

## Session 5 - Chemometrics and Remote sensing (Co-chairs: Beleites/Gorzsás)

### 05-01: Multivariate analytical strategies for spectral data of plants

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This plenary lecture aims to give an introduction to multivariate analysis, with a brief overview of selected techniques applicable to spectral data common in plant sciences. The techniques covered include common supervised and non-supervised methods, such as principal component analysis, multivariate curve resolution, partial least squares based techniques (including discriminant analyses) and clustering tools. The focus is on providing a guide by which multivariate analytical strategies can be chosen. The lecture is intended specifically for people with little to no background in chemometrics, to help them select the most suitable multivariate analytical technique based on the goal of the analysis and the type of the collected data. Real life examples are used to illustrate different aspects of the techniques, primarily based on vibrational (Fourier-transform infrared (FTIR) and Raman) spectra, but the discussed techniques are of general purpose and thus directly applicable to other types of spectral data spectra. The provided examples outline the handling of continuous sequential spectra [1], independent batch spectra [2,3] and hyperspectral image data [4] from the field of plant sciences.

#### References

- [1] GILLGREN, T., and A. GORZSÁS, 2016: Wood Science and Technology, **50**, 567-580.
- [2] FELTEN, J., HALL, H., JAUMOT, J., TAULER, R., DE JUAN, A., and A. GORZSÁS, 2015: Nature Protocols, **10**, 217-240.
- [3] SERK, H., GORZSÁS, A., TUOMINEN, H., and E. PESQUET, 2015: Plant Signaling and Behavior, **10**.
- [4] GORZSÁS, A., STENLUND, H., PERSSON, P., TRYGG, J., and B. SUNDBERG, 2011: Plant Journal, **66**, 903-914.