Walkup MS Report

Data File	SE-570 (AC)_Neg_LoopInjection_MS_07370.d	**Sample Name**	SE-570 (AC)
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6545 QTof	**User Name**	Susana Estopina-Duran
Acq Method	Neg_LoopInjection_MS.m	**Acquired Time**	8/29/2019 9:11:14 PM
IRM Calibration Status	Success	**DA Method**	Neg_LoopInjection_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Neg_LoopInjection_MS
Formula	C15H22O	**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)

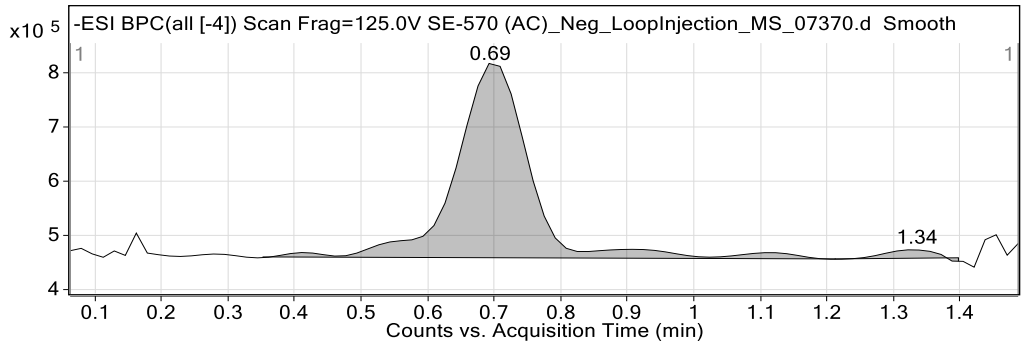

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.69	2816947	100.00	97.40	493.1205	0.150
1.34	75058	2.66	2.60	1033.9874	0.100

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: C15 H22 O	0.95	277.1839	218.1650	218.1671	-9.36	77.05

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

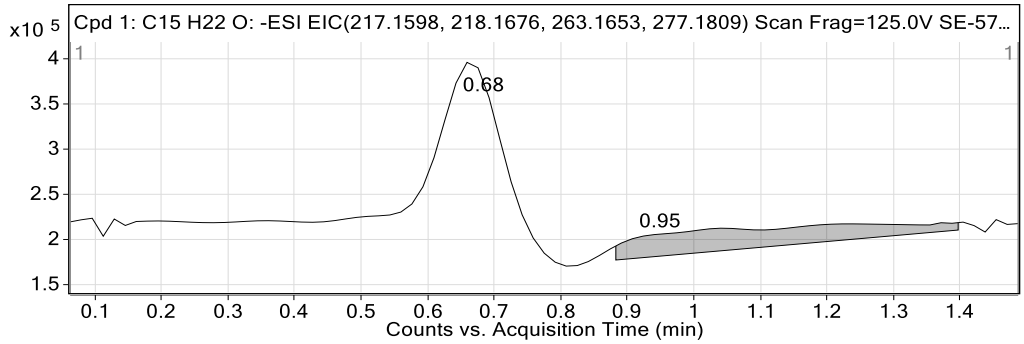

Figure: Extracted ion chromatogram (EIC) of compound.

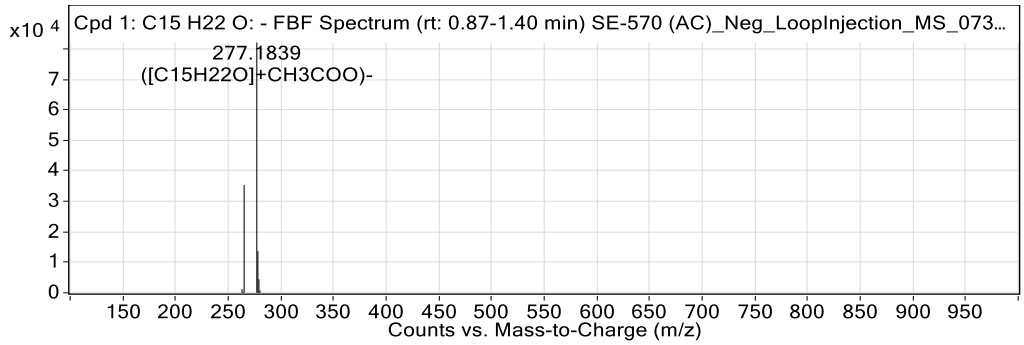

Figure: Full range view of Compound spectra and potential adducts.

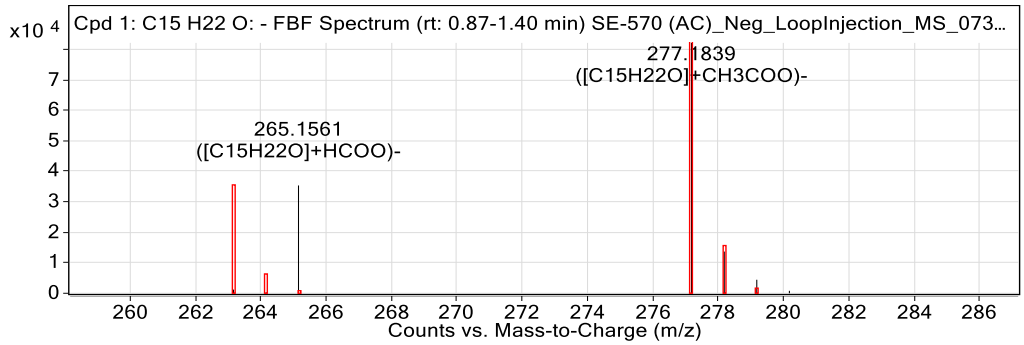

Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
263.1674	1	1201.7	C15H22O	(M+HCOO)-
264.1668	1	305.3	C15H22O	(M+HCOO)-
265.1561	1	35335.2	C15H22O	(M+HCOO)-
277.1839	1	82058.9	C15H22O	(M+CH3COO)-
278.1871	1	13665.9	C15H22O	(M+CH3COO)-
279.1823	1	4432.9	C15H22O	(M+CH3COO)-
280.1805	1	810.6	C15H22O	(M+CH3COO)-

--- End Of Report ---

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