Short Communication

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Comprehensive LC-MS reference library: Construction strategy and application in metabolic profiling and metabolomics

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Abstract

Unambiguous metabolite identification is an essential but yet unresolved problem in mass spectrometrybased (MS) metabolomics assays. It is particularly critical in studies of rich metabolic matrices such as those present in plant extracts. Generating a comprehensive mass spectra library from highly pure reference compounds isolated from an extensive repertoire of plant species is currently the most reliable strategy for advance in MS based identification of natural products. To address the issue of generating large MS libraries in a high-throughput manner, two computational pipelines were developed: one allows an automated construction of a reference library from LC-MS injections of authentic chemical standards and the other, termed, allows for an efficient and accurate matching of high resolution experimental LC-MS data to the reference library data. We applied the presented methods by injecting a comprehensive collection of several thousands of plant secondary (specialized) metabolites using a UPLC-qTOF MS in the MSE mode in order to generate a large and structurally diverse MS spectra library, termed. In this presentation, I will demonstrate the experimental methods used for the rapid generation of the WEIZMASS library: the main considerations during sample preparation and the choice of instrumentation parameters for the rapid construction of such a large MS reference library. I will highlight the building blocks of the software pipelines used and, present the chemical rationale behind the computational algorithms. Finally, I will demonstrate the application of the WEIZMASS library for identification of secondary metabolites in different plant extracts.

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Biography

Ilana Rogachev is a trained Analytical Chemist, an expert in Metabolomics, specializing in the analysis of natural products using LC-MS and GC-MS instruments. Her knowledge in the analysis of complex plant extracts and in structural identification of natural products formed the basis of the chosen experimental methods and the analytical rationale behind the computational algorithms used to create the WEIZMASS library.

