Supplementary File S4. Identification of metabolites. Chromatograms and spectra of study samples and pure chemical standards.

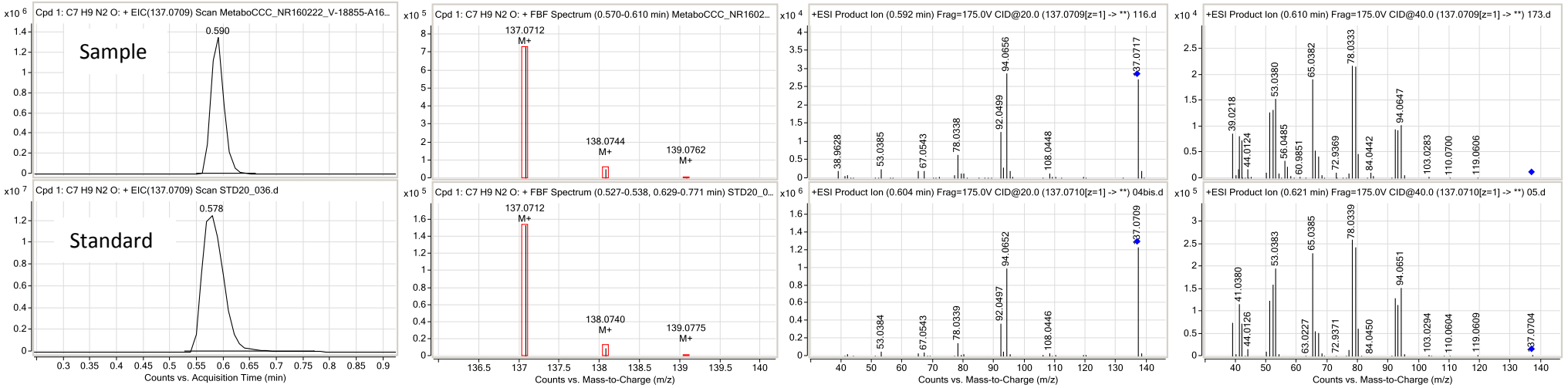
General notes:

Chromatograms and spectra are from representative study samples and pure chemical standards when available.

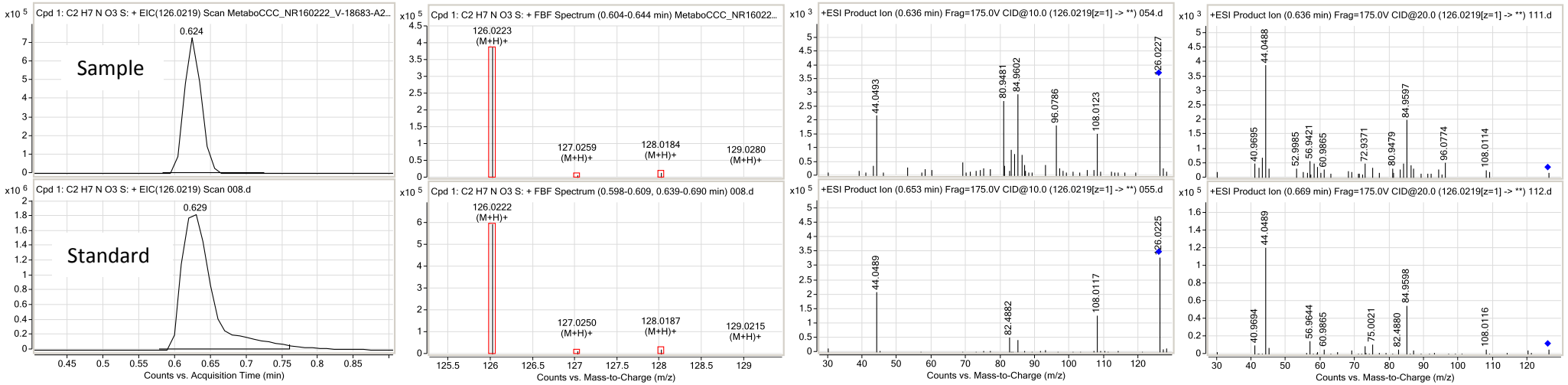
All chemical standards were from IROA Technologies' Mass Spectrometry Metabolite Library, except Phenylacetylglutamine (MetaSci), Decanoylcarnitine (Sigma), Glycochenodeoxycholic acid (Sigma), Indole-3-propionic acid (MetaSci), Indoleacetic acid (Sigma), Isatin (Sigma), Propionylcarnitine (Sigma), Tetradecanoylcarnitine (Sigma), and γ-CEHC (Chem Cruz)

- 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.

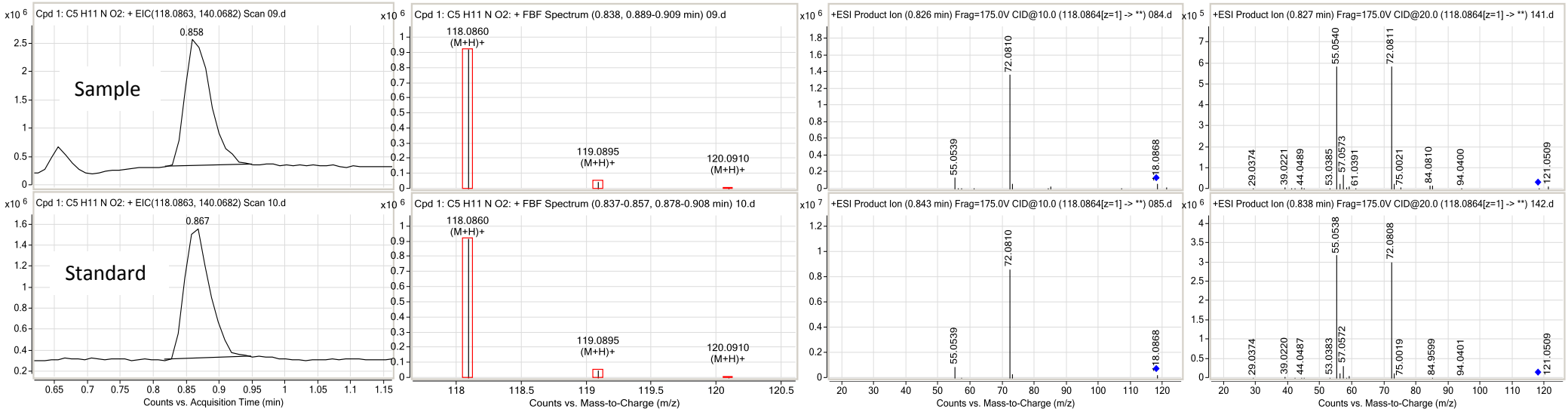
1-Methylnicotinamide



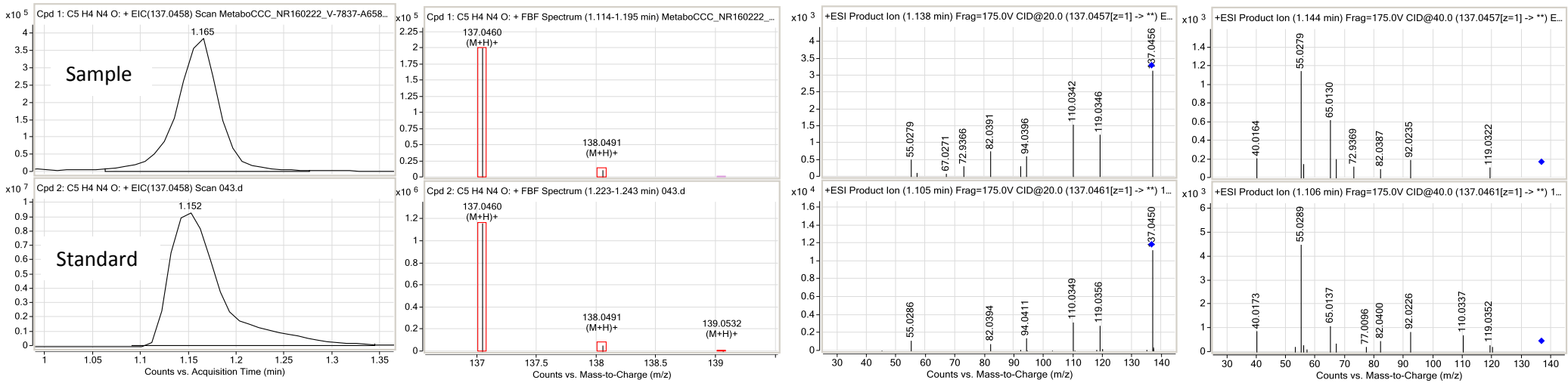
Taurine



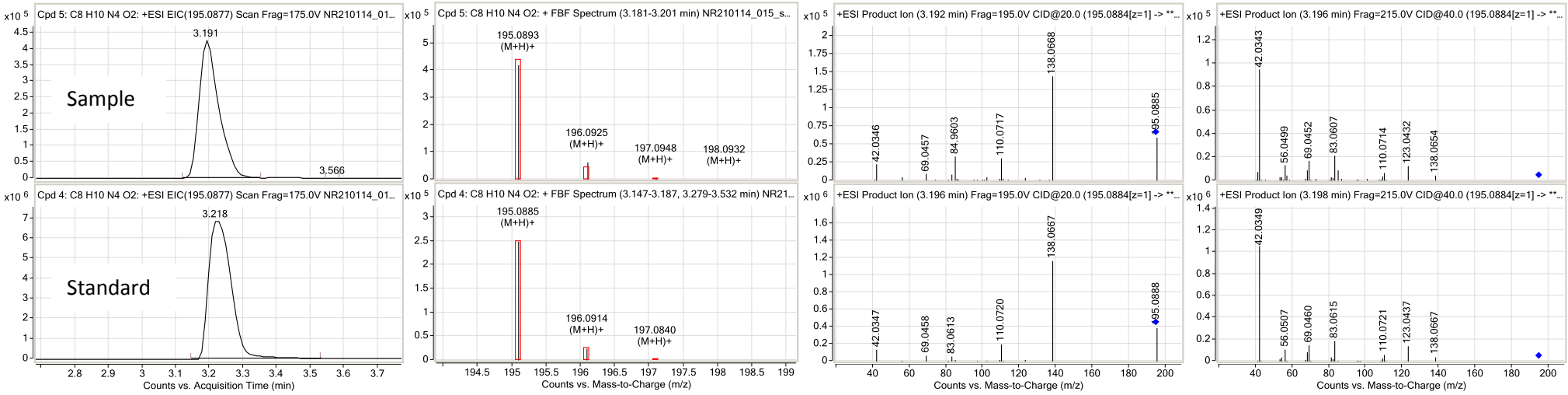
Valine



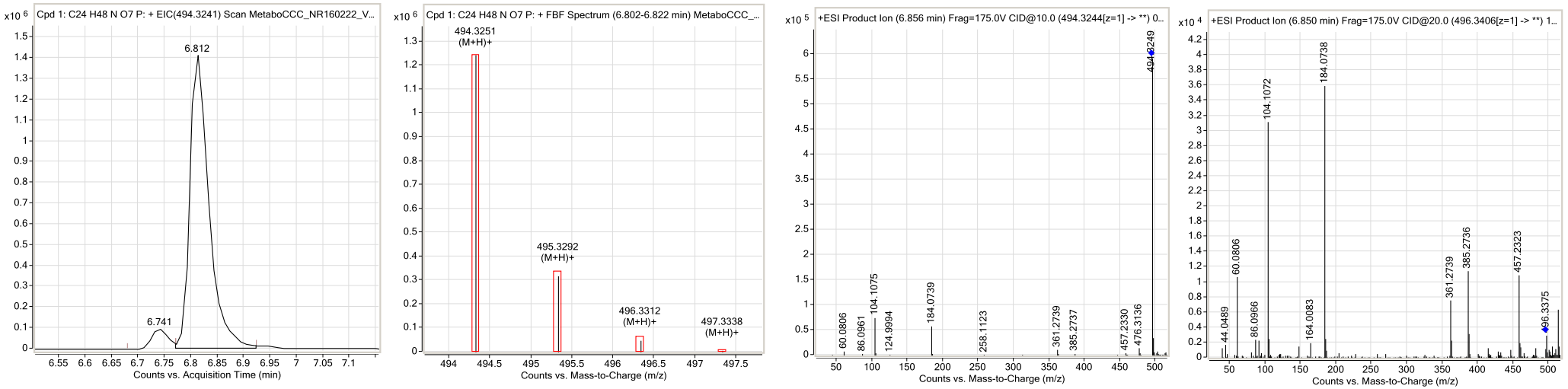
Hypoxanthine



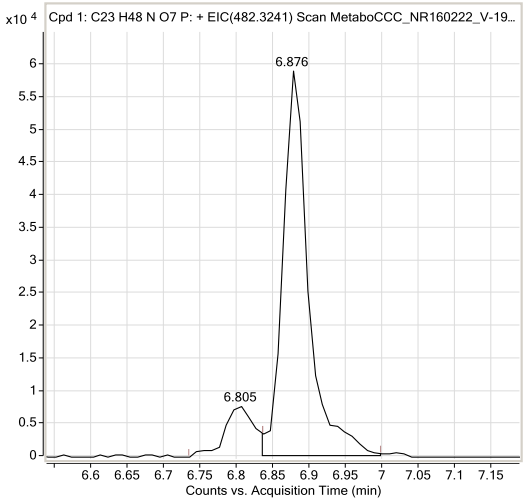
Caffeine

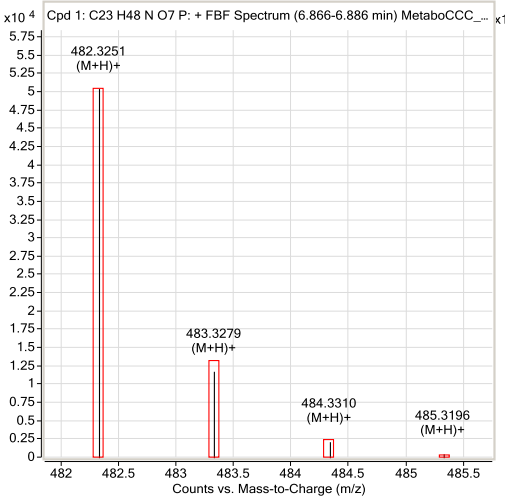


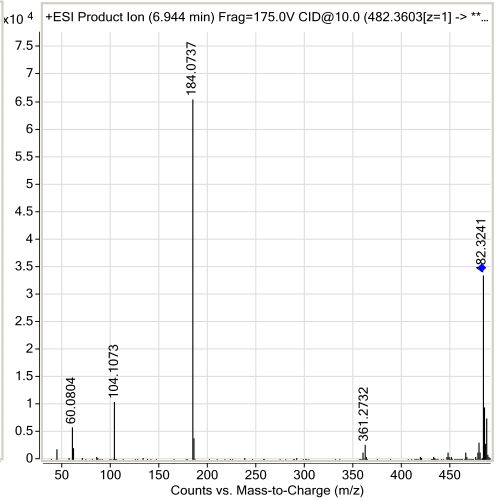
LysoPC (16:1)

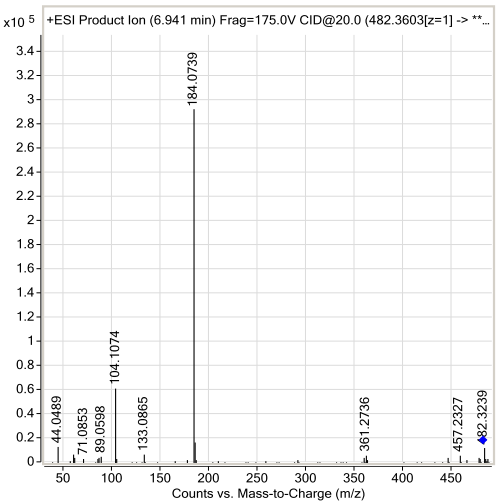


LysoPC (15:0)

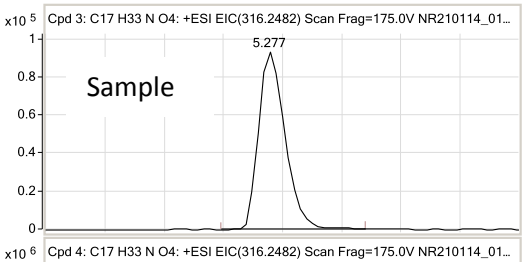


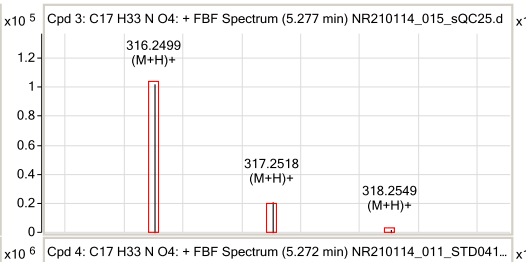


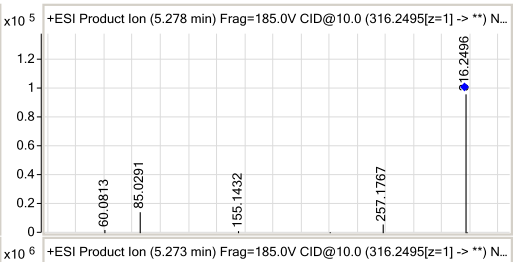


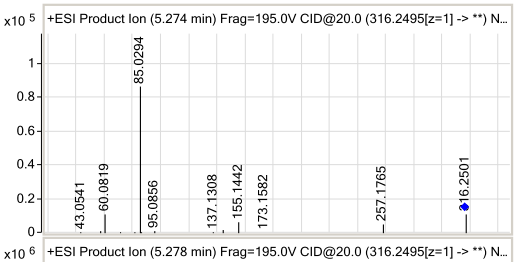


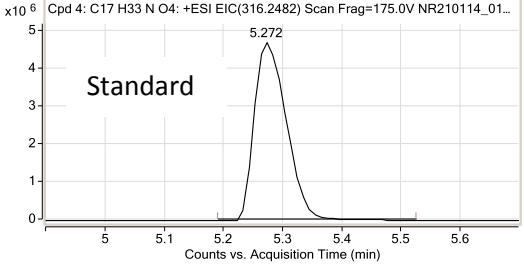
Decanoylcarnitine (C10:0)

