

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-42_P1-D-6_01_5268.d
Method lc_qtof_directospos.m
Sample Name US-42
Comment Sv: DCM + MeOH + HCOOH
Cecilia Attorresi

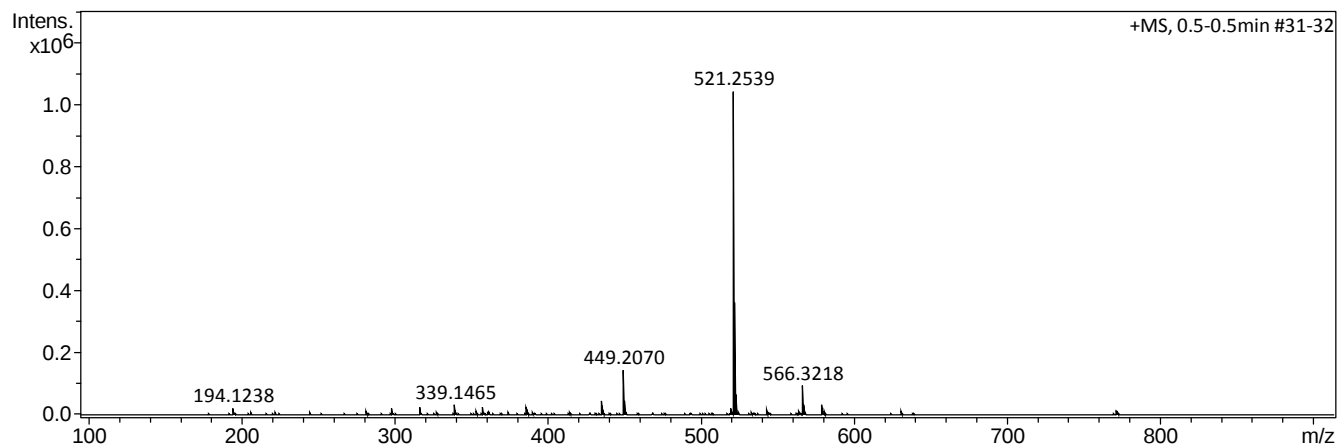
Acquisition Date 7/28/2022 1:44:33 PM

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	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 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
521.2539	1	C29H29N8O2	521.2408	-25.2	0.9	1	0.00	19.5	even	ok
	2	C28H29N10O	521.2520	-3.6	2.3	2	34.63	19.5	even	ok
	3	C30H37N2O6	521.2646	20.5	5.0	3	0.00	13.5	even	ok
	4	C31H37O7	521.2534	-1.0	5.2	4	100.00	13.5	even	ok
	5	C27H29N12	521.2633	17.9	5.2	5	0.00	19.5	even	ok
	6	C31H33N6O2	521.2660	23.1	8.4	6	0.00	18.5	even	ok
	7	C32H33N4O3	521.2547	1.5	10.8	7	78.72	18.5	even	ok
	8	C28H33N4O6	521.2395	-27.7	11.3	8	0.00	14.5	even	ok
	9	C27H33N6O5	521.2507	-6.2	13.3	9	11.73	14.5	even	ok
	10	C33H33N2O4	521.2435	-20.0	13.4	10	0.00	18.5	even	ok
	11	C26H33N8O4	521.2619	15.4	15.4	11	0.01	14.5	even	ok
	12	C35H37O4	521.2686	28.2	21.2	12	0.00	17.5	even	ok
	13	C34H29N6	521.2448	-17.4	24.4	13	0.00	23.5	even	ok
	14	C26H37N2O9	521.2494	-8.7	25.0	14	1.94	9.5	even	ok
	15	C25H37N4O8	521.2606	12.8	27.0	15	0.07	9.5	even	ok
	16	C37H33N2O	521.2587	9.3	34.7	16	1.06	22.5	even	ok
	17	C38H33O2	521.2475	-12.3	37.2	17	0.09	22.5	even	ok
	18	C24H41O12	521.2593	10.2	38.7	18	0.46	4.5	even	ok