

Qualitative Compound Report

Analysis Info

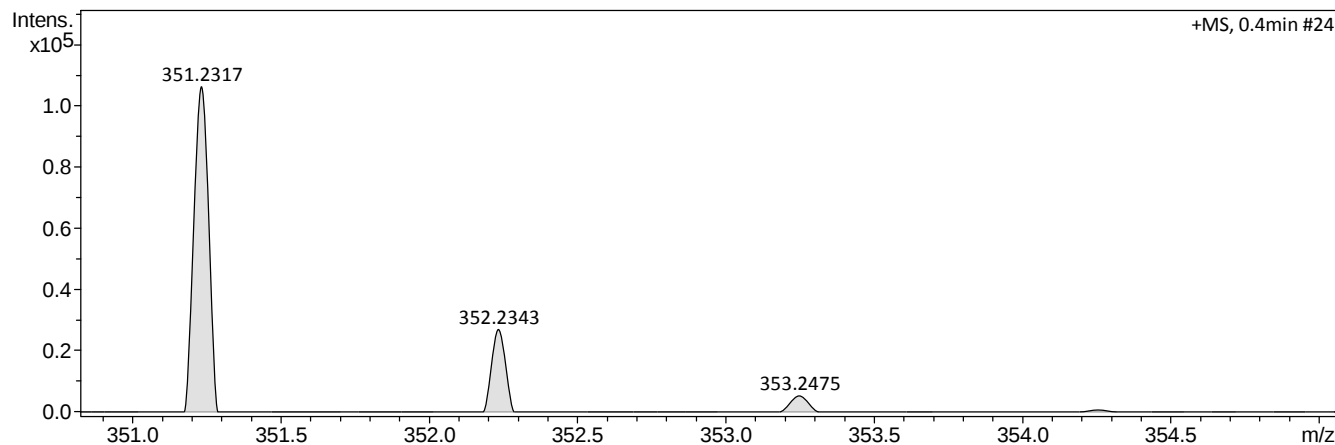
Analysis Name D:\Data\ggc\24-021401_P1-C-1_01_8634.d
 Method lc_qtof_directospos.m
 Sample Name 24-021401
 Comment LG108a
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 2:44:42 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
351.2317	1	C24H31O2	351.2319	0.3	8.7	1	100.00	9.5	even	ok

Mass Spectrum List Report

Analysis Info

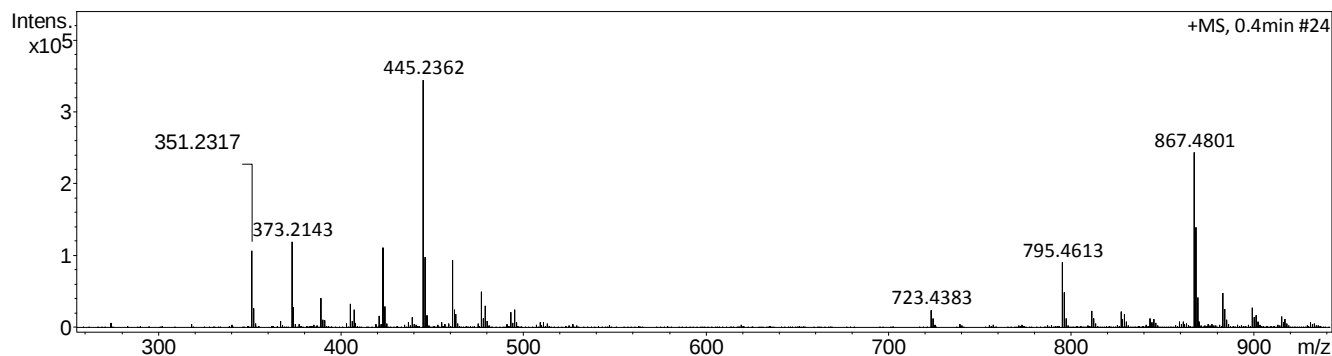
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 Method lc_qtof_directospos.m
 Sample Name 24-021401
 Comment LG108a
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 2:44:42 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	351.2317	106075	30.9
2	352.2343	26873	7.8
3	373.2143	119203	34.8
4	374.2188	28579	8.3
5	389.2081	41104	12.0
6	405.2033	32611	9.5
7	407.2192	24712	7.2
8	423.2480	110547	32.2
9	424.2507	29076	8.5
10	445.2362	342866	100.0
11	446.2391	97721	28.5
12	461.2293	93011	27.1
13	462.2328	25041	7.3
14	463.2160	18939	5.5
15	477.2259	49359	14.4
16	479.2367	30493	8.9
17	493.2189	21608	6.3
18	495.2348	25085	7.3
19	723.4383	24076	7.0
20	795.4613	90738	26.5
21	796.4622	48506	14.1
22	811.4502	23101	6.7
23	827.4502	22305	6.5
24	829.4582	18596	5.4
25	867.4801	243141	70.9
26	868.4834	139337	40.6
27	869.4821	41338	12.1
28	883.4713	47612	13.9
29	884.4726	25335	7.4
30	899.4663	27945	8.2

Qualitative Compound Report

Analysis Info

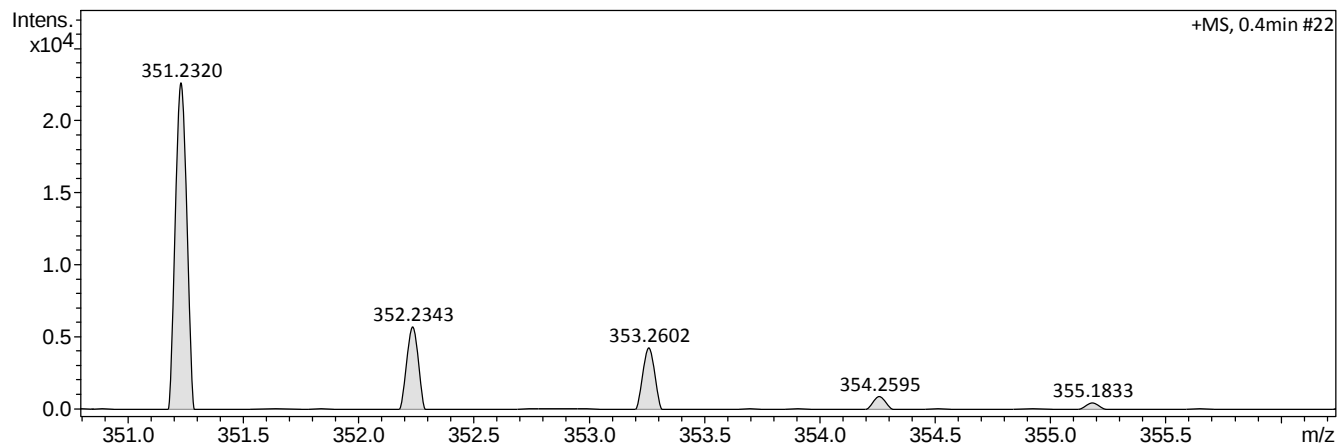
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 Method lc_qtof_directospos.m
 Sample Name 24-021402
 Comment LG108e
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 2:49:49 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
351.2320	1	C24H31O2	351.2319	-0.3	22.9	1	100.00	9.5	even	ok