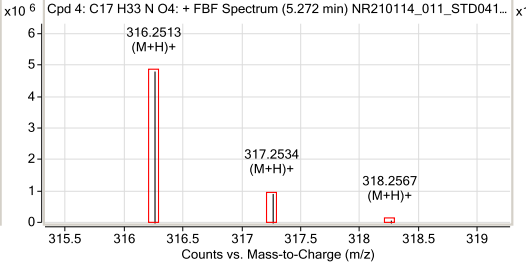


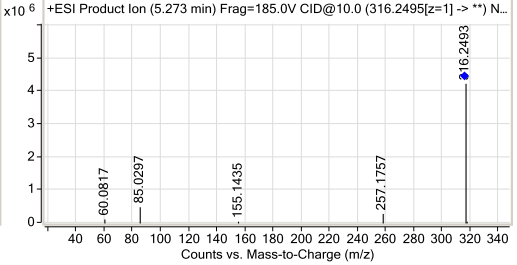


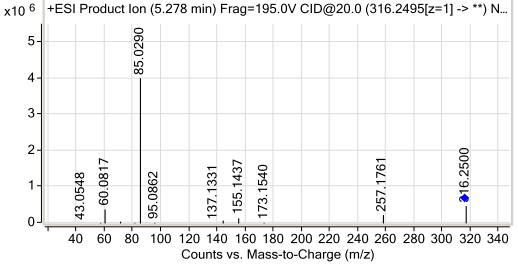




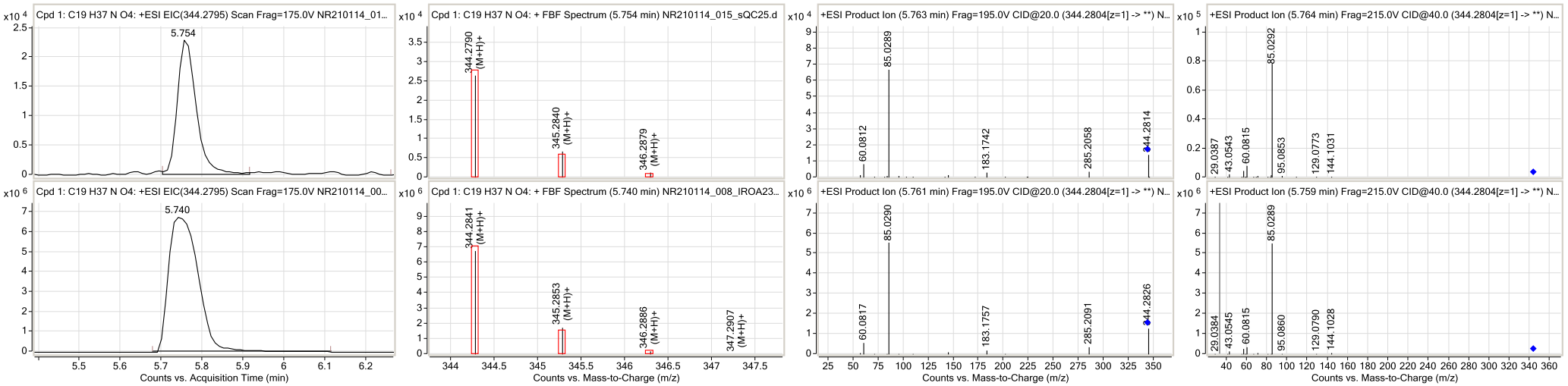




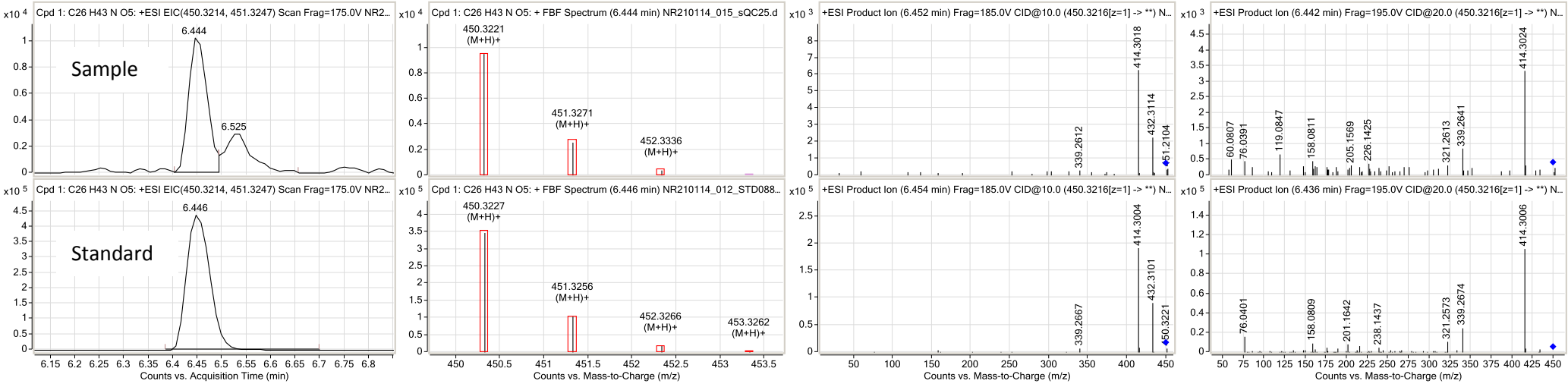




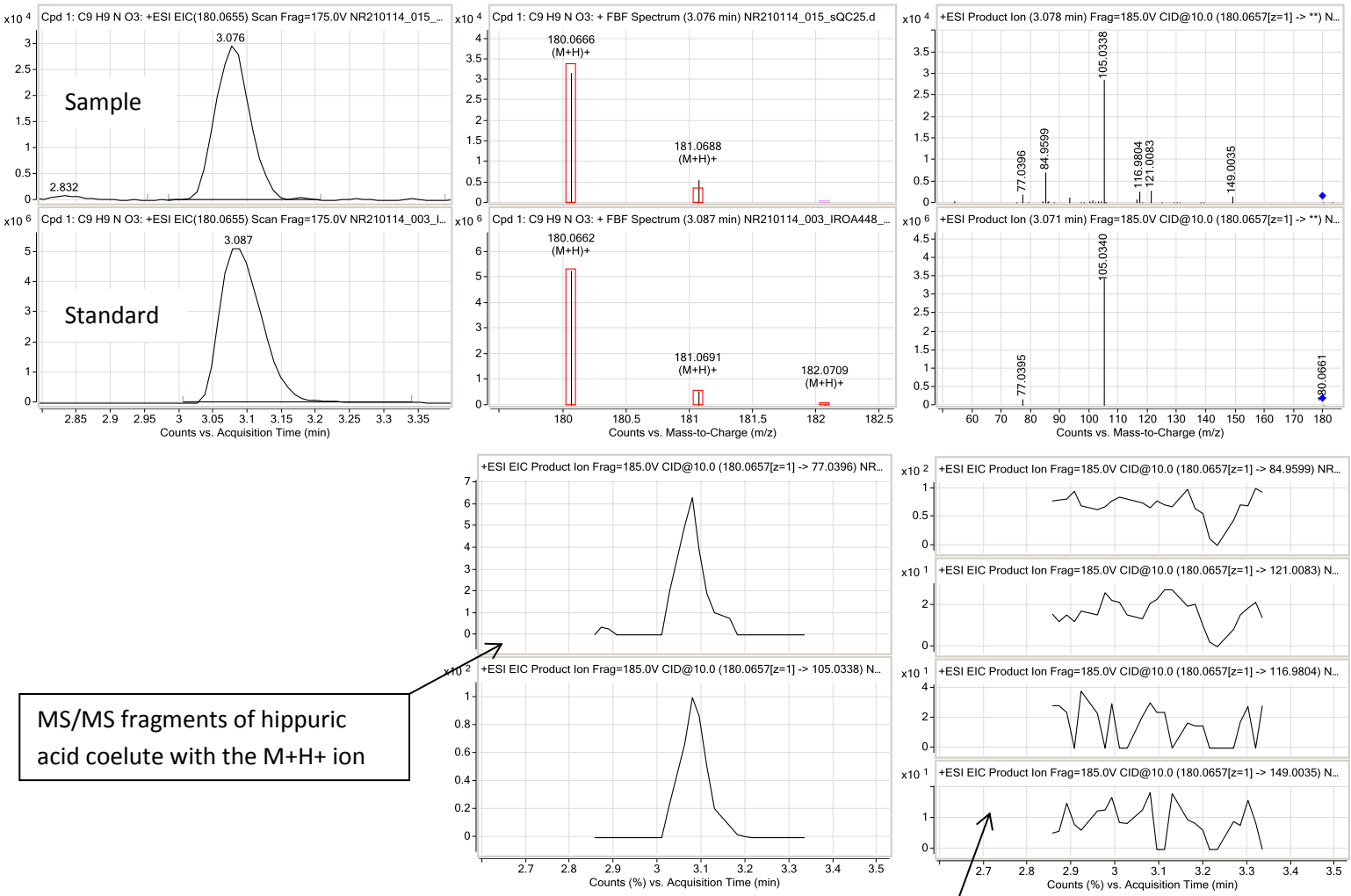
Dodecanoylcarnitine (C12:0)



Glycochenodeoxycholic acid



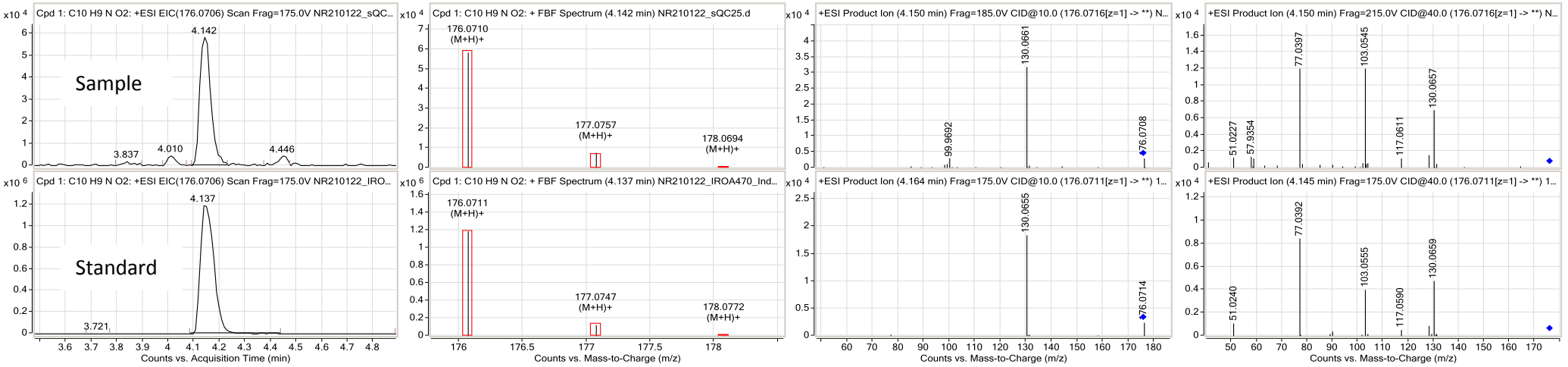
Hippuric acid



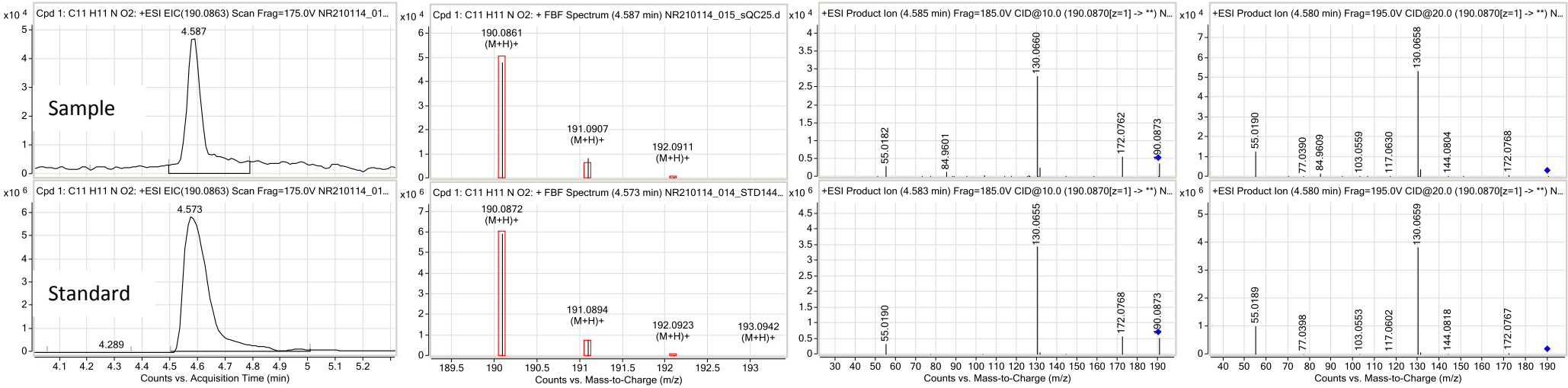
MS/MS fragments of hippuric acid coelute with the M+H+ ion

