

## Identification of metabolites

### General notes:

- Chromatograms and spectra are from representative study samples and pure chemical standards when available. All chemical standards were from IROA Technologies' Mass Spectrometry Metabolite Library (MSMLS)
- Chromatograms and isotope patterns: Find Compounds by Formula searches in Agilent MassHunter Qualitative Analysis B.06.00 SP1
- Isotope patterns: Red rectangles represent an isotope pattern calculated from the elemental composition (shown in the title of each spectra) , bars inside the rectangles show the observed isotope peaks
- MS/MS spectra: Precursor is indicated with a blue dot above the ion. Collision energy is on top of the spectra, e.g. CID@20.0.

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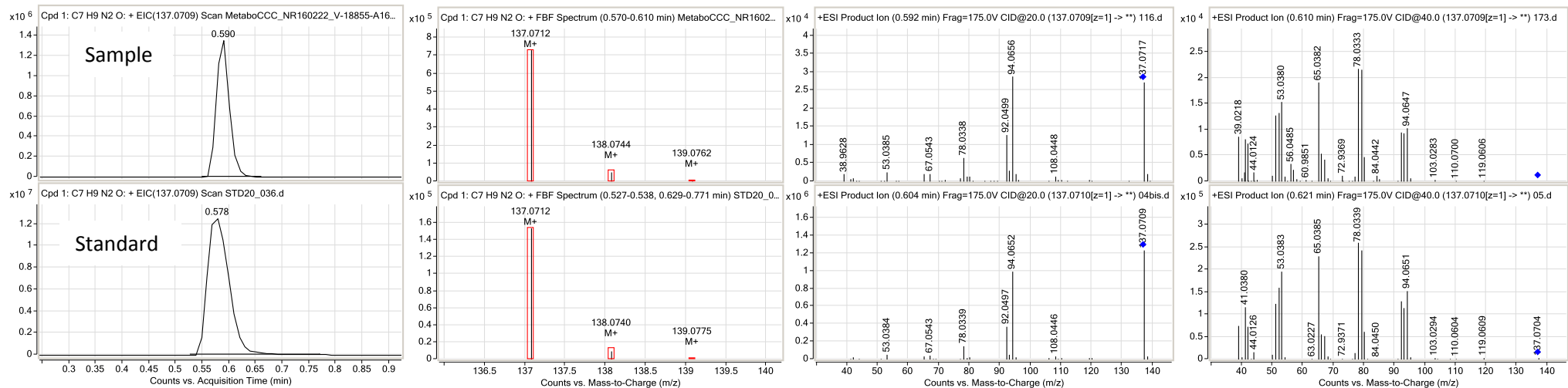
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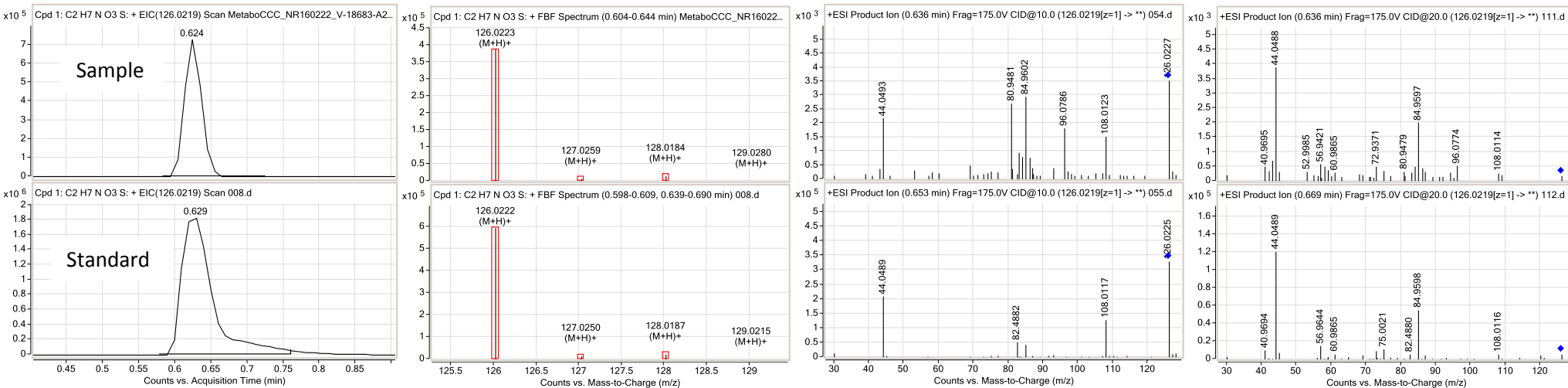
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# 1-Methylnicotinamide