Mass Spectrum List Report

Analysis Info

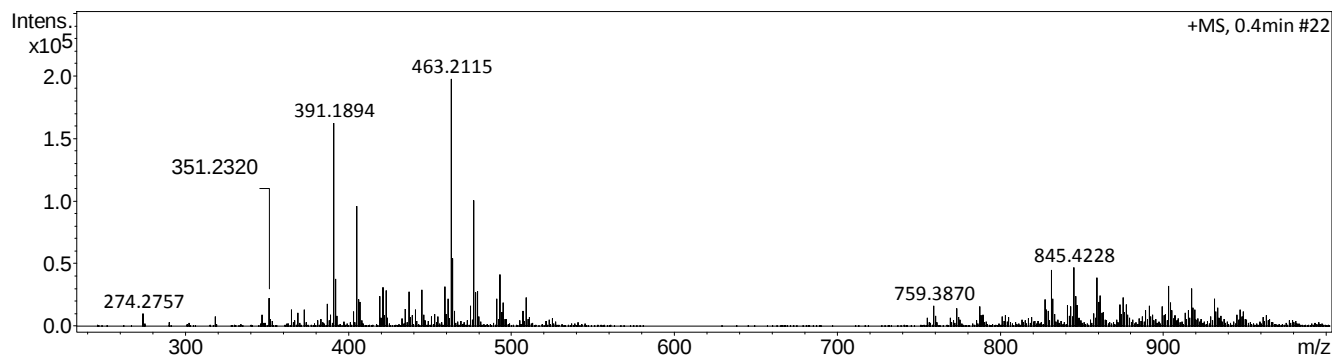
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 Method lc_qtof_directospos.m
 Sample Name 24-021402
 Comment LG108e
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 2:49:49 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	351.2320	22567	11.5
2	391.1894	161995	82.2
3	392.1937	37726	19.1
4	405.2031	95851	48.6
5	406.2058	21557	10.9
6	419.2000	23928	12.1
7	421.1999	31061	15.8
8	423.2254	28435	14.4
9	437.2111	27410	13.9
10	445.2334	29124	14.8
11	459.2157	31481	16.0
12	461.2282	21830	11.1
13	463.2115	197047	100.0
14	464.2142	54006	27.4
15	477.2260	100515	51.0
16	478.2284	26883	13.6
17	479.2127	28301	14.4
18	491.2128	22104	11.2
19	493.2189	41180	20.9
20	509.2174	23071	11.7
21	831.4068	45104	22.9
22	832.4115	22148	11.2
23	845.4228	46954	23.8
24	846.4258	24116	12.2
25	859.4310	38673	19.6
26	861.4211	24332	12.3
27	875.4200	23281	11.8
28	903.4234	32450	16.5
29	917.4414	30200	15.3
30	931.4476	22119	11.2

Qualitative Compound Report

Analysis Info

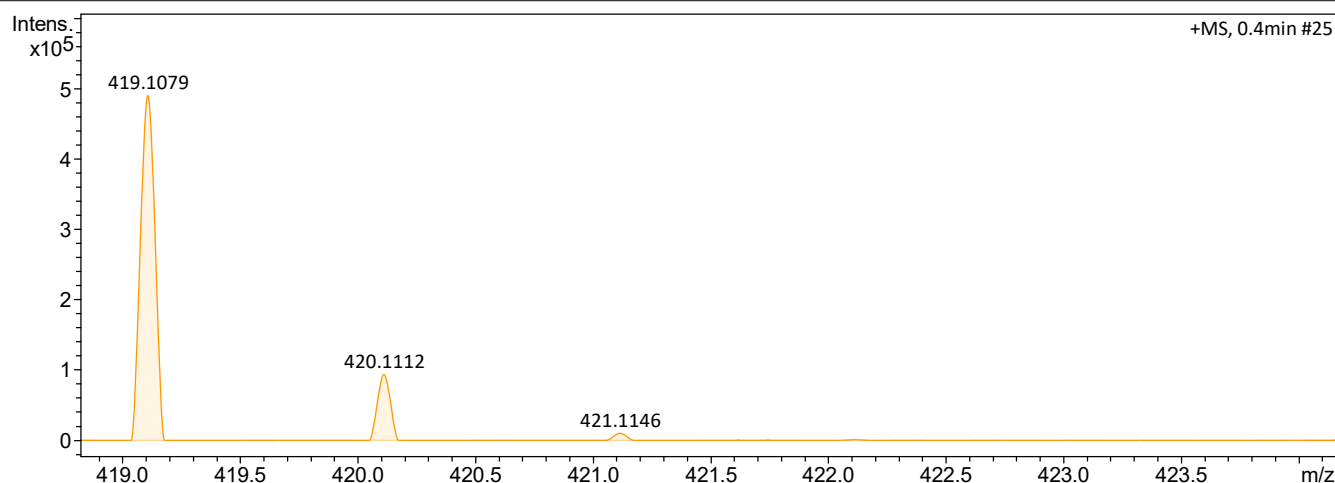
Analysis Name C:\Data\24-021403_P1-C-3_01_8636.d
 Method lc_qtof_directospos.m
 Sample Name 24-021403
 Comment LG067b2
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 14:54:56

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
419.1079	1	C18H28IO3	419.1078	-0.3	5.1	1	100.00	4.5	even	ok

Qualitative Compound Report

Analysis Info

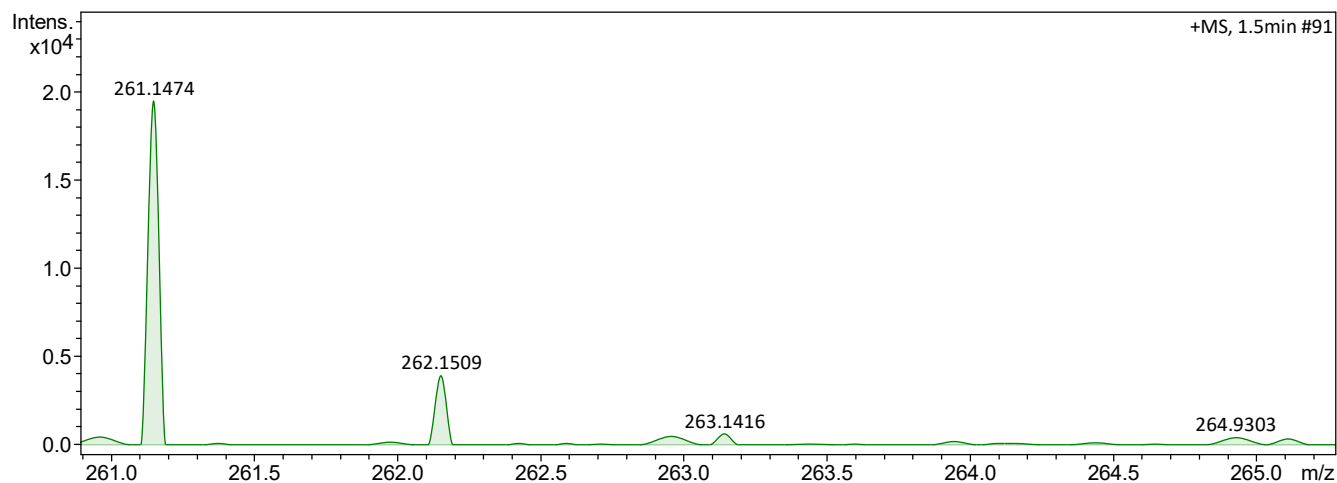
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 Method lc_qtof_directospos.m
 Sample Name 24-021404
 Comment TAC-014b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:00:03

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
261.1474	1	C16H21O3	261.1485	4.5	18.4	1	100.00	6.5	even	ok

