

Qualitative Compound Report

Analysis Info

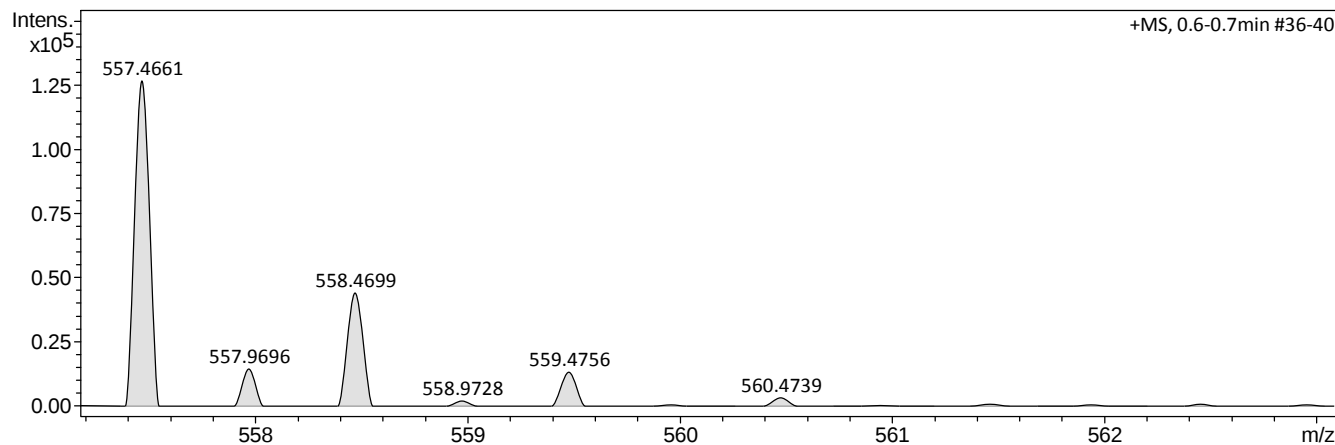
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 Method lc_qtof_directospos.m
 Sample Name 24-030404
 Comment Solano-R6-2
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 2:46:52 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
557.4661	1	C35H61N2O3	557.4677	2.9	26.8	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

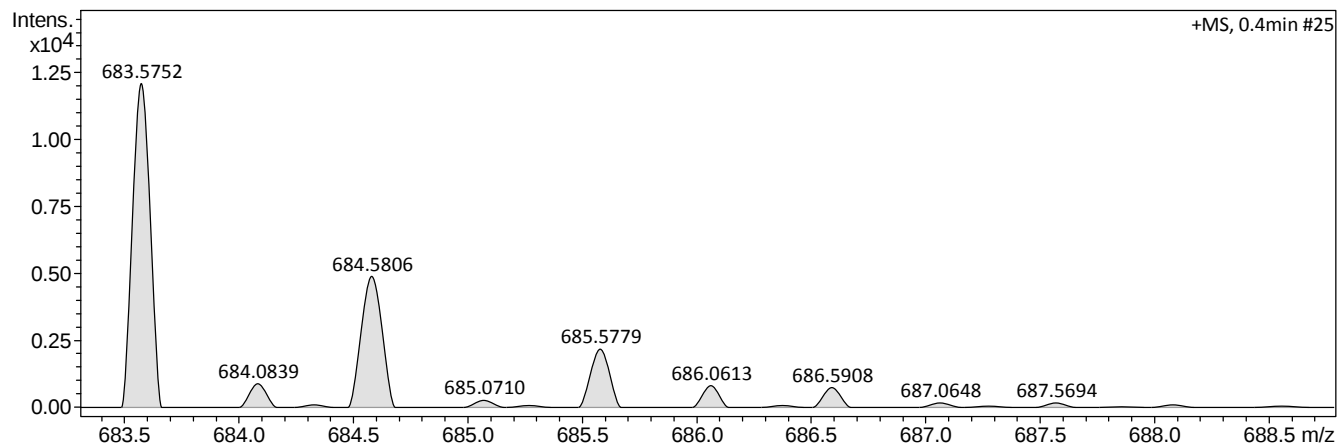
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 Method lc_qtof_directospos.m
 Sample Name 24-030405
 Comment Solano-AcOc-1
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 2:52:00 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
683.5752	1	C43H75N2O4	683.5721	-4.4	52.6	1	100.00	7.5	even	ok

