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Reverse metabolomics - Metabolomics in drug discovery: Connecting metabolomic profiles with phylogenetic, medicinal and flavoring properties

Ludger A Wessjohann
Leibniz Institute of Plant Biochemistry, Germany

How can we find out, which compounds in complex matrices, e.g. a plant extract, carries a certain flavoring or medicinal property? How can we do this without either (1) isolating all compounds, or (2) using bioassay guided fractionation. Method 1 requires extensive dereplication, and method 2 is limited to fast assays. Both are unsuitable to cover additive or synergistic effects.

Commonly metabolomics, especially in the plant sciences, is used to identify metabolite pattern differences on the basis of changed "properties", with properties commonly relating to genetic differences or treated vs. untreated organisms. By reversing this approach, we use metabolite patterns of different organisms to evaluate which properties are correlating with modified metabolite patterns.

In order to do so, requirements are different from comparative metabolomics, where precise repetition of processing, e.g. the extraction scheme of a plant, is of importance. In reverse metabolomics, annotation and quantification is more relevant, and different (new) methods of computational evaluation are required. Therefore, we initially compared and developed LC-MS, 1D- and 2D-NMR profiling methods for the secondary metabolome of several medicinal plant species, to relate this to phylogeny and origin (for adulteration ID). In a second step we compared and developed computational methods to correlate the profiles with, e.g., inflammation reduction, cytotoxic (anti-cancer)or antibiotic properties, and to identify the most likely property-relevant group parameters or even single constituents, which will allow selecting the best plants or origins for a desired property like beer bitterness in hops. Eventually the method was successfully transferred to different applications with commercial partners, such as identifying constituent combinations or even single metabolites responsible for antibiotic properties of fungi, anti-Alzheimer activity of algae, or even for the savery steak taste in grilled beef.

Biography

Ludger A Wessjohann studied Chemistry in Germany, UK and Norway, and a postdoctoral fellow (AvH) with Prof. Paul Wender at Stanford University (USA), working on the total synthesis of Taxol®. After professorships in Munich (D) and Amsterdam (NL), he became director and in 2010 managing director of the Leibniz Institute of Plant Biochemistry, and in parallel holds a chair at the University Halle. He focuses on the analysis, synthesis and application of natural products and derivatives, and has 270 publications and 20 patents. He is co-founder of four companiesand received several honors, e.g. the Microsoft IT Founders Award, honorary membership of the Argentinean Society of Synthetic Organic Chemistry etc.

wessjohann@ipb-halle.de