Qualitative Compound Report

Analysis Info

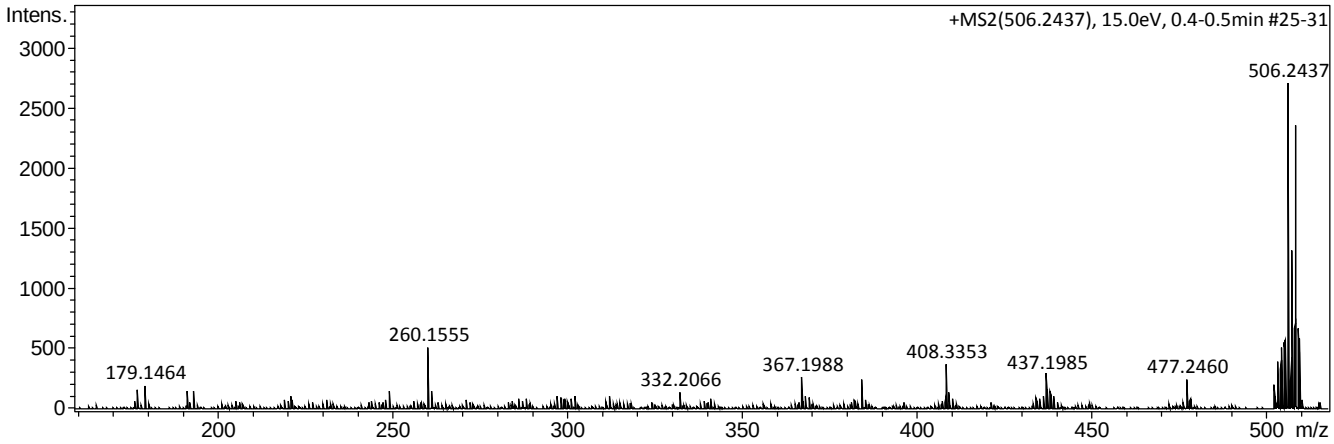
Acquisition Date 8/2/2023 9:41:38 AM

Analysis Name	D:\Data\ggc\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		

UMYMFOR CONICET FCEN - UBA

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
179.1464	1	C9H20FO2	179.1442	-12.2	n.a.	1	100.00	-0.5	even	ok
	2	C12H19O	179.1430	-18.6	n.a.	2	35.04	3.5	even	ok
191.1527	1	C9H20FN2O	191.1554	14.0	577.0	1	55.06	0.5	even	ok
	2	C12H19N2	191.1543	8.1	578.3	2	100.00	4.5	even	ok
249.1319	1	C15H18FO2	249.1285	-13.5	n.a.	1	100.00	6.5	even	ok
	2	C18H17O	249.1274	-18.1	n.a.	2	26.14	10.5	even	ok
260.1555	1	C15H19FN3	260.1558	0.8	65.1	1	100.00	7.5	even	ok
	2	C11H22N3O4	260.1605	19.0	88.9	2	0.57	2.5	even	ok
312.1362	1	C14H19FN3O4	312.1354	-2.4	n.a.	1	100.00	6.5	even	ok
	2	C17H18N3O3	312.1343	-6.0	n.a.	2	48.66	10.5	even	ok
	3	C22H18NO	312.1383	6.8	n.a.	3	40.23	14.5	even	ok
	4	C19H19FNO2	312.1394	10.5	n.a.	4	14.25	10.5	even	ok
332.2066	1	C20H27FNO2	332.2020	-13.7	n.a.	1	100.00	7.5	even	ok
	2	C22H26N3	332.2121	16.7	n.a.	2	24.11	11.5	even	ok
	3	C23H26NO	332.2009	-17.1	n.a.	3	19.33	11.5	even	ok
367.1988	1	C22H27N2O3	367.2016	7.7	n.a.	1	100.00	10.5	even	ok
	2	C19H28FN2O4	367.2028	10.8	n.a.	2	30.02	6.5	even	ok
	3	C27H27O	367.2056	18.6	n.a.	3	0.39	14.5	even	ok
437.1985	1	C29H26FN2O	437.2024	8.8	n.a.	1	100.00	17.5	even	ok
477.2460	1	C29H34FN2O3	477.2548	18.5	n.a.	1	100.00	13.5	even	ok
506.2437	1	C29H33FN3O4	506.2450	2.4	n.a.	1	100.00	14.5	even	ok