

Walkup MS Report



Data File	GZ02ONOO-reacted_Neg_5mins_MS_03007.d	Sample Name	GZ02ONOO-reacted
Sample Type	Sample	Position	P1-A8
Instrument Name	6545 QTof	User Name	Georgia Zacharia
Acq Method	Neg_5mins_MS.m	Acquired Time	3/12/2019 2:05:38 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C10H8O4,C10H16N2O3S,C20H22N2O6S	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)

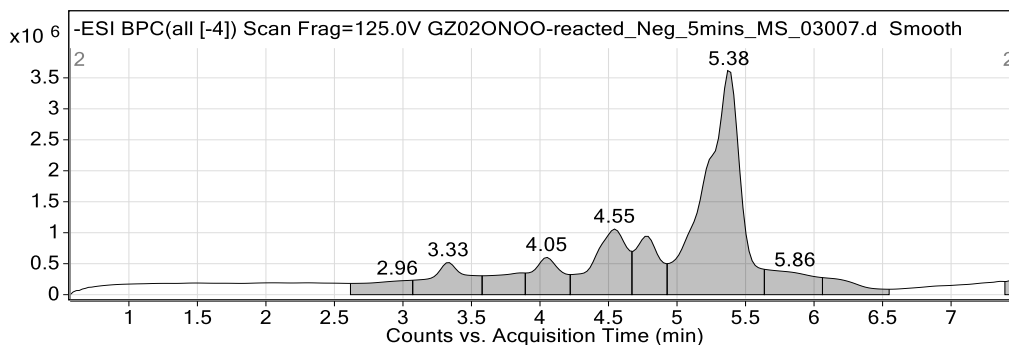


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
2.96	5557695	8.36	3.92	181.0684	0.350
3.33	10282466	15.46	7.25	191.0322	0.260
3.86	6157812	9.26	4.34	175.0379	0.230
4.05	8749881	13.16	6.17	252.9477	0.200
4.55	18266188	27.46	12.89	420.2473	0.230
4.78	11548031	17.36	8.15	266.1015	0.180
5.38	66509119	100.00	46.92	311.1674	0.250
5.86	8897405	13.38	6.28	181.0711	0.350
6.20	5125542	7.71	3.62	181.0712	0.310
7.43	668718	1.01	0.47	181.0711	0.050

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: C10 H8 O4	3.33	191.0349	192.0421	192.0423	-0.60	99.69
Cpd 2: C10 H16 N2 O3 S	3.76	303.1055	244.0898	244.0882	6.86	52.95
Cpd 3: C20 H22 N2 O6 S	4.12	417.1131	418.1200	418.1199	0.39	99.06

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

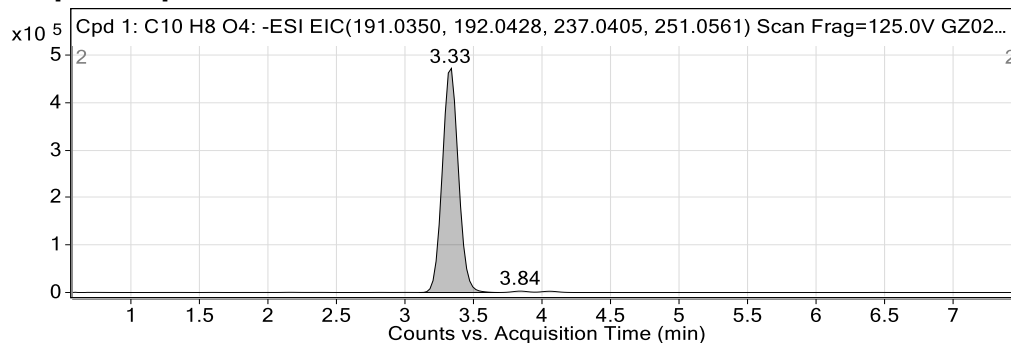


Figure: Extracted ion chromatogram (EIC) of compound.