Mass Spectrum List Report

Analysis Info

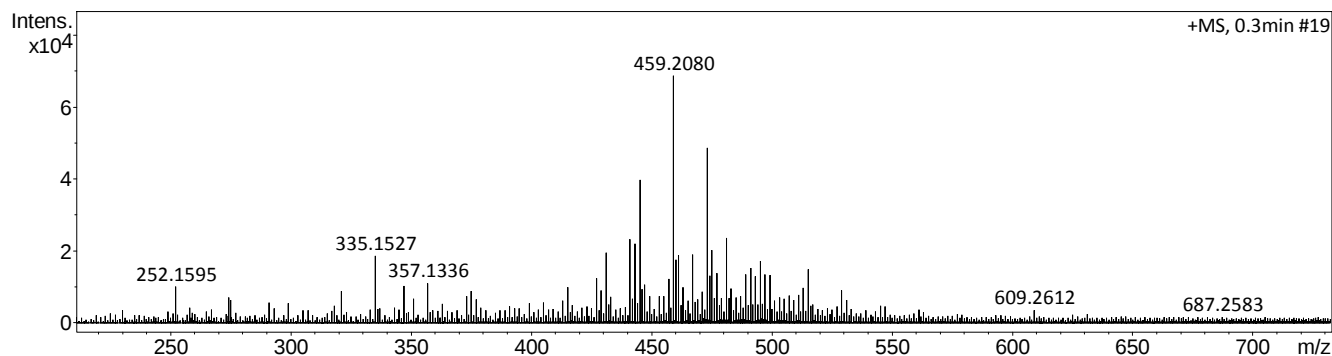
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 Method lc_qtof_directospos.m
 Sample Name 24-030406
 Comment RED CARB
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/25/2024 1:30:07 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	252.1595	10146	14.8
2	335.1527	18684	27.3
3	347.1509	10212	14.9
4	357.1336	10983	16.0
5	415.2083	9926	14.5
6	427.2008	12350	18.0
7	431.2057	19450	28.4
8	441.1942	23213	33.9
9	443.2072	21926	32.0
10	445.2227	39676	57.9
11	447.2132	10665	15.6
12	457.1979	12288	17.9
13	459.2080	68470	100.0
14	460.2107	17537	25.6
15	461.2159	18717	27.3
16	463.1953	9907	14.5
17	467.2066	19006	27.8
18	473.2201	48504	70.8
19	474.2227	13191	19.3
20	475.2100	20119	29.4
21	477.2161	13877	20.3
22	481.2027	23479	34.3
23	489.2126	13485	19.7
24	491.2205	15288	22.3
25	493.2176	12877	18.8
26	495.2068	17153	25.1
27	497.1995	13511	19.7
28	499.2124	13276	19.4
29	513.2084	9830	14.4
30	515.2140	14840	21.7

Mass Spectrum List Report

Analysis Info

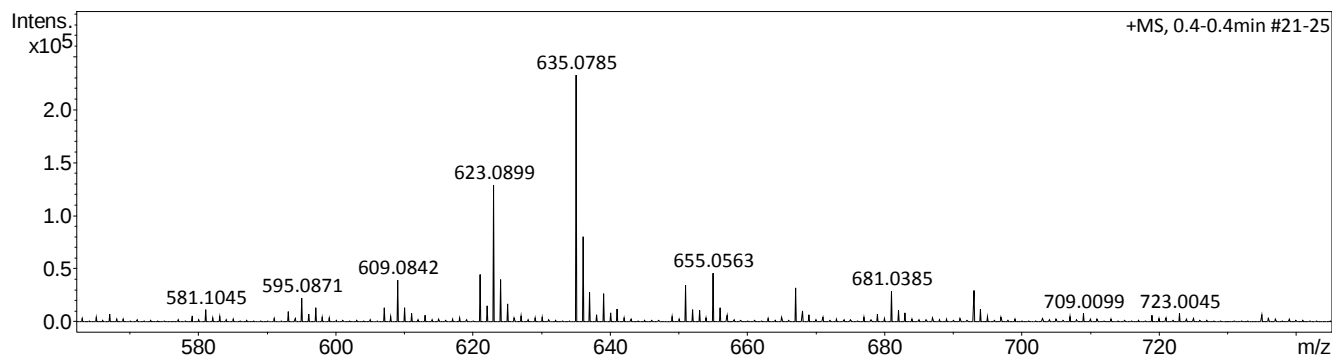
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 Sample Name 24-030407
 Comment ACETILADO
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:02:16 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	581.1045	11683	5.0
2	593.0964	9596	4.1
3	595.0871	22494	9.7
4	597.0942	13597	5.9
5	607.0740	13475	5.8
6	609.0842	39112	16.9
7	610.0853	13268	5.7
8	621.0773	44544	19.2
9	622.0794	14928	6.4
10	623.0899	128401	55.3
11	624.0930	39822	17.2
12	625.0820	17318	7.5
13	635.0785	231998	100.0
14	636.0799	79973	34.5
15	637.0703	28073	12.1
16	639.0666	26804	11.6
17	640.0687	8799	3.8
18	641.0622	12446	5.4
19	651.0571	34388	14.8
20	652.0570	11820	5.1
21	653.0453	11094	4.8
22	655.0563	45656	19.7
23	656.0580	13566	5.8
24	667.0393	31968	13.8
25	668.0401	10355	4.5
26	681.0385	29296	12.6
27	682.0385	11203	4.8
28	683.0245	8911	3.8
29	693.0243	29685	12.8
30	694.0286	11979	5.2

