

Walkup Analysis Report



Data Filename	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

Walkup Sample Description

Formula C15H22O

Stream Name LC 1

Info.

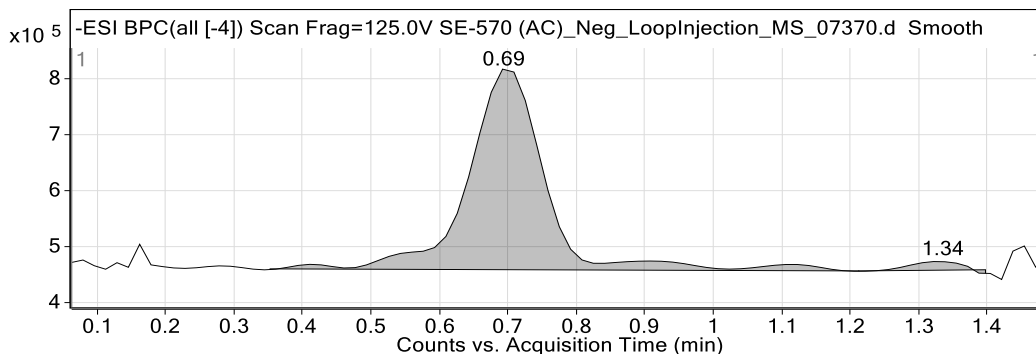
Walkup Method Neg_LoopInjection_MS

Walkup Method Description Negative mode ionization using loop injection

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

User Chromatograms

Fragmentor Voltage 125 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.35	0.69	1.21	321423	2816947	100
2	1.21	1.34	1.4	12748	75058	2.66

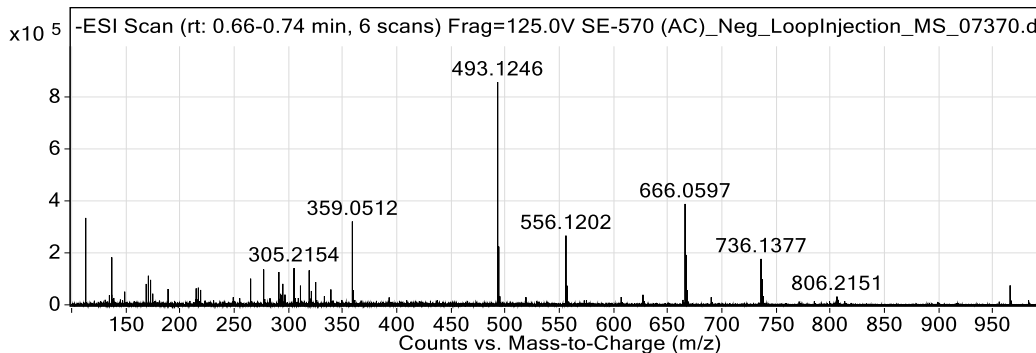
User Spectra

Spectrum Source
Peak (1) in "- BPC(all [-4]) Scan"

Fragmentor Voltage
125

Collision Energy
0

Ionization Mode
ESI



Peak List

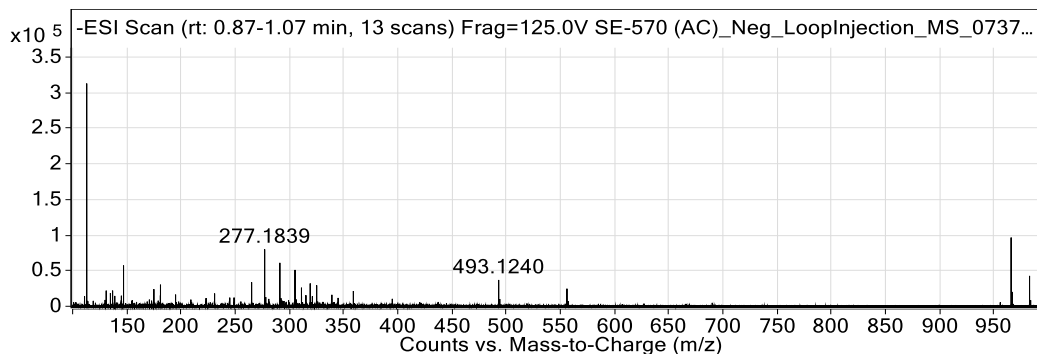
m/z	z	Abund
61.9883		200808.28
112.9857		334096.35
137.0241	1	193397.33
359.0512	1	341620.7
493.1246	1	875114.47

