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LC-MS-based profiling of winter wheat – method development and validation

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Wheat was one of the first domesticated food crops and its cultivation reaches far back into history. Today, wheat is grown on more land area than any other crop including rice, maize or potatoes and continues to be one of the most important food sources for humans. 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 (**A**ssessment of **w**heat cropping systems from an economical, **eco**logical and the **s**ociety's perspective) project aims to assess different breeding strategies for winter wheat. The project identifies advantages and disadvantages of eight different genotypes (high-yield, disease resistant and drought-tolerant cultivars) cultivated with different plant protection strategies (organic vs. conventional farming systems) at five locations around Germany. The assessment will focus on economical, ecological and socio-economic impacts, as well as on the quality of wheat samples.

To investigate cultivar- and cropping system-specific metabolite changes in winter wheat, UHPLC/ESI-QTOF-MS-based metabolite profiling studies are in progress. To cover a wide range of metabolites with different polarity, three analytical methods will be used to provide information about polar, semipolar and nonpolar compounds. In the chromatographic method specific UHPLC columns (HILIC, C18 and C8), suited for metabolites of different polarity, are used.

Comprehensive long-term analysis of metabolites in complex biological matrices like winter wheat is a challenging task for quality assurance. To ensure reliable metabolomic data with high reproducibility, validation strategies become an important part during method development of non-targeted metabolomic studies. To optimize the analytical conditions overall and investigate parameters like accuracy, precision, recovery, matrix effects, test compounds, which cover a broad spectrum of chemical diversity, were used in the validation process. The test compounds provide important data about the methods and instrumental setup and build the basic information for the next step the profiling of wheat samples. Furthermore the validation involves assessment of chemometric models and normalization methods which are applied to the huge data sets.

With the established methods and optimized analytical conditions cultivar- and cropping system-specific metabolite changes can be analysed and interpreted with knowledge about the variability of precision, accuracy and suitability of the instrumental system.