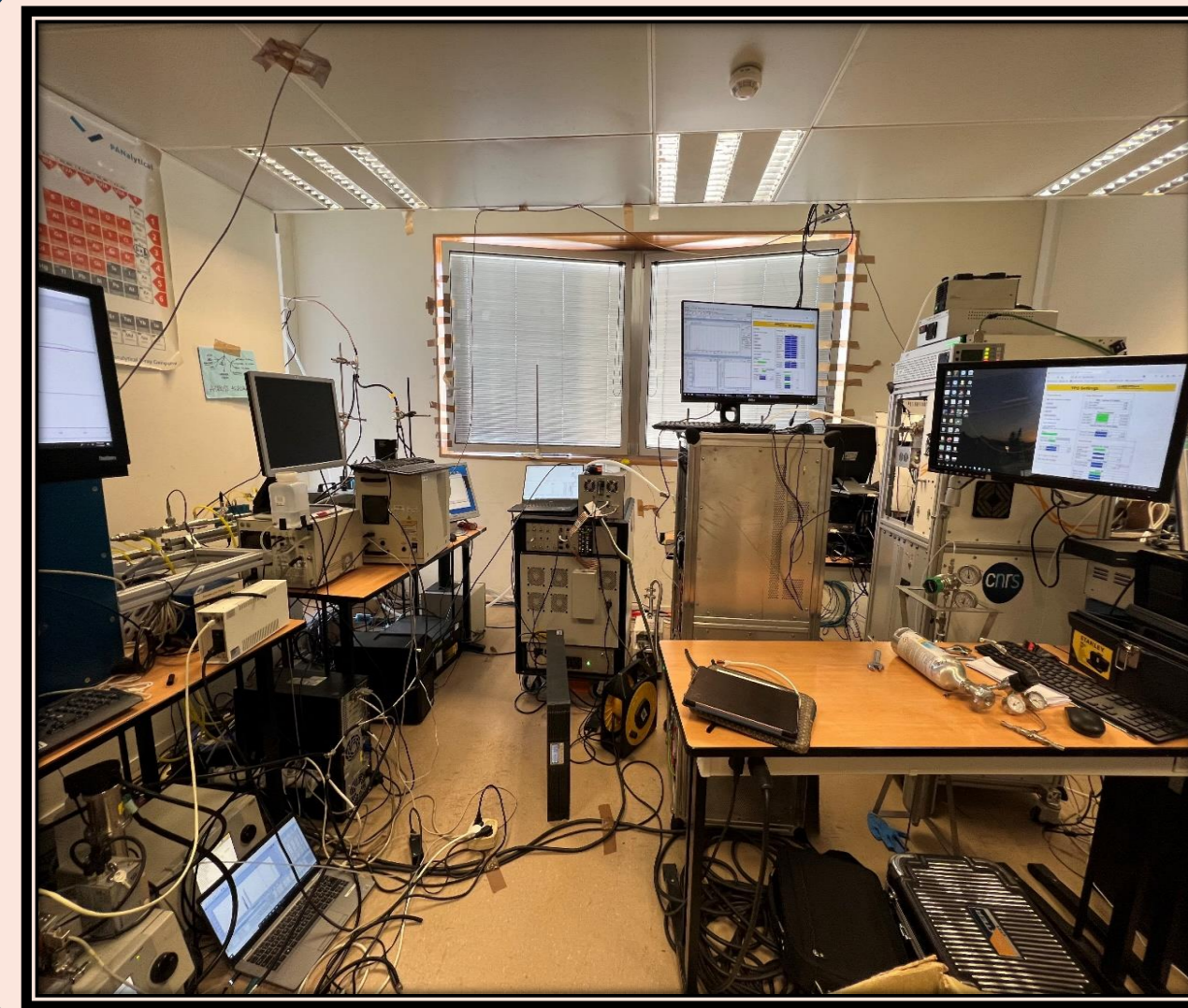


Sampling Location

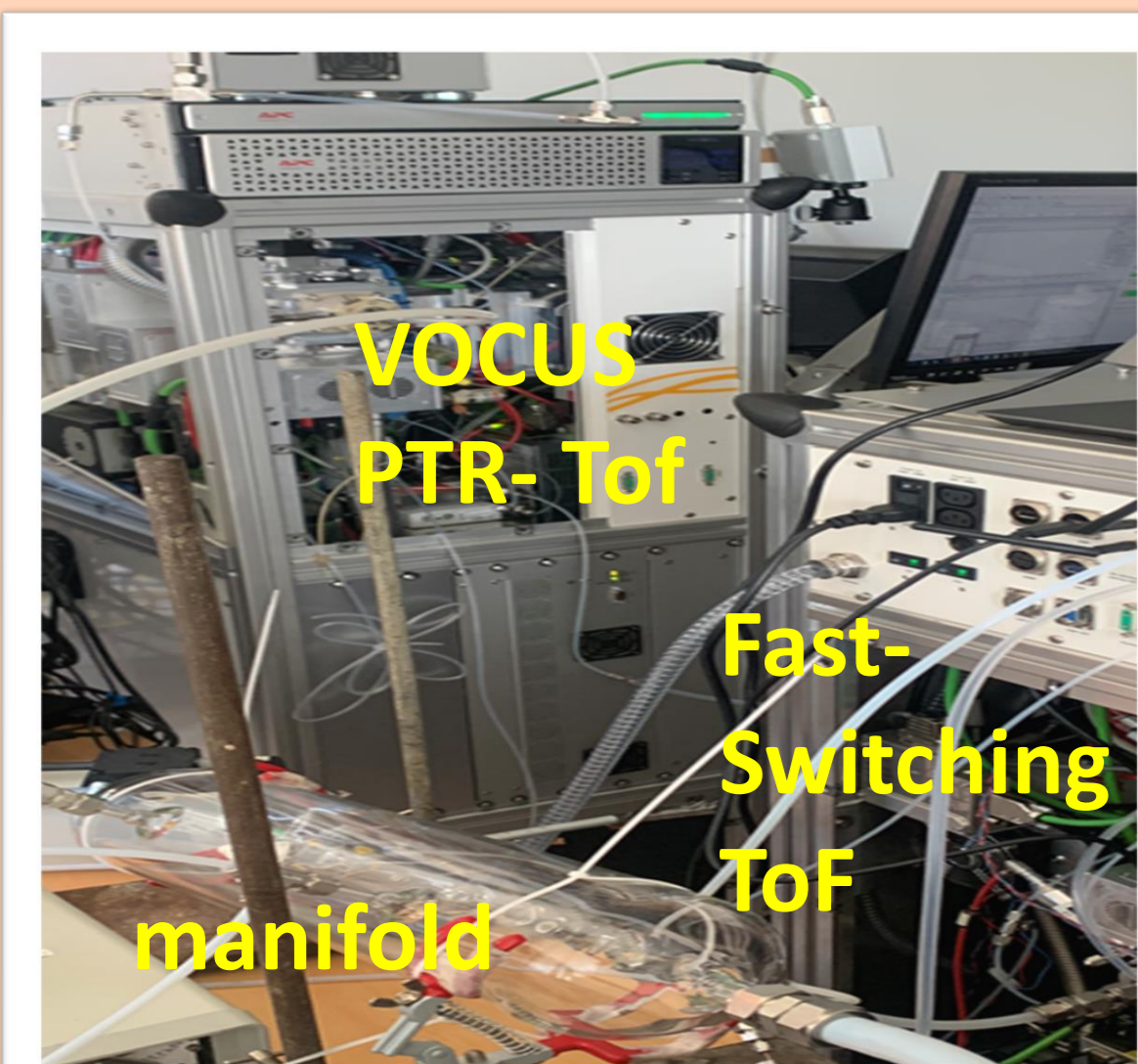


Ambient air measurements performed at Université Paris Cité (48.83°N, 2.38°E) sampling at about 25m above ground level in summer season from 13-06-2022 to 12-07-2022.

What are siloxanes and their environmental implications?