Qualitative Compound Report

Analysis Info

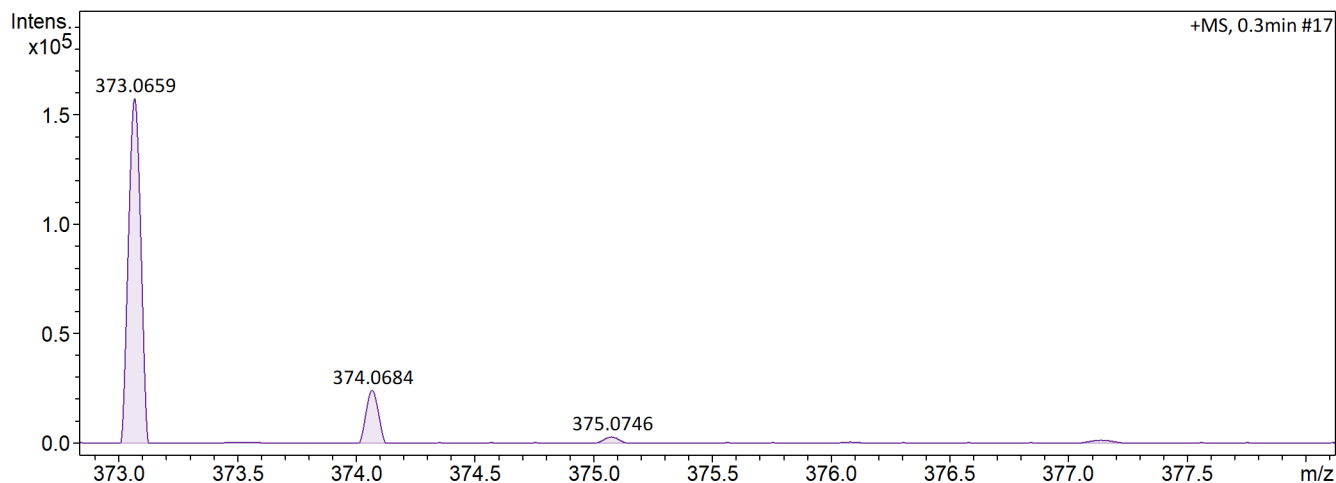
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 Method lc_qtof_directospos.m
 Sample Name 24-021405
 Comment LG035a
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:05:10

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
373.0659	1	C16H22IO2	373.0659	0.1	12.8	1	100.00	5.5	even	ok

Qualitative Compound Report

Analysis Info

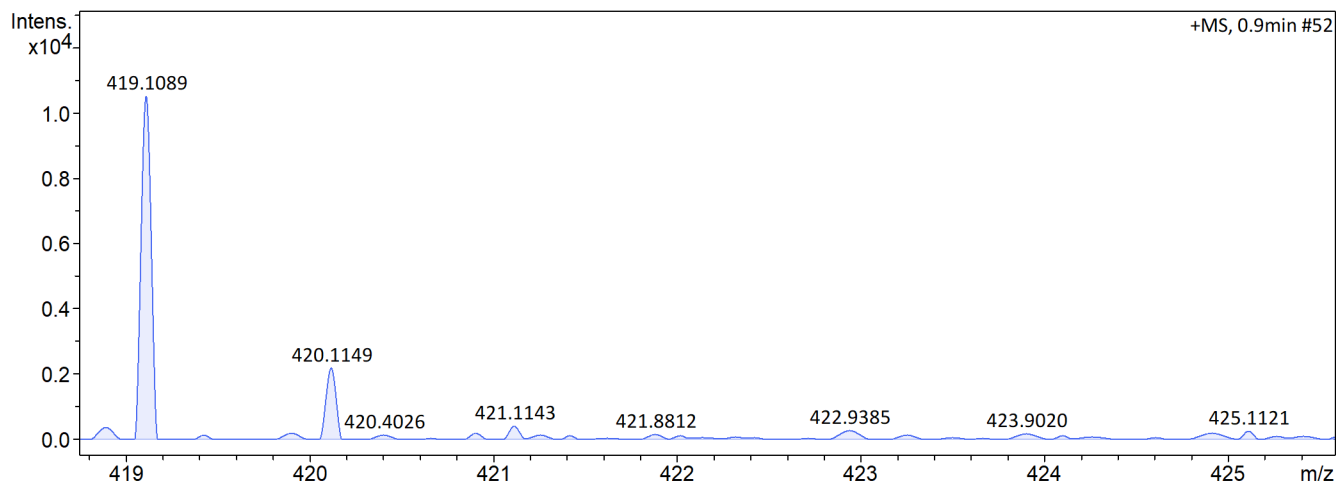
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 Method lc_qtof_directospos.m
 Sample Name 24-021406
 Comment LG053b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:10:17

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
419.1089	1	C18H28IO3	419.1078	-2.7	9.2	1	100.00	4.5	even	ok

Mass Spectrum List Report

Analysis Info

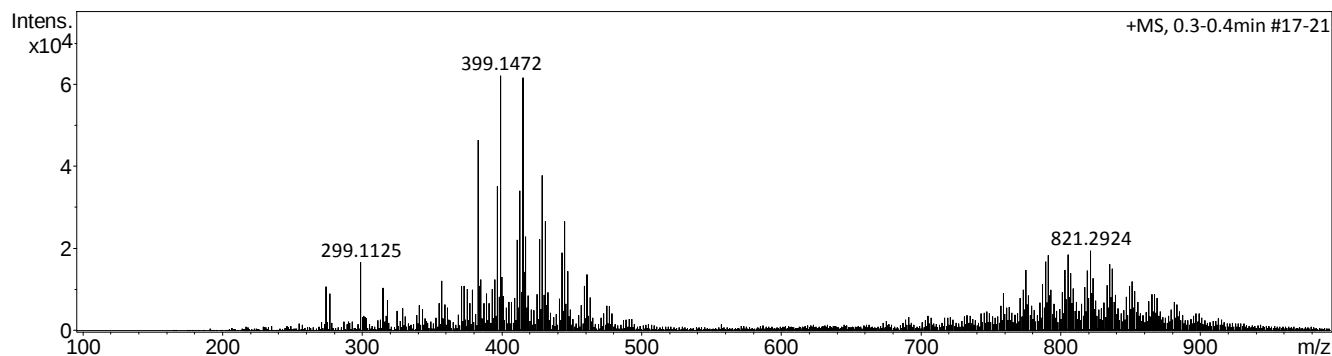
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 Method lc_qtof_directospos.m
 Sample Name 24-021407
 Comment LG088b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 3:15:24 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	299.1125	16551	26.7
2	383.1507	46215	74.6
3	385.1318	12461	20.1
4	395.1502	12435	20.1
5	397.1526	35050	56.6
6	399.1472	61912	100.0
7	400.1480	13076	21.1
8	411.1445	22089	35.7
9	413.1509	34060	55.0
10	415.1449	61482	99.3
11	416.1472	14270	23.0
12	417.1506	22752	36.7
13	427.1381	22165	35.8
14	429.1472	37687	60.9
15	431.1481	26561	42.9
16	443.1327	18872	30.5
17	445.1406	26505	42.8
18	447.1459	14496	23.4
19	461.1349	13588	21.9
20	775.2941	14789	23.9
21	789.3009	16724	27.0
22	791.2997	18262	29.5
23	803.3017	14776	23.9
24	805.3005	18449	29.8
25	807.2893	13929	22.5
26	819.2975	14650	23.7
27	821.2924	19475	31.5
28	823.2870	12687	20.5
29	835.2907	16176	26.1
30	837.2915	15091	24.4

