

Walkup MS Report



Data File	mlo446_Pos_LoopInjection_MS_fragile2_03648.d	Sample Name	mlo446
Sample Type	Sample	Position	P1-A1
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Pos_LoopInjection_MS_fragile2.m	Acquired Time	4/9/2019 2:47:17 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	C26H26BN2O3Br	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)

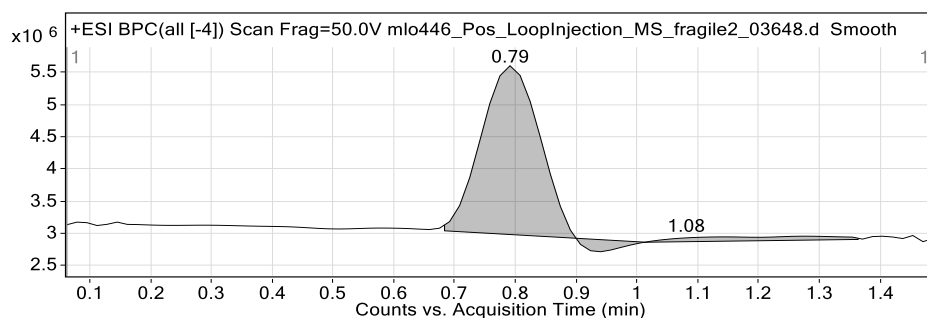


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.79	16741486	100.00	93.72	107.0402	0.130
1.08	1120920	6.70	6.28	64.0151	0.320

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: C26 H26 B Br N2 O3	0.80	507.1284	503.1259	503.1256	0.55	99.10

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

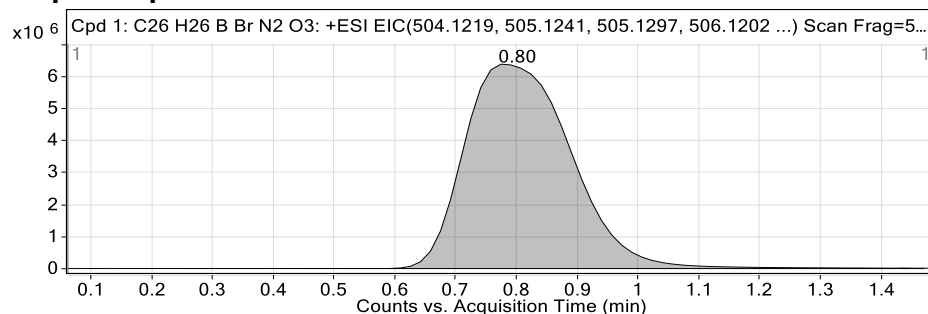


Figure: Extracted ion chromatogram (EIC) of compound.

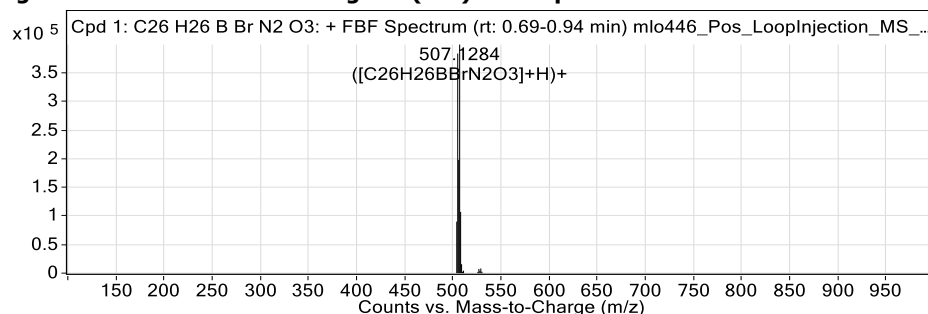


Figure: Full range view of Compound spectra and potential adducts.

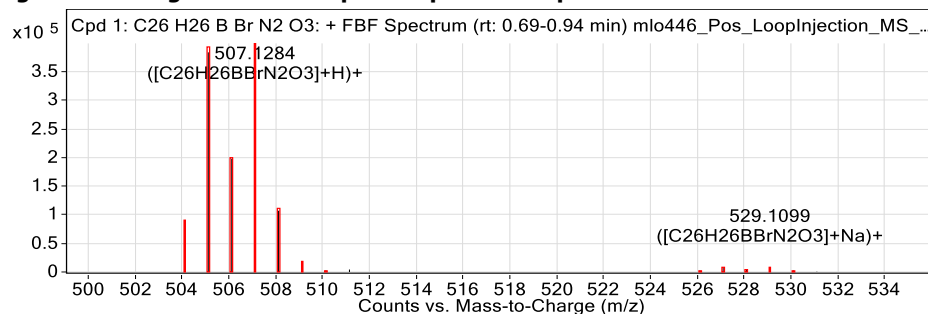


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
504.1326	1	89983.6	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
505.1300	1	383825.0	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
506.1319	1	197941.1	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
507.1284	1	399473.1	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
508.1309	1	107032.7	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
509.1354	1	15649.5	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
511.1585	1	4266.4	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+H)+
526.1148	1	2082.2	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+Na)+
527.1113	1	7279.1	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+Na)+
529.1099	1	8159.8	C ₂₆ H ₂₆ BrN ₂ O ₃	(M+Na)+

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