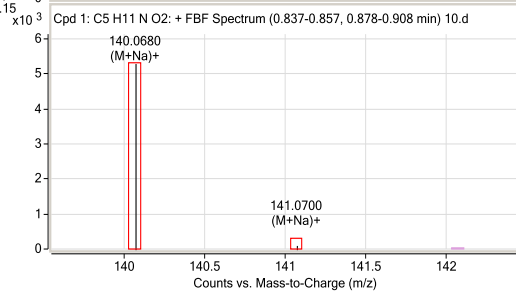
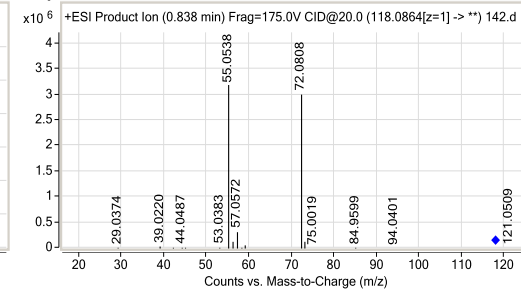
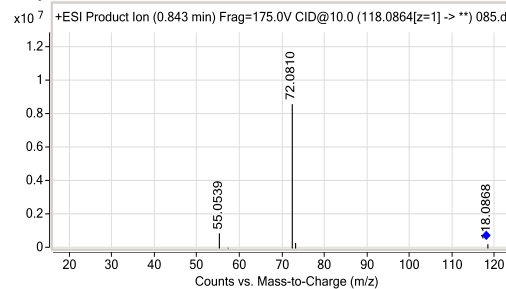
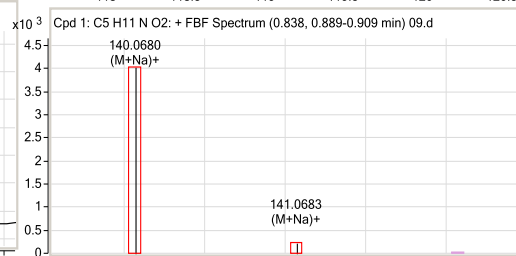
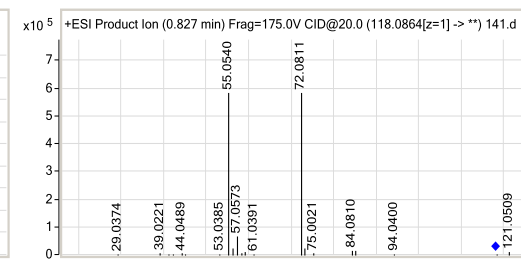
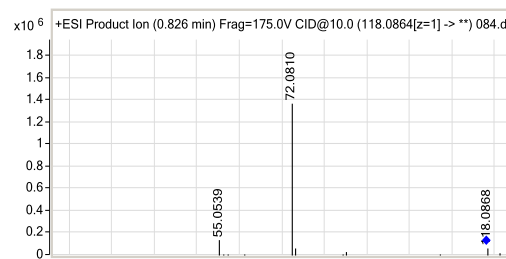
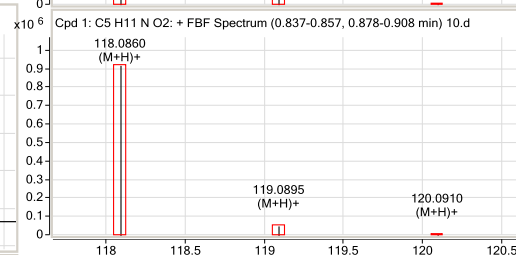
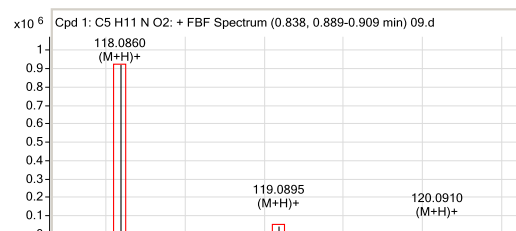


# Taurine

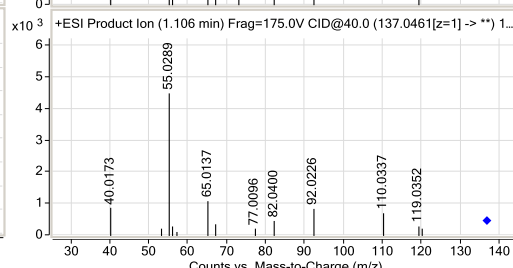
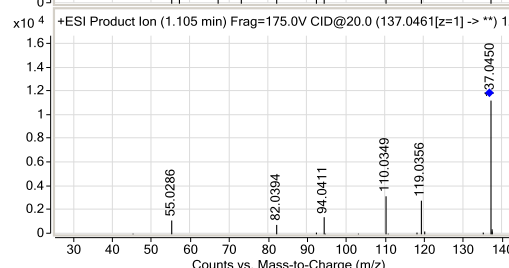
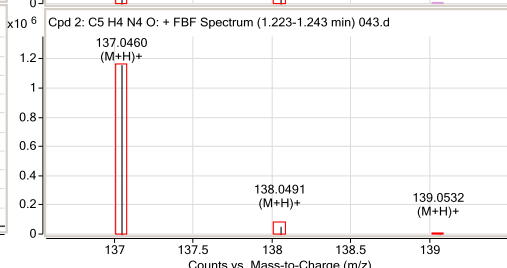
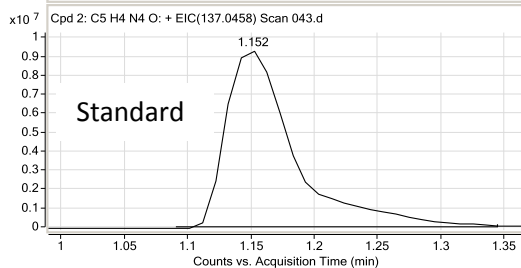
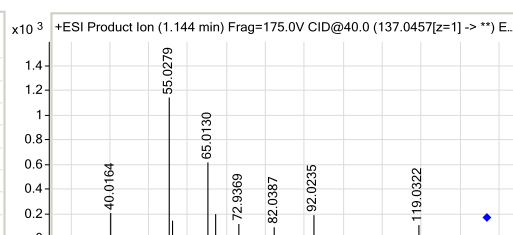
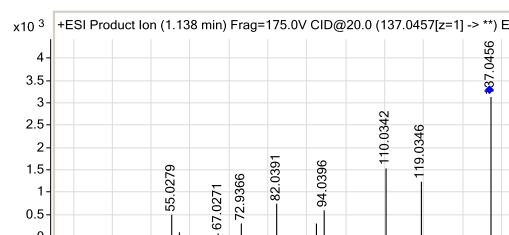
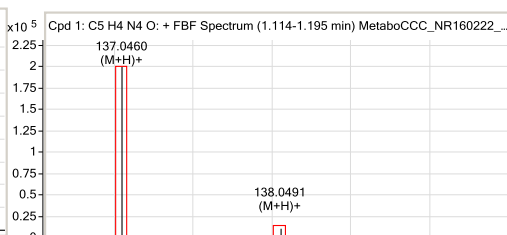
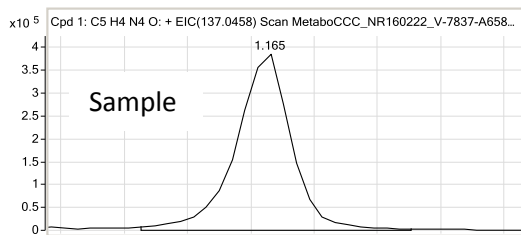