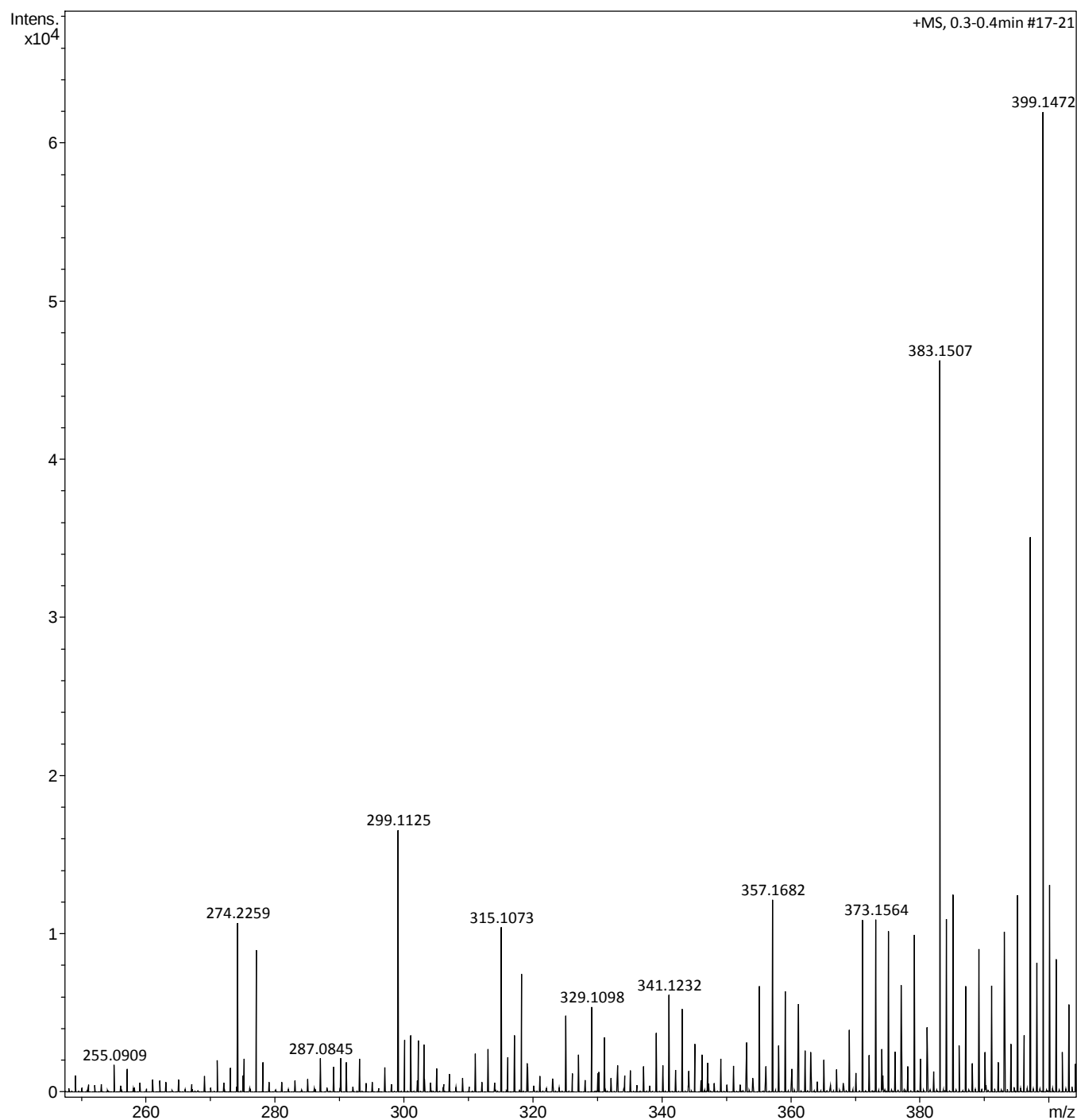
Generic Display Report

Analysis Info

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 Method lc_qtof_directospos.m
 Sample Name 24-021407
 Comment LG088b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 3:15:24 PM

Operator ELB
 Instrument microTOF-Q II



Qualitative Compound Report

Analysis Info

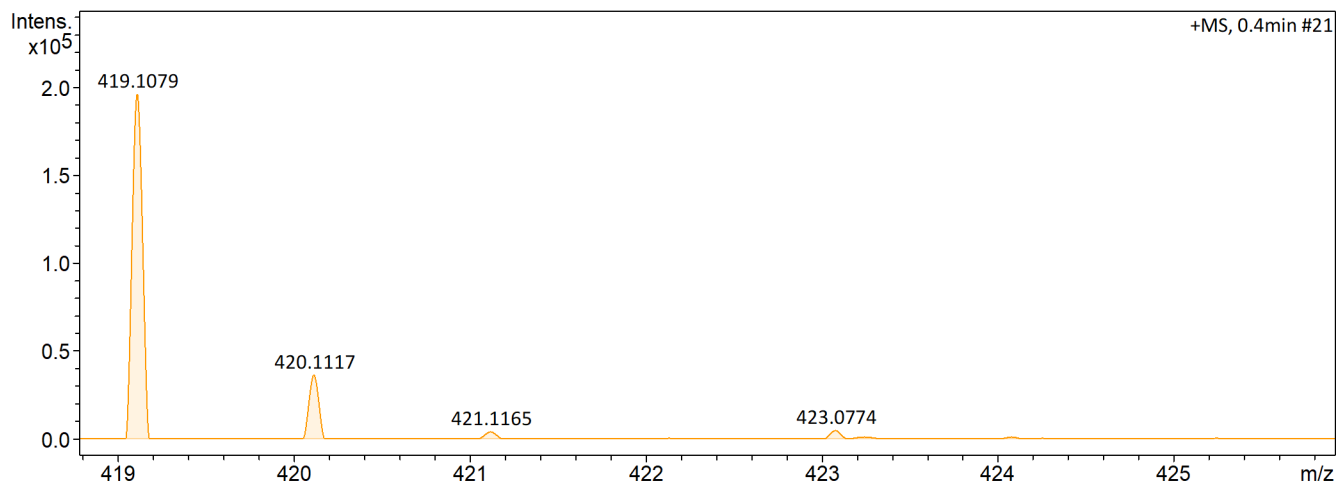
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 Method lc_qtof_directospos.m
 Sample Name 24-021408
 Comment LG054d
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:20:32

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
419.1079	1	C18H28IO3	419.1078	-0.4	7.7	1	100.00	4.5	even	ok

Qualitative Compound Report

Analysis Info

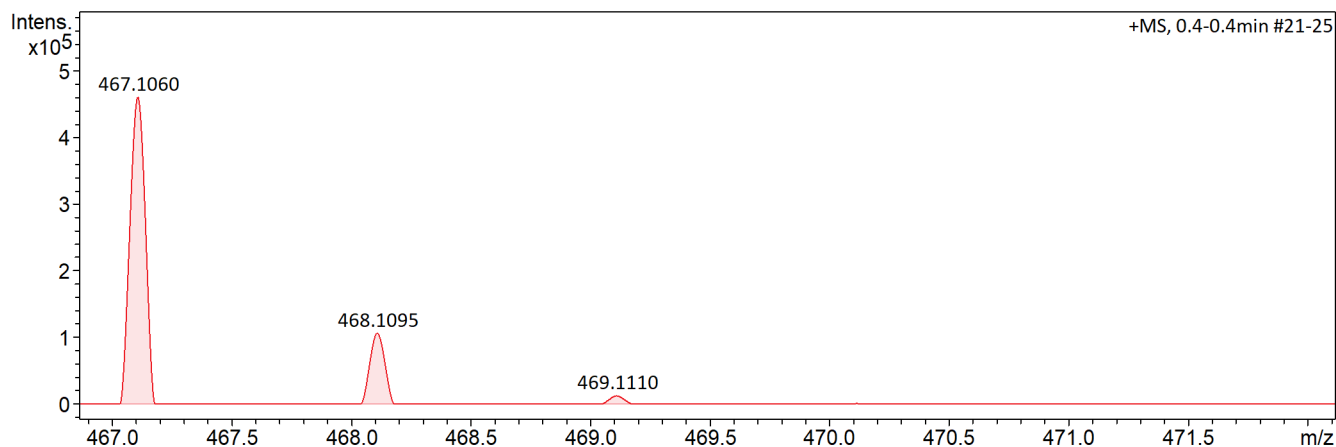
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 Method lc_qtof_directospos.m
 Sample Name 24-021409
 Comment LG065c2
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:25:41

