

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-44 ta repeticion_P1-B-1_01_7425.d
Method lc_qtof_directospos mrm atorressi.m
Sample Name US-44 ta repeticion
Comment Sv: MeOH + HCOOH
Cecilia Attoresi

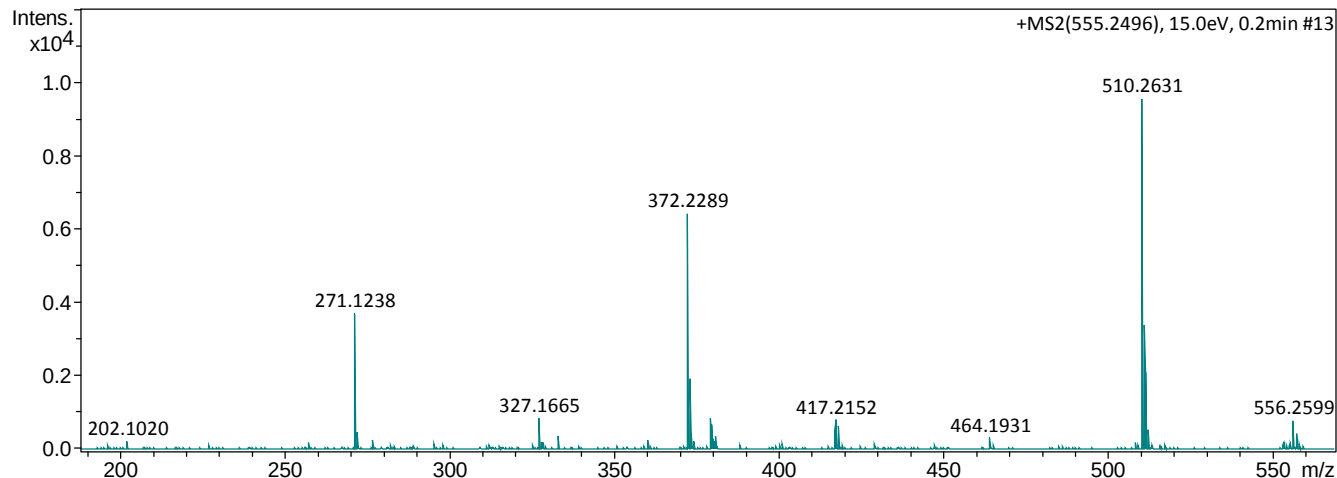
Acquisition Date 6/14/2023 1:39:43 PM

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
202.1020	1	C13H13FN	202.1027	3.2	n.a.	1	100.00	7.5	even	ok
	2	C10H15FO3	202.1000	-10.1	n.a.	2	41.08	3.0	odd	ok
	3	C13H14O2	202.0988	-15.7	n.a.	3	14.89	7.0	odd	ok
	4	C8H13FN3O2	202.0986	-16.7	n.a.	4	12.12	3.5	even	ok
271.1238	1	C13H18FNO4	271.1214	-8.7	17.5	1	40.92	5.0	odd	ok
	2	C16H17NO3	271.1203	-13.0	34.6	2	9.22	9.0	odd	ok
	3	C16H16FN2O	271.1241	1.1	35.4	3	100.00	9.5	even	ok
	4	C19H15N2	271.1230	-3.1	53.9	4	45.43	13.5	even	ok
327.1665	1	C19H23N2O3	327.1703	11.8	17.4	1	72.35	9.5	even	ok
	2	C20H22FNO2	327.1629	-10.8	18.7	2	100.00	10.0	odd	ok
	3	C16H24FN2O4	327.1715	15.3	18.9	3	16.17	5.5	even	ok
	4	C22H21N3	327.1730	20.0	31.2	4	1.06	14.0	odd	ok
	5	C23H21NO	327.1618	-14.3	34.0	5	17.52	14.0	odd	ok
333.1377	1	C18H20FNO4	333.1371	-1.8	n.a.	1	100.00	9.0	odd	ok
	2	C24H17N2	333.1386	2.8	n.a.	2	84.93	17.5	even	ok
	3	C21H19NO3	333.1359	-5.3	n.a.	3	50.04	13.0	odd	ok
	4	C21H18FN2O	333.1398	6.2	n.a.	4	39.75	13.5	even	ok
360.1853	1	C20H25FN2O3	360.1844	-2.5	n.a.	1	100.00	9.0	odd	ok
	2	C23H23FN3	360.1871	4.9	n.a.	2	57.85	13.5	even	ok
	3	C28H24	360.1873	5.5	n.a.	3	49.93	17.0	odd	ok
	4	C23H24N2O2	360.1832	-5.7	n.a.	4	46.95	13.0	odd	ok
	5	C25H25FO	360.1884	8.6	n.a.	5	18.39	13.0	odd	ok
	6	C19H26N3O4	360.1918	18.1	n.a.	6	0.18	8.5	even	ok
372.2289	1	C27H29F	372.2248	-10.9	5.0	1	8.72	13.0	odd	ok
	2	C26H30NO	372.2322	9.0	7.7	2	18.83	12.5	even	ok
	3	C23H31FNO2	372.2333	12.0	24.8	3	3.51	8.5	even	ok
	4	C23H32O4	372.2295	1.8	26.5	4	100.00	8.0	odd	ok
	5	C21H30N3O3	372.2282	-1.8	32.9	5	84.77	8.5	even	ok
	6	C18H31FN3O4	372.2293	1.2	51.4	6	56.25	4.5	even	ok
417.2152	1	C31H29O	417.2213	14.6	264.4	1	17.56	17.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
	2	C30H27NO	417.2087	-15.6	268.9	2	5.31	18.0	odd	ok
	3	C29H27N3	417.2199	11.4	271.4	3	60.81	18.0	odd	ok
	4	C28H30FO2	417.2224	17.3	283.4	4	0.26	13.5	even	ok
	5	C27H28FNO2	417.2099	-12.8	287.8	5	3.85	14.0	odd	ok
	6	C26H28FN3O	417.2211	14.1	290.4	6	1.24	14.0	odd	ok
	7	C26H29N2O3	417.2173	4.9	291.6	7	100.00	13.5	even	ok
	8	C23H30FN2O4	417.2184	7.7	310.4	8	3.52	9.5	even	ok
464.1931	1	C33H24N2O	464.1883	-10.3	34.6	1	25.88	23.0	odd	ok
	2	C31H27FNO2	464.2020	19.2	35.9	2	0.01	18.5	even	ok
	3	C30H25FN2O2	464.1895	-7.9	36.9	3	100.00	19.0	odd	ok
	4	C31H28O4	464.1982	11.0	38.0	4	15.21	18.0	odd	ok
	5	C29H26N3O3	464.1969	8.1	39.0	5	83.06	18.5	even	ok
	6	C30H26NO4	464.1856	-16.1	39.1	6	0.26	18.5	even	ok
	7	C26H27FN3O4	464.1980	10.6	56.2	7	8.84	14.5	even	ok
510.2631	1	C32H33FN3O2	510.2551	-15.6	8.8	1	0.01	17.5	even	ok
	2	C33H35FN2O2	510.2677	9.1	12.0	2	3.01	17.0	odd	ok
	3	C33H36NO4	510.2639	1.6	12.5	3	100.00	16.5	even	ok
556.2599	1	C33H35FN3O4	556.2606	1.2	93.9	1	100.00	17.5	even	ok