

Mass Spectrum SmartFormula Report

Analysis Info

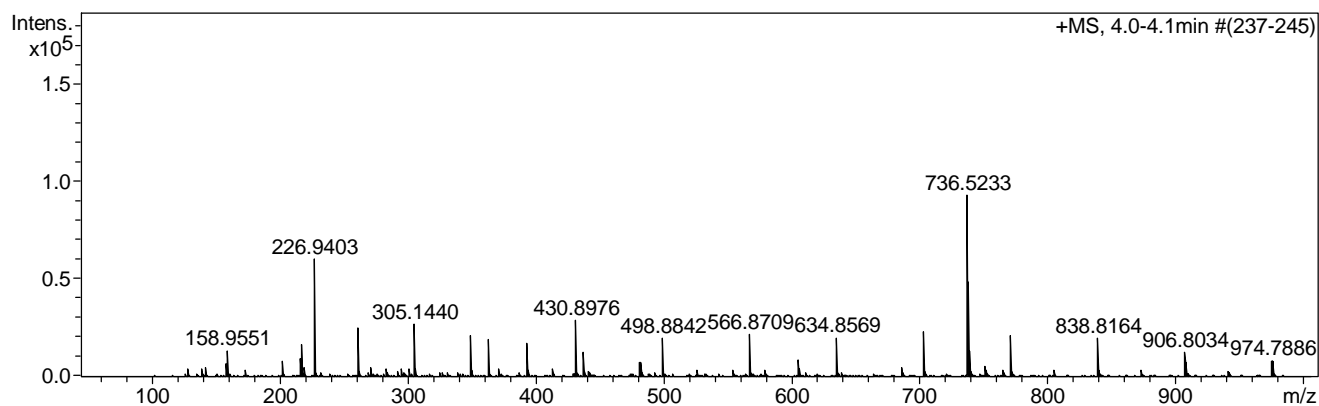
Analysis Name E:\Data2\Kilian\pCF3KBu000001.d
Method Tune_low_pos.m
Sample Name pCF3KBu
Comment

Acquisition Date 2018-02-16 14:03:51

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 ma	rdb	e ⁻ Conf	N-R ule
253.0803	1	C 5 H 13 F 3 N 6 Na O	0.00	253.0995	19.3	76.1	44.0	0.5	even	ok
	2	C 12 H 13 F 3 Na O	100.00	253.0811	0.8	3.2	75.1	4.5	even	ok
	3	C 8 H 13 F 3 N 5 O	0.00	252.1067	-973.6	-3847.0	774.8	3.5	even	ok