

Straubing, December 18, 2023

Master's Thesis Topic

Development of an Automated Background and Overlap Correction in 1H-NMR Spectra of Dandelion

The demand for natural rubber for the production of tires and many other rubber products is increasing worldwide and has so far been met exclusively from the latex of the tropical rubber tree. It is expected that this source will no longer be able to meet global demand within this decade. To avoid further deforestation of tropical rainforests for rubber plantations, all major tire manufacturers worldwide are looking for alternative rubber plants.

The Russian dandelion (*Taraxacum koksaghyz*) produces latex of a suitable quality. However, the plant is very weak-growing, has small roots and the wild material only has a rubber content of 2-3%. Initial tests have shown that the combination of Russian dandelion with common dandelion (*Taraxacum officinale*) can increase root mass by a factor of 10. The suitability of combining common dandelion and Russian dandelion is the subject of current research with the aim of establishing dandelion as an alternative source of rubber.

Metabolomics, the study of small molecules involved in cellular processes, has emerged as a powerful tool in understanding the complex metabolic pathways of plants [1]. Within this framework, 1H NMR spectroscopy serves as a non-destructive and versatile technique for identifying metabolites. However, challenges arise in the form of background distortions and signal overlaps, potentially leading to inaccuracies in metabolite identification.

This master's thesis addresses these challenges by developing an automated background and overlap correction in the 1H NMR spectra. This should significantly improve the precision of metabolite identification and quantification in dandelion spectra. The quality of the determined metabolite concentrations is an essential prerequisite for a reliable analysis of the plant metabolome in the context of metabolomics-assisted breeding [2].

Basic knowledge of at least one programming language (preferably R or Python) is required. The work is supervised by Prof. Dr. Clemens Thielen (Professorship of Complex Networks) in collabora-

tion with Prof. Dr. Andreas Krumpel (Weihenstephan-Triesdorf University of Applied Sciences, Professorship of Physics and Mathematics) and lifespın GmbH in Regensburg; it is suitable for different master's programs (Chemical Biotechnology, Technology of Biogenic Resources, Biomass Technology, or related areas). If you are interested, please send an email to clemens.thielen@tum.de or andreas.krumpel@hswt.de.

References

- [1] Roy R. et al. Emwas, A.-H., *NMR spectroscopy for metabolomics research*, *Metabolites* **9** (2019), no. 7, 123.
- [2] A. R. Fernie and N. Schauer, *Metabolomics-assisted breeding: A viable option for crop improvement?*, *Trends in Genetics* **25** (2009), no. 1, 39–48.