



# Applications



## > Food & Flavor Science:

### Real-Time Aroma Release Monitoring Analysis of Complex Flavors < 1 pptv

#### FOOD & FLAVOR ANALYSIS WITH PTR-MS

Aroma and its perception can influence buying decisions. It is therefore indispensable for the industry to understand what we smell and taste when e.g. drinking a cup of coffee or enjoying a fresh strawberry, at the very moment the flavor molecules hit our receptors.

Flavor and taste of food can also vary over time, depending on raw materials or production processes etc. For a consistent brand image however, the aroma quality of food should remain stable.

Coping with requirements such as very high time resolution, basically real-time and direct air sampling are challenges to traditional analytical techniques.

In order to provide scientists and the industry with a better understanding of sensory perception, IONICON provides real-time VOC analyzers and is the market leader in Proton Transfer Reaction – Mass Spectrometry (PTR-MS).

#### MAJOR REASONS FOR USING PTR-TOFMS

- ▶ Monitoring of real-time variations in aroma
- ▶ Head-space analysis without sample preparation
- ▶ Direct mouth- & nose-space air analysis
- ▶ Rapid screening of complex aroma systems
- ▶ Suitable for chemometric datamining

#### PTR-TOFMS SERIES

- > High time-resolution and sensitivity
- > High mass resolution
- > Rapid screening for complex aroma
- > Real-time high-throughput sampling

Find out more:

[www.ionicon.com/food-flavor](http://www.ionicon.com/food-flavor)

## REAL-TIME FOOD & FLAVOR RELEASE ANALYSIS WITH PTR-TOF 6000 X2

In food and flavor science researchers are often confronted with highly complex matrices. Thus, in order to separate compounds of interest from other compounds which share the same nominal  $m/z$  but have a different chemical composition (isobars), very high mass resolution is of utmost importance. The benchmark for highest mass resolution for substance separation is the IONICON PTR-TOF 6000 X2 which reaches over 6200  $m/\Delta m$  (see Fig. 1). PTR-TOFMS unlike quadrupole based analyzers can separate isobars well and are therefore ideally suited for the measurement of complex aroma systems.

### HIGH MASS RESOLUTION

To demonstrate the benefit of this outstanding resolution we analyzed the nosespace of a person who had consumed some freshly brewed coffee. It is well known that vanillin and 4-ethylguaiacol are important isobaric aroma compounds at nominal  $m/z$  153 (protonated molecules). However, by looking at the mass spectrum around  $m/z$  153 in Fig. 2 one can see that there are in fact four ions which share this nominal mass (black line). For a low resolution instrument (e.g. quadrupole-based), all four ions would be merged into one broad mass spectral peak and only the intensity of the sum of them could be measured. The high mass resolution of the PTR-TOF 6000 X2 enables separation of all four ions. With IONICON's sophisticated data processing software the intensities are automatically deconvoluted (grey and blue lines; the orange line is the sum of the deconvoluted peaks, which perfectly reproduces the original data) and vanillin and 4-ethylguaiacol can be quantified independently, without parasitic influence of the two additional isobars.

### HIGH SENSITIVITY & THROUGHPUT

High sensitivity is particularly important when compounds of extremely low abundance have to be quantified with high time resolution. Utilizing the high sensitivity PTR-TOF 6000 X2 we analyzed the nosespace of a person before (blank) and after drinking freshly brewed coffee. In Fig. 3 concentration values of a flavor compound at  $m/z$  149.063 are shown during this experiment with a time resolution of 700 ms. Although this important aroma compound is present only in trace concentrations below 1 ppbv, the high sensitivity and low limit-of-detection of the PTR-TOF 6000 X2 allow for online quantification of the aroma development over numerous breath cycles after swallowing the coffee in real-time.

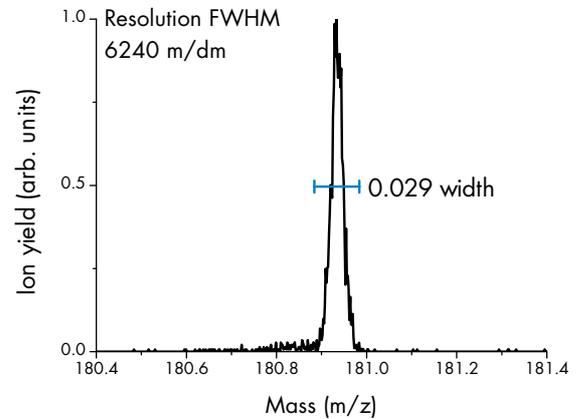


Fig. 1: Mass resolution of trichlorobenzene peak, detected by a PTR-TOF 6000 X2 instrument: over 6200  $m/\Delta m$  (FWHM).

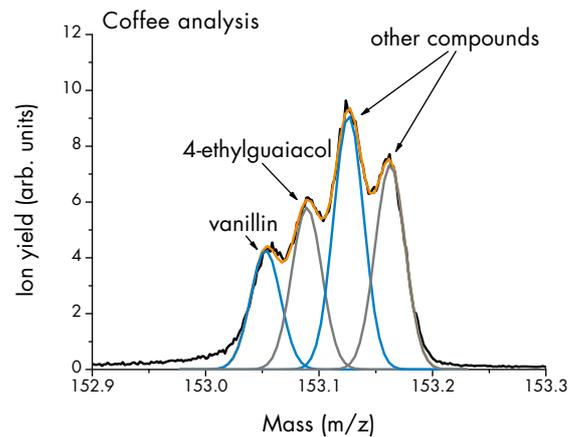


Fig. 2: Nose-space air analysis of coffee flavor demonstrates high mass resolving power of PTR-TOF 6000 X2.

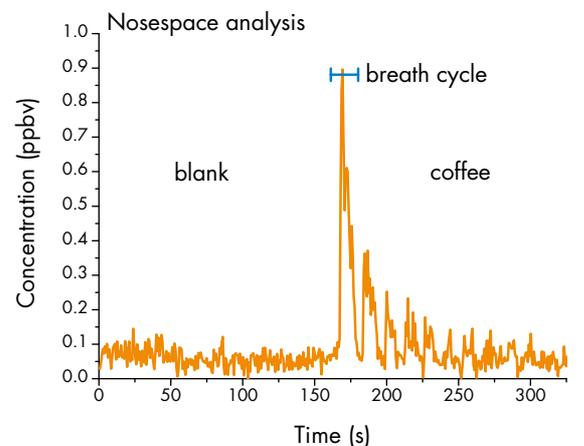


Fig. 3: Quantification of 3-mercapto-3-methylbutyl formate at  $m/z$  149.063 with a time resolution of 700 ms and a concentration < 1 ppbv.