

# Walkup MS Report



<b>Data File</b>	Cou-Bpin-Br + ONOO0_Neg_5mins_MS_06528.d	<b>Sample Name</b>	Cou-Bpin-Br + ONOO0
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A1
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Maria Odyniec
<b>Acq Method</b>	Neg_5mins_MS.m	<b>Acquired Time</b>	7/23/2019 9:51:05 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Neg_5mins_MS.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Walkup Sample Description</b>		<b>Walkup Method</b>	Neg_5Mins_C18
<b>Formula</b>	C10H7BrO3	<b>Walkup Method Description</b>	Negative mode ionization using C18 column chromatography
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

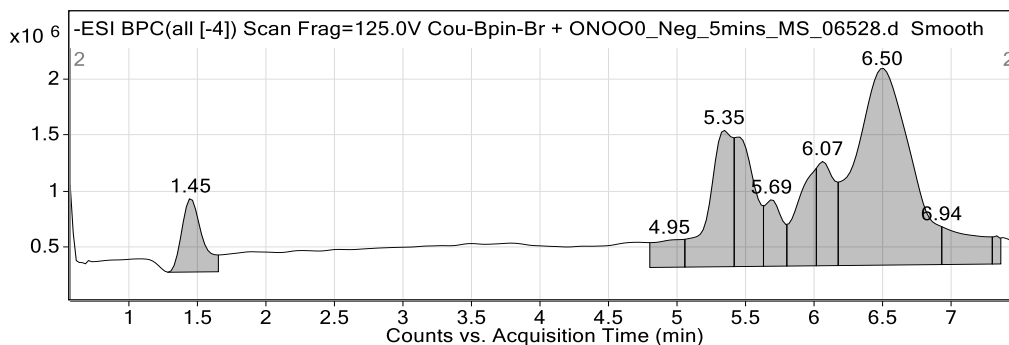


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
1.45	6862831	14.11	6.00	1033.9822	0.150
4.95	3652502	7.51	3.19	1033.9859	0.200
5.35	14930189	30.70	13.05	1033.9865	0.180
5.45	11612353	23.88	10.15	1033.9873	0.150
5.69	5250982	10.80	4.59	1033.9872	0.150
5.93	8264946	16.99	7.23	1033.9879	0.170
6.07	8188168	16.84	7.16	1033.9881	0.130
6.50	48636907	100.00	42.52	1033.9885	0.440
6.94	6078722	12.50	5.31	1033.9885	0.300
7.33	907204	1.87	0.79	1033.9889	0.060

## Compound Table

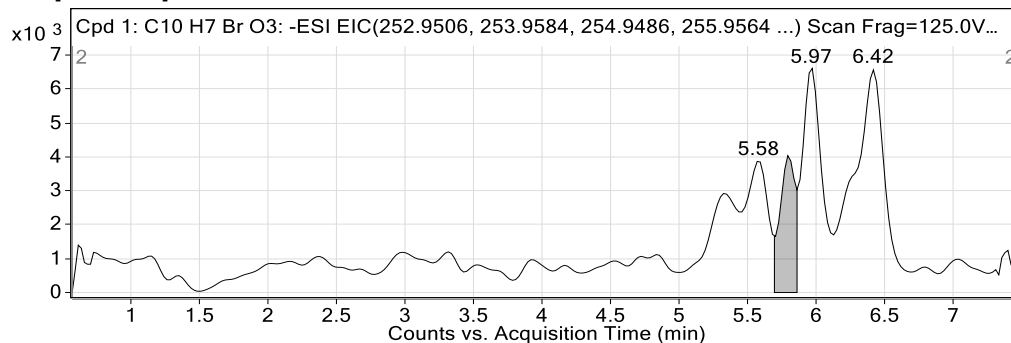
Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C10 H7 Br O3	5.80	252.9505	253.9569	253.9579	-3.60	83.05

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

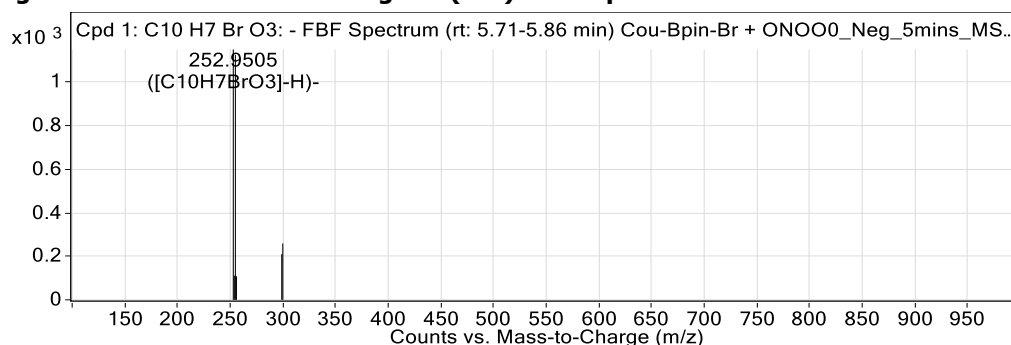
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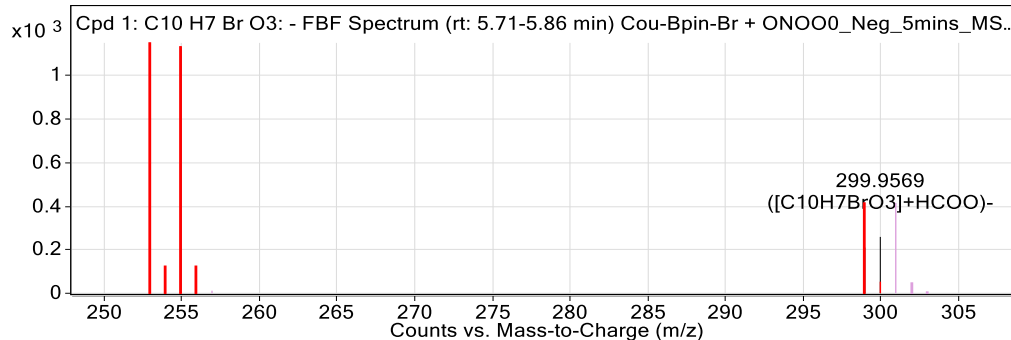
## Compound specific information



**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
252.9505	1	1150.9	C10H7BrO3	(M-H)-
253.9498	1	110.7	C10H7BrO3	(M-H)-
254.9468	1	1126.4	C10H7BrO3	(M-H)-
255.9493	1	108.4	C10H7BrO3	(M-H)-
298.9604	1	210.0	C10H7BrO3	(M+HCOO)-
299.9569	1	259.1	C10H7BrO3	(M+HCOO)-

--- End Of Report ---