

Walkup MS Report



Data File	mlo436_Neg_LoopInjection_MS_fragile_03864.d	Sample Name	mlo436
Sample Type	Sample	Position	P1-A7
Instrument Name	6545 QToF	User Name	Maria Odyniec
Acq Method	Neg_LoopInjection_MS_fragile.m	Acquired Time	4/24/2019 2:21:08 PM
IRM Calibration Status	Success	DA Method	Neg_LoopInjection_MS_fragile.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_LoopInjection_MS_fragile
Formula	C30H36NO8	Walkup Method Description	Lower fragmentor and Rf voltages in negative mode loop injection for fragile ions
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

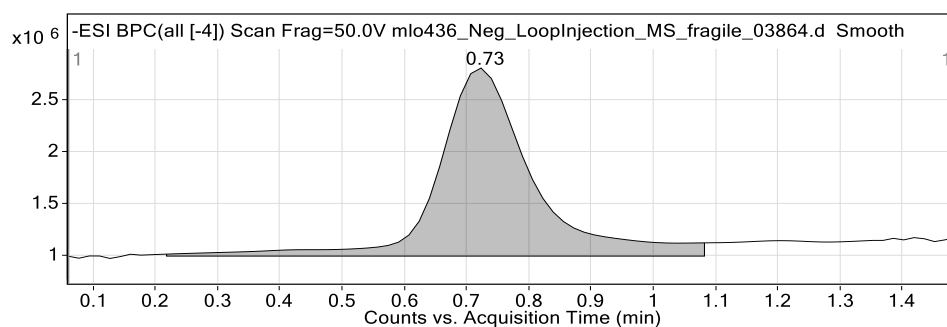


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.73	19169985	100.00	100.00	112.9840	0.180

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: C30 H36 B N O8	0.73	594.2513	548.2559	548.2570	-2.13	79.19

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

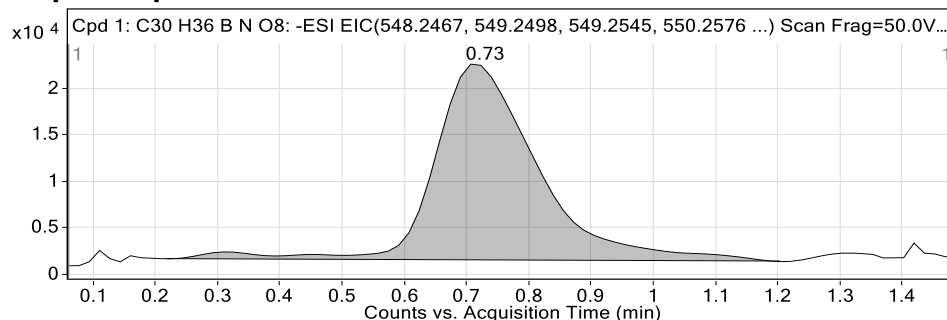


Figure: Extracted ion chromatogram (EIC) of compound.

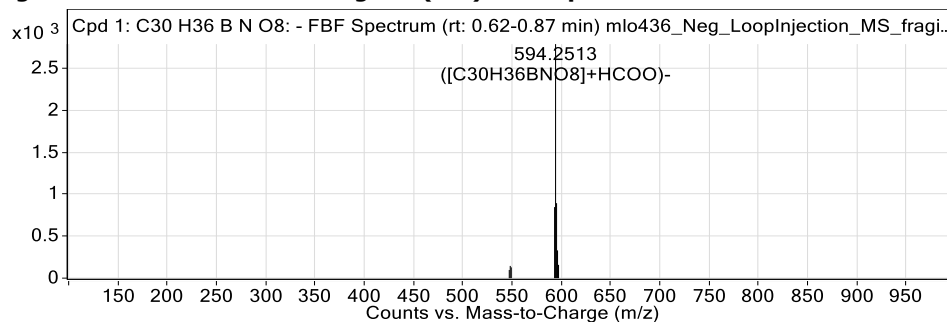


Figure: Full range view of Compound spectra and potential adducts.

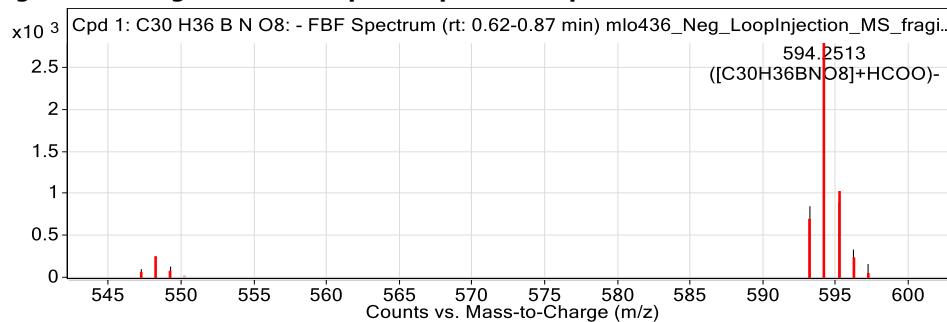


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
547.2608	1	97.3	C ₃₀ H ₃₆ BNO ₈	(M-H)-
548.2395	1	145.6	C ₃₀ H ₃₆ BNO ₈	(M-H)-
549.2737	1	128.3	C ₃₀ H ₃₆ BNO ₈	(M-H)-
593.2545	1	846.3	C ₃₀ H ₃₆ BNO ₈	(M+HCOO)-
594.2513	1	2787.9	C ₃₀ H ₃₆ BNO ₈	(M+HCOO)-
595.2525	1	893.3	C ₃₀ H ₃₆ BNO ₈	(M+HCOO)-
596.2484	1	330.6	C ₃₀ H ₃₆ BNO ₈	(M+HCOO)-
597.2547	1	158.2	C ₃₀ H ₃₆ BNO ₈	(M+HCOO)-

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