

Qualitative Compound Report

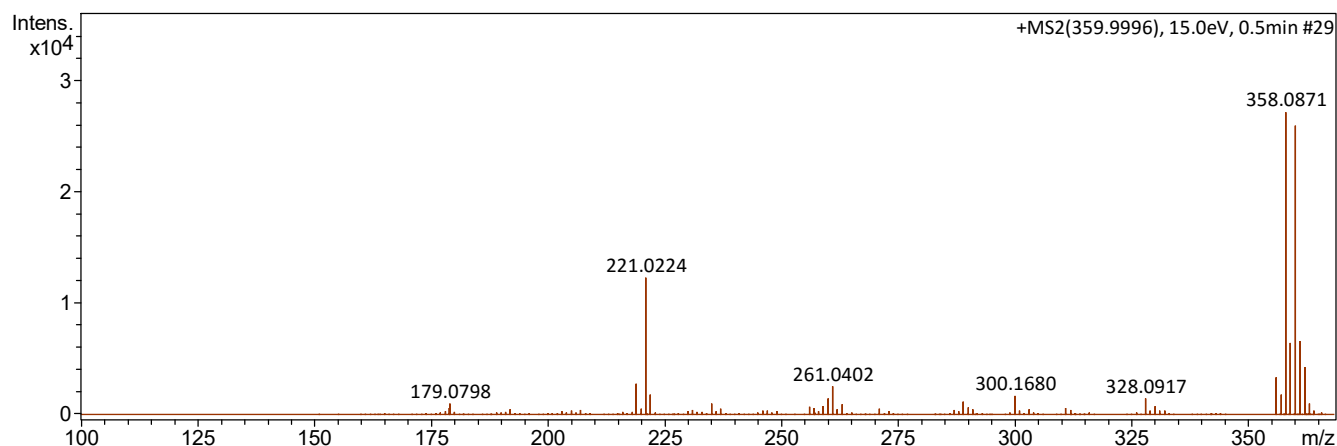
Analysis Info

Analysis Name D:\Data\US-47 toluenocrudo de rxn a ta_P1-C-5_01_7738.d
Method lc_qtof_directospos mrm atorressi us-47 tolueno.m Operator ELB
Sample Name US-47 toluenocrudo de rxn a ta Instrument micrOTOF-Q II
Comment Sv: MeOH + HCOOH
Cecilia Attoresi

Acquisition Date 2/8/2023 9:41:38 a. m.

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
179.0798	1	C9H11N2O2	179.0815	9.8	68.3	1	100.00	5.5	even	ok
221.0224	1	C12H3N3O2	221.0220	-2.0	1.5	1	100.00	13.0	odd	ok
	2	C15H3F2	221.0197	-12.2	11.3	2	18.27	13.5	even	ok
	3	C17H3N	221.0260	16.2	25.7	3	5.53	17.0	odd	ok
235.0867	1	C15H11N2O	235.0866	-0.5	78.3	1	100.00	11.5	even	ok
	2	C12H12FN2O2	235.0877	4.3	96.5	2	29.41	7.5	even	ok
261.0402	1	C17H5F2N	261.0385	-6.8	11.1	1	100.00	15.0	odd	ok
	2	C19H5N2	261.0447	17.2	23.7	2	5.12	18.5	even	ok
311.0000	1	C19HF2N2O	311.0051	16.5	271.3	1	100.00	19.5	even	ok
328.0917	1	C17H12F2N3O2	328.0892	-7.5	35.3	1	100.00	12.5	even	ok
360.1526	1	C19H20F2N3O2	360.1518	-2.2	26.0	1	100.00	10.5	even	ok