

41^e journées françaises de spectrométrie de masse

30 June - 3 July 2025, Montpellier, France

PTR-TOF-MS : Addressing Instrumental and Computational Challenges

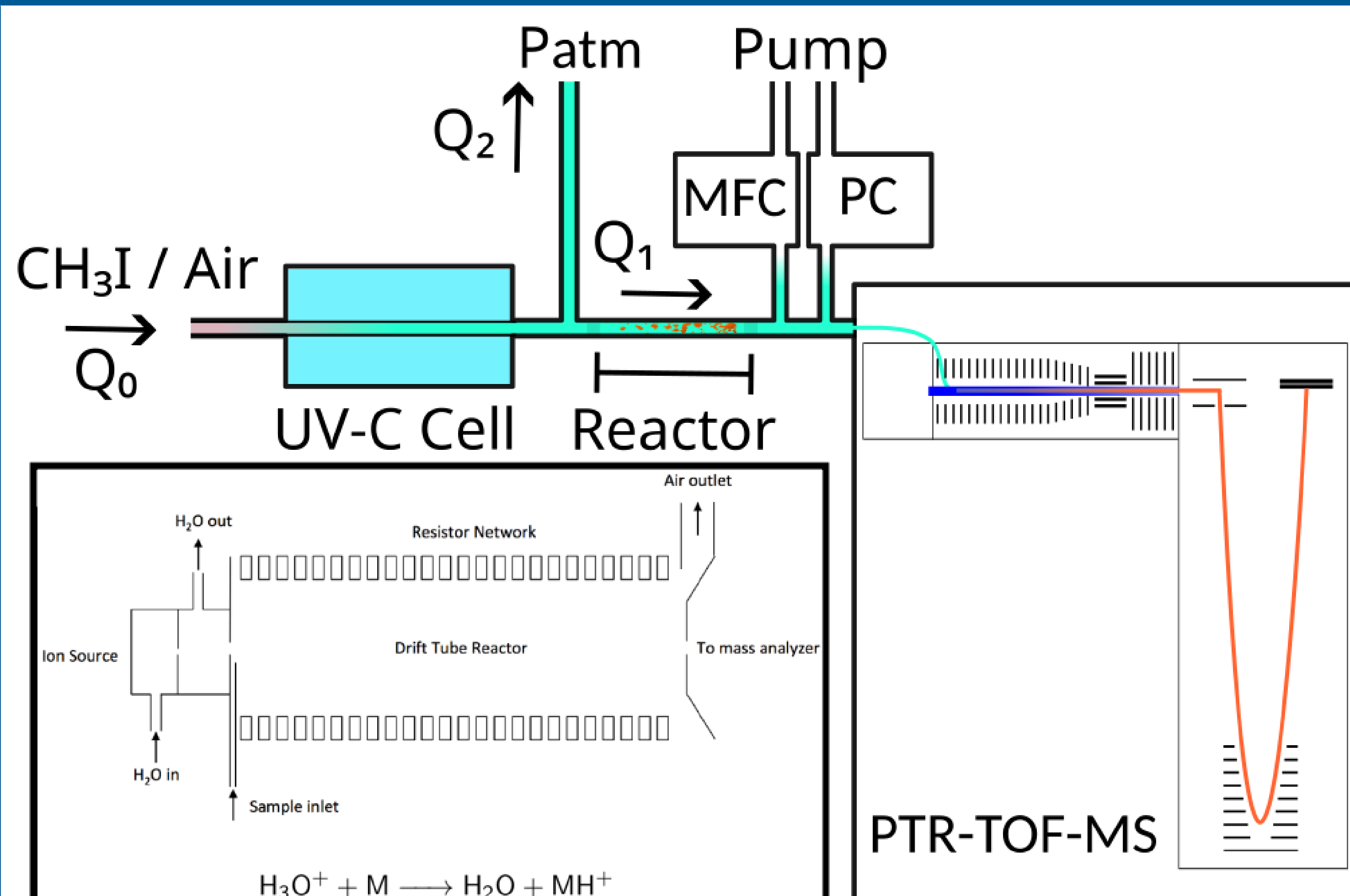
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MassSpec.jl, a Julia package for Proton-Transfer Reaction Time-of-Flight Mass Spectrometry data processing.