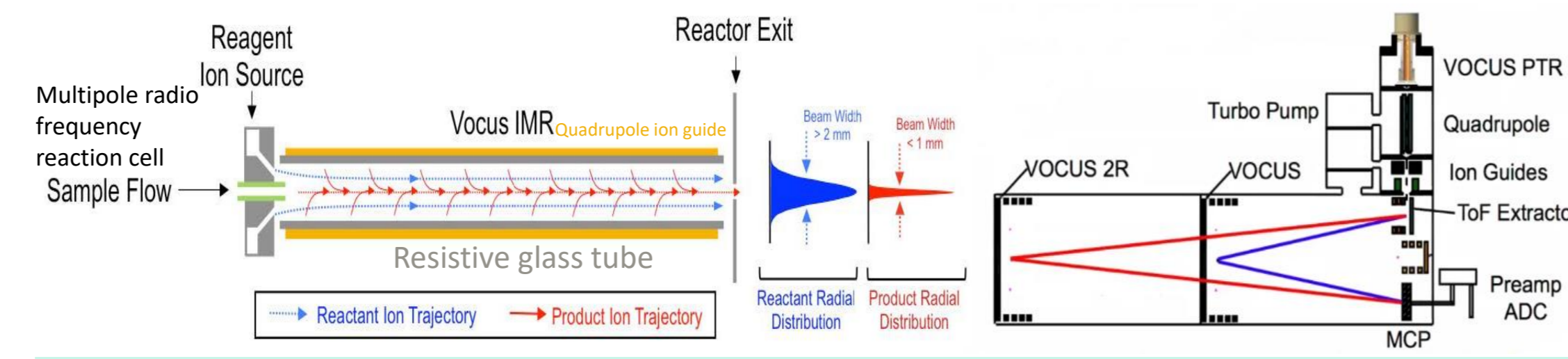
- **Cyclic volatile methyl Siloxanes (cVMS)** are silicon-based organic compounds of anthropogenic origin.
- Annual global output: 45-227*10⁴ tons
- Utilized extensively in **industrial, automotive, consumer, and personal care products.**⁽¹⁾
- 90% of the environmentally released cVMS diffuse directly into the atmosphere.⁽²⁾
- **Persistent and bioaccumulative** in the environment.
- **EU restricted use of cVMS** in certain cosmetic and personal care products, with recommendations in 2021 to restrict use in certain industrial processes.⁽³⁾

Instruments Used



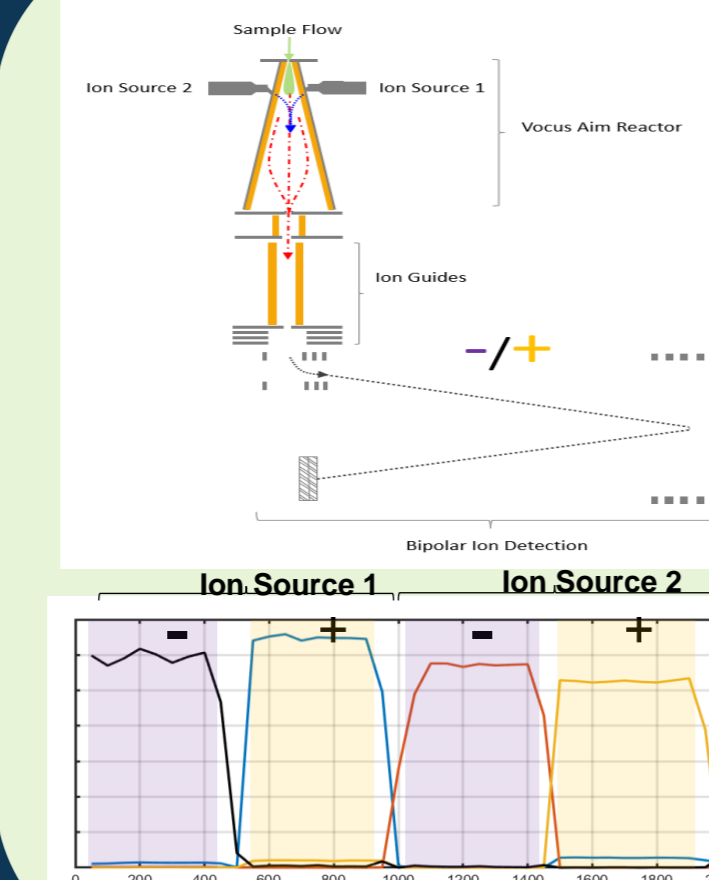
- Two time of flight mass spectrometers deployed:
 1. VOCUS PTR-ToF
 2. Fast-polarity Switching ToF
- Ambient air sampled via a Teflon tube, connected to a manifold.