Mass Spectrum List Report

Analysis Info

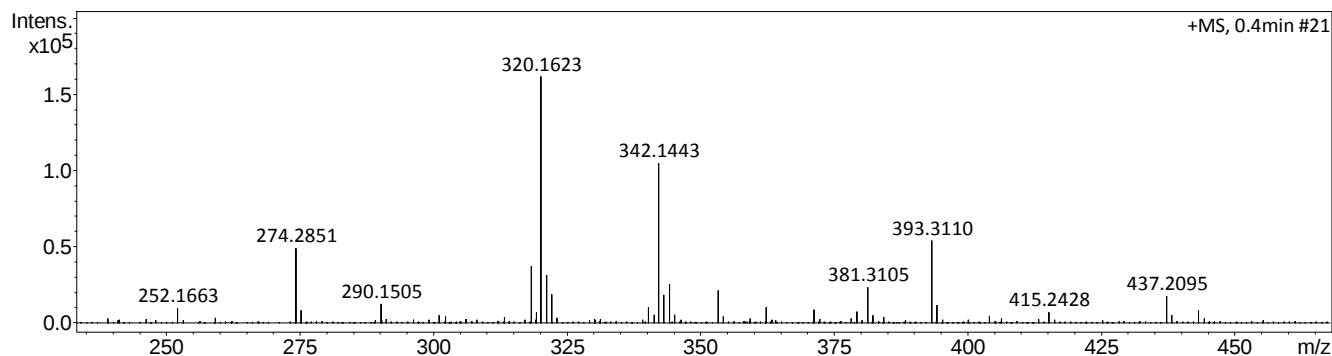
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 Method lc_qtof_directospos.m
 Sample Name 24-030408
 Comment LACTAMA
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/25/2024 1:35:18 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	252.1663	9458	5.9
2	274.2851	48878	30.3
3	275.2878	8203	5.1
4	290.1505	12675	7.9
5	301.1521	5043	3.1
6	318.3114	37361	23.2
7	319.3156	7181	4.5
8	320.1623	161343	100.0
9	321.1651	31399	19.5
10	322.1745	18722	11.6
11	340.2942	10636	6.6
12	341.3076	5529	3.4
13	342.1443	104562	64.8
14	343.1470	18485	11.5
15	344.1592	25514	15.8
16	345.1607	5281	3.3
17	353.2799	21454	13.3
18	362.3397	10290	6.4
19	371.3275	8974	5.6
20	379.2958	7480	4.6
21	381.3105	23609	14.6
22	382.3124	5225	3.2
23	393.3110	53938	33.4
24	394.3159	11595	7.2
25	404.1142	4598	2.8
26	415.2428	7006	4.3
27	437.2095	17488	10.8
28	438.2136	4914	3.0
29	443.2763	8313	5.2
30	763.6321	5196	3.2

Mass Spectrum List Report

Analysis Info

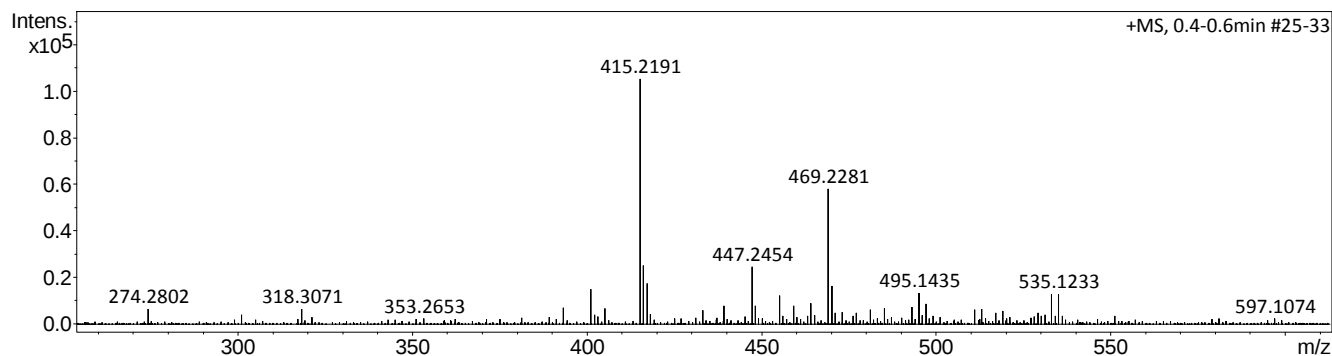
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 Method lc_qtof_directospos.m
 Sample Name 24-030409
 Comment BROMADO
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/25/2024 1:40:25 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	252.1616	6417	6.1
2	274.2802	6663	6.3
3	318.3071	6633	6.3
4	393.3008	6989	6.7
5	401.2027	14913	14.2
6	405.1963	6922	6.6
7	415.2191	104999	100.0
8	416.2218	25057	23.9
9	417.2332	17371	16.5
10	439.2131	7963	7.6
11	447.2454	24544	23.4
12	448.2467	7873	7.5
13	455.2135	12196	11.6
14	459.2430	7961	7.6
15	464.2714	8866	8.4
16	469.2281	58001	55.2
17	470.2304	16449	15.7
18	481.2272	6349	6.0
19	485.2244	6889	6.6
20	493.1320	7427	7.1
21	495.1435	13488	12.8
22	497.1455	8793	8.4
23	511.1418	6327	6.0
24	513.1463	6430	6.1
25	533.1259	12843	12.2
26	535.1233	12880	12.3
27	901.4504	11576	11.0
28	915.4671	31701	30.2
29	916.4707	15223	14.5
30	917.4651	6309	6.0

