	281.0298	6302	10.9
10	299.0453	8009	13.8
11	353.2399	7164	12.4
12	355.0449	24765	42.8
13	356.0461	7826	13.5
14	357.0428	4571	7.9
15	371.0766	6301	10.9
16	381.2680	6242	10.8
17	429.0568	15263	26.4
18	430.0593	6887	11.9
19	431.0571	5172	8.9
20	455.1568	9784	16.9
21	503.0712	8238	14.2
22	504.0753	4365	7.5
23	523.2855	6121	10.6
24	553.1831	16783	29.0
25	554.1856	5402	9.3
26	556.1360	4116	7.1
27	609.2428	24207	41.9
28	610.2485	10218	17.7
29	671.2356	3755	6.5
30	685.3918	5428	9.4

Qualitative Compound Report

Analysis Info

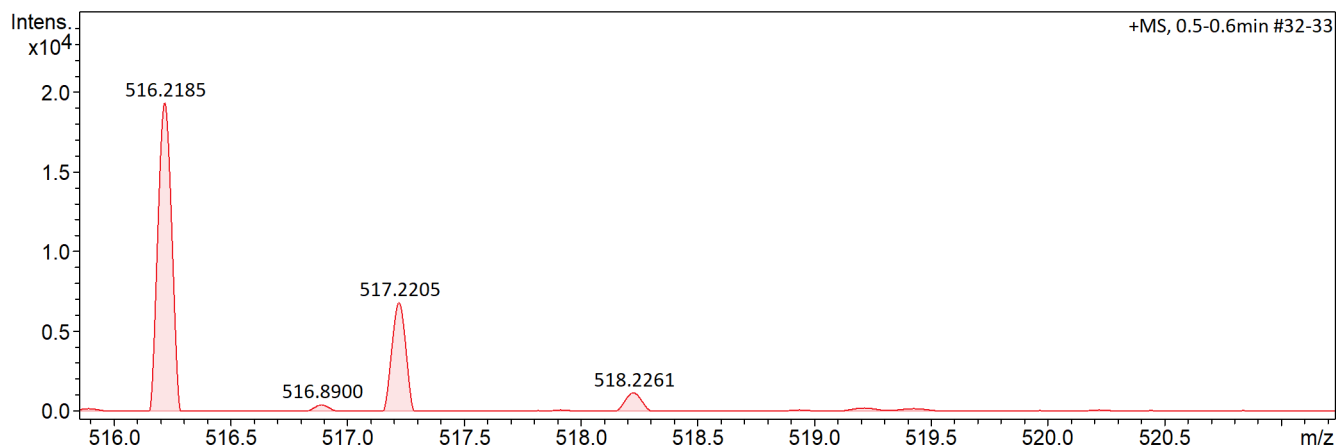
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 Sample Name 24-092007
 Comment AE25
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:42:24

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
516.2185	1	C35H26N5	516.2183	-0.5	25.4	1	100.00	25.5	even	ok

Mass Spectrum List Report

Analysis Info

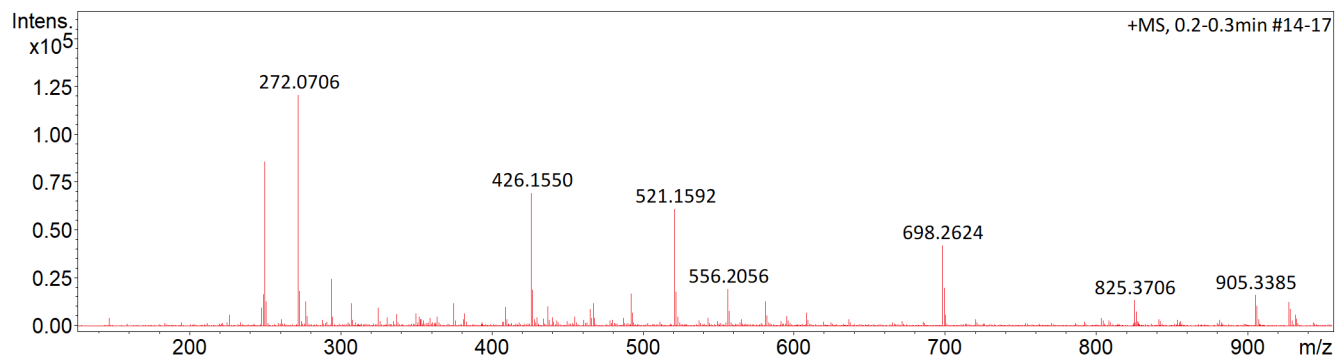
Analysis Name C:\Data\24-092008_P1-B-8_01_9457.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092008
 Comment AE23
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:47:31