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494.1278	1	223660.26
556.1202	1	271845.18
666.0597	1	392909.9
667.0621	1	191949.02
1033.9881	1	879530.22

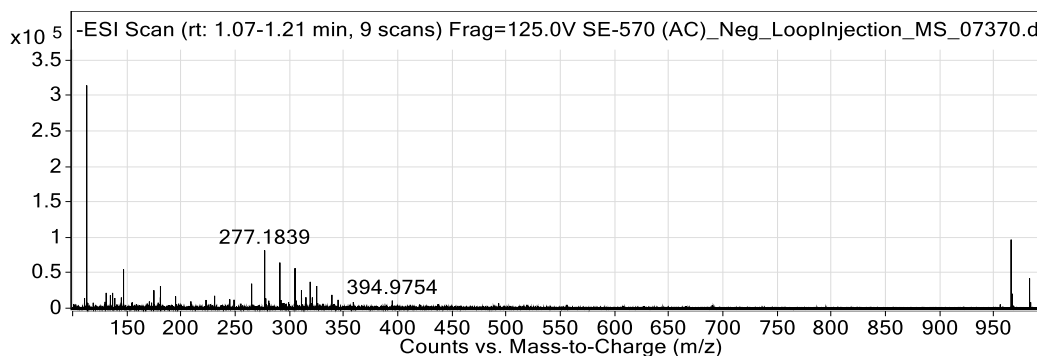
Spectrum Source Peak (2) in "- BPC(all [-4]) Scan" **Fragmentor Voltage** 125 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.9882		89755.8
68.9956		83580.1
112.9857		312903.73
146.9655		58110.86
277.1839	1	80209.58
291.1995	1	65503.06
305.2152	1	51083.32
965.9997	1	96602.62
1033.9881	1	878738.5
1034.9909	1	180527.73

Spectrum Source Peak (3) in "- BPC(all [-4]) Scan" **Fragmentor Voltage** 125 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

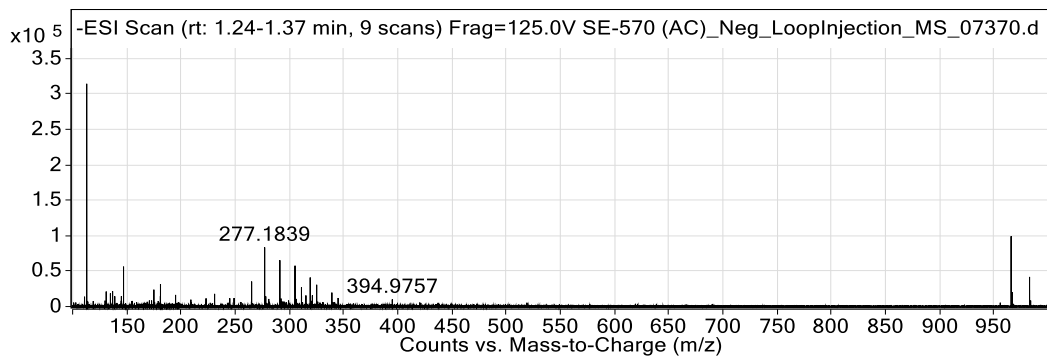
m/z	z	Abund
61.9882		78277.43
68.9956		84301.66
112.9857		314206.81
146.9655		55621.13
277.1839	1	81753.92
291.1995	1	69049.54
305.2152	1	56478.59