Mass Spectrum List Report

Analysis Info

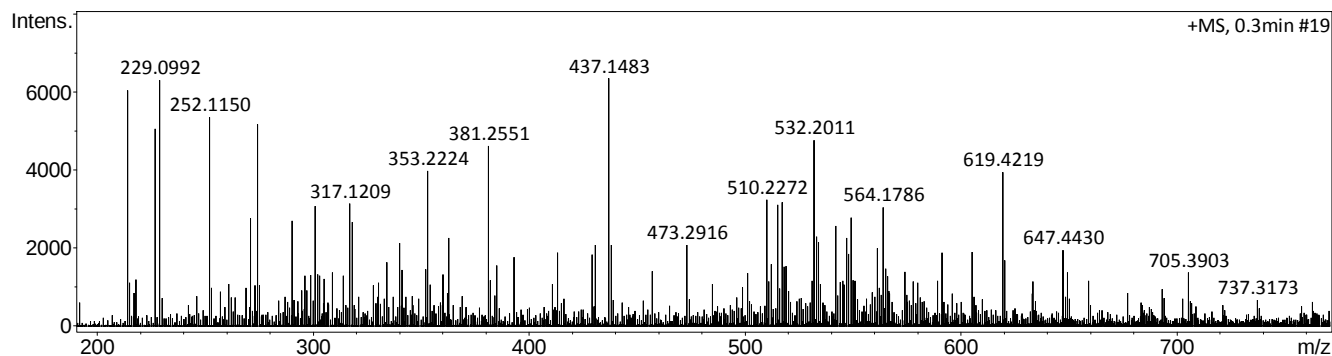
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 Method lc_qtof_directospos.m
 Sample Name 24-030410
 Comment 2F3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:17:42 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	214.0817	6027	95.2
2	226.9113	5054	79.8
3	229.0992	6288	99.3
4	252.1150	5339	84.3
5	271.0867	2758	43.5
6	274.2299	5164	81.5
7	290.2247	2704	42.7
8	301.0998	3079	48.6
9	317.1209	3130	49.4
10	318.2570	2664	42.1
11	340.2372	2124	33.5
12	353.2224	3968	62.7
13	362.8868	2254	35.6
14	381.2551	4599	72.6
15	430.8680	2077	32.8
16	437.1483	6333	100.0
17	438.1557	2071	32.7
18	473.2916	2071	32.7
19	510.2272	3231	51.0
20	515.1828	3105	49.0
21	517.1965	3173	50.1
22	517.3012	2498	39.4
23	532.2011	4749	75.0
24	533.1944	2295	36.2
25	534.2124	2149	33.9
26	542.2101	2568	40.5
27	547.1663	2251	35.5
28	549.1795	2773	43.8
29	564.1786	3035	47.9
30	619.4219	3931	62.1

Qualitative Compound Report

Analysis Info

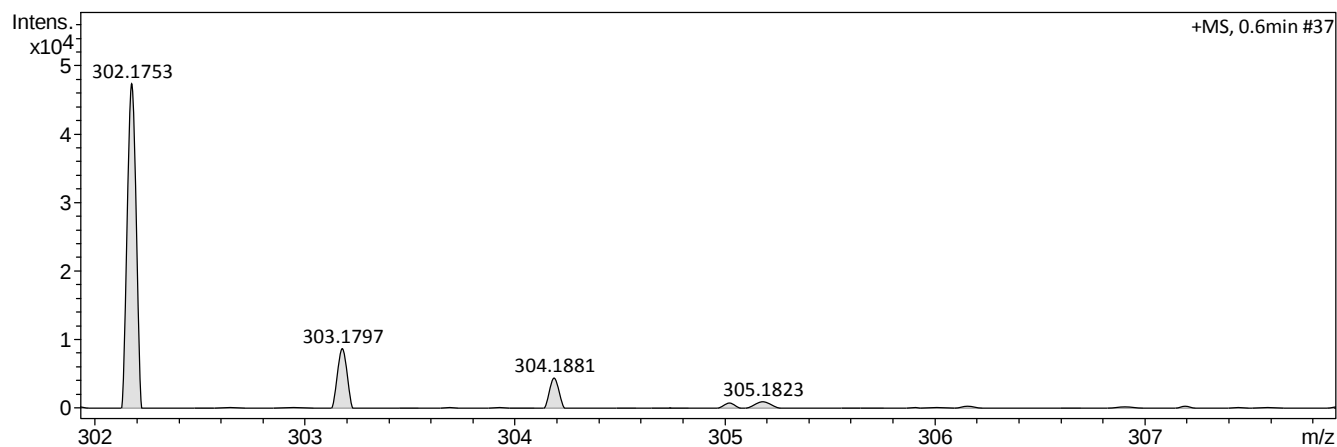
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 Method lc_qtof_directospos.m
 Sample Name 24-030411
 Comment 9F3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:22:49 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
302.1753	1	C18H24NO3	302.1751	-0.6	40.5	1	100.00	7.5	even	ok

