Analysis of spatially resolved isotopic images assessed by LA-ICP-MS by using isotope pattern deconvolution and data reduction by means of ArcGIS

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Chemical imaging using laser ablation in combination with inductively coupled plasma mass spectrometry (LA-ICP-MS) has evolved into a powerful tool for the investigation of the spatial distribution of elements and isotopes in biological tissues. Double coupling of specific mass spectrometers allows for the simultaneous assessment of elemental and isotopic information. Certain challenges concerning the spatial resolution, limits of detection and the accurate quantification are still considered as critical. Data evaluation of isotopic patterns composed of either a mixture of different natural isotopic sources or a blend of natural and enriched (i.e. isotope spikes) isotopic sources may pose a nontrivial problem to unravel. This is especially the case when the quantities of the individual contributing sources are unknown.

Isotope pattern deconvolution (IPD) is a mathematical tool, which allows for deconvolving the isotope pattern in a mixed or spiked sample without knowing the quantities of different isotope sources as well as the degree of impurities and species-interconversion. So far, IPD has mainly found application in tracer studies in various fields, ranging from biological applications to studies in forensics and environmental sciences. The objective of this paper is to evaluate and summarize the analytical aspects for isotope pattern deconvolution and reports on the crucial factors to be considered when performing isotope pattern deconvolution.

In addition ArcGIS® is introduced as tool for a spatially based data reduction and for multilayer matching and analysis of data obtained by different techniques. The presented work is based on experiments on the natural isotopic variation and isotopic spike distribution of strontium and magnesium isotopes using (laser ablation) multicollector inductively coupled plasma mass spectrometry ((LA)-MC ICP-MS).