

Evaluating the potential of the wheat aleurone fraction in humans using ^1H NMR-based metabolomic analysis

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Epidemiological evidence indicates that the increased consumption of whole grain foods is associated with a decreased prevalence of several chronic diseases including obesity, diabetes, CVD and cancer⁽¹⁾. Whole grain comprises the endosperm and the outer bran layer. The bran includes the aleurone, which is particularly rich in bioactive components that may contribute to the beneficial effects of whole grains. Metabolomics is an untargeted technique that can investigate acute and chronic alterations in metabolite profiles, and thus has the potential for elucidating the overall biochemical effects of the potentially protective components present in aleurone. However, until now, metabolomics has only been used to evaluate whole grain using animal models^(2,3). Thus, the aim of this study was to use the ^1H NMR-based metabolomic analysis to identify alterations in postprandial human urinary metabolite profiles after consumption of a wheat aleurone meal, compared to a control meal.

A wheat aleurone meal and a control meal (balanced for fibre and macronutrients) were prepared by boiling with water, and consumed warm by subjects (7 male; 7 female) after an overnight fast, 1 week apart, using a randomized crossover design. Urine samples were collected at baseline, and at 1 and 2 h post consumption. For each urine sample, ^1H NMR spectra were acquired with 32 000 data points and 128 scans over a spectral width of 8 kHz using a 500 MHz DRX NMR spectrometer (Bruker Biospin, Karlsruhe, Germany) with the use of a Noesyprsat pulse sequence. The SIMCA-P+11.5 software package was used to carry out statistical analysis.

Partial least square discriminant analysis (PLS-DA) of these ^1H NMR spectra revealed clear differences between the 1 h postprandial urinary metabolome profiles following aleurone consumption compared to the control. The PLS-DA model had $R^2 = 0.36$ and $Q^2 = 0.41$. Compared to the control, at 1 h, the aleurone meal, showed a urinary metabolome profile with significantly elevated citrate, dimethylamine, lactate, *N*-acetylaspartate and *N*-acetylaspartylglutamate and significantly decreased creatine. Results indicate that wheat aleurone can influence postprandial urinary metabolite profiles. However, further work is needed to elucidate the significance of these effects in relation to the health benefits of whole grain.

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