

Qualitative Compound Report

Analysis Info

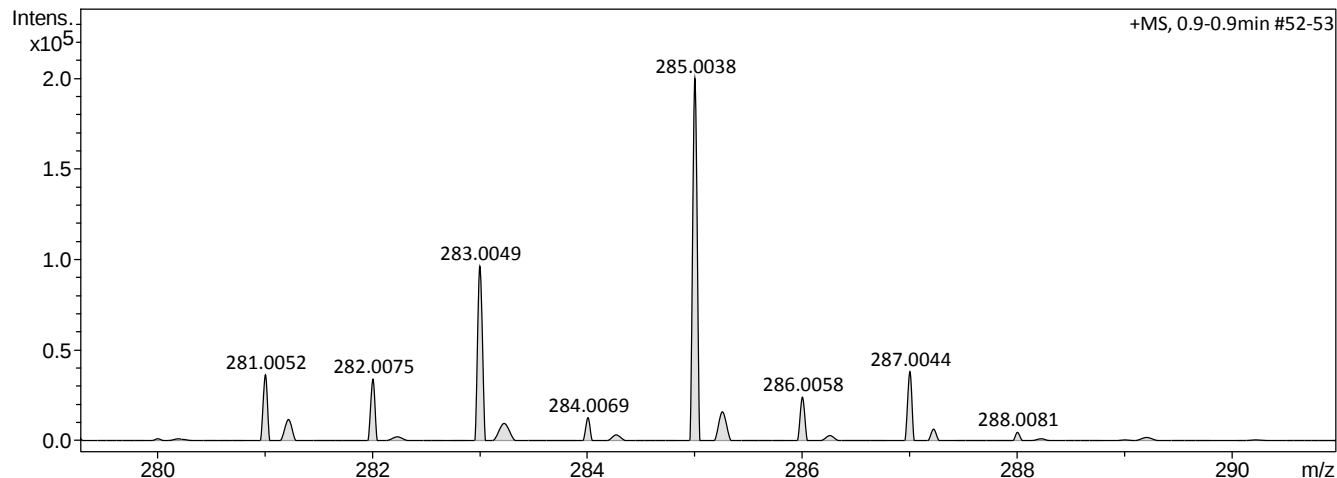
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 Method APCI.m
 Sample Name BPG-VI-45A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 1:20:11 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
285.0038	1	C ₁₂ H ₁₃ O ₃ Se	285.0024	-4.5	7.7	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

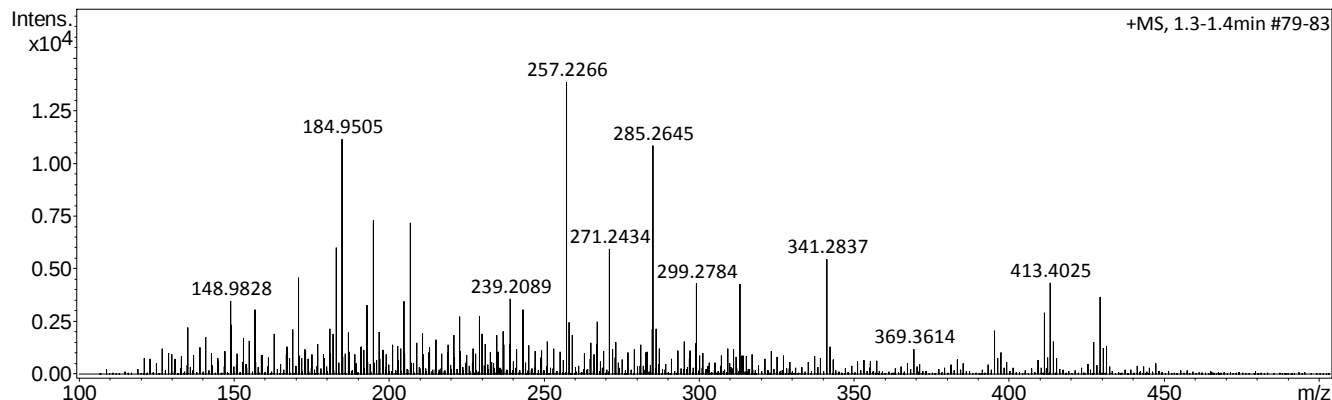
Analysis Name D:\Data\ggc\24-031524.d
 Method APCI.m
 Sample Name BPG-VI-47B
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 3:01:43 PM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	135.0701	2224	16.1
2	148.9828	3441	24.9
3	149.0886	2336	16.9
4	156.9161	3075	22.2
5	168.9365	2120	15.3
6	170.9313	4572	33.1
7	180.9468	2153	15.6
8	182.9477	5998	43.4
9	184.9505	11120	80.4
10	192.9383	3262	23.6
11	194.9378	7295	52.8
12	204.9248	3462	25.0
13	206.9241	7164	51.8
14	222.9410	2721	19.7
15	229.1810	2743	19.8
16	239.2089	3564	25.8
17	243.2036	3050	22.1
18	257.2266	13828	100.0
19	258.2298	2469	17.9
20	267.2399	2494	18.0
21	271.2434	5925	42.8
22	284.9910	2126	15.4
23	285.2645	10841	78.4
24	286.2682	2163	15.6
25	299.2784	4306	31.1
26	313.2672	4260	30.8
27	341.2837	5446	39.4
28	411.3890	2924	21.1
29	413.4025	4343	31.4
30	429.4010	3672	26.6

Qualitative Compound Report

Analysis Info

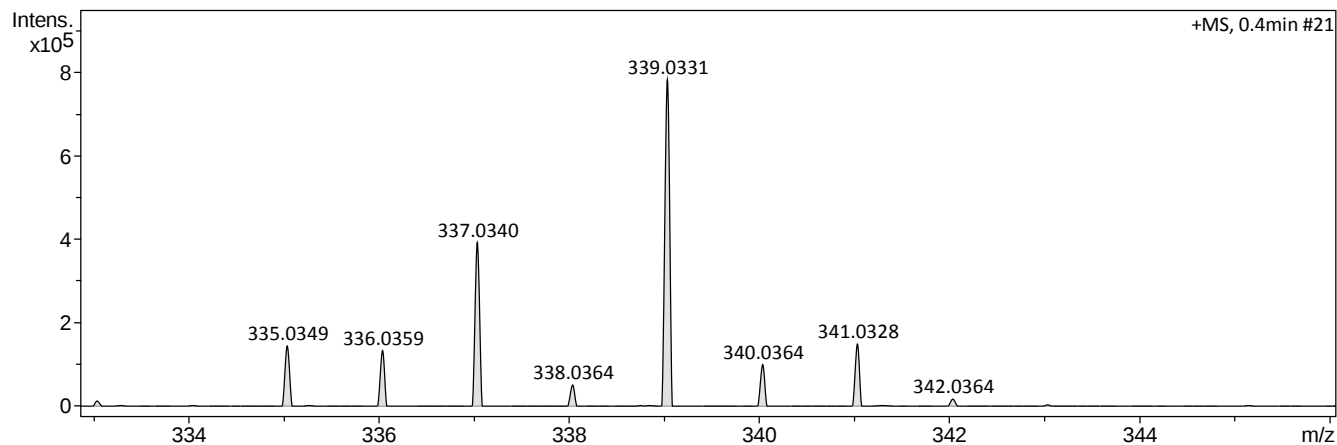
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 Method lc_qtof_directospos.m
 Sample Name 24-031524
 Comment BPG-VI-47B
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 2:46:34 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
339.0331	1	C ₁₂ H ₁₉ O ₆ Se	339.0341	3.2	4.4	1	100.00	3.5	even	ok