Mass Spectrum List Report

Analysis Info

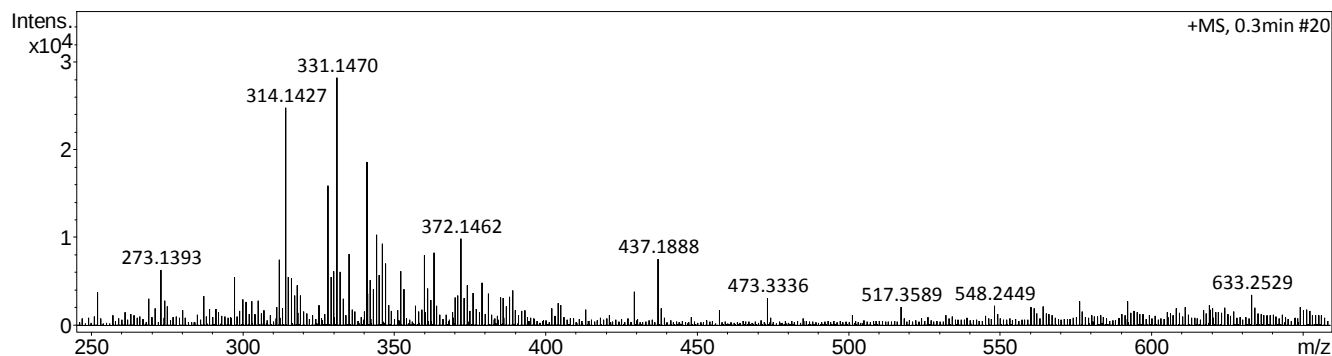
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 Method lc_qtof_directospos.m
 Sample Name 24-030412
 Comment 3F3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:27:57 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	273.1393	6303	22.4
2	297.2356	5476	19.4
3	312.1283	7443	26.4
4	314.1427	24759	87.9
5	315.1429	5512	19.6
6	316.0943	5332	18.9
7	318.1062	4508	16.0
8	328.1235	15858	56.3
9	329.1310	5463	19.4
10	330.1431	6132	21.8
11	331.1470	28176	100.0
12	332.1430	6082	21.6
13	335.1409	8078	28.7
14	341.1333	18569	65.9
15	342.1251	5135	18.2
16	343.1413	4124	14.6
17	344.1228	10256	36.4
18	345.1267	5701	20.2
19	346.1312	9289	33.0
20	347.1404	7023	24.9
21	352.1737	6112	21.7
22	353.2595	4136	14.7
23	360.1156	7974	28.3
24	361.1343	4210	14.9
25	363.1383	8227	29.2
26	372.1462	9838	34.9
27	374.1298	4511	16.0
28	379.1413	4827	17.1
29	389.1487	3964	14.1
30	437.1888	7514	26.7

Mass Spectrum List Report

Analysis Info

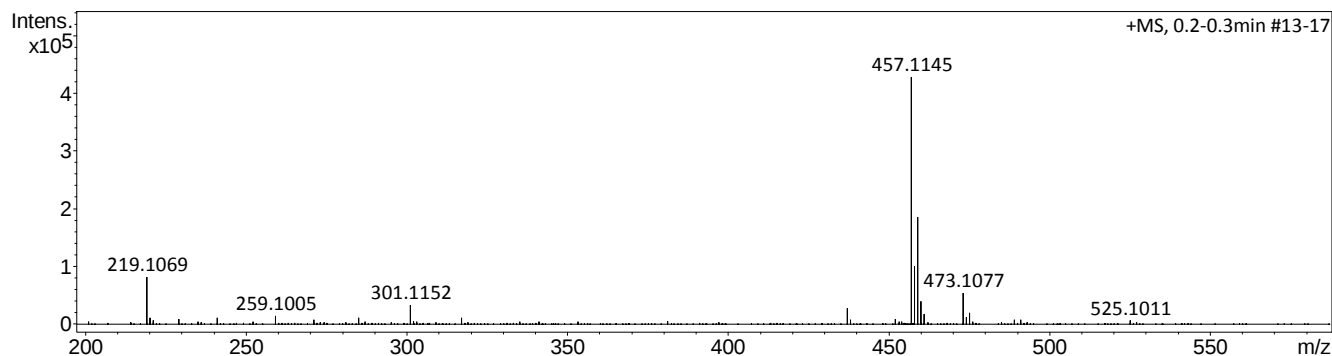
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 Method lc_qtof_directospos.m
 Sample Name 24-030413
 Comment 19F3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:33:06 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	219.1069	81841	19.2
2	220.1093	11077	2.6
3	221.1214	6762	1.6
4	229.0963	8681	2.0
5	241.0897	10799	2.5
6	259.1005	14681	3.4
7	271.1364	7188	1.7
8	285.1182	10879	2.5
9	301.1152	32633	7.6
10	317.1147	11353	2.7
11	437.2049	27945	6.5
12	438.2061	7710	1.8
13	452.1593	8894	2.1
14	457.1145	427236	100.0
15	458.1168	100618	23.6
16	459.1156	185673	43.5
17	460.1177	40049	9.4
18	461.1242	17423	4.1
19	473.1077	53845	12.6
20	474.1114	12280	2.9
21	475.1068	19512	4.6
22	489.1075	7520	1.8
23	491.0878	7643	1.8
24	891.2285	36689	8.6
25	892.2297	18794	4.4
26	893.2303	33828	7.9
27	894.2347	13752	3.2
28	895.2345	12047	2.8
29	907.2239	7629	1.8
30	909.2239	6290	1.5

