



Library-Based Discovery of Bioactive Natural Products - from Screening to Medicinal Chemistry

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Abstract

The lecture will introduce the concept, and practical use, of preformatted libraries of extracts as a starting point for discovery of bioactive natural products. The combination of library-based screening and miniaturized tracking of bioactivity with the aid of HPLC-based activity profiling will be explained. Information content and practical use of activity profiles and parallel detection modes in HPLC (PDA-ELSD-MS) for prioritization of active extracts will be explained with examples from our work. The discovery of piperine as a new scaffold for GABA_A receptor modulators, and the subsequent cycles of optimization of the structure by medicinal chemistry will be discussed in more detail. Finally, data from a retrospective analysis of outcomes from several screening campaigns with our extract library will be shown, in particular data relating traditional knowledge and taxonomic diversity to hit rates in screening and discovery of new bioactive molecules.

Keywords: bioactive, natural products, bioactive molecules

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