Qualitative Compound Report

Analysis Info

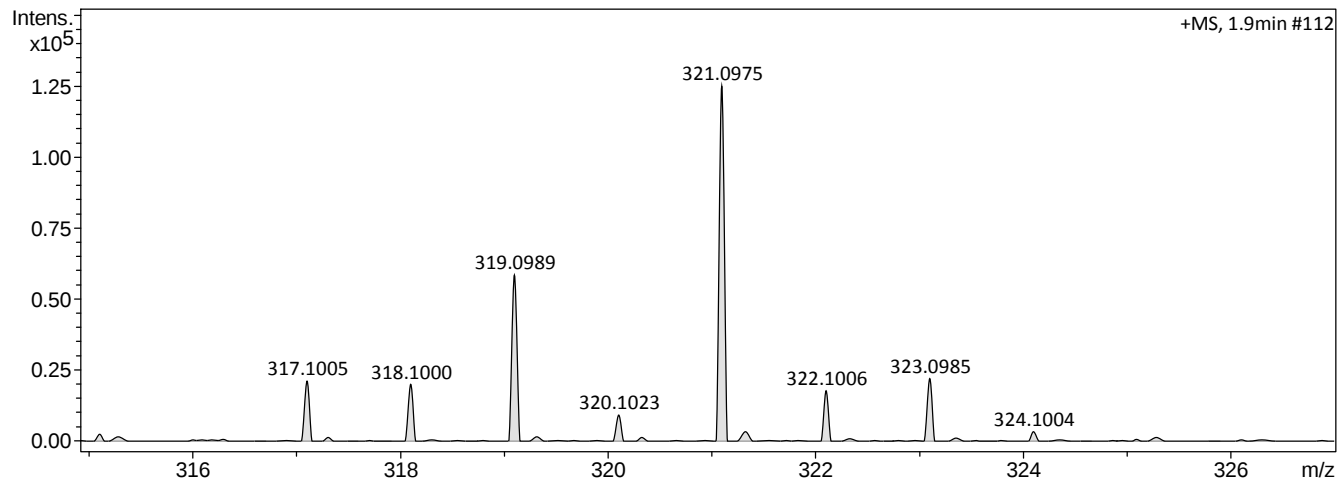
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 Method APCI.m
 Sample Name BPG-VI-49A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 1:01:28 PM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
321.0975	1	C14H25O3Se	321.0963	-3.3	16.6	1	100.00	2.5	even	ok

Mass Spectrum List Report

Analysis Info

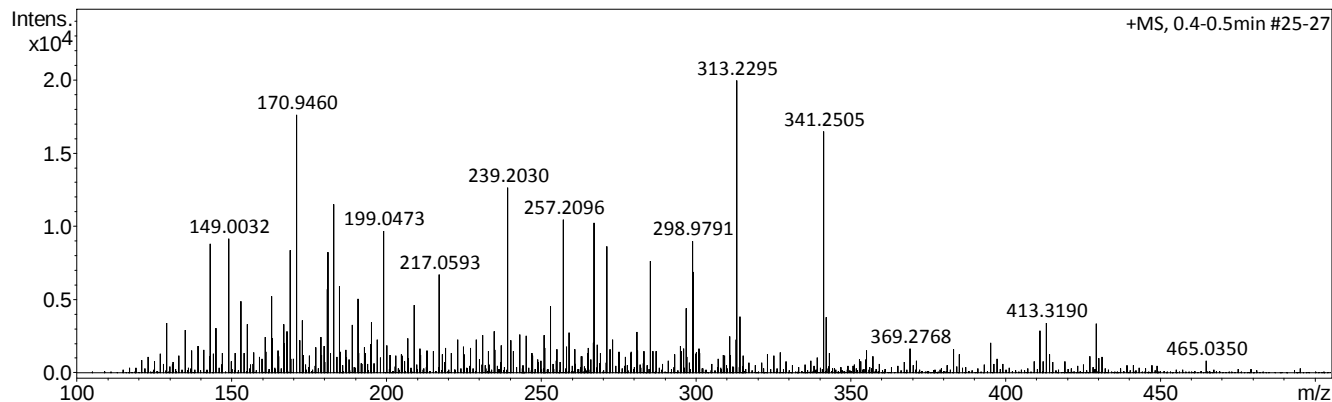
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 Method APCI.m
 Sample Name BPG-VI-52F
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 3:10:08 PM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	143.0655	8778	44.1
2	149.0032	9131	45.8
3	153.0516	4875	24.5
4	162.9434	5234	26.3
5	168.9485	8367	42.0
6	170.9460	17584	88.3
7	171.0582	14734	74.0
8	172.9441	3582	18.0
9	180.9480	5705	28.6
10	181.0713	8249	41.4
11	182.9482	11515	57.8
12	184.9555	5942	29.8
13	190.9340	5037	25.3
14	195.0913	3463	17.4
15	199.0473	9673	48.6
16	208.9583	4641	23.3
17	217.0593	6729	33.8
18	239.2030	12613	63.3
19	252.9786	4554	22.9
20	257.2096	10438	52.4
21	267.2287	10219	51.3
22	271.2220	8637	43.4
23	285.2354	7607	38.2
24	296.9782	4393	22.1
25	298.9791	8955	45.0
26	299.2483	6900	34.6
27	313.2295	19917	100.0
28	314.2332	3851	19.3
29	341.2505	16432	82.5
30	342.2533	3786	19.0