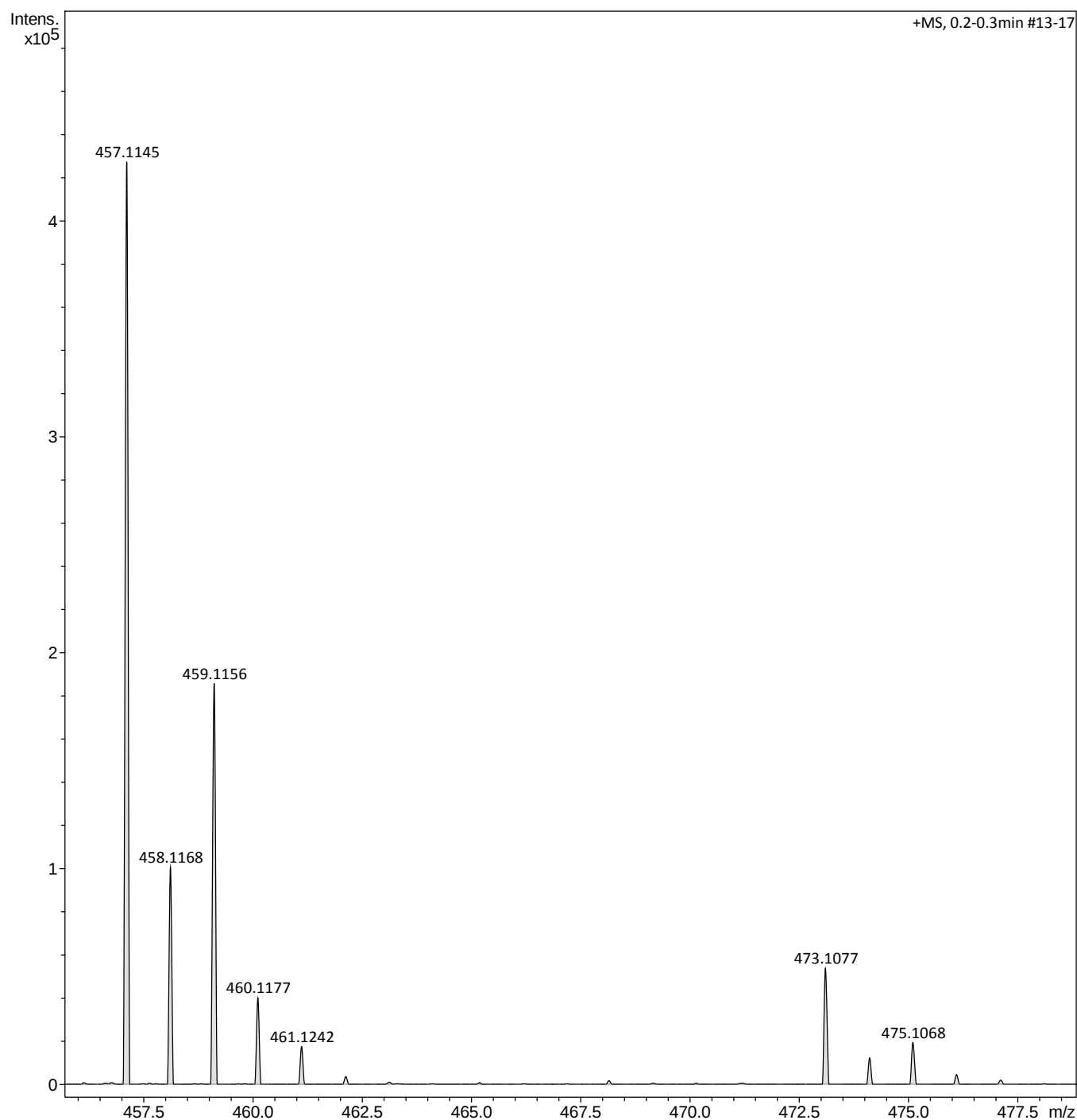
Generic Display Report

Analysis Info

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 Method lc_qtof_directospos.m
 Sample Name 24-030413
 Comment 19F3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:33:06 PM

Operator ELB
 Instrument micrOTOF-Q II



Qualitative Compound Report

Analysis Info

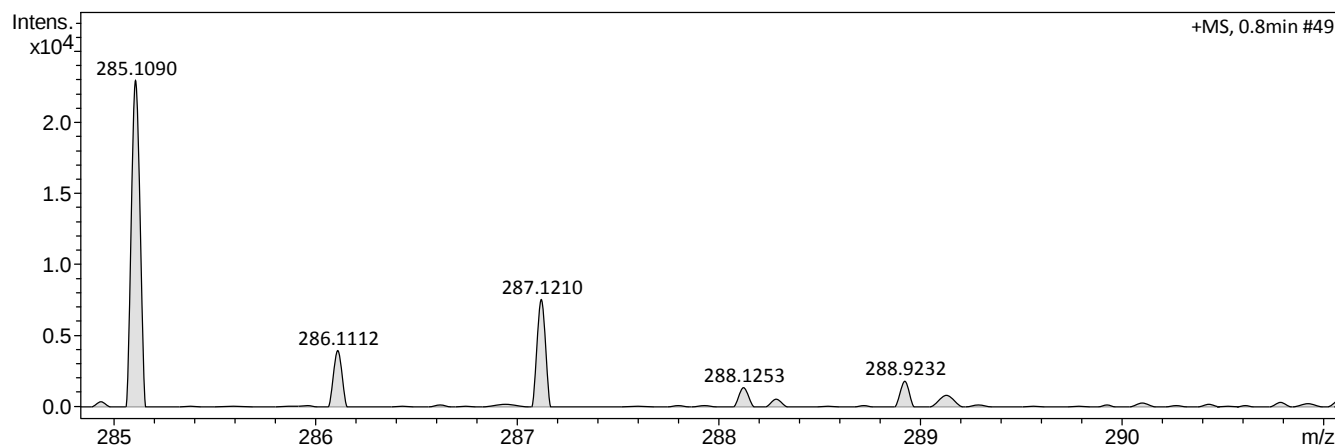
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 Comment 19F5
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:38:15 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
285.1090	1	C15H18NaO4	285.1097	2.7	177.1	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