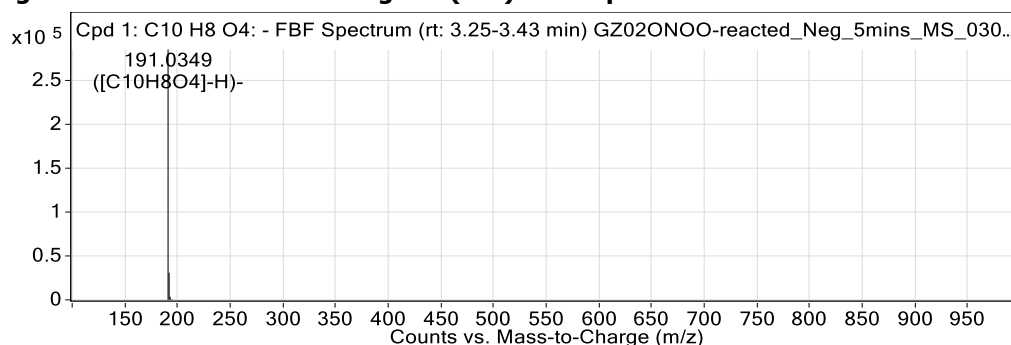


Figure: Full range view of Compound spectra and potential adducts.

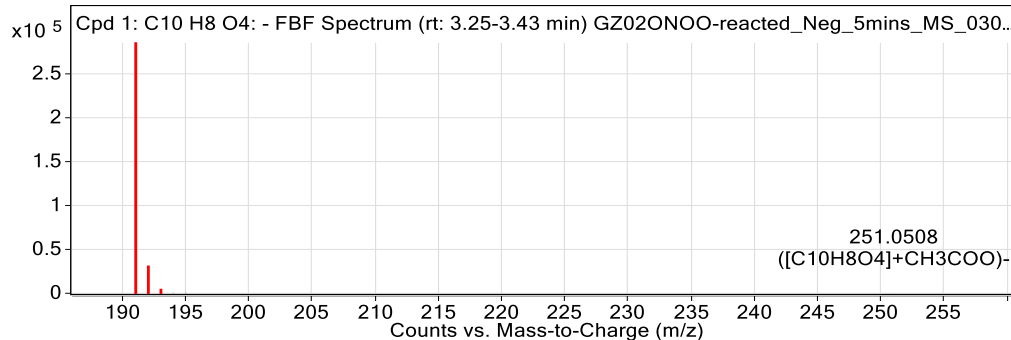


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
191.0349	1	285913.5	C ₁₀ H ₈ O ₄	(M-H)-
192.0380	1	30991.7	C ₁₀ H ₈ O ₄	(M-H)-
193.0398	1	3518.9	C ₁₀ H ₈ O ₄	(M-H)-
194.0441	1	361.9	C ₁₀ H ₈ O ₄	(M-H)-
195.0288	1	422.0	C ₁₀ H ₈ O ₄	(M-H)-
251.0508	1	91.9	C ₁₀ H ₈ O ₄	(M+CH ₃ COO)-

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Compound specific information

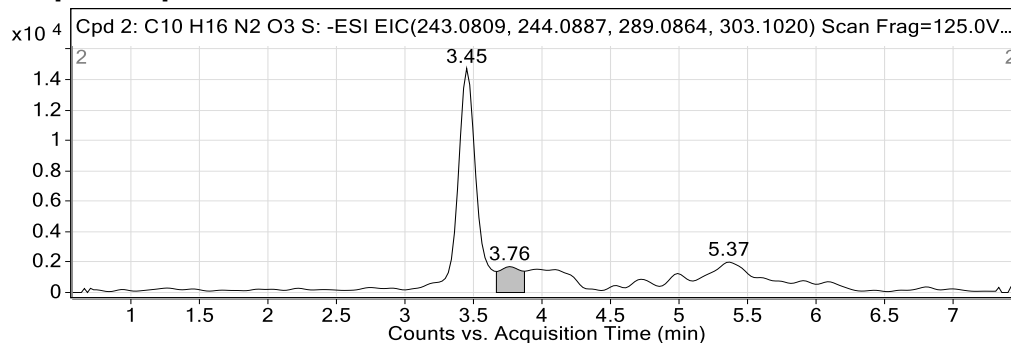


Figure: Extracted ion chromatogram (EIC) of compound.

