

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-44 MRM 556.d
Method Tune_low_format 210120.m
Sample Name US-44 MRM 556
Comment Ceci

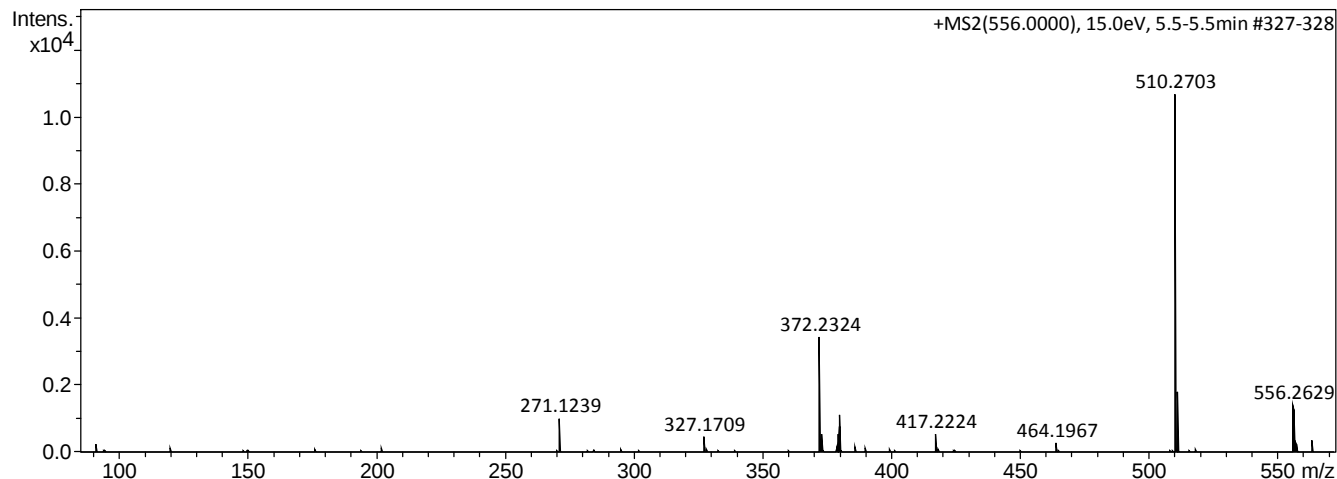
Acquisition Date 4/11/2023 10:05:16 AM

Operator ELB
Instrument micrOTOF-Q II



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	1500 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
271.1239	1	C16H16FN2O	271.1241	0.8	n.a.	1	100.00	9.5	even	ok
	2	C19H15N2	271.1230	-3.4	n.a.	2	69.88	13.5	even	ok
	3	C13H18FNO4	271.1214	-9.1	n.a.	3	23.64	5.0	odd	ok
327.1709	1	C16H24FN2O4	327.1715	1.7	n.a.	1	100.00	5.5	even	ok
	2	C19H23N2O3	327.1703	-1.8	n.a.	2	97.25	9.5	even	ok
	3	C22H21N3	327.1730	6.4	n.a.	3	37.95	14.0	odd	ok
	4	C19H22FN3O	327.1741	9.9	n.a.	4	13.62	10.0	odd	ok
372.2324	1	C18H31FN3O4	372.2293	-8.4	36.9	1	39.33	4.5	even	ok
	2	C23H32O4	372.2295	-7.9	62.0	2	22.31	8.0	odd	ok
	3	C23H31FNO2	372.2333	2.4	62.9	3	100.00	8.5	even	ok
	4	C26H30NO	372.2322	-0.7	81.6	4	67.49	12.5	even	ok
417.2224	1	C28H30FO2	417.2224	0.1	n.a.	1	100.00	13.5	even	ok
	2	C31H29O	417.2213	-2.6	n.a.	2	59.88	17.5	even	ok
	3	C26H28FN3O	417.2211	-3.1	n.a.	3	53.05	14.0	odd	ok
	4	C29H27N3	417.2199	-5.8	n.a.	4	22.89	18.0	odd	ok
	5	C23H30FN2O4	417.2184	-9.5	n.a.	5	4.82	9.5	even	ok
464.1967	1	C29H26N3O3	464.1969	0.3	n.a.	1	100.00	18.5	even	ok
	2	C26H27FN3O4	464.1980	2.8	n.a.	2	41.41	14.5	even	ok
	3	C31H28O4	464.1982	3.2	n.a.	3	48.57	18.0	odd	ok
510.2703	1	C33H35FN2O2	510.2677	-5.1	106.3	2	100.00	17.0	odd	ok
556.2629	1	C33H35FN3O4	556.2606	-4.0	86.4	1	100.00	17.5	even	ok