



METABOLOMIC-BASED APPROACH ON WINE AUTHENTICATION: A CASE STUDY ON VARIETAL DISCRIMINATION

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Wine metabolomics constitutes a powerful discipline towards wine authenticity assessment through the simultaneous exploration of multiple classes of compounds in the wine matrix. Over the last decades, wines from autochthonous Greek grape varieties have become increasingly popular among wine connoisseurs, attracting great interest for their authentication and chemical characterization. In this work a case study is presented, where 46 red wine samples from Agiorgitiko and Xinomavro grape varieties were collected from wineries in two important winemaking regions of Greece during two consecutive vintages and analyzed using ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry (UHPLC-QToF-MS). A targeted metabolomics methodology was developed, including the determination and quantification of 28 phenolic compounds from different classes (hydroxycinnamic acids, hydroxybenzoic acids, stilbenes and flavonoids). Moreover, 86 compounds were detected and tentatively identified via a robust suspect screening workflow using an in-house database of 420 wine related compounds. Supervised chemometric techniques were employed to build an accurate and robust model to discriminate between two varieties.

Keywords: wine; metabolomics; HRMS; chemometrics; biomarkers

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