

Qualitative Compound Report

Analysis Info

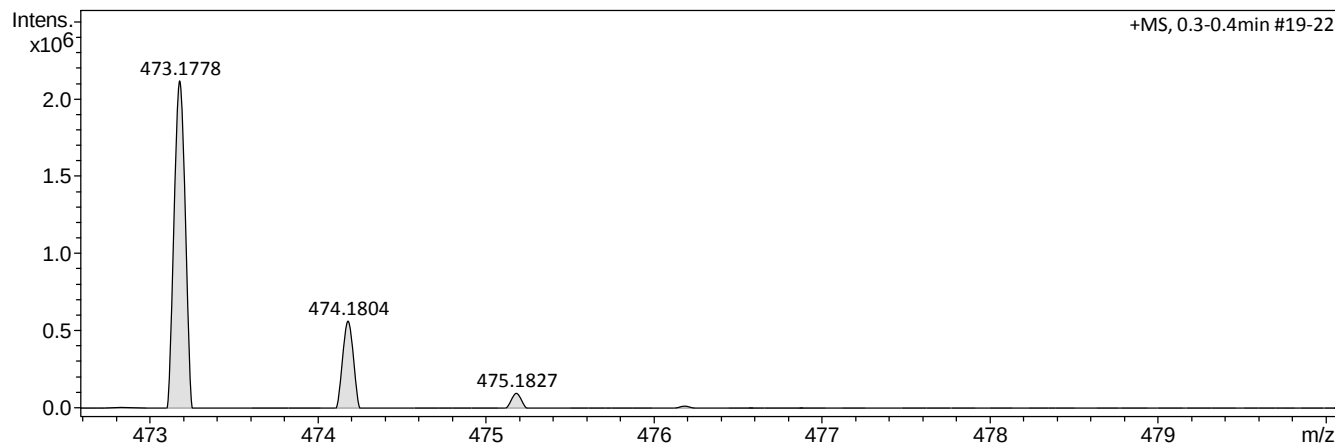
Analysis Name D:\Data\ggc\24-111503_P1-D-1_01_9777.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-111503
 Comment IABD17
 Sv: DCM + MeOH + HCOOH
 Ivan Alejandro Barri - UNLP

Acquisition Date 11/26/2024 11:52:26 AM

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
473.1778	1	C23H30NaO9	473.1782	0.8	5.7	2	100.00	8.5	even	ok

Mass Spectrum List Report

Analysis Info

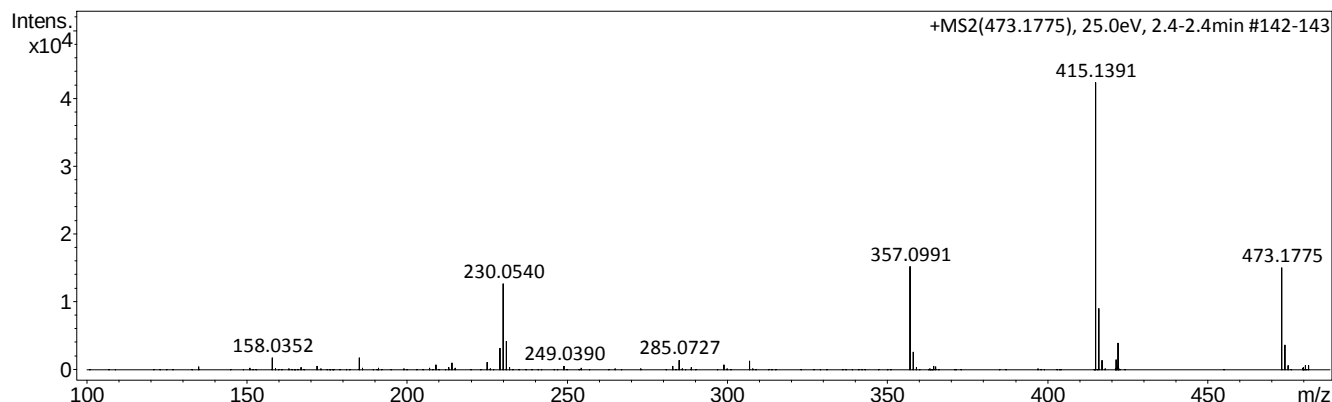
Analysis Name D:\Data\ggc\24-111503000001.d
 Method tunelow300924.m
 Sample Name IABD17
 Comment Sv: DCM + MeOH + HCOOH
 Barri - UNLP