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
467.1060	1	C22H28IO3	467.1078	3.9	8.0	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

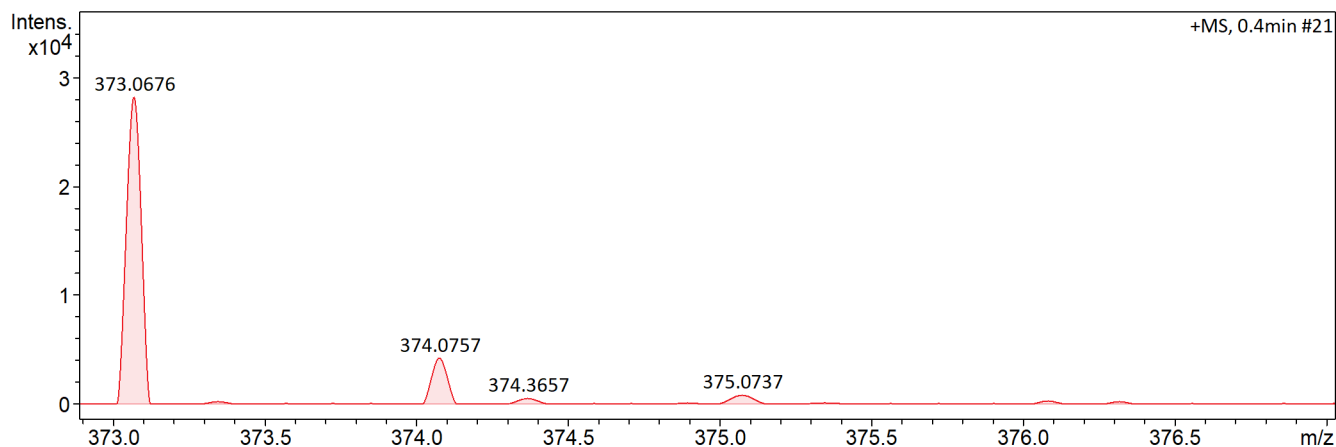
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 Method lc_qtof_directospos.m
 Sample Name 24-021410
 Comment LG040d
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:30:47

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
373.0676	1	C16H22IO2	373.0659	-4.6	15.9	1	100.00	5.5	even	ok

Mass Spectrum List Report

Analysis Info

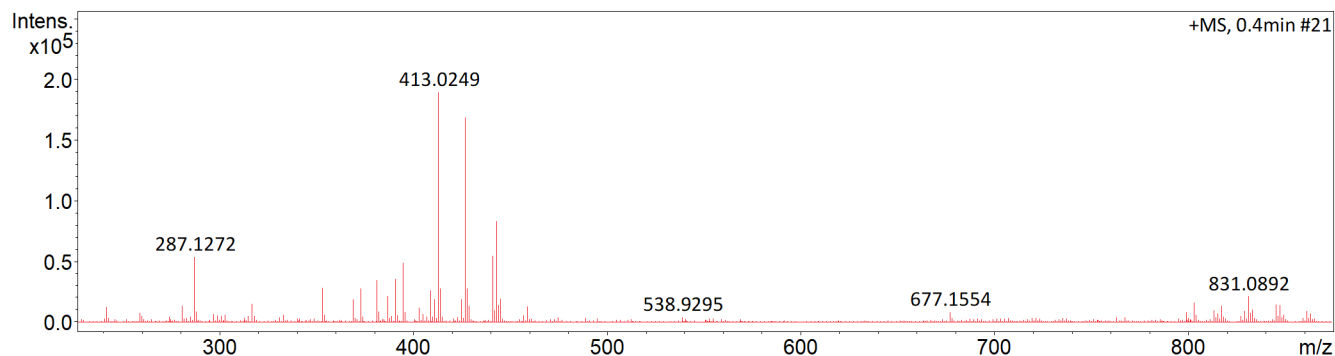
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 Method lc_qtof_directospos.m
 Sample Name 24-021410
 Comment LG040d
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:30:47

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	242.1303	12221	6.5
2	281.1163	13278	7.0
3	287.1272	53672	28.4
4	317.1349	14713	7.8
5	353.2675	28723	15.2
6	369.0359	18663	9.9
7	373.0676	28177	14.9
8	381.2997	34881	18.5
9	387.0453	21125	11.2
10	391.0236	35920	19.0
11	395.0507	49077	26.0
12	403.0420	11861	6.3
13	409.0277	26304	13.9
14	411.0449	18619	9.9
15	413.0249	188847	100.0
16	414.0280	27857	14.8
17	425.0267	18344	9.7
18	427.0397	168474	89.2
19	428.0431	28100	14.9
20	429.0433	13030	6.9
21	441.0531	54724	29.0
22	443.0356	83355	44.1
23	444.0388	13932	7.4
24	445.0477	18889	10.0
25	459.0384	12601	6.7
26	803.0599	15774	8.4
27	817.0737	13192	7.0
28	831.0892	21016	11.1
29	845.0933	14462	7.7
30	847.0820	13825	7.3

Qualitative Compound Report

Analysis Info

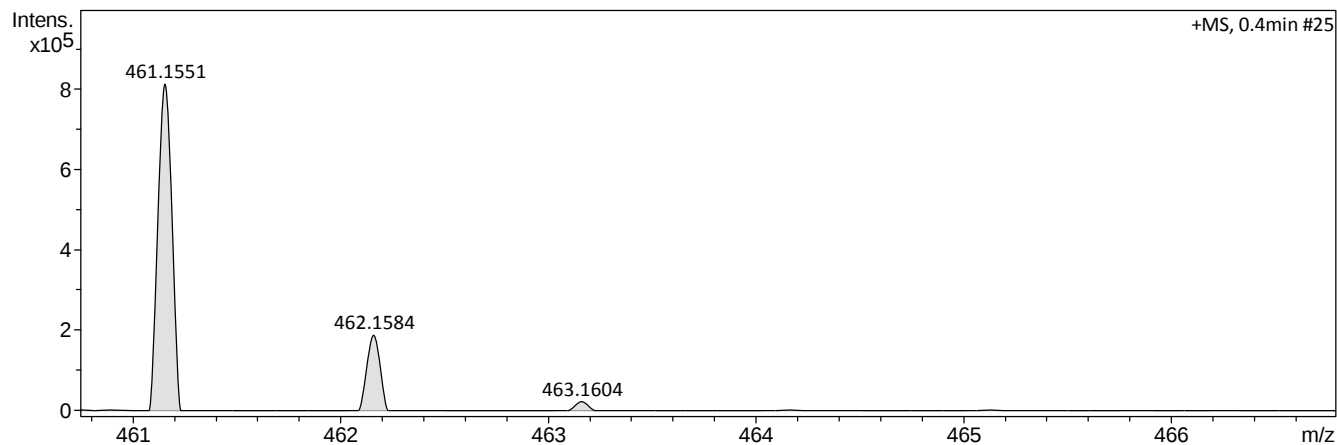
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 Method lc_qtof_directospos.m
 Sample Name 24-021411
 Comment TAC-033b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 3:35:54 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
461.1551	1	C21H34IO3	461.1547	-0.8	3.3	1	96.20	4.5	even	ok

