

Walkup MS Report



Data File	esipt-br + ONOO-_Neg_LoopInjection_MS_06201.d	Sample Name	esipt-br + ONOO-
Sample Type	Sample	Position	P1-A4
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS.m	Acquired Time	7/12/2019 12:44:34 PM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_LoopInjection_MS
Formula	C13H9BrN2O	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)

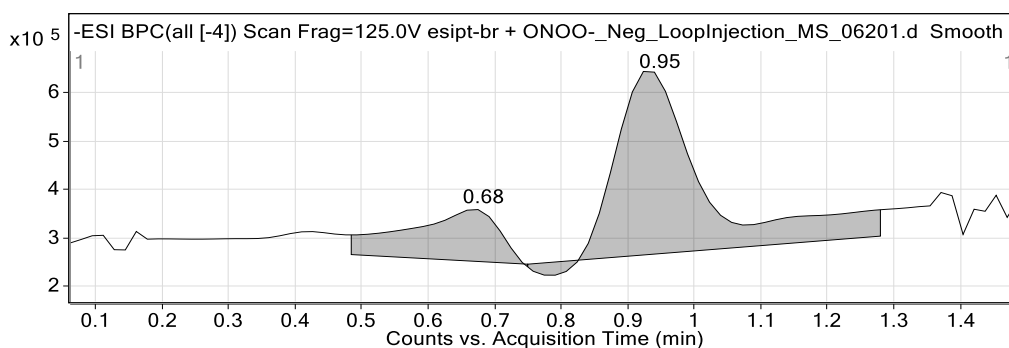


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.68	1012517	29.91	23.02	1033.9715	0.170
0.95	3385387	100.00	76.98	286.9762	0.180

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: C13 H9 Br N2 O	0.68	286.9821	287.9893	287.9898	-1.72	99.69

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

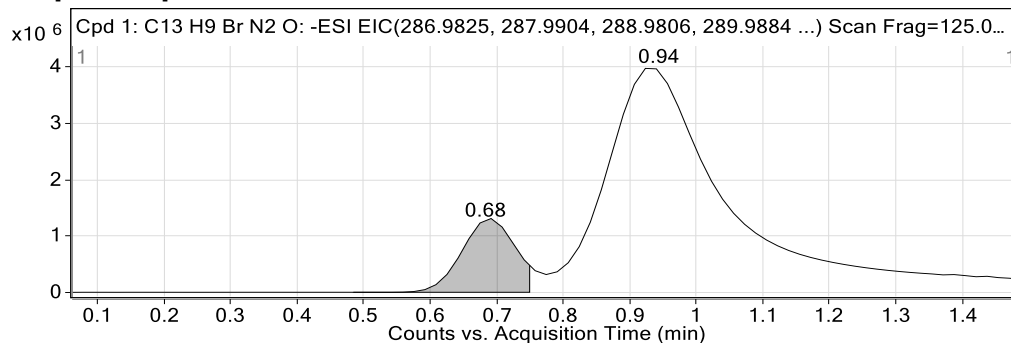


Figure: Extracted ion chromatogram (EIC) of compound.

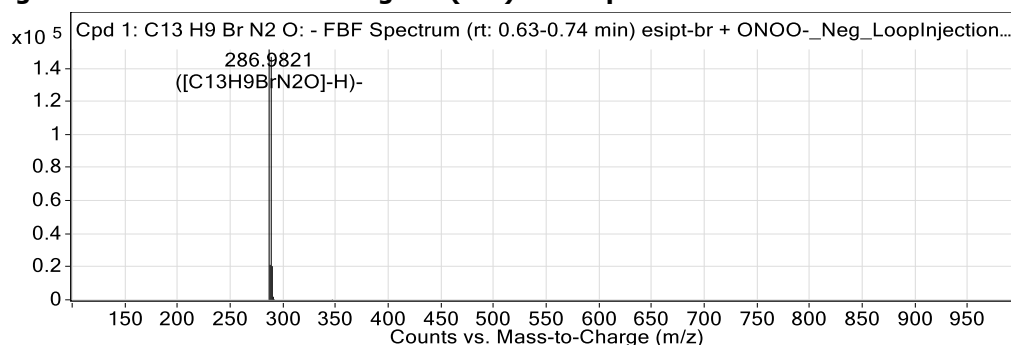


Figure: Full range view of Compound spectra and potential adducts.

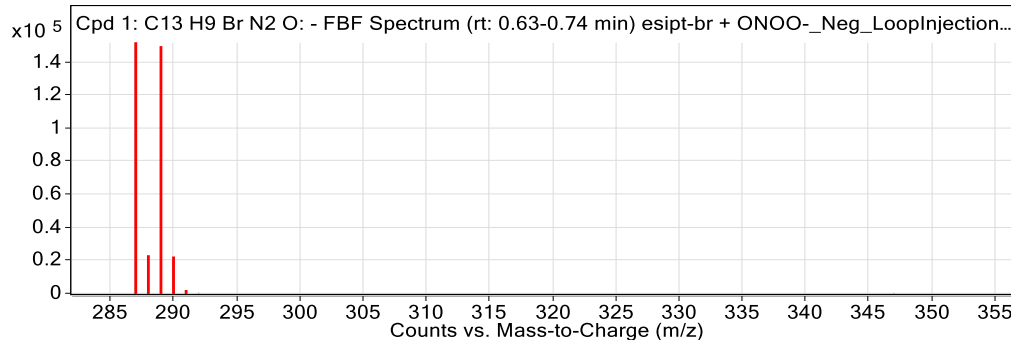


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
286.9821	1	151397.3	C ₁₃ H ₉ BrN ₂ O	(M-H)-
287.9850	1	21145.5	C ₁₃ H ₉ BrN ₂ O	(M-H)-
288.9801	1	146932.5	C ₁₃ H ₉ BrN ₂ O	(M-H)-
289.9827	1	20360.6	C ₁₃ H ₉ BrN ₂ O	(M-H)-
290.9850	1	1835.3	C ₁₃ H ₉ BrN ₂ O	(M-H)-
291.9915	1	236.9	C ₁₃ H ₉ BrN ₂ O	(M-H)-
347.0129	1	188.0	C ₁₃ H ₉ BrN ₂ O	(M+CH ₃ COO)-

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