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Short communication

Spectroscopy analysis of phenolic and sugar patterns in a food grade chestnut tannin

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ABSTRACT

Tannin of chestnut (*Castanea sativa Mill.*) wood, commonly used in winemaking was characterised with a spectroscopy qualitative approach that revealed its phenolic composition: several vibrational diagnostic bands assigned using the Attenuated Total Reflectance-Infrared Spectroscopy, and fragmentation patterns obtained using the Laser-Desorption–Ionization Time-of-Flight technique evidenced polygalloylglucose, e.g. castalagin/vescalagin-like structures as the most representative molecules, together with sugar moieties. The implication of these findings on winemaking application and the potential influence of the chemical structure on the sensory properties of wine are discussed.

1. Introduction

The wood of *Castanea sativa Mill.* European (i.e. chestnut) is approximately composed of 40% cellulose, 20% hemicellulose, 25% lignin, and 10% ellagitannins, which are hexahydroxydiphenic acid molecules esterified with glucose (Mosedale, Charrier, & Janin, 1996; Nonier et al., 2005). Although the tannin fraction exhibits high variability between botanical species (Nonier et al., 2005; Prida & Puech, 2006), the chestnut extractable fraction is mainly represented by monomeric and oligomeric phenolic compounds, mostly vescalagin and castalagin, grandinin and roburin E (Salminen, Ossipov, Loponen, Haukioja, & Pihlaja, 1999), together with galloyl glucosyilated phenolic compounds (Lampire et al., 1998).

The chestnut tannin is currently used in industrial application (Navarrete, Pizzi, Pasch, Rode, & Delmotte, 2010; Ping, Pizzi, Guo, & Brosse, 2012), and it is commonly added in winemaking as fining coadiuvant (OIV 2009). The chemistry of hydrolysable tannins in wine is mainly affected by their solubility in water system, e.g. wine, their reaction with oxygen (Versari, du Toit, & Parpinello, 2013), and interaction with proteins (Mané et al., 2007). The sensory impact of chestnut tannins in wine is controversial as some chemical compounds derived from ellagitannins influences the composition of wine itself; in particular, there is a need for a detailed characterisation of the molecular structures responsible for wine bitterness and astringency (Puech, Prida, & Isz, 2007).

In this preliminary study a new commercial food grade ellagitannin extracted from chestnut wood was analysed for its composition in monomers and polymeric fractions (phenolics, polysaccharides, lignin residues) with the combined use of Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) and Matrix-Assisted Laser Desorption/Ionization Time-of-Flight (MALDI-TOF) spectroscopies, thus allowing to recognize molecular patterns which influences sensory perception. Preliminary results aim to propose an effective analytical approach for the study of the impact of natural extracts in wine, to provides complementary information to analytical techniques routinely used, including HPLC (Mattivi, Vrhovsek, Masuero, & Trainotti, 2009), in view of future and more extended characterisation of oenological tannins commercially available.

2. Materials and methods

A food grade commercial tannin powder from wood of *C. sativa Mill.* (i.e. chestnut) was divided into three sub-samples and each replicate analysed with ATR-FTIR and MALDI-TOF spectroscopies according to our procedures previously described in details (Ricci, Parpinello, Olejar, Kilmartin, & Versari, 2015; Lagel, Pizzi,

