



***Mass Spectrometry &
Grapes, Wines, Spirits***

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High resolution mass approaches for wine and oenological products analysis

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In the last years, high resolution mass spectrometry (HRMS) has achieved resounding success thanks to high selectivity and sensitivity of analyses. Differently from classical unit-mass-resolution MS/MS approach, HRMS provides more information on sample composition through the collection of full-scan spectra and the possibility to perform retrospective data analysis. Consequently, even without defining a compound-specific tuning, HRMS data can be used for identification of suspect compounds or for structural elucidation of unknowns thanks to the definition of accurate mass of both precursor and product ions and of their isotope patterns. In addition, non-targeted and suspect screening approaches can be used to provide the fingerprint of biological systems in order to more easily identify potential adulteration.

Glycosides are important and widespread secondary metabolites of plant kingdom, whose great structural variety is attributed to the broad selection of aglycones - mainly belonging to terpenoid, steroid, flavonoid, quinonoid, lignan, simple phenols and isothiocyanate - and to the different stereochemical configurations of their sugar components. They can be employed in natural medicine or cosmetic and are widely appreciated as bioactive compounds of food commodities. Indeed, glycosides can be hydrolysed to the corresponding aglycones during food transformation and have the same antioxidant properties of the corresponding free and esterified forms. However the knowledge related both to their chemical structure and their occurrence in foods and beverages is as for now incomplete, showing that a deeper analysis on glycosides is mandatory.

The aim of this work was to deepen the comprehension of the three different HRMS approaches (non-targeted, suspect and targeted screening), examining both their potentiality and limits in the analysis of compounds of interest in different matrices. This work studied the Neutral Loss experiment as instrument for the non-targeted screening analysis of glycosides, and investigated the selectivity and sensitivity of HRMS approach in the targeted analysis of free and glycosylated low-molecular weight phenolic compounds and in the suspect screening analysis of the latter. In particular, this work examined the distribution of selected compounds in skin, pulp and seeds of hybrid and *Vitis vinifera* grapes and their transfer from grapes to wine during winemaking; it studied the occurrence of glycosylated low-molecular weight phenolic compounds in tannins of different botanical origin, in order to evaluate a

possible phenolic enrichment of wine after tannin use; it investigated the free phenolic composition of wood barrels, in order to evaluate phenolic enrichment during ageing, and the effect of different barrel sanitation treatments on the phenolic transfer from wood to wines stored inside them; and finally, it studied the free and glycosylated low-molecular weight phenolic profile of Primitivo di Manduria and Negroamaro wines of different vintages, in order to evaluate the effect of wine ageing.

In conclusion, combining non-targeted, suspect and targeted approaches with the efficiency and time saver of on-line SPE clean-up in reducing matrix interference allowed to achieve efficient tools for the study and broad description of different oenological products. Even changing chemical characteristics of compounds under investigation, the settled approaches can be tune and optimized in order to correctly identify and, when possible, quantify new molecules.