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Occasional Comment

Plant chemophenetics – A new term for plant chemosystematics/plant chemotaxonomy in the macro-molecular era

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ABSTRACT

Plant chemosystematic or chemotaxonomic studies based purely on the profiles of small molecules have become obsolete as tools to study phylogenetic relationships of higher plants due to the advent of the much more powerful (macro-) molecular techniques and new methods of data analysis established in parallel to these techniques. A new term is herein proposed for the field of studies aimed at the exploitation of characteristic arrays of specialized natural products of plant taxa: plant chemophenetics. Chemophenetic studies as defined here are studies aimed at describing the array of specialized secondary metabolites in a given taxon. Thus, chemophenetic studies contribute to the phenetic description of taxa, similar to anatomical, morphological, and karyological approaches, which have already been recognized as of major importance for establishing "natural" systems, and which continue to be of the utmost importance for the description of organisms classified with the help of modern molecular methods.

During a brief period, facilitated by the wide access to new methods in analytical natural products chemistry, chemosystematics/chemotaxonomy appeared to be a promising tool to help in solving challenges in establishing a natural classification of higher plants (Alston and Turner, 1963; Fairbrothers et al., 1975; Waterman and Gray, 1987). This hope faded as it became more and more apparent that chemosystematic characters in higher plants are, as with all other phenetic characters, affected by ecological stress factors, thus are subject to phenomena of parallel evolution (Wink, 2003; Reimann et al., 2004). However, as chemosystematics/chemotaxonomy lost validity as a 'stand-alone' means to establish phylogenetic relationships for higher plants, the advent of (macro-) molecular DNA-based classification systems (Palmer et al., 1988; Savolainen and Chase, 2003) occurred. This approach has gone from strength to strength, culminating in the now firmly established system developed by the scientists of the angiosperm phylogeny group (APG, 1998, 2003, 2009, 2016).

The original definition of biochemical systematics, chemosystematics, and/or chemotaxonomy encompassed all micro- and macro-molecular chemical characters (Giannasi and Crawford, 1986; Reynolds, 2007). However, the escalation of DNA-sequence based macro-molecular phylogenetics generally restricted the usage of these terms to micro-molecular compounds, while DNA sequence data were now generally named "molecular data"; a term which originally had been used in a much wider sense, including, for example, protein sequence data (Loomis and Smith, 1990). Nowadays, the term chemosystematics sometimes has a negative connotation for scientists not familiar with the field and using the term in project applications or publications is often met with rejection. For applied chemosystematic studies, modern, fashionable terms, such as 'bioprospecting' are at hand (Soejarto et al., 2005). In contrast, purely scientific chemosystematic studies mainly focused on the elucidation and exploitation of the array of plant natural products in a given taxon are currently hard to name, because the term chemosystematic, though scientifically valid, today might imply that the acquired data are intended to be used as a means to establish phylogenetic systems. This would nowadays be naïve and is usually not the aim of the authors of such studies. Nonetheless, a combination of phytochemical and macro-molecular characters can be of pronounced interest, and can, for example, help in the characterization of clades so far only supported by DNA sequence data (Enke et al., 2012). Another application for a combination of micro- and macro-molecular data is the systematic search for new sources of rare natural products (Çiçek et al., 2012).

Therefore, a new term to describe chemosystematic studies not aimed at elucidating phylogenetic relationships, but at describing the array of natural products of a given taxon, and using these for a phenetic characterization of clades found by DNA-sequence based methods seems needed. Because such studies phenetically characterize the chemistry of the studied organisms, the term **chemophenetics** is proposed for this field of science.

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Important note

Vajda et al. (2017) recently used the term 'chemo-phenetic' in a similar context but in a slightly different sense. These authors used Fourier transform infrared spectra, originating from mixtures of aliphatic (alkene/alkane) and cyclic (aromatic, phenolic) compounds contained in samples of cuticles of fossil and modern *Ginkgo* and fossil and modern conifers, to group the analyzed taxa based on their IR spectra. The authors used the term 'chemo-phenetic' for this kind of analysis, because the taxon-specific spectra were depending on the relative amounts of the compounds; these were reflected by different intensities of the respective spectral bands. Apart from this one occurrence, the term does not seem to exist yet in the scientific literature.

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