

# LC-MS-based metabolite profiling of winter wheat grains

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Wheat was one of the first domesticated food crops and its cultivation reaches far back into history. Today, wheat is one of the major crops and an important source for nutrients like carbohydrates and proteins. Whole grains contain besides starch and protein various phytochemicals from the primary and secondary metabolism. The essential role of wheat as a foodstuff comes along with the indispensability to ensure sufficient and secure crop production for worldwide nutrition.

The AWECOS (Assessment of wheat cropping systems from an economical, ecological and the society's perspective) project aims to assess different breeding strategies for winter wheat. The project identifies advantages and disadvantages of eight different genotypes cultivated with different plant protection strategies at five locations around Germany. The assessment will focus on economical, ecological and socio-economic impacts, as well as on the phytochemical quality of wheat samples.

To investigate environment-specific metabolite changes in winter wheat grains, UHPLC/ESI-QTOF-MS based metabolite

profiling studies were carried out. To cover a wide range of metabolites with different polarity, two analytical methods were used to provide information about semipolar and nonpolar compounds. In the chromatographic method specific UHPLC columns (C18 and C8), suited for metabolites of different polarity, were used. The coupling of UHPLC to a high resolution mass spectrometer allows separation, annotation and relative quantification of numerous wheat metabolites. Around 250 semipolar compounds including vitamins, free amino acids, lignans, benzoxazinoids and flavanoids as well as 150 nonpolar phytochemicals like alkyresorcinols, sterols, phospholipids and triglycerides could be annotated.

A non-targeted data analyses approach in positive and negative ion mode combined with analyses of variance were used to investigate metabolite changes. The results show significant environment-specific differences in the metabolite patterns and the discriminability of the profiles on basis of a principal component analyses.



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