PhD DISSERTATION PROJECTS

Study of Chemical and Sensory Markers for Precision Oenology as a Component of the Decision Support System (DSS) for Wineries

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This PhD thesis research project aims to study chemical and sensory markers that wineries can use in a DSS to improve wine production and quality. Precision oenology, which optimizes winemaking operations using data-driven methodologies and DSS, is one of the two sides of aspects connecting the right product for the right consumer. The other side would be the development of non-invasive method for fingerprinting bottled wine products to ensure their authenticity and consumers expectations. The project will be developed in collaboration with wineries and providers of analytical non-invasive devices.

Studio di marcatori chimici e sensoriali per l'enologia di precisione come componente del sistema di supporto decisionale (DSS) per le aziende

Questo progetto di ricerca per la tesi di dottorato mira a studiare i marcatori chimici e sensoriali che le aziende vinicole possono utilizzare in un DSS per migliorare la produzione e la qualità del vino. L'enologia di precisione, che ottimizza le operazioni di vinificazione utilizzando metodologie guidate dai dati e DSS, è una delle due facce degli aspetti che collegano il prodotto giusto al consumatore giusto. L'altro aspetto è lo sviluppo di un metodo non invasivo per la rilevazione dell’impronta digitale dei prodotti vinicoli imbottigliati, per garantirne l'autenticità e le aspettative dei consumatori. Il progetto sarà sviluppato in collaborazione con aziende vinicole e fornitori di dispositivi analitici non invasivi.

# **1. State-of-the-Art**

Wine production is a multi-stage process that starts with grape growth and harvest, and continues through fermentation, ageing, and bottling. Numerous elements, such as grape variety, *terroir*, viticulture practices, winemaking methods, and ageing circumstances, have an impact on the wine's quality and sensory qualities (Reynolds, 2022). Precision oenology is a burgeoning field of study that employs chemical and sensory markers to analyze and monitor different facets of wine production. Winemakers can make informed decisions regarding grape selection, fermentation techniques, maturation, and overall wine quality by identifying specific markers (Poggesi et al., 2021). As the wine industry strives to produce high-quality wines, the application of precision oenology has become increasingly vital. However, consumers and manufacturers alike continue to worry about the authenticity of wine sold in bottles. Financial costs for producers and damage to consumer trust can occur from fraudulent tactics like adulteration, mislabeling, and counterfeiting (Popović et al., 2021, Merkytė et al., 2020b). Therefore, it is important to create technologies for fingerprinting bottled wine products to satisfy consumers' demands for authenticity.

Numerous studies have focused on the development of analytical methodologies for wine analysis. Typically, these techniques involve the identification and quantification of chemical compounds in wine samples. Liquid chromatography coupled with mass spectrometry (LC/MS) and Gas chromatography-mass spectrometry (GC-MS) are the common techniques for identifying non-volatile and volatile organic compounds in wines, which can reveal large information on the winemaking technology, grape variety, and vintage (Lukić et al., 2022, Merkytė et al., 2020a).

Recently, non-invasive technologies, such as near-infrared spectroscopy (NIRS) and mid-infrared spectroscopy (MIRS), have acquired popularity due to their ability to enable rapid and non-destructive analysis of wine samples. These techniques can be used to learn key information about the wine, using chemical and sensory markers, such as its vintage, grape variety, and place of origin. Non-invasive procedures significantly reduce wine sample damage, allowing for repeated evaluations without harming product quality. In addition, changes in the molecular vibrations of chemical compounds in wine samples can allow the identification and quantification of diverse substances (Hu et al., 2019). Moreover, these methodologies are being already used to reveal the chemical composition of wine, such as its sugar and acid content, as well as the presence of specific compounds, such as tannins and flavonoids.

Non-invasive chemical and sensory marker studies will assist create a comprehensive wine fingerprint database to match the right product for the right consumer. The DSS can use the database to optimize winemaking operations and improve wine quality. This database may additionally include wine's provenance, vintage, grape variety, chemical, and sensory markers. which can help to provide accurate product information and help consumers buy the right wine product. In addition, an exhaustive database can serve as a reference for future analyses of wine, which can aid in the detection of wine fraud.

