

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\US-46_P1-F-9_01_5713.d
Method lc_qtof_directospos.m
Sample Name US-46
Comment Sv: MeOH + HCOOH
Attorressi

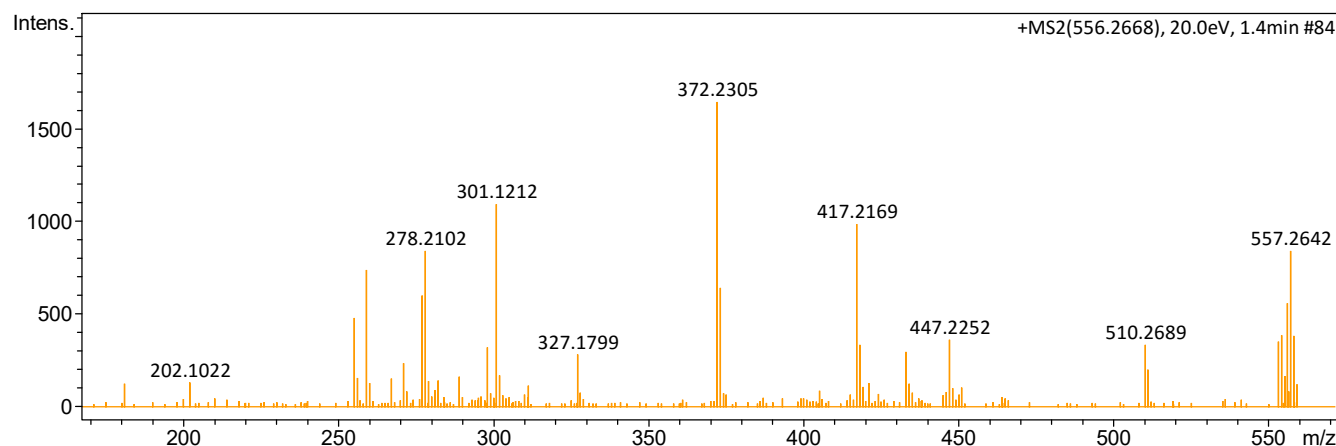
Acquisition Date 4/10/2022 10:13:05 a. m.

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
181.1034	1	C11H14FO	181.1023	-6.2	n.a.	1	100.00	4.5	even	ok
202.1022	1	C13H13FN	202.1027	2.2	n.a.	1	100.00	7.5	even	ok
255.1520	1	C13H20FN2O2	255.1503	-6.5	100.8	1	100.00	4.5	even	ok
259.1244	1	C15H16FN2O	259.1241	-1.0	9.5	1	100.00	8.5	even	ok
	2	C18H15N2	259.1230	-5.4	19.7	2	43.95	12.5	even	ok
278.2102	1	C17H28NO2	278.2115	4.6	20.3	1	100.00	4.5	even	ok
301.1212	1	C16H16FN3O2	301.1221	2.9	22.0	1	100.00	10.0	odd	ok
	2	C19H15N3O	301.1210	-0.9	39.7	2	86.86	14.0	odd	ok
	3	C21H17O2	301.1223	3.5	46.7	3	47.47	13.5	even	ok
372.2305	1	C26H30NO	372.2322	4.5	64.2	1	100.00	12.5	even	ok
	2	C23H32O4	372.2295	-2.7	82.6	2	77.33	8.0	odd	ok
	3	C21H30N3O3	372.2282	-6.3	88.2	3	23.92	8.5	even	ok
	4	C18H31FN3O4	372.2293	-3.2	105.8	4	24.00	4.5	even	ok
417.2169	1	C26H29N2O3	417.2173	1.0	45.0	1	100.00	13.5	even	ok
	2	C23H30FN2O4	417.2184	3.7	60.5	2	32.12	9.5	even	ok
433.2131	1	C26H29N2O4	433.2122	-2.1	206.5	1	100.00	13.5	even	ok
	2	C26H28FN3O2	433.2160	6.8	208.9	2	17.62	14.0	odd	ok
	3	C29H27N3O	433.2149	4.1	221.9	3	14.17	18.0	odd	ok
447.2252	1	C27H31N2O4	447.2278	5.8	32.8	1	100.00	13.5	even	ok
	2	C31H28FN2	447.2231	-4.8	49.0	2	95.44	18.5	even	ok
510.2689	1	C33H35FN2O2	510.2677	-2.4	118.5	1	100.00	17.0	odd	ok