1st International Symposium on Metabolomics in Mexico
25-26 June, 2015
Guadalajara, Mexico

METABOLOMICS OF MEDICINAL PLANTS AND FOOD PRODUCTS. WHAT CAN BE ACHIEVED AND WHAT SHOULD BE ACHIEVED.

Jan Schripsema
Grupo Metabolômica, Laboratório de Ciências Quimicas, Universidade Estadual do Norte Fluminense,
Av. Alberto Lamego, 2000, Parque California, Campos dos Goytacazes, RJ – 28013-602, Brazil.
E-mail: jan@uenf.br or jan.schripsema@gmail.com
Key words: Metabolomics, medicinal plants, food

Metabolomics has been defined as “the area of research which strives to obtain complete metabolic fingerprints, to detect differences between them and to provide hypothesis to explain those differences”[1].

Since the first paper on plant metabolomics using NMR[2], which we published in 1991, long before the term metabolomics was invented, much progress has been made in the analytical techniques. In NMR the sensitivity increased about 1000-fold and nowadays nanogram quantities can be detected. Despite this progress the number of metabolites identified in typical metabolomics experiments using NMR has not increased accordingly. In 1991 sixteen metabolites were identified in the spectra, a number comparable to what in modern papers is related. With GC-MS and LC-MS much more compounds are detectable, but the identification is more difficult.

One of the medicinal plants investigated in our laboratory is known under the popular name “carqueja”. The name carqueja was given by Portuguese colonizers to many different species of the genus *Baccharis,* which were similar to a medicinal plant from Portugal, which despite its morphological similarity is not at all related. Many commercial samples from carqueja were obtained for a comparison with NMR-based metabolomics. In order to increase the number of compounds to be detected in the fingerprints obtained by NMR spectroscopy a two-phase extraction method was used. The comparison of the fingerprints of the series of commercial samples revealed large differences. E.g. in certain samples high quantities of flavonoids were observed, while in other samples these could not even be detected.

Also in the analysis of the food products chocolate and butter, a two-phase extraction was applied, yielding fingerprints for both the apolar and polar fraction. The extracts were completely complementary and its analysis revealed details about the production processes, quality and additives.

In NMR based metabolomics the spectra are generally processed by binning or bucketing before multivariate data analysis. This leads to a tremendous loss of information and improvements are necessary to come to a better spectral processing. Ideally the spectra should be resolved in the individual component spectra and improved data bases and spectral processing will help in this process. In the analysis of Cashew nut shell liquid it was possible to calculate the individual components by a simulation of the mixture spectrum from the individual component spectra.

1. Schripsema, J, Dagnino, D. (2014). Metabolomics: Experimental Design, Methodology and Data Analysis. *Encyclopedia of Analytical Chemistry*. 1–17.
2. Schripsema, J, Verpoorte, R. (1991). Investigation of extracts of plant cell cultures by proton nuclear magnetic resonance spectroscopy. *Phytochem. Anal*. 2: 155-162.