Implementing VIS-NIR spectroscopy as a rapid and non-intrusive technique for assessing anthocyanin and phenolic concentrations in *Vitis vinifera* L. Grenache whole grape berries.

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Abstract (250 words)

Anthocyanins and phenolic compounds play a crucial role in winemaking, contributing to the profile, flavor, color, texture, and stability of wine. Grape clusters, specifically *Vitis vinifera* L. cv. Grenache, were handpicked from a commercial vineyard sited in Tudelilla, La Rioja, Spain (42°18' 52.26", Long. -2°7' 59.15", Alt. 582 m) on five distinct dates from veraison to harvest during the 2015 season. Non-contact spectral measurements were conducted on intact grape berries using a VIS-NIR spectrometer operating in the 570 - 1000 nm spectral range under controlled laboratory conditions, positioned at a distance of 25 cm from the berries. The quantification of 16 anthocyanins and phenols in 120 grape clusters was performed using HPLC, established as the reference method for validating the spectral tool. Data exploration and prediction of phenolic concentration in grape berries were conducted through Principal Component Analysis (PCA) and Modified Partial Least Squares (MPLS) regression. The best calibration and cross-validation models were built for total monomeric anthocyanins, nonacylated anthocyanins and cyanidin 3-glucoside with determination coefficients (R^2_{cv} values above 0.86, while the standard errors of cross validation (SECV) were 0.058 mg/g, 0.052 mg/g and 0.001 mg/g respectively. Of the other phenolic groups, the model for total flavanol yielded R^2_{cv} = 0.66 and SECV = 0.023 mg/g. This technology shows high potential for the selection and classification of berries throughout ripening in the vineyard or upon grape reception at the winery. Its application could help tailoring the oenological fate of grape berries to various wine qualities or styles.

Keywords: Berry ripening, Non-invasive technologies, Anthocyanin, Phenols, Chemometrics.