

## NON-TARGET SCREENING OF WATER WITH HIGH RESOLUTION MASS SPECTROMETRY: PERSPECTIVES FROM A COLLABORATIVE TRIAL

**SCHYMANSKI E.L.<sup>1</sup>, SINGER H.P.<sup>1</sup>, SLOBODNIK J.<sup>2</sup>, IPOLYI I. M.<sup>2</sup>, OSWALD P.<sup>2</sup>,  
KRAUSS M.<sup>3</sup>, SCHULZE T.<sup>3</sup>, HAGLUND P.<sup>4</sup>, LETZEL T.<sup>5</sup>, GROSSE S.<sup>5</sup>, THOMAIDIS N.S.<sup>6</sup>,  
ZWIENER C.<sup>7</sup> and HOLLENDER J.<sup>1</sup>**

<sup>1</sup>Eawag: Swiss Federal Institute for Aquatic Science and Technology, Überlandstrasse 133, 8600 Dübendorf, Switzerland. <sup>2</sup>Environmental Institute, s.r.o., Okružná 784/42, 972 41 Koš, Slovak Republic. <sup>3</sup>Helmholtz Centre for Environmental Research - UFZ, Permoserstraße 15, 04318 Leipzig, Germany. <sup>4</sup>Umeå University, Linnaeus väg 6, 90187 Umeå, Sweden.

<sup>5</sup>Technische Universität München, Chair of Urban Water Systems Engineering, Am Coulombwall 8, 85748 Garching, Germany. <sup>6</sup>University of Athens, Department of Chemistry, Panepistimiopolis Zografou, 157 71 Athens, Greece. <sup>7</sup>Eberhard Karls University of Tübingen, Environmental Analytical Chemistry, Hoelderlinstr. 12, 72074 Tübingen, Germany.

E-mail: emma.schymanski@eawag.ch

In 2013/2014, a collaborative non-target screening trial was organised by the NORMAN Association of environmental monitoring laboratories, in response to the request from members to harmonize and provide guidance on non-target screening in Europe. A total of 18 institutes from 12 European countries analysed an extract of the same water sample collected from the River Danube with either one or both of liquid and gas chromatography (LC, GC) coupled with mass spectrometric (MS) detection; the latter mostly with low resolution methods. The LC-MS(/MS) results revealed interesting trends on the use of high resolution screening techniques applying target, suspect and non-target workflows to identify substances in environmental samples. A total of 625 target results were reported (347 unique compounds). For suspects and non-targets, 631 tentatively-identified substances were reported, 553 with a defined structure (the remaining as substance class or undefined isomer). In total 649 unique compounds were reported as target, suspect or non-targets, while carbamazepine and atrazine were reported most frequently. For the GC-MS, 64 target results were reported for 55 compounds; a further 295 results were reported as library matches (255 unique compounds in total). Of the 858 unique compounds overall, 46 were reported in both LC and GC, approximately 5.4 %. Specific examples highlight major challenges such as isobaric, co-eluting substances and dependence on target and suspect lists (e.g. terbutylazine, sebutylazine, simazine and transformation products), formula assignment (surfactants), the use of retention information and the confidence of identification. Approaches and methods applicable to unit resolution data also show especially what data analysis features are not yet (sufficiently) established for LC-MS-based techniques. While most substances were identified using high resolution data with target and suspect screening approaches, some participants proposed tentative non-target identifications, some of which could be revised using evidence from results reported by other participants. This comprehensive dataset revealed that non-target analytical techniques are already considerably harmonized between the participants, but the data processing remains time-consuming. Although the dream of a “fully-automated identification workflow” remains elusive in the short-term, important steps in this direction have been taken, exemplified in the growing popularity of suspect screening approaches. Major recommendations arising from this trial to improve non-target screening include better integration and connection of desired features into software packages, the exchange of target and suspect lists and the contribution of more spectra from standard substances into (openly accessible) databases.

**Keywords:** Non-target screening, high resolution mass spectrometry, LC-MS, suspect screening, surface water

## REFERENCES

**Schymanski, E.L.**, Singer, H.P., Slobodnik, J., Ipolyi, I.M., Oswald, P., Krauss, M., Schulze, T., Haglund, P., Letzel, T., Grosse, S., Thomaidis, N.S., Bletsou, A., Zwiener, C., Ibáñez, M., Portolés, T., de Boer, R., Reid, M.J., Onghena, M., Kunkel, U., Schulz, W., Guillon, A., Noyon, N., Leroy, G., Bados, P., Bogialli, S., Stipanichev, D., Rostkowski, P., Hollender, J. (2015) Non-target screening with high resolution mass spectrometry: Critical review using a collaborative trial on water analysis, *Analytical & Bioanalytical Chemistry*, 407 (21), 6237-6255. DOI: [10.1007/s00216-015-8681-7](https://doi.org/10.1007/s00216-015-8681-7)