
The potential of very high-field ^1H and ^{13}C NMR spectroscopy for food composition analysis in liquid and solid-state: case study of coffee.

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Résumé

Fast magic-angle spinning (MAS; > 40 kHz), very high magnetic fields (17.6 – 21.1 Tesla) and the resort to cryoprobes can significantly enhance both resolution and sensitivity in NMR analysis¹. While very high-resolution configurations of NMR instrument have been reported in literature for medical applications^{2,3,4}, the latter type of equipment is however not easily available to food scientists due to its high cost. As an example, to date, the highest field used to analyse coffee composition was 14 Tesla for liquid state⁵ as well as for solid state with a rotating speed of 12 kHz⁶. Yet, the food science community could take advantage of this cutting-edge technology to address analytical challenges it cannot overcome with lower performance spectrometers.

In this study, the composition of green and roasted coffee beans, coffee extracts and spent ground coffee was investigated using two very high field NMR spectrometers: a 21.1 Tesla instrument (^1H Larmor frequency of 900 MHz) equipped with a cryoprobe on the one hand for liquid-state analyses (coffee extracts), and a 18.8 Tesla equipment (800 MHz; MAS frequency up to 60 kHz) on the other hand for solid-state investigations (coffee beans and spent ground coffee). ^1H and ^{13}C NMR spectra were compared with those obtained using a more conventional configuration (400 MHz spectrometer, MAS frequency of 5-10 kHz) to study the impact of (i) roasting on coffee bean and coffee extract composition, and (ii) extraction on spent ground coffee composition.

This work enabled to highlight the gain in analytical performance obtained by using very high magnetic fields for the analysis of coffee beans, coffee extracts and spent ground coffee. In particular, the increase in resolution and sensitivity makes it possible to observe new resonances, that can serve for authentication purposes or to study process impact on product composition. In the case of coffee, there is a particular interest of using very high field solid-state NMR for the characterization of spent ground coffee.

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