Characterization of isomers selenium containing compounds and determination of isomer ratio from Se-rich yeast water extract using electrospray ionization and Ion Mobility Mass Spectrometry

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Selenium (Se) is an essential trace element. Its toxicity is dose and chemical form dependent. Se-rich yeast is one of the most popular forms of organic Se supplement. Speciation analyses of organic Se containing compounds received a recent interest since putative protective effects for cancer prevention were suggested for supranutritional level of organic Se by Clark and coworkers [1].

N-2,3-dihydroxypropionyl-selenocystathionine ($[M+H]^+$:$C_{10}H_{19}N_2O_7Se^+$, *m/z*: 359) was identified in Se-rich yeast water extract by three dimensional liquid chromatography using Inductively Coupled Plasma Mass Spectrometry (ICP MS) and ElectroSpray Ionization (ESI) tandem mass spectrometry parallel detection by Dernovics and coworkers [2]. Two perfectly coeluting Se isomers at m/z: 359 were suggested to explain the MS/MS mass spectra.

An additional dimension of separation combining an ion mobility cell and a mass analyzer (IM-MS) was investigated to resolve the coeluting isomers. The SynaptG2 HDMS (Waters ®) is equipped with a Traveling-Wave Ion Mobility Spectrometry (TWIMS) cell and Time of Flight (ToF) mass analyzer. The TWIMS cell is resolving the ions according to their respective cross section by pushing the ions using successive electric waves inside a slightly pressurized cell.

N-2,3-dihydroxypropionyl-selenocystathionine was purified using size exclusion and anion exchange liquid chromatography. Two different ions with Se isotope pattern at *m/z*: 359 were separated and detected by nanoESI IM-MS. The structural identification of each isomer was established using MS/MS mass spectra acquisition and was in accordance with the results of Dernovics and coworkers. Moreover a semi quantitative determination of isomer ratio was performed using nanoESI IM-MS. The non equivalent ratio of isomers could support a metabolic origin of the 2,3-dihydroxypropionyl adduct.

[1] Clark *et al.*, Journal of the American Medical Association (1996) 276, 1957-1963
[2] Dernovics *et al.*, Metallomics (2009) 1, 317–329