VOCUS PTR-ToF-MS



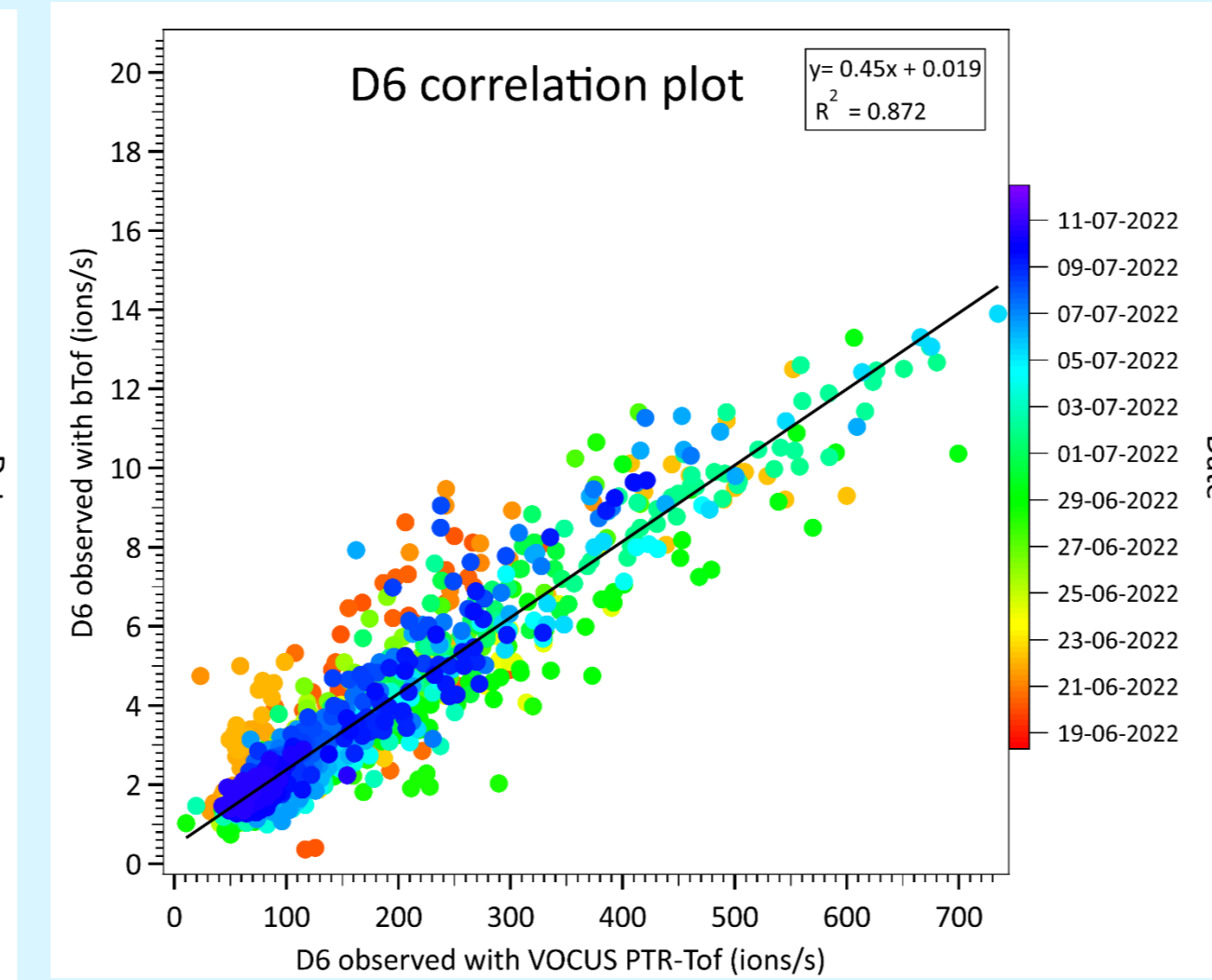
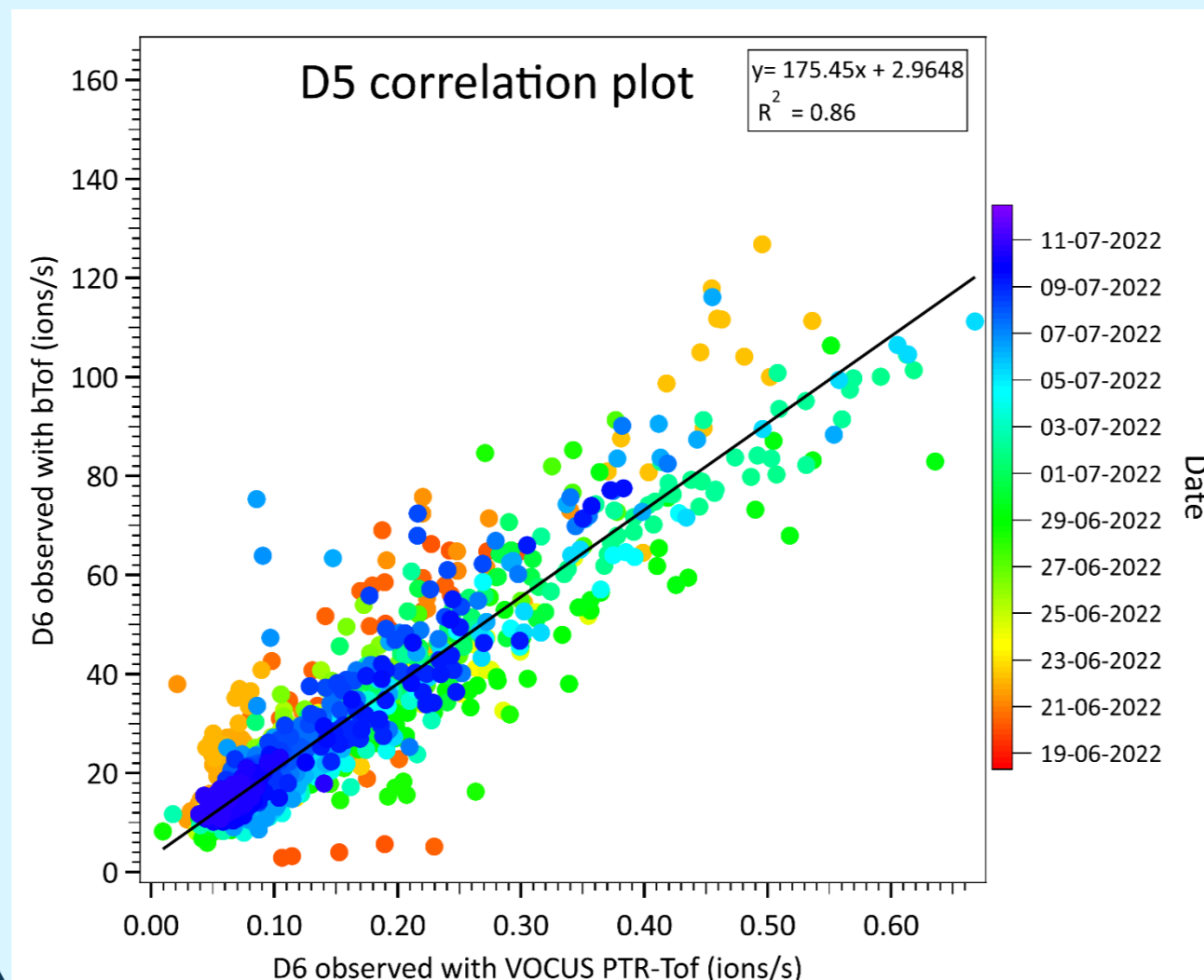
- Mass resolution: 12000
- Analytes proton affinity > reagent ion H₃O⁺/(H₂O)H₃O⁺ are detected as positively charged [M]H⁺ via proton transfer.

