

Walkup MS Report



Data File	mlo428_Pos_LoopInjection_MS_fragile2_02140.d	Sample Name	mlo428
Sample Type	Sample	Position	P1-A4
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Pos_LoopInjection_MS_fragile2.m	Acquired Time	2/7/2019 5:43:36 PM
IRM Calibration Status	Success	DA Method	Pos_LoopInjection_MS_fragile2.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Pos_LoopInjection_MS_fragile
Formula	C33H39BN2O8S	Walkup Method Description	Lower fragmentor and Rf voltages in positive 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)

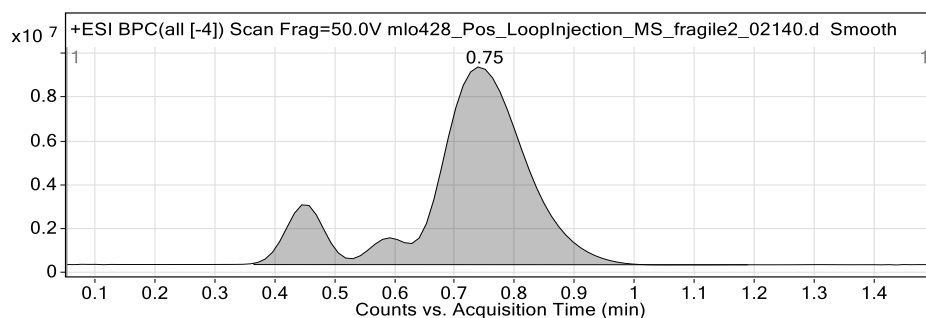


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	101262781	100.00	100.00	107.0415	0.210

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: C33 H39 B N2 O8 S	0.79	657.2422	633.2580	633.2556	3.68	99.26	No H adduct

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

Walkup MS Report

Compound specific information

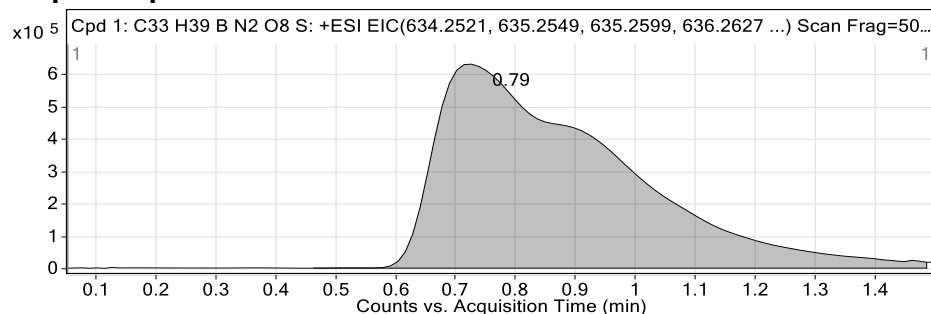


Figure: Extracted ion chromatogram (EIC) of compound.

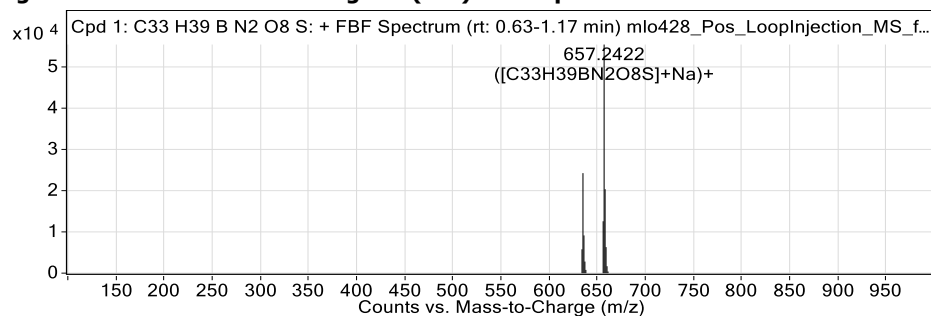


Figure: Full range view of Compound spectra and potential adducts.

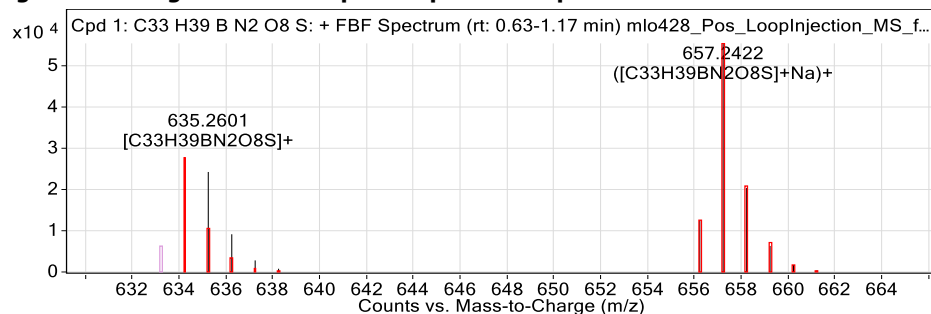


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
634.2632	1	5787.8	C ₃₃ H ₃₉ BN ₂ O ₈ S	M+
635.2601	1	24267.7	C ₃₃ H ₃₉ BN ₂ O ₈ S	M+
636.2629	1	9152.8	C ₃₃ H ₃₉ BN ₂ O ₈ S	M+
637.2627	1	2806.4	C ₃₃ H ₃₉ BN ₂ O ₈ S	M+
638.2617	1	783.6	C ₃₃ H ₃₉ BN ₂ O ₈ S	M+
656.2448	1	12588.8	C ₃₃ H ₃₉ BN ₂ O ₈ S	(M+Na)+
657.2422	1	55473.1	C ₃₃ H ₃₉ BN ₂ O ₈ S	(M+Na)+
658.2449	1	20371.4	C ₃₃ H ₃₉ BN ₂ O ₈ S	(M+Na)+
659.2449	1	6312.5	C ₃₃ H ₃₉ BN ₂ O ₈ S	(M+Na)+
660.2463	1	1675.8	C ₃₃ H ₃₉ BN ₂ O ₈ S	(M+Na)+

--- End Of Report ---