Additional fragments in the MS/MS spectrum are unrelated to hippuric acid

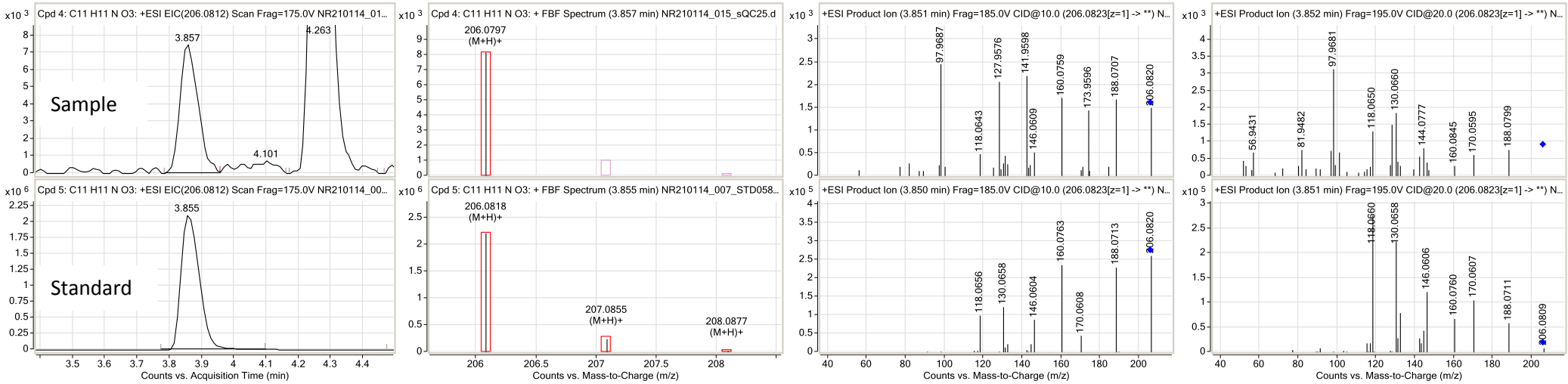
Indoleacetic acid

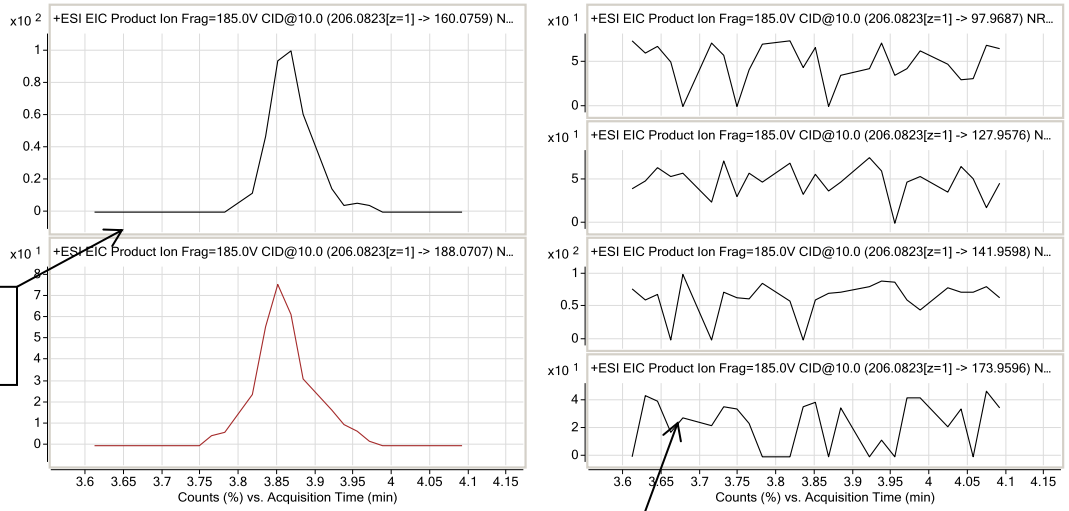


Indole-3-propionic acid



Indolelactic acid

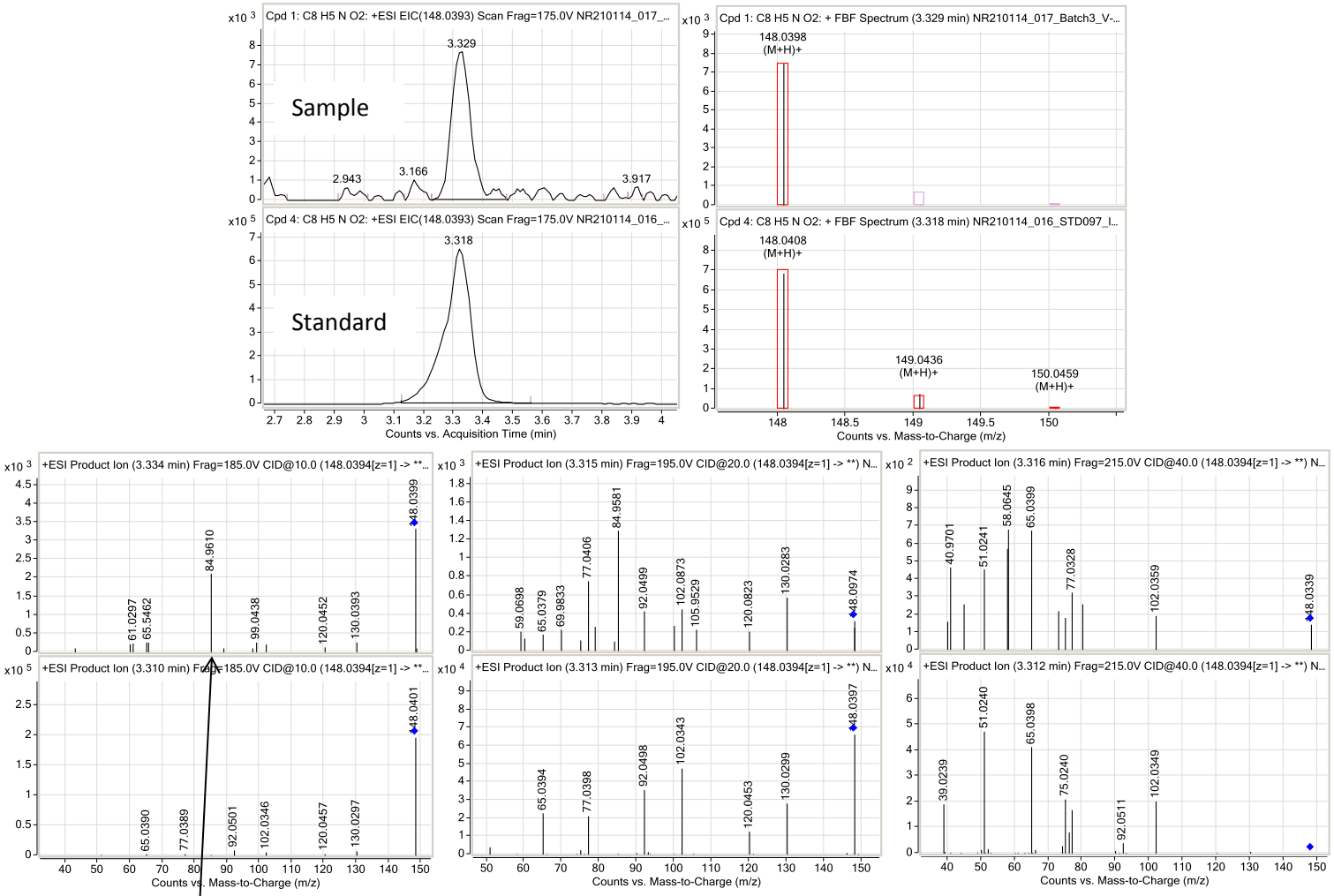




MS/MS fragments of indolelactic acid coelute with the M+H+ ion

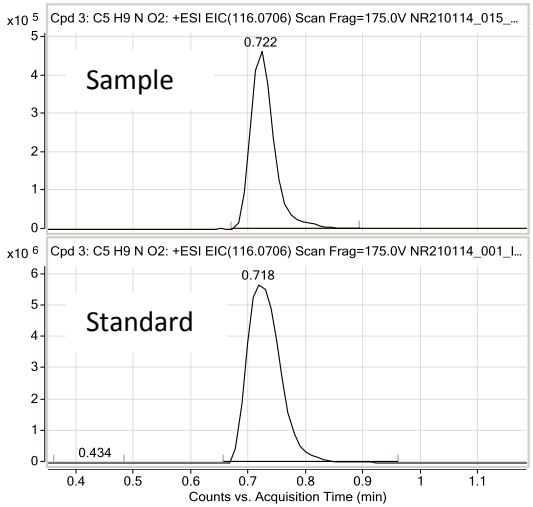
Additional fragments seen in the MS/MS spectra are unrelated to indolelactic acid

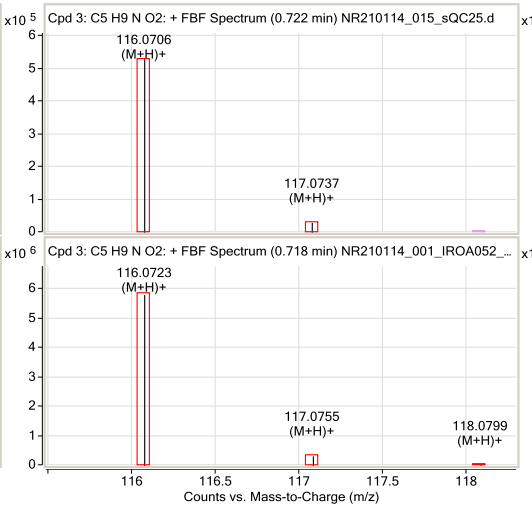
Isatin

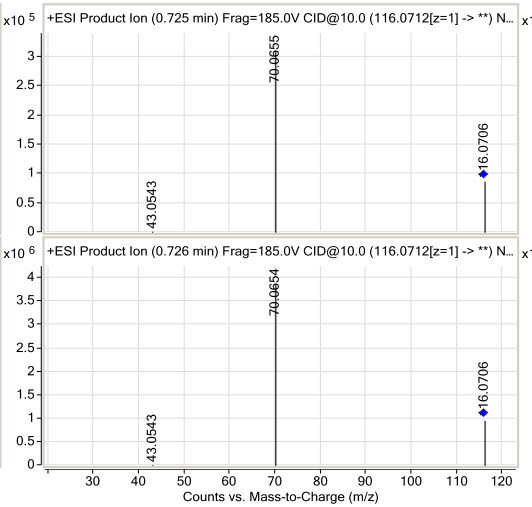


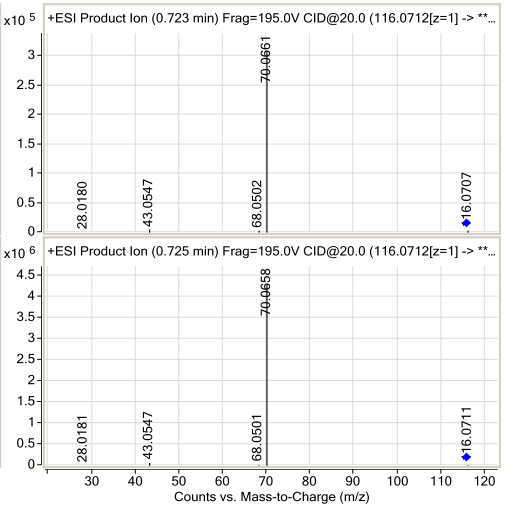
Due to low precursor ion intensity, some unrelated background ions (e.g. *m/z* 84.9610 can be seen (see hippuric acid for details)

Proline

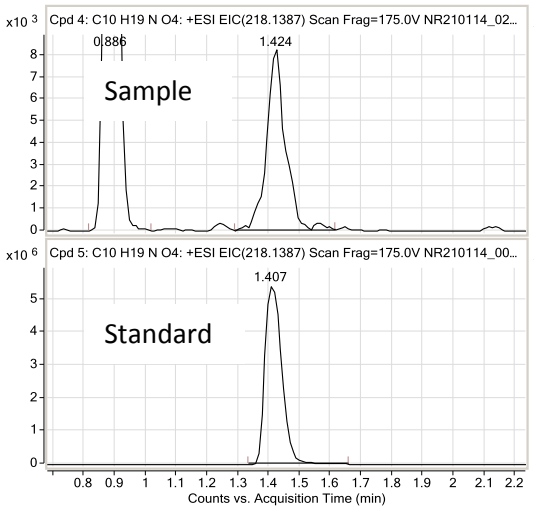


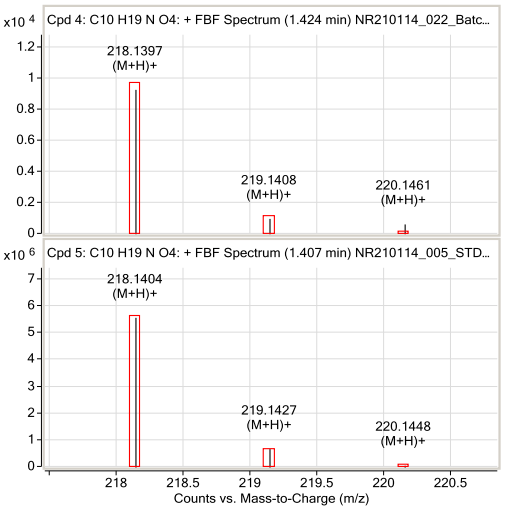


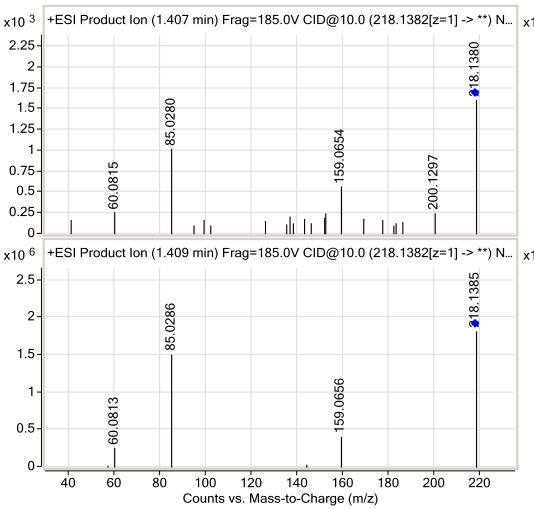


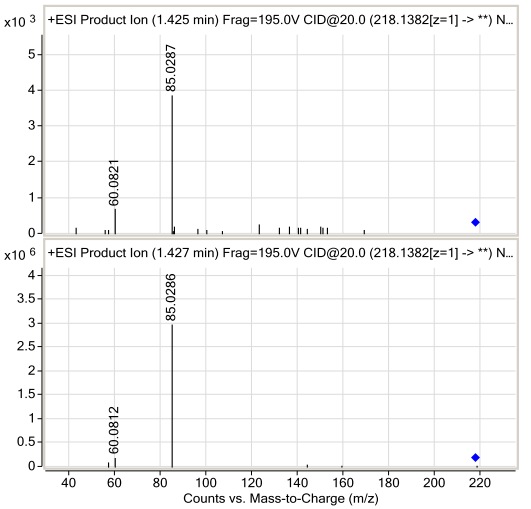


Propionylcarnitine (C3:0)

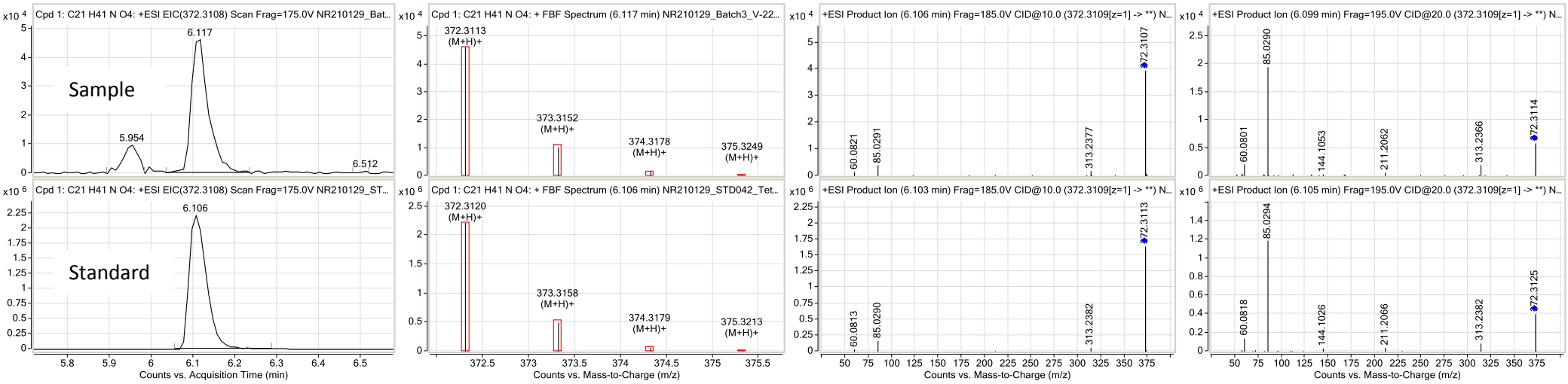




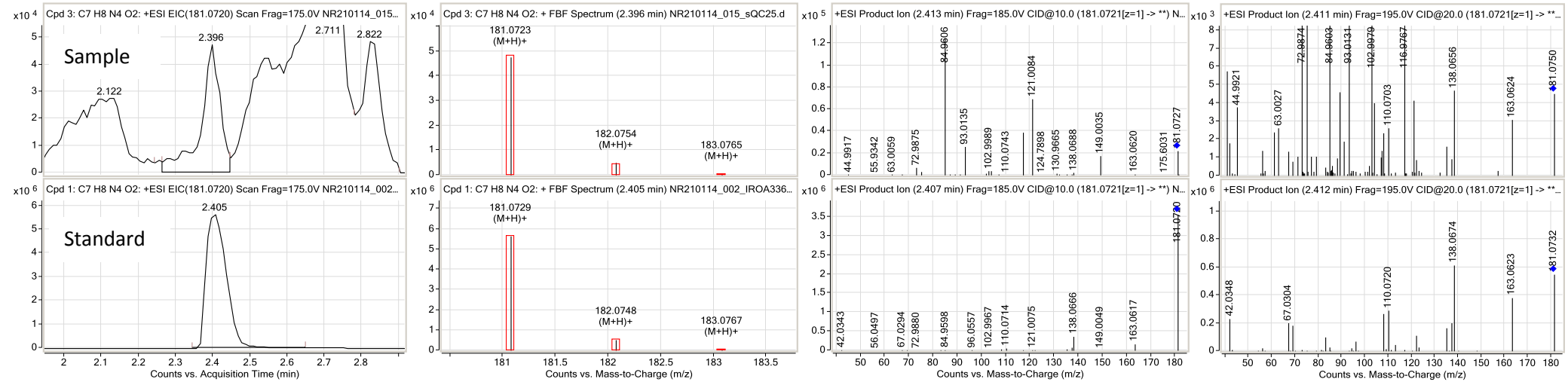




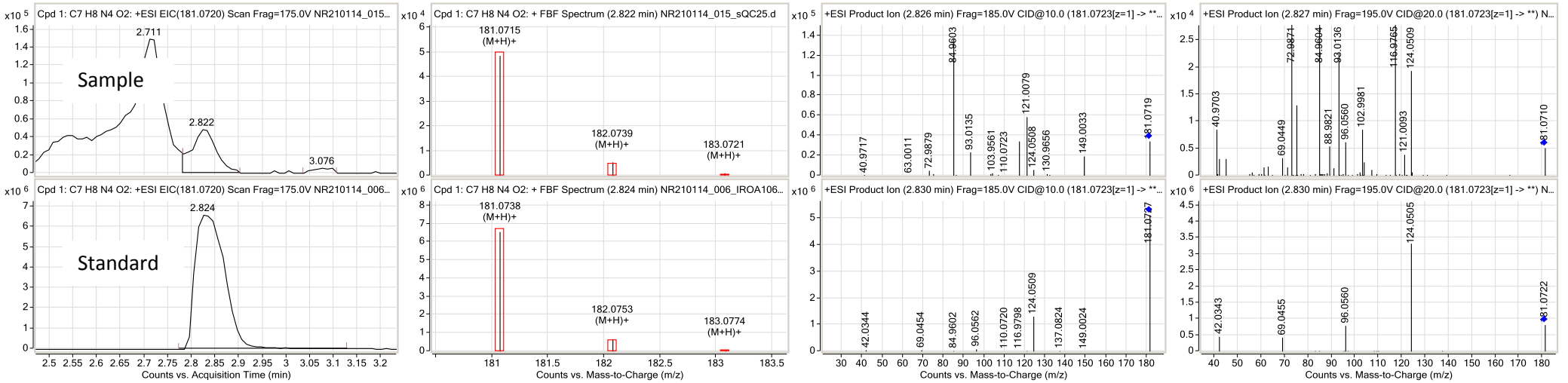
Tetradecanoylcarnitine (C14:0)



