

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\US-45 ta repeticion_P1-C-3_01_7736.d
Method lc_qtof_directospos mrm atorressi us-45.m
Sample Name US-45 ta repeticion
Comment Sv: MeOH + HCOOH
Cecilia Attodesi

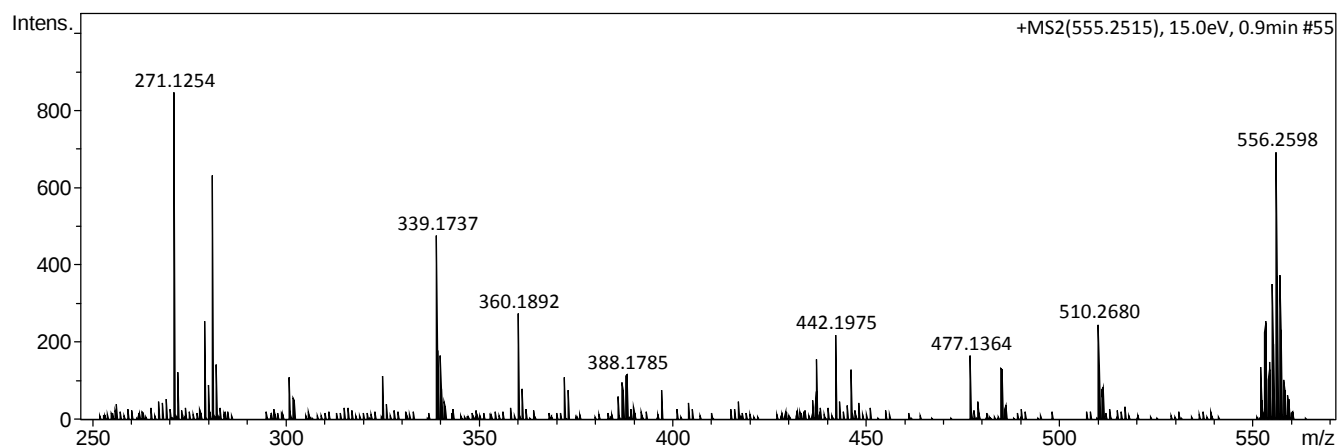
Acquisition Date 8/2/2023 9:31:19 AM

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
271.1254	1	C16H16FN2O	271.1241	-4.7	24.9	1	100.00	9.5	even	ok
	2	C19H15N2	271.1230	-8.9	43.1	2	27.23	13.5	even	ok
281.1298	1	C19H18FO	281.1336	13.7	17.2	1	9.72	10.5	even	ok
	2	C22H17	281.1325	9.7	17.4	2	31.48	14.5	even	ok
	3	C17H17N2O2	281.1285	-4.6	23.2	3	81.86	10.5	even	ok
	4	C14H18FN2O3	281.1296	-0.6	39.3	4	100.00	6.5	even	ok
301.0774	1	C19H10FN2O	301.0772	-0.9	n.a.	1	100.00	15.5	even	ok
	2	C22H9N2	301.0760	-4.7	n.a.	2	53.81	19.5	even	ok
325.1823	1	C18H26FO4	325.1810	-4.3	n.a.	1	100.00	5.5	even	ok
	2	C21H25O3	325.1798	-7.8	n.a.	2	42.21	9.5	even	ok
339.1737	1	C25H23O	339.1743	1.9	50.2	1	100.00	14.5	even	ok
	2	C22H24FO2	339.1755	5.3	66.2	2	29.11	10.5	even	ok
	3	C20H23N2O3	339.1703	-9.9	73.9	3	5.54	10.5	even	ok
	4	C17H24FN2O4	339.1715	-6.5	91.4	4	7.72	6.5	even	ok
360.1892	1	C23H23FN3	360.1871	-6.0	n.a.	1	100.00	13.5	even	ok
	2	C19H26N3O4	360.1918	7.1	n.a.	2	72.54	8.5	even	ok
	3	C24H26NO2	360.1958	18.3	n.a.	3	0.36	12.5	even	ok
388.1785	1	C27H22N3	388.1808	5.9	n.a.	1	100.00	18.5	even	ok
	2	C24H23FN3O	388.1820	8.8	n.a.	2	34.20	14.5	even	ok
437.1930	1	C30H26FO2	437.1911	-4.4	n.a.	1	100.00	17.5	even	ok
	2	C33H25O	437.1900	-7.0	n.a.	2	49.84	21.5	even	ok
	3	C25H26FN2O4	437.1871	-13.6	n.a.	3	0.89	13.5	even	ok
	4	C28H25N2O3	437.1860	-16.2	n.a.	4	0.12	17.5	even	ok
	5	C32H25N2	437.2012	18.7	n.a.	5	0.01	21.5	even	ok
442.1975	1	C32H25FN	442.1966	-2.2	n.a.	1	100.00	20.5	even	ok
	2	C28H28NO4	442.2013	8.5	n.a.	2	12.86	15.5	even	ok
	3	C27H25FN3O2	442.1925	-11.3	n.a.	3	1.99	16.5	even	ok
	4	C30H24N3O	442.1914	-13.9	n.a.	4	0.34	20.5	even	ok
446.1608	1	C32H20N3	446.1652	9.8	n.a.	1	100.00	24.5	even	ok
	2	C29H21FN3O	446.1663	12.3	n.a.	2	20.33	20.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
	3	C30H21FNO2	446.1551	-12.9	n.a.	3	13.88	20.5	even	ok
	4	C33H20NO	446.1539	-15.4	n.a.	4	2.61	24.5	even	ok
477.1364	1	C33H18FN2O	477.1398	7.0	n.a.	1	100.00	25.5	even	ok
485.1444	1	C31H21N2O4	485.1496	10.6	n.a.	1	100.00	22.5	even	ok
510.2680	1	C33H36NO4	510.2639	-8.1	n.a.	1	100.00	16.5	even	ok
	2	C32H36N3O3	510.2751	13.9	n.a.	2	1.05	16.5	even	ok
556.2598	1	C33H35FN3O4	556.2606	1.5	91.9	1	100.00	17.5	even	ok