Operator EB - MV
 Instrument / Ser# 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



#	m/z	I	I %
1	248.0610	9382	7.8
2	249.1035	16206	13.5
3	250.0878	85608	71.3
4	251.0896	12746	10.6
5	272.0706	120059	100.0
6	273.0736	18440	15.4
7	277.1338	12664	10.5
8	294.0498	24723	20.6
9	307.0920	11492	9.6
10	325.1331	9478	7.9
11	375.1106	11601	9.7
12	409.1516	9639	8.0
13	426.1550	69082	57.5
14	427.1595	18960	15.8
15	437.1829	9841	8.2
16	465.1692	8614	7.2
17	467.1850	11488	9.6
18	492.1797	16500	13.7
19	521.1592	60856	50.7
20	522.1629	17629	14.7
21	556.2056	19242	16.0
22	557.2069	7776	6.5
23	581.2012	12732	10.6
24	698.2624	41907	34.9
25	699.2635	19930	16.6
26	825.3706	13370	11.1
27	905.3385	15959	13.3
28	906.3419	10365	8.6
29	927.3281	12353	10.3
30	928.3316	8609	7.2

Qualitative Compound Report

Analysis Info

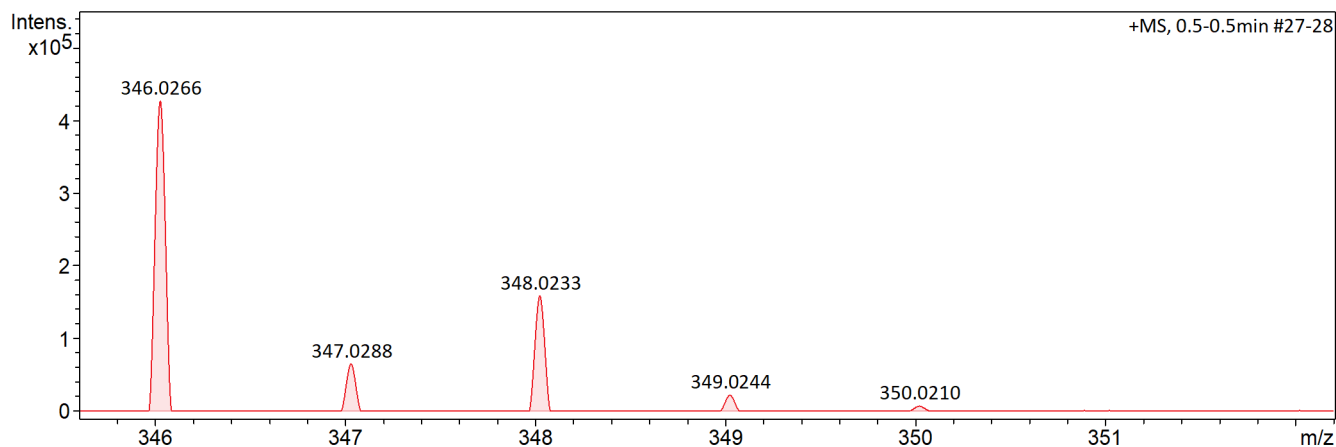
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 Method lc_ms directos tunelow300924.m
 Sample Name 24-092009
 Comment MAC-III-39'
 Sv: DCM + MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:52:39

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
346.0266	1	C15H14CINNaO3S	346.0275	2.8	14.7	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