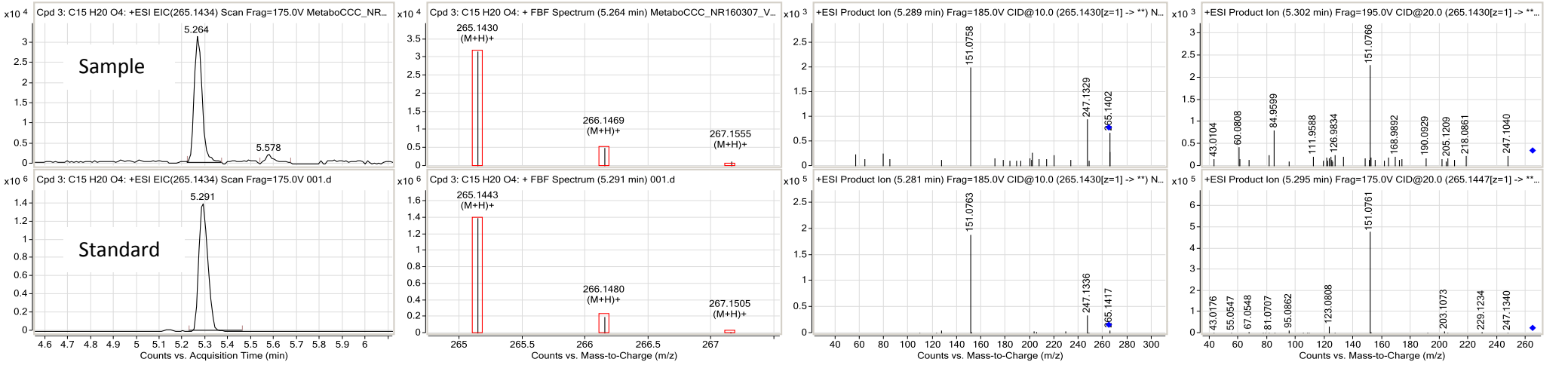
Theobromine



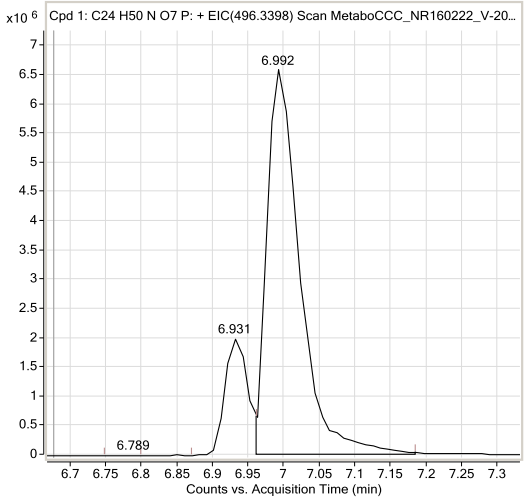
Theophylline

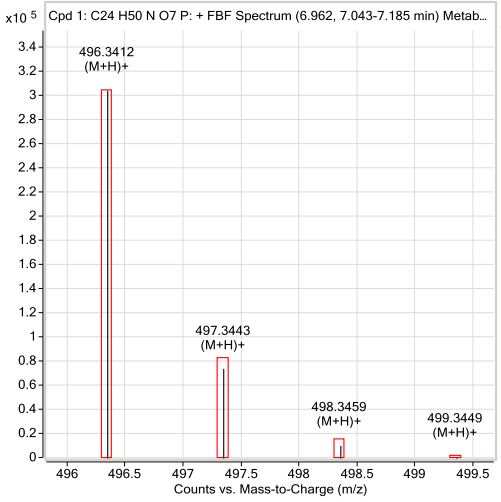


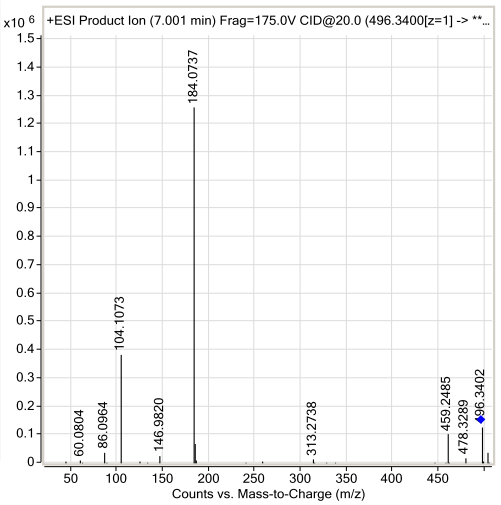
γ-CEHC

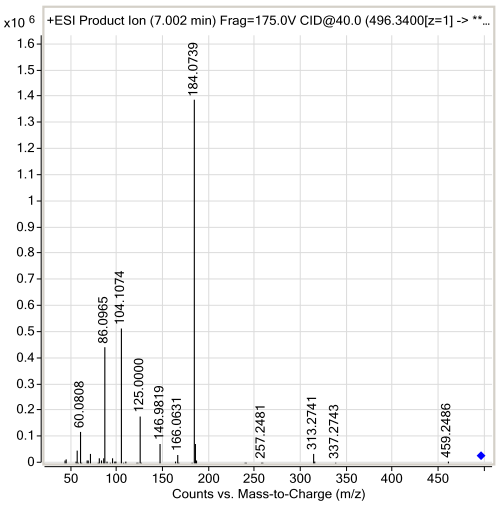


LysoPC (16:0)

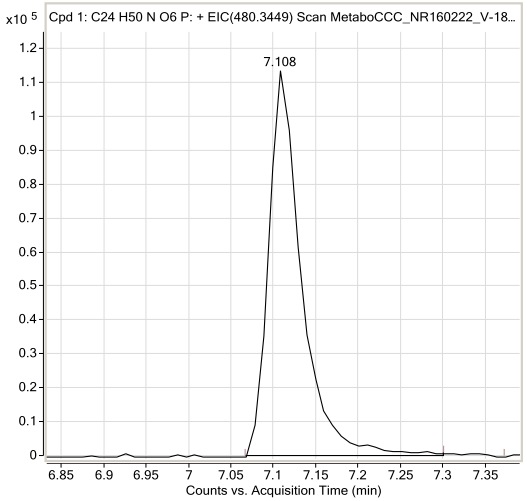


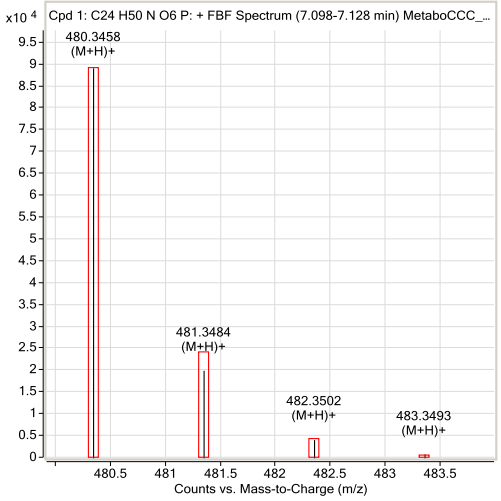


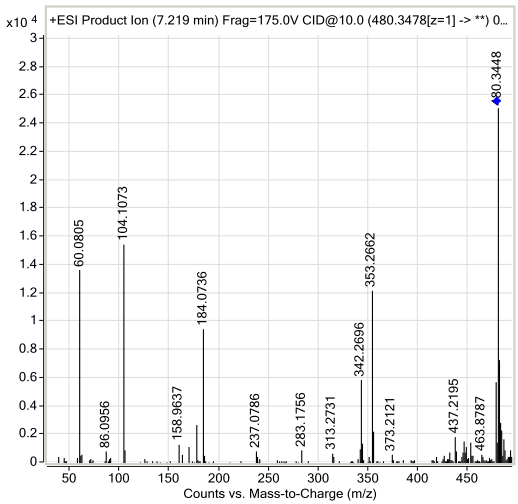


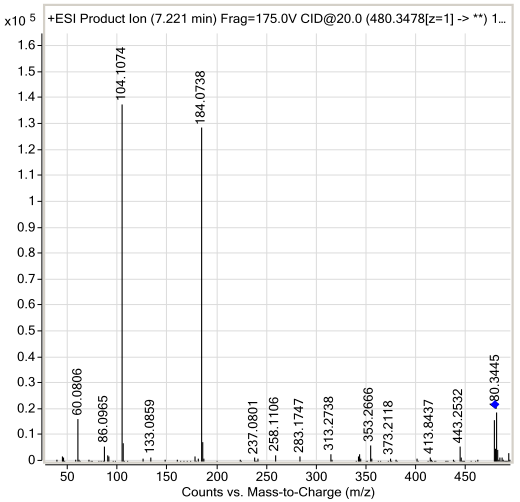


LysoPC (P-16:0)

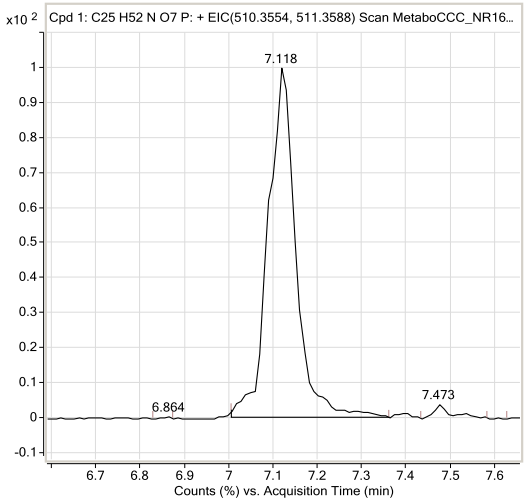


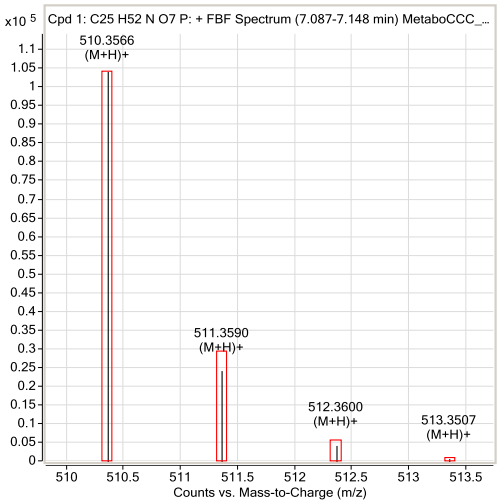


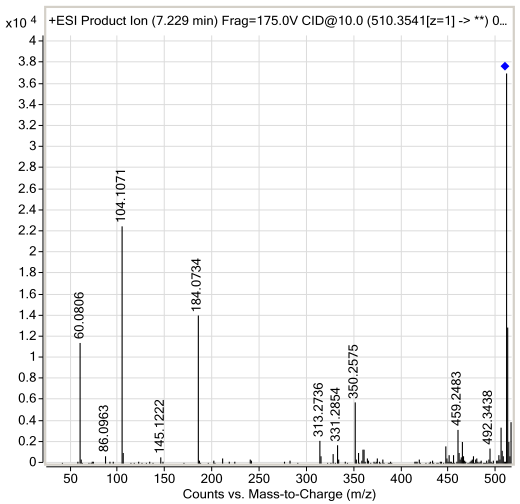


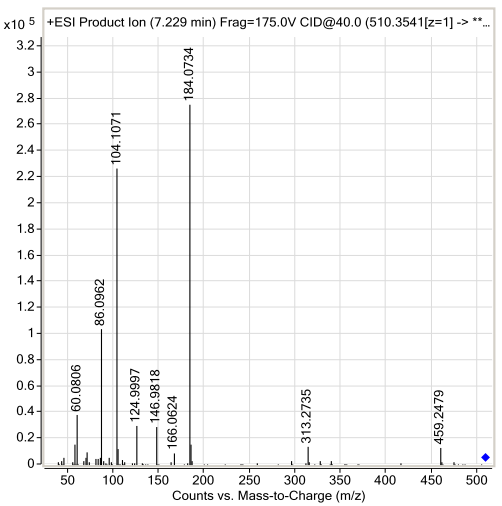


LysoPC (17:0)

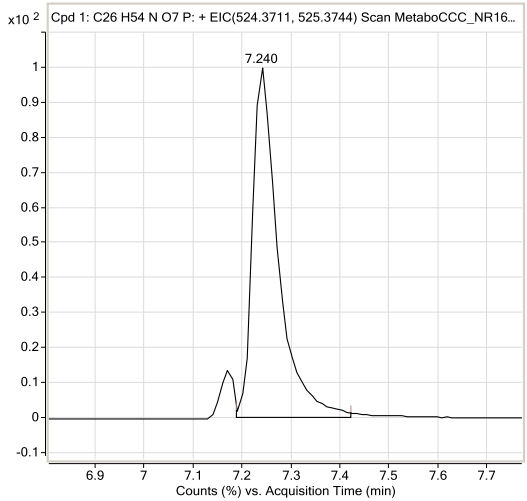


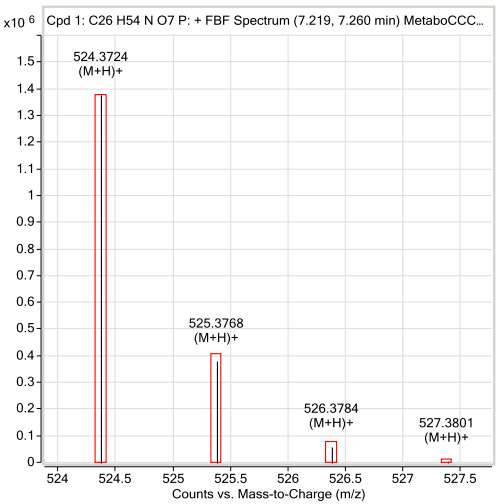


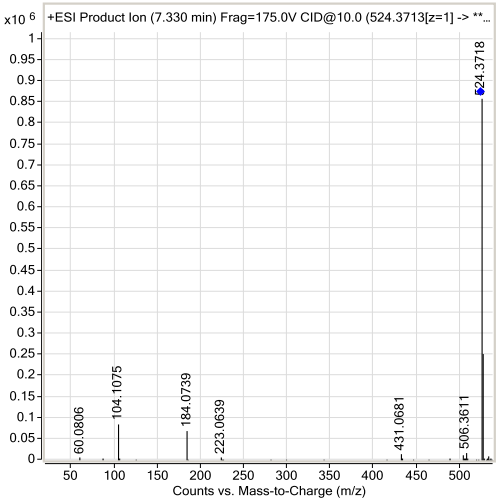


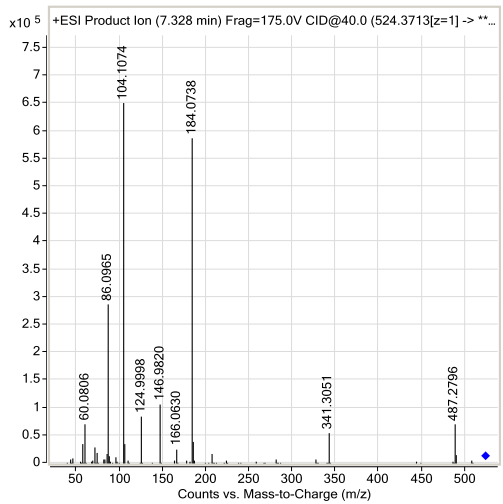


LysoPC (18:0)



