Highly-accurate untargeted metabolomics mass spectrometry approach to determine the elemental composition of Satureja Montana essential oil

Alessandro Maccelli, Dipartimento di Chimica e Tecnologie del Farmaco, Università degli Studi di Roma La Sapienza, P.le A. Moro 5-00185 Roma, Italy

Metabolomics is a rapidly growing and expanding subdiscipline in systems biology. The metabolome provides much information about the functional status of an organism and the environmental influences. Several approaches have been used to describe chemical diversity between different samples. One of these is the metabolic profiling, where the analysis is focused to the identification of different metabolites in complex biological matrices. The high sensibility and specificity of high resolution mass spectrometry (HR-MS) conducted by a Fourier-transform ion cyclotron resonance (FTICR) mass spectrometer coupled to an electrospray ionization (ESI) source have been applied to obtain the untargeted fingerprint profile of *Satureja Montana* essential oil. The analytical workflow allowed to identify carvacrol as the main component of this complex mixture, together with other terpenoids, such as p-cymene and thymol, responsible of the synergic antimicrobial action. An exhaustive characterization also occurred, identifying minority compounds such as fatty acids, free organic acids and secondary metabolites deriving from the metabolic pathways of the main terpenoids.