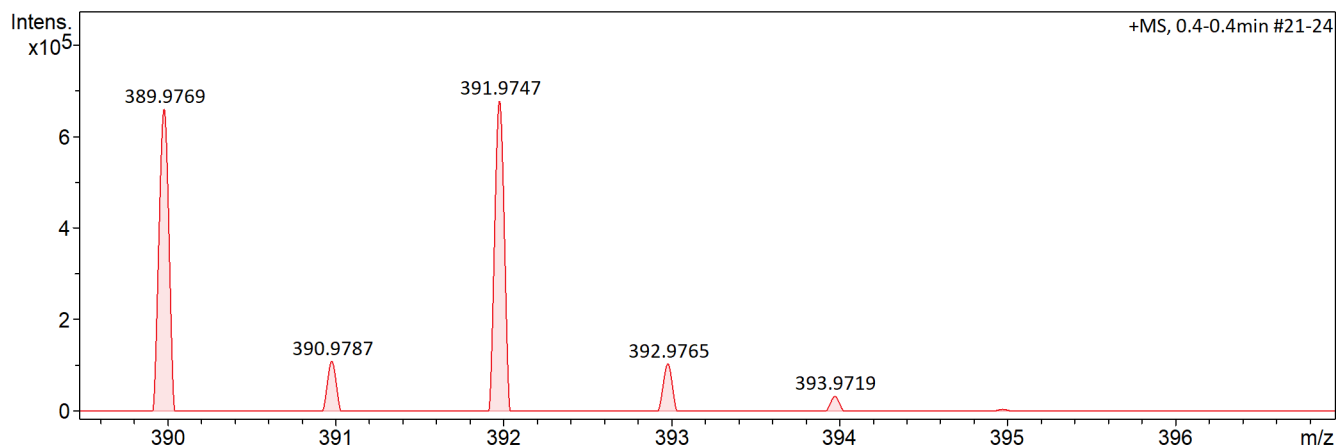
Analysis Name C:\Data\24-092010_P1-C-1_01_9459.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092010
 Comment MAC-IV-1'
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 15:57:50

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
391.9747	1	C15H14BrNNaO3S	389.9770	0.8	13.1	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

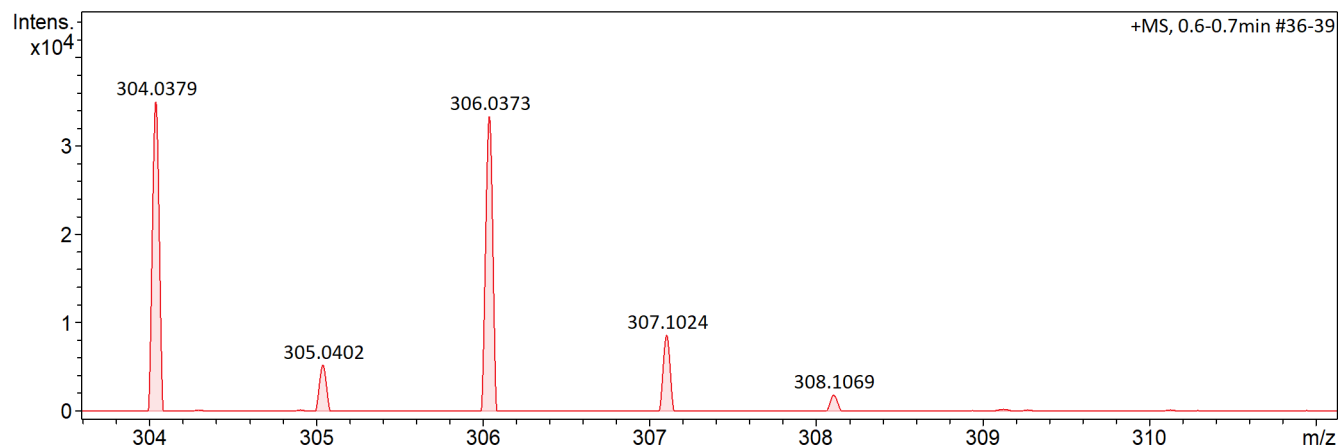
Analysis Name C:\Data\24-092011_P1-C-2_01_9460.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092011
 Comment MAC-IV-3-F3-8
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 16:02:58

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



Mass Spectrum List Report

Analysis Info

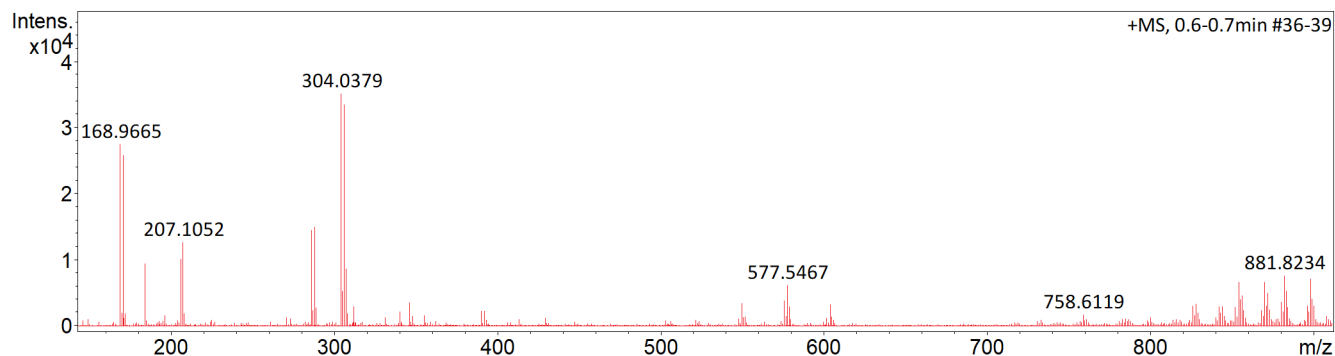
Analysis Name C:\Data\24-092011_P1-C-2_01_9460.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092011
 Comment MAC-IV-3-F3-8
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 16:02:58

