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Development of a multi-element method using an ICP-QQQ-MS to characterize the chemical status of surface water bodies

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An instantaneous assessment of the chemical status of surface water bodies provides the ability to better predict the water quality, react in time, and be able to backtrack sources. Also, it is widely accepted that knowledge of the natural chemistry of surface waters is fundamental for identifying anthropogenic pollution (Menzie et al., 2009). The chemical composition of water bodies is controlled by various factors (i.e. atmospheric, geological, biological, etc.). However, the main impact beside anthropogenic pollution is the geological background (e.g. Filella et al., 2014).

To monitor and understand the chemical status it is necessary to measure, with the best possible reliability, a wide spectrum of inorganic analytes. Inductively coupled plasma mass spectrometry (ICP-MS) is widely-accepted as versatile instrument in trace element determination due to its low detection limits, fast multi-element ability and wide dynamic range. The appearance of various polyatomic interferences, low analyte abundance and low sensitivity due to high ionization energy are major challenges in accomplishing precise, routine suitable, multi-element analysis to quantify all target elements which often requires complex pre-measurement treatments. The triple quadrupole ICP-MS (ICP-QQQ-MS; resp. ICP-MS/MS) is a promising tool to overcome some of these limitations. Therefore, our aim was to create a multi-element method with about 65 major and trace elements for surface water. In contrast to existing ICP-MS methods, a single-run-measurement of all analytes is envisaged, including also challenging elements like B, C, P, S, Hg, and REE without a pre-concentration or matrix removal step. The development exhibits very low Limits of Quantification for Rhine and Moselle river water (e.g. REE < 10 ppt).

Our method is based on certified reference material, single element standards (traceable to NIST) and samples from the Rhine and Moselle rivers (Germany). Single element optimized methods were adjusted to the multi-element monitoring purpose. We optimized different collision/reaction cell modes (O₂, He, H₂) to eliminate isobaric, polyatomic and/or double charged interferences

and the multi-element calibration cross check for memory effects and uncertainties. Hence, we developed a powerful method for surface water quality monitoring and hydro-chemical fingerprinting adaptable to the specific user requirements.

Filella, M., Pomian-Szednicki, I., Nirel, P.M., 2014. Development of a powerful approach for classification of surface waters by geochemical signature. *Water Res* 50, 221-228.

Menzie, C.A., Ziccardi, L.M., Lowney, Y.W., Fairbrother, A., Shock, S.S., Tsuji, J.S., Hamai, D., Proctor, D., Henry, E., Su, S.H., 2009. Importance of considering the framework principles in risk assessment for metals. *Environ. Sci. Technol.* 43, 22, 8478-8482.