NEXT-GEN PTR-MS TASTES CHOCOLATE

The chocolate benchmark: benefits for complex aroma real-time analysis
with new high-performance IONICON PTR-TOF instruments

One of the main fields of application of proton transfer reaction–mass spectrometry (PTR–MS) is food and flavor science. Here, we present a recent study on one of the world's most popular foods: chocolate. We demonstrate how IONICON's Next-Gen PTR-TOFMS take chocolate analysis to the next level.

Direct sample injection without the need for any sample preparation, real-time quantification, extremely high sensitivity, and detection limits in the low pptv region within less than one second are just the perfect prerequisites for in-vivo and in-vitro foodstuff analysis. PTR-MS unites all of these benefits. Thus it is not surprising that over the past 25 years, countless PTR-MS studies have been published on samples ranging from various drinks, dairy products, fruits and vegetables, meat, snacks, and, of course, chocolate.

IONICON's Next-Gen PTR-TOFMS: chocolate analysis with unmatched insights

Real-time nosespace analysis during the consumption of chocolate is very challenging for analytical instrumentation because the nosespace gas not only consists of chocolate compounds, but also of chemicals present in room air and substances originating from human metabolism. Many of these compounds are isobars with only small differences in exact m/z but huge differences in intensity.

IONICON's PTR-TOF 10k, which offers a mass resolution of 10,000 to 15,000 m/Δm, is ideally placed to meet this challenge. We find that above 10,000 m/Δm, up to nine peaks per nominal m/z can be identified in chocolate nosespace. With such an excellent mass resolution, we can quantify the release of trimethylpyrazine – one of the key aroma compounds of chocolate – into the test subject's nosespace, while the close isobar C_9H_{14} is present in room air at high concentration.

The PTR-TOF 10k perfectly separates relevant isobars, and thus takes selectivity to the next level. It also enables aroma monitoring with sub-second time resolution in the pptv region.

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 high-quality data is required. In a proof-of-concept test, we sampled the headspace above differently flavored chocolate pieces at room temperature. After only 1s 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.
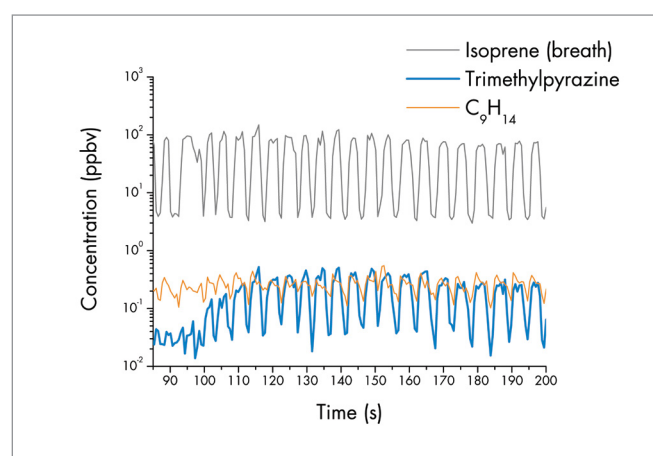

Figure 1. Real-time quantification of trimethylpyrazine in nosespace during the consumption of chocolate.

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