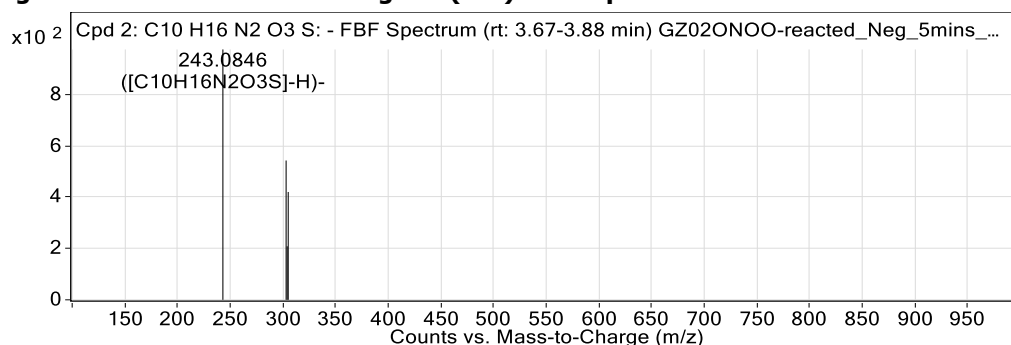


Figure: Full range view of Compound spectra and potential adducts.

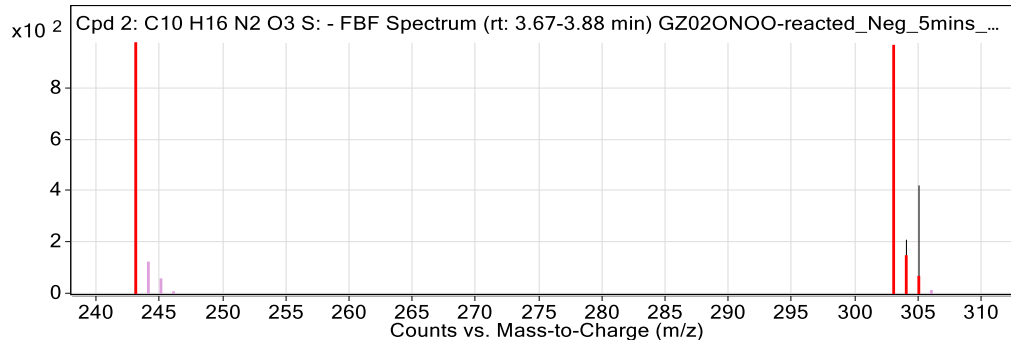


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
243.0846	1	974.4	C ₁₀ H ₁₆ N ₂ O ₃ S	(M-H)-
303.1055	1	542.3	C ₁₀ H ₁₆ N ₂ O ₃ S	(M+CH ₃ COO)-
304.1036	1	208.4	C ₁₀ H ₁₆ N ₂ O ₃ S	(M+CH ₃ COO)-
305.0968	1	419.7	C ₁₀ H ₁₆ N ₂ O ₃ S	(M+CH ₃ COO)-

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Compound specific information

