

L4. Investigation of main contamination sources of heavy metal ions in fish, sediments and waters from catalonia rivers using different multiway data analysis methods

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Comparison of different multiway data analysis methods including Principal Component Analysis and Multivariate Curve Resolution Matrix Augmentation bilinear model based methods, and PARAFAC and TUCKER3 trilinear model based methods is performed in the analysis of a three-way data set formed by the analysis of 11 metal ions in 17 river samples of fish, sediment and water at the same site locations of Catalonia (NE, Spain). Adaptation of Multivariate Curve Resolution for the fulfillment of PARAFAC and TUCKER3 trilinear models is shown the flexibility of this method to handle data of different structures and fulfilling different type of constraints. Although the way how the results are obtained using these different chemometric methods is different, it is shown that the same main interpretation and conclusions may be derived independently of the chemometric method used for the analysis although a more simplified interpretation is obtained in some cases using multilinear models specially if reduction of the number of components in one of the modes is possible