Acquisition Date 11/29/2024 2:41:50 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 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	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	158.0352	1798	4.3
2	172.0473	505	1.2
3	185.0571	1789	4.2
4	209.0764	735	1.7
5	214.0601	1026	2.4
6	225.0704	1095	2.6
7	229.0466	3141	7.4
8	230.0540	12664	29.9
9	231.0603	4169	9.9
10	249.0390	537	1.3
11	283.1005	546	1.3
12	285.0727	1350	3.2
13	299.0912	758	1.8
14	307.0791	1297	3.1
15	357.0991	15164	35.8
16	358.1003	2616	6.2
17	364.6157	536	1.3
18	415.1391	42307	100.0
19	416.1402	8958	21.2
20	417.1415	1361	3.2
21	421.3888	760	1.8
22	421.5521	1454	3.4
23	421.6395	574	1.4
24	422.0227	3902	9.2
25	422.0959	3050	7.2
26	473.1775	14981	35.4
27	474.1810	3597	8.5
28	475.1879	604	1.4
29	480.6789	654	1.5
30	481.5654	617	1.5

Qualitative Compound Report

Analysis Info

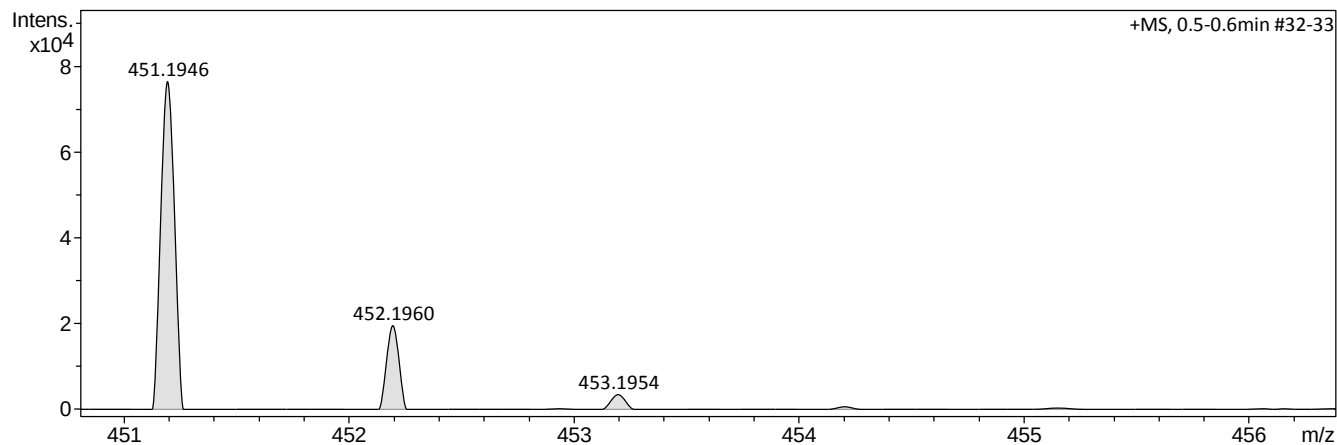
Analysis Name D:\Data\ggc\24-111504_P1-D-2_01_9778.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-111504
 Comment IABD23
 Sv: DCM + MeOH + HCOOH
 Ivan Alejandro Barri - UNLP

Acquisition Date 11/26/2024 11:57:32 AM

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
451.1946	1	C23H31O9	451.1963	3.6	2.6	1	100.00	8.5	even	ok

