

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name C:\Users\amlab\Desktop\amlab drop\Kilian\Backup\2016-05-25\THT-oSMePh000001.d
Method Tune_low_pos.m
Sample Name THT-oSMePh
Comment

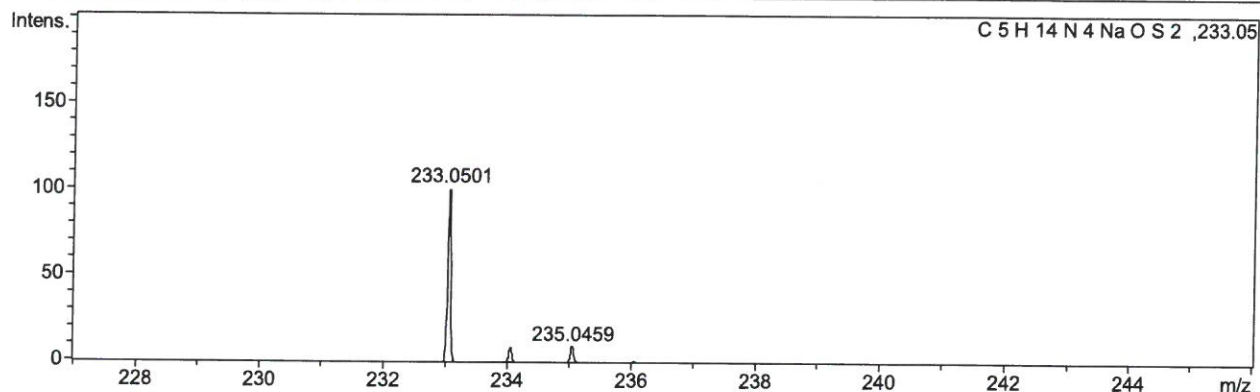
Acquisition Date 2016-03-24 14:51:34

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]	mSig	rdb	e ⁻ Conf	N-R
233.0501	1	C 6 H 14 N 2 Na O 2 S 2	0.00	233.0389	-11.2	-48.2	1.0	0.5	even	ok
	2	C 5 H 14 N 4 Na O S 2	100.00	233.0501	0.0	0.0	1.9	0.5	even	ok
	3	C 7 H 14 Na O 3 S 2	0.00	233.0277	-22.5	-96.4	2.9	0.5	even	ok
	4	C 11 H 14 Na S 2	0.02	233.0429	-7.2	-30.9	24.4	4.5	even	ok

