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HR MAS NMR: Profiling Metabolites in Single-Kernels

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The functionality and nutritional value of cereals for food and industrial purposes is mainly determined by the composition of starch, fibers and proteins, the protein/starch relationship, the architecture of starch and the content and structure of cell wall fibers. Therefore, it is of supreme importance to obtain detailed knowledge about composition of the mature grain. Generally, using high resolution magic angle spinning nuclear magnetic resonance (HR MAS NMR), it is possible to measure NMR spectra from small pieces of solids, including plant tissue with no other pretreatment than washing in locking solvent. This paper demonstrates the development of HR MAS NMR single seed measurements and the analysis will be exemplified in studies of wheat and several barley β -glucan mutants. In order to profile the various metabolites within the seed, both 1D and 2D NMR measurements were performed. Also, considerations about spinning speed, temperature and locking solvent are discussed, as these experimental concerns may influence the resulting spectra. The problems and limitations of the method especially concerning large immobile molecules within the sample are summarized and exemplified. It is hypothesized that the lack of expected signals in some species indicates partial immobilization of compounds that appears to be either genotypic or water content dependent.