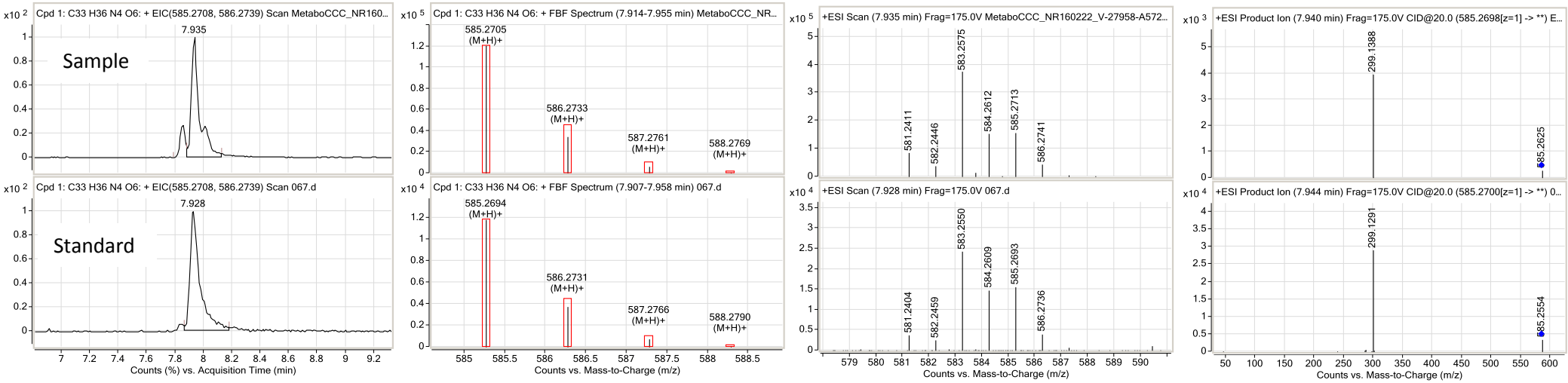






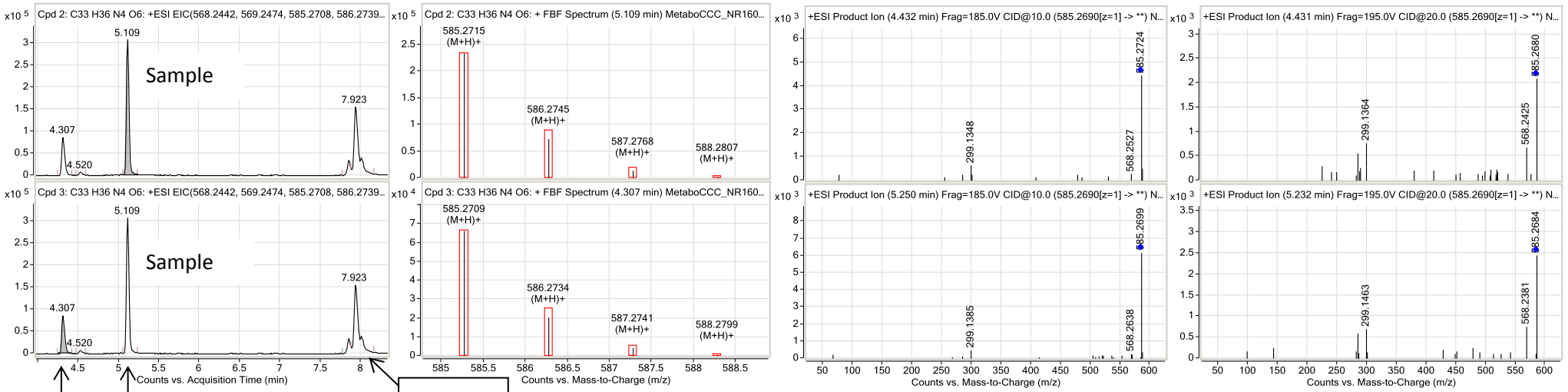
Bilirubin

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



Bilirubin isomers 1 and 2:

Two bilirubin isomers, possible photodegradation products (for details, see Ennever *et al.* J Clin Invest. 1987;79:1674 and Pediatr Res. 1985;19:205)

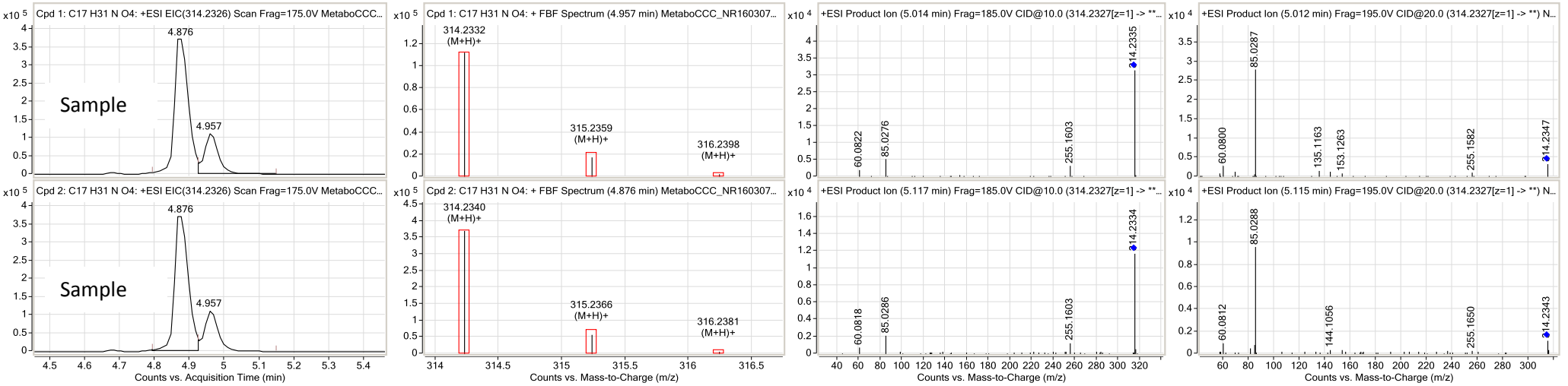


Two structural isomers of bilirubin that can be formed by light exposure.

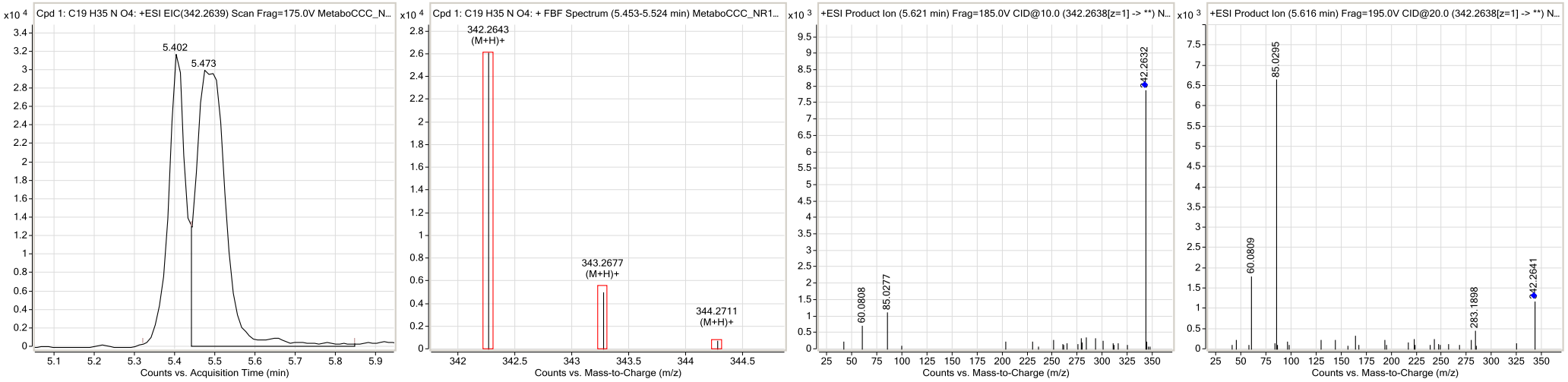
Isotope patterns and MS/MS spectra matching with those of bilirubin.

Detailed identification using the same instrumentation and method: Stepien *et al.*, Int J Cancer 2021;148:609-25

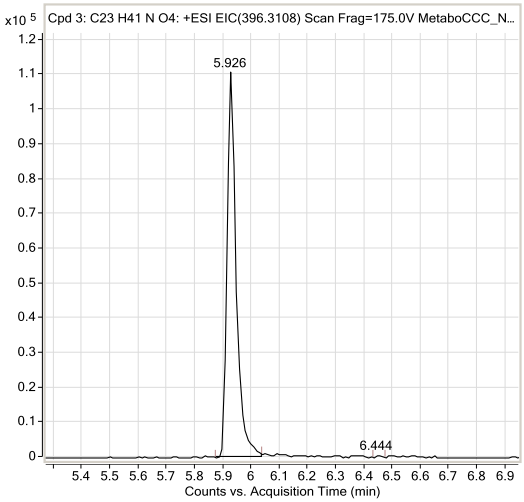
Decenoylcarnitine (C10:1), isomer 1 and 2

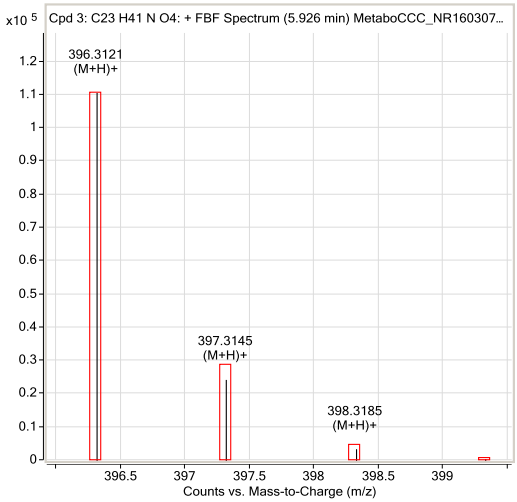


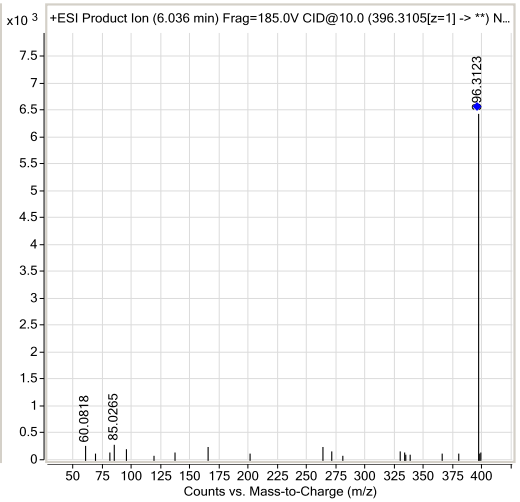
Dodecenoylcarnitine (C12:1)

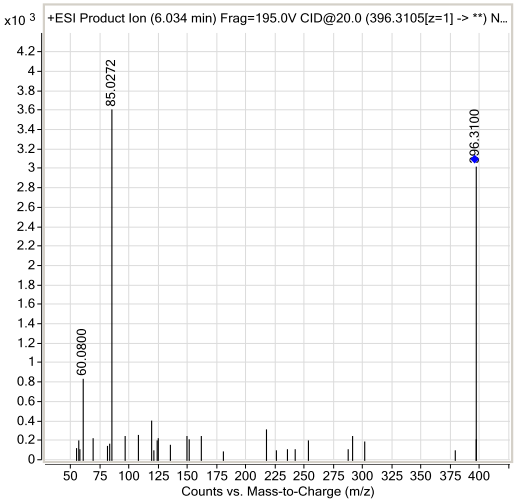


Hexadecadienoylcarnitine (C16:2)

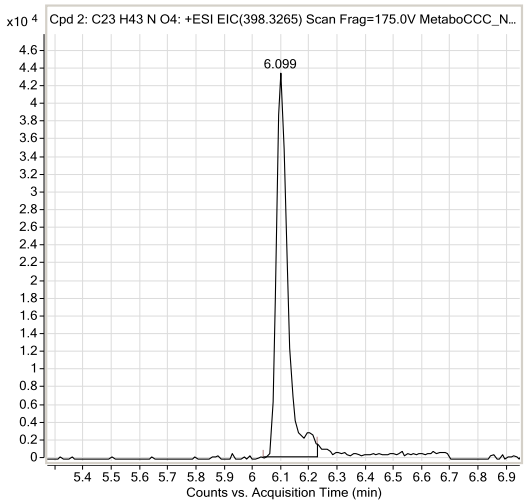


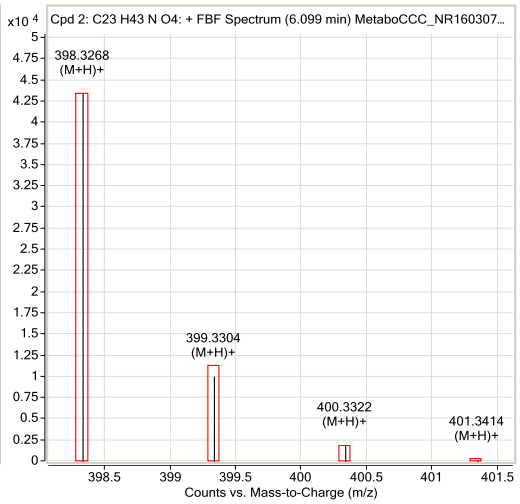


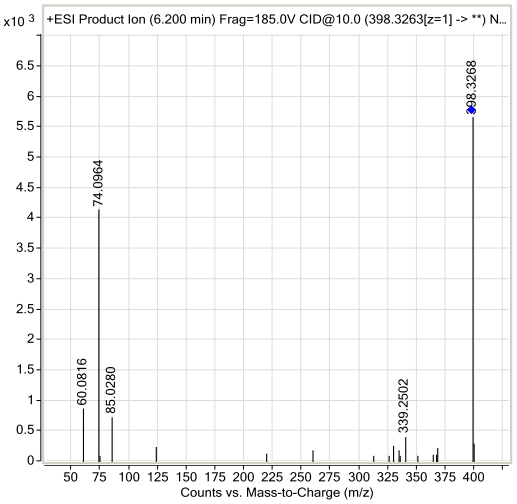


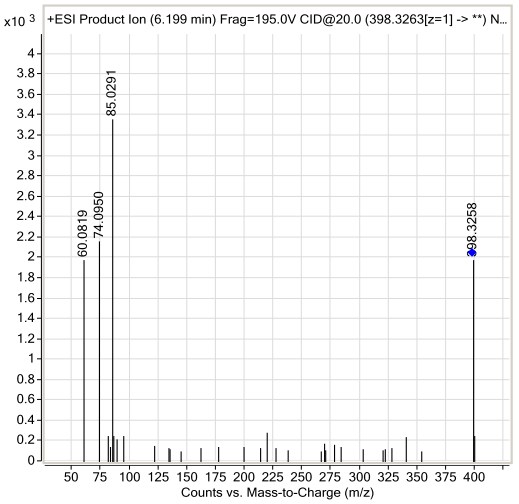


Hexadecenoylcarnitine (C16:1)

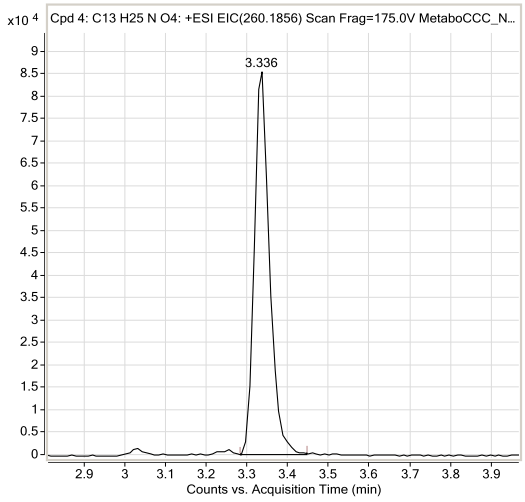


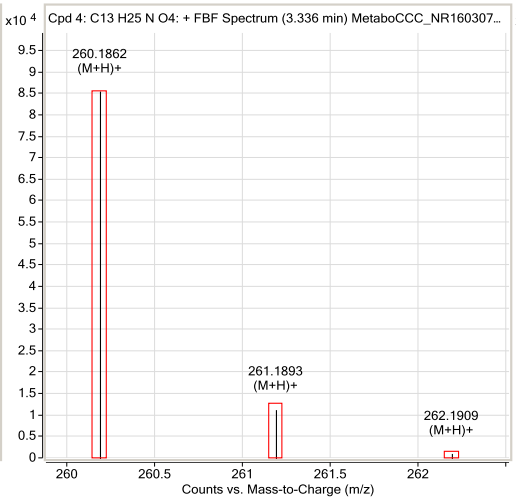


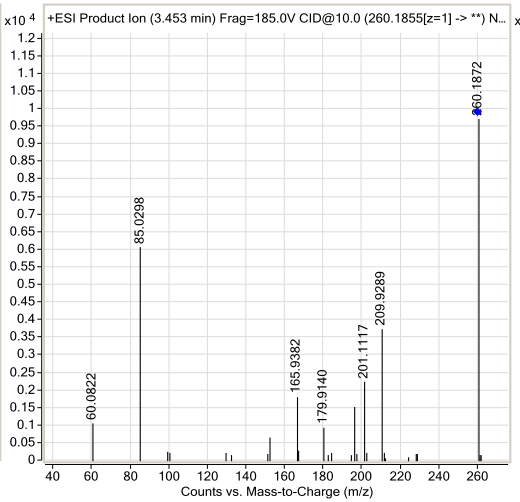


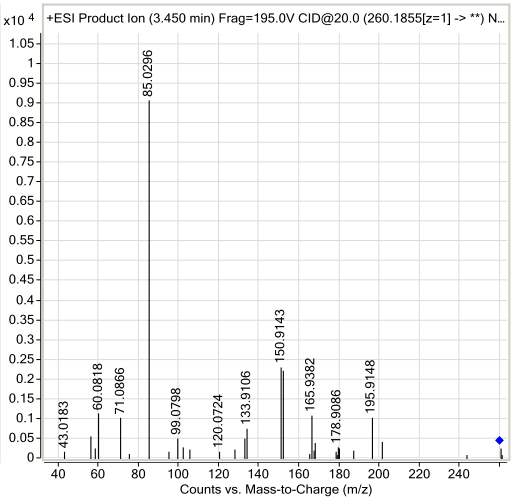


Hexanoylcarnitine (C6:0)