Fast-Polarity Switching ToF-MS (Vocus B)

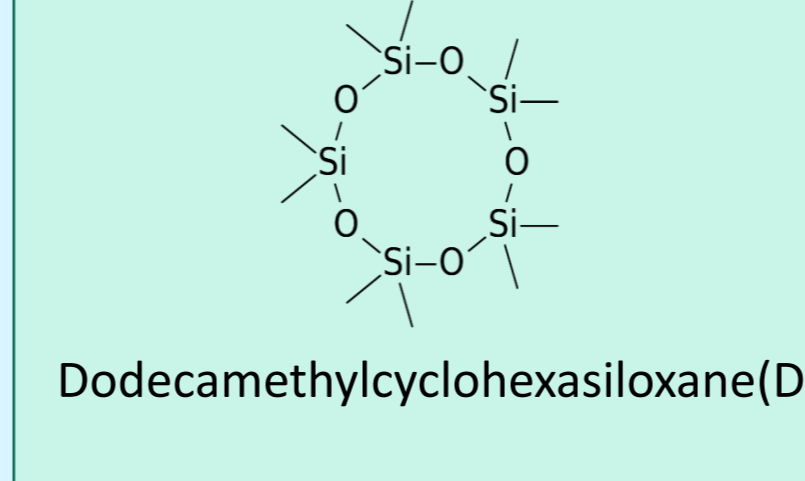
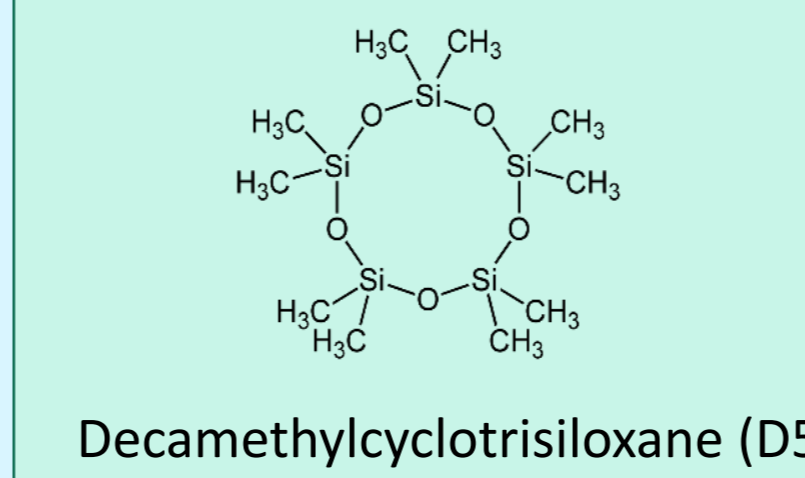
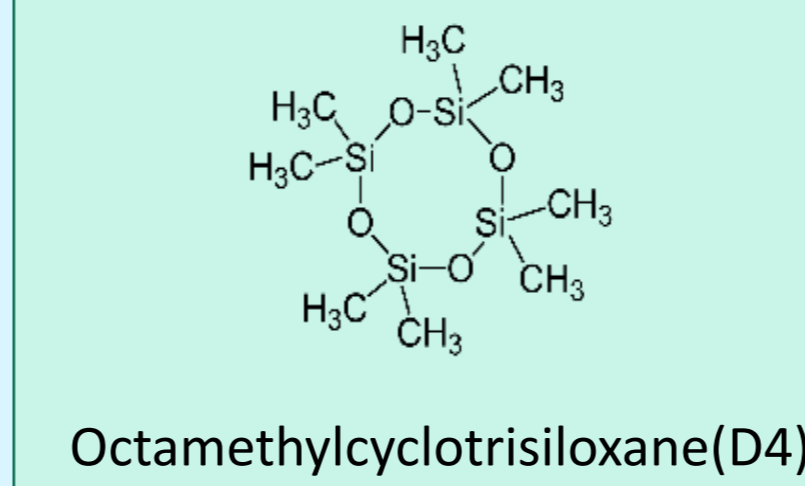
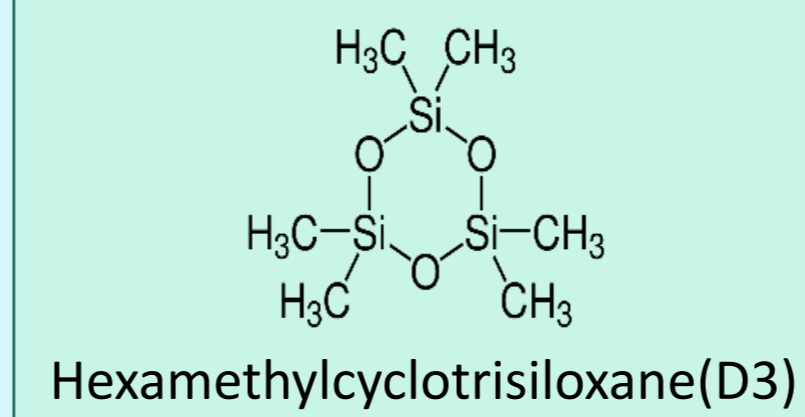


