# Olefins Quantification Using Paternò–Büchi Derivatization and High-Resolution Mass Spectrometry

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 project aims to develop and optimize a workflow for olefin quantification in complex hydrocarbon mixtures using the Paternò–Büchi (PB) photochemical derivatization reaction combined with UHPLC-HRMS. Olefins are critical components in sustainable aviation fuel (SAF) and other petrochemical products, yet their characterization remains challenging due to coelution and high degree of spectral similarity in conventional analytical methods. The PB reaction offers a promising approach for selective derivatization of C=C bonds, for improved detection and potential quantification of olefins.

## Scientific Background

Current sustainable aviation fuel production routes rely on olefins as intermediates, but analytical characterization of olefins in complex mixtures is limited [1]. Traditional GC-based methods cannot fully resolve olefins from cyclic paraffins or analyze high-carbon-number hydrocarbons [2]. The PB reaction, a [2+2] cycloaddition between an excited carbonyl compound and compound

[1] Wenya Hu et al., "Selective Characterization of Olefins by Paternò-Büchi Reaction with Ultrahigh Resolution Mass Spectrometry," *Analytical Chemistry* 95, no. 41 (2023): 15342–49, https://doi.org/10.1021/acs.analchem.3c02966.

[2] Kuangnan Qian and Frank P. Di Sanzo, "Detailed Analysis of Olefins in Processed Petroleum Streams by Combined Multi-Dimensional Supercritical Fluid Chromatography and Field Ionization Time-of-Flight Mass Spectrometry," *Energy and Fuels* 30, no. 1 (2016): 98–103, https://doi.org/10.1021/acs.energyfuels.5b01921.

containing C=C bond under UV light, has been successfully applied in lipidomics for double bond localization. This thesis will adapt and optimize PB derivatization for olefins characterization, screening carbonyl reagents, solvents, and reaction conditions to maximize conversion and analytical performance.

## Objectives

- Development and optimization of PB derivatization conditions for olefins in fuel-relevant matrices.
- Screening of carbonyl reagents, solvents, and additives for improved conversion and selectivity.
- Establishing UHPLC-HRMS workflow for PB product detection.
- Investigation of kinetic parameters for different olefin classes.
- Method validation using surrogate standards and application to real fuel samples.

## Key Learnings

You will learn how to:

- Perform photochemical derivatization reactions and optimize analytical workflows.
- Operate UHPLC-HRMS and interpret high-resolution mass spectrometry data.
- Apply advanced data analysis techniques for complex mixtures.
- Collaborate within a multidisciplinary team focused on sustainable fuel analytics.

## General Tasks

During this project, you will:

- Conduct PB reactions under controlled UV irradiation using various reagents and solvents.
- Prepare and purify surrogate standards for method validation.
- Perform UHPLC-HRMS analysis.
- Analyze kinetic data and evaluate reaction efficiency.
- Document findings in a written thesis according to university guidelines.

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.