Applications

> Food & Flavor Science:

Chocolate aroma analysis with Next-Gen PTR-TOF instruments

ADVANTAGES OF NEXT-GEN PTR-TOF

The use of PTR-MS for the investigation of the food chemistry of chocolate is well established. Therefore, this application is predestined to demonstrate the amazing benefits of IONICON's latest instrumental developments, which generally take PTR-MS to the next level.

Recently, we performed an extensive food and flavor study comparing our ultimate-resolution trace VOC analyzer PTR-TOF 10k and equally high resolving but even more sensitive FUSION PTR-TOF 10k, to a common high-resolution PTR-TOF instrument. While the 10k instruments are equipped with the ioniTOF 10k platform which enables mass resolutions of 10 000 – 15 000 m/Δm, the comparison device was tuned to more common 5 000 m/Δm. The aim of the study was to identify the main advantages of exceptionally high mass resolution but also what extreme sensitivity can achieve for food and flavor science.

FUSION PTR

- > Ultimate sensitivity
- > Ultra-high mass resolution
- > Resolving complex flavor matrix
- > Real-time high-throughput sampling

Find out more:
www.ionicon.com/food-flavor

NEXT-GEN PTR-TOF PERFORMANCE
MORE RESOLUTION, MORE SELECTIVITY

Both, the PTR-TOF 10k and the FUSION PTR-TOF 10k offer Next-Gen mass resolution between 10 000 and 15 000 m/Δm.

The level of analytical detail which is revealed by stepping up from 5 000 to 15 000 m/Δm is nearly unbelievable. Fig. 1 shows the example of nominal m/z 147 in the mass spectrum of exhaled breath after the consumption of salt-caramel flavored chocolate. Where previously only two slightly "deformed" peaks were visible, with Next-Gen mass resolution no less than nine peaks can be separated and easily identified. The resolved isobars comprise important aroma constituents like benzalacetone (C10H10O) and butyl lactate (C7H14O3) as well as metabolism and lab-air compounds.

The invaluable advantage of this selectivity becomes even more obvious during the analysis of nosespace air. Trimethylpyrazine (C7H10N2; protonated m/z 123.092) is of utmost interest, as it belongs to the key aroma compounds of cocoa and chocolate. The isobar C9H14 on the other hand is an omnipresent VOC which can be detected at high concentrations in indoor air. With 5 000 m/Δm the two molecules can hardly be distinguished, while at 10 000 m/Δm two clearly separated peaks are visible in the mass spectrum (Fig. 2).

With the PTR-TOF 10k, where the two isobars can be quantified independently, the concentration of trimethylpyrazine in blank nosespace (up to cycle ~100 s in Fig. 3) is only at about 20 pptv, i.e. the signal is not masked by C9H14 from room air. Therefore, the release of trimethylpyrazine into the nosespace can be effectively monitored with sub-second time resolution.

MORE SENSITIVITY, MORE SPEED

The FUSION PTR-TOF 10k is equipped with a revolutionary reaction chamber and outperforms common PTR-MS devices with a stunning sensitivity of up to 80 000 cps/ppbv. In food and flavor research such an extreme sensitivity can be crucial when the available time per measurement is strongly limited but still high quality data need to be produced.

In a proof-of-concept test, we sampled the headspace above differently flavored chocolate pieces at room temperature. After only 1 s of measurement time, the relative errors of the relevant aroma compounds were already below 1 percent. This means that even in the 100 ms region, excellent data quality can still be expected.

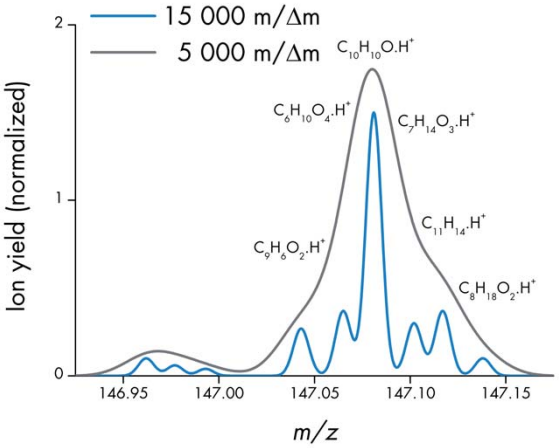

Fig. 1: Mass spectra comparison based on data from a PTR-TOF 10k; with 15 000 m/Δm nine peaks can be separated and identified.

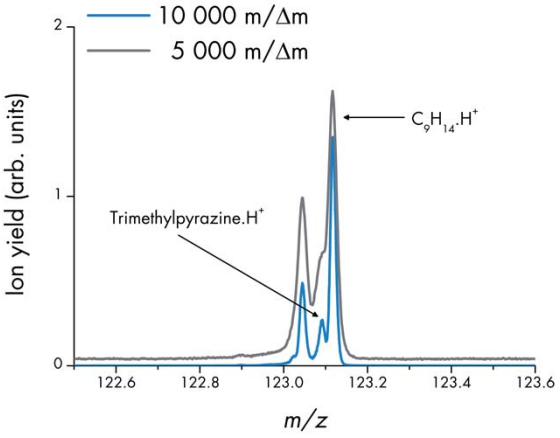

Fig. 2: Nosespace analysis - Trimethylpyrazine peak clearly visible at 10 000 m/Δm, whereas at 5 000 m/Δm it is masked by the dominant room air isobar C9H14.

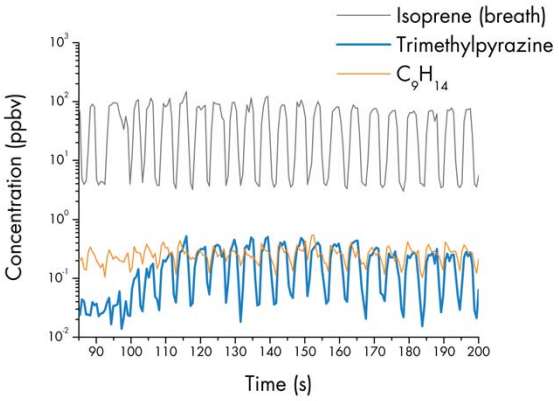

Fig. 3: Real-time quantification of trimethylpyrazine in nosespace during the consumption of chocolate.