



Wine metabolomics: a complete workflow

Panagiotis Arapitsas[#], Daniele Perenzoni, Andrea Angeli and Fulvio Mattivi

Department of Food Quality and Nutrition, Research and Innovation Centre, Fondazione Edmund Mach (FEM),
Via E. Mach 1, 38010, San Michele all'Adige, Italy

[#] Presenting and Corresponding author: Panagiotis Arapitsas, email: panagiotis.arapitsas@fmach.it

ABSTRACT

Metabolomics was very fast recognized as a powerful tool in analytical chemistry and biology for its ability to generate new hypotheses. The opportunity to work under a holistic and unsupervised approach, with simple sample preparation and short wet-lab times, attracted many researchers. On the other hand, building up an unbiased untargeted method is a tricky and delicate issue, which requires multidisciplinary knowledge and experience, while the time needed for data analysis is multiplied in respect to the targeted methods. Probably the biggest actual problem in Metabolomics is the lack of standardization and guidelines; which causes many different invalidated workflows and methods -often inadequate-, prolonged data analysis periods, and many expensive unpublished metabolomics experiments because of the poor and insufficient data quality.

To overcome these problems is essential a systematic control of every step during the workflow, and a good knowledge of the sample nature and the instrumentations capabilities. In this wine metabolomics project we present a complete, 3 years, workflow which include the follow steps:

1. Experimental design
2. LC-MS method optimization/adaptation
3. Sample preparation optimization
4. LC-MS analysis (including daily controls of system stability and data quality)
5. Different QC strategies evaluation
6. Quality control of the final data
7. Marker discovery
8. Dealing with false positive and false negative
9. Markers annotation
10. New compounds identification
11. Markers validation
12. Hypotheses generation

From this experience it was clear that in metabolomics, and in contrast to targeted methods, the wet-lab represents a very small part of the total project time (5-10%), but since this is "heart" and the most delicate component of the work maximum attention is necessary to avoid long data analysis and problematic data quality.

Between the results of this project, were new hypotheses and knowledge about the red wine quality decrease during domestic storage.

REFERENCE

[1] Arapitsas P, Speri G, Angeli A, Perenzoni D, and Mattivi F. 2014. Metabolomics, Online, DOI: 10.1007/s11306-014-0638-x