Initially developed as a side project during a postdoctoral contract in atmospheric chemistry at KTH Stockholm, MassSpec.jl now provides an easy-to-use solution for PTR-MS data automation. This package is distributed under MIT license. Complete documentation is available.

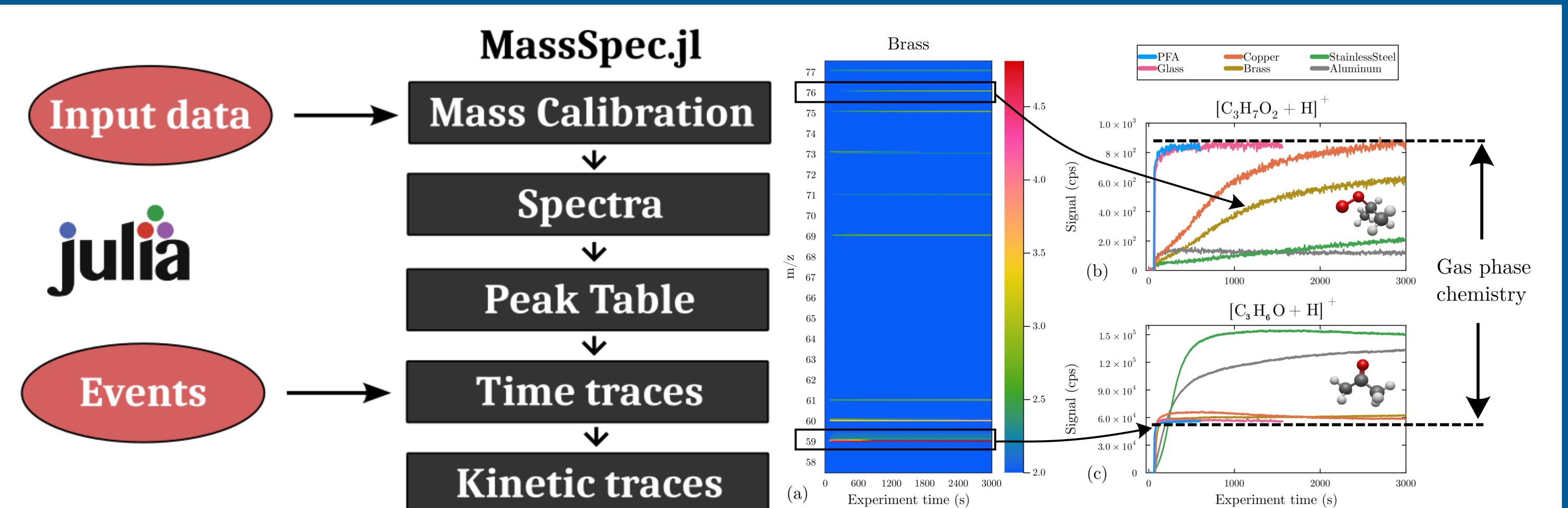
The experimental setup



Our main challenges

- High Data Volume:** Time-dependent mass spectra acquired every second. Approximately 1 GB of raw data acquired per hour.
- Detection of Reactive Intermediates:** Specific challenges in identifying and quantifying short-lived species such as peroxy radicals ($\text{CH}_3\text{OO}^\bullet$), which have low concentrations (sub-ppb) and overlapping signals.
- Complexity of the Chemical Network:** Detection of hundreds of volatile organic compounds (VOCs) in polluted environments, leading to highly congested mass spectra.

