

Walkup MS Report



Data File	mlo462_Pos_LoopInjection_MS_fragile2_04494.d	Sample Name	mlo462
Sample Type	Sample	Position	P1-A1
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Pos_LoopInjection_MS_fragile2.m	Acquired Time	5/29/2019 12:31:48 PM
IRM Calibration Status	Success	DA Method	Pos_LoopInjection_MS_fragile2.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Pos_LoopInjection_MS_fragile
Formula	C33H31BN4O3	Walkup Method Description	Lower fragmentor and Rf voltages in positive mode loop injection for fragile ions
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

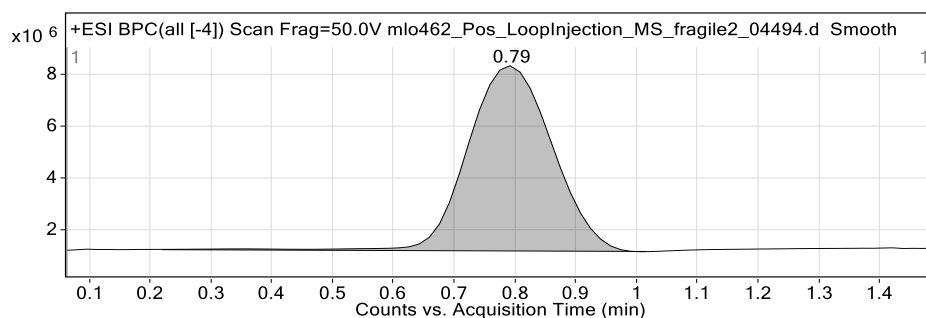


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.79	69245951	100.00	100.00	85.0580	0.160

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)	Error flag
Cpd 1: C33 H31 B N4 O3	0.98	543.2562	541.2582	541.2526	10.46	73.47	m/z tolerance

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

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Compound specific information

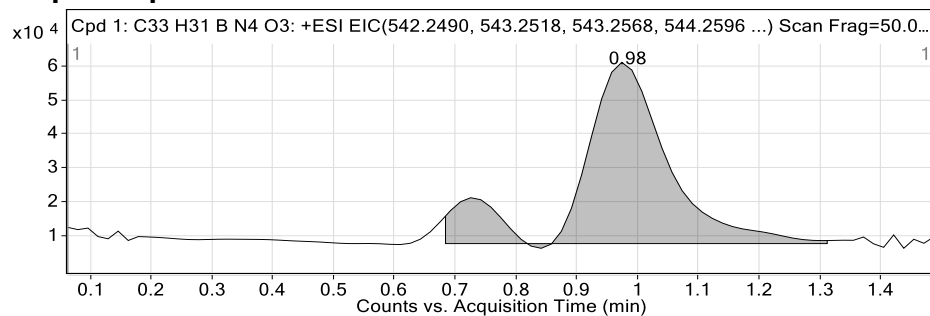


Figure: Extracted ion chromatogram (EIC) of compound.

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