# Valine

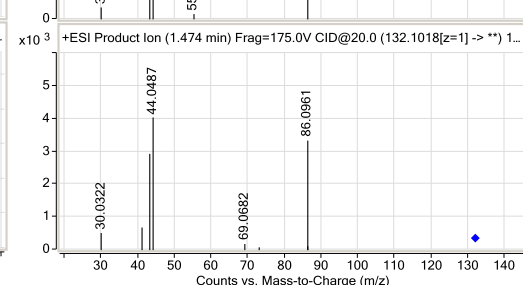
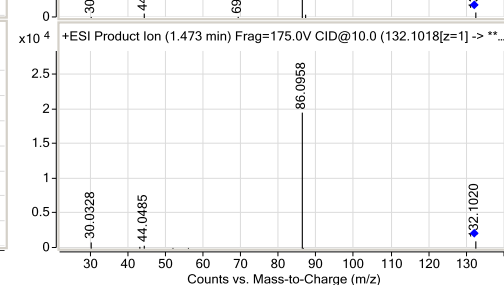
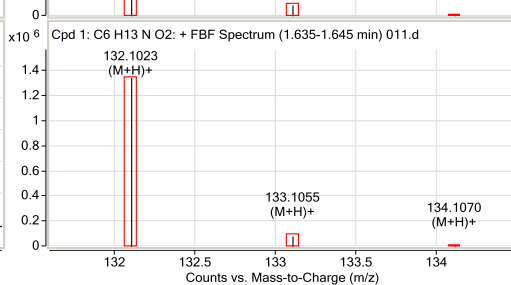
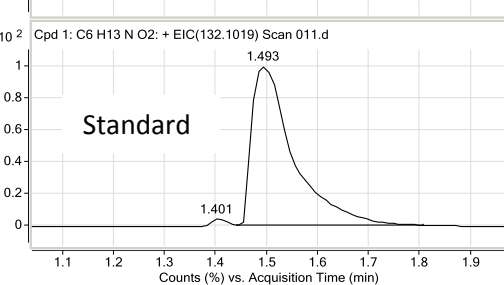
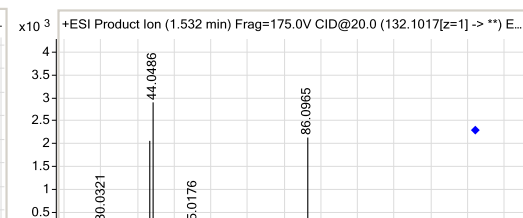
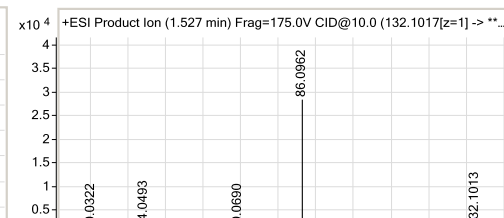
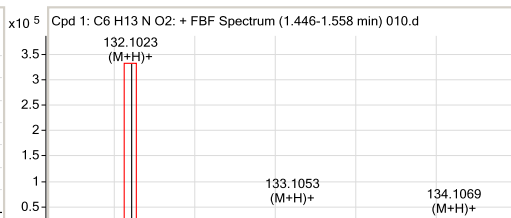
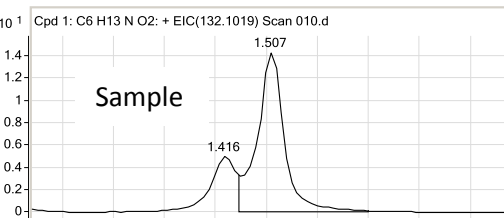
Valine was found as  $[M+Na]^+$  due to saturation of the principal ion  $[M+H]^+$ . MS/MS spectra acquired from  $[M+H]^+$



## Hypoxanthine

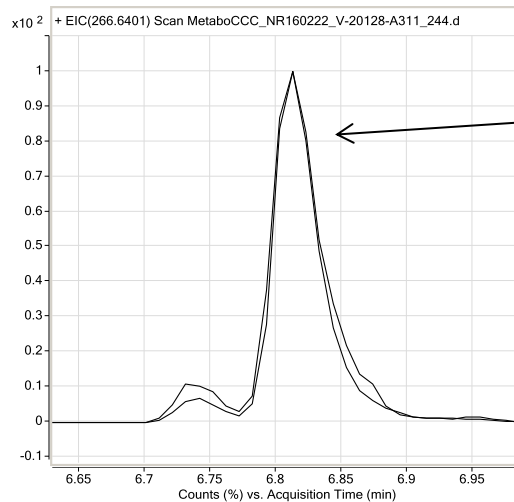
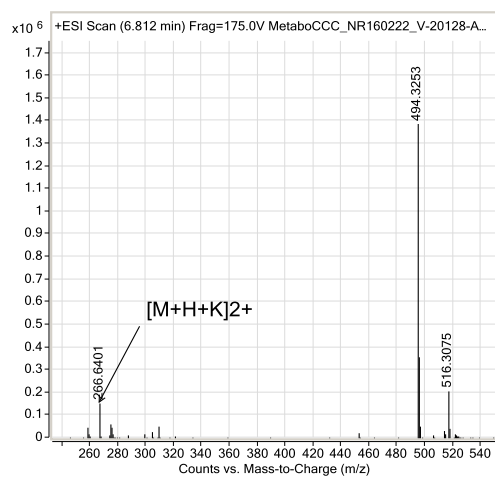


