

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

Sample Name US-47 toluenocrudo de rxn a ta

Comment Sv: MeOH + HCOOH

Cecilia Attoresi

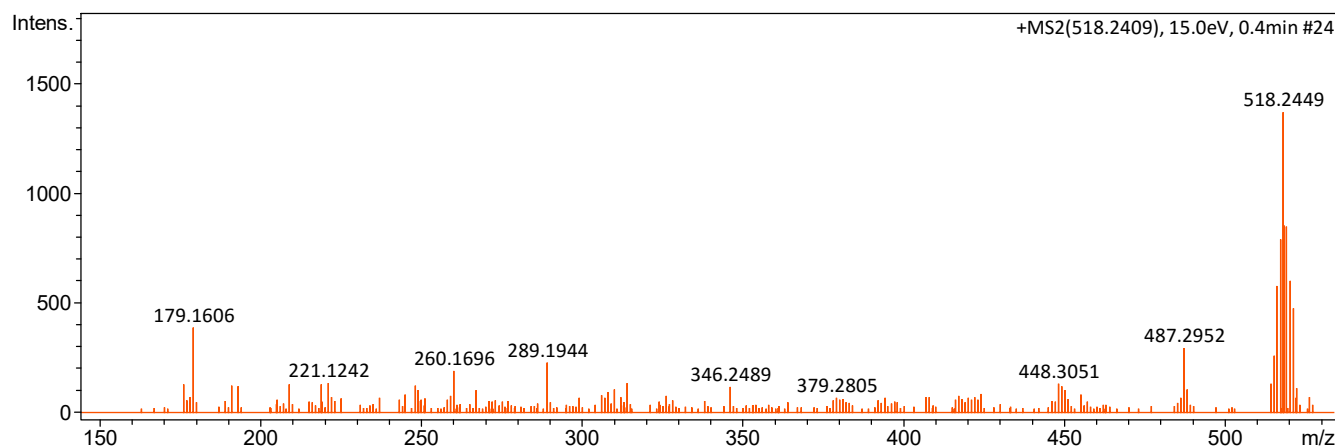
Acquisition Date 2/8/2023 9:41:38 a. m.

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
221.1242	1	C16H15N	221.1199	-19.6	200.8	1	100.00	10.0	odd	ok
	2	C13H16FNO	221.1210	-14.4	219.2	2	72.02	6.0	odd	ok
	3	C12H17N2O2	221.1285	19.1	223.1	3	15.57	5.5	even	ok
260.1696	1	C16H21FN2	260.1683	-5.0	n.a.	1	100.00	7.0	odd	ok
	2	C12H24N2O4	260.1731	13.2	n.a.	2	16.61	2.0	odd	ok
	3	C13H23FNO3	260.1656	-15.3	n.a.	3	9.06	2.5	even	ok
	4	C16H22NO2	260.1645	-19.7	n.a.	4	2.03	6.5	even	ok
267.2137	1	C15H26FN3	267.2105	-11.9	141.3	1	38.28	4.0	odd	ok
	2	C17H28FO	267.2119	-6.9	144.5	2	100.00	3.5	even	ok
	3	C20H27	267.2107	-11.1	157.3	3	16.34	7.5	even	ok
289.1944	1	C17H24FN3	289.1949	1.7	11.1	1	100.00	7.0	odd	ok
	2	C17H25N2O2	289.1911	-11.6	13.5	2	11.19	6.5	even	ok
	3	C19H26FO	289.1962	6.3	13.6	3	42.52	6.5	even	ok
	4	C14H26FN2O3	289.1922	-7.6	25.4	4	24.94	2.5	even	ok
	5	C22H25	289.1951	2.4	27.2	5	64.35	10.5	even	ok
	6	C13H27N3O4	289.1996	18.0	29.1	6	0.77	2.0	odd	ok
314.1650	1	C21H20N3	314.1652	0.6	n.a.	1	100.00	13.5	even	ok
	2	C15H23FN2O4	314.1636	-4.3	n.a.	2	54.67	5.0	odd	ok
	3	C18H21FN3O	314.1663	4.3	n.a.	3	54.55	9.5	even	ok
	4	C23H22O	314.1665	4.9	n.a.	4	47.88	13.0	odd	ok
	5	C18H22N2O3	314.1625	-7.9	n.a.	5	23.32	9.0	odd	ok
	6	C20H23FO2	314.1677	8.5	n.a.	6	19.50	9.0	odd	ok
346.2489	1	C20H32N3O2	346.2489	0.0	n.a.	1	100.00	6.5	even	ok
	2	C22H34O3	346.2502	3.9	n.a.	2	50.12	6.0	odd	ok
	3	C19H35FO4	346.2514	7.2	n.a.	3	21.32	2.0	odd	ok
	4	C25H32N	346.2529	11.6	n.a.	4	4.40	10.5	even	ok
	5	C22H33FNO	346.2541	14.9	n.a.	5	0.97	6.5	even	ok
379.2805	1	C25H35N2O	379.2744	-16.2	n.a.	1	100.00	9.5	even	ok
424.2534	1	C26H33FN2O2	424.2521	-3.2	n.a.	1	100.00	11.0	odd	ok
	2	C29H32N2O	424.2509	-5.9	n.a.	2	42.34	15.0	odd	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
518.2449	1	C30H33FN3O4	518.2450	0.0	n.a.	1	100.00	15.5	even	ok