Flexibility and performance of modular "ioniTOF" Time-of-Flight platform used in PTR-TOF and APi-TOF systems

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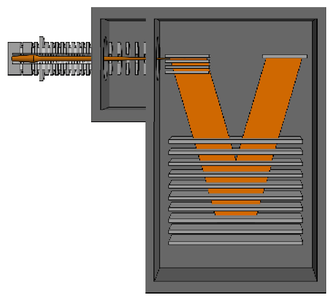
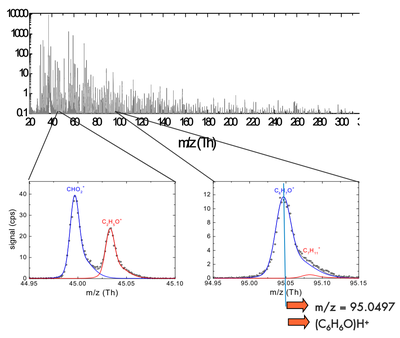
Proton-Transfer-Reaction - Mass Spectrometry



- PTR: Proton Transfer Reaction
  - "Soft" ionization of VOCs
    - low fragmentation
    - simple quantification
  - Real-time < 100 ms
  - Linearity over 6 orders of magnitude
  - High sensitivity, LOD < 1 pptv

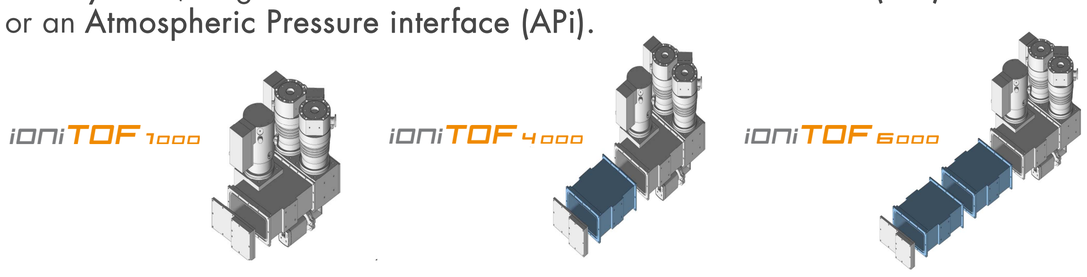


$$H_3O^+ + VOC \rightarrow VOC.H^+ + H_2O$$

- MS: Time-of-Flight Mass Spectrometry
  - High mass resolution
  - Separation of isobars
  - Identification of chemical composition

Modular Design – Fit for Flexibility

Time-Of-Flight (TOF) mass spectrometers are state of the art in fields of application where whole mass spectra are needed with high time and mass resolution [1]. Here we present a novel approach of an in-house developed **modular** TOF platform (**ioniTOF**) which can be coupled with **various sources** and **inlet systems**, e.g with an established **Proton-Transfer-Reaction (PTR) ion source** or an **Atmospheric Pressure interface (APi)**.

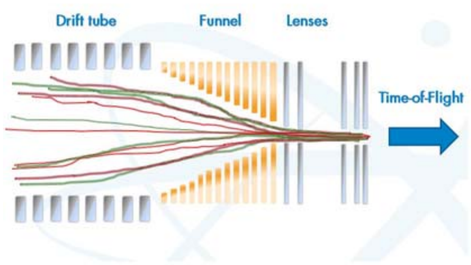


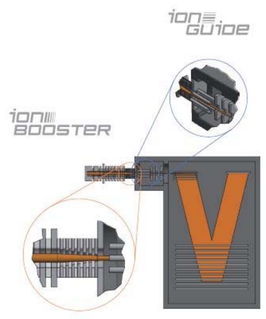
Fight path:	about 25 cm	about 45 cm	about 65 cm

- **Compact** orthogonal TOF analyzer with a length of **25 cm**
- **Ion mirror** doubles the flight path ➔ **high mass resolution** despite **small dimensions**
- **Module** of about **20 cm length** ➔ **Extension of the flight path** and **increase of the mass resolution**

Ion Funnel and Ion Guide

- Ion-funnel technology: **ION BOOSTER**
- Series of ring electrodes with **decreasing orifices** and applied **RF field**
- Combination with a Hexapole as **ION GUIDE** is possible
- **Modular design ➔ easy upgrading** of existing PTR-MS instruments
- Focusing of ions and improvement of ion transmission
- In-house built TOF platform





Performance Comparison

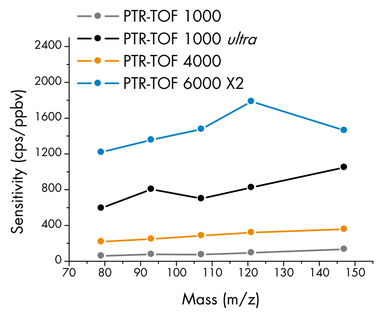


Figure 1: The **sensitivities (cps/ppbv)** are obtained by analysis of compounds from a certified gas standard (TO-14A).

