

^1H NMR-based metabonomics applied in the elucidation of biochemical effects of consumption of whole grain cereals

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Consumption of whole grain cereals has been associated with many health benefits, including a reduction of the risk of cardiovascular disease, diabetes, obesity and some cancers. The objective of the present work was to examine ^1H NMR-based metabonomics as a tool to elucidate the biochemical effects in biofluids after the consumption of whole grain products using the pig as a model. Two diets with similar levels of dietary fibre and macronutrients, but with contrasting levels of whole grain and plant phytochemicals, were prepared from whole grain rye (WGR) and non-whole grain wheat (NGW) and fed pigs in a cross-over design. Plasma and urine samples were collected after 5 and 7 days on each diet, respectively. ^1H NMR spectra were acquired on a Bruker Avance 400 MHz spectrometer. PLS-DA on NMR spectra obtained for plasma samples revealed that the spectral region at 3.25 ppm dominates the differentiation between the two diets. Spiking experiments and LC-MS analyses of the plasma verified that this spectral difference could be ascribed to a significantly higher content of betaine in WGR plasma samples compared with NGW samples. In addition, PLS-DA on NMR spectra obtained for urine samples revealed changes in the intensities of spectral regions which could be ascribed to differences in the content of betaine and creatinine between the two diets, and LC-MS analyses verified a significantly lower content of creatinine in WGR urine samples compared with NGW samples. The results demonstrates that ^1H NMR-based metabonomics is an excellent tool for exploring the biochemical effects of a diet with a high content of whole grain cereals, which can contribute in elucidating the health benefits of a whole grain-based diet.