



How stereochemistry influences the taste of wine: Isolation, characterization and sensory evaluation of lyoniresinol stereoisomers



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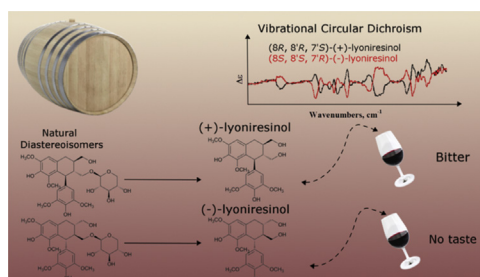
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HIGHLIGHTS

- Targeted screening by LC–HRMS was used to search for stereoisomers of lyoniresinol.
- *Epi*-lyoniresinol was isolated and identified for the first time in *Quercus* genus.
- Two lyoniresinol enantiomers were separated.
- Vibrational circular dichroism was used to determine their absolute configuration.
- Among lyoniresinol isomers in wine, only (+)-lyoniresinol exhibits bitterness.

GRAPHICAL ABSTRACT



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ABSTRACT

Wine expresses its beauty by sending a sensory message to the taster through molecules coming from grapes, yeast metabolism or oak wood. Among the compounds released during barrel aging, lyoniresinol has been recently reported as a relevant contributor to wine bitterness. As this lignan contains three stereogenic carbons, this work aimed at investigating the influence of stereochemistry on wine taste by combining analytical and sensorial techniques. First, an oak wood extract was screened by Liquid Chromatography–High Resolution Mass Spectrometry to target isomers separable in a symmetric environment and a diastereoisomer called *epi*-lyoniresinol was isolated for the first time. Then, an original racemic resolution based on natural xylose-derivatives was carried out to obtain lyoniresinol enantiomers. Chiroptical spectroscopic measurements associated with theoretical calculations allowed the unambiguous determination of their absolute configuration. The taste properties of all these stereoisomers revealed that only one lyoniresinol enantiomer is strongly bitter whereas the other one is tasteless and the diastereoisomer is slightly sweet. The presence of these three compounds was established in an oaked Bordeaux wine by chiral and non-chiral chromatography, suggesting the significant influence of stereochemistry on wine taste.

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1. Introduction

Among the aesthetic pleasures in life, wine tasting plays a special role in that, unlike music, poetry or paintings, wine is physically absorbed by the taster. Therefore, even though cognitive processing is primordial [1,2], the emotion caused by wine tasting is above all due to direct contact between wine stimuli and the taster's sensory receptors. These stimuli are volatile and non-volatile compounds that are responsible for the odors and tastes of wine, respectively. The identification of such taste-active molecules has been a subject of intense research for decades, demonstrating that they can be released from grapes, synthesized by micro-organisms during fermentation or chemically modified during bottle storage [3]. Oak wood is another source of active molecules; during barrel aging, both volatile and non-volatile compounds are released from wood to wine, whose organoleptic properties are thus highly modified [4]. Recently, a lignan from oak wood called lyoniresinol was shown to exhibit bitterness [5]. Another study showed that lyoniresinol is present in wines aged in new oak barrels at concentrations higher than its perception threshold (1.5 mg/L in white wine), establishing its key contribution to the increase in bitterness observed during oak aging [6].

Since the presence of functional groups can modulate the sensory attributes of wine molecules [7], natural derivatives of lyoniresinol have also been sought in oak wood extract. Galloyl, glucosyl and xylosyl derivatives were thus discovered, some of them exhibiting bitterness but with a lower intensity than lyoniresinol [6].

Beyond functional groups, stereochemistry also plays an important role on organoleptic properties. This importance is well known for numerous volatile compounds whose absolute configuration influences both the intensity and the nature of the aroma (*S*- and *R*-enantiomers of limonene smell of lemon and orange, respectively [8]). Similarly, stereochemistry also influences taste attributes. For the first time in 1886, Piutti isolated *D*-asparagine, the enantiomer of *L*-asparagine, demonstrating that these compounds are sweet and tasteless, respectively [9]. After this discovery, other compounds were shown to have different taste characteristics according to their stereochemistry, such as naringin diastereoisomers with their distinct bitterness [10], and alapyridaine enantiomers whose dextrorotary form has a sweet taste whereas the levorotatory form has no taste at all [11].