## Leucine

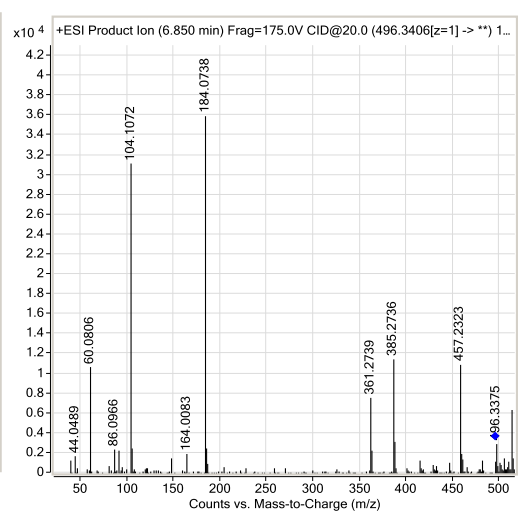
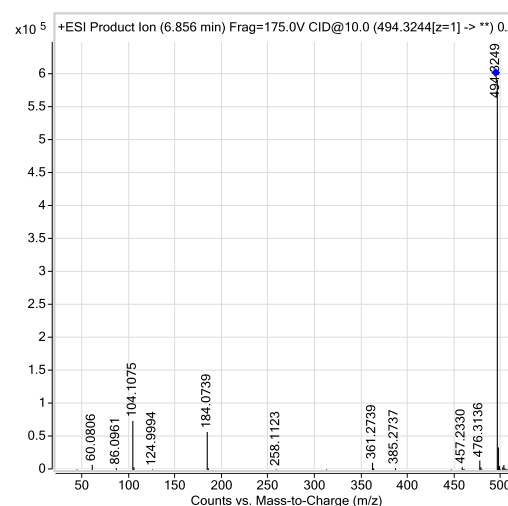
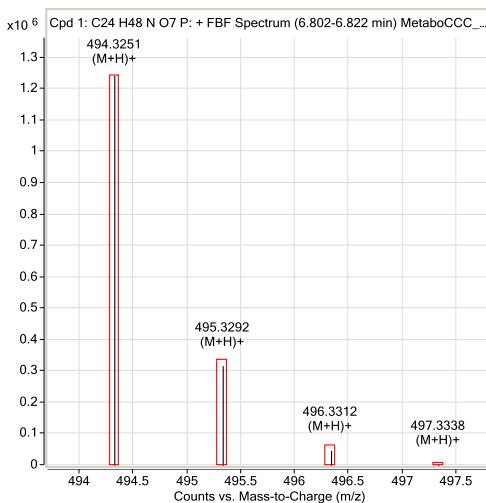
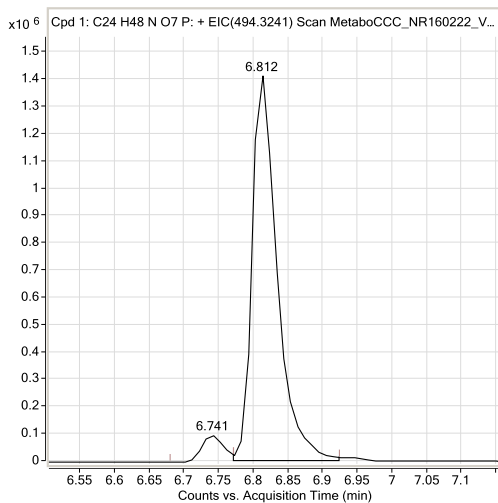


# LysoPC(16:1)

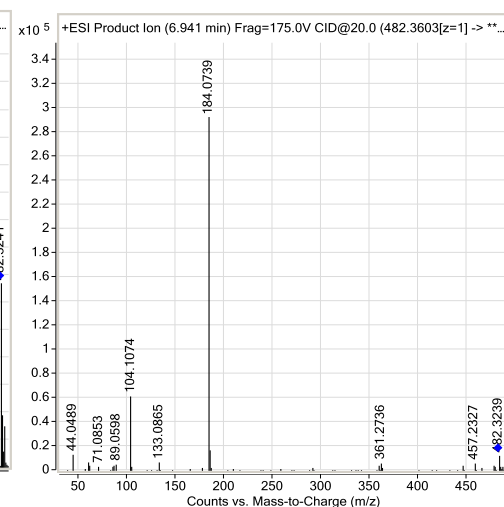
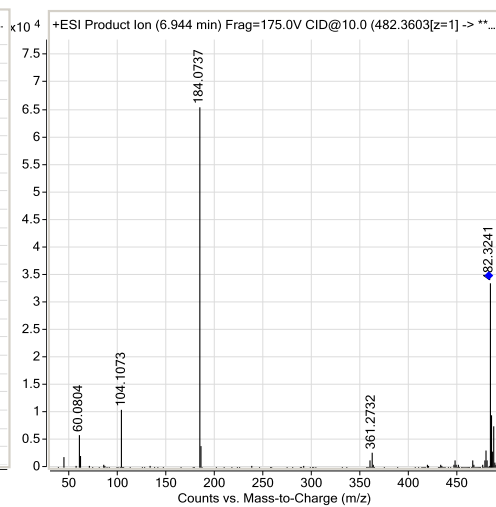
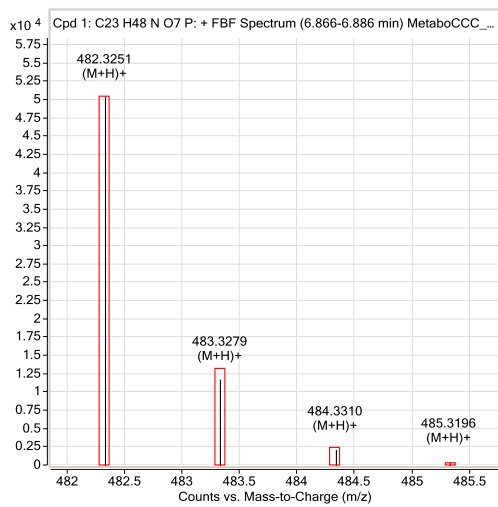
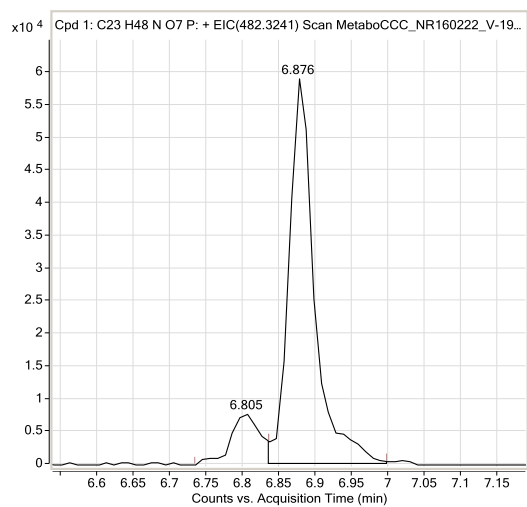
LysoPC(16:1) found as  $[M+H+K]^{2+}$ . MS/MS was acquired from  $[M+H]^+$



