

# Spatio-temporal analysis of metabolite profiles during barley germination

Jan Kölling<sup>1</sup>, Karin Gorzolka<sup>2</sup>, Karsten Niehaus<sup>2</sup>, Tim W. Nattkemper<sup>1</sup>

<sup>1</sup>*Biodata Mining Group, Bielefeld University*

<sup>2</sup>*Proteome and Metabolome Research, Bielefeld University*

koelling@cebitec.uni-bielefeld.de

Mass spectrometry imaging generates a series of localized mass spectra from discrete positions on a tissue or thin-film, thereby providing comprehensive information on molecular composition and spatial distribution in a single experiment. This allows for an untargeted and simultaneous measurement of a wide variety of molecules.

To study a biological process over time and space, multiple MSI measurements can be conducted and combined into a time series. The sample preparation and imaging process are destructive for the sample, therefore each time point needs to be represented by a different specimen. As a result the sample morphology is different for each time point and spatial distribution can not be directly compared. Inter and intra sample variance of the signal intensity is also an issue.

After standard MSI preprocessing steps we use H<sup>2</sup>SOM clustering of manually selected mass signals for all time points with our previously developed tool WHIDE [KLA<sup>+</sup>12]. The resulting hierarchy of cluster prototypes is further analyzed to identify spatio-temporal patterns across the time series.

The approach was applied to localize metabolites during the barley germination process which is of high scientific and agricultural interest.

## References

- [KLA<sup>+</sup>12] Jan Kölling, Daniel Langenkämper, Sylvie Abouna, Michael Khan, and Tim W Nattkemper. WHIDEa web tool for visual data mining colocation patterns in multivariate bioimages. *Bioinformatics*, 28(8):1143–1150, 2012.