Mass Spectrum List Report

Analysis Info

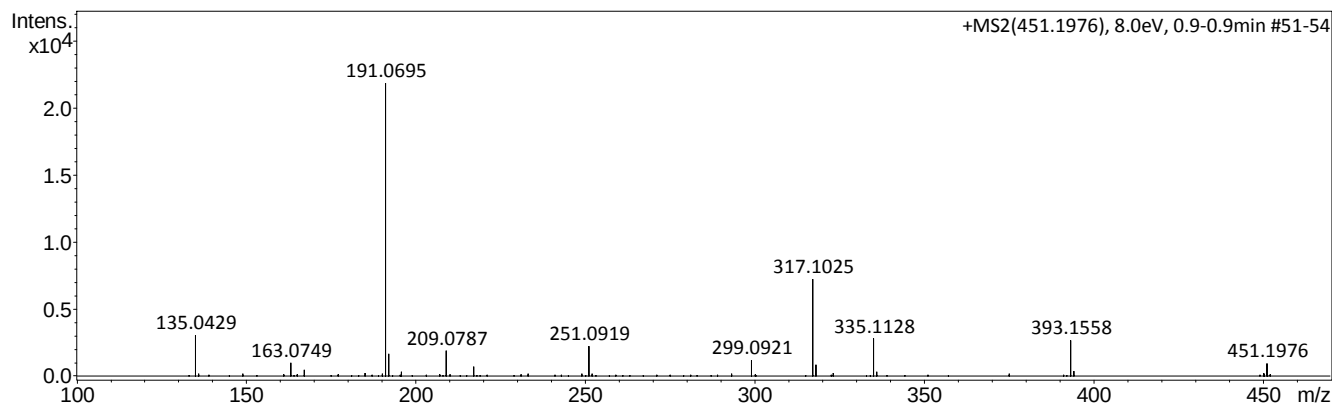
Analysis Name D:\Data\ggc\24-111504.d
 Method tunelow300924.m
 Sample Name IABD23
 Comment Sv: DCM + MeOH + HCOOH
 Ivan Alejandro Barri - UNLP

Acquisition Date 11/27/2024 12:12:18 PM

Operator EB - MV
 Instrument / Ser# microTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 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	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	135.0429	3074	14.1
2	136.0470	227	1.0
3	149.0601	190	0.9
4	163.0749	1026	4.7
5	167.0688	475	2.2
6	185.0822	239	1.1
7	190.0851	225	1.0
8	191.0695	21837	100.0
9	192.0739	1685	7.7
10	195.7607	344	1.6
11	207.0656	177	0.8
12	209.0787	1904	8.7
13	210.0858	185	0.8
14	217.0873	743	3.4
15	233.0783	211	1.0
16	249.1022	207	0.9
17	251.0919	2256	10.3
18	252.1007	211	1.0
19	293.1011	190	0.9
20	299.0921	1208	5.5
21	317.1025	7231	33.1
22	318.1035	867	4.0
23	323.1626	253	1.2
24	335.1128	2837	13.0
25	336.1180	359	1.6
26	375.1450	198	0.9
27	393.1558	2660	12.2
28	394.1557	393	1.8
29	450.2066	236	1.1
30	451.1976	984	4.5

Qualitative Compound Report

Analysis Info

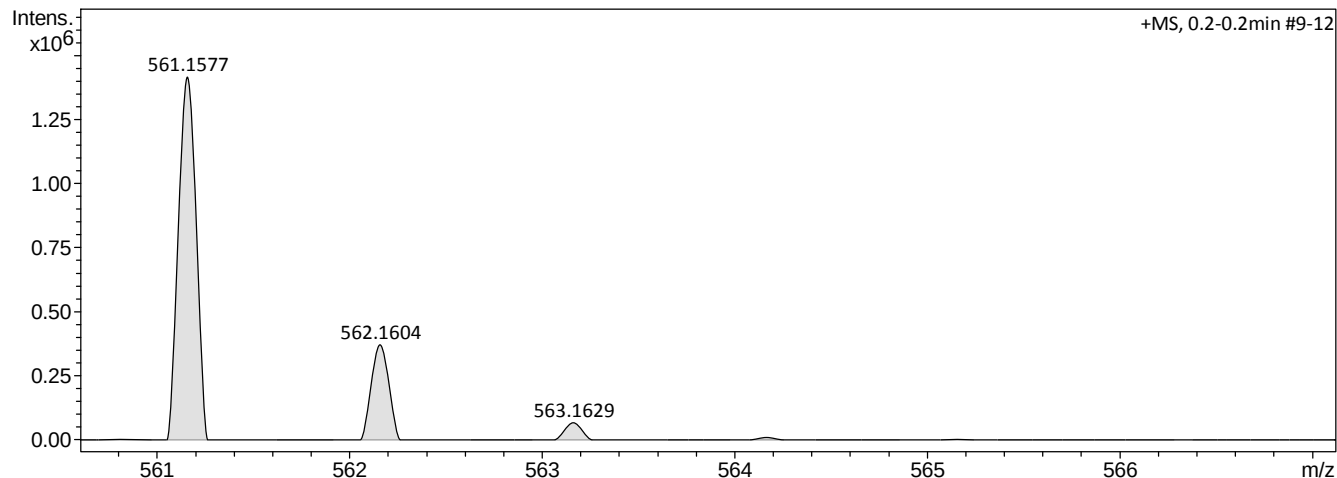
Analysis Name D:\Data\ggc\24-111505000001.d
 Method tunelow300924.m
 Sample Name IABD33
 Comment Sv: DCM + MeOH + HCOOH
 Barri - UNLP

