Sustainable Production of 5-Nitrovanillin from Lignin in Biphasic Systems

Supervision: Saša Bjelić (group leader)

Research group: Advanced Analytics Platform

Time scope: 6–9 months

Start: as soon as possible

Work location: Paul Scherrer Institute, 5232 Villigen, Switzerland

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Prospective candidates should currently be enrolled in a Master's program in chemistry, chemical engineering, technical chemistry, or environmental science.

Scope of the Thesis

This thesis will explore the sustainable production of 5-nitrovanillin from lignin using biphasic oxidative depolymerization (BPD) systems. The work will investigate different nitrate salts and nitric acid as nitrating agents, evaluate the effect of cations on nitration efficiency, and use vanillin as a model compound to study reaction pathways. The project will also assess the feasibility of producing 5-nitrovanillin from lignin-derived vanillin.

Scientific Background

Lignin is a significant natural resource – it is the most abundant naturally occurring aromatic polymer on Earth. Lignin is also a major side-product from the pulp and paper industry and cellulosic ethanol production, with about 50 million tons of lignin produced [1]. One of the promising approaches to its valorization is biphasic oxidative depolymerization. It combines oxidative depolymerization in an acidic aqueous phase with simultaneous extraction of aromatic monomers into an organic phase, protecting them from over-oxidation and repolymerization. Understanding how different nitrate salts and nitric acid influence nitration pathways is essential for developing a selective and sustainable process. Using vanillin as a model compound provides mechanistic insights, although real lignin systems may behave differently. Producing 5-nitrovanillin from lignin

[1] Omar Y. Abdelaziz et al., "On the Oxidative Valorization of Lignin to High-Value Chemicals: A Critical Review of Opportunities and Challenges," *ChemSusChem* 15, no. 20 (2022), https://doi.org/10.1002/cssc.202201232.

or lignin-derived vanillin offers a fossil-free alternative to conventional synthesis routes, but economic viability and market demand must be considered.

Key Learnings

You will learn how to:

• Design and execute biphasic nitration experiments with various nitrate sources.

• Quantify vanillin and 5-nitrovanillin using UHPLC-HRMS.

• Understand nitration pathways in lignin and model systems.

• Evaluate sustainability and market feasibility for nitro-aromatic production.

General Tasks

During this project, you will:

- Screen different nitrating agents in biphasic systems.
- Conduct model compound studies using vanillin to elucidate nitration mechanisms.
- Extend experiments to lignin feedstock and compare product yields and selectivity.
- Quantify 5-nitrovanillin formation using UHPLC-HRMS and validate analytical methods.
- Assess sustainability metrics and perform preliminary market analysis for 5-nitrovanillin.
- Document protocols, datasets, and conclusions in the final thesis.

Your results will be reported in a written thesis conforming with the rules of the respective university you are enrolled in. Depending on the quality of the results, they could be included in future publications in scientific publications.