Integrated metabolomics approaches for berry fruit used in nutraceutical formulations

Abstract

The species under investigation during these three years of PhD course were: *Fragaria ananassa*, *Fragaria vesca*, *Morus alba*, *Morus nigra* and *Myrtus communis*. All these species are characterized by the production of small fruits, and all of them are plant species that can be used for the formulation of plant food supplements, in fact they are reported into the official list of Italian legislation (DM 9 luglio 2012- G.U. 21-7-2012, serie generale n. 169, and update on March 27, 2014). Some of them are recognized as traditional food products of Italian region, like *Fragaria vesca*, that is typical of Campania region and *Myrtus communis*, that is typical of Sardinia.

Targeted and *untargeted* metabolomics approaches were applied to investigate the effect of environment, genotype, or both on variation of many metabolites in these plant species.

The final goal of a metabolomics analysis is the identification and quantification of all metabolites in a given organism in addition to the assessment of the metabolic relationship among them. The most widely used techniques, known as *metabolite profiling*, consist in the analysis of the maximum number of metabolites in a given sample. Mass spectrometry coupled to separative techniques such as HPLC, GC, or capillary electrophoresis is used for this purpose. The analysis of the large data sets generated by LC-MS requires data processing tools such as those based on multivariate data analysis. These techniques are robust to noise and missing data and enable one to deal with correlated variables; different software such as the commercially available Markerlynx (Micromass Ltd., Manchester, U.K.) or freeware such as metAlign (Plant Reaserch International, Wageningen, The Netherlands) MzMine or XCMS perform the automatic extraction, alignment, and retention time correction of chromatographic peaks within individual mass to charge value using different algorithms.

In the present work liquid chromatography coupled to high resolution mass spectrometry and in conjunction with multivariate data analysis were applied to investigate the metabolic composition of the different berry species; with these approaches we could confirm that metabolomics represent a useful tool to evaluate the contribution of environmental and genetic factors to the differences in metabolite composition or content of berry fruits; Additionally, this technique can be also used for food control.

Moreover with the characterization of polar compounds we could also assert the berry fruits as important food product with a recognized value in the production of food supplements.