

Title ^1H NMR metabolic fingerprints of grape berries produced in different plots in Bordeaux, France
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Abstract

Sugars, organic acids, amino acids and phenolics are important determinants of grape berry quality. The aim of this study was to determine the metabolite profiles of skin and pulp tissues from mature berries of ‘Cabernet franc’, ‘Cabernet Sauvignon’ and ‘Sauvignon blanc’ in relation to their growing conditions. Proton nuclear magnetic resonance (^1H NMR) allows one to quantify many different compounds in berry extracts at a single time. Grape berries were collected at harvest in 2002 from grapevines cultivated in different soil types and climates near Bordeaux, France. After an ethanolic-water extraction, the ^1H NMR spectra of water-soluble extracts of the pulp and skin were run in 15 minutes. Discriminant analyses were performed on spectra data after segmentation into 190 spectra domains of 0.04 ppm between 0 to 8 ppm. Principal component analysis and partial least square analysis of skin spectra significantly discriminated ripe fruit of grapevines grown on different soils. The ^1H NMR spectra of pulp were less discriminating. The resonances, contributing to significant discrimination, were attributed to sugars and amino acids. In conclusion, ^1H NMR analysis of berry skin extracts discriminates berries from different locations more efficiently than classical biochemical analyses based on sugar, acidity and nitrogen measurements. This technique should improve the study of environmental effects on grape berry quality by metabolite profiling.