- It is a chemical ionisation mass spectrometer.
- By combining VOCUS and AIM reactor, allows ultra fast reagent ion and polarity switching.
- Analytes observed were adducted with C₆H₆⁺ or I⁻ or NH₄⁺.
- Siloxanes observed with NH₄⁺

How is the correlation between VOCUS and Vocus B for same species?

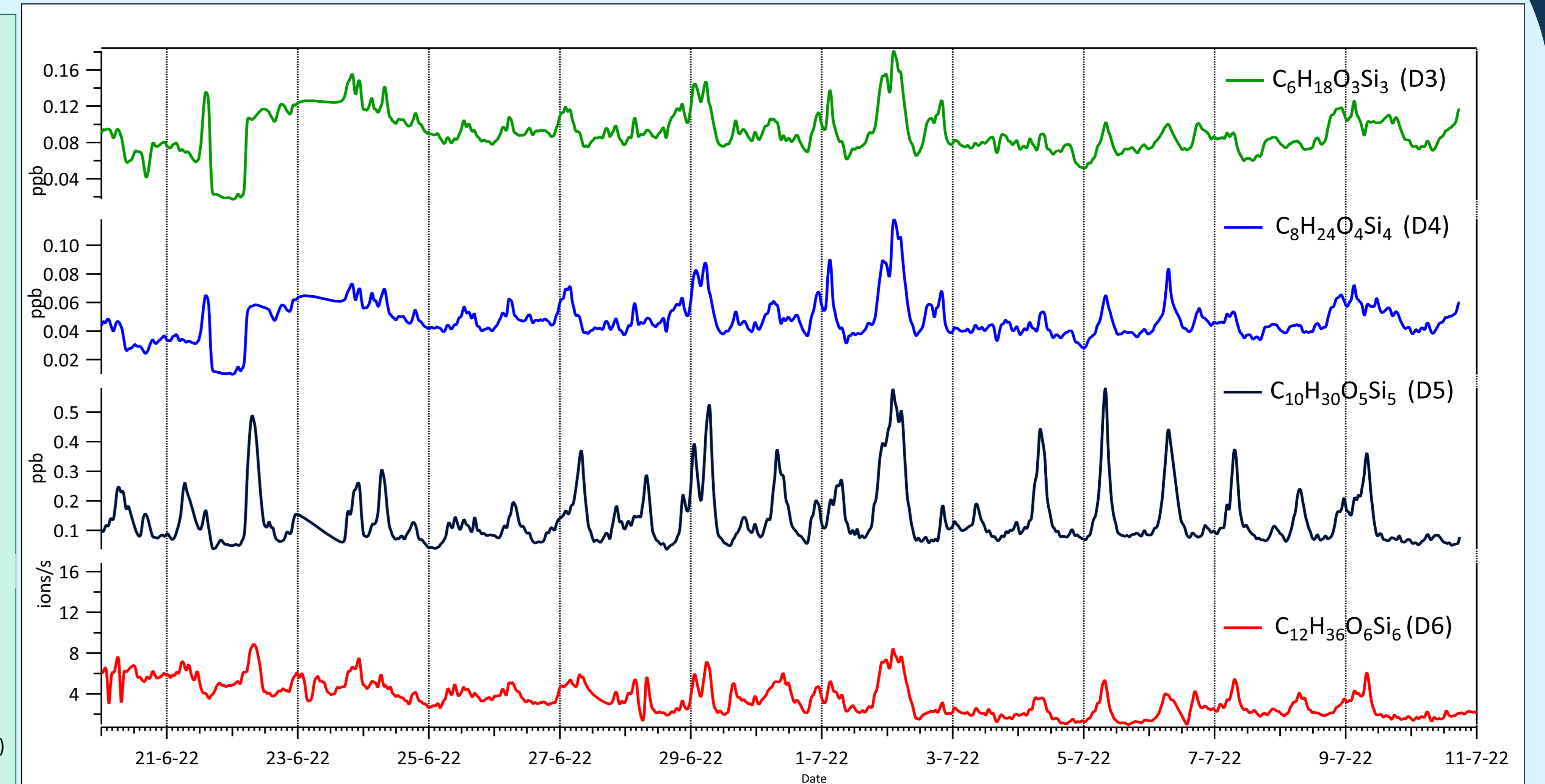


Siloxanes

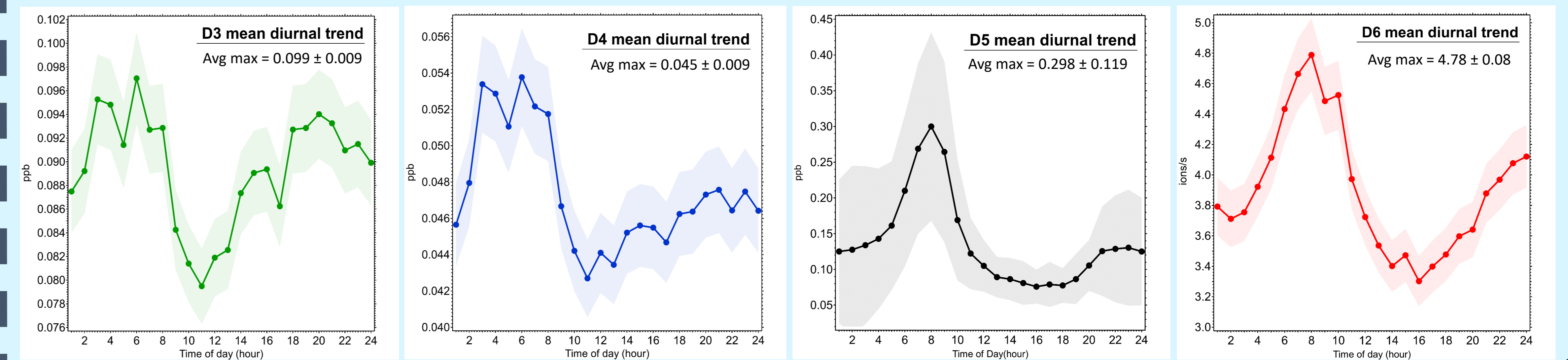


Results

Time series of observed siloxanes obtained with VOCUS PTR-ToF and Vocus B



Diurnal profiles of the observed siloxanes



Observations and Conclusions

- **HR-peak fitting** for the mass spectrum observed with both instruments was performed with Tofware (v 3.3.0), run in Igor Pro 8 environment.
- Hexamethylcyclotrisiloxane (D3), Octamethylcyclotrisiloxane (D4), Decamethylcyclotrisiloxane (D5) and Dodecamethylcyclotrisiloxane (D6), cVMS were observed.
- Observed intensities were **well correlated** for both instruments.
- **Diurnal trends** are apparent for cVMS.

- Concentrations peaked early in the morning reaching to an **averaged maximum of 0.298 ± 0.119 ppb for D5**.
- A minimum value is observed in the afternoon followed by a slight increase during the night.

FURTHER QUESTIONS?

- What are the oxidation mechanisms, pathways and oxidation products of siloxanes?
- What are the main sources of cyclic siloxanes?

