Automated chemometric procedure for quantitative and qualitative analysis of confocal Raman images

Carlo G. Bertinetto¹, Leonardo Galvis¹, Anne Jokela², Tapani Vuorinen¹, Perttu Virkajärvi³

¹Department of Forest Products Technology, School of Chemical Technology, Aalto University, P.O. Box 16300, 00076 Aalto, Espoo, Finland
²Department of Biology, University of Oulu, P.O. Box 3000, 90014, Oulu, Finland
³MTT Agrifood Research, Halolantie 31 A, 71750, Maaninka, Finland

SCOPE
This poster illustrates a chemometric procedure for the analysis of confocal Raman images. It can identify and map several sample components easily and with no a priori knowledge. Most of its operations are performed automatically.

CONFOCAL RAMAN SPECTROSCOPY (CRS)
CRS couples Raman spectroscopy with an optical microscope. It allows for fast, label-free and non-invasive spectral imaging.

CHEMOMETRIC TREATMENT AND ANALYSIS
Data pre-processing
- RAW data
- Pre-processed data
- SVD
- Band-Target Entropy Minimization (BTEM)

Spectral unmixing
- Post-screening of BTEM solutions
- Spectra of pure components
- Leastsquares fit
- Distribution maps

Examples of processed images
Barley kernels
- Optical image
- Starch
- Protein
- B-glucan
- Starch anisotropy
- Protein?
- Ferulic acid

Timothy grass stem
- Optical image
- Cellulose
- Lignin
- Ferulic acid
- Embedding resin
- Background
- Residual baseline distortion + some lignin signal
- Anisotropy?

CONCLUSION
The presented chemometric procedure can correct the most common noises and distortions of Raman signals and obtain the spectra of the pure components in the sample, requiring very little user intervention and no expertise in chemometrics. It can detect components with overlapping peaks and small signal, which are often not found with other methods. It is useful for both qualitative and quantitative analysis.

REFERENCES

CONTACT:
Carlo G. Bertinetto
Post-doc researcher
carlo.bertinetto@aalto.fi