

## **Profiling techniques and targeted analyses in the quest for differentiation of organic versus conventional DOK wheat**

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Organic and conventional wheat grain from several growing seasons of the field trial was investigated using profiling methods and targeted analyses. The aim of the work was to determine, whether there were consistent differences in grain constituents of the various growing systems and, whether these differences could be used to analytically differentiate organic and conventional wheat grain.

Targeted analysis of wheat grain comprised determination of a number of minerals, crude protein content, phosphate levels, antioxidative capacity, levels of phenols, fibre, fructan, oxalate and phytic acid. Levels of these substances fell into a range that is known to occur in other wheat crops, indicating that wheat from the trial was not exceptional. Clear-cut differences were observed for non-fertilised wheat, which was significantly lowest in thousand seed weight, protein and significantly highest in total oxalate. For the majority of the nutritionally important substances analysed, there were no significant differences between bio-dynamic, organic, and conventional growing systems.

Profiling techniques enable the detection of a wide range of substances in biological samples. In combination with bioinformatic evaluation tools a fast and easy comparison of large datasets is possible. Together these techniques are useful for biomarker searching, in extracts of wheat grain. 2D-gel-electrophoresis and MALDI-TOF-MS/MS analysis was used for protein profiling of wheat grain extracts. Within a set of several hundred proteins a small number of proteins was identified that had significantly different levels in organic and conventional wheat in individual growing seasons and cultivars. Across cultivars and growing seasons expression differences of individual proteins were not stable. When all identified gliadins and glutenins were viewed as a group of proteins, this group was elevated in conventional wheat. Similarly, a group of  $\alpha$ -amylase inhibitors was increased in one growing season in organic wheat.

Metabolite profiles were generated with GC-MS from methanol extracts of finely ground wheat grains. Using this technique approximately 50 metabolites and 250 unidentified metabolites (TAGs) per wheat sample were detected. Monitoring of the cultivar Runal revealed four metabolites that had significantly different concentrations in all three analysed harvest years. Across 11 varieties of the 2007 harvest year, 5 metabolites and 11 TAGs showed significantly different concentrations between the cultivation forms. PCA performed on metabolite data for the individual varieties and for individual growing seasons revealed a clustering according to the cultivation forms. However, PCA of metabolites and TAGs of combined data of all 11 varieties and growing seasons did not result in such a clustering.

For both, analysis of protein and metabolite profiles, it was apparent that cultivar and effects of the growing season were much stronger than the effect of the growing system. On the basis of these results an analytical differentiation of organic and conventional wheat appears very challenging.