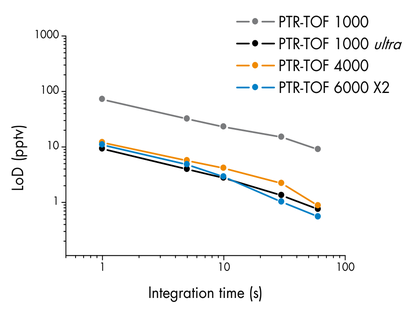


Figure 2: **Limit-of-Detection (LoD)** is calculated using the **3σ** (standard deviation) method for integration times between 1 and 60 s.

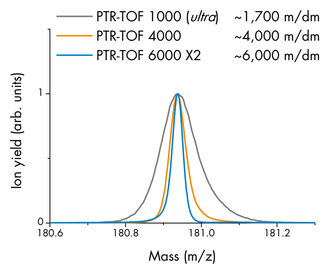
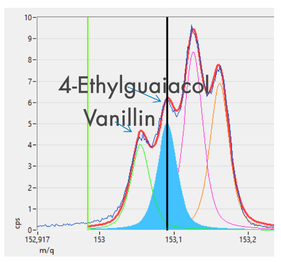


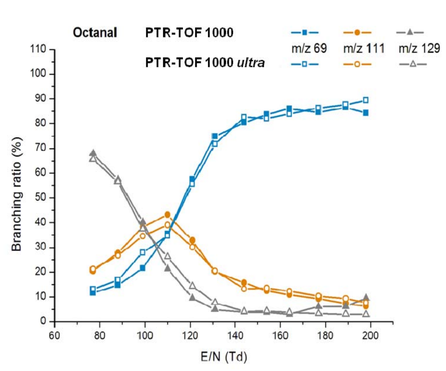
Figure 3:
Left: Mass resolution for protonated Trichlorobenzene (m/z 181). The resolutions are calculated by the FWHM method.
Right: Nosespace data of a coffee study demonstrating the high mass resolution of the PTR-TOF 6000 X2. In this example isobaric compounds in the coffee flavor can be clearly separated.

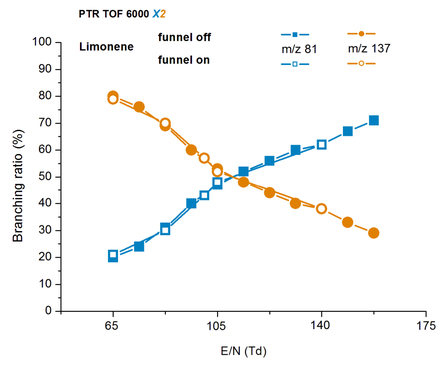


	Funnel	Ion-Guide	TOF
PTR-TOF 1000			compact
PTR-TOF 1000 *ultra*	✓		compact
PTR-TOF 4000		✓	high resolution
PTR-TOF 6000 X2	✓	✓	very high resolution

Straight forward ion chemistry

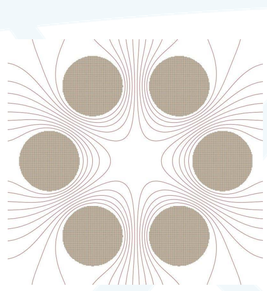
How does the RF field of the ion funnel influence the ion chemistry during the ionization process?
We analyzed the fragmentation pattern of compounds whose product ion branching ratios strongly depend on the reduced electric field in the drift tube **(E/N)**. Two such compounds, **octanal** and **limonene,** were measured with and without ion funnel (**see Figure below**). By adjusting the RF amplitude and the DC voltages of the ion funnel in the **PTR-TOF 1000 *ultra*** and the **PTR-TOF 6000 X2** we could reproduce the branching ratios with an error well below 10%. Our modular ion funnel clearly improves the instrumental sensitivity while not considerably changing the ion chemistry. Branching ratios and calculated concentrations remain accurate.

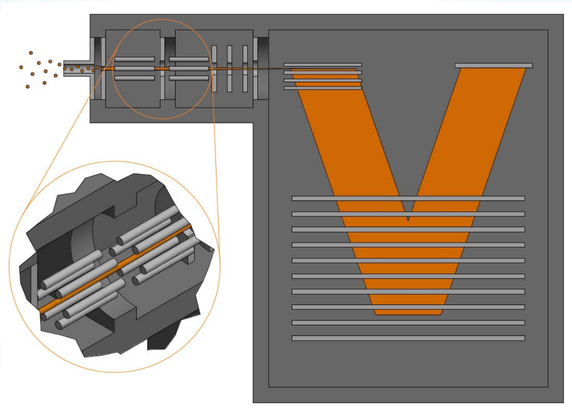




APi-TOF

We have developed a novel **Atmospheric Pressure interface (APi; see scheme below)** for the analysis of positive as well as negative ions in the environment. The system, which has been designed to be coupled with the ioniTOF platform, consists of an atmospheric pressure interface with a **critical orifice** for contact free sample introduction and a hexapole ion guide for **high ion transmission** efficiency over a broad m/z range (in contrast to common quadrupole ion guides). By combining two virtually identical versions of this setup with opposite polarity into one rugged and compact instrument, **both ion polarities can be detected simultaneously in real-time**.





References

[1] A.M. Ellis, C.A. Mayhew, In: Proton Transfer Reaction Mass Spectrometry: Principles and Applications, Chichester, UK: John Wiley & Sons, Ltd (2014).

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