

Walkup MS Report



Data File	mlo408_Neg_LoopInjection_MS_00532.d	Sample Name	mlo408
Sample Type	Sample	Position	P1-A1
Instrument Name	6545 QToF	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS.m	Acquired Time	11/20/2018 9:18:04 AM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_LoopInjection_MS
Formula	C14H10N2O2	Walkup Method Description	Negative mode ionization using loop injection
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

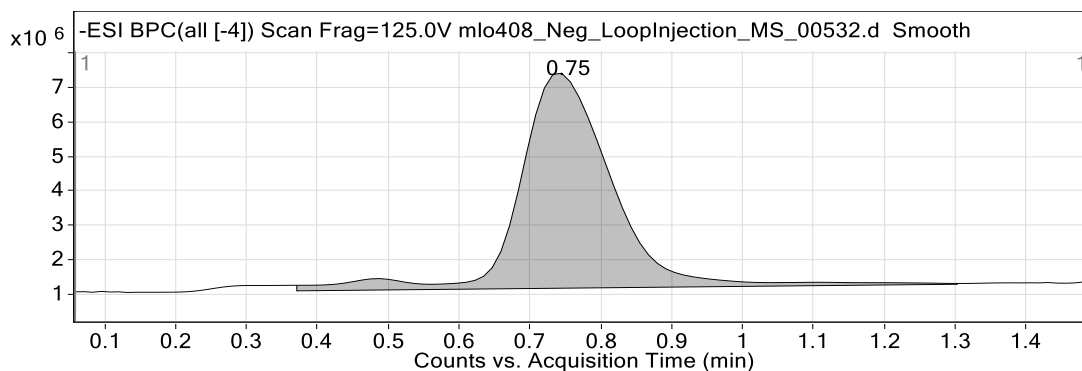


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	56875152	100.00	100.00	112.9868	0.190

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: C14 H10 N2 O2	0.76	237.0669	238.0742	238.0742	-0.28	97.54

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Compound specific information

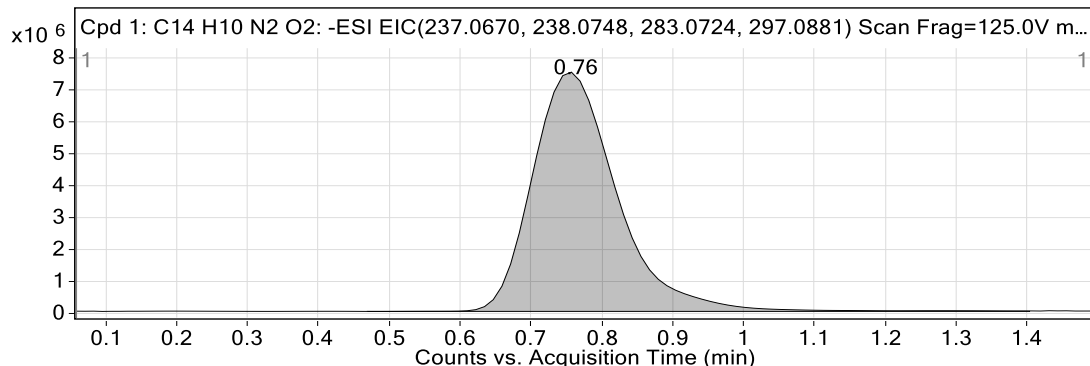


Figure: Extracted ion chromatogram (EIC) of compound.

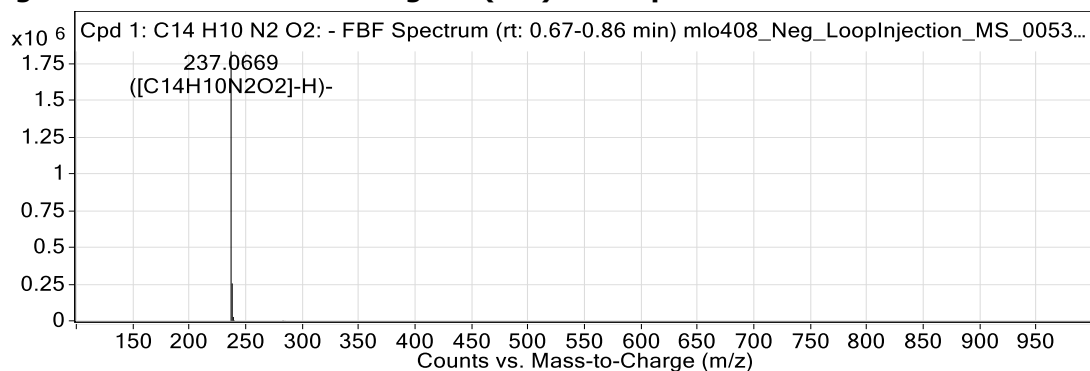


Figure: Full range view of Compound spectra and potential adducts.

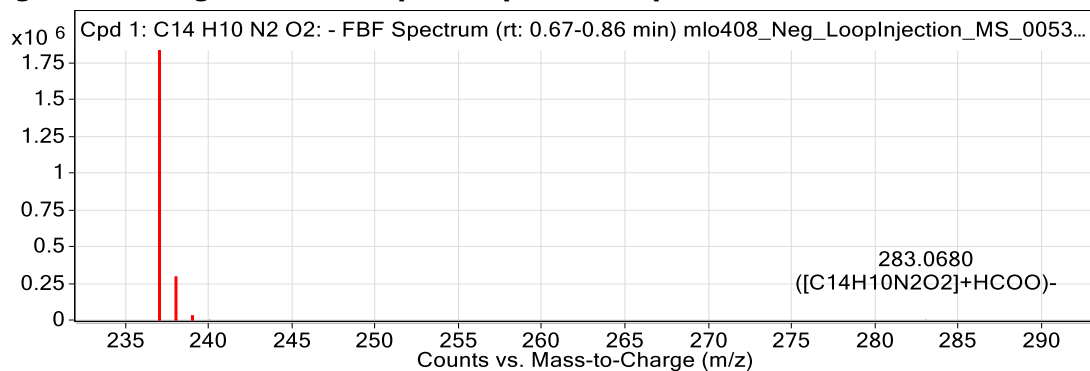


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
237.0669	1	1834098.6	C ₁₄ H ₁₀ N ₂ O ₂	(M-H)-
238.0702	1	254616.0	C ₁₄ H ₁₀ N ₂ O ₂	(M-H)-
239.0724	1	26267.5	C ₁₄ H ₁₀ N ₂ O ₂	(M-H)-
240.0739	1	2035.5	C ₁₄ H ₁₀ N ₂ O ₂	(M-H)-
283.0680	1	1953.6	C ₁₄ H ₁₀ N ₂ O ₂	(M+HCOO)-
284.0711	1	341.9	C ₁₄ H ₁₀ N ₂ O ₂	(M+HCOO)-
285.0695	1	334.6	C ₁₄ H ₁₀ N ₂ O ₂	(M+HCOO)-

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