Mixture analysis by NMR: From an identification tool to quantitative analysis and a profiling technique

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The high degree of chemical diversity of natural products has attracted attention for a long time as a plentiful resource of bioactive chemicals. While multiplicity is a key advantage of natural products, it has also become an obstacle to their exploitation as sustainable resources. This is because this innate variation in the chemical profile of organisms and changes of metabolite levels results in complex experimental conditions. In this way, the diversity of both chemicals and organisms as well as biological variation, the promising side of natural products, is easily converted into a disadvantage, actually the first hurdle to be tackled by natural products researchers. Thus to extract the maximum potential from natural products, it is necessary to use methods that can handle the great diversity both in quantitative and qualitative characters of diverse metabolites is required.

One of the approaches that has gained momentum in the last years, is metabolomics., the comprehensive profiling of all the metabolites in organisms. This approach reflects the shift in trend in life sciences that has shifted to more holistic methods involving the observation of living organisms as they stand. Diverse omics technologies are part of systems biology: genomics, transcriptomics, proteomics and metabolomics [1]. Metabolomics is an omics technology and in the last years there has been an increased application to many fields of biology such as functional genomics, physiology, toxicology, and the generation of a natural products research [2]. Indeed, metabolomics takes a part to provide holistic information of whole metabolome network [2, 3]. Recent advances in analytical chemistry, combined with multivariate data analysis, has brought us closer to the final goal of metabolomics, comprehensive evaluation of all metabolites in living organisms particularly plants.

Among the available analytical platforms, NMR has been considered to be one of the most promising, since it covers all the metabolites in a short time despite its inherent low sensitivity as compared with MS-based technology. In addition to the clear advantages of NMR such as the broad range of detected metabolites, the ease of data handling for further statistic treatment and the robustness of the generated signals has resulted attractive for metabolomists.

In this presentation, the profiling competence of NMR for natural products will be shown. All practical aspects such as sample preparation, the NMR parameters used for profiling and quantitative work and possible NMR protocols for mixture analysis will be discussed with some case studies.

[1] Lubbe A. *et al.*, in: Metabolomics in Practice Successful Strategies to Generate and Analysis Metabolic Data, (Eds.: Lämmerhofer M., Weckwerth W.), Weinheim: Wiley-VCH, **2013**; ch. 9, pp. 209–238.
[2] Verpoorte R. *et al.*, *Phytochem. Rev.* **2008**, *7* (1), 525–537.
[3] Kim H.K. *et al.*, *Trend. Biotechnol.* **2011**, *29*, 267-275.