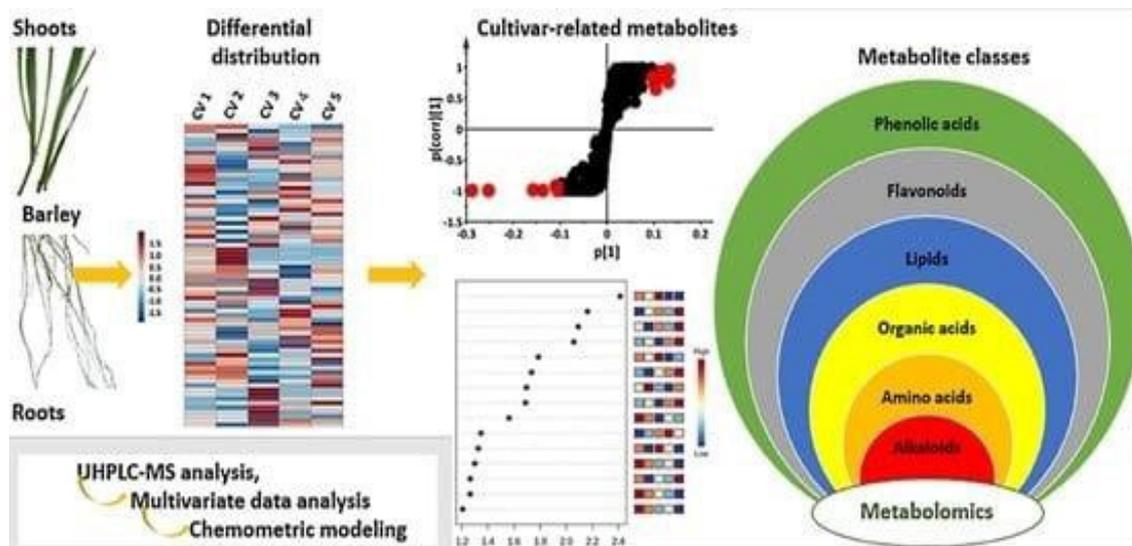


Metabolomes as a measure of the phenotype: The case for barley cultivar identification

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Metabolomics Approach and Chemometric Tools for Differentiation of Barley Cultivars and Biomarker Discovery

Introduction: One of the ultimate goals of plant breeding is the development of new crop cultivars capable of withstanding increasing environmental stresses, to sustain the constantly growing population and economic demands. Investigating the chemical composition of the above and underground tissues of cultivars is crucial for the understanding of common and specific traits thereof.

Methodology: Using an untargeted metabolomics approach together with appropriate chemometrics tools, the differential metabolite profiles of leaf and root extracts from five cultivars of barley ('Erica', 'Elim', 'Hessekwa', 'S16' and 'Agulhas') were explored and potential signatory biomarkers were revealed. The study was conducted on seedlings grown for 21 days under identical controlled conditions. An ultra-high performance liquid chromatography coupled to high-resolution mass spectrometry (UHPLC-HRMS) was employed to analyse hydromethanolic leaf and root extracts of barley cultivars. Furthermore, unsupervised and supervised learning algorithms were applied to mine the generated data and to pinpoint cultivar-specific metabolites.

Results and Conclusion: Among all the classes of metabolites annotated, phenolic acids and derivatives formed the largest group and also represented the most discriminatory metabolites. In roots, saponarin, an important allelochemical differentially distributed across cultivars, was the only flavonoid annotated. The application of an untargeted metabolomics approach in phenotyping grain crops such as barley was demonstrated, and the metabolites responsible for differentiating between the selected cultivars were revealed. The study provides insights into the chemical architecture of barley, an agro-economically relevant cereal crop; and reiterates the importance of metabolomics tools in plant breeding practices for crop improvement.

References: Hamany Djande, C. Y., et al. (2021). A Metabolomics Approach and Chemometric Tools for Differentiation of Barley Cultivars and Biomarker Discovery. *Metabolites*, 11, 578.

Keywords: *Hordeum vulgare*; barley; cultivar differentiation; liquid chromatography; mass spectrometry; metabolomics; multivariate data analysis; phenotyping; secondary metabolites; signatory metabolites.