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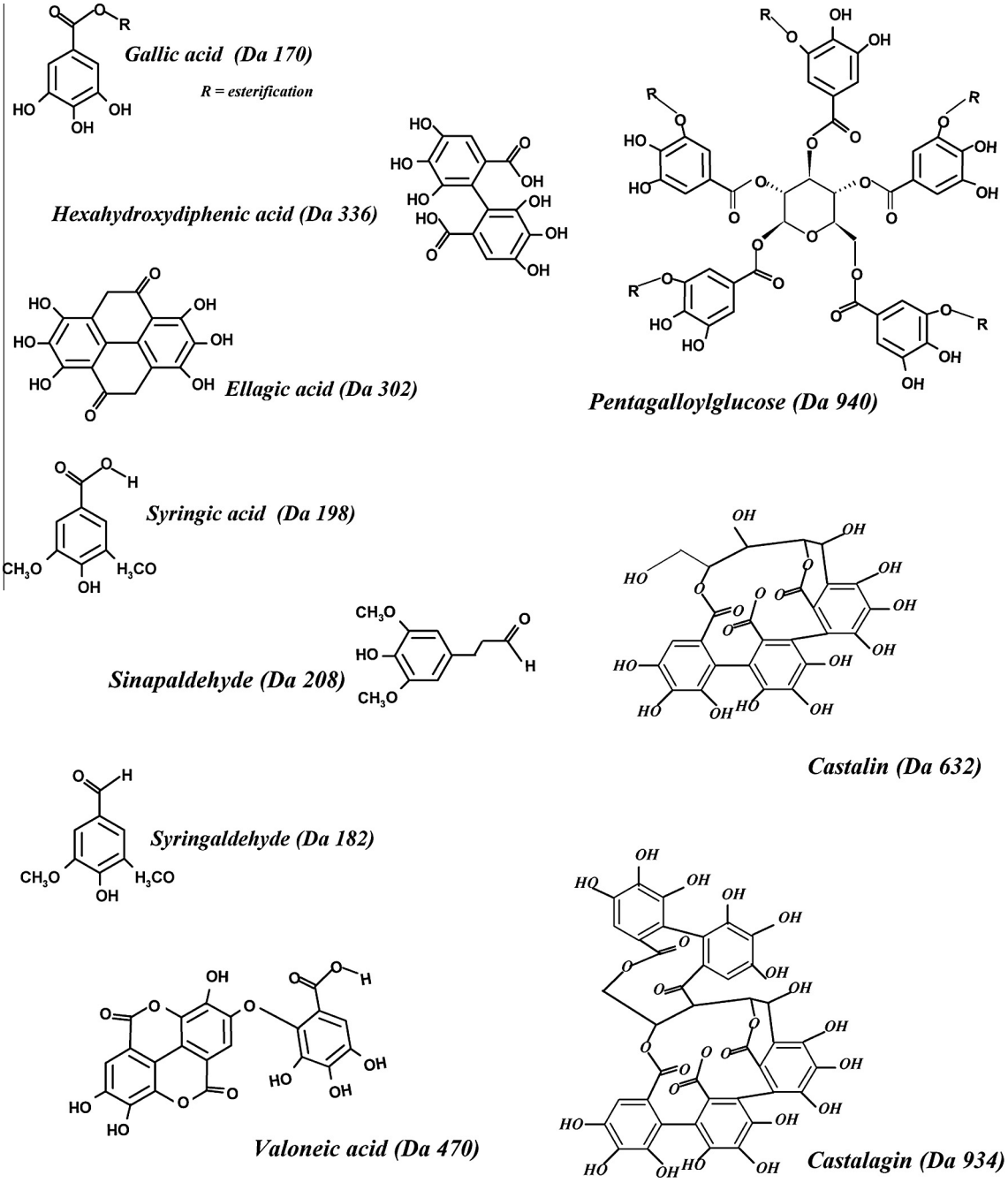

Fig. 1. Molecular structure of selected compounds identified in MALDI-TOF spectroscopy.

& Giovando, 2014). Purified water (18-Ohm), acetone (HPLC grade, 99.98%), 2,5-dihydroxybenzoic acid (99%) and phosphorus red reference standard (99.999%) for MALDI-TOF analyses were purchased by Acros (Acros Organics, NJ, US).

3. Results and discussion

3.1. ATR-FTIR spectroscopy

The ATR-FTIR spectrum of chestnut tannin, obtained using the average of 128 scans per samples, revealed the presence of several functional groups that are typical of hydrolysable tannins, mostly located in the middle-infrared spectral range (Table 1). Five bands were considered diagnostic of chestnut tannin, including 1600,

Table 1
ATR-FTIR vibrational peaks attribution in the middle-infrared range (4000–760 cm^{-1}) for the characterisation of commercial oenological tannin from *Castanea sativa Mill.* wood.

Peak (cm^{-1})	Attribution
3700–2900	OH stretching; aromatic CH stretching
2972; 2934	Aliphatic CH_3; CH_2 stretching
1736	Phenyl ester linkage vibration
1718	Carbonyl C=O stretching
1600	Aromatic C=C *sym* stretching
1509	Ring in-plane bending
1447	Aromatic C=C *antisym* stretching
1309	Saturated C–C chains stretching
1197	Aliphatic C–O *sym* stretching
1032	Aliphatic C–O *antisym* stretching
780	Phenolic OH wagging; aromatic out-of-plane bending
762	Glycosides ring breathing