

Walkup MS Report



Data File	mlo416 ONOO_Neg_LoopInjection_MS_fragile_01391.d	Sample Name	mlo416 ONOO
Sample Type	Sample	Position	P1-A2
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS_fragile.m	Acquired Time	1/10/2019 2:53:54 PM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS_fragile.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_LoopInjection_MS_fragile
Formula	C46H43BCIN3O7, C14H12N2O2, C19H16ClNO4	Walkup Method Description	Lower fragmentor and Rf voltages in negative mode loop injection for fragile ions
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

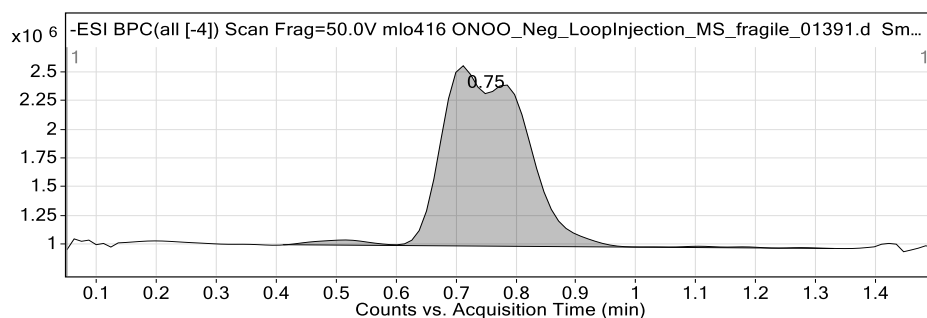


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	15399040	100.00	100.00	112.9838	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 (%)	Error flag
Cpd 1: C46 H43 B Cl N3 O7	1.15	795.2957	794.2910	794.2919	-1.18	5.25	low score
Cpd 2: C14 H12 N2 O2	0.71	239.0810	240.0882	240.0899	-6.91	80.89	
Cpd 3: C19 H16 Cl N O4	0.98	402.0765	357.0823	357.0768	15.39	16.43	m/z tolerance

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

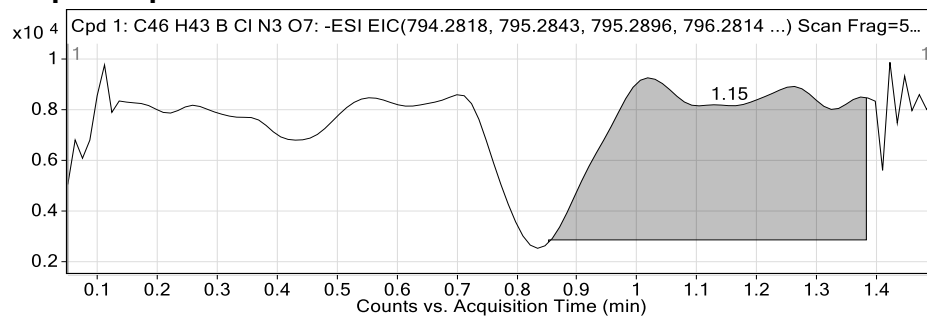


Figure: Extracted ion chromatogram (EIC) of compound.

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

Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

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Compound specific information

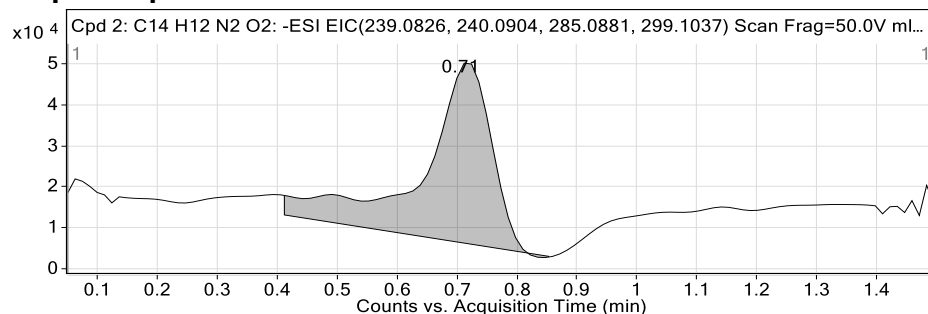


Figure: Extracted ion chromatogram (EIC) of compound.

