

# Walkup MS Report



<b>Data File</b>	Cou-TPP_Neg_5mins_MS_06340.d	<b>Sample Name</b>	Cou-TPP
<b>Sample Type</b>	Sample	<b>Position</b>	P1-C3
<b>Instrument Name</b>	6545 QTof	<b>User Name</b>	Maria Odyniec
<b>Acq Method</b>	Neg_5mins_MS.m	<b>Acquired Time</b>	7/16/2019 4:59:21 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, C22H22O2P, C32H28O5P	<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)

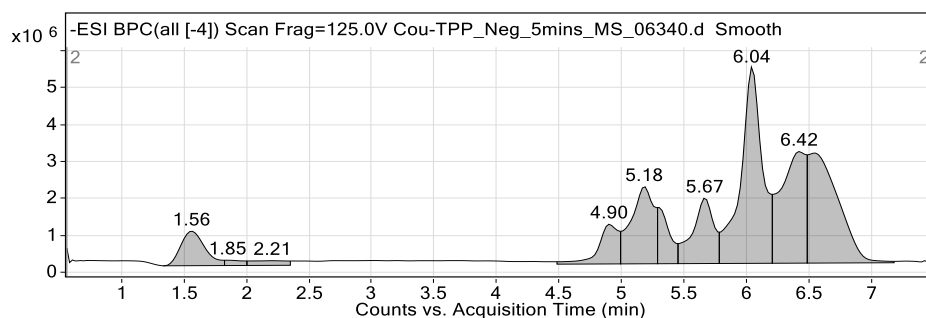


Figure 1: Base peak chromatogram

## User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
1.56	12666591	19.68	5.22	1033.9885	0.210
1.85	1432165	2.23	0.59	112.9860	0.140
2.21	2536726	3.94	1.05	1033.9885	0.270
4.90	12007368	18.66	4.95	191.0354	0.160
5.18	26645586	41.40	10.99	612.0225	0.180
5.29	9876903	15.35	4.07	138.0202	0.110
5.67	21051980	32.71	8.68	221.1554	0.170
6.04	64359154	100.00	26.55	389.1807	0.170
6.42	41880505	65.07	17.28	277.1834	0.200
6.54	49975750	77.65	20.61	132.9242	0.270

## 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	4.88	191.0350	192.0422	192.0423	-0.13	99.83	
Cpd 2: C22 H22 O2 P	5.29	350.1331	349.1339	349.1357	-5.18	55.68	
Cpd 3: C32 H28 O5 P	5.18	582.1741	523.1583	523.1674	-17.50	46.53	m/z tolerance

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

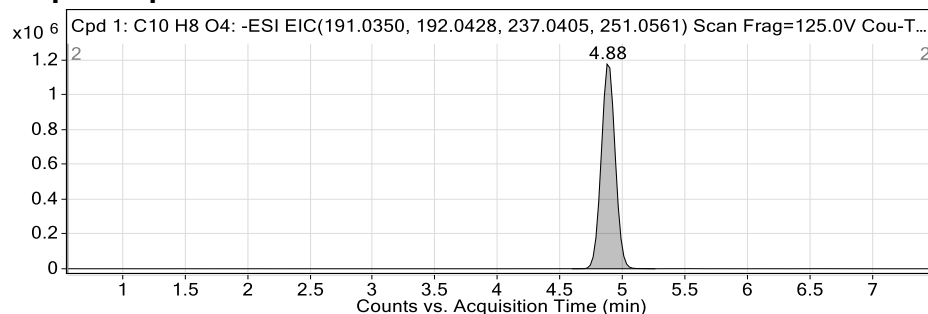


Figure: Extracted ion chromatogram (EIC) of compound.

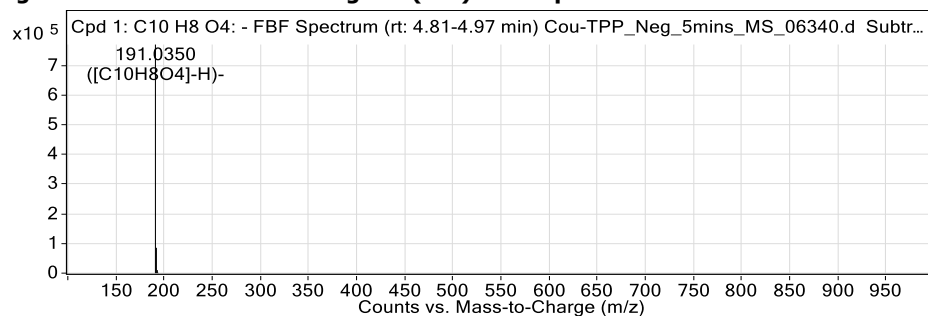


Figure: Full range view of Compound spectra and potential adducts.

