

Qualitative Compound Report

Analysis Info

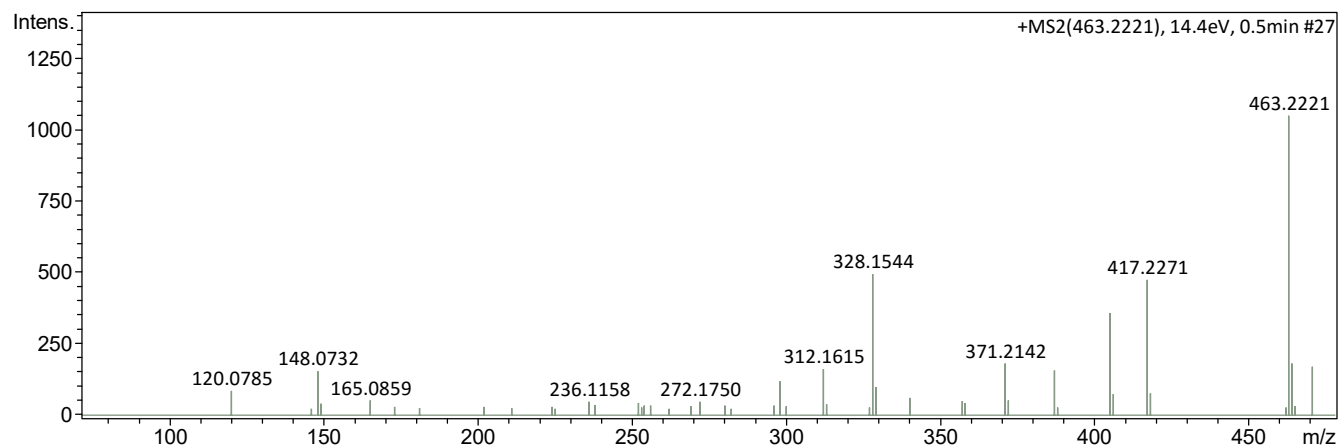
Analysis Name D:\Data\US-2_P1-C-2_01_2080.d
Method tune_pos_formate lcms.m
Sample Name US-2
Comment Glu-C6F13
Sv: DCM + MeOH
Erwin Mora / Alberto Postigo

Acquisition Date 30/10/2019 12:18:15 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
120.0785	1	C5H12O3	120.0781	-3.4	n.a.	1	100.00	0.0	odd	ok
148.0732	1	C6H12O4	148.0730	-1.3	107.2	1	100.00	1.0	odd	ok
165.0859	1	C5H13N2O4	165.0870	6.4	n.a.	1	100.00	0.5	even	ok
202.0404	1	C15H6O	202.0413	4.5	n.a.	1	100.00	13.0	odd	ok
236.1158	1	C12H16N2O3	236.1155	-1.2	450.3	1	100.00	6.0	odd	ok
272.1750	1	C13H24N2O4	272.1731	-7.3	n.a.	1	100.00	3.0	odd	ok
	2	C18H24O2	272.1771	7.5	n.a.	2	95.70	7.0	odd	ok
298.1447	1	C18H20NO3	298.1438	-3.1	177.1	1	100.00	9.5	even	ok
	2	C21H18N2	298.1465	5.9	190.3	2	20.81	14.0	odd	ok
312.1615	1	C22H20N2	312.1621	2.0	17.9	1	100.00	14.0	odd	ok
	2	C19H22NO3	312.1594	-6.6	21.4	2	37.67	9.5	even	ok
328.1544	1	C19H22NO4	328.1543	-0.2	19.1	1	100.00	9.5	even	ok
	2	C22H20N2O	328.1570	7.9	33.7	2	14.13	14.0	odd	ok
340.1538	1	C20H22NO4	340.1543	1.7	n.a.	1	100.00	10.5	even	ok
	2	C23H20N2O	340.1570	9.5	n.a.	2	13.48	15.0	odd	ok
371.2142	1	C25H27N2O	371.2118	-6.6	23.3	1	100.00	13.5	even	ok
387.2092	1	C25H27N2O2	387.2067	-6.4	67.8	1	100.00	13.5	even	ok
405.2193	1	C25H29N2O3	405.2173	-5.1	50.3	1	100.00	12.5	even	ok
417.2271	1	C27H31NO3	417.2298	6.5	85.6	1	100.00	13.0	odd	ok
463.2221	1	C27H31N2O5	463.2227	1.3	67.4	1	100.00	13.5	even	ok