

Walkup MS Report



Data File	GZ01-reactionNOO-_Neg_5mins_MS_02824.d	Sample Name	GZ01-reactionNOO-
Sample Type	Sample	Position	P1-A5
Instrument Name	6545 QTof	User Name	Georgia Zacharia
Acq Method	Neg_5mins_MS.m	Acquired Time	3/6/2019 2:36:05 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description	fluorescence experiments Mitochondrialtargeting with peroxynitrite titration studies	Walkup Method	Neg_5Mins_C18
Formula	C10H8O4,C23H24O2P,C33H3 005P	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)

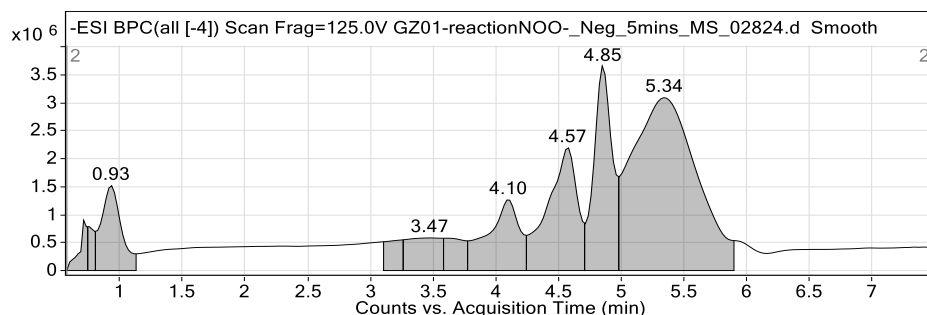


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.72	3838557	3.48	1.52	175.0397	0.070
0.75	2742827	2.48	1.09	175.0398	0.060
0.93	16959676	15.36	6.72	252.9497	0.160
3.19	5000578	4.53	1.98	181.0715	0.130
3.47	11089968	10.04	4.39	181.0714	0.290
3.61	6466811	5.86	2.56	181.0714	0.170
4.10	22402007	20.29	8.88	251.1281	0.230
4.57	36261316	32.84	14.37	420.2493	0.230
4.85	37231231	33.72	14.75	277.1805	0.150
5.34	110406639	100.00	43.74	132.9229	0.520

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: C10 H8 O4	0.95	191.0353	192.0435	192.0423	6.26	64.75	
Cpd 2: C23 H24O2 P				2727.7695			no EIC peaks
Cpd 3: C33 H30 O5 P	0.77	536.1707	537.1790	537.1831	-7.52	46.75	low score

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

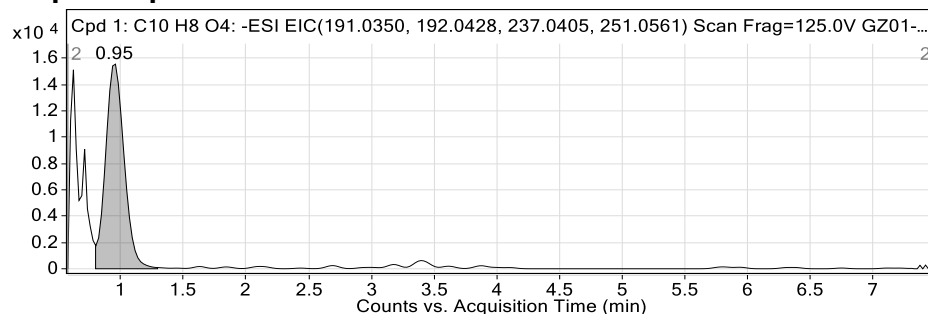


Figure: Extracted ion chromatogram (EIC) of compound.