# **2. PhD Thesis Objectives and Milestones**

The main objective of this research proposal is to investigate the chemical and sensory markers and use of non-invasive techniques to optimize winemaking practices and improve wine quality and integrate those techniques into DSS.

A1) **Chemical Analysis of collected samples from wineries:** Wine samples from several wineries will be gatheredto identify and quantify aroma compounds and their precursors in bottled wine samples using advanced analytical techniques, such as GC-MS, GCxGC-MS, and LC-MS. The effectiveness of different non-invasive fingerprinting techniques for wine products will be investigated. These methods will include spectroscopic techniques; specifically, near-infrared spectroscopy using the portable spectrometer.

A2) **Identification of Potential Markers:** To identify potential markers or combinations of markers that can be used to validate the authenticity of wine products. The markers discovered will be determined according to their sensitivity, specificity, and robustness.

A3) **Method Development and Validation:** To develop and validate a reliable method for applying the identified markers by using multivariate statistical approaches. The approach will be tested on a variety of wine products from various areas and vintages. To assess its efficacy, the created method will be compared to existing methods for wine authenticity from a supply chain traceability perspective.

A4) **Addition to Decision Support System (DSS):** To advise the design of a DSS to help wineries streamline their processes and produce higher-quality wine. Winemaking procedures like grape selection, fermentation, ageing, and blending tactics will be informed by data because of the DSS's integration of chemical and sensory markers revealed in the research.

A5) **Writing and Editing** the PhD thesis, scientific papers and oral and/or poster communications.

***Table 1***Gantt diagram for this PhD thesis project.

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| Activity Months | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** | **12** | **13** | **14** | **15** | **16** | **17** | **18** | **19** | **20** | **21** | **22** | **23** | **24** |
| A1) | ***Chemical Analysis*** |   |   |   |  |  |  |  |   |   |  |  |  |  |   |  |  |  |  |   |   |  |  |  |  |
|  | 1) Advanced Analytical Techniques |   |  |   |  |  |  |  |   |   |  |  |  |  |   |  |  |  |  |   |   |  |  |  |  |
|  | 2) Non-invasive Techniques |   |  |   |  |  |  |  |   |   |  |  |  |  |   |  |  |  |  |   |   |  |  |  |  |
| A2) | ***Identification of Potential Markers*** |   |   |   |  |  |  |  |   |   |  |  |  |  |   |   |   |  |   |   |   |  |  |  |  |
|  | 1) Potential Markers Identification |   |   |   |  |  |  |  |   |   |  |  |  |  |   |   |  |  |  |   |   |  |  |  |  |
|  | 2) Sensitivity and Specificity |   |  |   |  |  |  |  |   |   |  |  |  |  |   |  |   |  |   |   |   |  |  |  |  |
| A3) | ***Method Development*** |   |  |   |   |   |   |  |   |   |   |   |   |  |   |  |  |  |  |   |   |   |   |   |  |
|  | 1) Method Validation |   |  |   |   |   |  |  |   |   |   |   |  |  |   |  |  |  |  |   |   |   |   |  |  |
|  | 2) Efficacy Assessment |   |  |   |  |  |   |  |   |   |  |  |   |  |   |  |  |  |  |   |   |  |  |   |  |
| A4) | ***Addition to DSS*** |   |  |   |  |  |   |   |   |   |  |  |   |   |   |  |  |  |  |   |   |  |  |   |   |
|  | 1) Design of DSS |   |  |   |  |  |   |   |   |   |  |  |   |   |   |  |  |  |  |   |   |  |  |   |   |
|  | 2) Integration of Identified Markers |   |  |   |  |  |  |  |   |   |  |  |  |  |   |  |  |  |  |   |   |  |  |  |  |
| A5) | ***Thesis and Paper Preparation*** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |  |   |   |   |   |   |   |   |

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