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965.9997	1	96762.23
1033.9881	1	877837.76
1034.991	1	184764.1

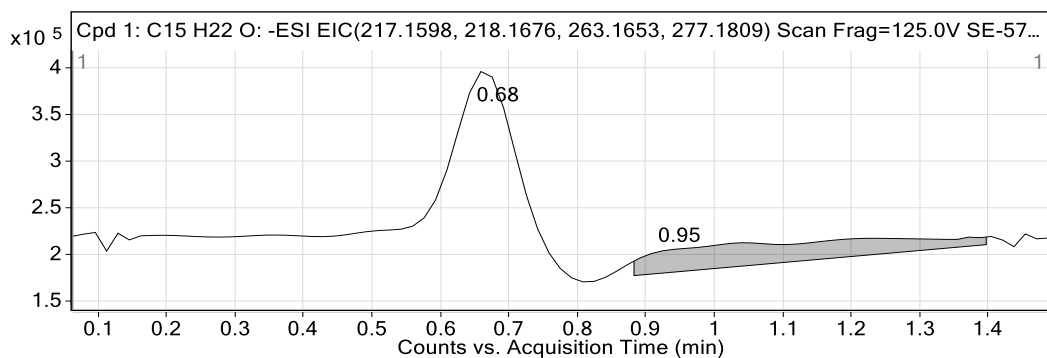
Spectrum Source Peak (4) in "- BPC(all [-4]) Scan" **Fragmentor Voltage** 125 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.9882		74536.99
68.9956		83869.75
112.9857		314312.89
146.9655		57167.43
277.1839	1	83689.19
291.1995	1	70296.98
305.2153	1	57711.74
965.9997	1	99230.58
1033.9881	1	879785.49
1034.991	1	183177.24

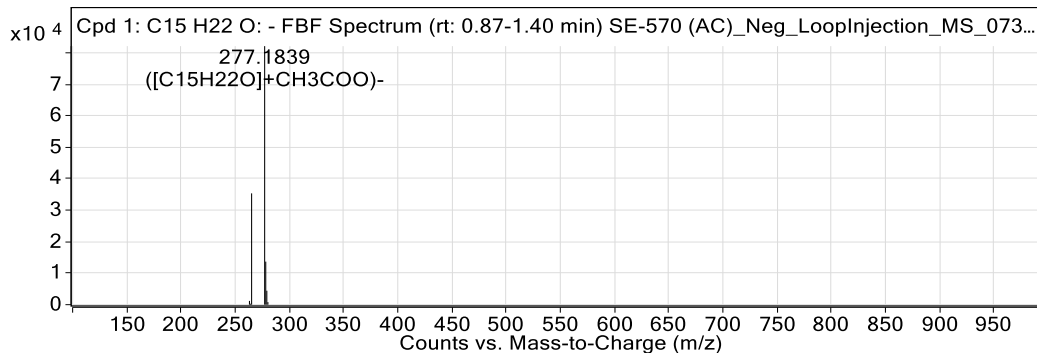
Compounds



Integration Peak List

Start	RT	End	Height	Area
0.35	0.68	0.82	179421	1656792
0.88	0.95	1.4	24278	569176

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Peak List

m/z	z	Abund	Formula	Ion
263.1674	1	1201.67	C ₁₅ H ₂₂ O	(M+HCOO)-
264.1668	1	305.25	C ₁₅ H ₂₂ O	(M+HCOO)-
265.1561	1	35335.17	C ₁₅ H ₂₂ O	(M+HCOO)-
277.1839	1	82058.94	C ₁₅ H ₂₂ O	(M+CH ₃ COO)-
278.1871	1	13665.85	C ₁₅ H ₂₂ O	(M+CH ₃ COO)-
279.1823	1	4432.89	C ₁₅ H ₂₂ O	(M+CH ₃ COO)-
280.1805	1	810.59	C ₁₅ H ₂₂ O	(M+CH ₃ COO)-

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