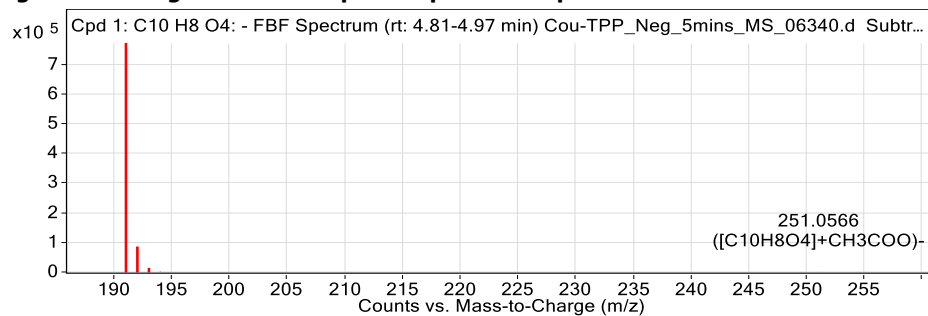


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

### Compound isotope peak List

m/z	z	Abund	Formula	Ion
191.0350	1	769481.1	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
192.0381	1	85273.9	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
193.0402	1	10040.2	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
194.0441	1	938.6	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	(M-H)-
251.0566	1	129.6	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

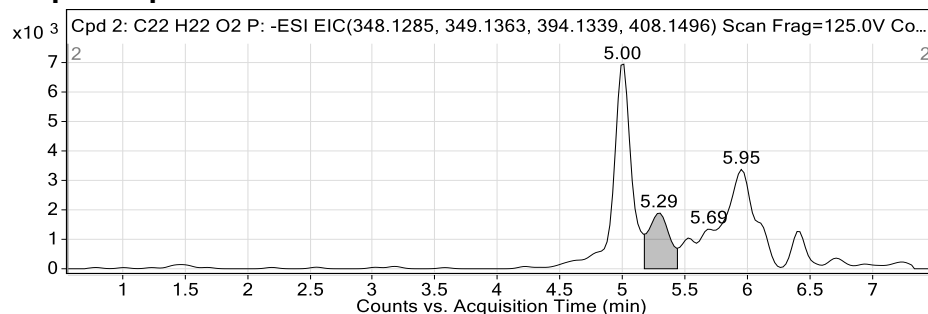


Figure: Extracted ion chromatogram (EIC) of compound.

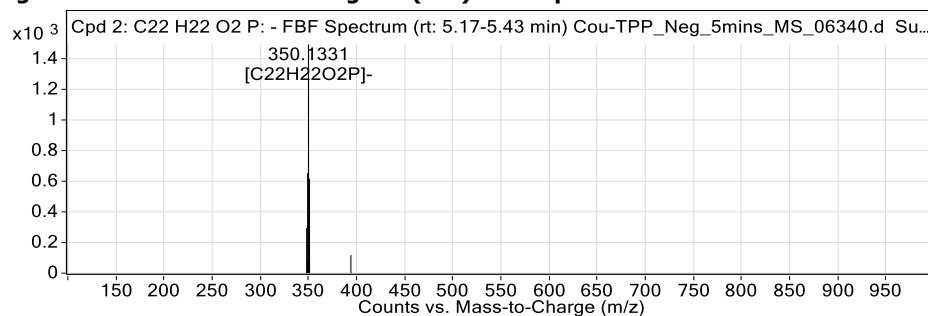


Figure: Full range view of Compound spectra and potential adducts.

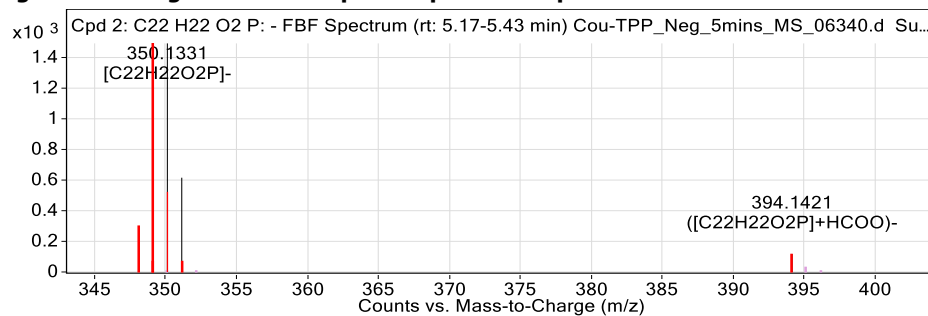


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

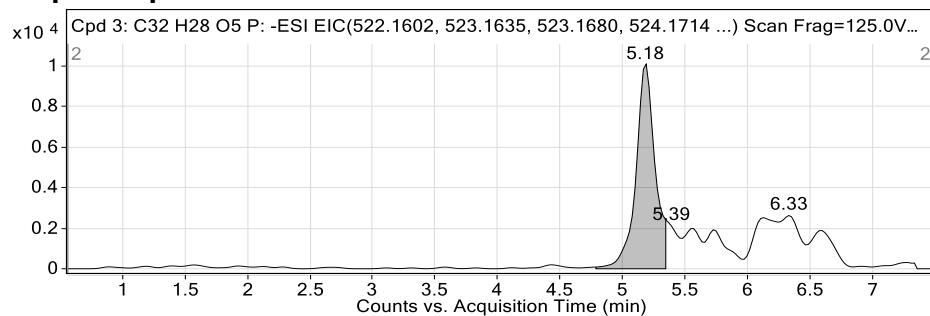
## Compound isotope peak List

m/z	z	Abund	Formula	Ion
348.1201	1	294.7	C22H22O2P	(M-H)-
349.1238	1	76.9	C22H22O2P	(M-H)-
349.1417	1	653.5	C22H22O2P	M-
350.1331	1	1494.3	C22H22O2P	M-
351.1468	1	616.3	C22H22O2P	M-
394.1421	1	117.7	C22H22O2P	(M+HCOO)-

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## Compound specific information



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

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