

Qualitative Compound Report

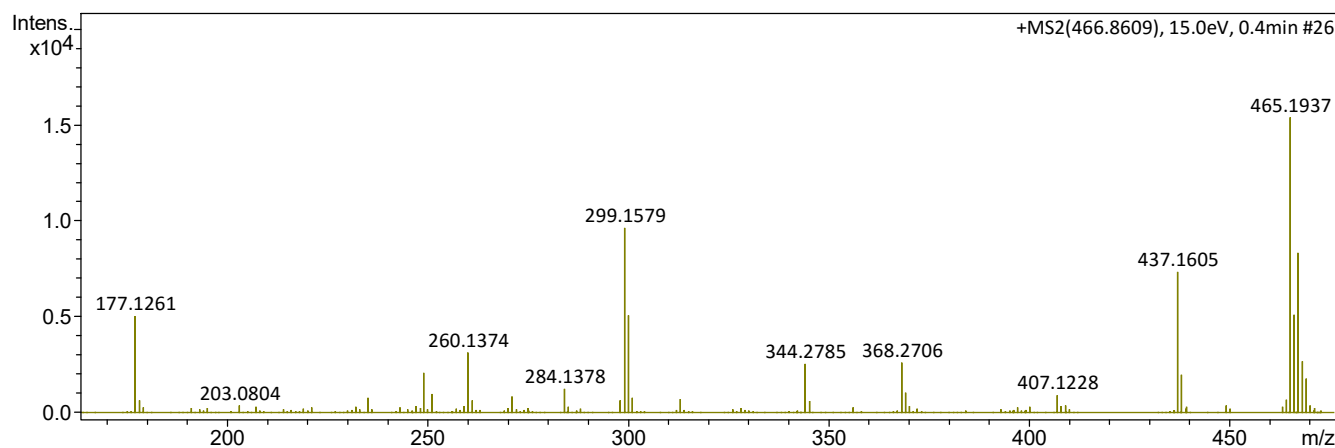
Analysis Info

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
177.1261	1	C12H17O	177.1274	7.2	27.7	1	100.00	4.5	even	ok
	2	C9H18FO2	177.1285	13.7	33.2	2	37.86	0.5	even	ok
	3	C7H17N2O3	177.1234	-15.5	37.6	3	25.51	0.5	even	ok
203.0804	1	C11H11N2O2	203.0815	5.3	n.a.	1	100.00	7.5	even	ok
	2	C8H13NO5	203.0788	-7.8	n.a.	2	72.48	3.0	odd	ok
	3	C8H12FN2O3	203.0826	11.0	n.a.	3	45.15	3.5	even	ok
235.1623	1	C14H20FN2	235.1605	-7.8	37.1	1	100.00	5.5	even	ok
	2	C11H22FNO3	235.1578	-19.2	57.1	2	3.71	1.0	odd	ok
	3	C10H23N2O4	235.1652	12.3	61.0	3	19.95	0.5	even	ok
249.0860	1	C9H14FN2O5	249.0881	8.4	17.6	1	69.62	3.5	even	ok
	2	C12H13N2O4	249.0870	3.8	35.0	2	100.00	7.5	even	ok
	3	C16H10FN2	249.0823	-15.1	58.1	3	4.74	12.5	even	ok
	4	C17H13O2	249.0910	20.0	61.2	4	0.92	11.5	even	ok
260.1374	1	C16H20O3	260.1407	12.8	22.6	1	24.72	7.0	odd	ok
	2	C13H21FO4	260.1418	17.2	39.0	2	4.37	3.0	odd	ok
	3	C11H20N2O5	260.1367	-2.7	46.9	3	100.00	3.0	odd	ok
271.1386	1	C20H17N	271.1356	-11.4	45.1	1	38.36	13.0	odd	ok
	2	C17H18FNO	271.1367	-7.2	46.3	2	100.00	9.0	odd	ok
	3	C14H20FO4	271.1340	-17.1	52.7	3	5.15	4.5	even	ok
	4	C13H21NO5	271.1414	10.2	54.2	4	39.30	4.0	odd	ok
284.1378	1	C21H18N	284.1434	19.7	17.0	1	2.45	13.5	even	ok
	2	C18H20O3	284.1407	10.3	31.6	2	49.82	9.0	odd	ok
	3	C15H21FO4	284.1418	14.3	48.2	3	9.25	5.0	odd	ok
	4	C13H20N2O5	284.1367	-3.9	56.1	4	100.00	5.0	odd	ok
299.1579	1	C21H19N2	299.1543	-12.1	169.6	1	100.00	13.5	even	ok
	2	C18H20FN2O	299.1554	-8.3	188.2	2	73.47	9.5	even	ok
	3	C15H22FNO4	299.1527	-17.2	208.0	3	0.65	5.0	odd	ok
	4	C14H23N2O5	299.1601	7.6	211.7	4	12.02	4.5	even	ok
313.1047	1	C18H17O5	313.1071	7.5	37.1	1	100.00	10.5	even	ok
	2	C18H16FNO3	313.1109	19.7	39.4	2	0.79	11.0	odd	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
	3	C21H15NO2	313.1097	16.1	44.7	3	4.01	15.0	odd	ok
	4	C22H14FO	313.1023	-7.6	47.3	4	73.20	15.5	even	ok
	5	C25H13	313.1012	-11.3	58.9	5	16.95	19.5	even	ok
407.1228	1	C26H16FN2O2	407.1190	-9.3	218.0	1	100.00	19.5	even	ok
437.1605	1	C25H24FNO5	437.1633	6.5	13.2	1	100.00	14.0	odd	ok
449.1845	1	C26H26FN2O4	449.1871	5.8	151.3	1	100.00	14.5	even	ok
467.1980	1	C26H28FN2O5	467.1977	-0.7	29.4	1	100.00	13.5	even	ok