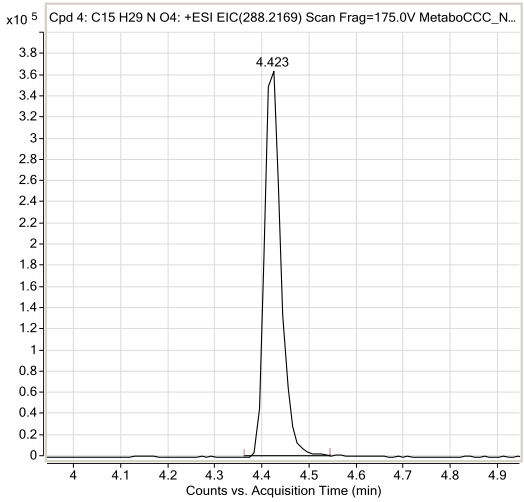


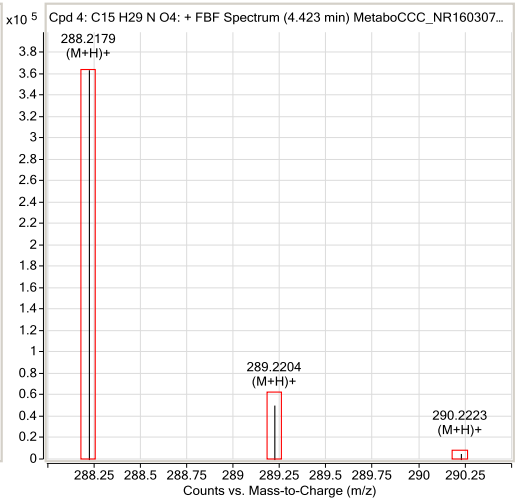


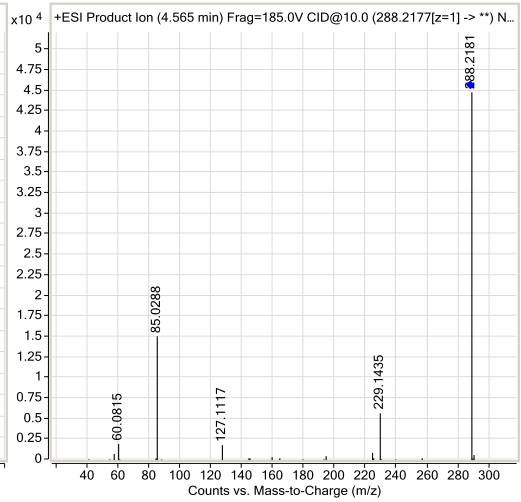


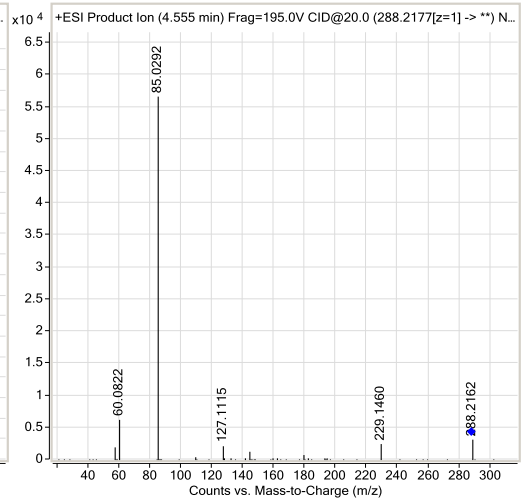


Octanoylcarnitine (C8:0)

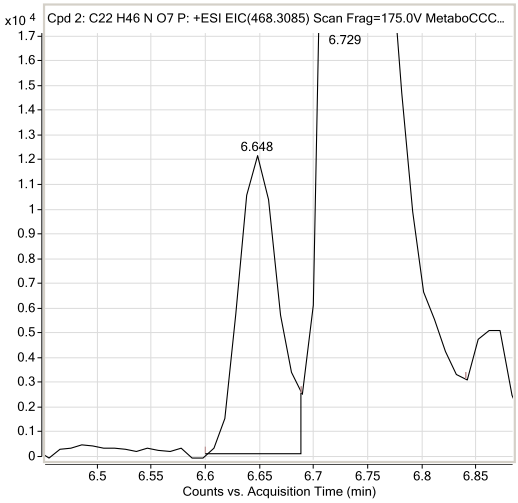


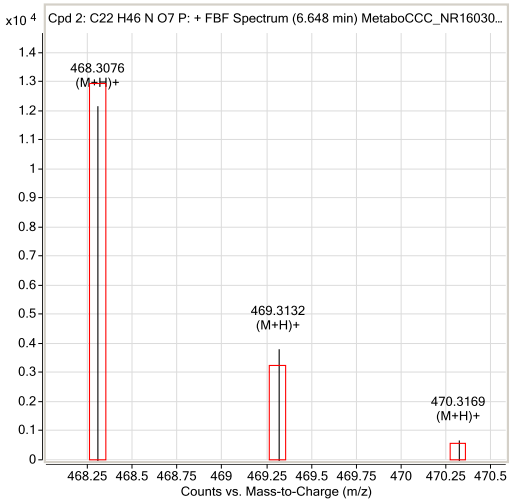


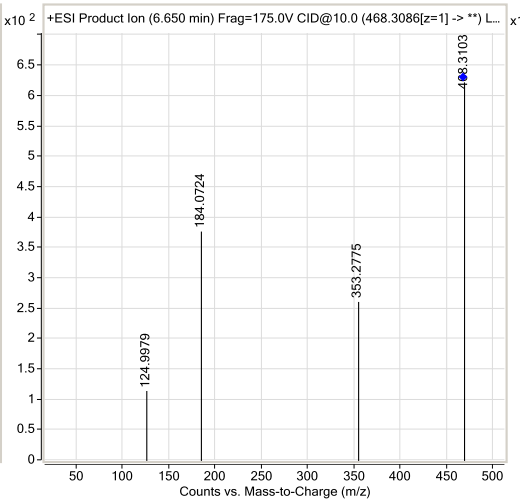


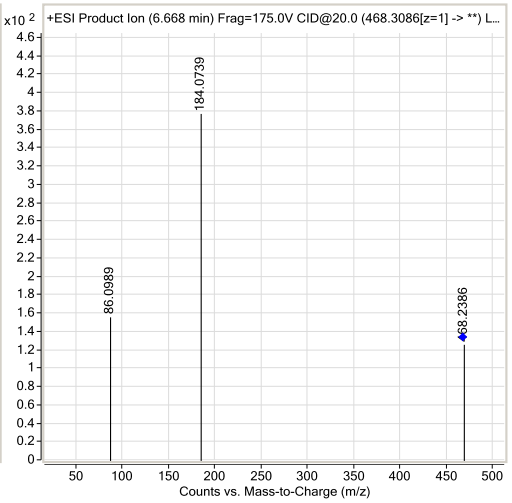


LysoPC (14:0) (isomer 1)

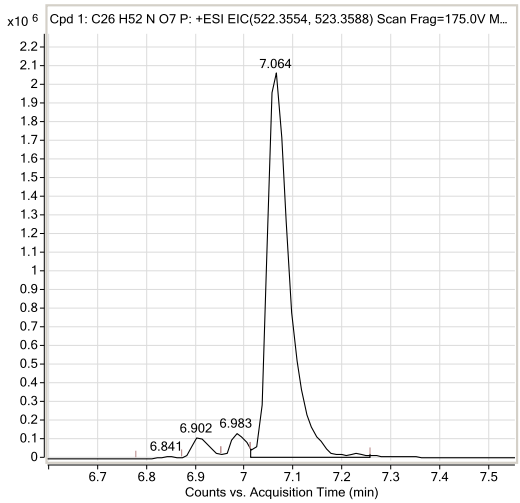


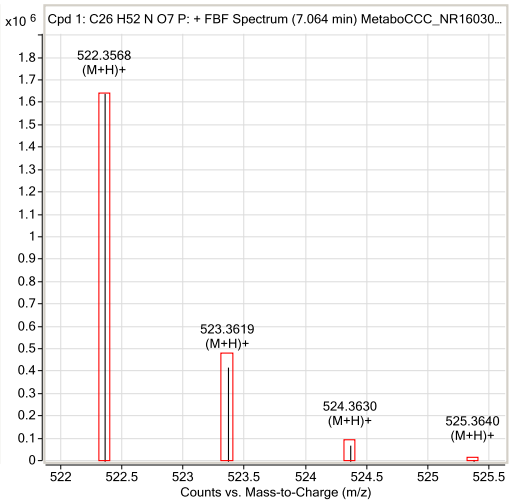


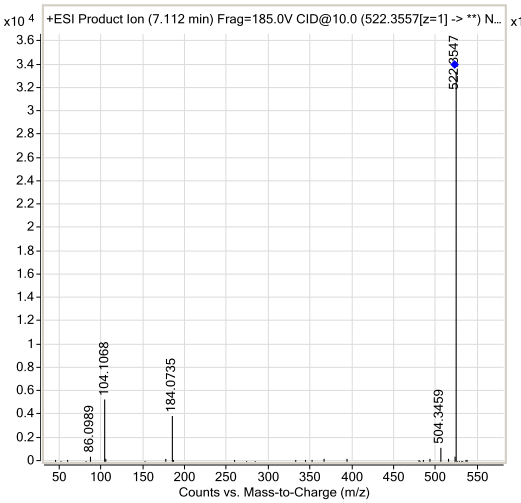


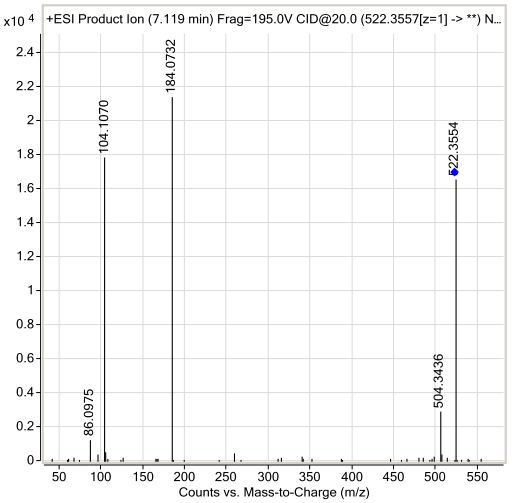


LysoPC (18:1)

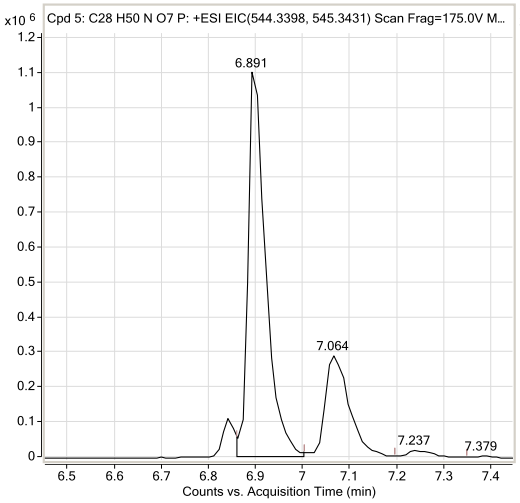


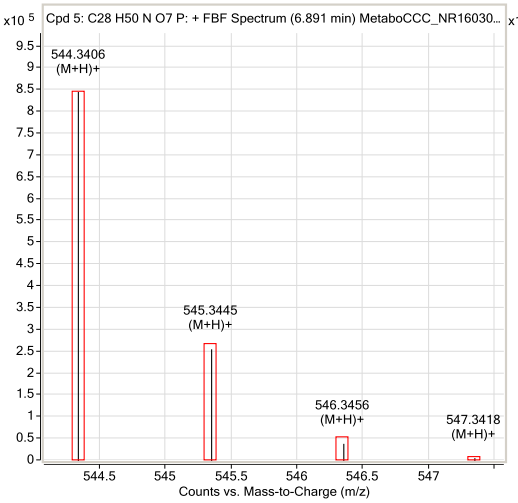


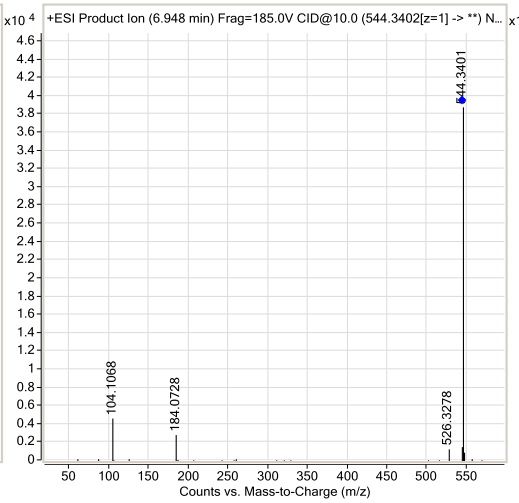


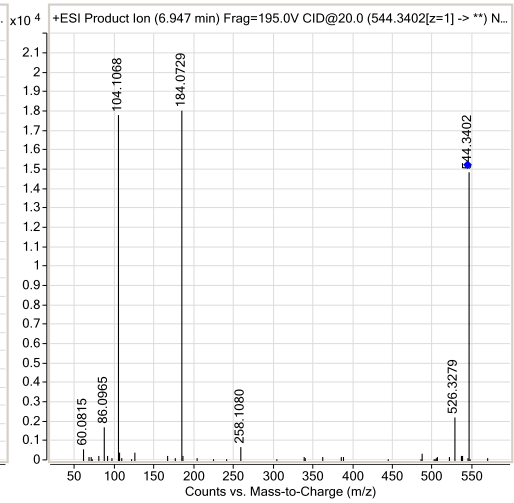


LysoPC (20:4)

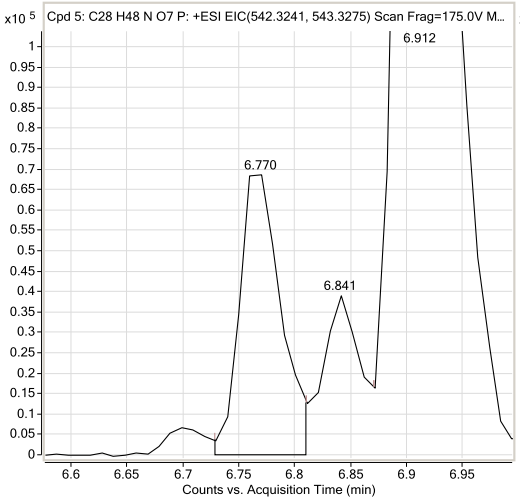


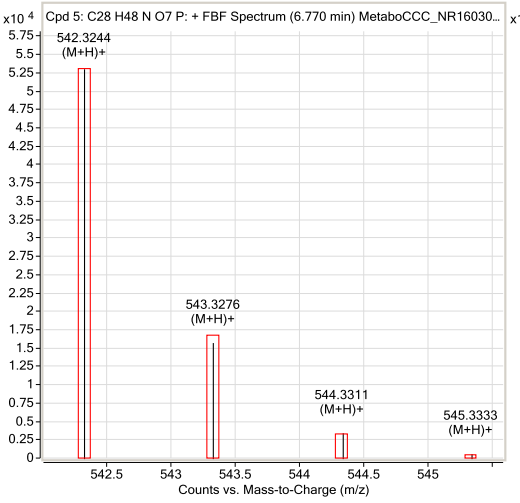


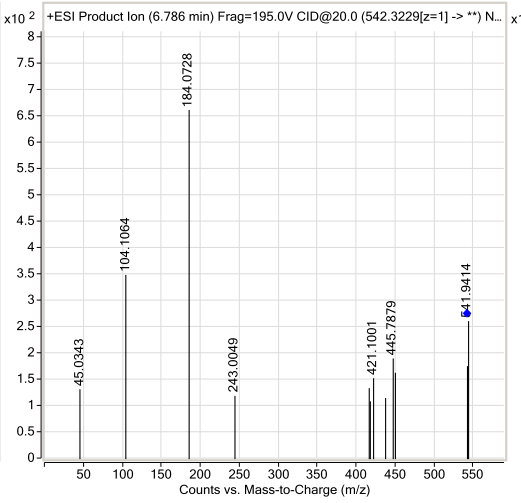


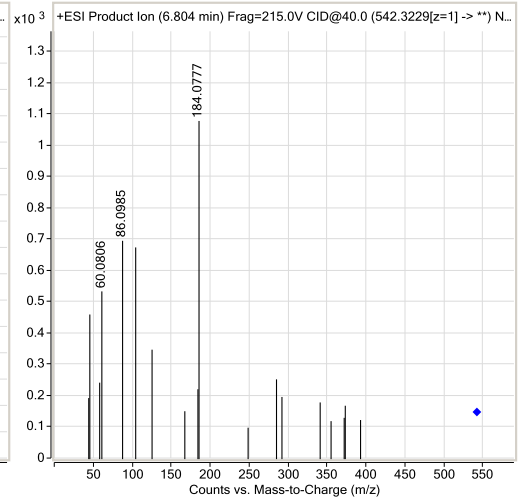


LysoPC (20:5)

