

Qualitative Compound Report

Analysis Info

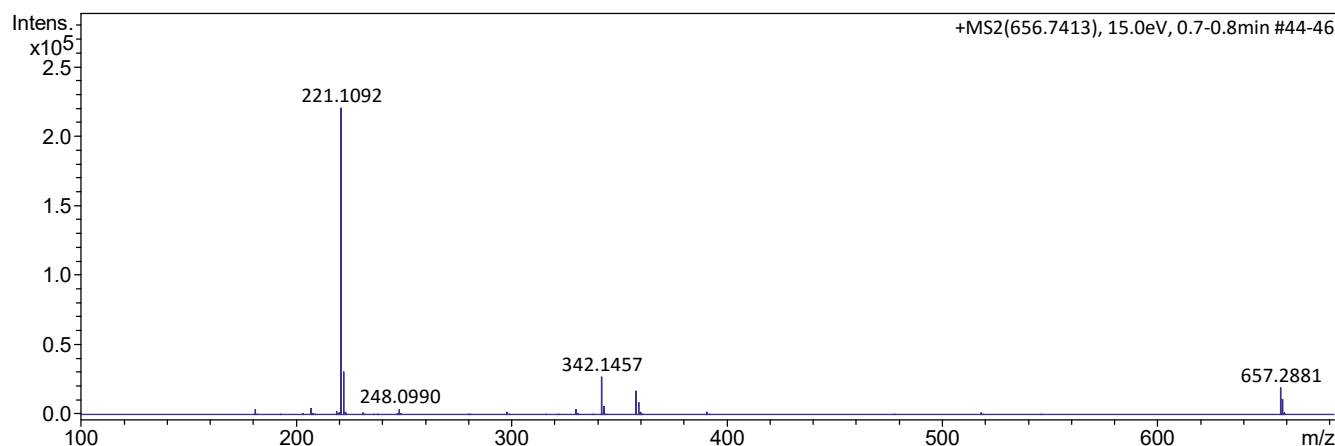
Analysis Name D:\Data\UStol-3_P1-C-4_01_8153.d
Method lc_qtof_directospos mrm atorressi 657.m
Sample Name UStol-3
Comment Sv: DCM + MeOH + HCOOH
Attores

Acquisition Date 18/10/2023 3:11:18 p. 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
181.0763	1	C12H9N2	181.0760	-1.3	5.4	1	100.00	9.5	even	ok
	2	C9H10FN2O	181.0772	5.0	23.9	2	50.08	5.5	even	ok
207.0916	1	C14H11N2	207.0917	0.4	55.9	1	100.00	10.5	even	ok
	2	C11H12FN2O	207.0928	5.9	59.9	2	48.98	6.5	even	ok
221.1092	1	C12H14FN2O	221.1085	-3.3	1.7	1	100.00	6.5	even	ok
	2	C15H13N2	221.1073	-8.5	18.6	2	35.63	10.5	even	ok
	3	C9H15F2N2O2	221.1096	1.8	18.6	3	85.84	2.5	even	ok
248.0990	1	C18H13F	248.0996	2.2	15.1	1	100.00	12.0	odd	ok
	2	C15H14F2O	248.1007	6.8	30.5	2	36.00	8.0	odd	ok
	3	C13H12F2N3	248.0994	1.4	36.4	3	67.30	8.5	even	ok
298.1474	1	C21H18N2	298.1465	-3.1	31.5	1	98.45	14.0	odd	ok
	2	C18H19FN2O	298.1476	0.7	43.9	2	100.00	10.0	odd	ok
330.1081	1	C19H16F2O3	330.1062	-5.8	4.1	1	42.75	11.0	odd	ok
	2	C17H14F2N3O2	330.1049	-9.9	4.4	2	12.94	11.5	even	ok
	3	C16H16N3O5	330.1084	1.0	10.4	3	100.00	10.5	even	ok
	4	C19H14N4O2	330.1111	9.1	11.1	4	15.16	15.0	odd	ok
	5	C22H15FO2	330.1051	-9.3	21.6	5	11.32	15.0	odd	ok
	6	C22H14F2N	330.1089	2.3	22.7	6	62.92	15.5	even	ok
342.1457	1	C21H20F2O2	342.1426	-9.0	7.4	1	15.98	11.0	odd	ok
	2	C18H19FN4O2	342.1487	8.7	8.9	2	17.15	11.0	odd	ok
	3	C20H22O5	342.1462	1.5	9.6	3	100.00	10.0	odd	ok
	4	C18H20N3O4	342.1448	-2.5	11.4	4	81.35	10.5	even	ok
	5	C21H18N4O	342.1475	5.4	13.2	5	41.69	15.0	odd	ok
	6	C23H20NO2	342.1489	9.3	20.2	6	11.28	14.5	even	ok
	7	C15H21FN3O5	342.1460	0.9	28.0	7	74.42	6.5	even	ok
358.1397	1	C24H18F2N	358.1402	1.4	142.1	1	100.00	15.5	even	ok
	2	C24H19FO2	358.1364	-9.3	143.2	2	11.32	15.0	odd	ok
	3	C21H18N4O2	358.1424	7.7	153.8	3	9.87	15.0	odd	ok
	4	C21H20F2O3	358.1375	-6.1	161.9	4	9.29	11.0	odd	ok
	5	C19H18F2N3O2	358.1362	-9.8	168.8	5	1.61	11.5	even	ok

Qualitative Compound Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
391.1847	6	C18H20N3O5	358.1397	0.2	173.5	6	14.05	10.5	even	ok
	1	C26H25F2O	391.1868	5.3	0.6	1	46.95	13.5	even	ok
	2	C24H23F2N3	391.1855	1.9	7.5	2	100.00	14.0	odd	ok
	3	C24H24FN2O2	391.1816	-7.9	8.6	3	17.10	13.5	even	ok
	4	C29H24F	391.1857	2.4	18.5	4	72.38	17.5	even	ok
518.2534	5	C21H25F2N2O3	391.1828	-4.9	27.4	5	31.17	9.5	even	ok
	1	C35H32F2N2	518.2528	-1.1	30.3	1	100.00	20.0	odd	ok
	2	C35H33FNO2	518.2490	-8.5	32.4	2	3.44	19.5	even	ok
	3	C34H34N2O3	518.2564	5.8	34.4	3	15.20	19.0	odd	ok
	4	C32H34F2NO3	518.2501	-6.3	41.3	4	10.09	15.5	even	ok
657.2881	5	C31H35FN2O4	518.2575	8.0	44.2	5	3.33	15.0	odd	ok
	1	C37H39F2N4O5	657.2883	0.4	70.5	1	100.00	19.5	even	ok