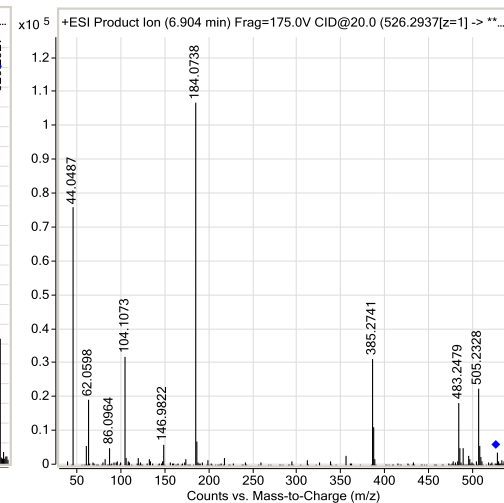
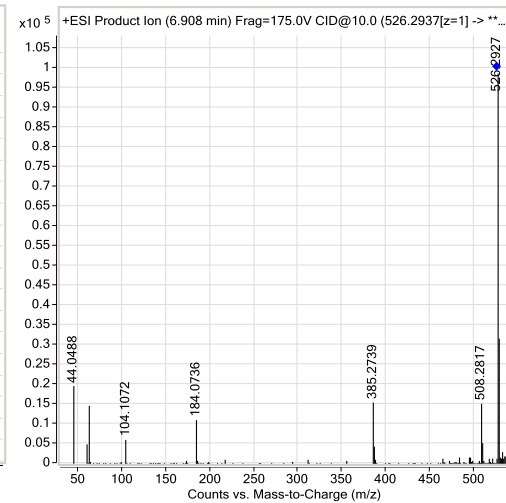
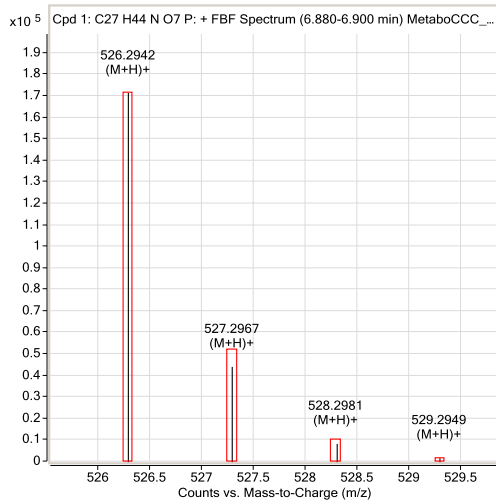
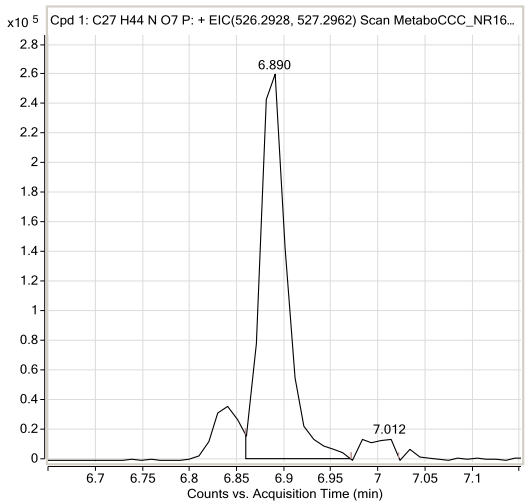
Overlaid chromatograms of  $[M+H+K]^{2+}$  and  $[M+H]^+$



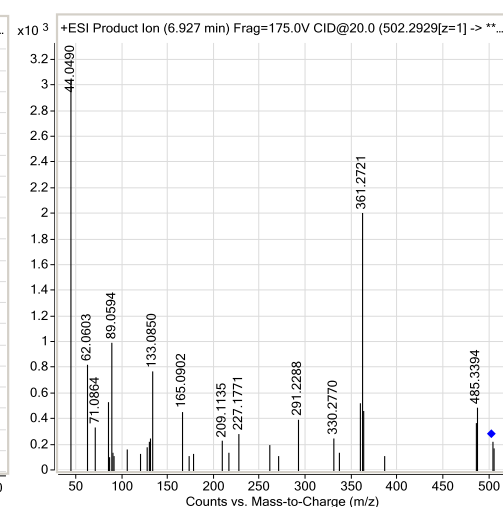
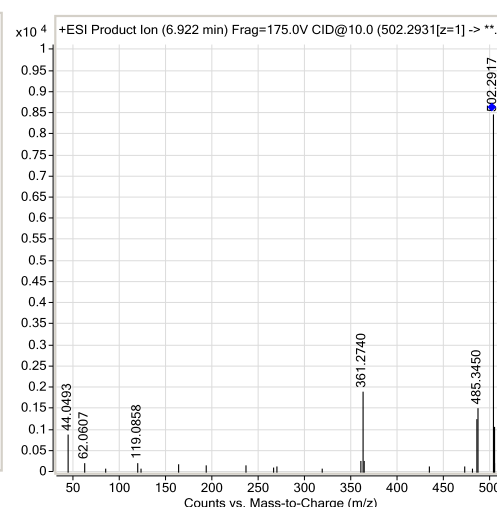
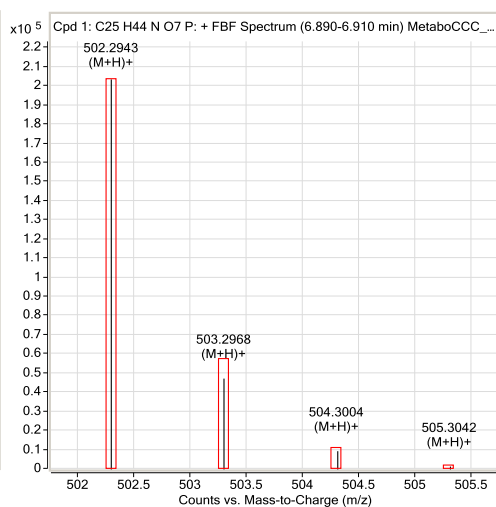
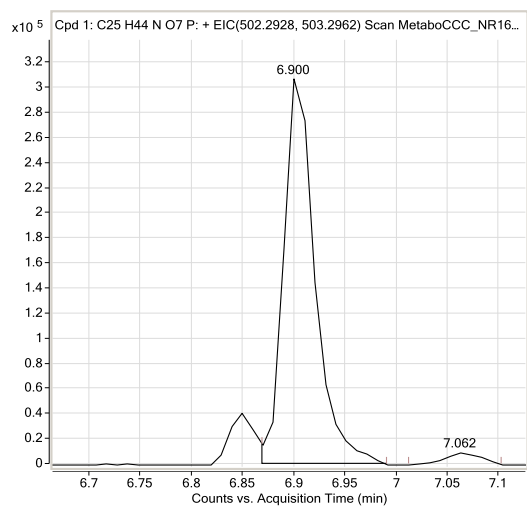
## LysoPC(15:0)



