

Qualitative Compound Report

Analysis Info

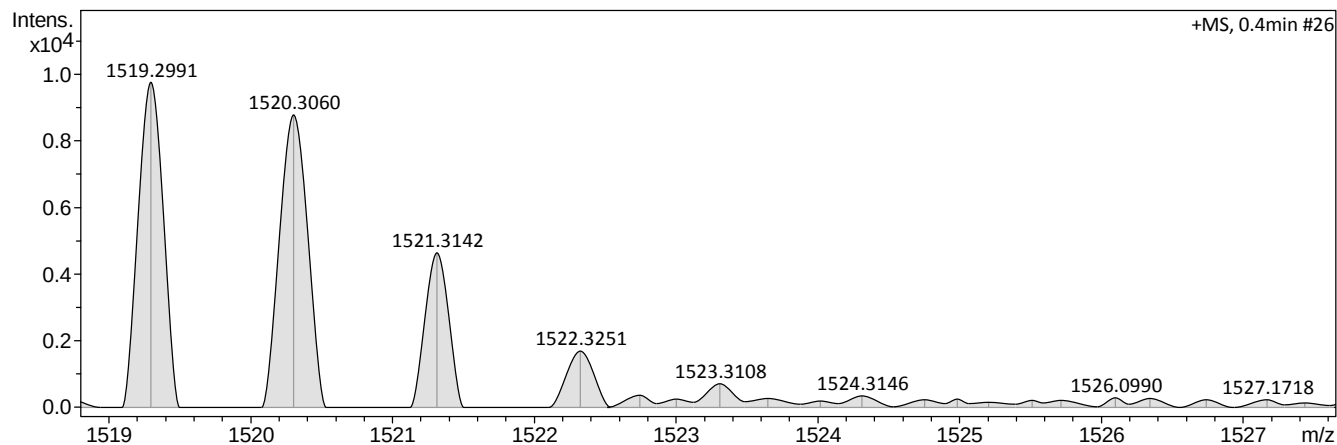
Analysis Name D:\Data\ggc\24-052401_P1-C-1_01_9239.d
 Method lc-qtof-directos pos masas altas.m
 Sample Name 24-052401
 Comment SOS807a
 Sv: DCM + MeOH + HCOOH
 Larghi

Acquisition Date 6/7/2024 1:34:58 PM

Operator MV
 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	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1800 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
1519.2991	1	C72H57F10N4O18S2	1519.2944	-3.1	206.3	6	11.52	41.5	even	ok

