

**Title** Novel aspects of grape berry ripening and post-harvest withering revealed by untargeted LC-ESI-MS metabolomics analysis

**Author** Ketti Toffali, Anita Zamboni, Andrea Anesi, Matteo Stocchero, Mario Pezzotti, Marisa Levi and Flavia Guzzo

**Citation** Metabolomics, 7, Number 3, 424-436, 2011

**Keywords** Grape metabolomics; O2PLS-DA; Grape berry ripening; Grape berry withering

### **Abstract**

We established a step-by-step, experiment-guided metabolomics procedure, based on LC-ESI-MS analysis, to generate a detailed picture of the changing metabolic profiles during late berry development in the important Italian grapevine cultivar Corvina. We sampled berries from four developmental time points and three post-harvest time points during the withering process, and used chromatograms of methanolic extracts to test the performance of the MetAlign and MZmine data mining programs. MZmine achieved a better resolution and therefore generated a more useful data matrix. Then both the quantitative performance of the analytical platform and the matrix effect were assessed, and the final dataset was investigated by multivariate data analysis. Our analysis confirmed the results of previous studies but also revealed some novel findings, including the prevalence of two specific flavonoids in unripe berries and important differences between the developmental profiles of flavones and flavanones, suggesting that specific individual metabolites could have different functions, and that flavones and flavanones probably play quite distinct biological roles. Moreover, the hypothesis-free multivariate analysis of subsets of the wide data matrix evidenced the relationships between the various classes of metabolites, such as those between anthocyanins and hydroxycinnamic acids and between flavan-3-ols and anthocyanins.

<http://www.springerlink.com/content/1667172j82626245/fulltext.pdf>