Qualitative Compound Report

Analysis Info

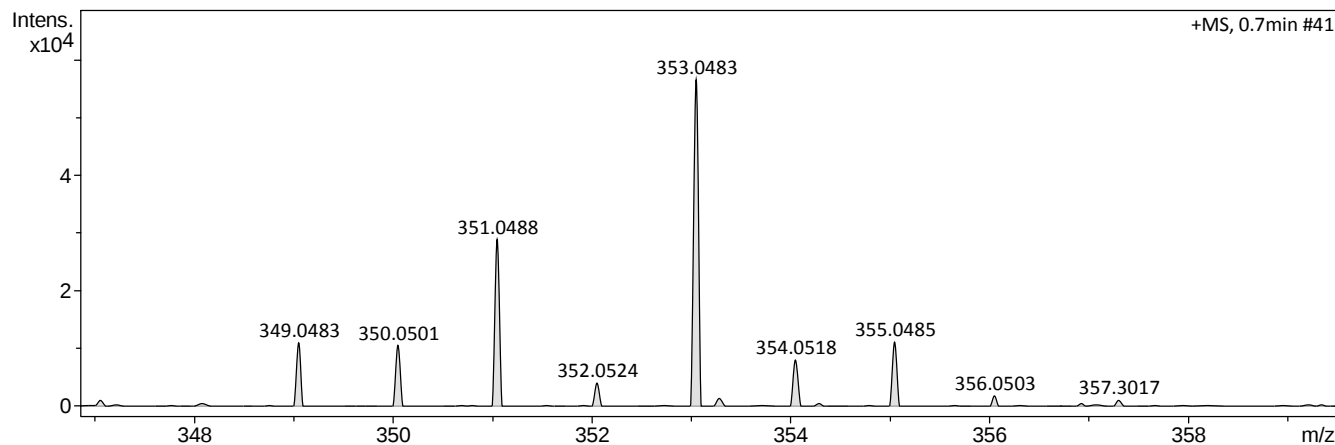
Analysis Name D:\Data\ggc\24-031526_P1-D-6_01_8823.d
 Method lc_qtof_directospos.m
 Sample Name 24-031526
 Comment BPG-VI-52F
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 2:56:50 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
353.0483	1	C13H21O6Se	353.0498	4.4	4.8	1	100.00	3.5	even	ok

Mass Spectrum List Report

Analysis Info

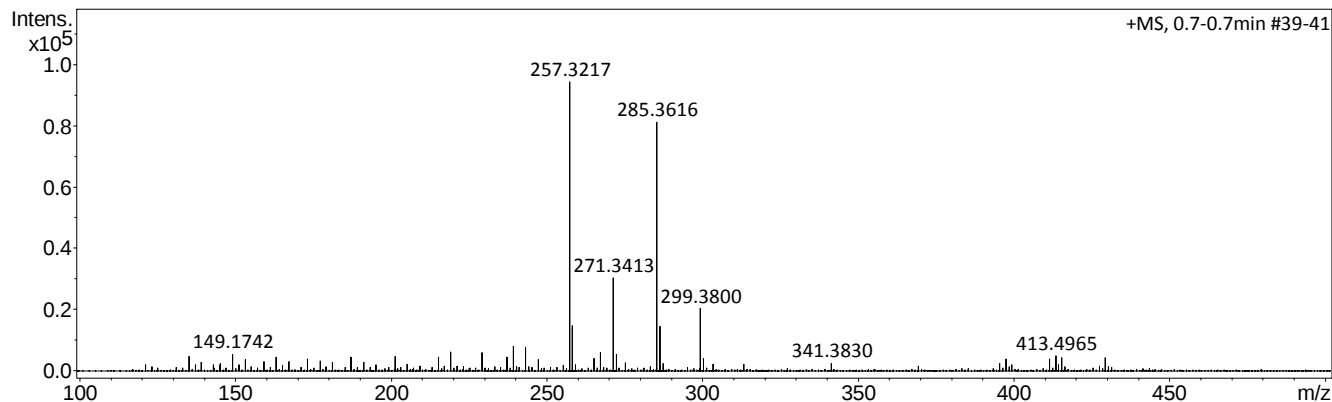
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 Method APCI.m
 Sample Name BPG-VI-61D
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 9:49:57 AM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	135.1535	4701	5.0
2	149.1742	5408	5.7
3	153.1708	3634	3.9
4	163.1928	4559	4.8
5	173.1988	3920	4.2
6	177.2113	3159	3.3
7	187.2196	4423	4.7
8	201.2393	4610	4.9
9	215.2592	4496	4.8
10	219.2714	6063	6.4
11	229.2797	6048	6.4
12	237.2881	4554	4.8
13	239.3055	7942	8.4
14	243.2999	7564	8.0
15	247.3095	3744	4.0
16	257.3217	94302	100.0
17	258.3242	14796	15.7
18	265.3254	4004	4.2
19	267.3436	6037	6.4
20	271.3413	30384	32.2
21	272.3446	5424	5.8
22	285.3616	81211	86.1
23	286.3649	14570	15.5
24	299.3800	20334	21.6
25	300.3834	4014	4.3
26	397.4945	3828	4.1
27	411.4837	3815	4.0
28	413.4965	4987	5.3
29	415.5107	4372	4.6
30	429.4960	4367	4.6

Qualitative Compound Report

Analysis Info

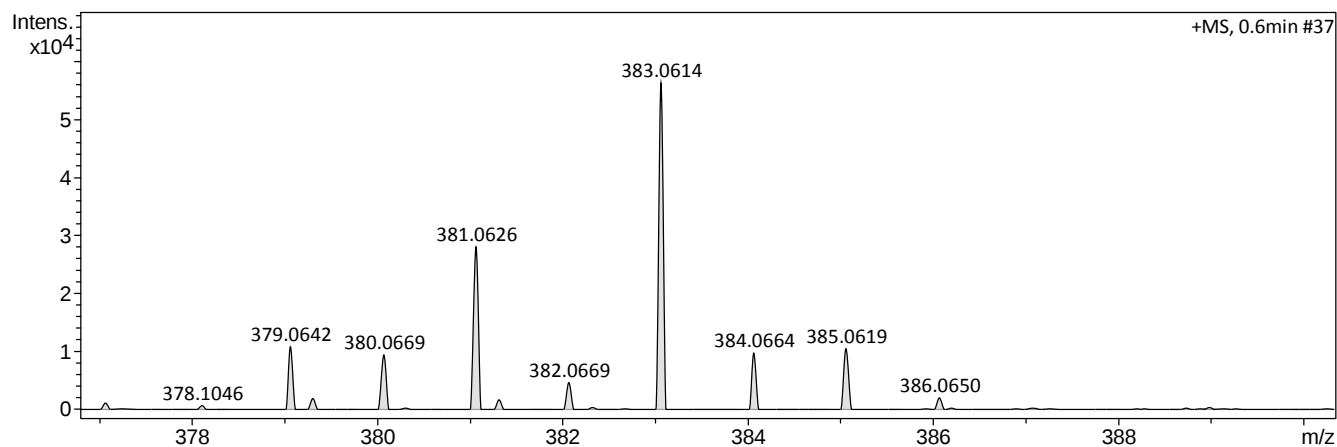
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 Sample Name 24-031527
 Comment BPG-VI-61D
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:01:58 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
383.0614	1	C14H23O7Se	383.0604	-2.6	8.9	1	100.00	3.5	even	ok

