

components. However, the persistence of the fully formulated nanocarrier (with all ingredients, including the AI) may not be known. Does this raise issues?

- Considering the variability in excipients and formulations, what is the correct reference material? AI alone is currently used for toxicity studies, not the formulations.
- Nano AI may be stabilised with e.g. surfactants: Does the fact that they are, or are associated with, a nanoparticle, make them different from a toxicological perspective?
- For a nanocarrier composed of ingredients that are already considered safe: are there ways to design bridging studies and potentially use existing toxicity data? How should the dose be compared? What data is needed for bridging? How does one determine dose? What tests/end points are needed?

Considering the above and many more questions that were raised at the Boston workshop, a follow up workshop was organised to coincide with the IUPAC Centenary Celebrations and General Assembly in July 2019. Ultimately, as an outcome of this project, we hope to develop well-considered views on some of the above challenges.

Reference

1. Walker, G; R.S. Kookana; N.E. Smith; M. Kah et al. *Journal of Agricultural and Food Chemistry*, 66(26): 6480-6486, 2017. DOI: 10.1021/acs.jafc.7b02373.

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Trace elements analysis of environmental samples with X-rays

An increasing number of scientists from around the world are using X-ray based methods for the analysis of trace elements in environmental samples. X-ray analyses can be successfully performed both at synchrotron facilities and in modern laboratories with dedicated instrumentation.

Synchrotron X-ray methods can provide information on both the concentration and the speciation of trace constituents and is being utilized to unravel many chemical processes and transformations. Synchrotron generated X-rays can also help scientists to elucidate reactions occurring over different lengths and time scales, usually not possible with conventional



Roberto Terzano (IUPAC Division VI secretary and Project Task Group) and other Task Group Members (from left: David Paterson, Gerald Falkenberg and Ryan Tappero) presenting awards to the winners of the "IUPAC Division VI Best Poster Prize."

laboratory instruments. In recent years, new beamlines dedicated to environmental analyses have been commissioned at synchrotron facilities around the world and new methodologies have been developed for fast and sensitive trace elements analyses in environmental matrices. However, the number of requests for beam-time at synchrotrons has also increased exponentially making it increasingly difficult to obtain access to these large facilities.

Nevertheless, recent technological improvements in X-ray optics and detectors (many of which were pioneered at synchrotron facilities) have been incorporated into modern analytical instruments. These

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incremental advancements allow in-house analyses using techniques previously available exclusively at synchrotron storage rings. The use of these sophisticated X-ray instruments allows scientists to generate robust data without a synchrotron light source, also very useful to justify future synchrotron experiments.

The objective of IUPAC Project 2016-019-2-600 is to inform the environmental scientific community about recent developments in trace elements analysis of environmental samples with X-rays, available at synchrotron beamlines and with in-house laboratory instrumentation. Specifically, we are sharing the latest developments in X-ray technology (sources, optics, detectors) and sample preparation for the analysis of trace elements in environmental samples. Our goal is to promote the use of X-ray based methods among environmental scientists by enhancing the network of users, method developers, beamline scientists and instrument manufacturers.

To this purpose, a Special Symposium entitled "Trace elements analysis of environmental samples with X-rays" was organized during the 14th International Conference on Biogeochemistry of Trace Elements—ICOBTE 2017, which took place in Zurich, Switzerland. Thirty abstracts were received from 16 countries, with keynote lectures given by Antonio Lanzarotti from the University of Chicago (USA) and Laszlo Vincze from the University of Ghent (Belgium). The symposium,

co-sponsored by Bruker GmbH (Germany), was attended by about 100 participants. Three poster prizes were awarded by IUPAC Division VI to young participants: Barbara Lopata (Poland), Kathryn Spiers (Germany) and Antonio Caporale (Italy).

The symposia focused on how advances in instrumentation could be applied to understand the fate of trace elements in a variety of environmental problems. The morning session was devoted to synchrotron applications, while the afternoon session mainly focused on laboratory scale methodologies. During these sessions, recent improvements in X-ray analyses were presented. In particular, new developments in the fields of X-ray diffraction, X-ray fluorescence, and X-ray absorption were discussed. The latest developments using 2D and 3D applications were introduced, with a special emphasis on spatially resolved microscopic and sub-microscopic analyses of minor and trace elements in environmental matrices.

After the symposium, the task group prepared an IUPAC Technical Report entitled "Recent advances in analysis of trace elements in environmental samples by X-ray based techniques". The report has been published in *Pure and Applied Chemistry* (June 2019, 91(6), pp. 1029-1063; doi: 10.1515/pac-2018-0605.)

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