Data processing workflow

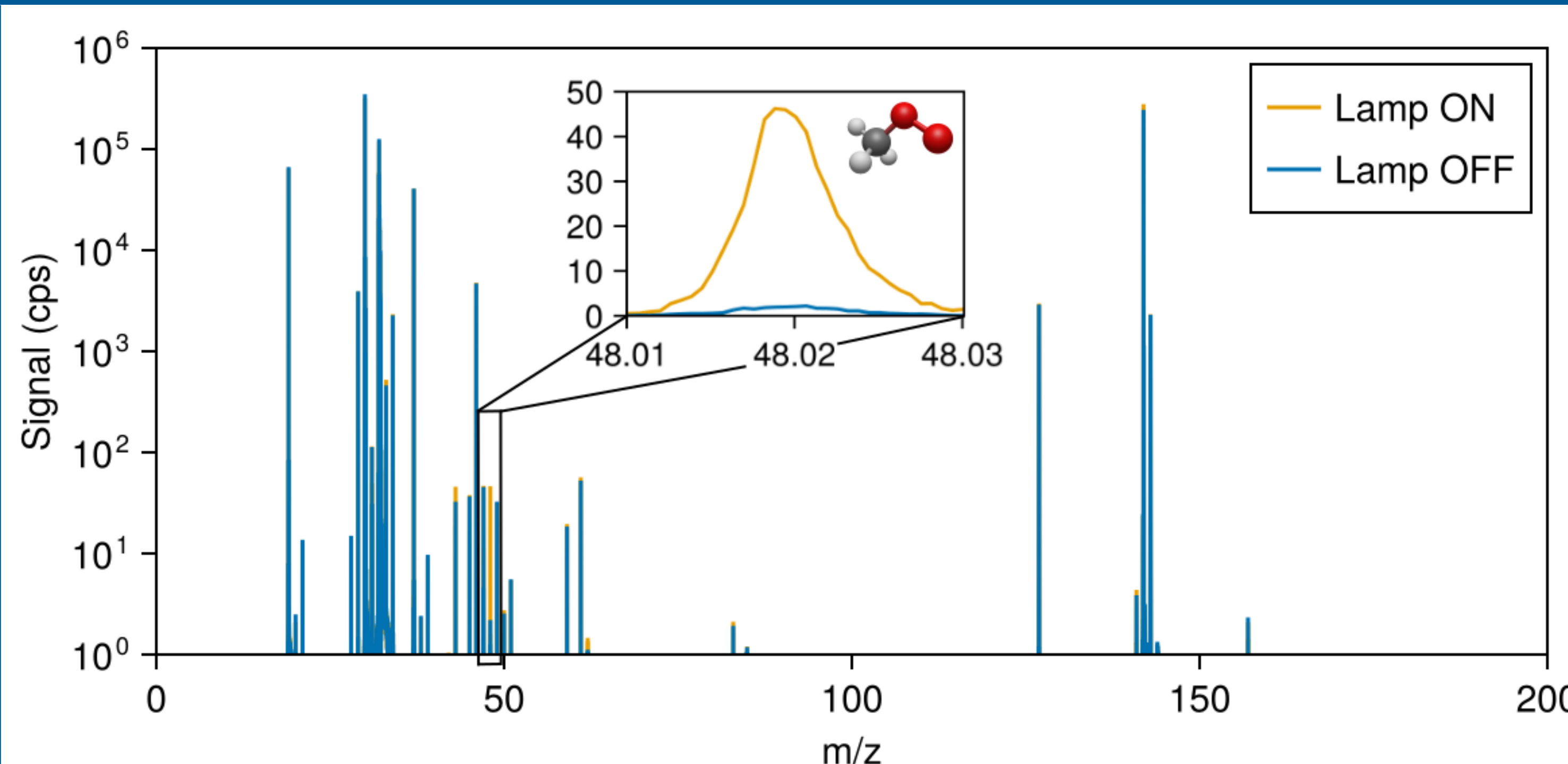


Some steps

Raw data is a big matrix: $\text{Timebin} \times \text{Acquisition}$.