Qualitative Compound Report

Analysis Info

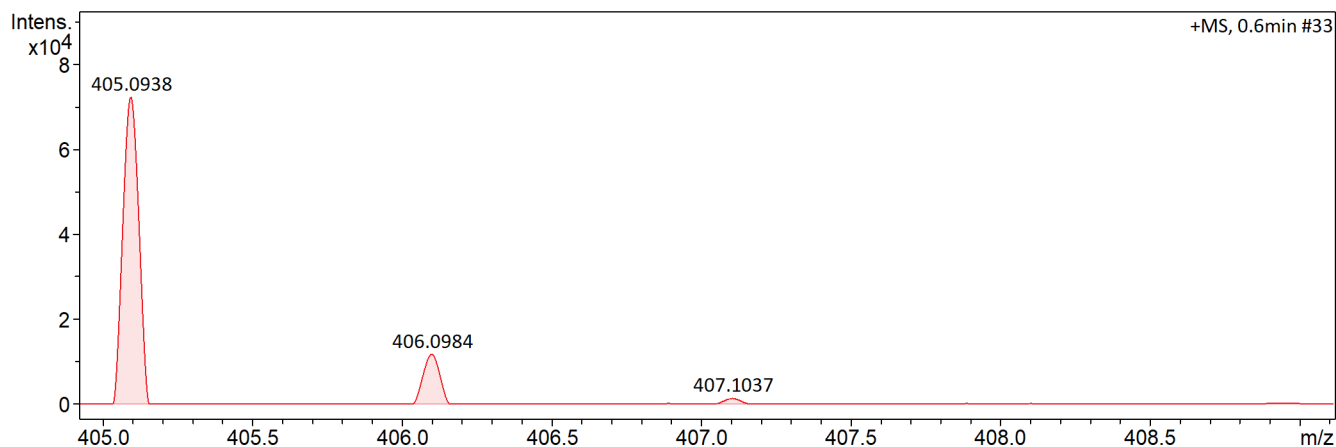
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 Method lc_qtof_directospos.m
 Sample Name 24-021412
 Comment LG059b2
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:40:59

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
405.0938	1	C17H26IO3	405.0921	-4.1	15.1	1	100.00	4.5	even	ok

Qualitative Compound Report

Analysis Info

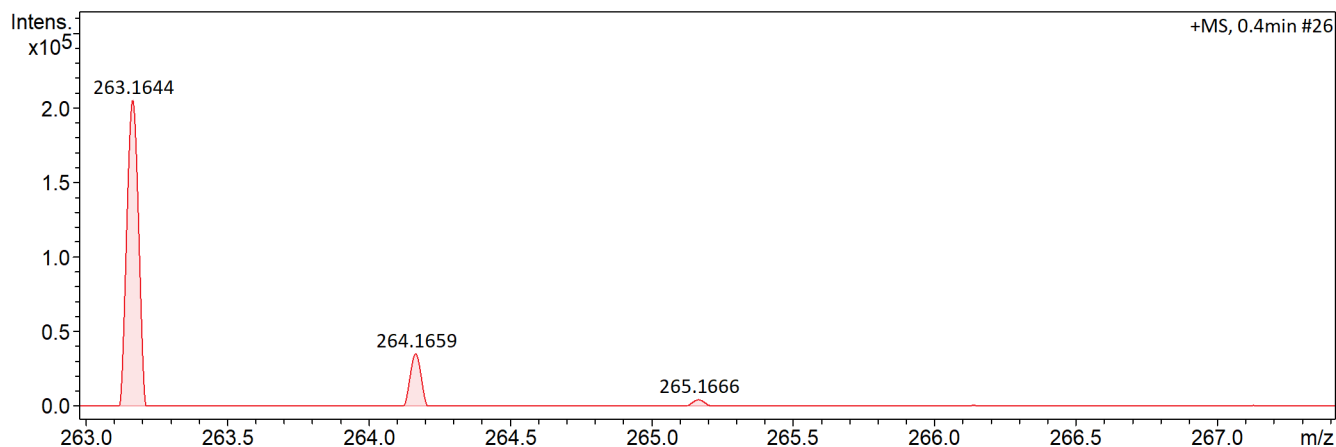
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 Method lc_qtof_directospos.m
 Sample Name 24-021413
 Comment LG035b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:46:07

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
263.1644	1	C16H23O3	263.1642	-0.7	2.6	1	100.00	5.5	even	ok

Qualitative Compound Report

Analysis Info

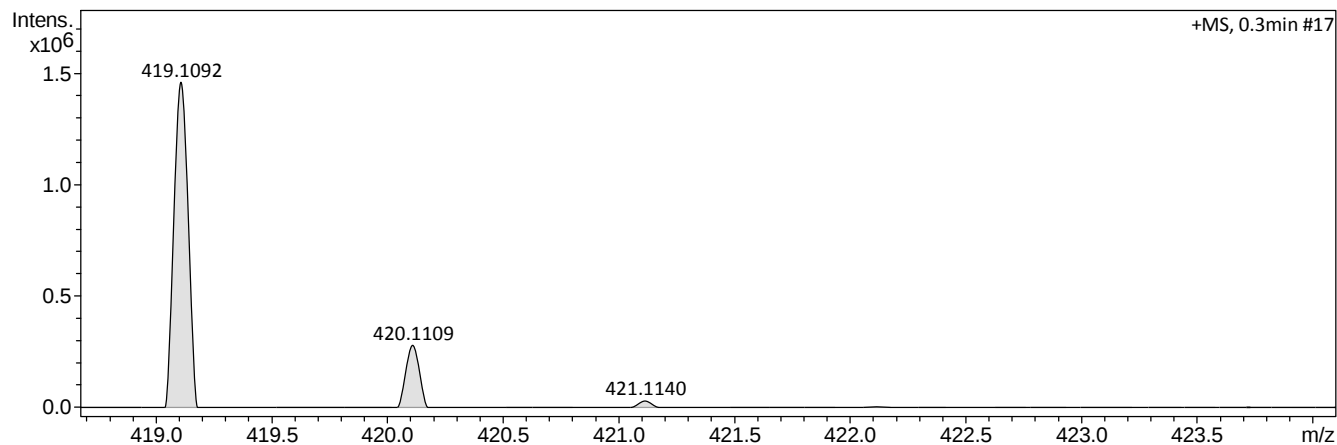
Analysis Name D:\Data\ggc\24-021414_P1-D-5_01_8647.d
 Method lc_qtof_directospos.m
 Sample Name 24-021414
 Comment FS007a2
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 3:51:15 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
419.1092	1	C18H28IO3	419.1078	-3.3	5.6	1	86.95	4.5	even	ok

Qualitative Compound Report

Analysis Info

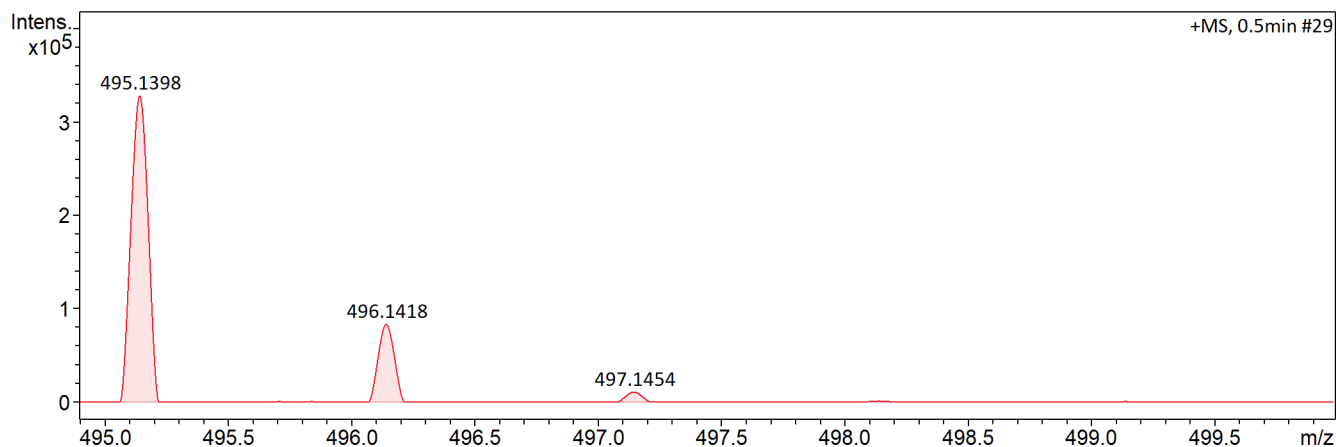
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 Method lc_qtof_directospos.m
 Sample Name 24-021415
 Comment LG111b
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 15:56:21

