

Walkup MS Report



Data File	MLO349 ONOO-_Neg_LoopInjection_MS_04396.d	Sample Name	MLO349 ONOO-
Sample Type	Sample	Position	P1-B3
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS.m	Acquired Time	5/23/2019 11:56:03 AM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_LoopInjection_MS
Formula	C10H8O4, C15H21Cl2O2N, C15H21Cl2NO, C7H6O	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)

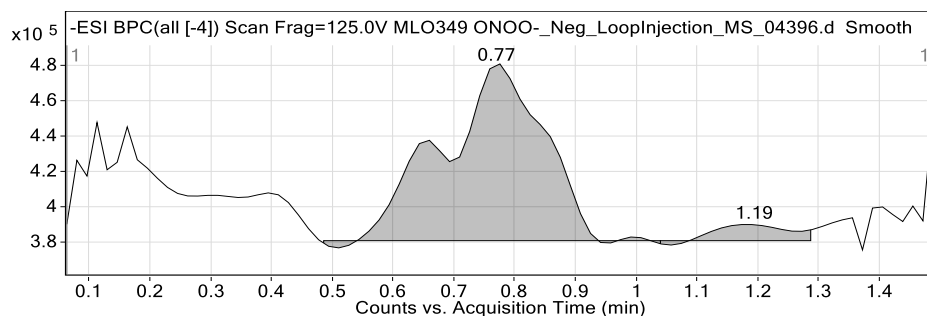


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.77	1165063	100.00	94.14	1033.9819	0.220
1.19	72525	6.23	5.86	1033.9819	0.150

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: C10 H8 O4	0.62	191.0367	192.0438	192.0423	8.08	59.38	
Cpd 2: C15 H21 Cl2 N O2				317.0949			m/z tolerance
Cpd 3: C15 H21 Cl2 N O				301.1000			m/z tolerance
Cpd 4: C7 H6 O	1.26	151.0413	106.0413	106.0419	-5.49	15.60	low score

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

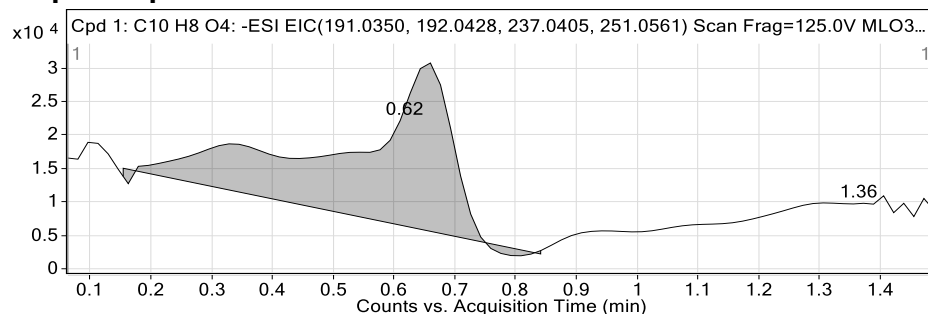


Figure: Extracted ion chromatogram (EIC) of compound.

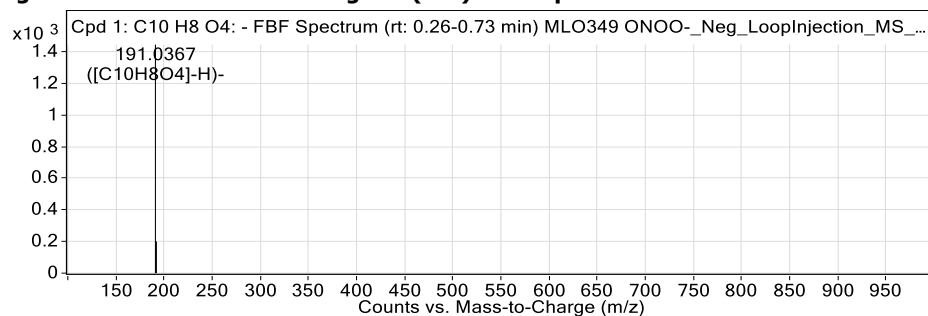


Figure: Full range view of Compound spectra and potential adducts.