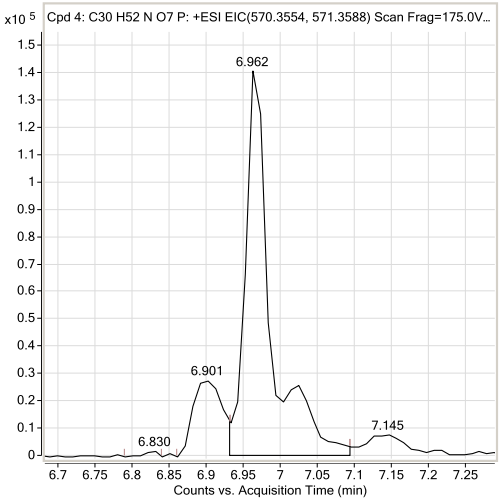


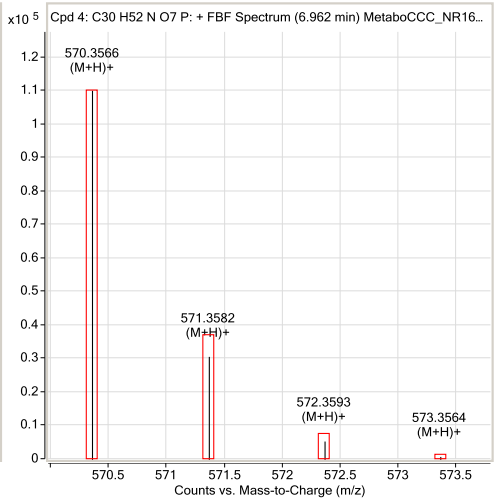


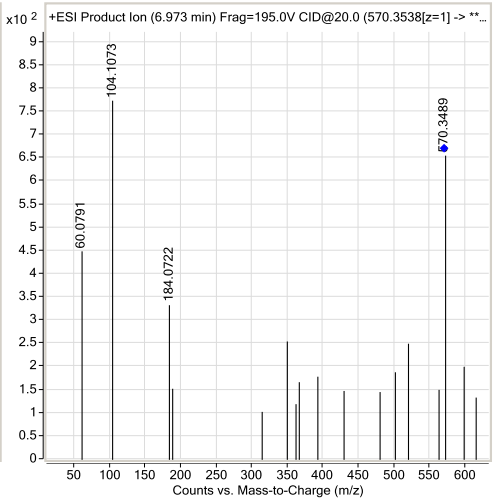


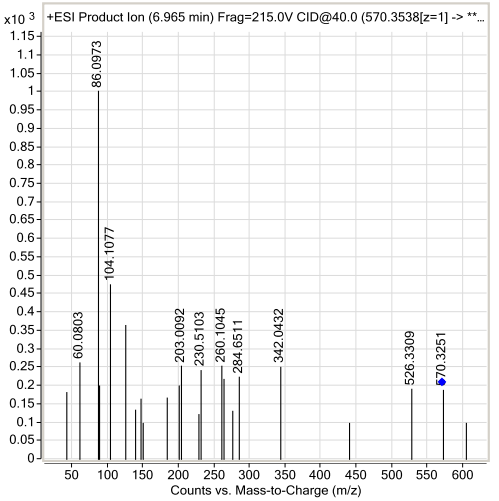


LysoPC (22:5)

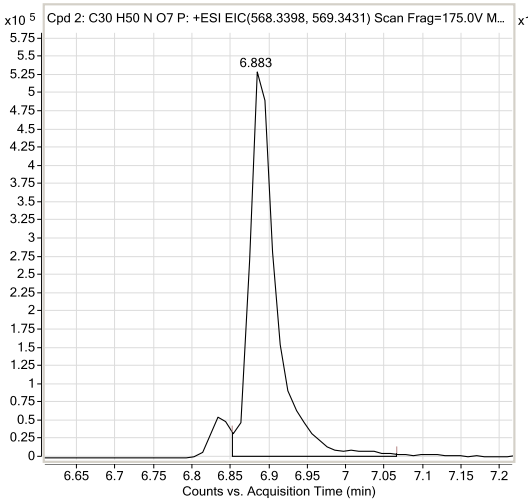


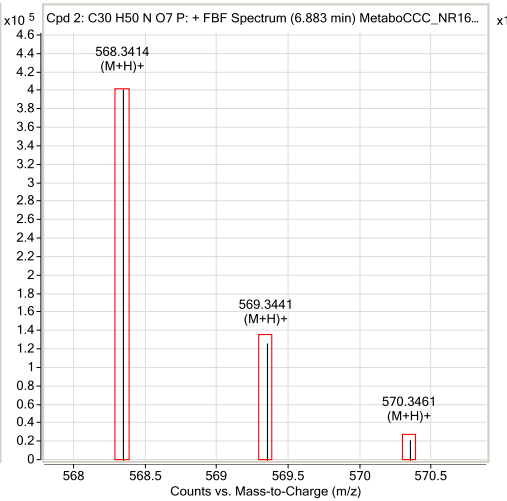


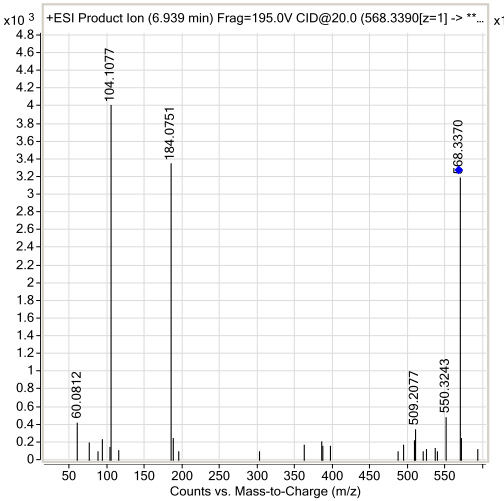


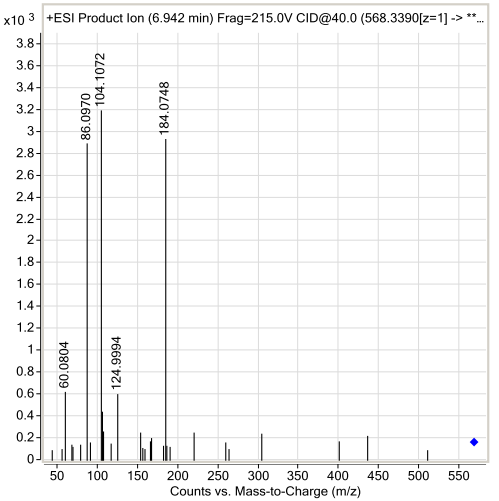


LysoPC (22:6)

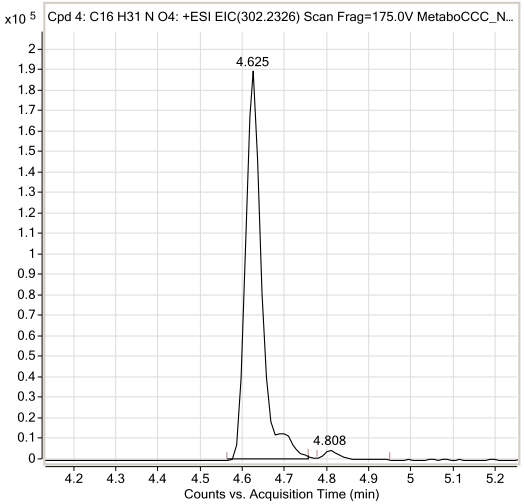


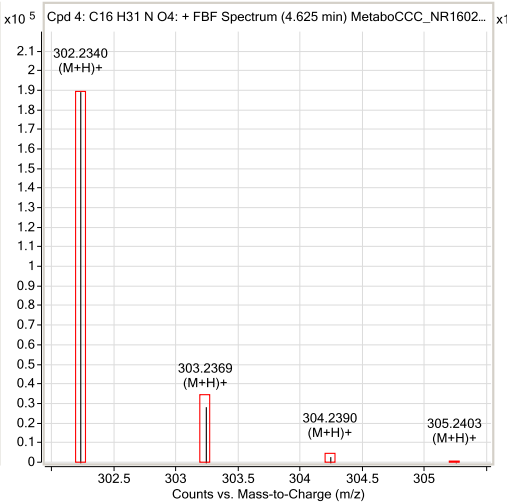


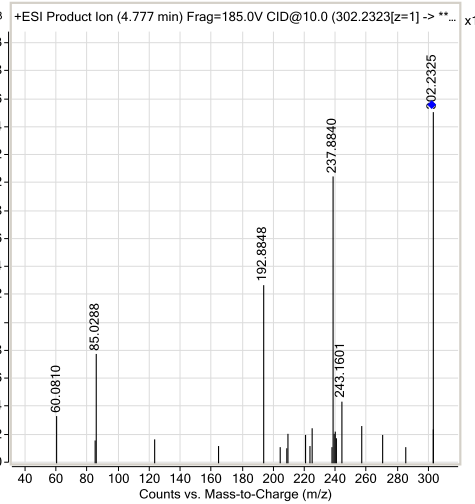


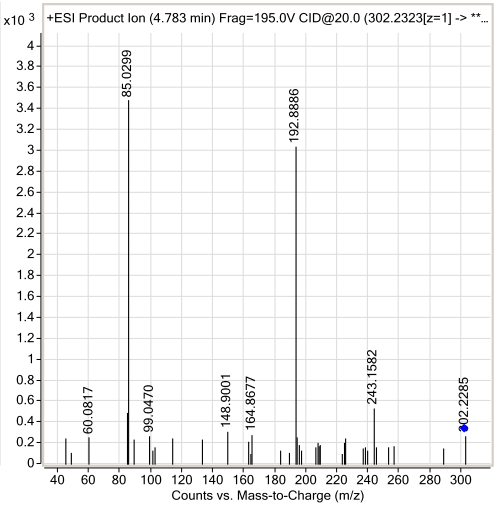


Nonanoylcarnitine (C9:0)

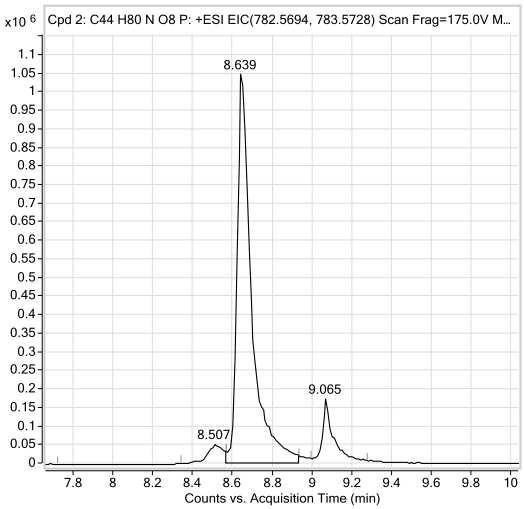


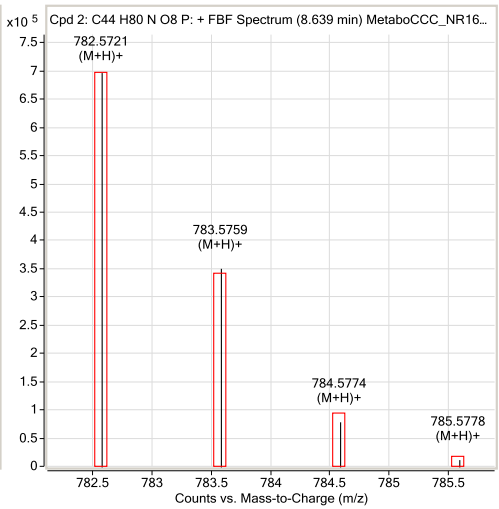


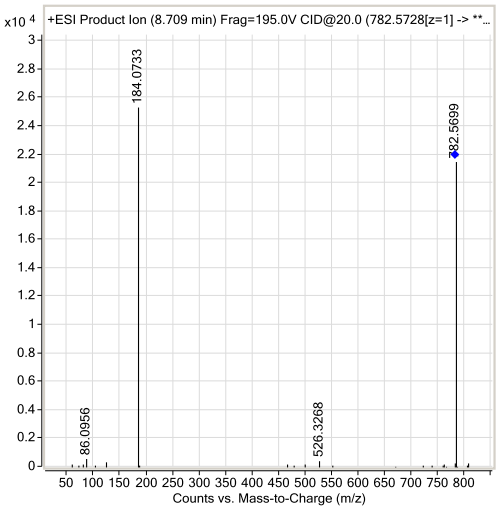


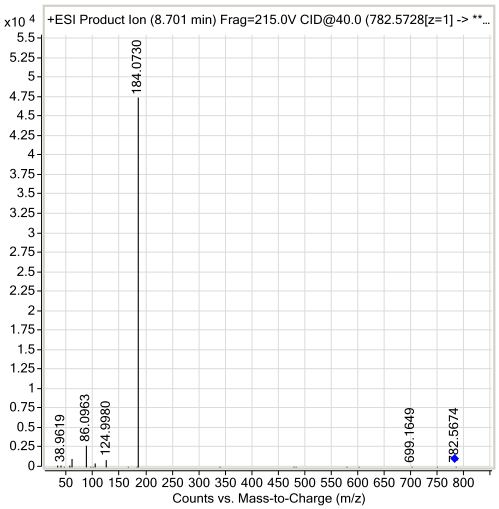


PC (36:4)

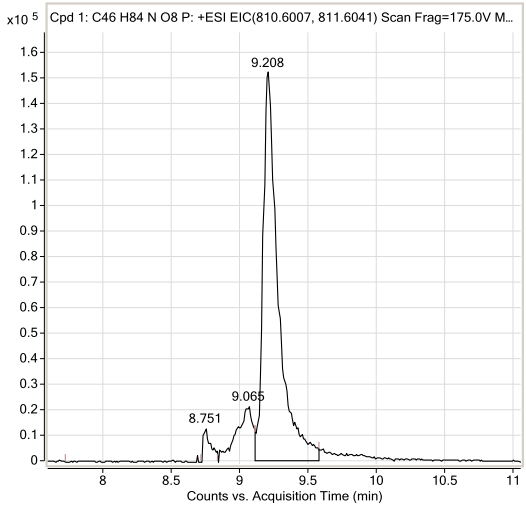


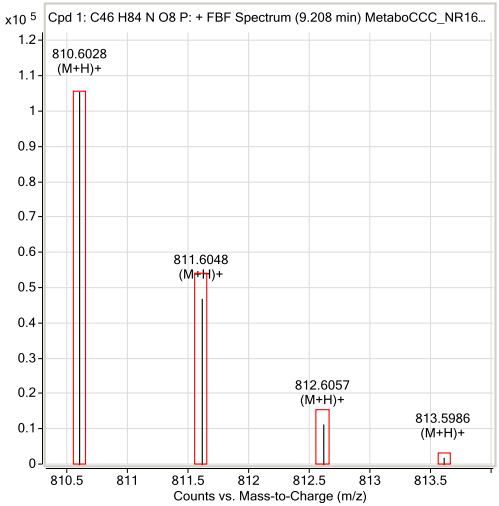


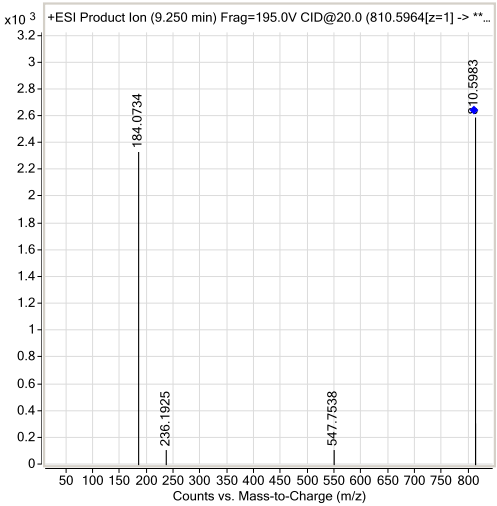


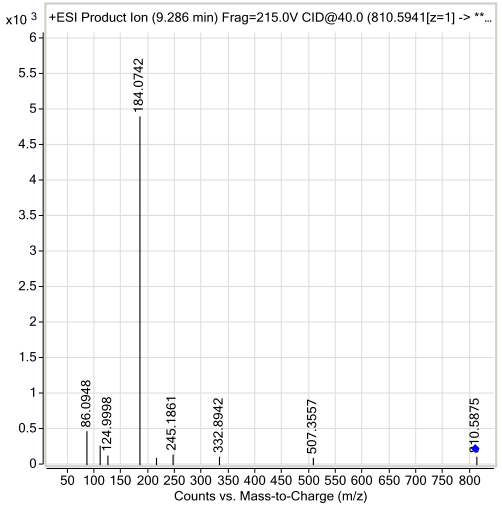


PC (38:4)

