High Resolution Magic Angle Spinning and Solid-State NMR spectroscopy methods to explore the metabolome of soybean genotypes upon abiotic stress

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Direct analysis by NMR is ideally suited to high-throughput metabolite profiling applications and has the advantage of detecting a wide range of metabolites in an inherently quantitative and unbiased manner. In this work, we explored the utility of using the High Resolution Magic Angle Spinning (HR-MAS) and Solid-State NMR (SSNMR) techniques to identify metabolic changes in soybean tissues subjected to water-deficient conditions. Control and water-deficient soybean leaves were analysed using 1D HR-MAS and SSNMR and the NMR data were submitted to Partial Least Square Discriminant Analysis (PLS-DA). Total RNA was extracted from the leaves for the transcriptomic analysis. The ^{1}H HR-MAS and CP-MAS $^{13}C\{^{1}H\}$ spectra of soybean leaves grown with and without water deficiency stress revealed striking differences in metabolites. A total of thirty metabolites were identified, and the impact of water deficiency on the metabolite profile of soybean leaves was to induce amino acid synthesis. High expression levels of genes required for amino acid biosynthesis were highly correlated with the compounds identified by ^{1}H HR-MAS. The integration of the 1H HR-MAS and SSNMR spectrum with the transcriptomic data provided a complete picture of the major changes in the metabolic profile of soybeans in response to water deficiency.