Mass Spectrum List Report

Analysis Info

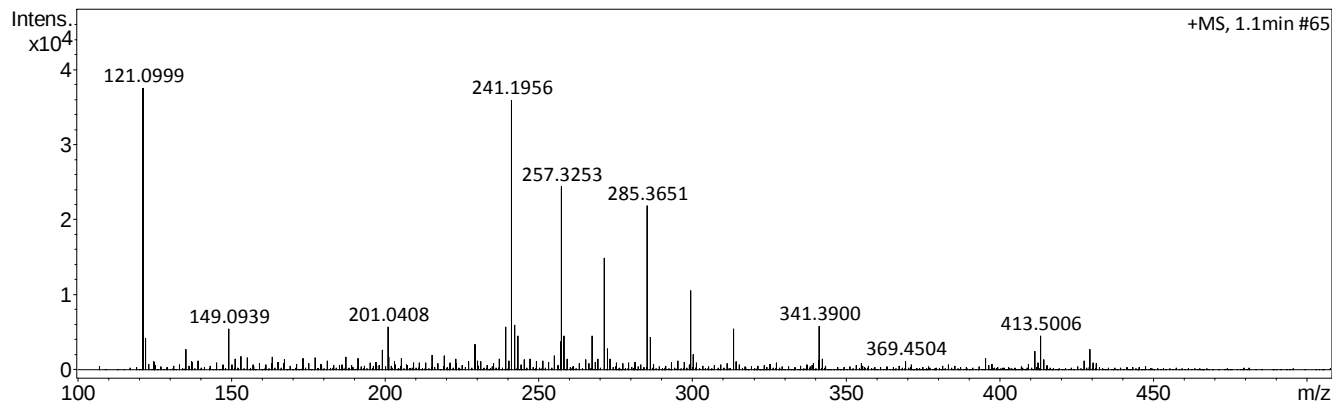
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 Method APCI.m
 Sample Name BPG-VI-75D
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 3:40:21 PM

Operator ELB
 Instrument / Ser# micrOTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	121.0999	37480	100.0
2	122.1042	4132	11.0
3	135.1292	2709	7.2
4	149.0939	5411	14.4
5	149.1726	2675	7.1
6	199.0409	2630	7.0
7	201.0408	5681	15.2
8	215.2593	1958	5.2
9	219.2715	1880	5.0
10	229.2807	3410	9.1
11	239.3062	5711	15.2
12	241.1956	35856	95.7
13	242.1995	5987	16.0
14	243.3020	4494	12.0
15	255.2239	1907	5.1
16	257.1968	3783	10.1
17	257.3253	24422	65.2
18	258.3280	4528	12.1
19	267.3482	4498	12.0
20	271.3464	14887	39.7
21	272.3488	2808	7.5
22	285.3651	21797	58.2
23	286.3691	4360	11.6
24	299.3821	10557	28.2
25	300.3872	2051	5.5
26	313.3687	5432	14.5
27	341.3900	5809	15.5
28	411.4886	2500	6.7
29	413.5006	4520	12.1
30	429.5042	2743	7.3

Qualitative Compound Report

Analysis Info

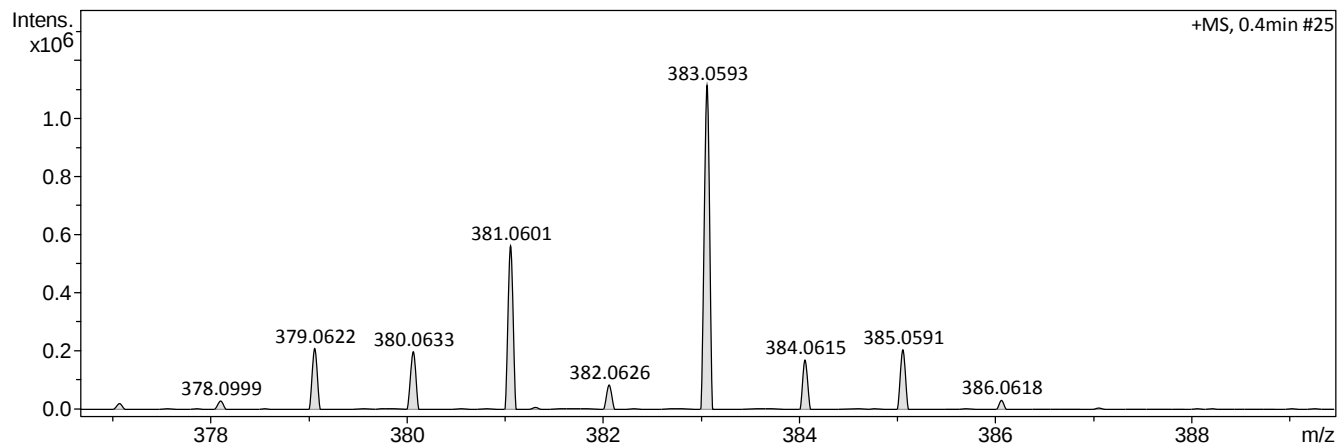
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 Method lc_qtof_directospos.m
 Sample Name 24-031528
 Comment BPG-VI-75D
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:07:06 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
383.0593	1	C14H23O7Se	383.0604	2.9	6.4	1	100.00	3.5	even	ok

Mass Spectrum List Report

Analysis Info

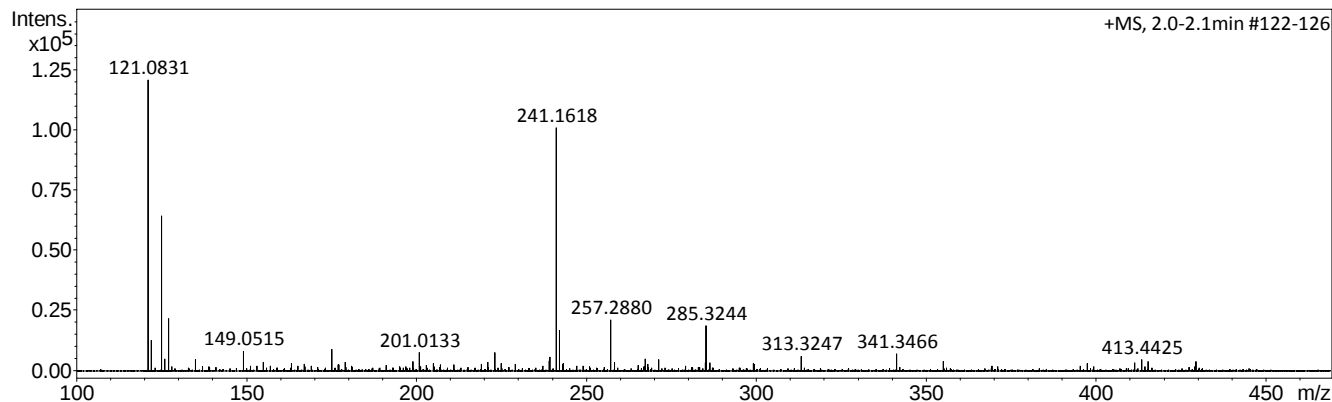
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 Sample Name BPG-VII-2C
 Comment SV: DCM
 Spanevello

