

Walkup MS Report



Data File	SE-496-3- (AC-2)_Neg_5mins_MS_07359.d	Sample Name	SE-496-3- (AC-2)
Sample Type	Sample	Position	P1-C4
Instrument Name	6545 QTof	User Name	Susana Estopina-Duran
Acq Method	Neg_5mins_MS.m	Acquired Time	8/29/2019 7:20:25 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C19H19BrO3	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)

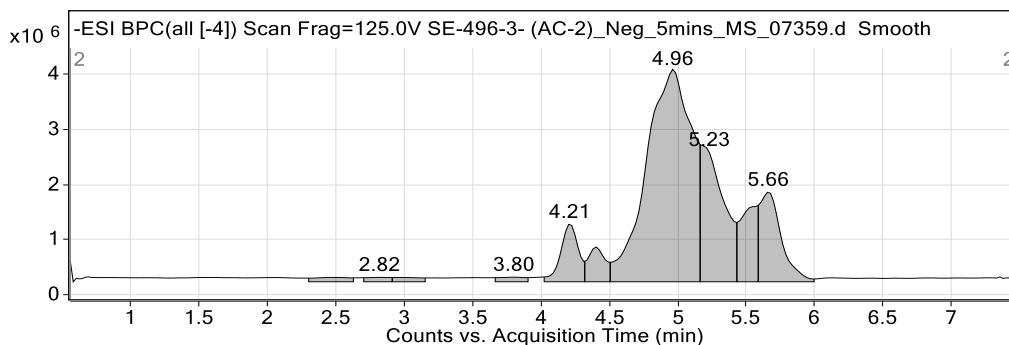


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
2.49	1442899	1.63	0.87	1033.9884	0.270
2.82	961176	1.08	0.58	1033.9881	0.170
2.98	1076091	1.21	0.65	1033.9872	0.200
3.80	1128688	1.27	0.68	1033.9884	0.190
4.21	9381256	10.58	5.63	230.9859	0.140
4.40	5435305	6.13	3.26	344.9791	0.130
4.96	88708217	100.00	53.26	265.1574	0.300
5.23	28790059	32.45	17.28	305.2159	0.210
5.52	11878281	13.39	7.13	305.2160	0.130
5.66	17761122	20.02	10.66	265.1496	0.160

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: C19 H19 Br O3	4.98	373.0446	374.0518	374.0518	0.19	99.70

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

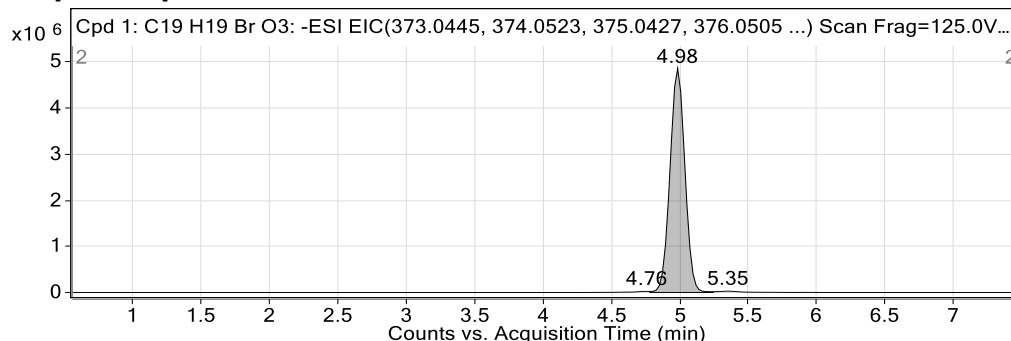


Figure: Extracted ion chromatogram (EIC) of compound.

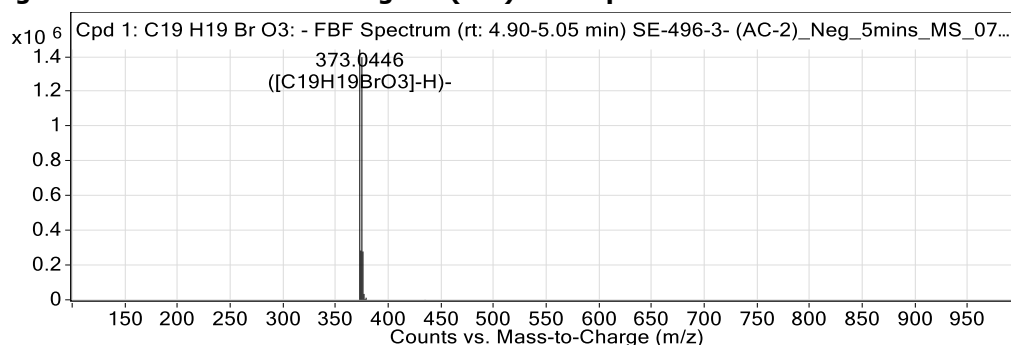


Figure: Full range view of Compound spectra and potential adducts.

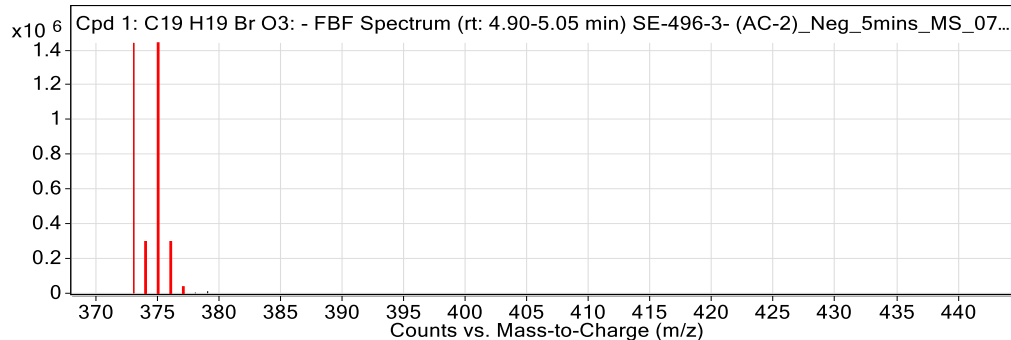


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
373.0446	1	1441312.4	C ₁₉ H ₁₉ BrO ₃	(M-H)-
374.0479	1	283829.0	C ₁₉ H ₁₉ BrO ₃	(M-H)-
375.0428	1	1396988.9	C ₁₉ H ₁₉ BrO ₃	(M-H)-
376.0460	1	278292.6	C ₁₉ H ₁₉ BrO ₃	(M-H)-
377.0483	1	33951.8	C ₁₉ H ₁₉ BrO ₃	(M-H)-
378.0512	1	4026.1	C ₁₉ H ₁₉ BrO ₃	(M-H)-
379.0491	1	12279.8	C ₁₉ H ₁₉ BrO ₃	(M-H)-
435.0512	1	543.8	C ₁₉ H ₁₉ BrO ₃	(M+CH ₃ COO)-
436.0743	1	44.8	C ₁₉ H ₁₉ BrO ₃	(M+CH ₃ COO)-

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