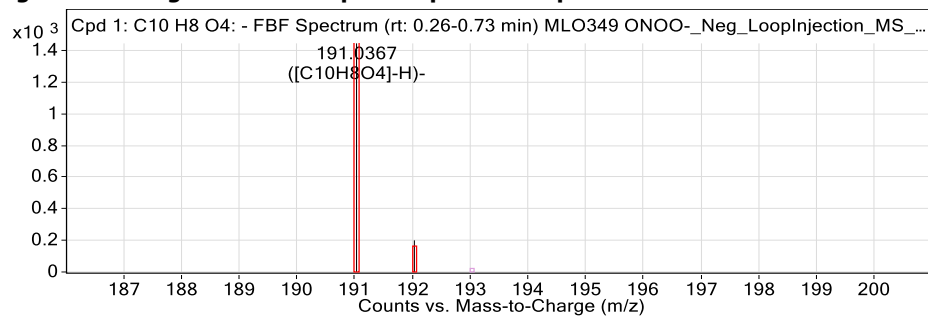


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
191.0367	1	1444.5	C ₁₀ H ₈ O ₄	(M-H)-
192.0384	1	199.8	C ₁₀ H ₈ O ₄	(M-H)-

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Compound specific information

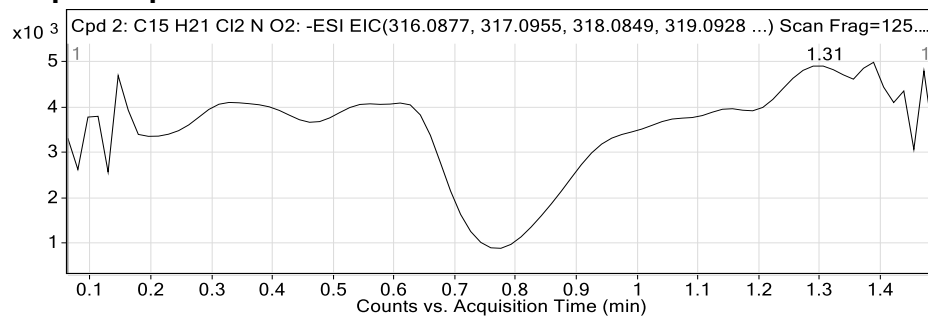


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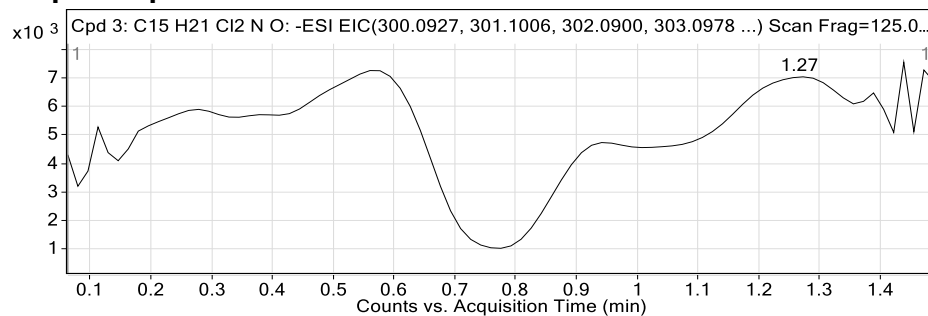


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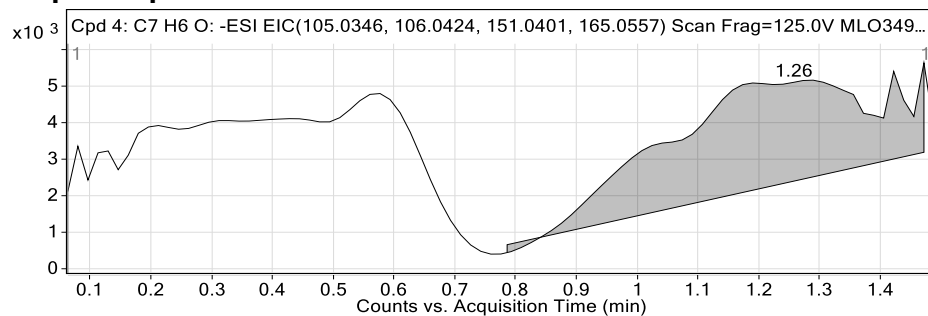


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