Acquisition Date 4/4/2024 3:54:11 PM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	121.0831	120629	100.0
2	122.0868	12579	10.4
3	125.0342	64277	53.3
4	126.0372	5009	4.2
5	127.0321	21563	17.9
6	135.1024	4590	3.8
7	149.0515	8053	6.7
8	155.0526	3492	2.9
9	175.0847	8914	7.4
10	178.9937	3647	3.0
11	199.0149	3813	3.2
12	201.0133	7594	6.3
13	221.0593	3580	3.0
14	223.0947	7592	6.3
15	239.0695	4137	3.4
16	239.2760	5662	4.7
17	241.1618	100641	83.4
18	242.1655	16885	14.0
19	257.2880	21161	17.5
20	258.2906	3604	3.0
21	267.3101	5008	4.2
22	271.3028	4551	3.8
23	285.3244	18761	15.6
24	313.3247	5870	4.9
25	341.3466	6927	5.7
26	355.1270	3888	3.2
27	413.4425	4618	3.8
28	415.4558	3893	3.2
29	429.4414	3860	3.2
30	663.5598	4440	3.7

Mass Spectrum List Report

Analysis Info

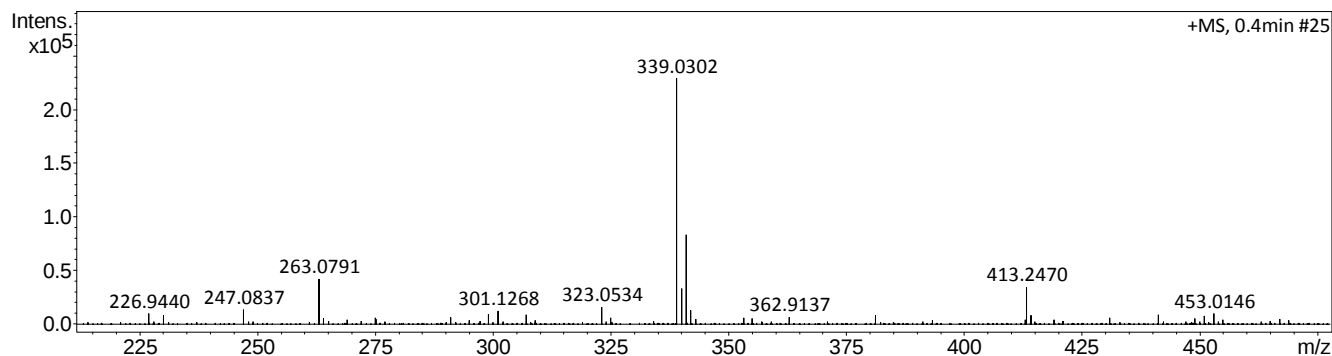
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 Method lc_qtof_directospos.m
 Sample Name 24-031529
 Comment BPG-VII-2C
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:12:16 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	226.9440	10179	4.4
2	230.1095	8503	3.7
3	247.0837	13446	5.9
4	263.0791	42033	18.4
5	275.0383	6018	2.6
6	291.1063	6685	2.9
7	299.0376	9638	4.2
8	301.1268	12324	5.4
9	307.0100	8832	3.9
10	323.0534	16016	7.0
11	325.0488	5754	2.5
12	339.0302	228860	100.0
13	340.0338	33420	14.6
14	341.0272	83355	36.4
15	342.0303	13117	5.7
16	353.2534	5830	2.5
17	362.9137	6340	2.8
18	381.2807	8291	3.6
19	413.2470	34356	15.0
20	414.2515	8456	3.7
21	430.8960	5711	2.5
22	441.2789	8746	3.8
23	451.0163	7367	3.2
24	453.0146	10222	4.5
25	655.0695	12810	5.6
26	657.0627	10712	4.7
27	685.4033	8266	3.6
28	729.2850	5760	2.5
29	764.5411	8087	3.5
30	1001.4418	7965	3.5

Mass Spectrum List Report

Analysis Info

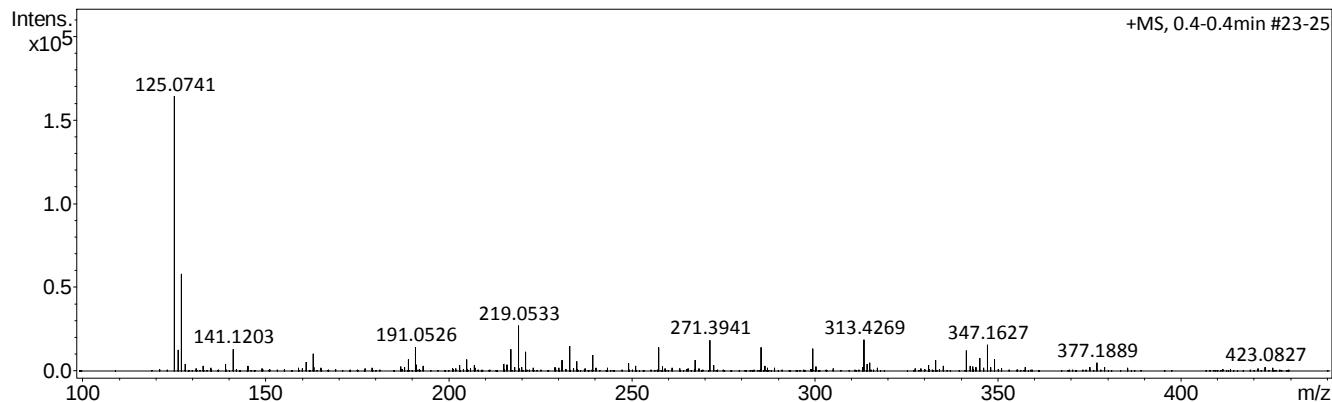
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 Method APCI.m
 Sample Name BPG-VII-1B
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 2:37:34 PM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	125.0741	163823	100.0
2	126.0782	12465	7.6
3	127.0730	57901	35.3
4	141.1203	12965	7.9
5	161.0435	5313	3.2
6	163.0434	10392	6.3
7	189.0518	6987	4.3
8	191.0526	14143	8.6
9	205.0326	7093	4.3
10	217.0528	12842	7.8
11	219.0533	27083	16.5
12	221.0565	11667	7.1
13	231.0762	6672	4.1
14	233.0757	14925	9.1
15	235.0752	5885	3.6
16	239.3528	9610	5.9
17	249.1442	4650	2.8
18	257.3719	14183	8.7
19	267.3968	6618	4.0
20	271.3941	18253	11.1
21	285.4159	14320	8.7
22	299.4392	13293	8.1
23	313.4269	18861	11.5
24	315.1226	5016	3.1
25	333.1402	6674	4.1
26	341.4699	12157	7.4
27	345.1625	7630	4.7
28	347.1627	15771	9.6
29	349.1603	6878	4.2
30	377.1889	4865	3.0