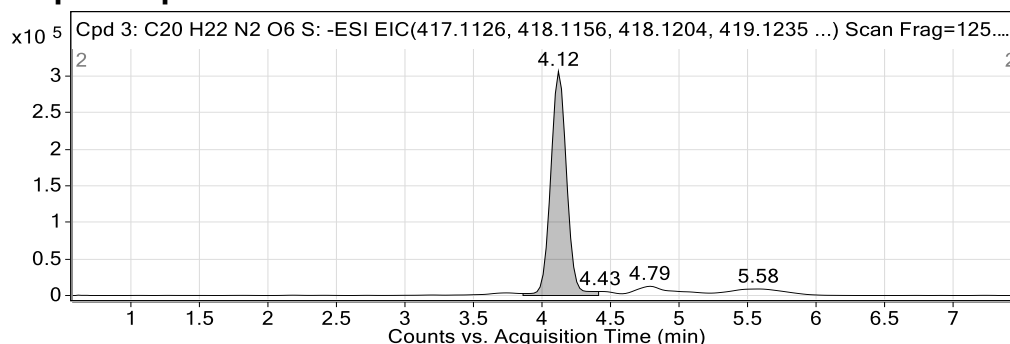


Figure: Extracted ion chromatogram (EIC) of compound.

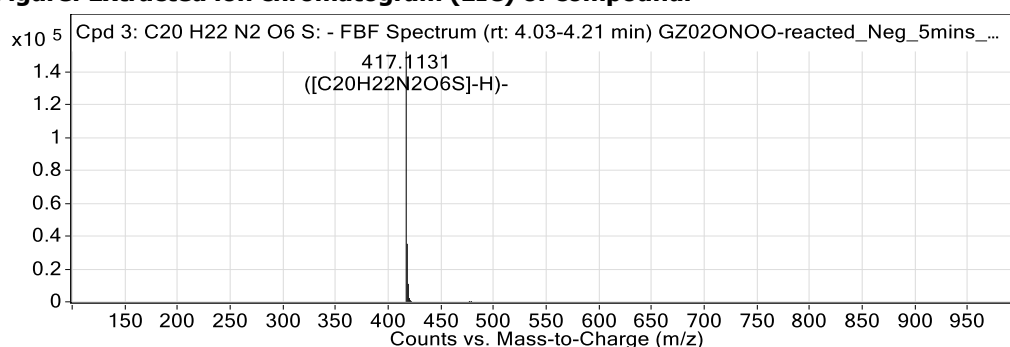


Figure: Full range view of Compound spectra and potential adducts.

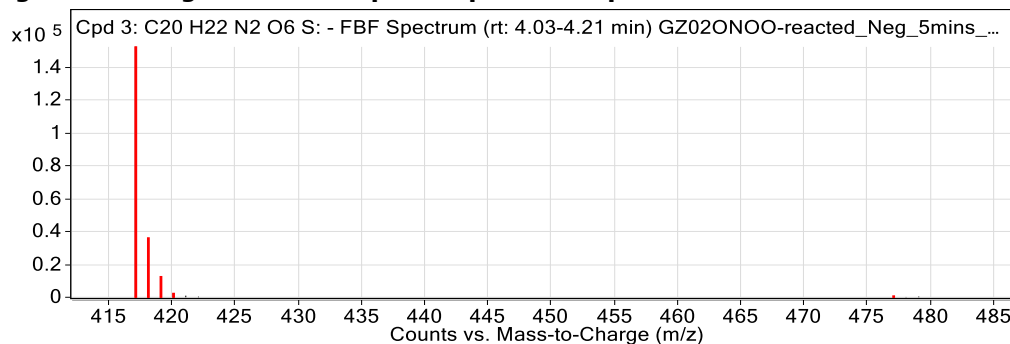


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
417.1131	1	152182.8	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
418.1158	1	35268.0	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
419.1130	1	10903.9	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
420.1136	1	2300.0	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
421.1023	1	987.2	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
422.1055	1	374.0	C ₂₀ H ₂₂ N ₂ O ₆ S	(M-H)-
477.1229	1	495.6	C ₂₀ H ₂₂ N ₂ O ₆ S	(M+CH ₃ COO)-
478.0900	1	192.9	C ₂₀ H ₂₂ N ₂ O ₆ S	(M+CH ₃ COO)-
479.0960	1	451.2	C ₂₀ H ₂₂ N ₂ O ₆ S	(M+CH ₃ COO)-

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