

# Different spectroscopic and physicochemical techniques for fingerprinting, characterization and quantification of lignocellulose with a specific focus on chemometric approaches

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## Summary

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*The overall goal of the project is the development of reliable spectroscopic and physicochemical methods in combination with multivariate analyses for the qualitative and quantitative assessment of lignocellulosic biomass and valorization products. The project addresses the following research questions: What are the main expected benefits and challenges of using spectroscopic methods together with chemometric analysis for qualitative and quantitative characterization of complex biopolymers? How to provide an effective extraction of the significant information from the multidimensional data and make reliable conclusions? How to improve the use of chemometric approaches in the field of biomass valorization?*

Research field:	Chemistry and biotechnology
Supervisors:	Dr. Tiit Lukk Dr. Maria Kulp
Availability:	This position is available.
Offered by:	School of Science Department of Chemistry and Biotechnology
Application deadline:	Applications are accepted between June 01, 2022 00:00 and June 30, 2022 23:59 (Europe/Zurich)

## Description

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Lignocellulosic biomass is a highly abundant renewable resource that can be converted into several types of high-value-added products, including chemicals, biofuels and advanced materials. Over the years, the development of new biomass processing technologies has attracted serious research attention, where analytical science plays crucial role in providing the biorefinery research with key information. Vibrational spectroscopy techniques such as near-infrared (NIR), midinfrared (MIR) and Raman spectroscopy can be applied as the first approach to obtain basic knowledge about biopolymers as well as a way to carry out qualitative and quantitative analyses. These techniques have the advantage of being rapid, easy-to-use and nondestructive in comparison to the tedious reference chemical and classical techniques, which require solvents and are time-consuming. Moreover, combined with multivariate analyses makes it easier to extract significant information from vast collected data sets, analyze those and make qualitative and quantitative conclusions.

The aims of the project are (1) to develop and apply different vibrational spectroscopy techniques to physicochemical characterization of raw lignocellulosic biomass, valorization process efficiency and quality of obtained products, and (2) to develop and apply different chemometric approaches for multidimensional data analysis, classification and prediction.

### Supervisors

Main supervisor: Dr. Maria Kulp  
Co-supervisor: Dr. Tiit Lukk

### Responsibilities and (foreseen) tasks

- Develop analytical procedures for qualitative and quantitative characterization of biomass and products and process efficiency (classic wet-chemistry and instrumental methods of analysis; MIR, NIR, NMR, UV spectroscopy);
- Apply chemometric methods for analysis of multidimensional data for *decomposition* - principal component analysis, parallel factor analysis; *regression* – multiple linear regression, partial least squares regression, artificial neural network, *classification* - PLS discriminant analysis, K-nearest neighbor etc.)

- Carry out planning and optimization of experiments using different experimental design approaches (e.g. response surface modelling).
- Contribute to the organization of research and practitioner workshops where project findings are presented

### **Applicants should fulfil the following requirements:**

- MSc degree in applied or analytical chemistry
- A clear interest in the topic of the position
- Previous experience in development of analytical procedures
- Experience in multidimensional statistic analysis
- Excellent English in communication and in writing, team working attitude
- Strong and demonstrable writing and analytical skills
- Capacity to work both as an independent researcher and as part of an international team
- Capacity and willingness to provide assistance in organizational tasks relevant to the project

### **The following experience is beneficial:**

- Previous experience in validation of analytical procedures
- Previous experience in quality assurance in chemical/instrumental analysis
- Working knowledge of Solo or other chemometric software
- Experience in chemistry of biopolymers is a plus

### **We offer:**

- 4-year PhD position in one of the largest, most internationalized and leading universities in Estonia
- The chance to do high-level research in the field of renewable raw materials valorization and contemporary analytical chemistry
- Opportunities for conference visits, research stays and networking with globally leading universities and research centers in the field of natural science and sustainable development

### **About the department**

The department of Chemistry and Biotechnology was created in the Faculty of Science in 2017, founding director was Ivar Järving. The institute merged the former Institute of Chemistry and the Institute of Gene Technology from the Faculty of Mathematics and Natural Sciences and the Institute of Food Science from the Faculty of Chemistry and Materials Technology. Recent scientific discoveries in chemistry, molecular biology and food technology have opened up completely new perspectives in fields as medicine, industry, agriculture and the environment.

### **Additional information**

For further information, please contact Dr. Maria Kulp [maria.kulp@taltech.ee](mailto:maria.kulp@taltech.ee) and Dr. Tiit Lukk [tiit.lukk@taltech.ee](mailto:tiit.lukk@taltech.ee) or visit <https://puidukeemia.ee/tooruhmad/puidupolumeeride-fraktsioneerimine-ja-analuutiline-keemia/> and [www.keemlab.ttu.ee](http://www.keemlab.ttu.ee)



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