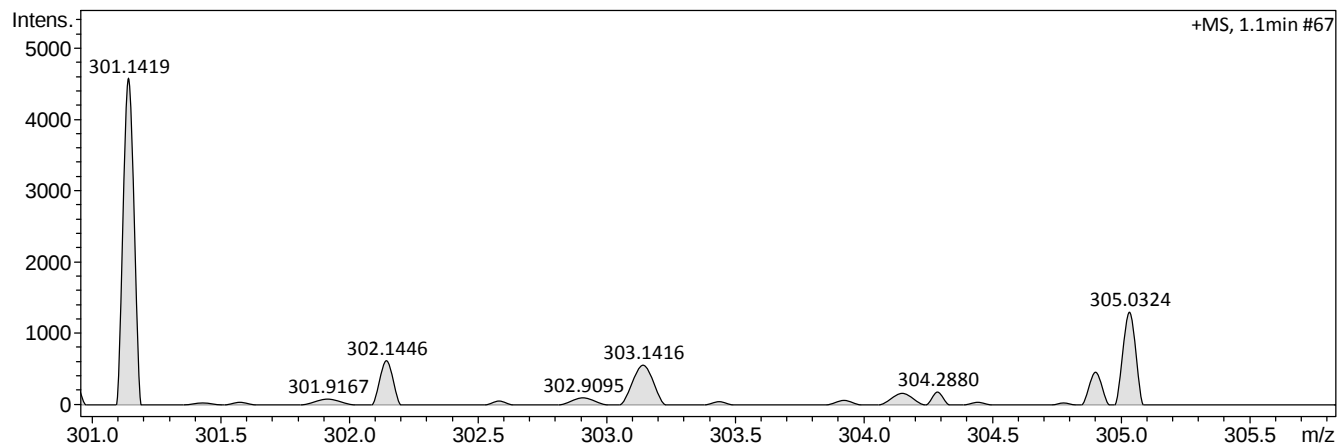
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 Sample Name 24-030415
 Comment 26X3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:43:23 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
301.1419	1	C16H22NaO4	301.1410	-2.8	61.4	1	100.00	5.5	even	ok

Mass Spectrum List Report

Analysis Info

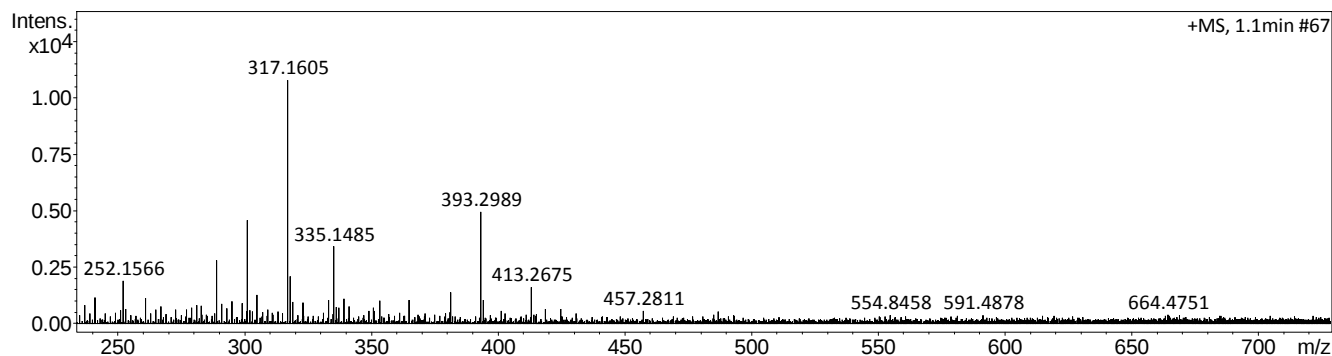
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 Sample Name 24-030415
 Comment 26X3
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:43:23 PM

Operator ELB
 Instrument / Ser# 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