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
495.1398	1	C24H32IO3	495.1391	-1.6	7.1	1	100.00	8.5	even	ok

Qualitative Compound Report

Analysis Info

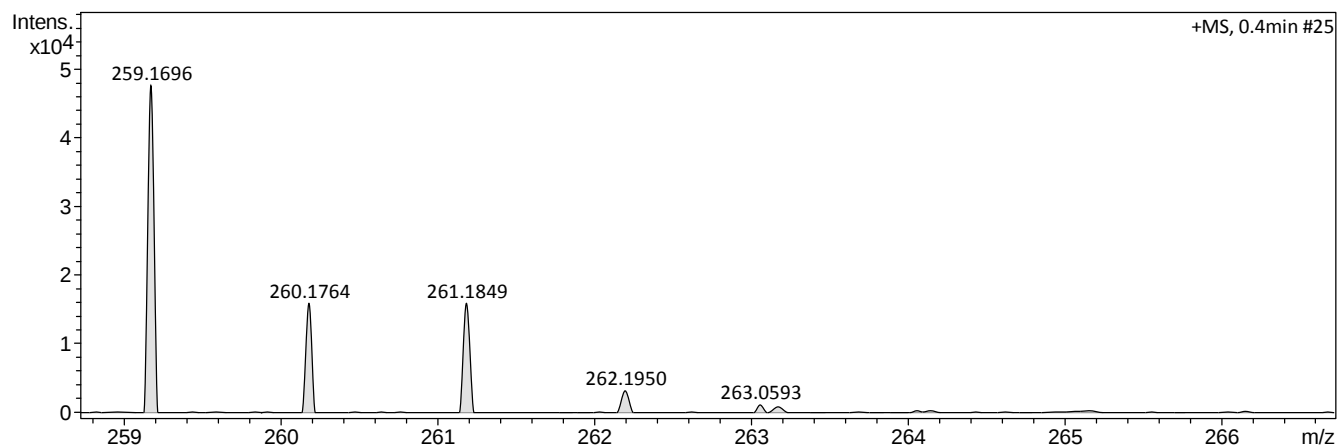
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 Method lc_qtof_directospos.m
 Sample Name 24-021416
 Comment MC010a
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 4:01:28 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
259.1696	1	C17H23O2	259.1693	-1.3	199.8	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

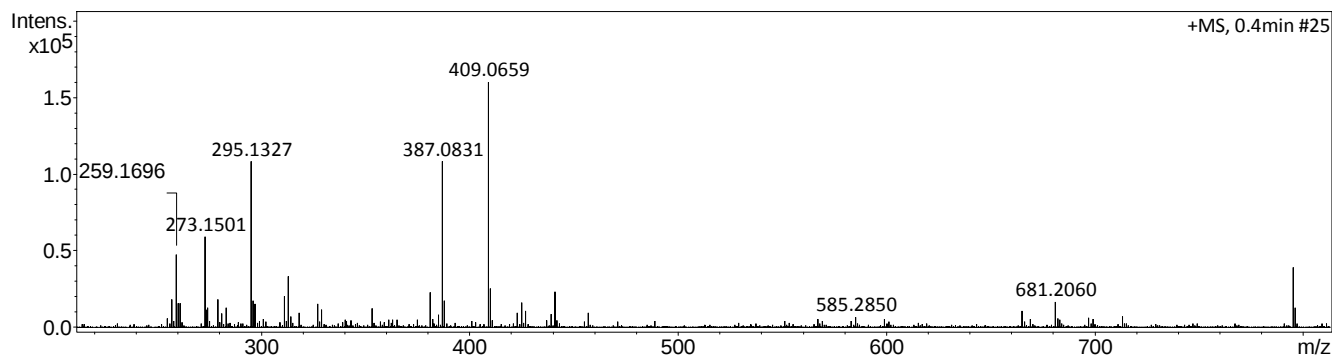
Analysis Name D:\Data\ggc\24-021416_P1-D-7_01_8649.d
Method lc_qtof_directospos.m
Sample Name 24-021416
Comment MC010a
Sv: MeOH + HCOOH
Martín J. Riveira

Acquisition Date 3/4/2024 4:01:28 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	257.1544	18247	11.4
2	259.1696	47520	29.8
3	260.1764	15896	10.0
4	261.1849	15866	9.9
5	273.1501	58818	36.9
6	274.1530	11576	7.3
7	274.2738	12821	8.0
8	279.1363	18015	11.3
9	283.1669	12805	8.0
10	295.1327	107991	67.7
11	296.1369	17500	11.0
12	297.1441	15225	9.5
13	311.1270	20246	12.7
14	313.1438	33154	20.8
15	327.1437	15311	9.6
16	329.1373	11436	7.2
17	353.2682	12387	7.8
18	381.3012	22945	14.4
19	387.0831	108259	67.8
20	388.0874	17578	11.0
21	409.0659	159577	100.0
22	410.0687	25237	15.8
23	425.0585	16305	10.2
24	427.0576	10899	6.8
25	441.0598	23311	14.6
26	457.0507	9489	5.9
27	665.2142	10581	6.6
28	681.2060	16549	10.4
29	795.1427	39082	24.5
30	796.1405	12719	8.0

Qualitative Compound Report

Analysis Info

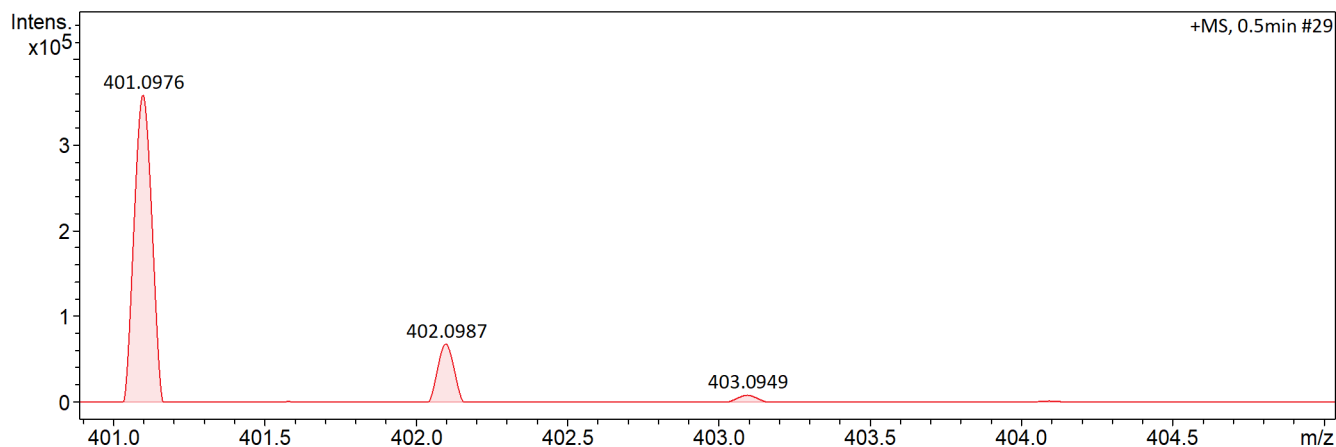
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 Method lc_qtof_directospos.m
 Sample Name 24-021417
 Comment FS007a1
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 4/3/2024 16:06:36

