High-resolution mass spectrometry: from algorithms to the great outdoors

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High-resolution mass spectrometry has become indispensable as a core technology in environmental analytics and metabolomics, providing broad chemical coverage and the potential to identify new compounds. I highlight contributions in diverse aspects of the field, from computational mass spectrometry to environmental applications. First, *RMassBank* [1], an automated workflow to generate high-quality MS^2 spectral library records including automatic recalibration, to support data contributions to the community-driven mass spectral database *MassBank*. Second, *MSNovelist* [2], a novel algorithm to propose chemical structures from MS^2 spectra based on chemical fingerprint prediction with *CSI:FingerID* and *de novo* structure generation with a recurrent neural network, making it possible to discover completely new structures not yet recorded in any chemical database. Third is *MS²field* [3], a transportable lab-in-the-field equipped with an Orbitrap mass spectrometer, a fully automated water sampling system, and live quantification, to monitor micropollutant contamination in near real-time and to acquire highly time-resolved time profiles with broad chemical coverage.

[1] M.A. Stravs, E.L. Schymanski, H.P.Singer, J. Hollender, *J Mass Spec*, **2013**, *48*, 89-99
[2] M.A. Stravs, K. Dührkop, S. Böcker, N. Zamboni, *Nat Meth*, **2022**, *19*, 865-870
[3] M.A. Stravs, C. Stamm, C. Ort, H. Singer, *Environ Sci Technol Lett*, **2021**, *8(5)*, 373-380