

# Walkup MS Report



<b>Data File</b>	MLO442_Pos_5mins_MS_04554.d	<b>Sample Name</b>	MLO442
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A6
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Maria Odyniec
<b>Acq Method</b>	Pos_5mins_MS.m	<b>Acquired Time</b>	6/3/2019 10:34:33 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Pos_5mins_MS.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Walkup Sample Description</b>		<b>Walkup Method</b>	Pos_5Mins_C18
<b>Formula</b>	C13H10N2S	<b>Walkup Method Description</b>	Positive mode ionization using C18 column chromatography
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

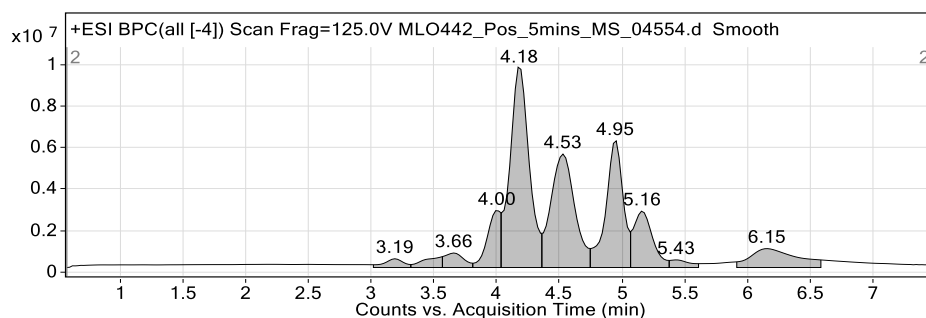


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
3.19	4548995	4.42	1.39	231.1216	0.160
3.43	5347725	5.20	1.63	275.1480	0.190
3.66	7367442	7.16	2.25	203.0938	0.160
4.00	19847776	19.29	6.06	185.1157	0.110
4.18	102904456	100.00	31.42	212.0861	0.160
4.53	72683002	70.63	22.20	398.2440	0.210
4.95	58679093	57.02	17.92	500.3121	0.140
5.16	28630190	27.82	8.74	413.2685	0.160
5.43	3961649	3.85	1.21	333.2421	0.180
6.15	23497454	22.83	7.18	141.9594	0.370

## Compound Table

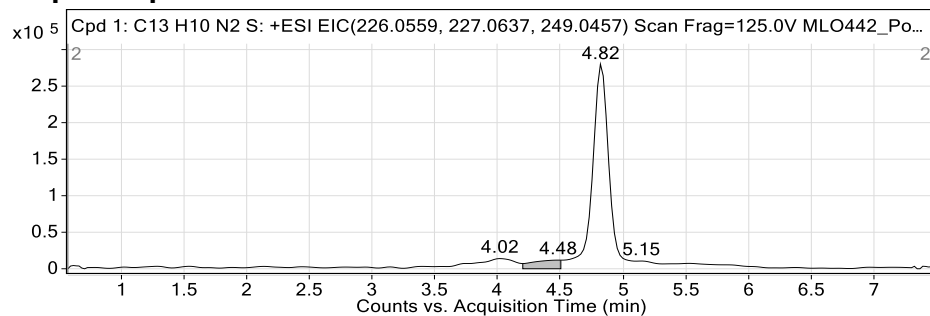
Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)	Error flag
Cpd 1: C13 H10 N2 S	4.48	227.0648	226.0561	226.0565	-1.45	47.99	low score

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.**

--- End Of Report ---