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
401.0976	1	C18H26IO2	401.0972	-1.1	5.3	1	100.00	5.5	even	ok

Qualitative Compound Report

Analysis Info

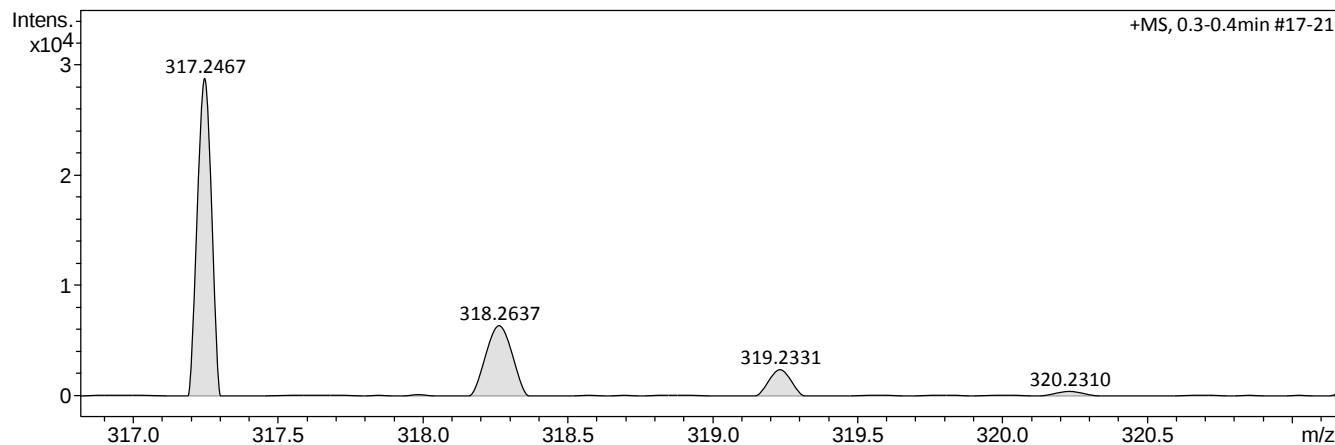
Analysis Name D:\Data\ggc\24-021418_P1-D-9_01_8651.d
 Method lc_qtof_directospos.m
 Sample Name 24-021418
 Comment LG095d
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 4:11:45 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
317.2467	1	C21H33O2	317.2475	2.4	n.a.	1	100.00	5.5	even	ok

Mass Spectrum List Report

Analysis Info

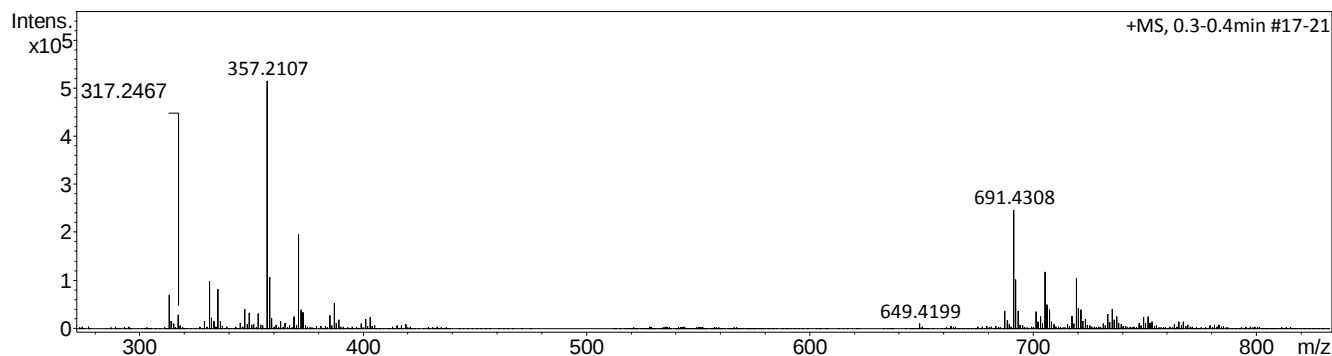
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 Method lc_qtof_directospos.m
 Sample Name 24-021418
 Comment LG095d
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 4:11:45 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	313.2220	69485	13.5
2	317.2467	28686	5.6
3	331.2327	97499	19.0
4	335.2270	81389	15.8
5	347.2261	40333	7.9
6	349.2391	32923	6.4
7	353.2164	32030	6.2
8	357.2107	513651	100.0
9	358.2138	106797	20.8
10	371.2260	196096	38.2
11	372.2279	39938	7.8
12	373.2106	33768	6.6
13	385.2051	26923	5.2
14	387.2187	53018	10.3
15	687.4338	37223	7.2
16	691.4308	246677	48.0
17	692.4316	102187	19.9
18	693.4302	37111	7.2
19	701.4507	35422	6.9
20	703.4335	24417	4.8
21	705.4428	117609	22.9
22	706.4481	50377	9.8
23	707.4294	39206	7.6
24	717.4399	26105	5.1
25	719.4554	104601	20.4
26	720.4559	41583	8.1
27	721.4471	39670	7.7
28	733.4391	30152	5.9
29	735.4476	40596	7.9
30	737.4448	24858	4.8

Qualitative Compound Report

Analysis Info

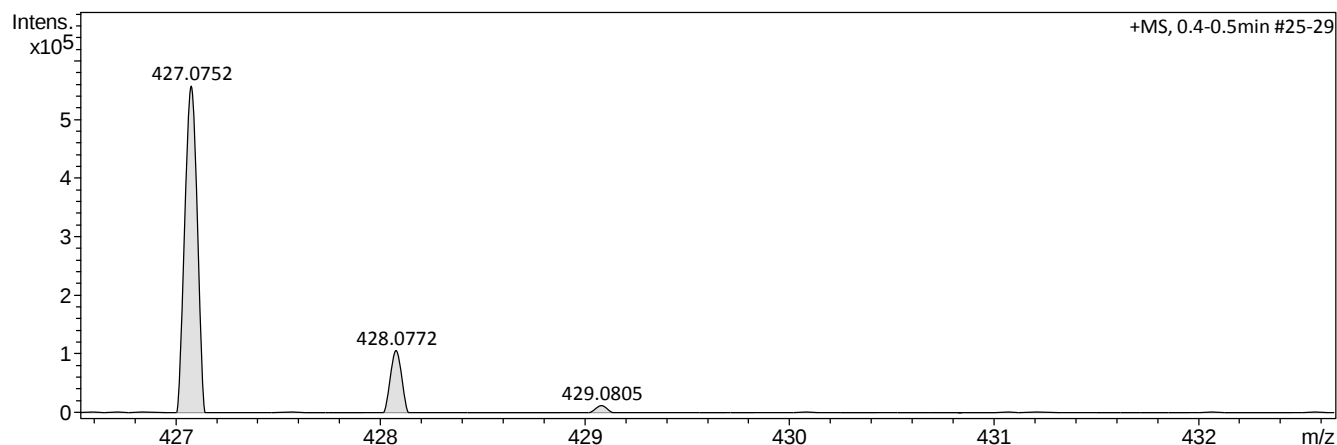
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 Method lc_qtof_directospos.m
 Sample Name 24-021419
 Comment LG071a
 Sv: MeOH + HCOOH
 Martín J. Riveira

Acquisition Date 3/4/2024 4:16:51 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
427.0752	1	C17H25INaO3	427.0741	-2.7	1.3	1	86.44	4.5	even	ok