

Walkup MS Report



Data File	mlo435_Neg_LoopInjection_MS_02838.d	Sample Name	mlo435
Sample Type	Sample	Position	P1-A1
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS.m	Acquired Time	3/7/2019 9:54:40 AM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description	coumarin-morpholine	Walkup Method	Neg_LoopInjection_MS
Formula	C17H19NO6	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)

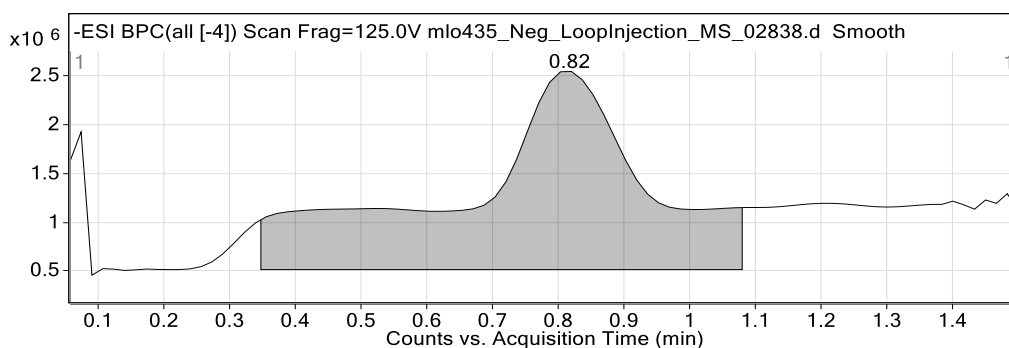


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.82	39138449	100.00	100.00	191.0325	0.290

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: C17 H19 N O6	0.83	332.1142	333.1214	333.1212	0.46	99.83

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

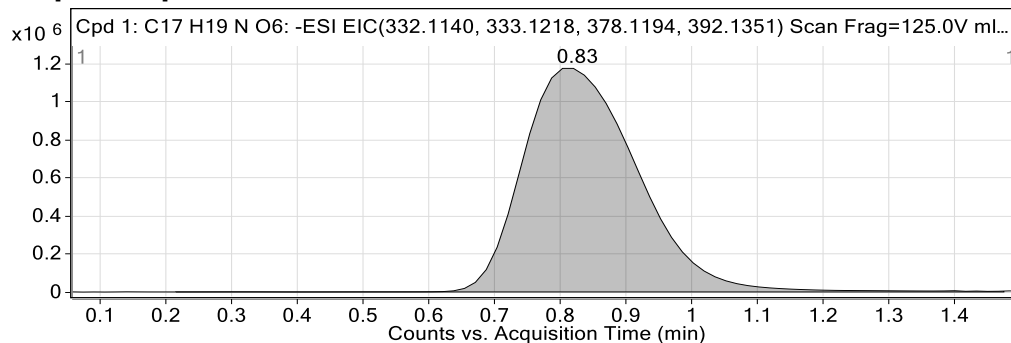


Figure: Extracted ion chromatogram (EIC) of compound.

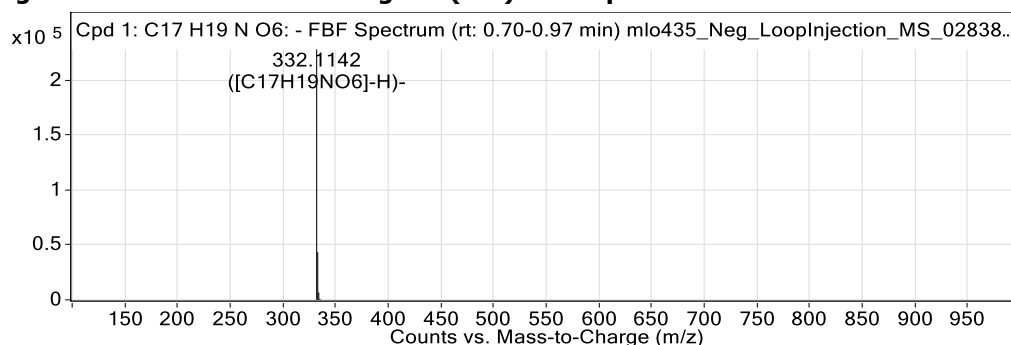


Figure: Full range view of Compound spectra and potential adducts.

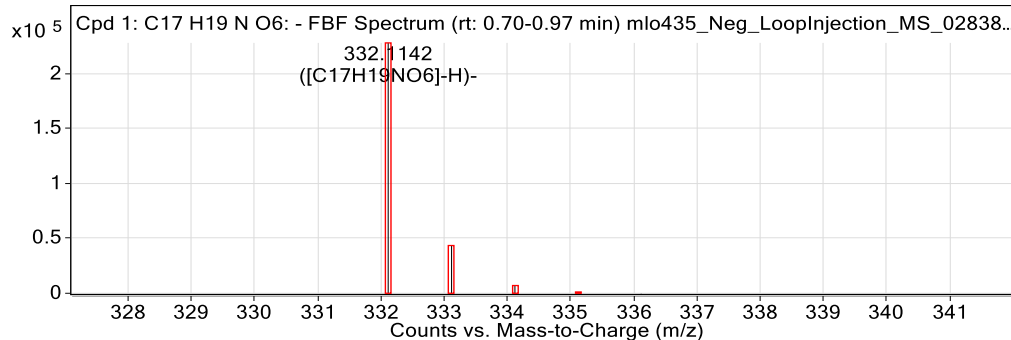


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
332.1142	1	228211.4	C ₁₇ H ₁₉ NO ₆	(M-H)-
333.1172	1	43469.4	C ₁₇ H ₁₉ NO ₆	(M-H)-
334.1195	1	6703.0	C ₁₇ H ₁₉ NO ₆	(M-H)-
335.1217	1	921.7	C ₁₇ H ₁₉ NO ₆	(M-H)-
336.1166	1	193.8	C ₁₇ H ₁₉ NO ₆	(M-H)-

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