

# Walkup MS Report



<b>Data File</b>	mlo459_Neg_LoopInjection_MS_04340.d	<b>Sample Name</b>	mlo459
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A3
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Maria Odyniec
<b>Acq Method</b>	Neg_LoopInjection_MS.m	<b>Acquired Time</b>	5/20/2019 3:24:22 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Neg_LoopInjection_MS.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Walkup Sample Description</b>		<b>Walkup Method</b>	Neg_LoopInjection_MS
<b>Formula</b>	C8H6O3	<b>Walkup Method Description</b>	Negative mode ionization using loop injection
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

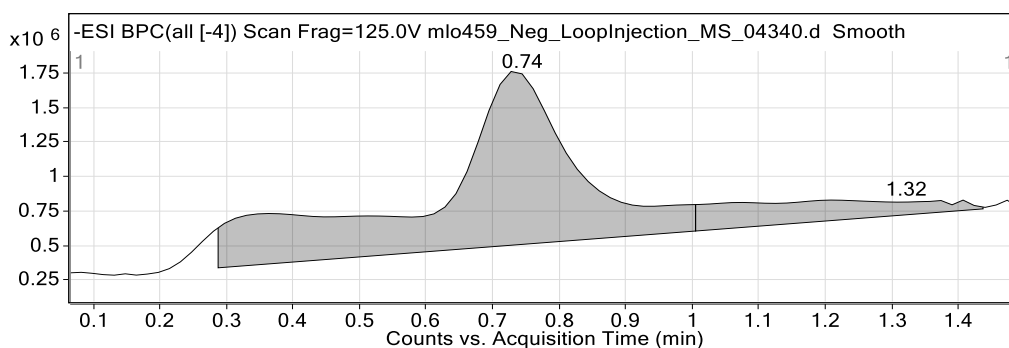


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.74	19440770	100.00	85.37	112.9860	0.260
1.32	3330661	17.13	14.63	1033.9930	0.560

## Compound Table

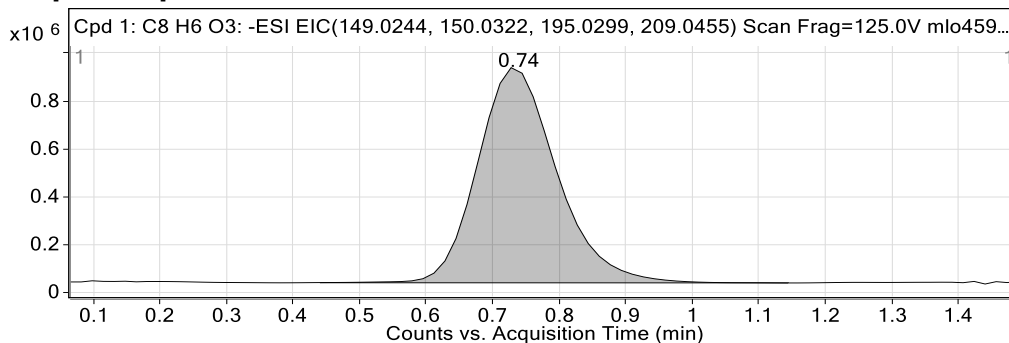
Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C8 H6 O3	0.74	149.0242	150.0315	150.0317	-1.59	99.67

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

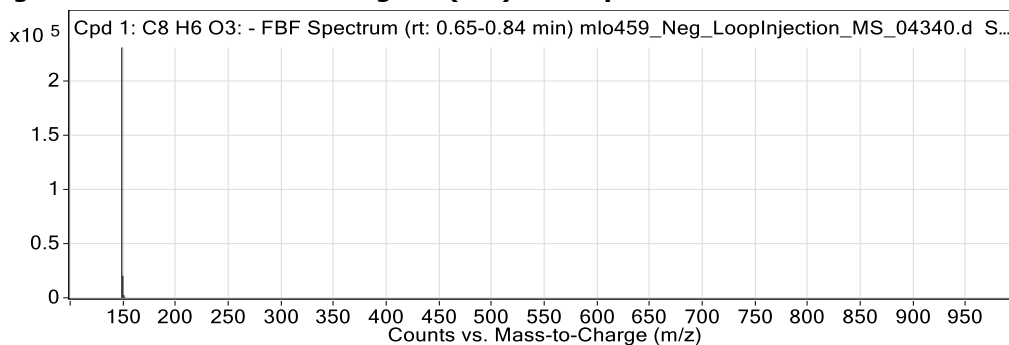
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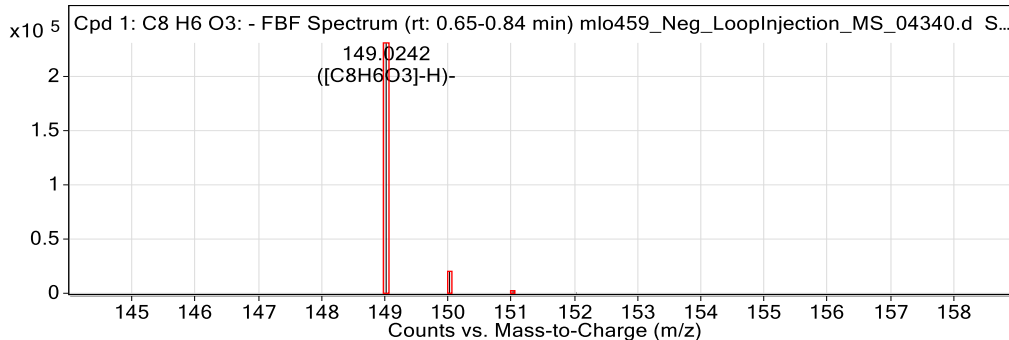
## Compound specific information



**Figure: Extracted ion chromatogram (EIC) of compound.**



**Figure: Full range view of Compound spectra and potential adducts.**



**Figure: Zoomed Compound spectra view**  
(red boxes indicating expected theoretical isotope spacing and abundance)

### Compound isotope peak List

m/z	z	Abund	Formula	Ion
149.0242	1	230760.7	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	(M-H)-
150.0273	1	20375.2	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	(M-H)-
151.0314	1	2441.4	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	(M-H)-
152.0350	1	534.0	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	(M-H)-

--- End Of Report ---