Acquisition Date 11/29/2024 2:52:38 PM

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
561.1577	1	C25H30NaO13	561.1579	0.2	12.5	1	100.00	10.5	even	ok

Mass Spectrum List Report

Analysis Info

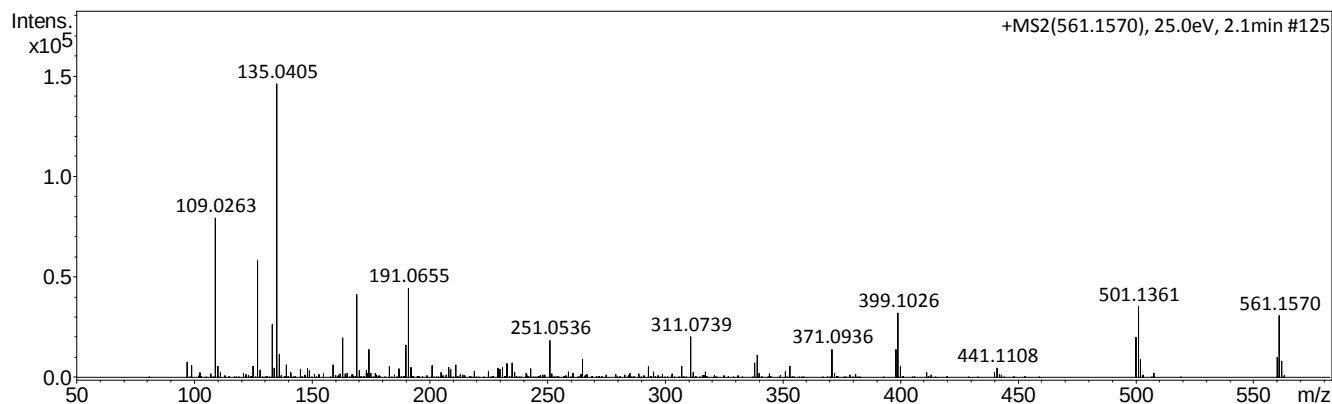
Analysis Name D:\Data\ggc\24-111505000001.d
 Method tunelow300924.m
 Sample Name IABD33
 Comment Sv: DCM + MeOH + HCOOH
 Barri - UNLP

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Operator EB - MV
 Instrument / Ser# microTOF-Q

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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	97.0271	7770	5.3
2	109.0263	79438	54.5
3	127.0361	58127	39.9
4	133.0601	26347	18.1
5	135.0405	145843	100.0
6	136.0439	11464	7.9
7	139.0340	6324	4.3
8	158.9936	6376	4.4
9	163.0673	19788	13.6
10	169.0472	41227	28.3
11	174.0883	13891	9.5
12	190.0831	16116	11.1
13	191.0655	44476	30.5
14	211.0574	6462	4.4
15	233.0412	7174	4.9
16	235.0571	7488	5.1
17	251.0536	18475	12.7
18	265.0648	9308	6.4
19	311.0739	20238	13.9
20	338.1004	7379	5.1
21	339.0870	11069	7.6
22	371.0936	14096	9.7
23	398.1196	13976	9.6
24	399.1026	32003	21.9
25	500.1465	20219	13.9
26	501.1361	35136	24.1
27	502.1372	8979	6.2
28	560.1722	10316	7.1
29	561.1570	30714	21.1
30	562.1573	8390	5.8