

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-47 ta T4-6_P1-C-6_01_7739.d
Method lc_qtof_directospos mrm atorressi us-47 tolueno.m
Sample Name US-47 ta T4-6
Comment Sv: MeOH + HCOOH
Cecilia Attoresi

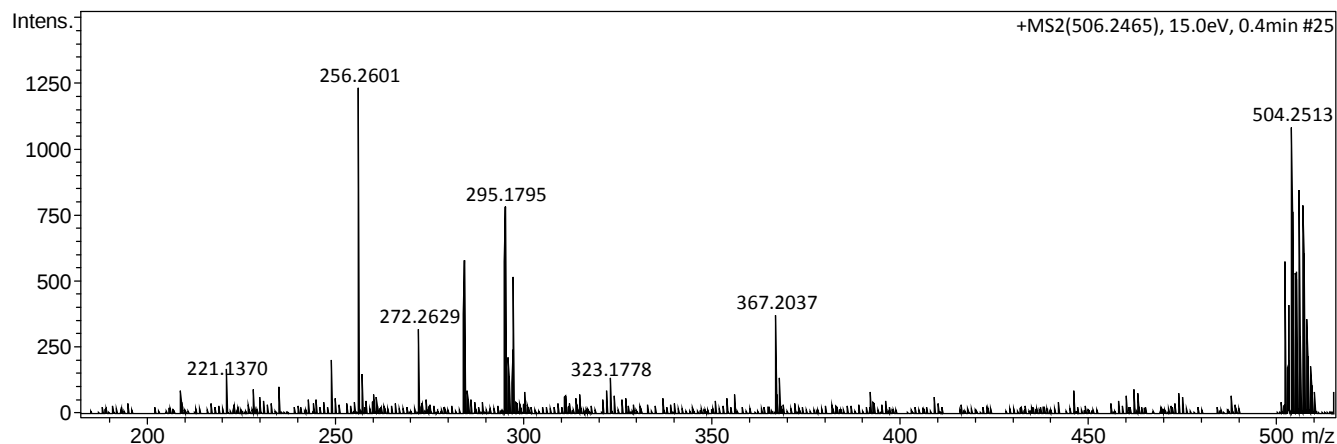
Acquisition Date 8/2/2023 9:46:46 AM

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
221.1370	1	C14H18FO	221.1336	-15.2	n.a.	1	100.00	5.5	even	ok
235.1302	1	C14H19O3	235.1329	11.5	n.a.	1	100.00	5.5	even	ok
	2	C11H20FO4	235.1340	16.4	n.a.	2	30.84	1.5	even	ok
249.1255	1	C10H18FN2O4	249.1245	-4.1	n.a.	1	100.00	2.5	even	ok
	2	C18H17O	249.1274	7.5	n.a.	2	57.96	10.5	even	ok
	3	C13H17N2O3	249.1234	-8.7	n.a.	3	45.79	6.5	even	ok
	4	C15H18FO2	249.1285	12.0	n.a.	4	21.93	6.5	even	ok
256.2601	1	C8H35FN3O4	256.2606	1.9	12.2	1	100.00	-7.5	even	ok
	2	C11H34N3O3	256.2595	-2.6	12.2	2	91.88	-3.5	even	ok
	3	C13H35FNO2	256.2646	17.6	18.9	3	2.61	-3.5	even	ok
	4	C16H34NO	256.2635	13.1	36.9	4	6.52	0.5	even	ok
272.2629	1	C13H35FNO3	272.2595	-12.1	n.a.	1	100.00	-3.5	even	ok
	2	C16H34NO2	272.2584	-16.3	n.a.	2	26.58	0.5	even	ok
295.1795	1	C19H23N2O	295.1805	3.5	35.9	1	100.00	9.5	even	ok
	2	C16H24FN2O2	295.1816	7.4	52.8	2	28.15	5.5	even	ok
297.2338	1	C17H30FN2O	297.2337	-0.4	n.a.	1	100.00	3.5	even	ok
	2	C20H29N2	297.2325	-4.2	n.a.	2	55.50	7.5	even	ok
323.1778	1	C17H24FN2O3	323.1765	-3.9	n.a.	1	100.00	6.5	even	ok
	2	C25H23	323.1794	5.1	n.a.	2	77.58	14.5	even	ok
	3	C20H23N2O2	323.1754	-7.4	n.a.	3	43.57	10.5	even	ok
	4	C22H24FO	323.1806	8.6	n.a.	4	30.92	10.5	even	ok
367.2037	1	C27H27O	367.2056	5.4	46.6	1	100.00	14.5	even	ok
	2	C24H28FO2	367.2068	8.5	61.4	2	22.92	10.5	even	ok
	3	C22H27N2O3	367.2016	-5.5	68.8	3	46.32	10.5	even	ok
	4	C19H28FN2O4	367.2028	-2.4	85.9	4	49.97	6.5	even	ok
504.2513	1	C31H35FNO4	504.2545	6.2	n.a.	1	100.00	14.5	even	ok
	2	C33H31FN3O	504.2446	-13.4	n.a.	2	0.63	19.5	even	ok
506.2465	1	C29H33FN3O4	506.2450	-3.0	n.a.	1	100.00	14.5	even	ok