Fast Analysis of Beer Aroma with GC-PTR-MS

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Terpenes and other aroma compounds determine the unique flavors that affect consumers' wine and beer preferences. Proton transfer reaction mass spectrometry (PTR-MS) is a fast and sensitive method for the analysis of volatile organic compounds (VOCs), including these aroma compounds. However, the analysis of alcoholic beverages by PTR-MS is challenging because the high-concentration of ethanol titrates the instrument, preventing the accurate measurement of lower concentration VOCs that are present in the liquid or headspace. Moreover PTR-MS cannot distinguish between isomers, such as different monoterpenes or sesquiterpenes, which have the same elemental composition but different molecular structures.

To quantify low concentration VOC isomers, a fast gas chromatogram (GC) - which can separate isomers - was coupled in line with a TOFWERK Vocus 2R PTR-TOF. As ethanol elutes from the GC well before most aroma compounds, quantitative flavor analysis of alcoholic beverages becomes possible.

Figure 1 demonstrates analysis of beer headspace with the Vocus GC-PTR-TOF.

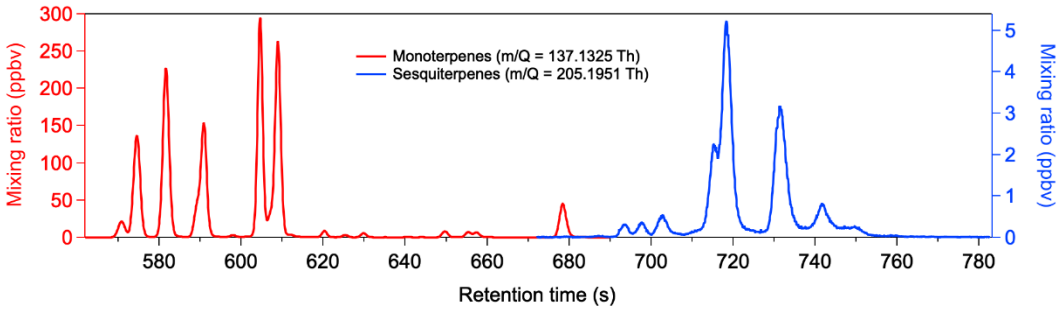

***Figure 1 GC-PTR-MS chromatograms of terpenes in the headspace of a beer sample**. Data were acquired with a Fast GC coupled to a Vocus 2R PTR-TOF. The overall analysis time was approximately 15 min. Beer headspace was sampled for 30 s before injection into the Fast GC column that was then ramped from room temperature to 225°C.*

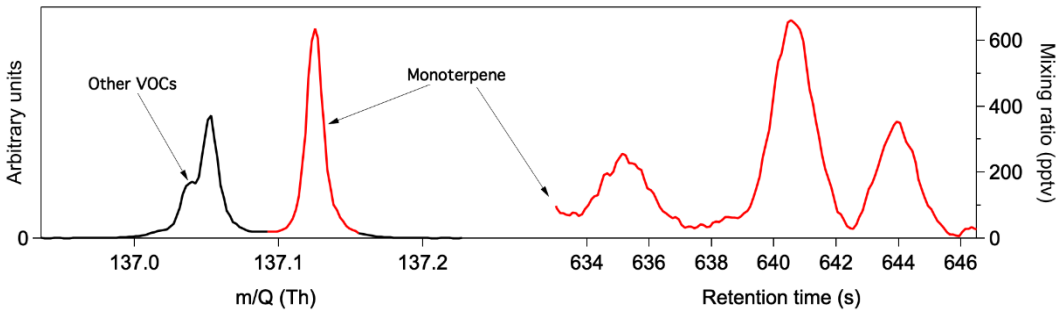

Figure 2. Mass spectral separation of terpenes from isobaric species. *In addition to the need for chromatographic separation of isomers, accurate characterization of terpenes (or other compound classes) by GC-PTR-MS requires that the mass analyzer can resolve any co-eluting compounds that have identical nominal mass and accurately identify species of interest based on exact mass. For example, these data show that at retention time 640 seconds the Vocus 2R resolves multiple compounds at nominal mass 137 Th and treats only the peak at 137.1325 Th as monoterpene signal.*

Mass spectral peaks at mass/charge 137.1325 Th and 205.1951 Th were determined to be monoterpenes and sesquiterpenes, respectively, by exact mass analysis. Figure 2 shows an example this analysis, whereby the TOF resolves terpenes from co-eluting VOCs having similar mass/charge. The numerous chromatographic peaks observed at each of these mass/charge values in Figure 1 are isomeric monoterpenes (red) and sesquiterpenes (blue).

Several isomers of each compound class are baseline separated allowing easy quantification. Detecting and resolving these low concentration species with fast GC relies on the high speed (10 mass spectra per second) and sensitivity (10000 cps/ppbv) of the Vocus PTR-TOF.

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