



Hes·so

Macrowine 2016

June 27 - 30, 2016 - CHANGINS (NYON), Switzerland

Conference programme

CHARACTERIZATION OF FREE AND GLYCOSIDICALLY BOUND SIMPLE PHENOLS IN HYBRID GRAPE VARIETIES USING LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS (Q-ORBITRAP)

Vitis vinifera is one of the most diffused grapevines over the world and it is the raw material for high quality wines production. The availability of more resistant interspecific hybrid vine varieties, developed from crosses between Vitis vinifera and other Vitis species, has generating much interest, also due to the low environmental effect of production. However, hybrid grape wine composition and varietal differences between interspecific hybrids are not well defined. Different studies revealed that wine consumption has health effects due to its high content of antioxidants, as phenolic compounds. In particular, simple phenols are appreciated not only for their physiological health benefits, including antioxidant, anti-inflammatory and cardioprotective effects, but also because they affect wines organoleptic profile and have a significant role in defining their nutritional characteristics. Glycosidically bound simple phenols are considered a natural stock of these compounds, because they can be hydrolyzed during the winemaking production releasing the corresponding free forms and constituting a potential contribution to final sensory profile. Adapting the method of Barnaba and colleagues, target and untargeted approaches were developed. On-line purification was performed with a HyperSep™ Retain PEP spe cartridge, the chromatographic separation was performed with an Acquity UPLC BEH C18 analytical column, managing a water-acetonitrile gradient from 5% to 100% of organic solvent. Mass spectra were acquired in full MS-data dependent MS/MS analysis at mass resolving power of 140.000, in negative ion mode and with a heated electrospray. The mass spectrometer operated using following parameters: spray voltage, 2.80 kV; sheath gas flow rate, 30 arbitrary units; capillary temperature, 310 °C. The aim of the study was to increase the understanding of hybrid grape varieties phenolic composition, combining on-line SPE clean-up for reducing matrix interference with an ultra-high liquid chromatography coupled to high resolution mass spectrometry. In particular, the phenolic composition of 4 hybrid (red: Cabernet Cantor and Prior; white: Muscaris and Solaris) and 2 European (red: Merlot; white: Chardonnay) grape varieties was investigated, focusing on free and glycosidically bound simple phenols and considering compounds distribution in pulp, skin and seeds. Through target approach 58 free simple phenols and 7 glucosidic precursors were quantified with quantification limits ranging from 0.001 to 1 mg Kg⁻¹, calibration R² of 0.99 for over 94% of compounds, and precision (R.S.D.%) always better than 12%. The untargeted approach was aimed to tentatively identify glycosylated precursors of selected free simple phenols in the forms of -hexoside, -pentoside, -hexoside-hexoside, -hexoside-pentoside, -pentoside-hexoside and -pentosidepentoside derivatives on the basis of accurate mass, isotopic pattern and MS/MS fragmentation.

Author	Email	Institution
*Chiara Barnaba	chiara.barnaba@fmach.it	Fondazione Edmund Mach
Giorgio Nicolini	giorgio.nicolini@fmach.it	Fondazione Edmund Mach
Mattia Giacomelli	mattia.giacomelli@fmach.it	Fondazione Edmund Mach
Roberto Larcher	roberto.larcher@fmach.it	Fondazione Edmund Mach
Tiziana Nardin	tiziana.nardin@fmach.it	Fondazione Edmund Mach