#	m/z	I	I %
1	162.9703	2195	20.4
2	214.9182	1734	16.1
3	220.9355	1528	14.2
4	226.9532	2247	20.9
5	237.1143	827	7.7
6	240.9915	1157	10.7
7	252.1566	1889	17.5
8	261.1102	1128	10.5
9	281.1490	814	7.6
10	282.9085	791	7.3
11	288.9257	2791	25.9
12	291.1266	884	8.2
13	295.1619	983	9.1
14	299.1185	901	8.4
15	301.1419	4565	42.4
16	305.0324	1290	12.0
17	317.1605	10766	100.0
18	318.1618	2094	19.5
19	319.1535	967	9.0
20	323.1383	948	8.8
21	333.1328	1042	9.7
22	335.1485	3420	31.8
23	339.1496	1119	10.4
24	353.2657	1035	9.6
25	365.1188	1044	9.7
26	381.2978	1388	12.9
27	393.2989	4941	45.9
28	394.3041	1065	9.9
29	413.2675	1628	15.1
30	838.6557	959	8.9

Qualitative Compound Report

Analysis Info

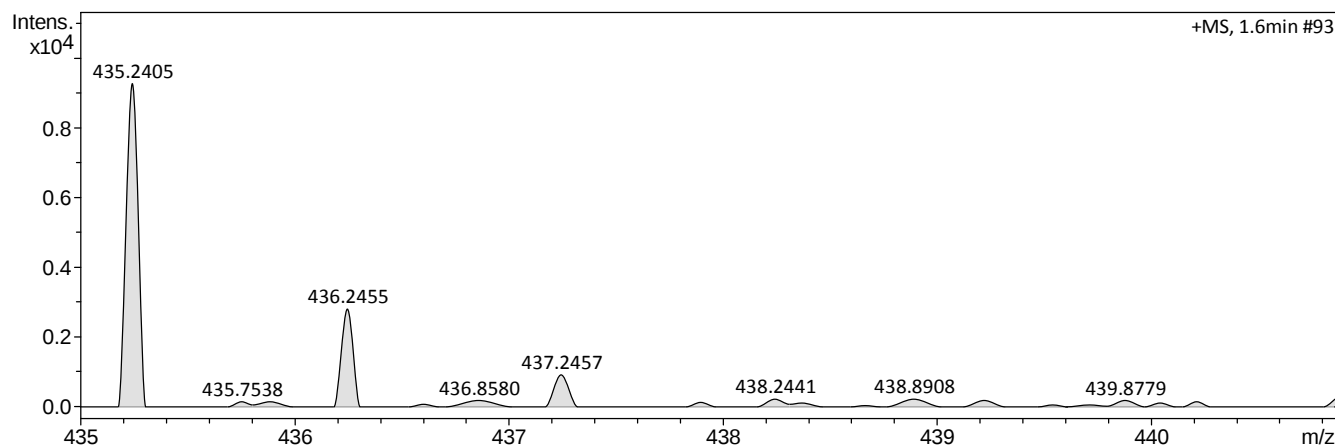
Analysis Name D:\Data\ggc\24-030416_P1-C-5_01_8725.d
 Method lc_qtof_directospos.m
 Sample Name 24-030416
 Comment 15F2
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:48:32 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
435.2405	1	C25H31N4O3	435.2391	-3.4	30.9	1	100.00	12.5	even	ok

Qualitative Compound Report

Analysis Info

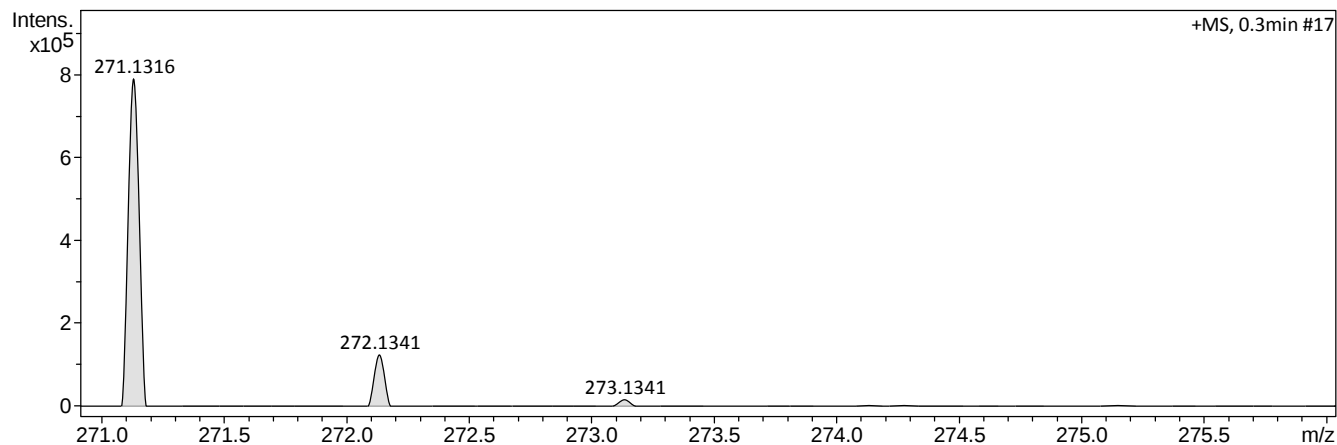
Analysis Name D:\Data\ggc\24-030417_P1-C-6_01_8726.d
 Method lc_qtof_directospos.m
 Sample Name 24-030417
 Comment Laurel1
 Sv: MeOH + HCOOH
 Manuela Garcia

Acquisition Date 3/18/2024 3:53:39 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
271.1316	1	C15H20NaO3	271.1305	-4.2	5.1	1	100.00	5.5	even	ok