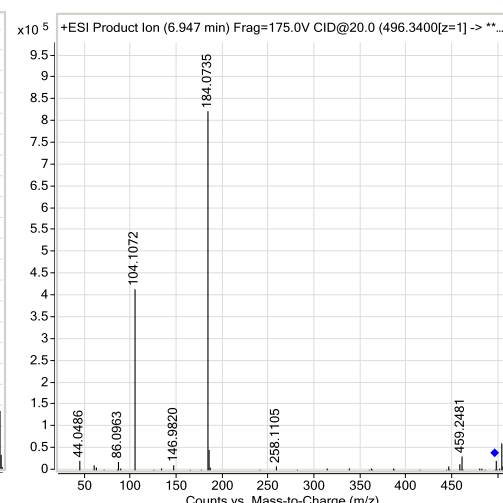
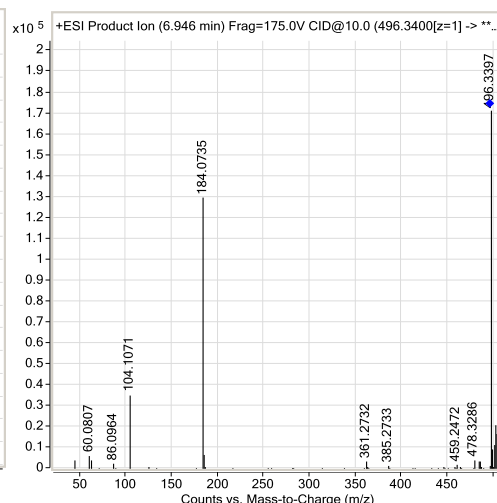
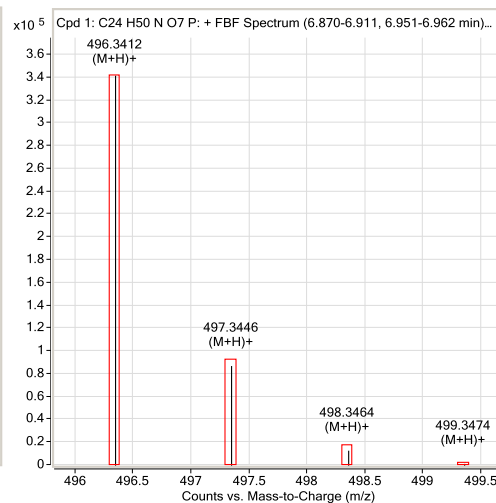
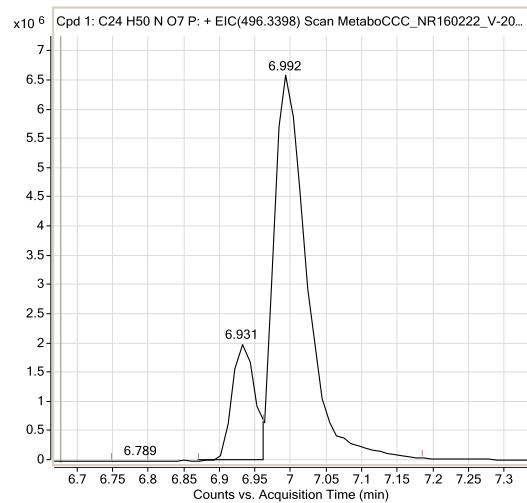
## LysoPE(22:6)



