Computational Mass Spectrometry-based Metabolomics for Phenotyping of Plant and Microbial Specialized Metabolism

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Plants and microorganisms have evolved to produce a myriad of chemicals to overcome environmental challenges. As metabolic pathways for these chemicals are unique to specific taxa, they are named specialized metabolism. As specialized metabolites are not only a valuable source of drug discovery but also a major means of intra- and interspecific interaction, they have been molecules of interest. Large-scale analysis on specialized metabolites has been limited, mainly due to the large chemical diversity of specialized metabolome in nature. However, recent advances in computational mass spectrometry enabled us to decompose complex metabolite mixtures into structural information [1]. In this presentation I will highlight how computational mass spectrometry-based metabolomics could enhance phenotyping of specialized metabolism in plants and microorganisms, showing several cases from our lab. High-throughput chemical diversity mapping of 78 Rhamnaceae plant species will be the first case [2]. Qualitative metabolomics-guided characterization of a UDP-xylosyltransferase with broad substrate specificity from wood-decaying fungi will be the second one [3], and applicability of the method for phenotyping of xenobiotics metabolism by human liver and symbiotic microorganisms will be also discussed [4].

References:
[1] Beniddir et al., *Nat Prod Rep* 38, 1967–1993 (2021)
[2] Kang et al., *Plant J* 98, 1134–1144 (2019)
[3] Jeong et al., *Proc Natl Acad Sci USA* 120, e2301007120 (2023)
[4] Yu et al., *Anal Chem* 94, 1456–1464 (2022)