

HR-MAS ^1H NMR Study of Hydration Water in Arabica Green Coffee: Relation to the Final Beverage Quality

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SUMMARY

The goal of this study was to determine the ability of high-resolution magic angle spinning (HR-MAS) NMR spectroscopy to assess the quality of green coffee before roasting. To this purpose, ten Arabica green coffee samples, half of which had produced good quality coffees (G samples) while the others resulted in worse tasting beverages (B samples), were analysed by HR-MAS ^1H NMR spectroscopy at high field (600 MHz) to determine their chemical composition and water hydration. From the proton NMR spectrum of each coffee powder a metabolic profile was obtained and a comparison between the average profile of G and B samples was made using different statistical methods. Principal component analysis (PCA) gave a good separation of G and B samples and this separation was mainly due to the amount of bound water. Two water signals, attributed to internal and external water, were in fact observable in the ^1H NMR spectrum at different chemical shift, after the addition of a small amount of water. Thus, more detailed information on the water structure was obtained by studying the position, intensity and shape of the NMR resonances as a function of the hydration. Finally, pulsed field gradient (PFG) HR-MAS ^1H NMR spectroscopy was applied to measure self-diffusion coefficients of water and oil molecules in the coffee powder. We showed that the externally added water diffuse in large pores within the powder particles whereas the fatty acids diffuse in a restricted environment within the coffee matrix.