Qualitative Compound Report

Analysis Info

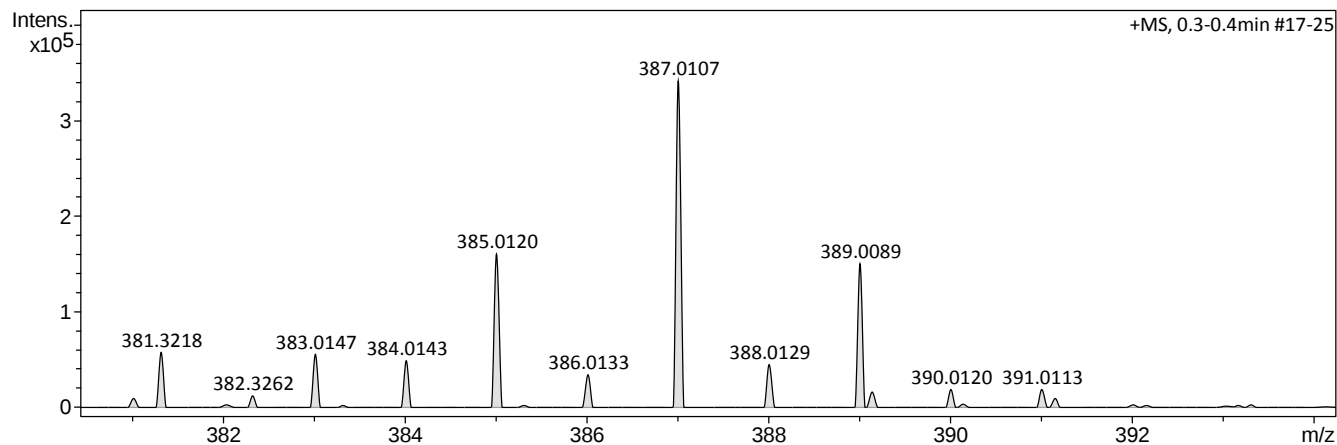
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 Method lc_qtof_directospos.m
 Sample Name 24-031530
 Comment BPG-VII-1B
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:17:22 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
387.0107	1	C ₁₃ H ₂₀ ClO ₆ Se	387.0108	-0.3	9.4	1	100.00	3.5	even	ok

Mass Spectrum List Report

Analysis Info

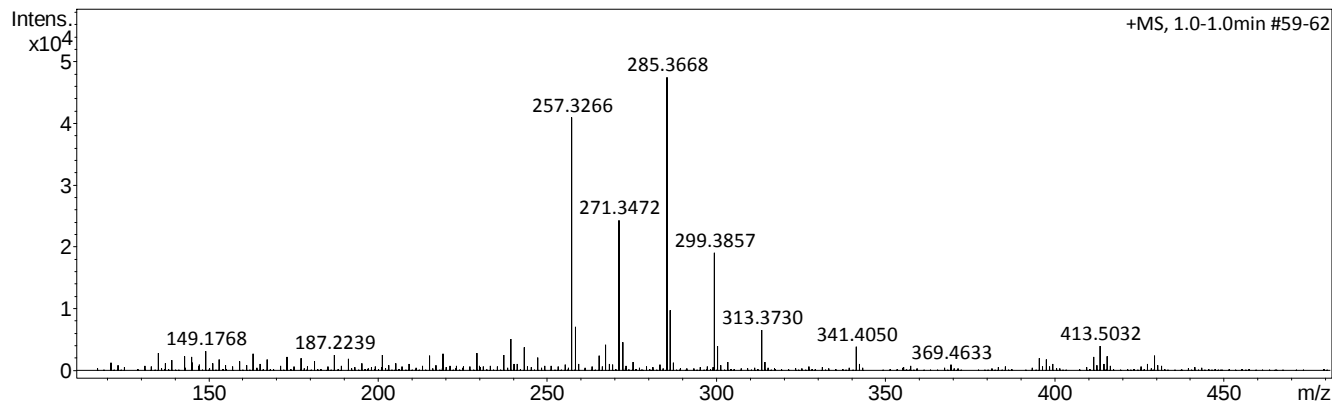
Analysis Name D:\Data\ggc\24-031531.d
 Method APCI.m
 Sample Name BPG-VII-6A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 10:01:15 AM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	135.1553	2806	5.9
2	142.9658	2356	5.0
3	144.9637	2263	4.8
4	149.1768	3091	6.5
5	163.1953	2695	5.7
6	173.2022	2231	4.7
7	187.2239	2561	5.4
8	201.2441	2548	5.4
9	215.2633	2409	5.1
10	219.2762	2761	5.8
11	229.2823	2834	6.0
12	237.2937	2541	5.4
13	239.3094	5111	10.8
14	243.3037	3733	7.9
15	257.3266	40874	86.2
16	258.3316	7073	14.9
17	265.3317	2412	5.1
18	267.3502	4134	8.7
19	271.3472	24306	51.3
20	272.3498	4553	9.6
21	285.3668	47414	100.0
22	286.3707	9729	20.5
23	299.3857	18983	40.0
24	300.3900	3958	8.3
25	313.3730	6528	13.8
26	341.4050	3847	8.1
27	411.4915	2240	4.7
28	413.5032	3939	8.3
29	415.5163	2293	4.8
30	429.5050	2402	5.1

Qualitative Compound Report

Analysis Info

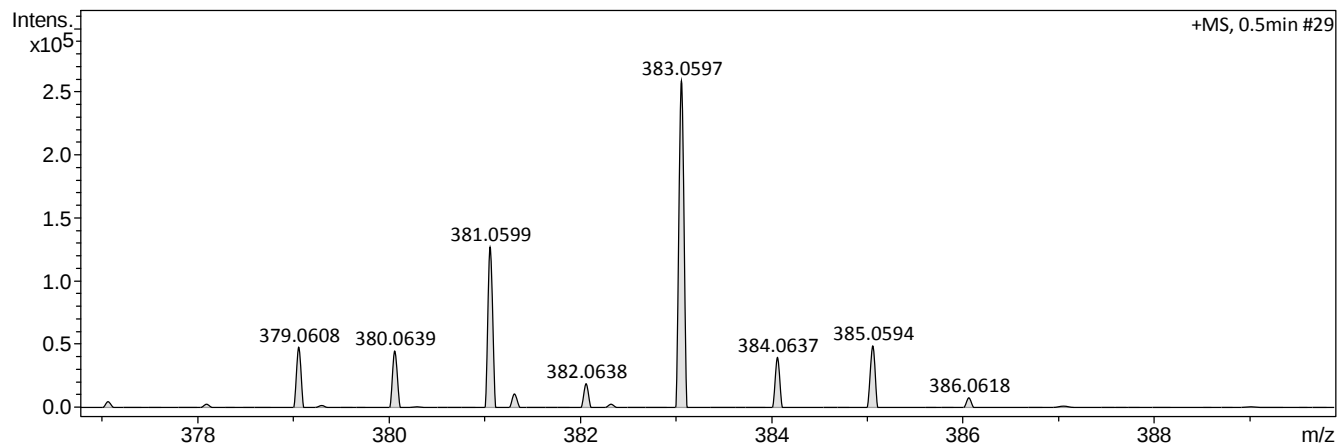
Analysis Name D:\Data\ggc\24-031531_P1-E-2_01_8828.d
 Method lc_qtof_directospos.m
 Sample Name 24-031531
 Comment BPG-VII-6A
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:22:30 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
383.0597	1	C14H23O7Se	383.0604	2.0	6.5	1	100.00	3.5	even	ok