Operator EB - MV
 Instrument / Ser# 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



#	m/z	I	I %
1	168.9665	27315	78.1
2	170.9646	25694	73.5
3	184.0738	9419	26.9
4	206.0977	10085	28.8
5	207.1052	12600	36.0
6	286.0268	14492	41.4
7	288.0244	14909	42.6
8	304.0379	34965	100.0
9	305.0402	5234	15.0
10	306.0373	33304	95.3
11	307.1024	8635	24.7
12	346.0349	3489	10.0
13	549.5061	3367	9.6
14	575.5277	3777	10.8
15	577.5467	6120	17.5
16	603.5601	3163	9.0
17	825.7488	3012	8.6
18	827.7654	3234	9.2
19	853.7867	6646	19.0
20	854.7846	3956	11.3
21	855.8027	4518	12.9
22	869.7762	6691	19.1
23	870.7809	3028	8.7
24	871.7830	4937	14.1
25	879.8186	3531	10.1
26	881.8234	7604	21.7
27	882.8363	5288	15.1
28	895.7888	3033	8.7
29	897.8033	7116	20.4
30	898.8059	4029	11.5

Qualitative Compound Report

Analysis Info

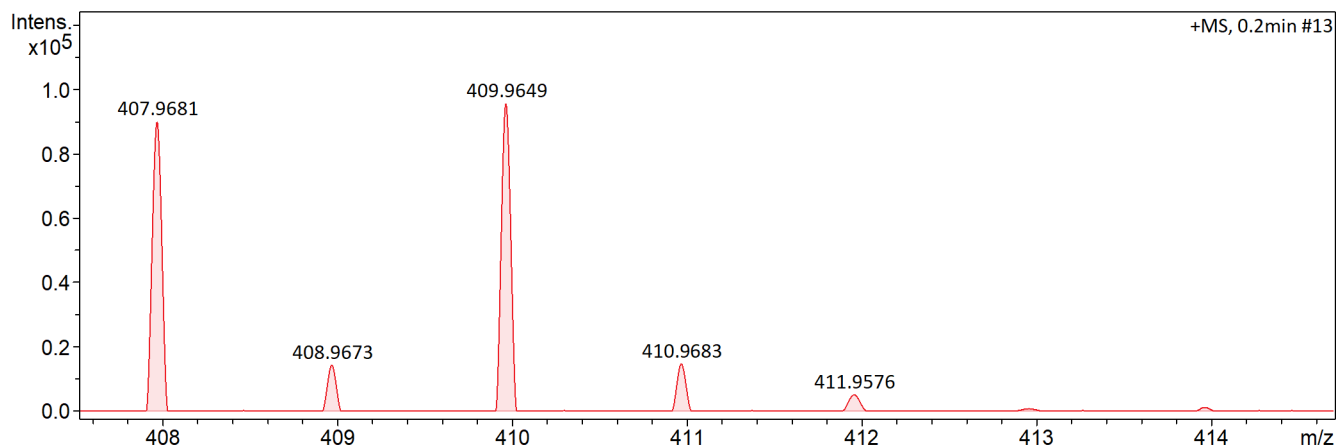
Analysis Name C:\Data\24-092012_P1-C-3_01_9461.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092012
 Comment MAC-IV-11'
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 16:08:07

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
409.9649	1	C15H13BrFNNaO3S	407.9676	1.8	16.3	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