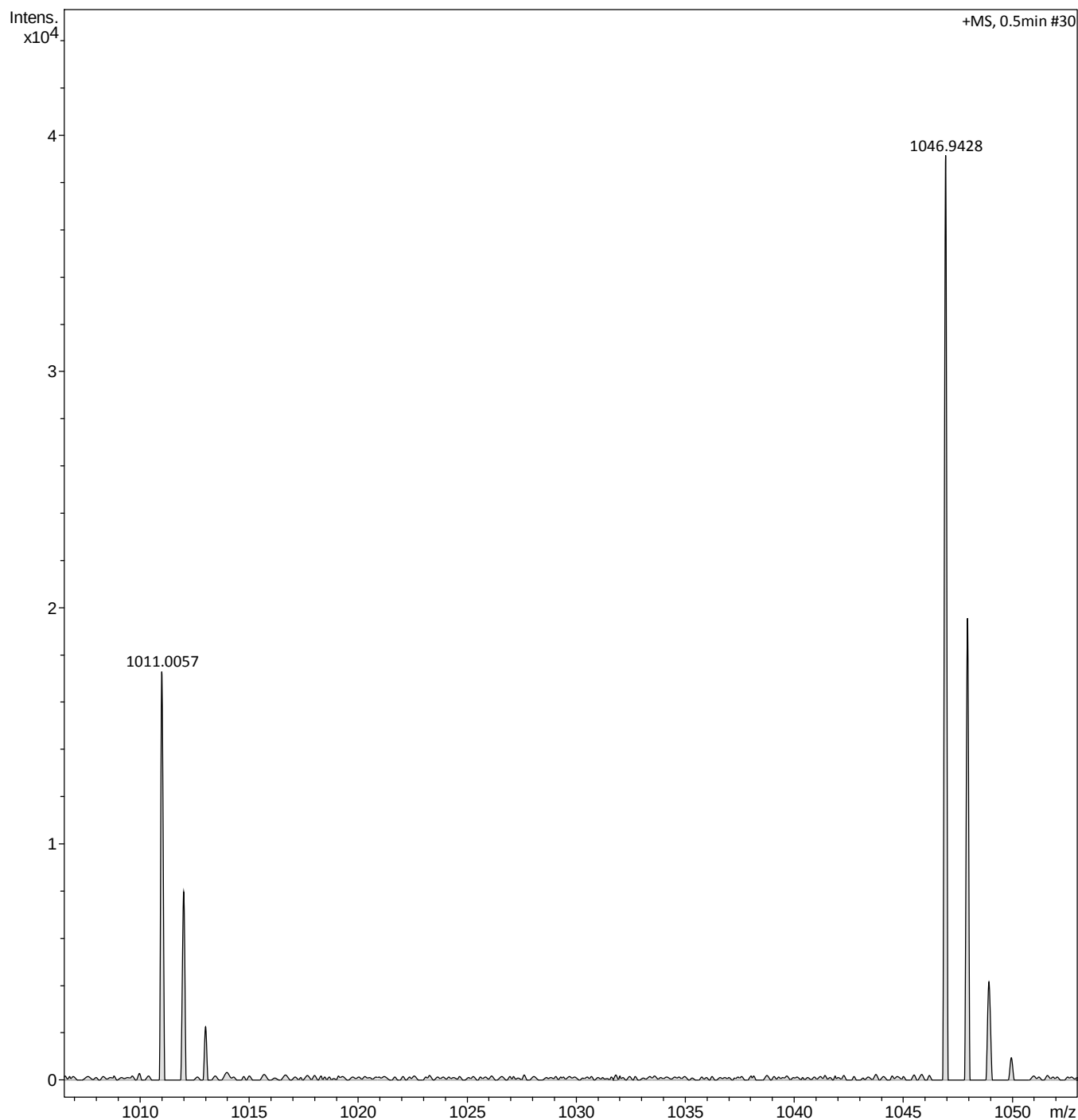
Generic Display Report

Analysis Info

Analysis Name D:\Data\ggc\24-052402_P1-C-2_01_9240.d
 Method lc-qtof-directos pos masas altas.m
 Sample Name 24-052402
 Comment SOS809k
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 6/7/2024 1:40:05 PM

Operator MV
 Instrument microTOF-Q II



Mass Spectrum List Report

Analysis Info

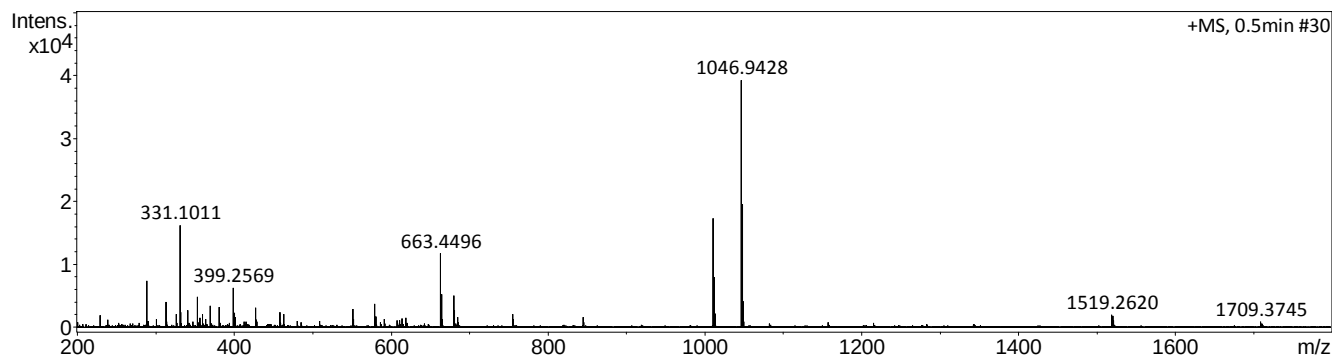
Analysis Name D:\Data\ggc\24-052402_P1-C-2_01_9240.d
 Method lc-qtof-directos pos masas altas.m
 Sample Name 24-052402
 Comment SOS809k
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 6/7/2024 1:40:05 PM

