

Mass Spectrum SmartFormula Report

Analysis Info

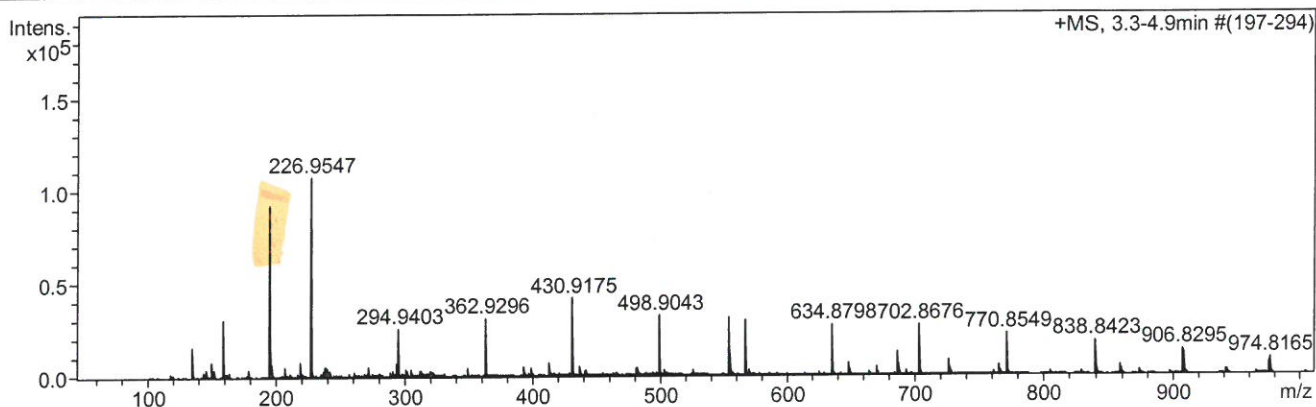
Analysis Name E:\Data2\Kilian\KC-5-manilineThiomorph000001.d
Method Tune_low_pos.m
Sample Name TMmanil
Comment

Acquisition Date 2016-11-11 11:32:10

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
195.0945	1	C 10 H 15 N 2 S	100.00	195.0950	0.5	2.6	20.3	4.5	even		ok
	2	C 10 H 14 N 2 S	0.00	194.0872	-4.5	-23.3	663.4	5.0	odd		ok