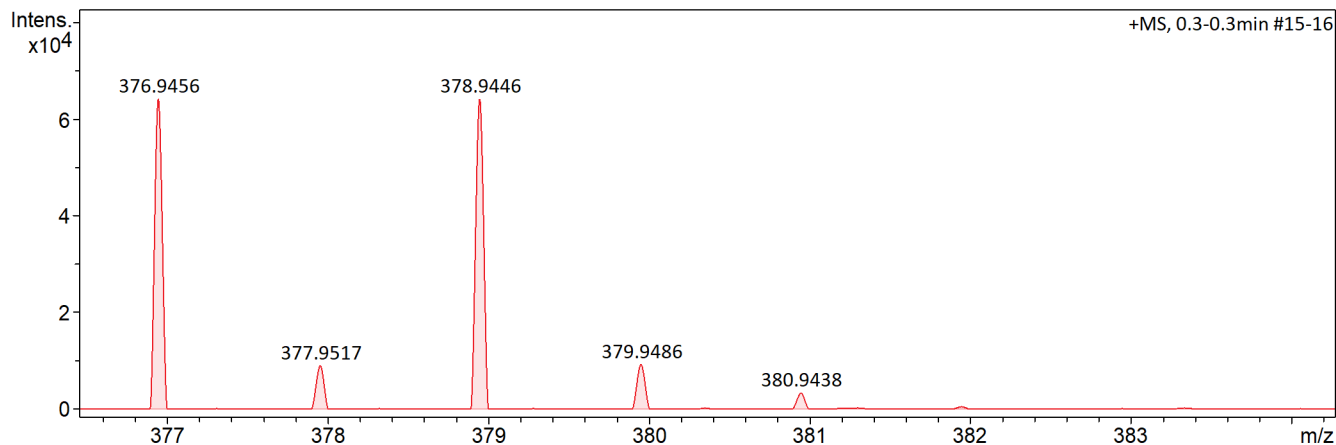
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 Sample Name 24-092013
 Comment MAC-IV-12
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 16:13:15

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
378.9446	1	C14H11BrNaO4S	376.9454	-3.3	19.9	1	100.00	8.5	even	ok

Mass Spectrum List Report

Analysis Info

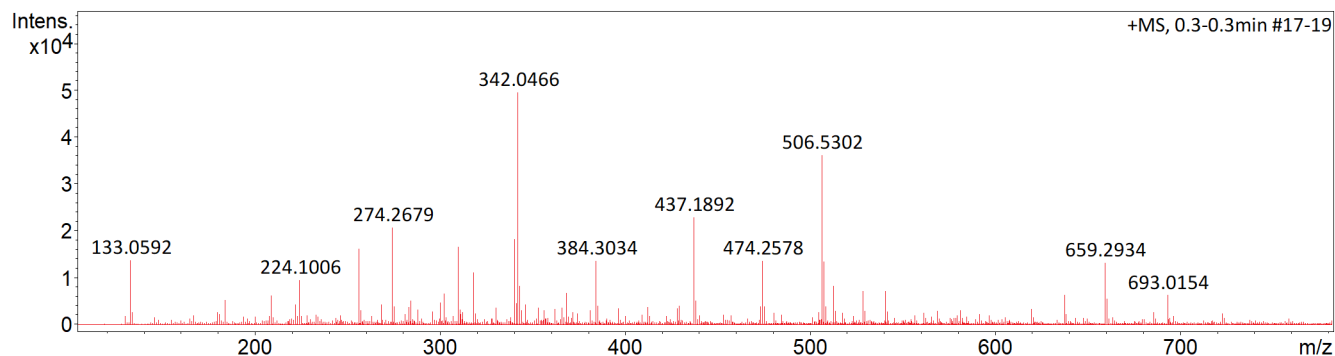
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 Method lc_ms directos tunelow300924.m
 Sample Name 24-092014
 Comment MAC-IV-26 t8
 Sv: MeOH + HCOOH
 Eugenia Buden

Acquisition Date 1/10/2024 16:18:21

Operator EB - MV
 Instrument / Ser# 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



#	m/z	I	I %
1	133.0592	13770	27.9
2	184.0682	5155	10.4
3	209.0773	6093	12.3
4	224.1006	9494	19.2
5	256.2571	16220	32.8
6	268.2914	4222	8.5
7	274.2679	20698	41.9
8	284.2861	5044	10.2
9	300.2837	4629	9.4
10	302.2964	6526	13.2
11	310.0464	16543	33.5
12	318.2927	11095	22.5
13	340.2772	18172	36.8
14	341.2759	4426	9.0
15	342.0466	49405	100.0
16	343.0504	8230	16.7
17	368.3080	6579	13.3
18	384.3034	13596	27.5
19	437.1892	22768	46.1
20	438.1900	5022	10.2
21	474.2578	13512	27.3
22	506.5302	36009	72.9
23	507.5308	13383	27.1
24	512.5044	8219	16.6
25	528.5094	7144	14.5
26	540.5350	7179	14.5
27	637.3149	6237	12.6
28	659.2934	13112	26.5
29	660.3000	5364	10.9
30	693.0154	6237	12.6