

Walkup MS Report



Data File	MLO414 + ONOO_Neg_5mins_MS_06072.d	Sample Name	MLO414 + ONOO
Sample Type	Sample	Position	P1-A11
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_5mins_MS.m	Acquired Time	7/10/2019 11:47:01 AM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C14H12N2O2	Walkup Method Description	Negative mode ionization using C18 column chromatography
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

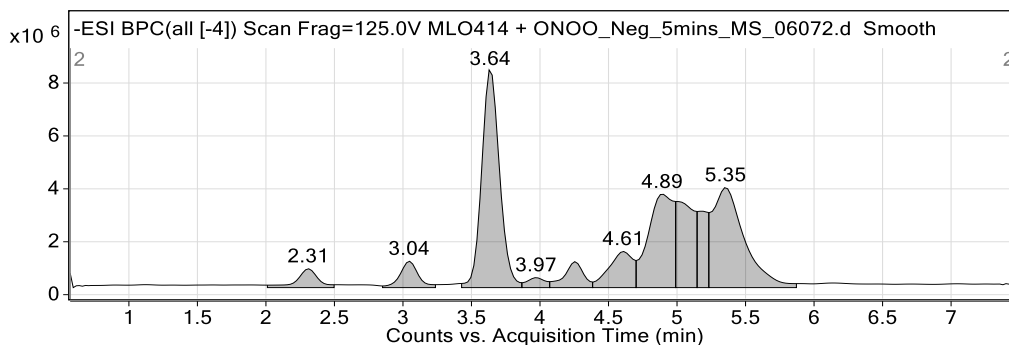


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
2.31	7792590	10.35	2.85	1033.9833	0.160
3.04	9251414	12.29	3.38	121.0288	0.140
3.64	75257789	100.00	27.53	239.0828	0.140
3.97	3493135	4.64	1.28	1033.9844	0.130
4.25	9563144	12.71	3.50	237.0659	0.150
4.61	16774836	22.29	6.14	420.2489	0.170
4.89	45519270	60.48	16.65	265.1567	0.190
5.04	29098276	38.66	10.65	291.1990	0.140
5.18	14789099	19.65	5.41	291.1991	0.070
5.35	61800179	82.12	22.61	305.2150	0.230

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 H12 N2 O2	3.97	239.0825	240.0897	240.0899	-0.74	99.62

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

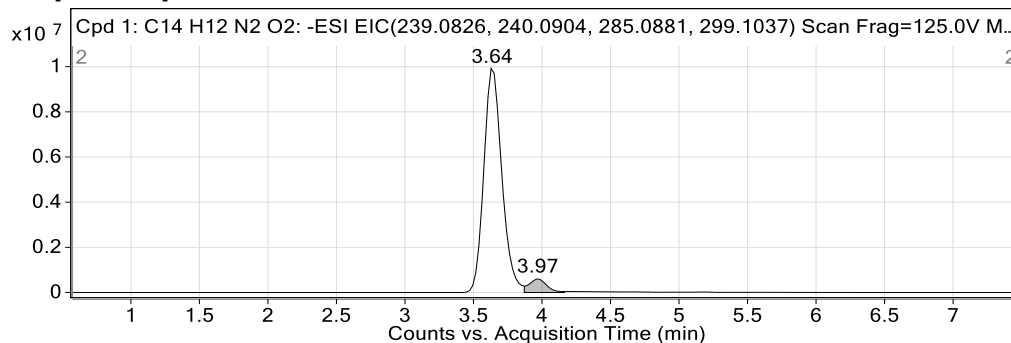


Figure: Extracted ion chromatogram (EIC) of compound.

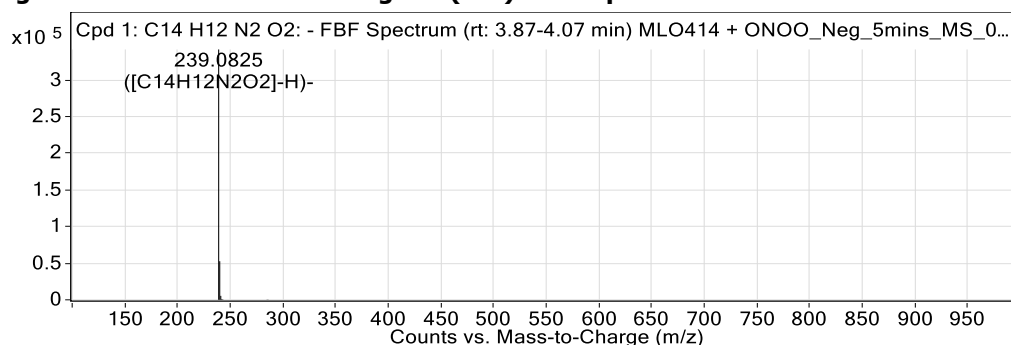


Figure: Full range view of Compound spectra and potential adducts.

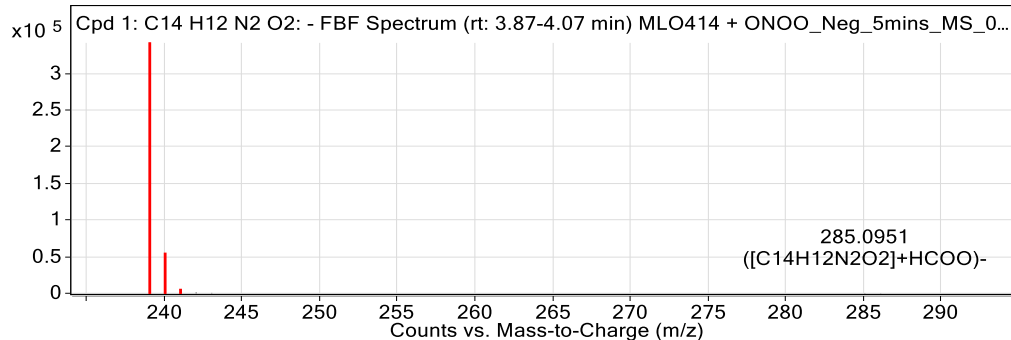


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
239.0825	1	341418.3	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
240.0855	1	52631.9	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
241.0875	1	5430.3	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
242.0619	1	956.9	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
243.0653	1	474.3	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
285.0951	1	295.9	C ₁₄ H ₁₂ N ₂ O ₂	(M+HCOO)-
286.1207	1	201.8	C ₁₄ H ₁₂ N ₂ O ₂	(M+HCOO)-

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