

# Walkup MS Report



<b>Data File</b>	GZ03ONOO-reacted_Neg_5mins_MS_03011.d	<b>Sample Name</b>	GZ03ONOO-reacted
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A9
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Georgia Zacharia
<b>Acq Method</b>	Neg_5mins_MS.m	<b>Acquired Time</b>	3/12/2019 2:14:05 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Neg_5mins_MS.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Walkup Sample Description</b>		<b>Walkup Method</b>	Neg_5Mins_C18
<b>Formula</b>	C10H8O4,C7H13NO3,C17H19NO6	<b>Walkup Method Description</b>	Negative mode ionization using C18 column chromatography
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

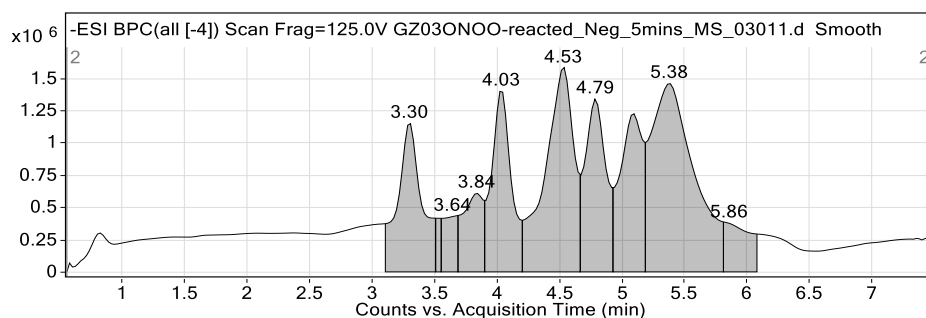


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
3.30	15363053	43.69	11.07	191.0343	0.180
3.51	1114033	3.17	0.80	181.0714	0.040
3.64	3412221	9.70	2.46	181.0714	0.130
3.84	6787102	19.30	4.89	175.0398	0.160
4.03	15312925	43.54	11.03	254.9479	0.150
4.53	25400941	72.23	18.30	420.2495	0.220
4.79	15490036	44.05	11.16	277.1803	0.170
5.09	15316313	43.55	11.04	265.1473	0.180
5.38	35165965	100.00	25.34	311.1681	0.330
5.86	5412278	15.39	3.90	181.0715	0.200

## 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	3.30	191.0349	192.0422	192.0423	-0.47	99.68	
Cpd 2: C7 H13 N O3				159.0895			no EIC peaks
Cpd 3: C17 H19 N O6	3.17	332.1133	333.1207	333.1212	-1.74	94.76	

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

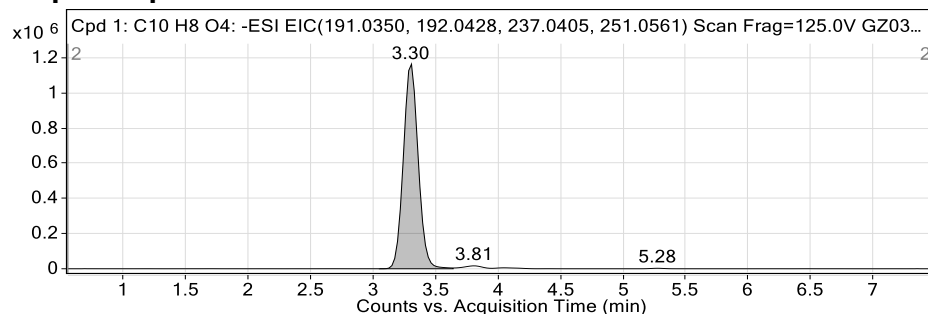


Figure: Extracted ion chromatogram (EIC) of compound.

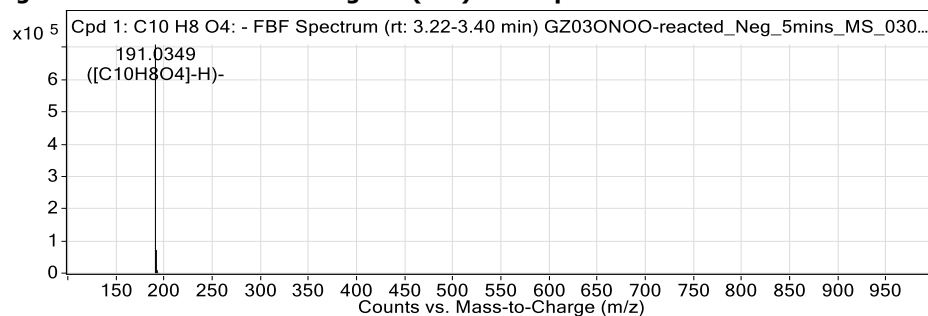


Figure: Full range view of Compound spectra and potential adducts.

