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Structural characterization of isobar selenium containing contaminant in a commercially available selenomethionine standard using electrospray – Ion Mobility Time of Flight Mass Spectrometry

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Selenium (Se) is an essential and trace element. Benefic effects of selenium are reported in cancer prevention for supra-nutritional dietary intake of organic selenium like Se-enriched yeast. To understand its biological significance in toxicology or nutrition, selenium speciation (quantification and structural identification of Se species) is needed. However, the lack of authentic standard or reference materials prevent the use of retention time matching based method with an elemental, robust and specific detector like Inductively Coupled Plasma Mass Spectrometry (ICP MS) to be used. The problem can be overcome by the use of molecular mass spectrometry like electrospray MS. Selenium have 6 isotopes and a characteristic isotope pattern. This pattern makes easier the identification of a selenium containing compound in the mass spectra. Unfortunately electrospray ionization suffers from poor ionization efficiencies and requires a very high degree of purification of the samples (e.g. multi-dimensional liquid chromatography) prior to structural characterization using tandem mass spectrometry.

A major selenium containing compound identified in various selenium-rich supplement or biological sample is selenomethionine, the selenium analogue of the methionine amino-acid. Selenomethionine standard is commercially available and is used as internal standard in quantitation and quality control purposes.

In this work, we evaluated the purity of this standard with Ion Mobility Mass Spectrometry (IM-MS). IM-MS is an emerging tool in molecular mass spectrometry. The general principles of IM-MS is to separate ions into a slightly pressurized cell (mobility cell). The acceleration potentials are pushing the ion into the mobility cell. The velocity of ions will slow down according to their respective cross section.

The commercially available selenomethionine standard was investigated using the Waters© Synapt G2. Synapt G2 is High Resolution Time of Flight mass spectrometer equipped with an electrospray ion source. The high resolution mode (*m/z*: 196 $R_{m/\Delta m}$:10.000, R_{FWHM}: 25.000) detected the presence of isobar compounds at m/z: 196. One was the ^{78}Se selenomethionine, the other was the ^{80}Se of a selenium containing contaminant. The two compounds were separated using the mobility cell. They produced fragment ions having almost similar mass at m/z: 181 but the identified contaminant fragmented more easily. This could explain why this impurity was not detected until now.

The structural characterization of this contaminant using the G2 in MS^E mode is proposed in this work. In addition, in the view of using selenomethionine as internal

standard in analytical chemistry, we estimated the bias induced by this interference for selenomethionine speciation studies.