- Mass calibration using 3 known peaks: $m(t) = \left(\frac{t-\beta}{\alpha}\right)^\gamma$.
- Averaging spectra with mass interpolation.
- Peak identification with peak borders defined at 2σ and molecular assignment such as: $\min(|m_i - \mu|)$, m_i is an exact mass in a catalog of about 1000 molecules, μ the expected value.
- Time traces extraction of identified peaks.
- Kinetic traces extraction, averaging time traces ranges.

Radical detection

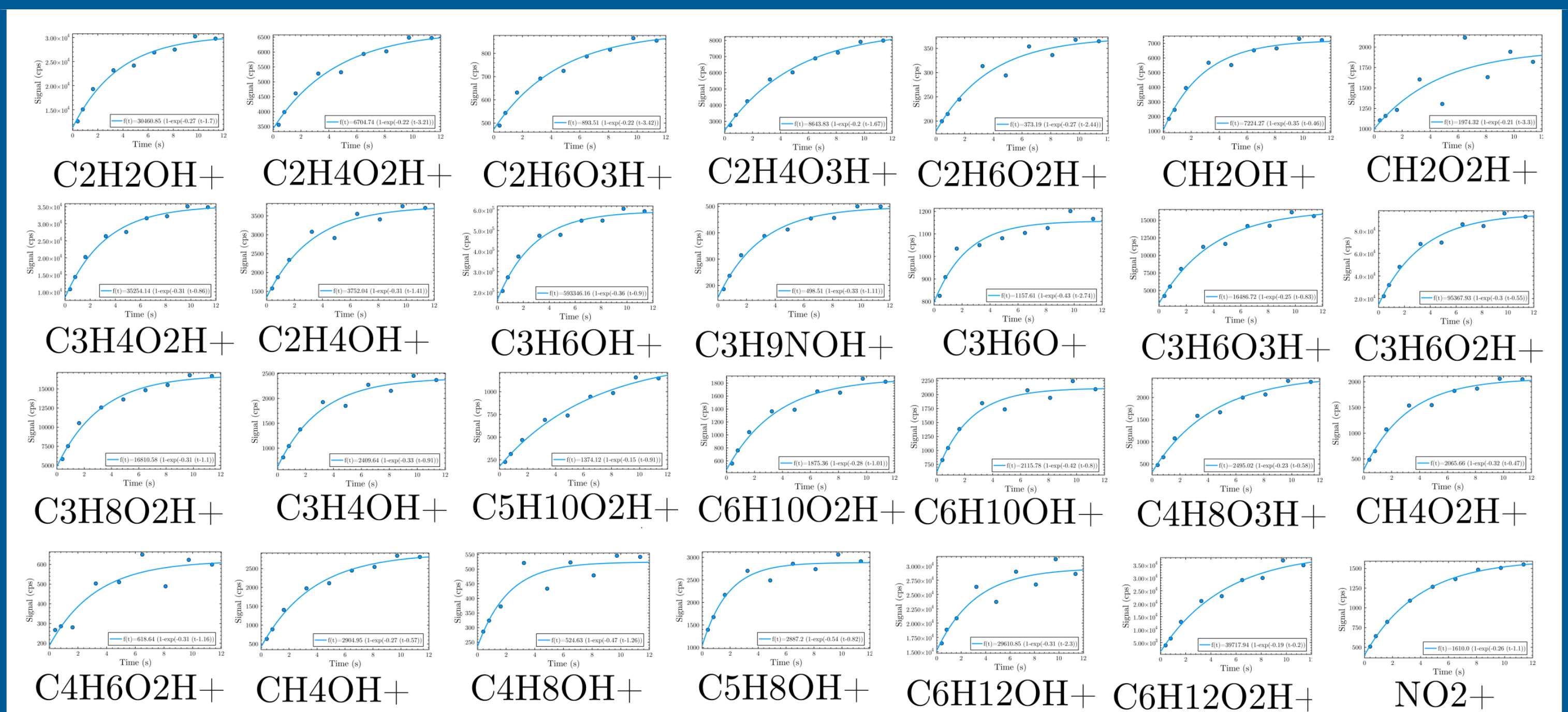


$\text{ROO}^\bullet$ unambiguously detected at ppb level (Durif et al. 2024).

