

# Walkup MS Report



<b>Data File</b>	mlo460 column_Neg_LoopInjection_MS_04474.d	<b>Sample Name</b>	mlo460 column
<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>	5/28/2019 10:02:34 AM
<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>	C20H14N4O	<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)

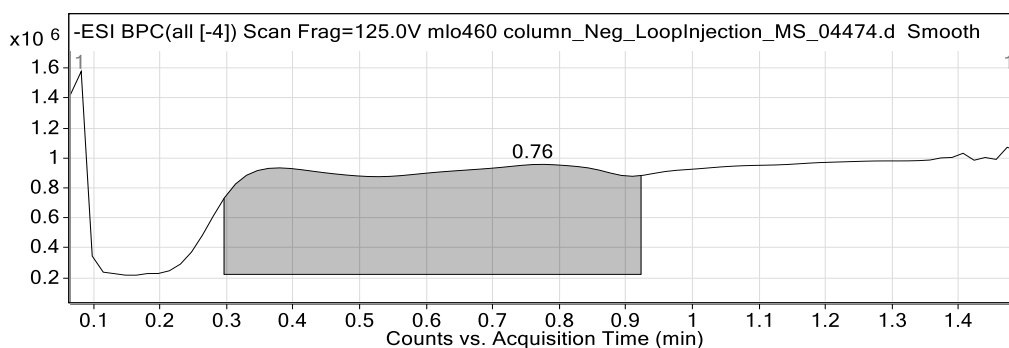


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.76	25812528	100.00	100.00	1033.9791	0.470

## 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: C20 H14 N4 O	0.75	325.1094	326.1166	326.1168	-0.37	99.58

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

# Walkup MS Report



## Compound specific information

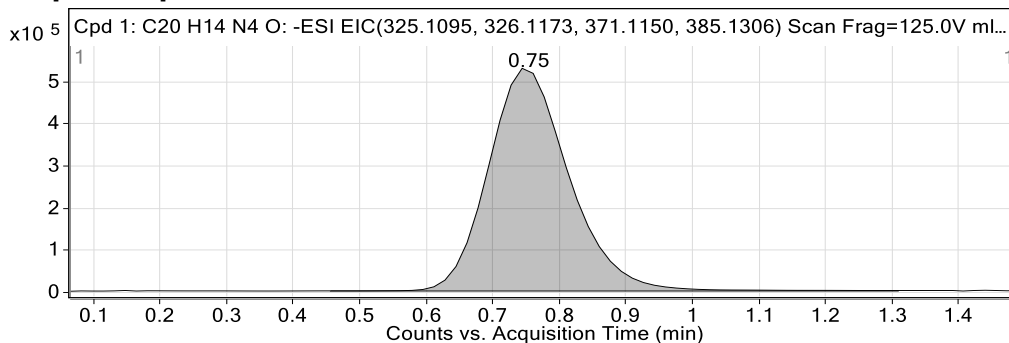


Figure: Extracted ion chromatogram (EIC) of compound.

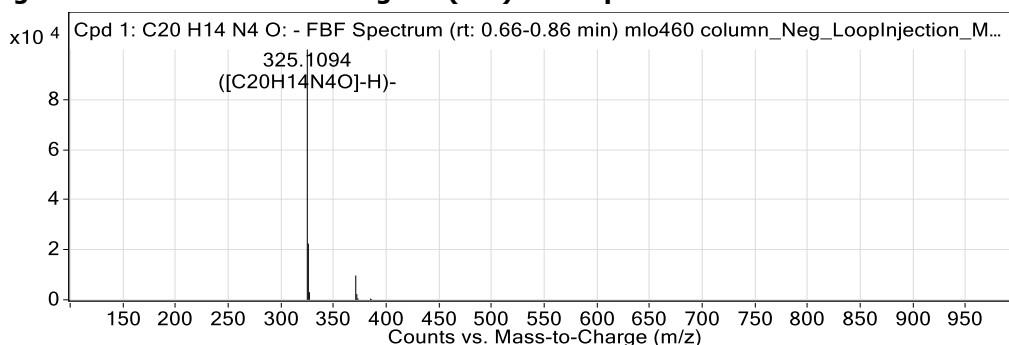


Figure: Full range view of Compound spectra and potential adducts.

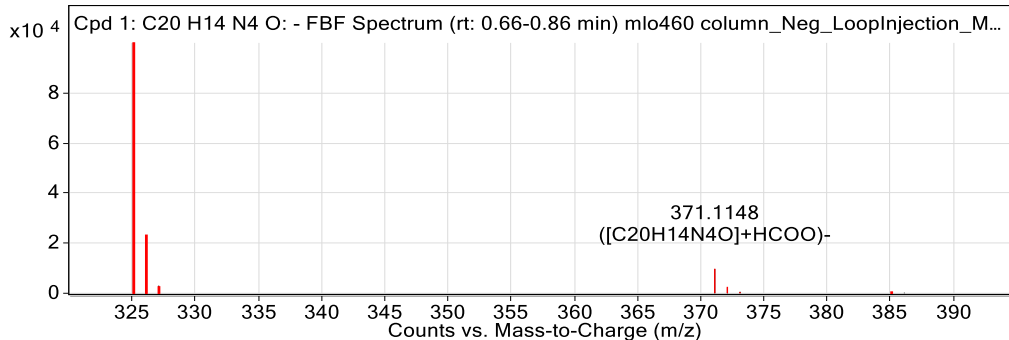


Figure: Zoomed Compound spectra view  
(red boxes indicating expected theoretical isotope spacing and abundance)

### Compound isotope peak List

m/z	z	Abund	Formula	Ion
325.1094	1	99969.8	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M-H)-
326.1123	1	22447.6	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M-H)-
327.1160	1	3044.2	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M-H)-
371.1148	1	9707.4	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M+HCOO)-
372.1187	1	2295.5	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M+HCOO)-
373.1199	1	611.1	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M+HCOO)-
385.1274	1	470.3	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M+CH <sub>3</sub> COO)-
386.1190	1	235.8	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub> O	(M+CH <sub>3</sub> COO)-

--- End Of Report ---