

Walkup MS Report



Data File	mlo424_Pos_LoopInjection_MS_02033.d	Sample Name	mlo424
Sample Type	Sample	Position	P1-A5
Instrument Name		User Name	Maria Odyniec
Acq Method	Pos_LoopInjection_MS.m	Acquired Time	2/4/2019 5:22:04 PM
IRM Calibration Status	Success	DA Method	Pos_LoopInjection_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Pos_LoopInjection_MS
Formula	C33H31O5P	Walkup Method Description	Positive mode ionization using loop injection
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

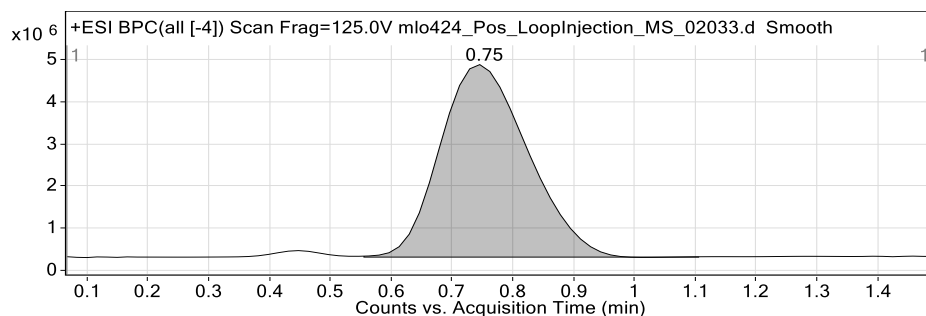


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	45731433	100.00	100.00	107.0415	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 (%)	Error flag
Cpd 1: C33 H31 O5 P	0.75	538.1856	538.1860	538.1909	-9.16	59.49	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

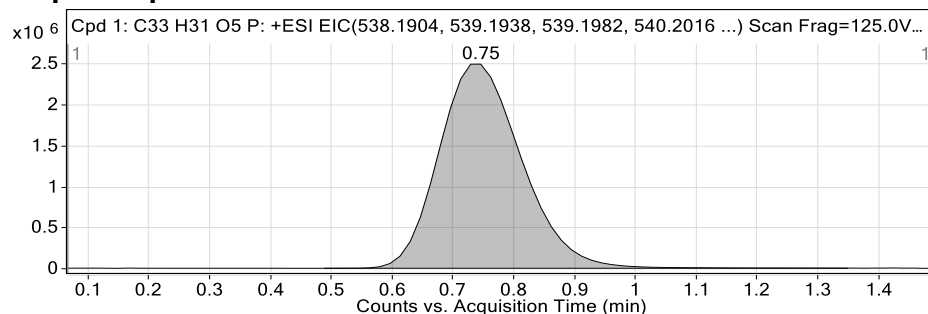


Figure: Extracted ion chromatogram (EIC) of compound.

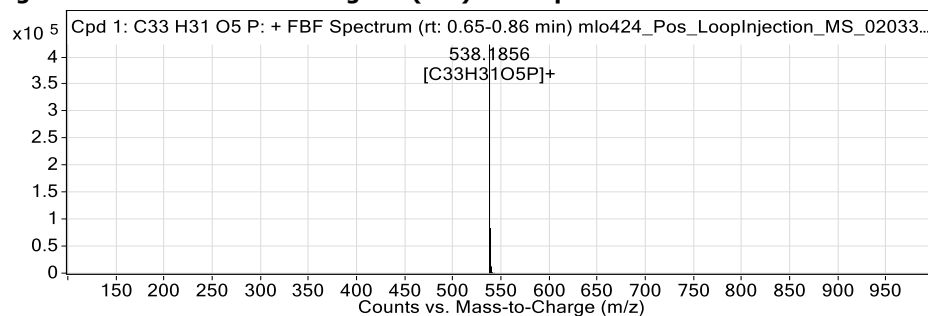


Figure: Full range view of Compound spectra and potential adducts.

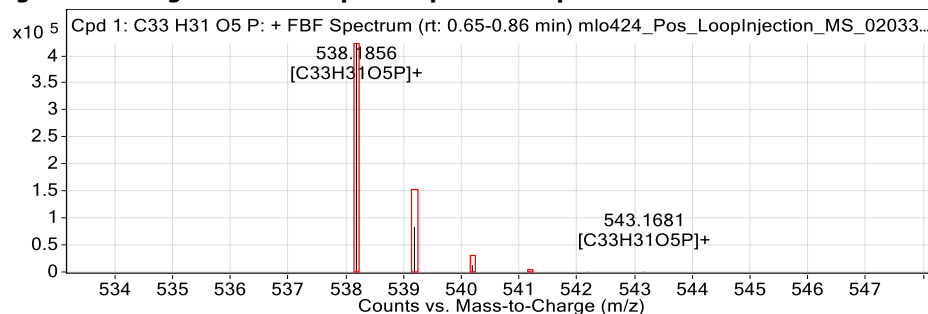


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
538.1856	1	422925.5	C33H31O5P	M+
539.1883	1	83508.2	C33H31O5P	M+
540.1911	1	12516.6	C33H31O5P	M+
541.1949	1	1625.1	C33H31O5P	M+
542.1968	1	342.2	C33H31O5P	M+
543.1681	1	605.4	C33H31O5P	M+

--- End Of Report ---