Walkup MS Report

Data File	SE-470-3 (AC)_Neg_5mins_MS_07361.d	**Sample Name**	SE-470-3 (AC)
Sample Type	Sample	**Position**	P1-C5
Instrument Name	6545 QTof	**User Name**	Susana Estopina-Duran
Acq Method	Neg_5mins_MS.m	**Acquired Time**	8/29/2019 7:28:48 PM
IRM Calibration Status	Success	**DA Method**	Neg_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Neg_5Mins_C18
Formula	C11H13I	**Walkup Method Description**	Negative mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

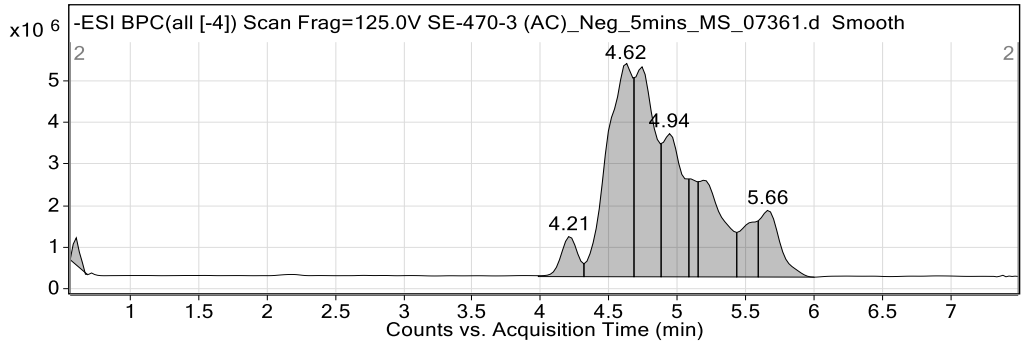

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.60	2168471	3.26	0.94	1033.9877	0.060
4.21	8172123	12.29	3.55	230.9862	0.130
4.62	66516947	100.00	28.89	246.9263	0.170
4.74	50865954	76.47	22.09	288.9739	0.140
4.94	35887132	53.95	15.59	265.1577	0.150
5.09	9442538	14.20	4.10	311.2023	0.070
5.19	28994177	43.59	12.59	305.2165	0.210
5.52	11689447	17.57	5.08	305.2160	0.130
5.66	16529040	24.85	7.18	265.1495	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 (%)
Cpd 1: C11 H13 I	4.96	331.0194	272.0052	272.0062	-3.65	97.64

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

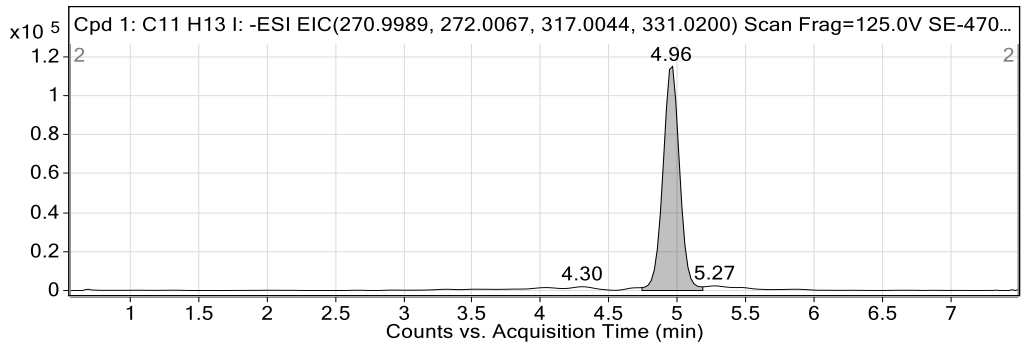

Figure: Extracted ion chromatogram (EIC) of compound.

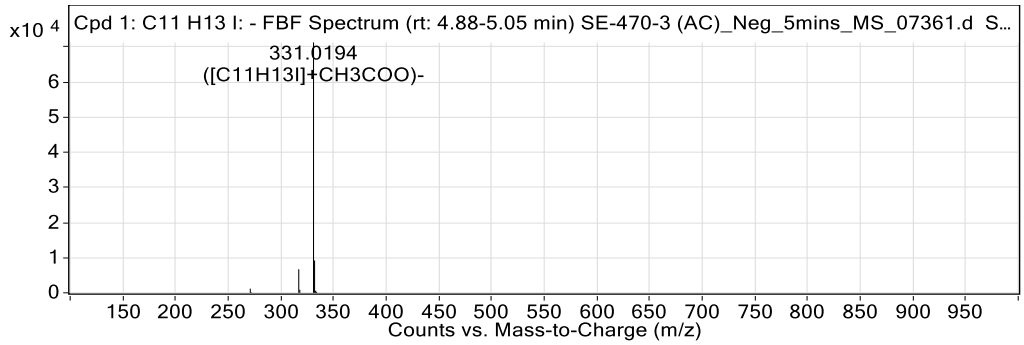

Figure: Full range view of Compound spectra and potential adducts.

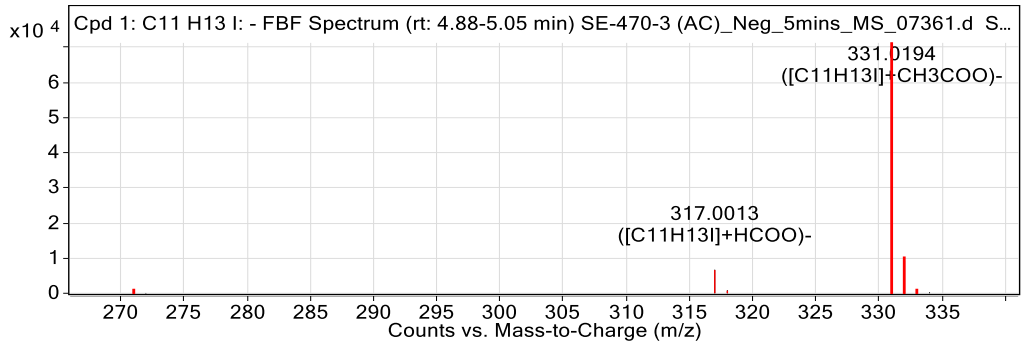

Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
270.9945	1	1178.4	C11H13I	(M-H)-
271.9664	1	82.1	C11H13I	(M-H)-
271.9991	1	72.2	C11H13I	M-
317.0013	1	6712.1	C11H13I	(M+HCOO)-
318.0052	1	872.9	C11H13I	(M+HCOO)-
331.0194	1	71251.4	C11H13I	(M+CH3COO)-
332.0229	1	9213.5	C11H13I	(M+CH3COO)-
333.0232	1	597.5	C11H13I	(M+CH3COO)-
334.0015	1	284.8	C11H13I	(M+CH3COO)-

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