

Walkup MS Report



Data File	SE-562 (AC)_Neg_5mins_MS_07367.d	Sample Name	SE-562 (AC)
Sample Type	Sample	Position	P1-A2
Instrument Name	6545 QTof	User Name	Susana Estopina-Duran
Acq Method	Neg_5mins_MS.m	Acquired Time	8/29/2019 7:53:59 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C25H20O3	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)

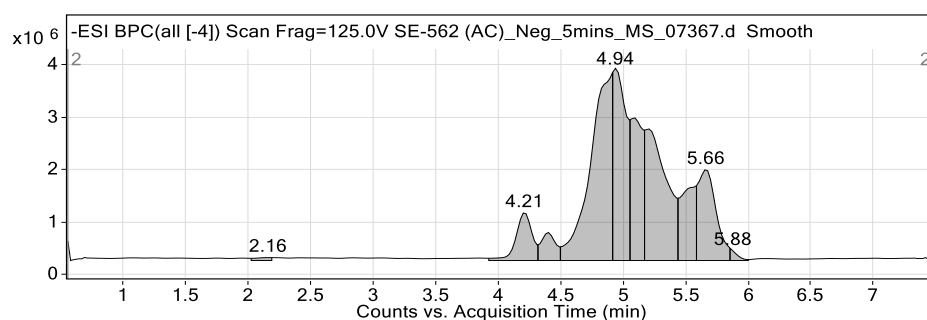


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
2.16	489788	1.14	0.30	1033.9879	0.130
4.21	8205995	19.08	5.09	230.9861	0.140
4.40	4282727	9.96	2.66	344.9790	0.120
4.80	43000580	100.00	26.67	277.1847	0.240
4.94	26815221	62.36	16.63	265.1577	0.120
5.09	18298547	42.55	11.35	311.2022	0.100
5.20	30077038	69.95	18.65	305.2161	0.200
5.52	11787196	27.41	7.31	305.2159	0.120
5.66	17446920	40.57	10.82	265.1495	0.150
5.88	828156	1.93	0.51	1033.9901	0.070

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)	Error flag
Cpd 1: C25 H20 O3	4.96	367.1345	368.1471	368.1412	15.83	98.16	m/z tolerance

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

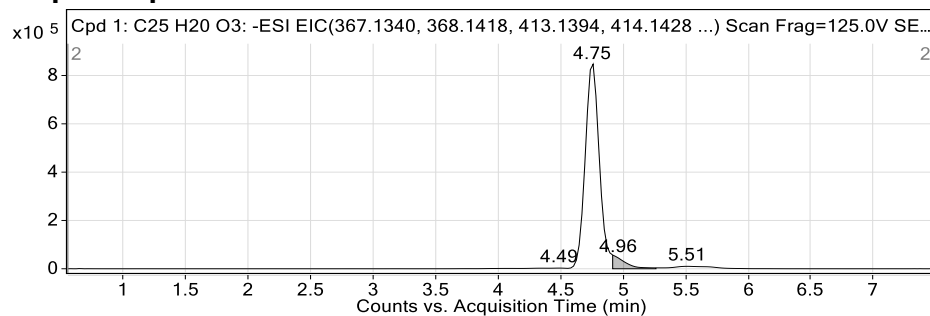


Figure: Extracted ion chromatogram (EIC) of compound.

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