

Walkup MS Report



Data File	MLO442 + ONOO- Neg_5mins_MS_03685.d	Sample Name	MLO442 + ONOO-
Sample Type	Sample	Position	P1-B2
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_5mins_MS.m	Acquired Time	4/11/2019 5:36:09 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C17H19N3O	Walkup Method Description	Negative mode ionization using C18 column chromatography
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

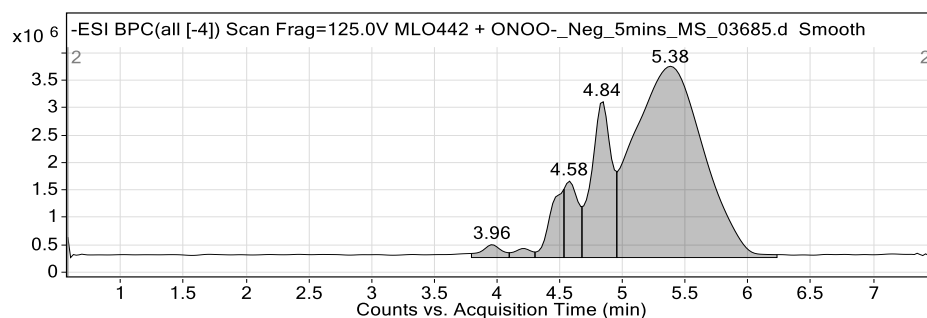


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
3.96	2591788	1.95	1.37	1033.9860	0.160
4.21	1575508	1.18	0.83	1033.9859	0.140
4.44	9434905	7.08	4.99	251.1285	0.150
4.58	10359177	7.77	5.48	420.2497	0.110
4.84	31858919	23.91	16.85	277.1806	0.160
5.38	133253111	100.00	70.48	132.9234	0.570

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: C17 H19 N3 O	4.16	280.1455	281.1504	281.1528	-8.58	42.04	low score

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

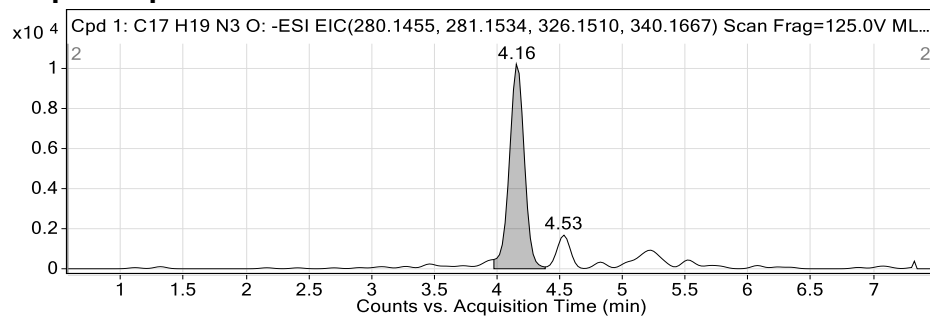


Figure: Extracted ion chromatogram (EIC) of compound.

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