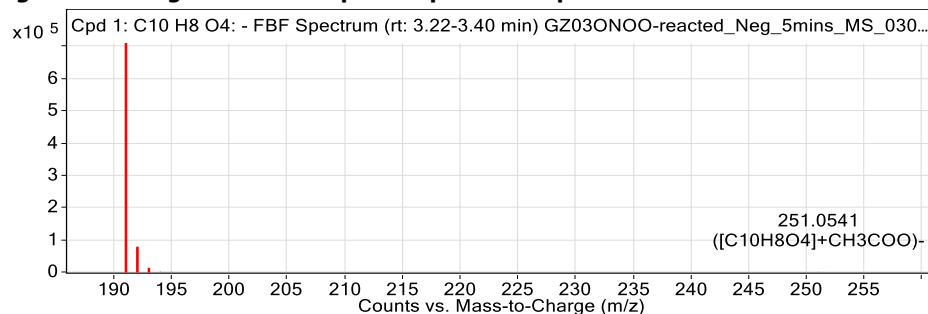


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

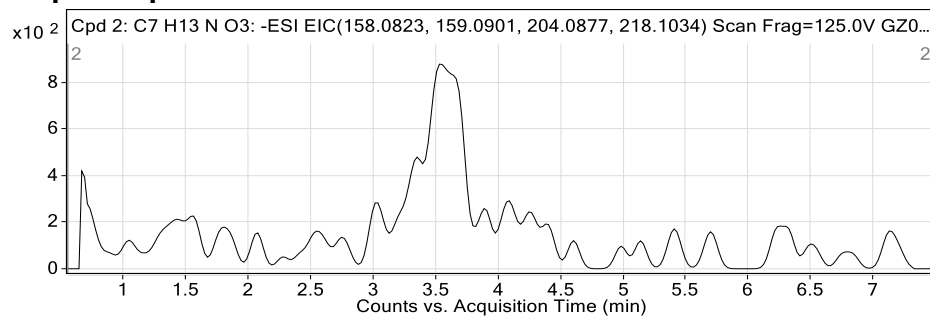
## Compound isotope peak List

m/z	z	Abund	Formula	Ion
191.0349	1	709069.1	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
192.0383	1	71925.7	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
193.0406	1	9100.2	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
194.0439	1	782.0	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
195.0296	1	659.4	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
251.0541	1	313.7	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M+CH <sub>3</sub> COO)-
252.0303	1	67.5	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M+CH <sub>3</sub> COO)-

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## Compound specific information



**Figure: Extracted ion chromatogram (EIC) of compound.**

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## Compound specific information

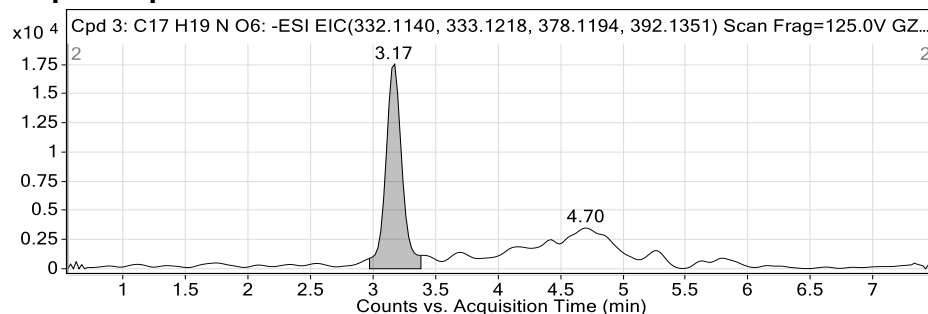


Figure: Extracted ion chromatogram (EIC) of compound.

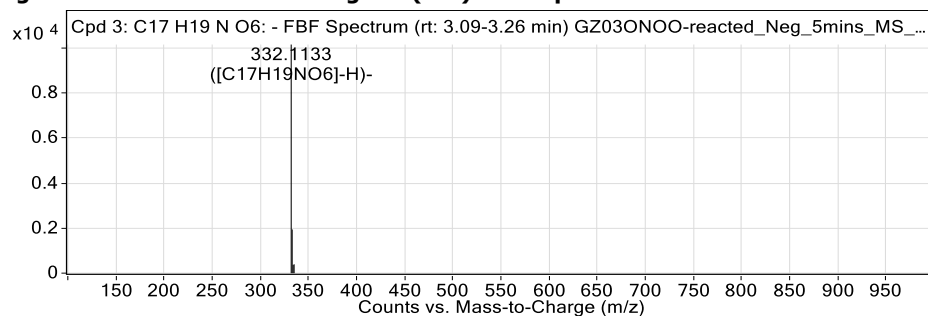


Figure: Full range view of Compound spectra and potential adducts.

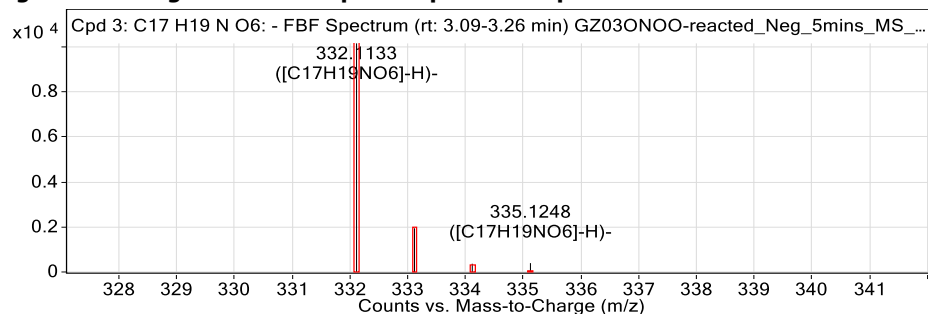


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

## Compound isotope peak List

m/z	z	Abund	Formula	Ion
332.1133	1	10151.8	C <sub>17</sub> H <sub>19</sub> NO <sub>6</sub>	(M-H) <sup>-</sup>
333.1169	1	1940.9	C <sub>17</sub> H <sub>19</sub> NO <sub>6</sub>	(M-H) <sup>-</sup>
334.1175	1	366.5	C <sub>17</sub> H <sub>19</sub> NO <sub>6</sub>	(M-H) <sup>-</sup>
335.1248	1	393.1	C <sub>17</sub> H <sub>19</sub> NO <sub>6</sub>	(M-H) <sup>-</sup>

--- End Of Report ---