Study unlocks mass spectrometry's potential for environmental science, agriculture and industry

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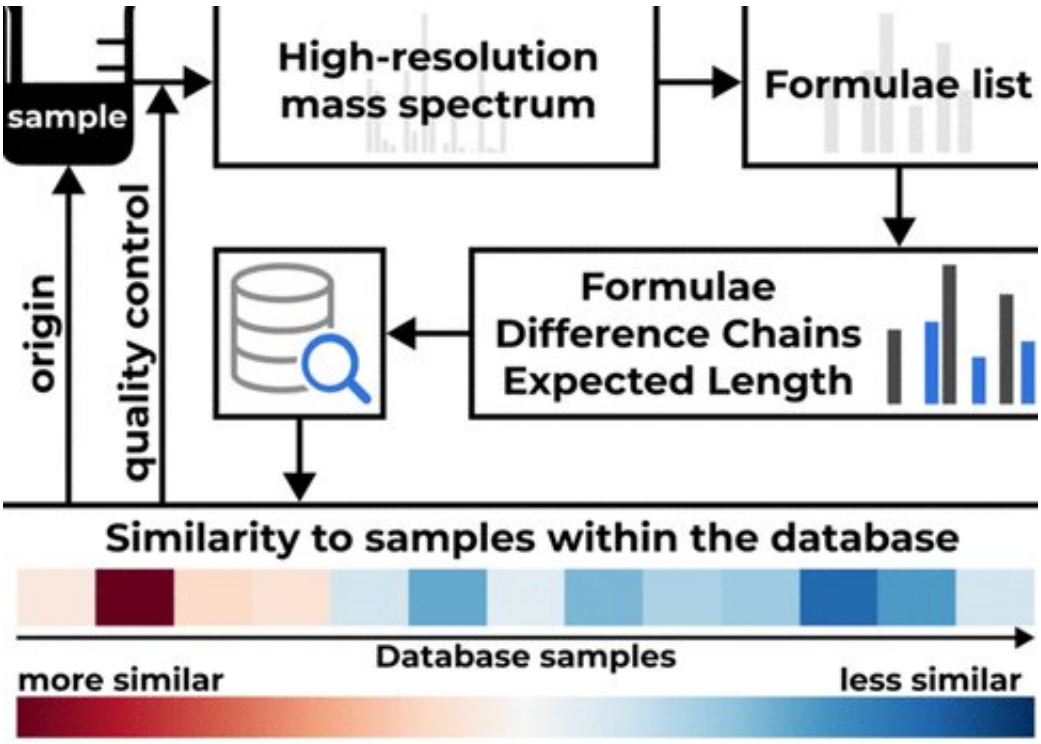

Graphical abstract. Credit: *Environmental Science & Technology* (2023). DOI: 10.1021/acs.est.2c08002

In a study published in *Environmental Science and Technology*, Skoltech researchers have proposed a novel metric and established an open-access database enabling the direct comparison of complex natural organic

matter samples analyzed using different mass spectrometry equipment.

Data on such samples have been accumulated in labs around the world for over two decades, but until now they could not be reliably compared beyond one research center, rendering them almost useless for predicting soil and water properties based on mass spectrometry results. This had virtually invalidated a powerful tool that could serve agriculture, the water processing industry, and climate research.

Natural organic matter, or NOM, is an essential component of any ecosystem: a river, a sea, or soil. It affects water and soil characteristics that are relevant to both industry and science, including agriculture, fish farming, drinking water supply, carbon capture, climate studies, and more. The only technique that can provide an overview of all the molecules in an NOM sample from the environment or an industrial facility—such as a fish farm—is high-resolution mass spectrometry. It involves ionizing the compound mixture and measuring the constituent ions' frequency of rotation in a magnetic field to identify them by the mass-to-charge ratio.

"Theoretically, you should be able to take the results of your mass spec analysis and be able to look up the soil or water organics characteristics you want. You would query a database and find a reasonably similar sample studied in a lab elsewhere in the world. And you could expect your sample to have similar properties to those of the reference sample," said the principal investigator of the study, Senior Research Scientist Alexander Zherebker of Skoltech Bio's Mass Spectrometry Laboratory, which is headed by study co-author Professor Evgeny Nikolaev.

"But there are two problems," the researcher went on. "First, such a database does not exist, or did not. Second, study after study has shown that for reasons having to do with sample complexity and instrument features, two different labs will very likely report strikingly different

compositions for one and the same sample."

To address this, Zherebker and his colleagues are proposing an alternative metric for characterizing NOM samples, which they found to be resistant to measurement errors and the minor distinctions known to exist between different mass spectrometry labs and hardware. The team also established and published a first-of-its-kind open database that will accumulate data on NOM samples characterized using the new metric.

The newly proposed metric abandons the attempt to capture the precise molecular composition of the sample. Instead, the researchers are specifying the NOM profile by looking at the source materials and products of a large number of chemical reactions known to occur in the environment.

Sure, this metric could not be used in some cases, for example to analyze the individual byproducts resulting from water disinfection. "But then again, such projects are often comfortably accomplished within a single laboratory, so the traditional approach will do," Zherebker said. "On the flip side, we have demonstrated that our metric enables two samples to be directly compared almost irrespective of where and by which group the data were collected, unlocking the so far unrealized potential of mass spectrometry in this domain."

As of now, the prototype database created by the authors of the study and freely available online only amounts to 14 samples and certainly requires expansion. That said, it already has multiple samples from various soil types and rivers from across the globe, and even one from an Antarctic lake. These are representative in the sense that they are the products of very different biogeochemical processes. The Antarctic sample, for example, is devoid of the plant-related components.

Besides serving as a reference for predicting the properties of an

arbitrary sample by comparison, the database could also be of use for assessing measurement quality. "If a laboratory runs the analysis on a well-studied reference sample and gets unexpected results, this means something's gone wrong and some corrections are in order for further measurements of unfamiliar samples to be deemed sound," Zherebker said.

More information: Anastasia Sarycheva et al, Formulae Differences Commence a Database for Interlaboratory Studies of Natural Organic Matter, *Environmental Science & Technology* (2023). DOI: 10.1021/acs.est.2c08002

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