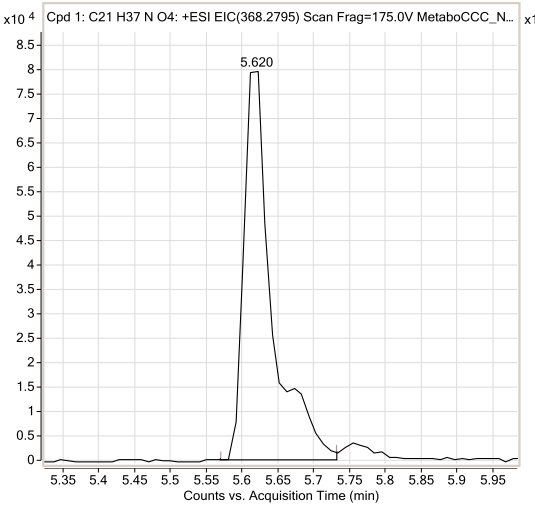


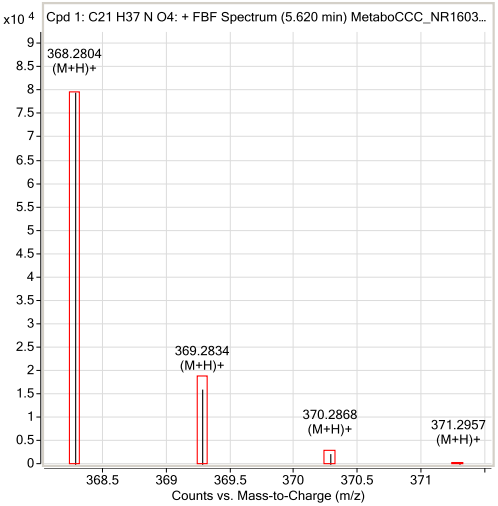


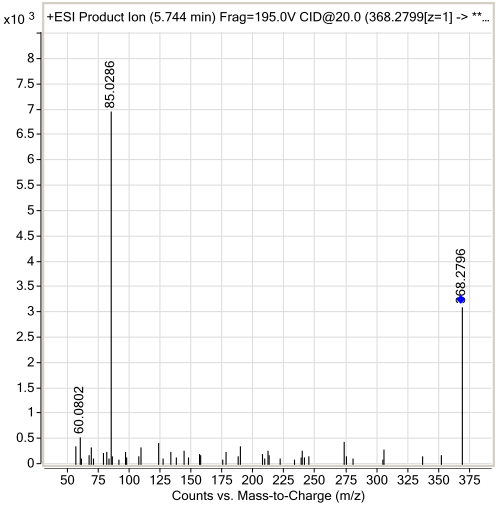


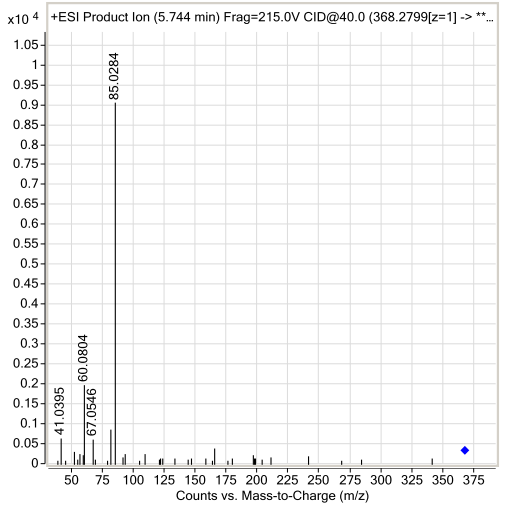


Tetradecadienoylcarnitine (C14:2)

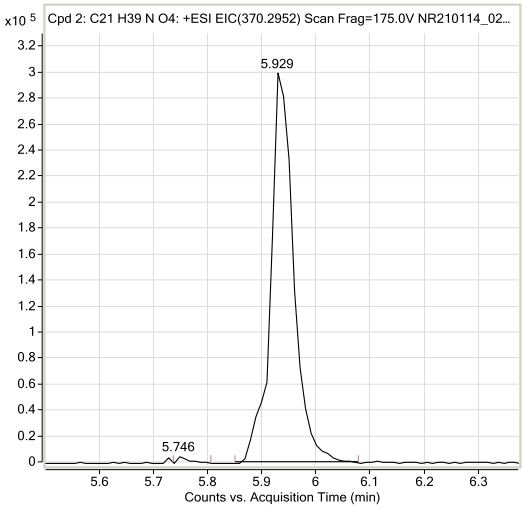


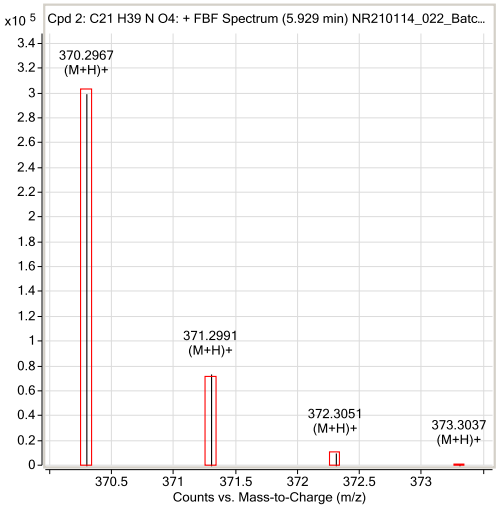


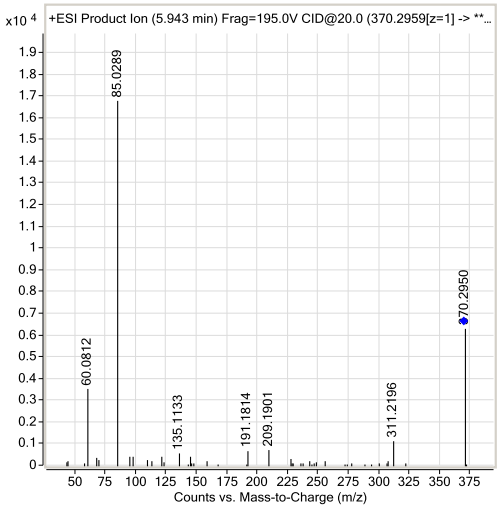


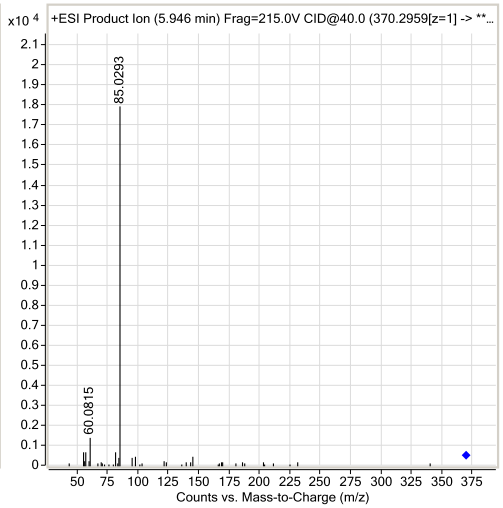


Tetradecenoylcarnitine (C14:1)

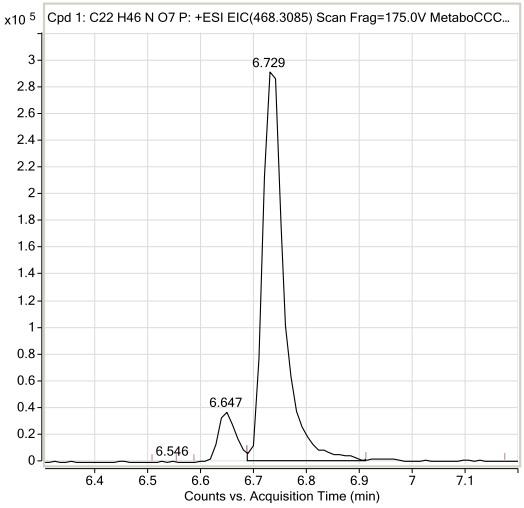


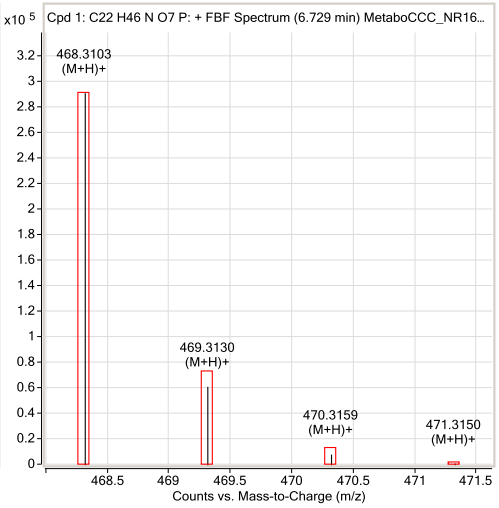


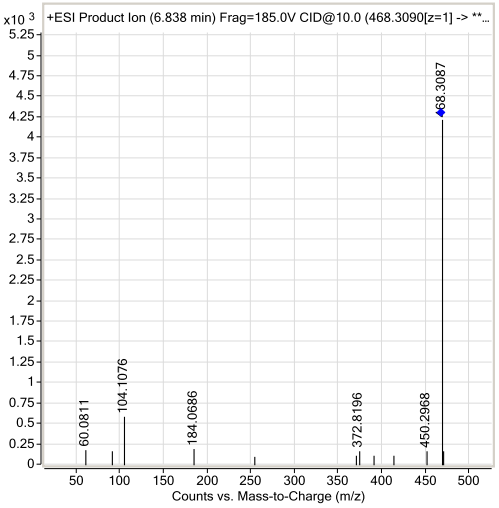


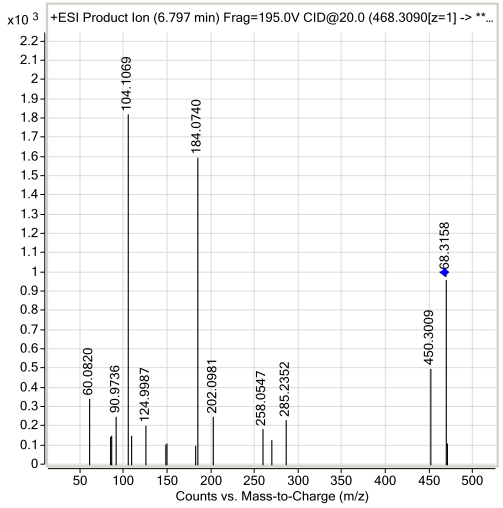


LysoPC (14:0) (isomer 2)

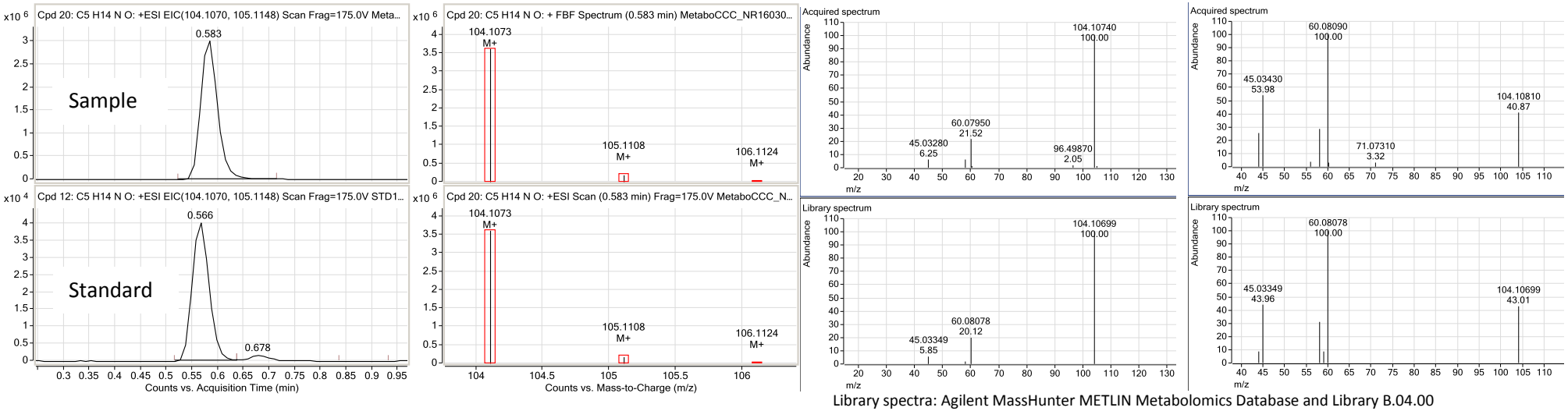






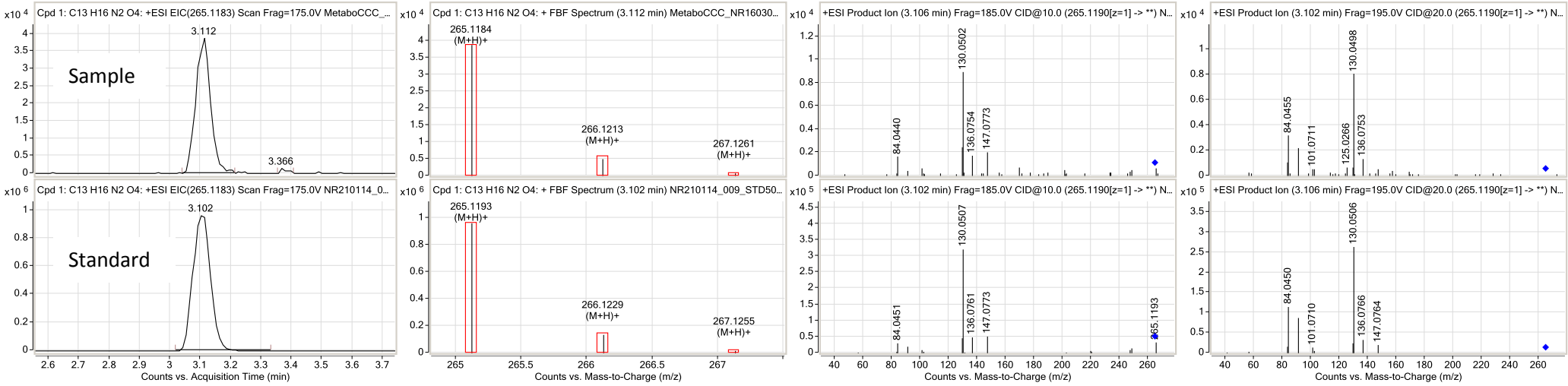


Choline

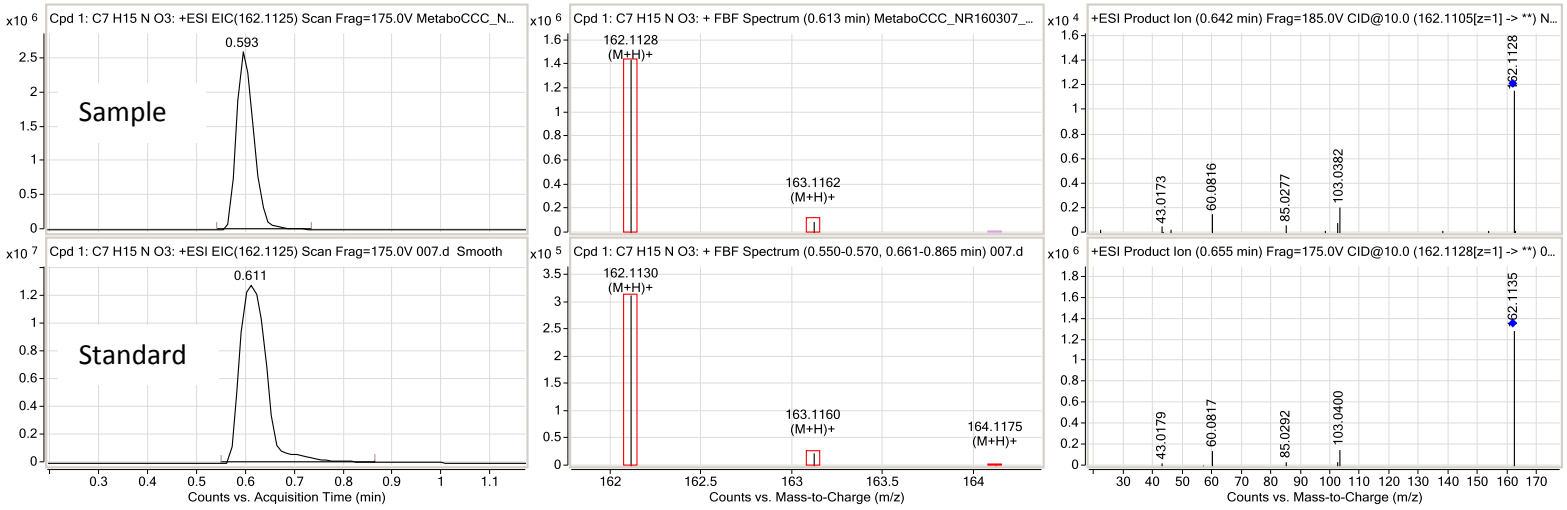


Library spectra: Agilent MassHunter METLIN Metabolomics Database and Library B.04.00

Phenylacetylglutamine



Carnitine



Docosahexaenoic acid