

Mass Spectrum SmartFormula Report

Analysis Info

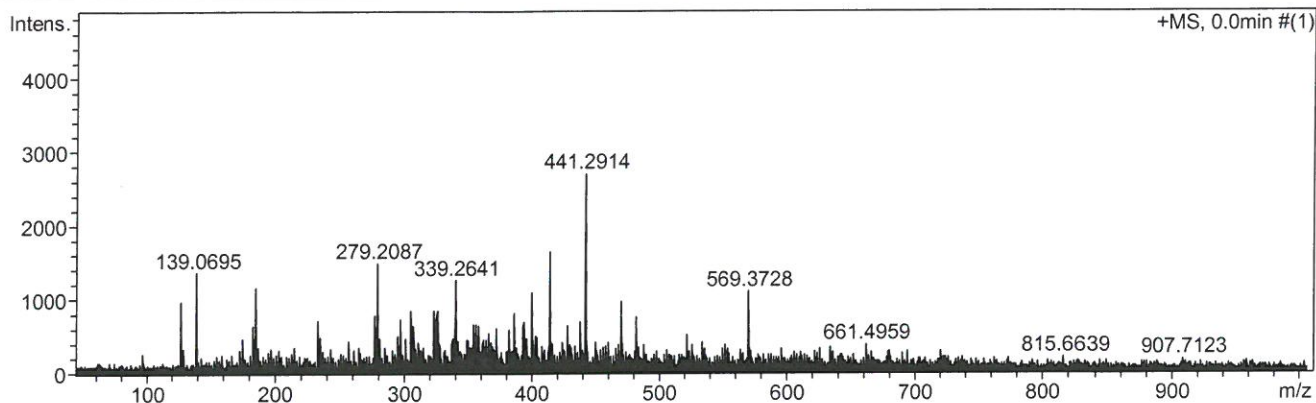
Analysis Name E:\Data2\Kilian\RMM123000004.d
Method Tune_low_pos.m
Sample Name RMM123
Comment PhSBnMe

Acquisition Date 2016-03-31 17:32:00

Operator Carin Larsson
Instrument / Ser# micrOTOF 125

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
215.0917	1	C 5 H 14 N O 6 S	0.00	216.0536	961.9	4472.2	50.7	-0.5	even		ok
	2	C 14 H 15 S	100.00	215.0889	-2.8	-13.1	251.8	7.5	even		ok
	3	C 10 H 15 O 3 S	0.00	215.0736	-18.1	-84.0	258.9	3.5	even		ok
	4	C 9 H 15 N 2 O 2 S	0.15	215.0849	-6.8	-31.8	260.6	3.5	even		ok
	5	C 8 H 15 N 4 O S	4.30	215.0961	4.4	20.4	264.9	3.5	even		ok
	6	C 7 H 15 N 6 S	0.00	215.1073	15.6	72.7	306.4	3.5	even		ok
	7	C 6 H 15 O 6 S	0.00	215.0584	-33.3	-154.9	308.8	-0.5	even		ok
	8	C 5 H 15 N 2 O 5 S	0.00	215.0696	-22.1	-102.7	310.6	-0.5	even		ok
	9	C 13 H 14 N S	0.00	216.0841	992.4	4614.0	474.5	7.5	even		ok
	10	C 9 H 14 N O 3 S	0.00	216.0689	977.2	4543.1	493.9	3.5	even		ok
	11	C 8 H 14 N 3 O 2 S	0.00	216.0801	988.4	4595.3	495.3	3.5	even		ok
	12	C 7 H 14 N 5 O S	0.00	216.0914	999.6	4647.5	573.6	3.5	even		ok