Developments to be addressed

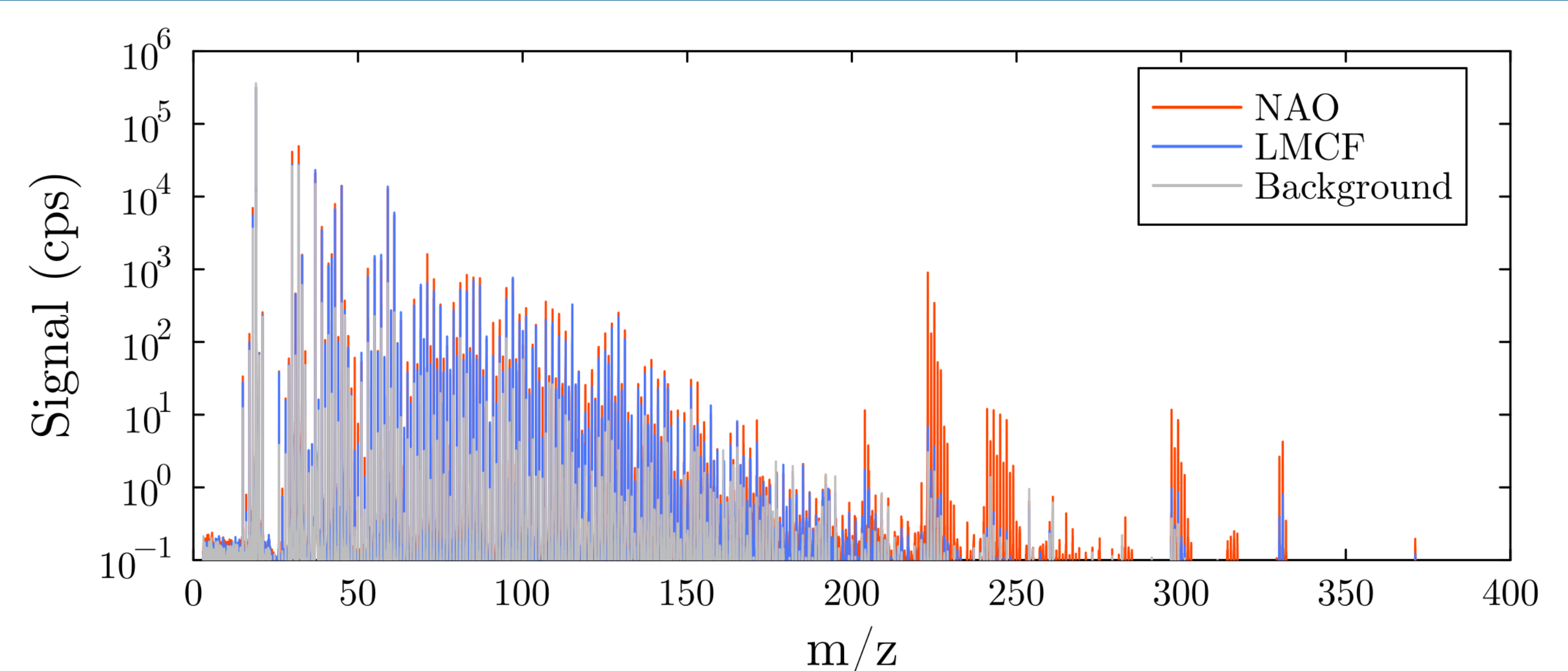
- Restructuring of input data files.
- Completion of clear documentation and code cleanup.
- Decoupling of core mass spectrometry processing from the kinetic modeling module.
- Coding a graphical interface for this program.
- Couple with AI tools to automatically compute a full PES explaining observed products.

Kinetic processing



Detected products of the ozonolysis of C_6H_{12} .

The most recent application



About 200 volatile organic compounds identified in brake wear emission (Durif et al., 2025).

Documentation:

<https://odurif.gitlab.io/MassSpec.jl/>