

ESI-MSⁿ in selenium speciation: focus on structure assessment

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Since the discovery of the essential role of selenium to mammals 40 years ago, only few selenium species were considered in selenium-speciation research [1, 2]. The reasons for this limited number of target compounds include the lack of commercial authentic standards allowing the development of analytical procedures and insufficient performance of instrumentation making it possible to detect, clean-up and identify any new species discovered in environmental and food matrices.

During the recent 3-4 years, the number of detected low molecular weight (< 1.0 kDa) and water soluble selenium species has increased considerably and exceeds the cumulated number of species of arsenic, mercury and tin dealt with in speciation research. There have been above 50 identified compounds and dozens of species still requiring unambiguous structure assignment. Clearly, the availability and continuous development of electrospray MS instrumentation were of crucial importance to achieve this level – however, dedicated sample preparation and orthogonal chromatographic purification protocols were as important as the progress in the ESI-MS technique itself.

Electrospray MS applied to selenium speciation research has considerably evolved from the triple quadrupole devices, through medium resolution time-of-flight instruments to the high resolution Fourier-transform MS using ion cyclotron resonance or orbital electrostatic trap (Orbitrap). These instruments were usually applied as chromatographic detectors, because the purity of selenium species was rarely high enough for infusion-type analyses. It is evident that the requirements regarding the purity of samples to introduce into an ESI-MS instrument strongly determined the preceding purification steps introducing the danger of modification of the selenium species.

The lecture presents a tutorial overview of the use of ESI-MS techniques in the identification of selenium species. The importance of data on collision induced dissociation and in-source fragmentation of known and unknown Se-species, accurate mass analyses, mass defect and isotopic pattern of selenium are discussed. Highlighting both successful and failed approaches in species detection and structure assignments will help to show selenium-related specific problems and solutions which may be faced when dealing with real world samples and with other elements.

[1] Lobinski, R.; Edmonds, J.S.; Suzuki, K.T.; Uden, P.C. *Pure Appl. Chem.*, 2000, 72, 447-461.

[2] Połatajko, A.; Jakubowski, N.; Szpunar, J. *J. Anal. At. Spectrom.*, 2006, 21, 639-654.