Operator MV
 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	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	289.0913	7435	19.0
2	313.2727	4009	10.2
3	326.1763	2138	5.5
4	331.1011	16185	41.4
5	331.2828	2299	5.9
6	332.1057	2450	6.3
7	341.3040	2746	7.0
8	353.2667	4843	12.4
9	359.3131	2118	5.4
10	369.1138	3426	8.8
11	381.2961	3215	8.2
12	399.2569	6292	16.1
13	400.2569	2343	6.0
14	427.2886	3189	8.2
15	458.1467	2451	6.3
16	463.1041	2140	5.5
17	551.4995	2954	7.6
18	579.5333	3725	9.5
19	663.4496	11705	29.9
20	664.4546	5217	13.3
21	680.4761	5050	12.9
22	681.4808	2693	6.9
23	755.3528	2099	5.4
24	1011.0057	17284	44.2
25	1012.0002	7965	20.4
26	1013.0104	2261	5.8
27	1046.9428	39121	100.0
28	1047.9482	19553	50.0
29	1048.9475	4154	10.6
30	1519.2620	2051	5.2

Mass Spectrum List Report

Analysis Info

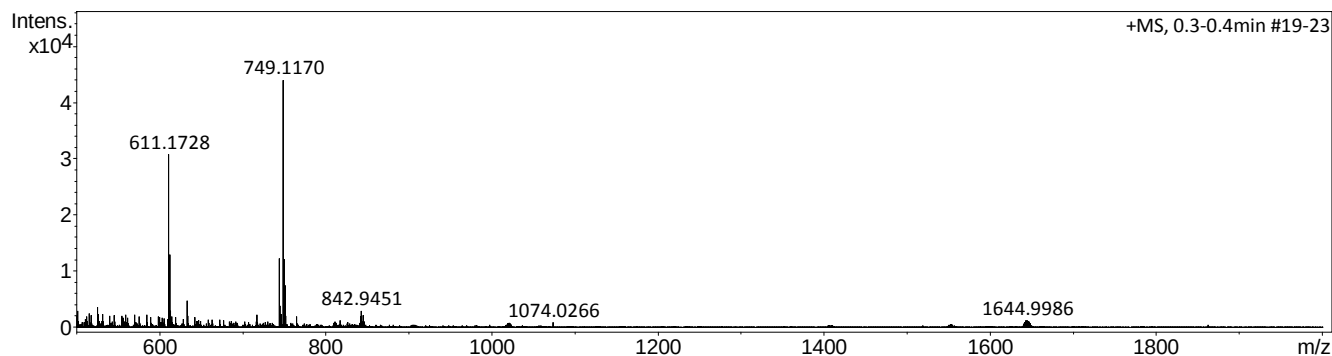
Analysis Name D:\Data\ggc\24-052403_P1-C-3_01_9244.d
 Method lc-qtof-directos pos masas altas hasta 2000.m
 Sample Name 24-052403
 Comment SOS834a
 Sv: DCM + MeOH + HCOOH
 Larghi