Qualitative Compound Report

Analysis Info

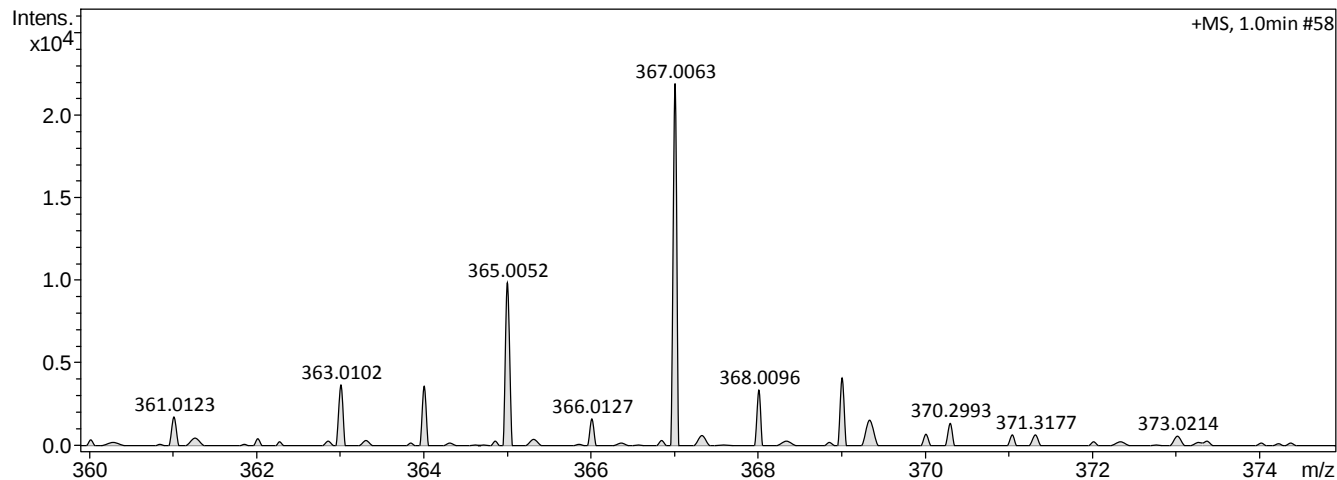
Analysis Name D:\Data\ggc\24-031532.d
 Method APCI.m
 Sample Name BPG-VII-20
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 10:10:01 AM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
367.0063	1	C14H14F3O3Se	367.0055	-2.1	28.7	1	100.00	6.5	even	ok

Mass Spectrum List Report

Analysis Info

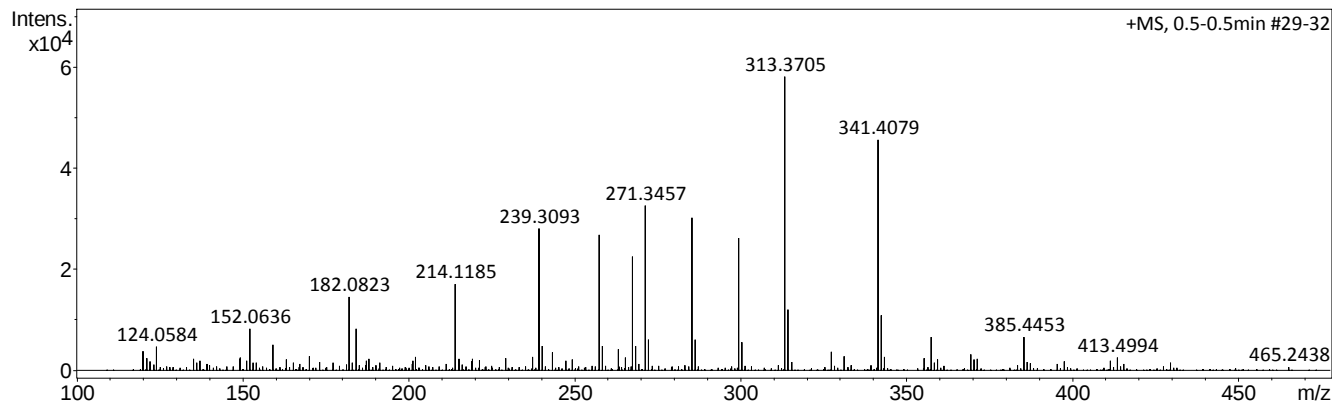
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 Method APCI.m
 Sample Name BPG-VII-27A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 10:34:56 AM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	120.0027	3836	6.6
2	124.0584	4713	8.1
3	152.0636	8254	14.2
4	159.0904	5153	8.9
5	170.0794	2842	4.9
6	182.0823	14531	25.0
7	184.0976	8214	14.2
8	214.1185	17128	29.5
9	239.3093	28100	48.4
10	240.3130	4859	8.4
11	243.3034	3608	6.2
12	257.3255	26790	46.2
13	258.3303	4890	8.4
14	263.1835	4219	7.3
15	267.3499	22504	38.8
16	268.3526	4812	8.3
17	271.3457	32565	56.1
18	272.3485	6134	10.6
19	285.3643	30153	52.0
20	286.3685	6050	10.4
21	299.3843	26145	45.1
22	300.3887	5631	9.7
23	313.3705	58008	100.0
24	314.3736	12060	20.8
25	327.3894	3746	6.5
26	341.4079	45568	78.6
27	342.4077	10844	18.7
28	357.4024	6637	11.4
29	369.4280	3157	5.4
30	385.4453	6566	11.3

Mass Spectrum List Report

Analysis Info

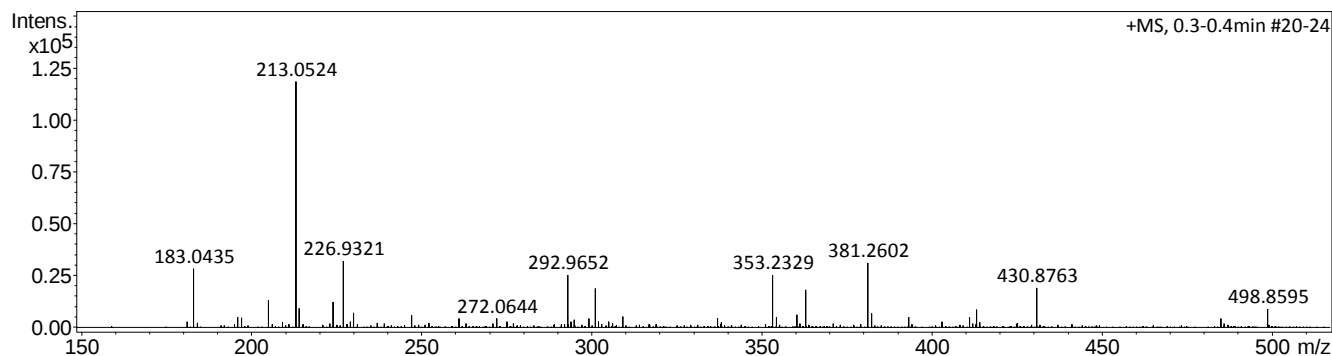
Analysis Name D:\Data\ggc\24-031533_P1-E-4_01_8830.d
 Method lc_qtof_directospos.m
 Sample Name 24-031533
 Comment BPG-VII-27A
 Sv: DCM + MeOH + HCOOH
 Spanevello