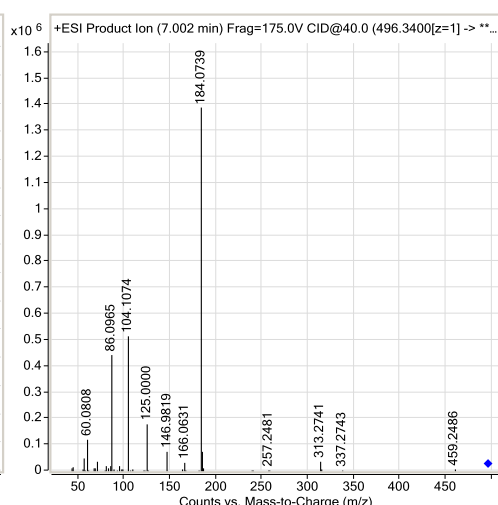
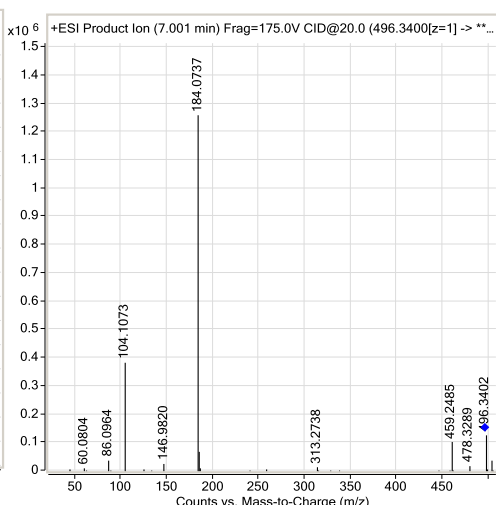
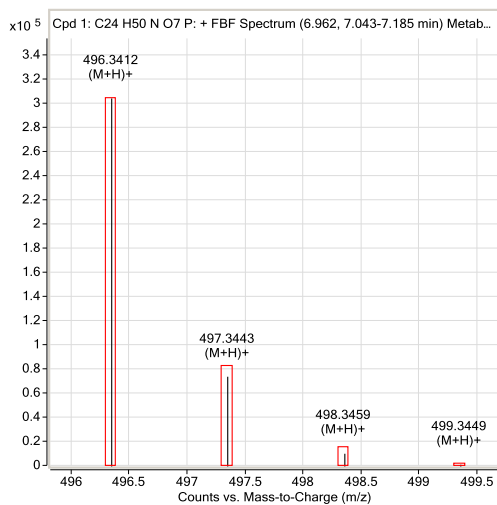
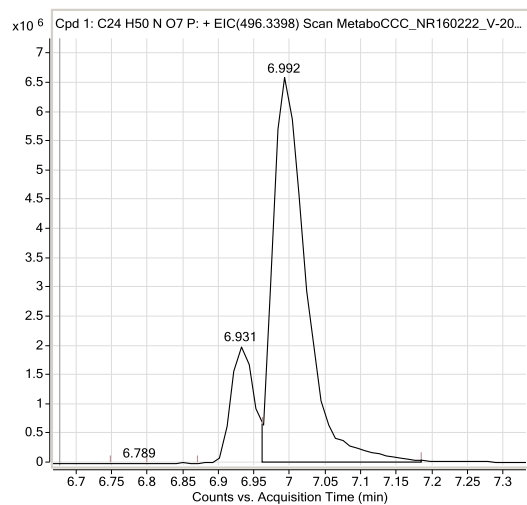
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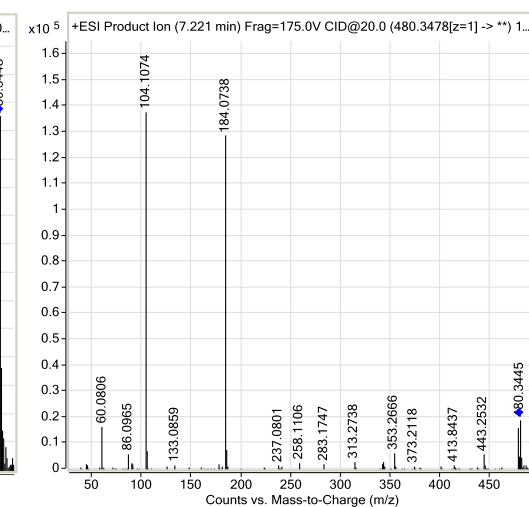
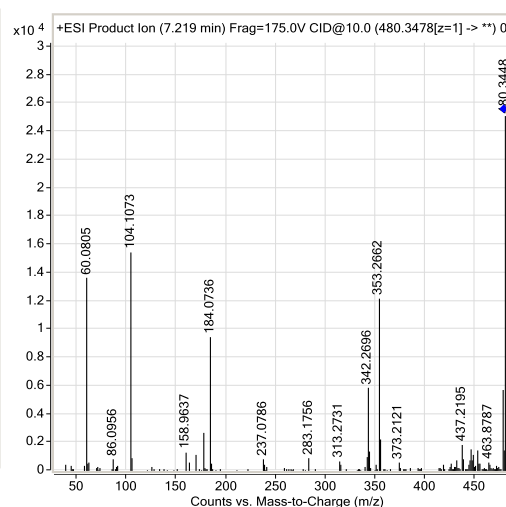
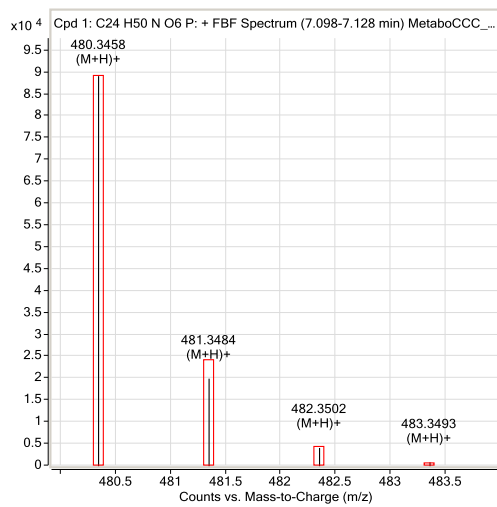
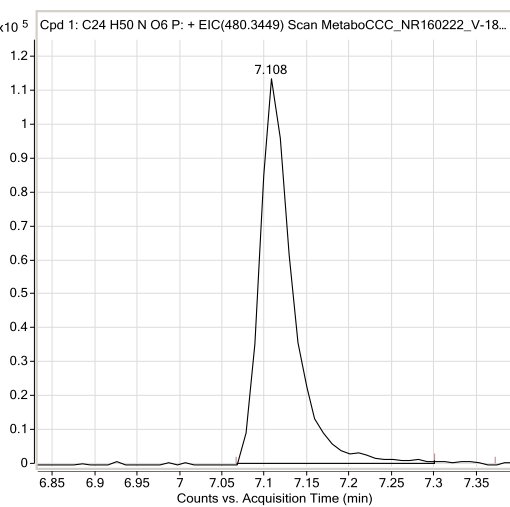
## LysoPC(16:0) isomer