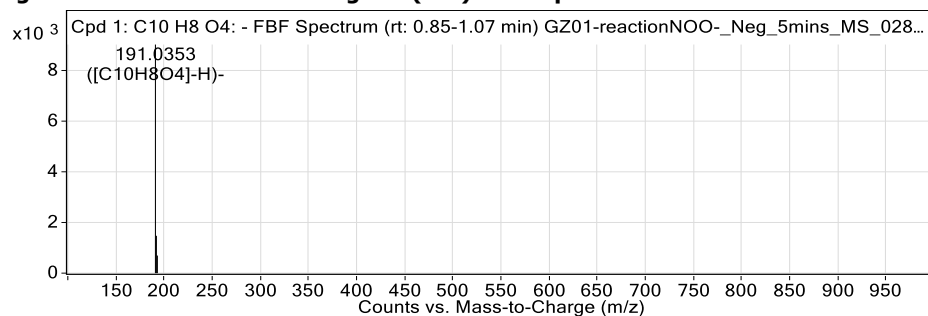


Figure: Full range view of Compound spectra and potential adducts.

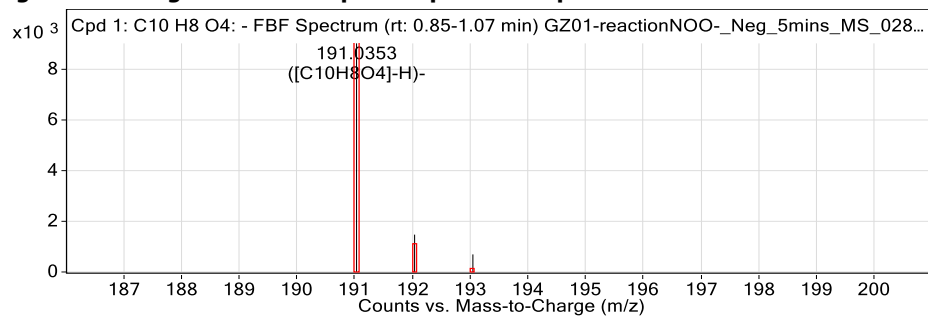


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
191.0353	1	9038.0	C10H8O4	(M-H)-
192.0407	1	1476.3	C10H8O4	(M-H)-
193.0500	1	695.0	C10H8O4	(M-H)-

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Compound specific information

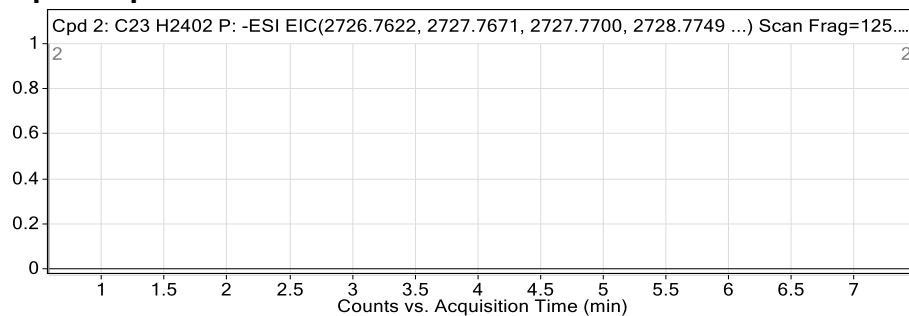


Figure: Extracted ion chromatogram (EIC) of compound.

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

Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

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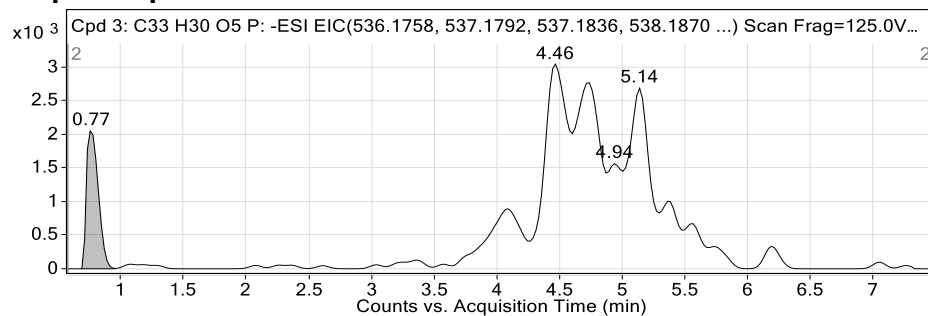


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Figure: Full range view of Compound spectra and potential adducts.

Figure: Zoomed Compound spectra view

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