Interestingly, lyoniresinol has three stereogenic centers, suggesting the potential existence of eight stereoisomers. Among the several plant species from which lyoniresinol has been isolated, it has been observed as a mixture of both *8R,8'R,7'S*- and *8S,8'S,7'R*-enantiomers with variable relative abundance [12]. In *Quercus* genus oak wood, specific optical rotation measurement indicated that the two enantiomers are present at similar concentrations [13]. Nevertheless, their individual gustatory properties have never been assessed. Furthermore, some lyoniresinol diastereoisomers have been identified in various plants [14–17] but never in the *Quercus* genus. Nonier et al. only evoked the presence of one lyoniresinol isomer in oak wood by comparing GC–MS spectra but no further investigations were carried out to verify this hypothesis [18,19].

Knowledge is therefore lacking about the existence of lyoniresinol isomers in oak wood and their organoleptic properties. Considering the strong bitterness developed by lyoniresinol in racemic mixture, the isolation, characterization and sensory study of such stereoisomers might be of particular relevance.

For this reason, we first sought lyoniresinol diastereoisomers in oak wood extract by targeted screening and Counter Current Chromatography (CCC) isolation guided by liquid chromatography

coupled with high resolution mass spectrometry (LC–HRMS). Then, an original enantiomeric resolution was implemented by hydrolysis of natural xyloside derivatives present in oak wood. Both enantiomers were isolated and their absolute configuration was determined unambiguously for the first time by means of chiroptical spectroscopic measurements. The gustatory properties of all the purified compounds were assessed and their presence in wine aged in oak barrels was studied to investigate whether the stereochemistry of lyoniresinol might influence the taste of wine and more generally the pleasure of the consumer.

2. Materials and methods

2.1. Chemicals and materials

Oak wood used in this study was heartwood staves of *Quercus petraea* from various French forests. The staves were 2-year air-dried and then reduced to chips by the cooperage industry (Seguin Moreau, Merpins, France). Two wines were used in this study: a non-oaked white Bordeaux 2013 (100% Sauvignon blanc, 13% vol. alc.) for sensory tests and a red Margaux 2012 (90% Cabernet Sauvignon and 10% Merlot, 13.5% vol. alc.) aged in new French oak barrels for 15 months for chemical analysis.

All solvents were HPLC grade (VWR International, Pessac, France) except acetonitrile used for HRMS analysis (Optima[®] LCMS grade, Fisher Scientific, Fair Lawn, USA) and deionized water (MilliQ, Millipore, Bedford, USA). Lyoniresinol, lyoniside ((+)-lyoniresinol 9'-O- β -xylopyranoside) and nudiposide ((-)-lyoniresinol 9'-O- β -xylopyranoside) were isolated as described previously by Marchal et al., 2014 [6].

2.2. Preparation of pre-purified oak wood extract

Oak wood extract was obtained from a hydro-alcoholic solution (50:50; EtOH/H₂O) of wood chips (250 g/L) for two weeks at room temperature. After a 0.45 μ m filtration, the hydro-alcoholic solution was concentrated *in vacuo* to remove ethanol. The aqueous solution was extracted three times with 200 mL of ethyl acetate (EtOAc). The combined organic layers were evaporated to dryness, suspended in water and freeze-dried to obtain a brownish free-flowing powder of EtOAc prepurified extract (1.9 g).

2.3. LC–HRMS analysis

The LC–HRMS apparatus consisted of an HTC PAL autosampler (CTC Analytics AG, Zwingen, Switzerland), an Accela U-HPLC system with quaternary pumps and an Exactive Orbitrap mass spectrometer equipped with a heated electrospray ionization HESI I probe (both from Thermo Fisher Scientific, Les Ulis, France). Liquid chromatography separation was carried out on a C18 column (Hypersil Gold 2.1 mm \times 100 mm, 1.9 μ m particle size, Thermo Fisher Scientific) with water (Eluent A) and acetonitrile (Eluent B) as mobile phases. The flow rate was set at 600 μ L/min and the injection volume was 5 μ L. Eluent B varied as follows: 0 min, 14%; 0.5 min, 14%; 1.5 min, 19%; 2 min, 19%; 4.5 min, 38%; 4.6 min, 98%; 6.9 min, 98%; 7 min, 14%; 8.6 min, 14%. Chiral chromatography analysis were performed on a Chiralpak[®] IB-3 column (2.1 mm \times 150 mm, 3 μ m particle size) with a flow rate set at 300 μ L/min and an isocratic elution mode (water/acetonitrile; 80:20; v/v).

Mass acquisitions were performed in negative Fourier transform mass spectrometry (FTMS) ionization mode. The chromatographic conditions as well as the ionization and spectrometric parameters are described in Supplementary Data.

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