## LysoPC(16:0)

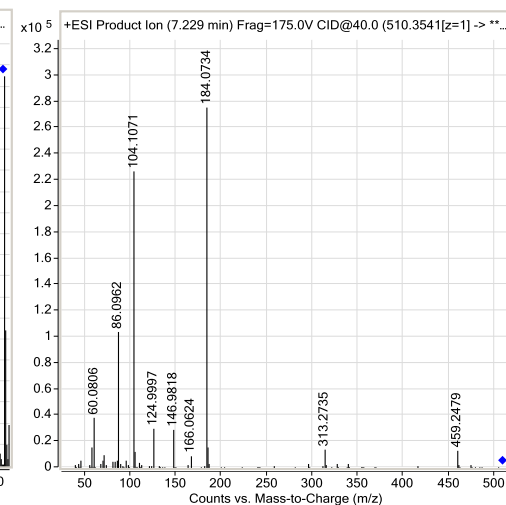
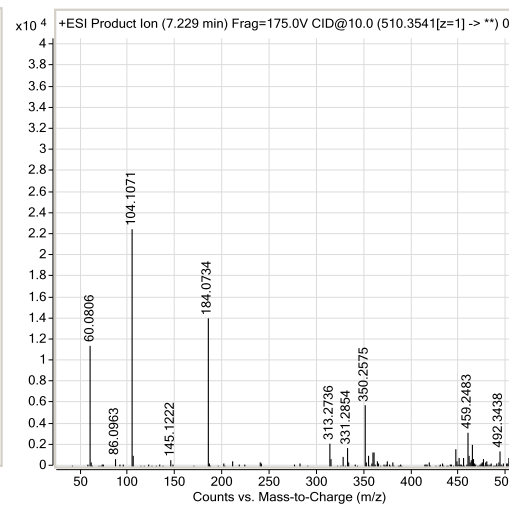
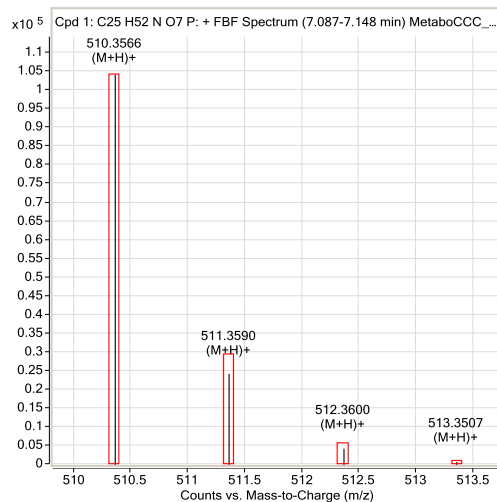
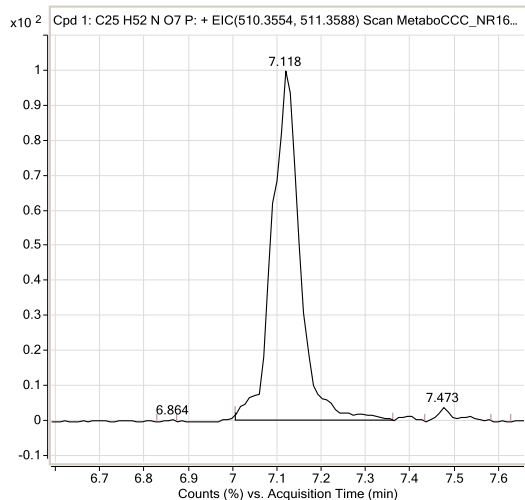


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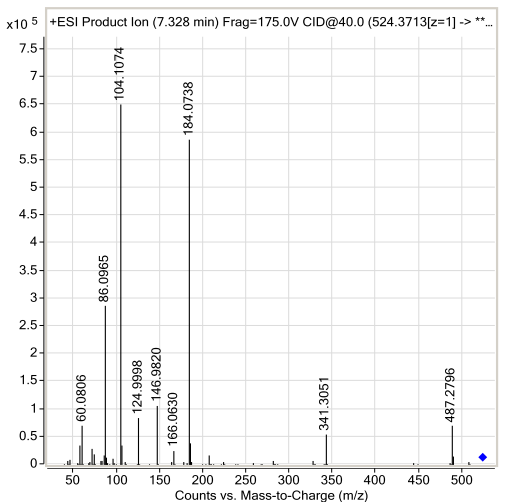
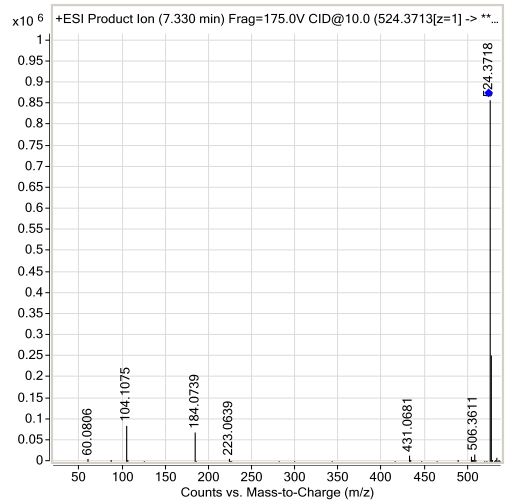
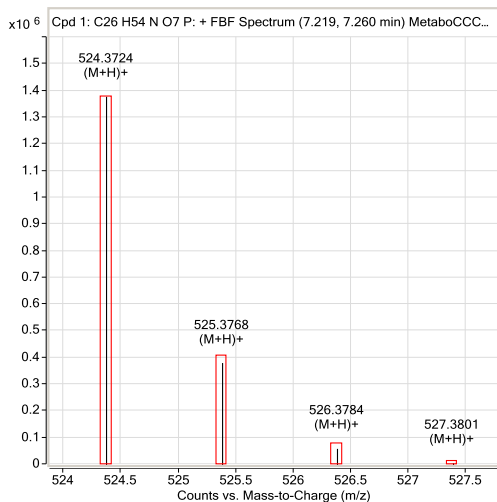
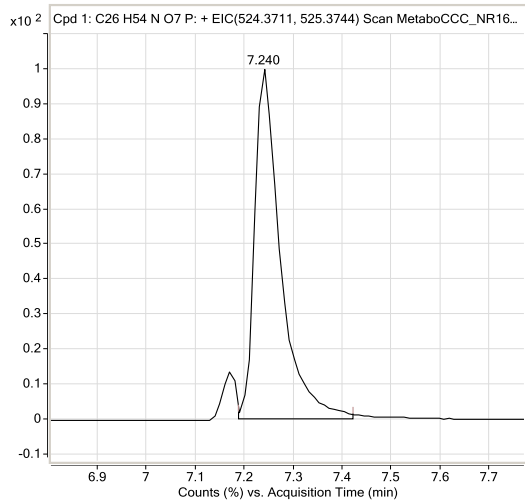




## LysoPC(17:0)



## LysoPC(18:0)



## Bilirubin

Bilirubin typically exhibits high number of ions in electrospray (see isotope patterns below). MS/MS was acquired from  $[M+H]^+$