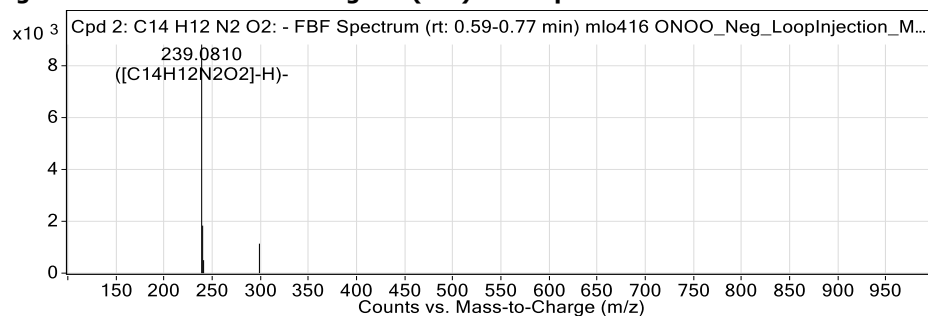


Figure: Full range view of Compound spectra and potential adducts.

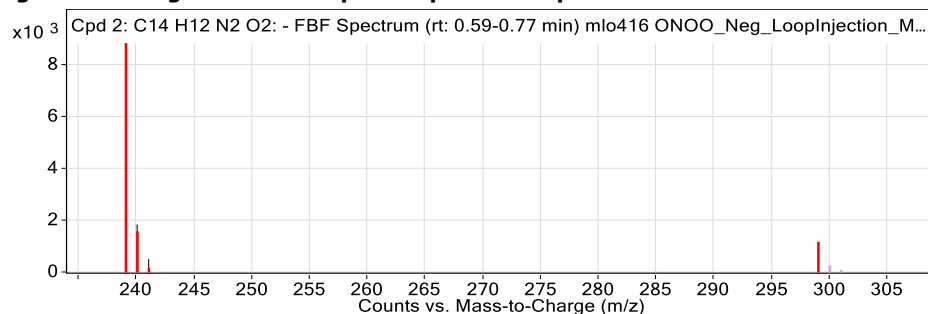


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
239.0810	1	8816.7	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
240.0855	1	1832.5	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
241.0869	1	500.3	C ₁₄ H ₁₂ N ₂ O ₂	(M-H)-
299.0988	1	1137.0	C ₁₄ H ₁₂ N ₂ O ₂	(M+CH ₃ COO)-

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Compound specific information

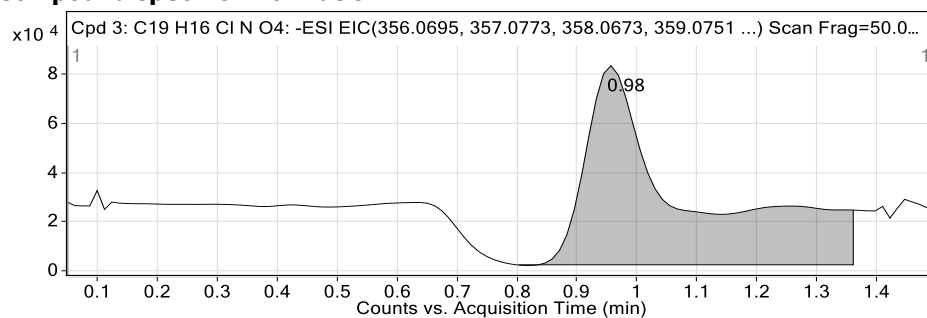


Figure: Extracted ion chromatogram (EIC) of compound.

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

Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

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