

# Walkup MS Report



<b>Data File</b>	MLO461 column 1_Neg_LoopInjection_MS_fragile_04476.d	<b>Sample Name</b>	MLO461 column 1
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Maria Odyniec
<b>Acq Method</b>	Neg_LoopInjection_MS_fragile.m	<b>Acquired Time</b>	5/28/2019 10:06:40 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Neg_LoopInjection_MS_fragile.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Walkup Sample Description</b>		<b>Walkup Method</b>	Neg_LoopInjection_MS_fragile
<b>Formula</b>	C30H27BN4O3	<b>Walkup Method Description</b>	Lower fragmentor and Rf voltages in negative mode loop injection for fragile ions
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

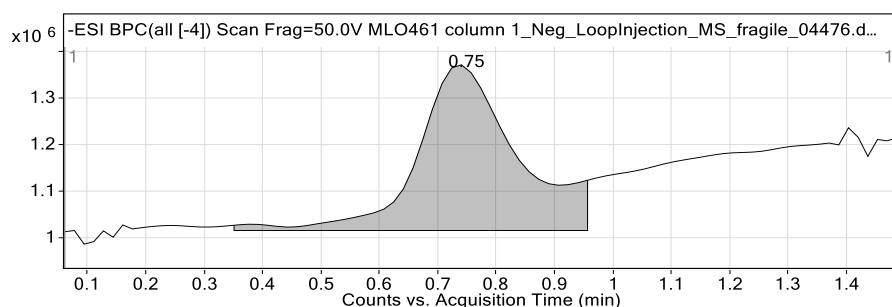


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	4199184	100.00	100.00	112.9835	0.200

## 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: C30 H27 B N4 O3	0.74	501.2105	501.2210	501.2213	-0.46	71.42

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

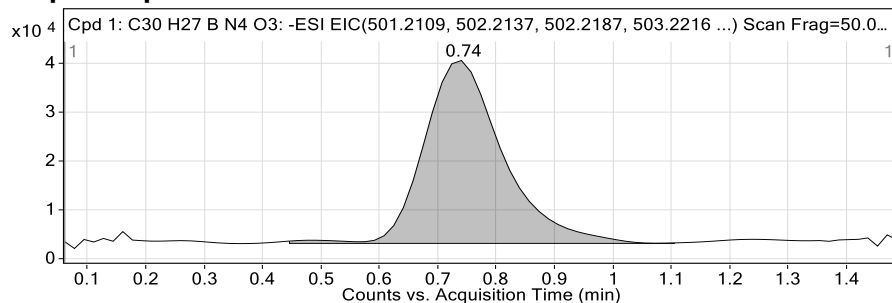


Figure: Extracted ion chromatogram (EIC) of compound.

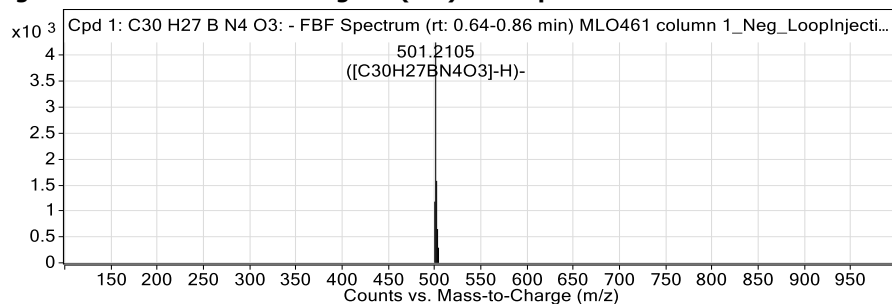


Figure: Full range view of Compound spectra and potential adducts.

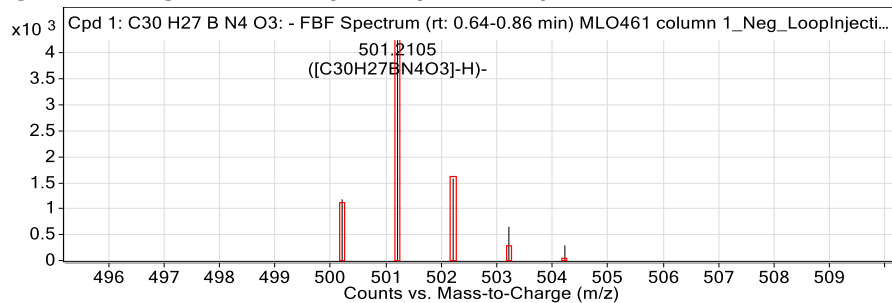


Figure: Zoomed Compound spectra view  
(red boxes indicating expected theoretical isotope spacing and abundance)

## Compound isotope peak List

m/z	z	Abund	Formula	Ion
500.2118	1	1180.3	C30H27BN4O3	(M-H)-
501.2105	1	4250.3	C30H27BN4O3	(M-H)-
502.2134	1	1580.8	C30H27BN4O3	(M-H)-
503.2175	1	651.9	C30H27BN4O3	(M-H)-
504.2270	1	291.9	C30H27BN4O3	(M-H)-

--- End Of Report ---