

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-47 toluenocrudo de rxn a ta_P1-C-5_01_7738.d

Acquisition Date 8/2/2023 9:41:38 AM

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

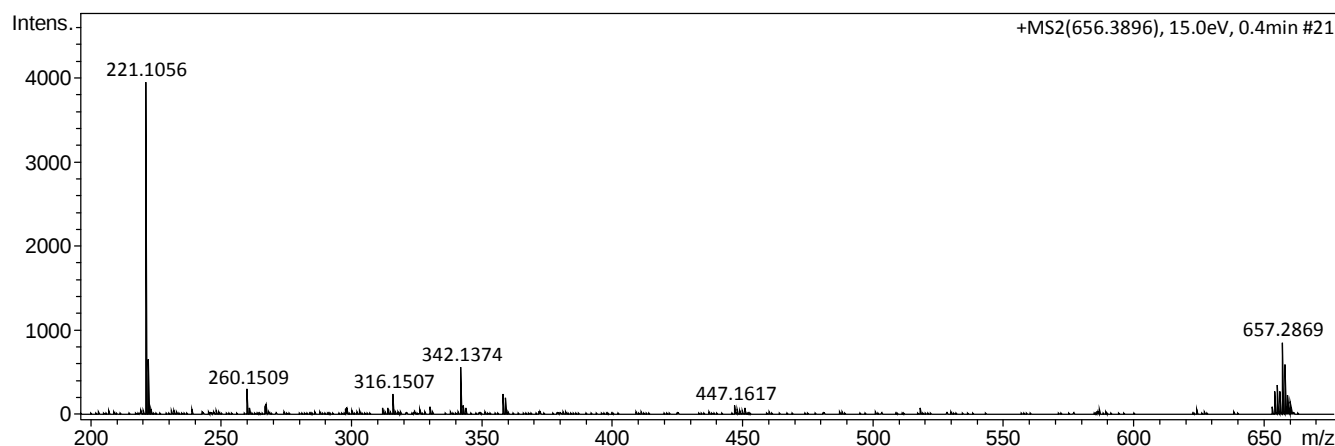
Comment Sv: MeOH + HCOOH

Cecilia Attoresi



Acquisition 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
221.1056	1	C15H13N2	221.1073	7.7	8.1	1	100.00	10.5	even	ok
	2	C12H14FN2O	221.1085	12.9	17.9	2	32.34	6.5	even	ok
	3	C10H13N4O2	221.1033	-10.5	25.7	3	44.02	6.5	even	ok
	4	C9H15F2N2O2	221.1096	18.1	35.6	4	6.36	2.5	even	ok
	5	C7H14FN4O3	221.1044	-5.3	43.7	5	62.49	2.5	even	ok
	6	C4H15F2N4O4	221.1056	-0.1	62.0	6	62.19	-1.5	even	ok
260.1509	1	C12H22NO5	260.1492	-6.3	n.a.	1	100.00	2.5	even	ok
	2	C15H19FN3	260.1558	18.7	n.a.	2	3.62	7.5	even	ok
	3	C13H20F2NO2	260.1457	-20.1	n.a.	3	2.18	3.5	even	ok
267.2043	1	C7H28FN4O5	267.2038	-1.7	n.a.	1	100.00	-4.5	even	ok
	2	C10H27N4O4	267.2027	-5.9	n.a.	2	51.89	-0.5	even	ok
	3	C15H27N2O2	267.2067	9.1	n.a.	3	27.00	3.5	even	ok
	4	C12H28FN2O3	267.2078	13.4	n.a.	4	8.89	-0.5	even	ok
	5	C9H29F2N2O4	267.2090	17.7	n.a.	5	2.20	-4.5	even	ok
	6	C11H25F2N4O	267.1991	-19.4	n.a.	6	1.18	0.5	even	ok
316.1507	1	C19H20F2NO	316.1507	0.2	n.a.	1	100.00	9.5	even	ok
	2	C22H19FN	316.1496	-3.4	n.a.	2	61.41	13.5	even	ok
	3	C18H22NO4	316.1543	11.6	n.a.	3	6.89	8.5	even	ok
	4	C14H20F2N3O3	316.1467	-12.5	n.a.	4	5.02	5.5	even	ok
	5	C15H23FNO5	316.1555	15.2	n.a.	5	1.67	4.5	even	ok
	6	C17H19FN3O2	316.1456	-16.1	n.a.	6	1.13	9.5	even	ok
	7	C20H18N3O	316.1444	-19.7	n.a.	7	0.19	13.5	even	ok
342.1374	1	C19H18F2N3O	342.1412	11.1	22.5	1	47.86	11.5	even	ok
	2	C19H20NO5	342.1336	-11.3	23.2	2	44.28	10.5	even	ok
	3	C22H17FN3	342.1401	7.8	39.8	3	100.00	15.5	even	ok
358.1294	1	C26H16NO	358.1226	-18.8	299.5	1	3.87	19.5	even	ok
	2	C25H16N3	358.1339	12.5	301.6	2	100.00	19.5	even	ok
	3	C23H17FNO2	358.1238	-15.6	317.6	3	2.67	15.5	even	ok
	4	C22H17FN3O	358.1350	15.7	319.7	4	1.94	15.5	even	ok
	5	C20H18F2NO3	358.1249	-12.5	335.8	5	1.18	11.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
447.1617	6	C19H18F2N3O2	358.1362	18.9	338.0	6	0.02	11.5	even	ok
	1	C28H20FN4O	447.1616	-0.3	n.a.	1	100.00	20.5	even	ok
	2	C25H21F2N4O2	447.1627	2.2	n.a.	2	65.98	16.5	even	ok
	3	C31H19N4	447.1604	-2.9	n.a.	3	55.08	24.5	even	ok
	4	C27H24FO5	447.1602	-3.3	n.a.	4	64.80	15.5	even	ok
	5	C30H23O4	447.1591	-5.9	n.a.	5	26.71	19.5	even	ok
	6	C24H23N4O5	447.1663	10.2	n.a.	6	2.35	15.5	even	ok
	7	C30H21F2N2	447.1667	11.2	n.a.	7	1.30	20.5	even	ok
	8	C31H21F2O	447.1555	-13.9	n.a.	8	0.20	20.5	even	ok
	9	C34H20F	447.1544	-16.5	n.a.	9	0.03	24.5	even	ok
657.2869	10	C29H23N2O3	447.1703	19.2	n.a.	10	0.00	19.5	even	ok
	1	C37H39F2N4O5	657.2883	2.2	142.6	1	100.00	19.5	even	ok