Mass Spectrum Molecular Formula Report

Analysis Info

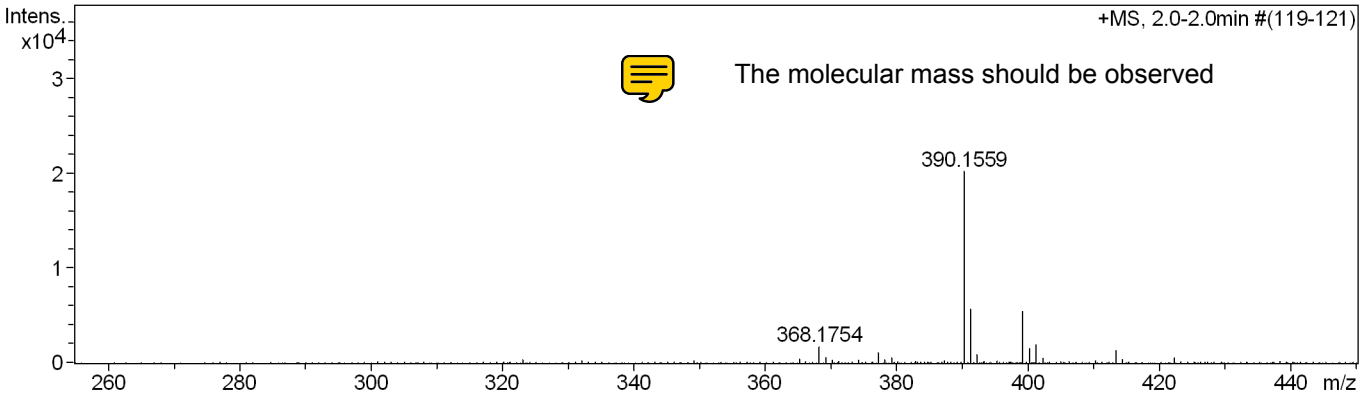
Analysis Name	D:\Data\ahmet\bil_60u_.d	Acquisition Date	7/16/2014 1:32:51 PM
Method	gok_tune_wide.m	Operator	bruker customer
Sample Name		Instrument / Ser#	micrOTOF-Q 55
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	5000 V	Set Dry Heater	180 °C
Scan Begin	250 m/z	Set End Plate Offset	-400 V	Set Dry Gas	4.0 l/min
Scan End	450 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

Generate Molecular Formula Parameter

Formula, min.	C22						
Formula, max.	N5-O2						
Measured m/z	368.175	Tolerance	1	mDa	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 24 H 22 N 3 O 1	0.085	368.1757	0.91	-2.48	0.33	15.50	ok	even

The mean error should be less than 5 ppm (minus, plus)

The molecular formula such as C24H22N3O1 should be calculated by the instrument.