

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\US-10_P1-D-1_01_2088.d
Method tune_pos_formate lcms.m
Sample Name US-10
Comment Sv: agua + metanol
Dr. Oscar Varela

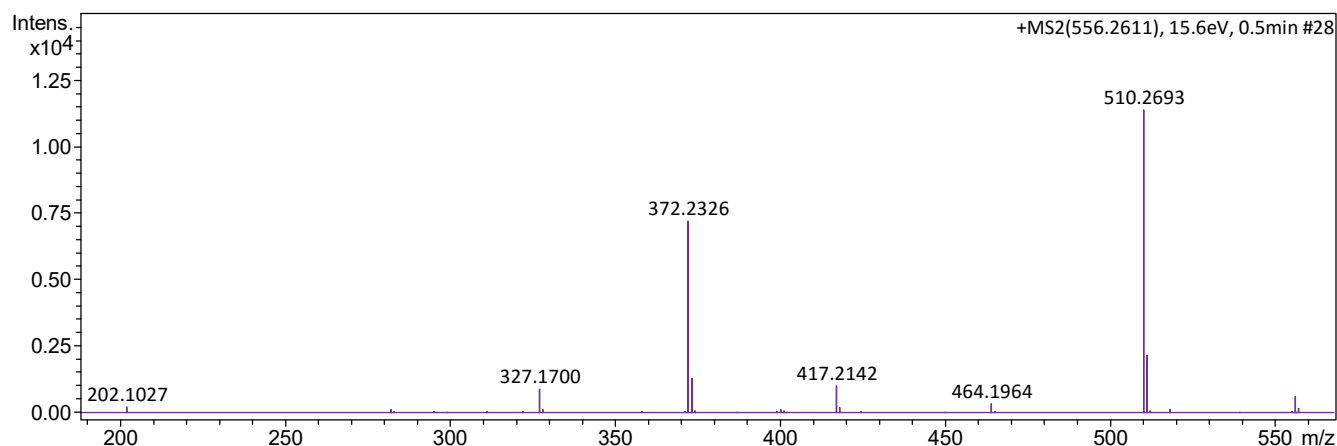
Acquisition Date 30/10/2019 12:59:24 p. m.

Operator GC
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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
202.1027	1	C13H13FN	202.1027	-0.2	n.a.	1	100.00	7.5	even	ok
327.1700	1	C16H24FN2O4	327.1715	4.5	33.4	1	87.98	5.5	even	ok
	2	C19H23N2O3	327.1703	1.0	51.4	2	100.00	9.5	even	ok
	3	C22H21N3	327.1730	9.2	70.9	3	7.76	14.0	odd	ok
372.2326	1	C18H31FN3O4	372.2293	-9.0	20.2	1	24.89	4.5	even	ok
	2	C23H32O4	372.2295	-8.4	45.0	2	16.36	8.0	odd	ok
	3	C23H31FNO2	372.2333	1.8	45.8	3	100.00	8.5	even	ok
	4	C26H30NO	372.2322	-1.2	64.5	4	61.36	12.5	even	ok
417.2142	1	C23H30FN2O4	417.2184	10.1	39.3	1	47.92	9.5	even	ok
	2	C26H29N2O3	417.2173	7.3	56.9	2	100.00	13.5	even	ok
464.1964	1	C26H27FN3O4	464.1980	3.4	68.1	1	50.75	14.5	even	ok
	2	C29H26N3O3	464.1969	1.0	75.2	2	100.00	18.5	even	ok
	3	C31H28O4	464.1982	3.9	81.6	3	34.89	18.0	odd	ok
510.2693	1	C33H35FN2O2	510.2677	-3.1	94.7	1	100.00	17.0	odd	ok
556.2611	1	C33H35FN3O4	556.2606	-1.0	63.9	1	100.00	17.5	even	ok