Acquisition Date 4/3/2024 3:32:43 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	183.0435	28304	23.9
2	196.0212	4968	4.2
3	205.0628	13106	11.1
4	213.0524	118314	100.0
5	214.0604	9161	7.7
6	224.0496	12218	10.3
7	226.9321	32013	27.1
8	230.0977	7189	6.1
9	247.1385	5703	4.8
10	292.9652	25311	21.4
11	301.1057	18679	15.8
12	309.1724	5217	4.4
13	353.2329	25223	21.3
14	360.2872	6231	5.3
15	362.8948	18014	15.2
16	381.2602	30992	26.2
17	382.2636	6629	5.6
18	393.2612	5006	4.2
19	413.2235	8710	7.4
20	430.8763	19203	16.2
21	498.8595	8916	7.5
22	566.8398	9564	8.1
23	591.4382	7762	6.6
24	619.4667	7049	6.0
25	634.8181	8671	7.3
26	702.8026	11110	9.4
27	770.7657	7653	6.5
28	838.7641	10151	8.6
29	906.7229	5342	4.5
30	974.7219	5643	4.8

Qualitative Compound Report

Analysis Info

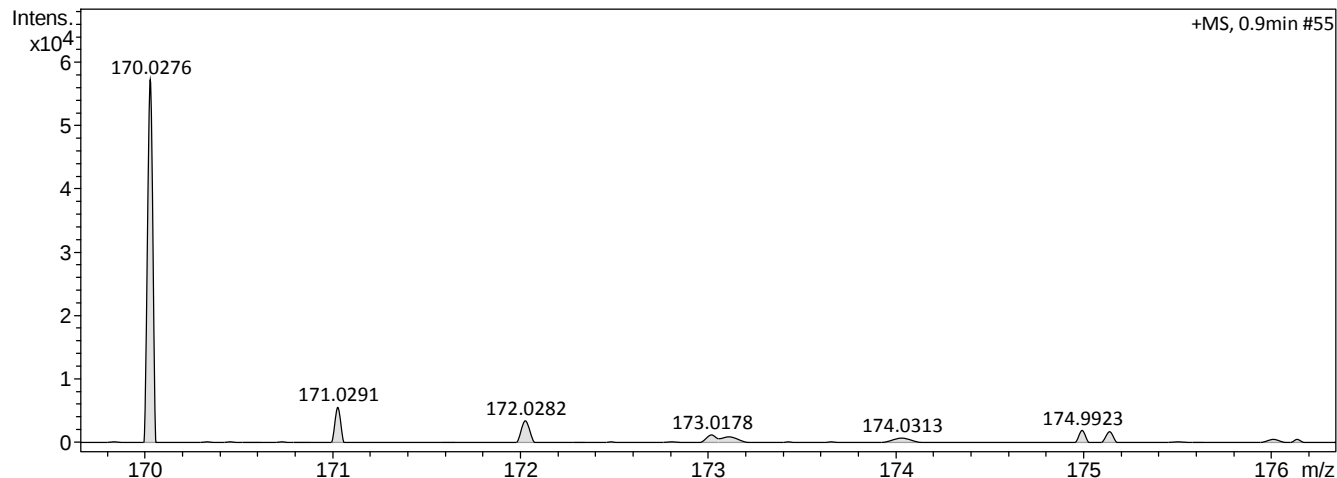
Analysis Name D:\Data\ggc\24-031534.d
 Method APCI.m
 Sample Name BPG-VII-27A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 10:44:46 AM

Operator ELB
 Instrument micrOTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
170.0276	1	C7H8NO2S	170.0270	-3.6	6.1	1	100.00	4.5	even	ok

Mass Spectrum List Report

Analysis Info

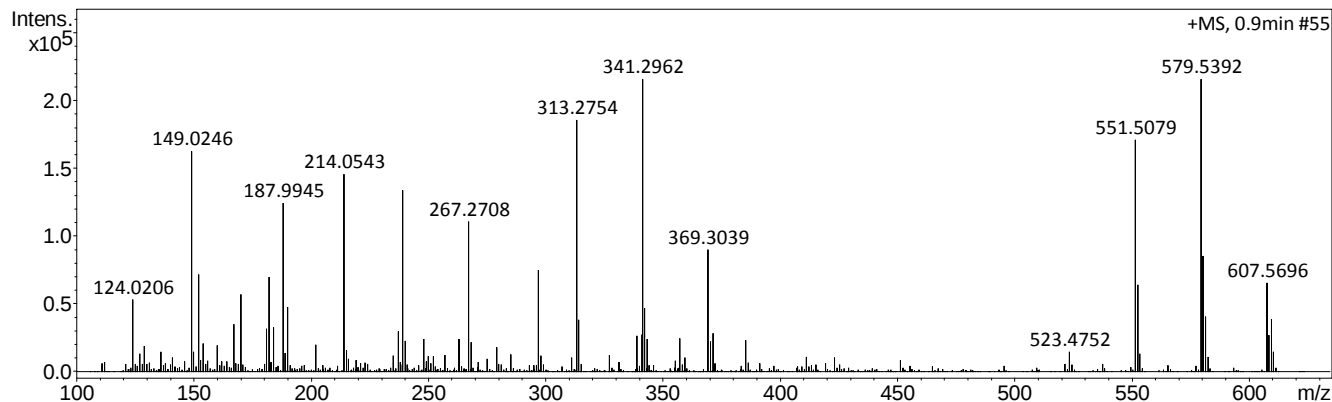
Analysis Name D:\Data\ggc\24-031534.d
 Method APCI.m
 Sample Name BPG-VII-27A
 Comment SV: DCM
 Spanevello

Acquisition Date 4/5/2024 10:44:46 AM

Operator ELB
 Instrument / Ser# microTOF-Q II

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	11.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	124.0206	53298	24.7
2	149.0246	162470	75.4
3	152.0176	71802	33.3
4	167.0345	34833	16.2
5	170.0276	57100	26.5
6	181.1226	31501	14.6
7	182.0281	69776	32.4
8	184.0419	32755	15.2
9	187.9945	124126	57.6
10	189.9906	47570	22.1
11	214.0543	145502	67.5
12	237.1861	29749	13.8
13	239.0992	31169	14.5
14	239.2381	133760	62.1
15	267.2708	110498	51.3
16	297.0919	75017	34.8
17	313.2754	185101	85.9
18	314.2806	38283	17.8
19	341.2962	215196	99.8
20	342.3003	46629	21.6
21	369.3039	89886	41.7
22	371.3162	28149	13.1
23	551.5079	170855	79.3
24	552.5102	64259	29.8
25	579.5392	215524	100.0
26	580.5411	85292	39.6
27	581.5266	40431	18.8
28	607.5696	65641	30.5
29	609.5514	38937	18.1
30	663.4560	34074	15.8