

Walkup MS Report



Data File	mlo427_Neg_5mins_MS_02087.d	Sample Name	mlo427
Sample Type	Sample	Position	P1-A10
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_5mins_MS.m	Acquired Time	2/6/2019 4:11:36 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C20H22N2O6S	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)

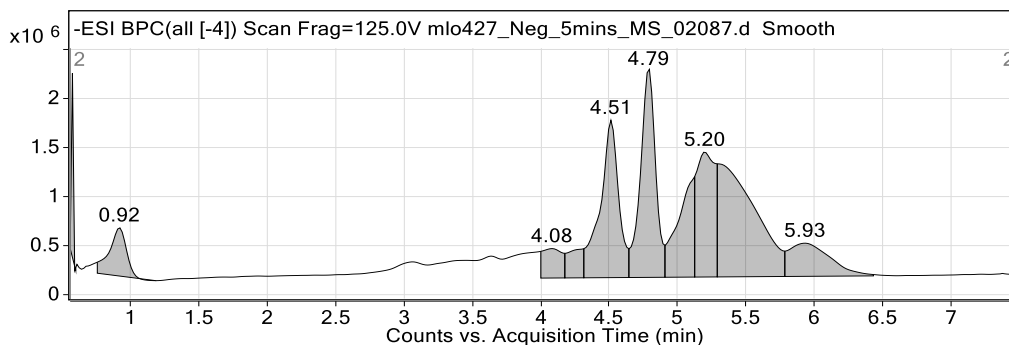


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.57	1837083	8.36	1.98	197.8083	0.020
0.92	4260835	19.39	4.60	417.1146	0.130
4.08	2977202	13.55	3.22	1033.9919	0.140
4.25	2315917	10.54	2.50	1033.9923	0.110
4.51	15221237	69.28	16.44	420.2517	0.140
4.79	16519777	75.19	17.84	277.1816	0.110
5.08	8544511	38.89	9.23	467.0896	0.160
5.20	11806843	53.74	12.75	299.2598	0.130
5.34	21970140	100.00	23.73	132.9235	0.350
5.93	7145177	32.52	7.72	1033.9908	0.350

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: C20 H22 N2 O6 S	3.64	417.1127	418.1199	418.1199	0.18	99.57

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

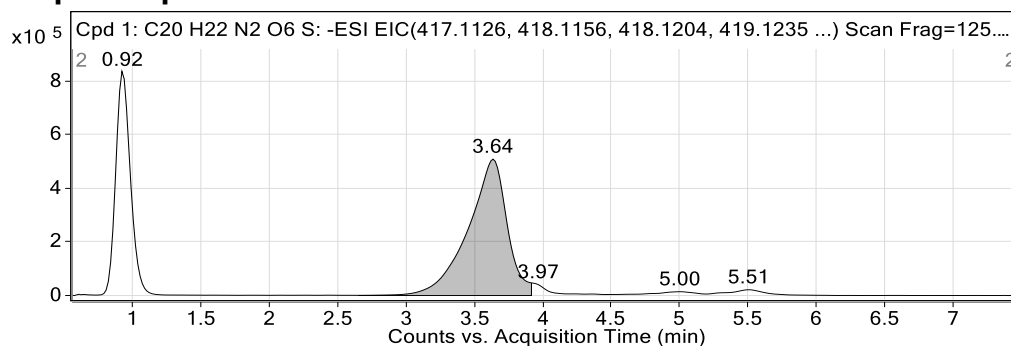


Figure: Extracted ion chromatogram (EIC) of compound.

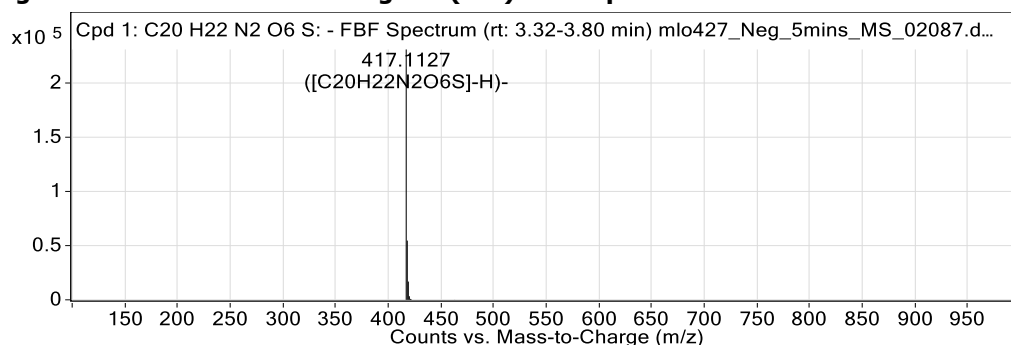


Figure: Full range view of Compound spectra and potential adducts.

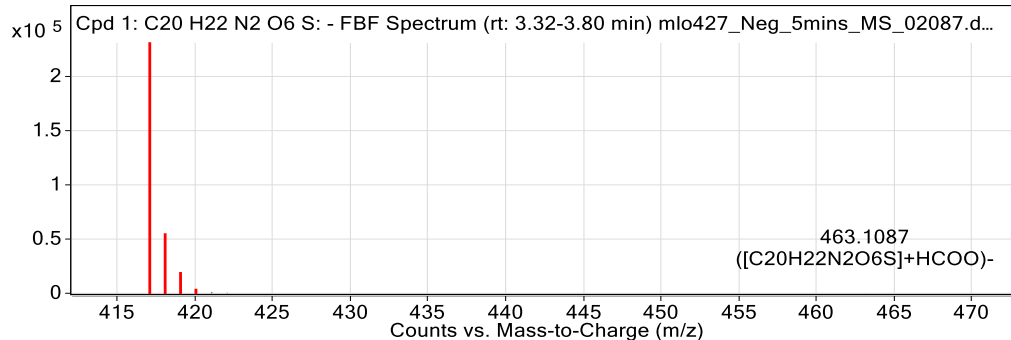


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
417.1127	1	231240.0	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
418.1157	1	54709.1	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
419.1134	1	16867.6	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
420.1147	1	3317.9	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
421.0938	1	842.8	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
422.0969	1	344.2	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
463.1087	1	52.7	C ₂₀ H ₂₂ N ₂ O ₆ S	(M+HCOO)-

--- End Of Report ---