

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name C:\Users\amlab\Desktop\amlab drop\Kilian\Backup\2016-05-25\KC-3-PhSMeiPr-re000001.d
Method Tune_low_pos.m
Sample Name KC-3-PhSMeiPr-re
Comment

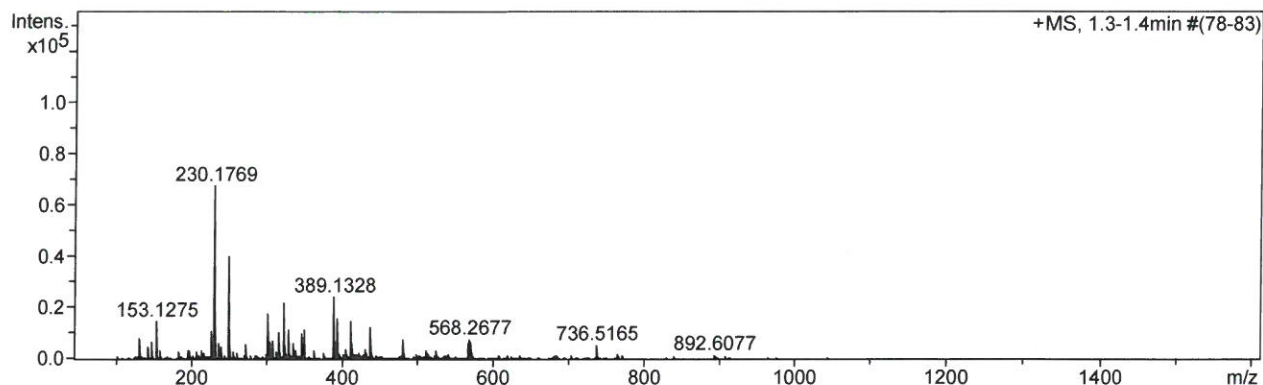
Acquisition Date 2015-12-18 11:09:48

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	1600 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
205.0456	1	C 10 H 14 K S	100.00	205.0448	-0.8	-3.8	178.1	3.5	even	ok
	2	C 6 H 14 K O 3 S	0.00	205.0295	-16.0	-78.2	192.5	-0.5	even	ok
	3	C 5 H 14 K N 2 O 2 S	0.65	205.0408	-4.8	-23.4	194.4	-0.5	even	ok