Acquisition Date 6/7/2024 2:53:29 PM

Operator MV
 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	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	501.1179	2049	4.7
2	501.3616	2984	6.8
3	515.3753	2499	5.7
4	517.3564	2135	4.9
5	525.1573	3636	8.3
6	526.4182	2352	5.4
7	531.3733	2368	5.4
8	540.4283	2068	4.7
9	545.3883	2110	4.8
10	554.4452	2086	4.8
11	559.4013	2270	5.2
12	570.4422	2324	5.3
13	575.3948	1983	4.5
14	584.4559	2279	5.2
15	611.1728	30703	70.0
16	612.1753	12882	29.4
17	613.1808	2981	6.8
18	633.1515	4813	11.0
19	634.1591	2083	4.8
20	717.1438	2271	5.2
21	744.1588	12290	28.0
22	745.1628	3903	8.9
23	746.1591	2330	5.3
24	749.1170	43845	100.0
25	750.1199	12161	27.7
26	751.1182	7535	17.2
27	752.1178	2087	4.8
28	841.9468	1983	4.5
29	842.9451	3002	6.8
30	844.9435	2198	5.0

Mass Spectrum List Report

Analysis Info

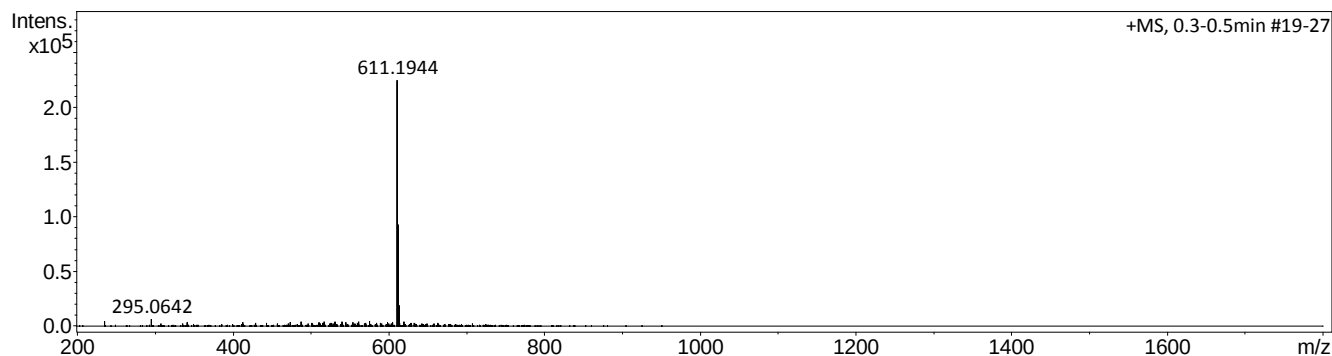
Analysis Name D:\Data\ggc\24-052404_P1-C-4_01_9242.d
 Method lc-qtof-directos pos masas altas.m
 Sample Name 24-052404
 Comment SOS835k
 Sv: MeOH + HCOOH
 Larghi

Acquisition Date 6/7/2024 1:50:24 PM

Operator MV
 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	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	235.2391	4603	2.1
2	295.0642	6831	3.0
3	341.0579	3719	1.7
4	413.0574	3838	1.7
5	443.3344	3185	1.4
6	473.3454	3671	1.6
7	487.3582	4484	2.0
8	501.3797	3223	1.4
9	510.4381	3570	1.6
10	515.3964	3278	1.5
11	517.3689	3982	1.8
12	526.4331	3376	1.5
13	531.3891	4480	2.0
14	540.4525	4070	1.8
15	545.4033	3716	1.7
16	554.4619	3764	1.7
17	561.3956	4251	1.9
18	570.4601	3285	1.5
19	575.4111	4721	2.1
20	584.4767	3222	1.4
21	598.4935	3504	1.6
22	605.4198	3565	1.6
23	611.1944	224246	100.0
24	612.1976	92769	41.4
25	613.1994	19359	8.6
26	614.2022	2954	1.3
27	614.4892	2969	1.3
28	619.4327	3977	1.8
29	628.5036	2947	1.3
30	663.4563	3012	1.3