

Rapid Quantification of “Brett” Off-Flavor Compounds in Wine

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Brettanomyces yeast live on grapes and oak barrel surfaces. Commonly called “Brett”, this yeast can introduce unwanted compounds into wine, most notably 4-ethylphenol (4-EP) and 4-ethylguaiacol (4-EG). Above certain concentrations, these off-flavor compounds yield unpleasant odors that are described with terms such as “barnyard.” Detection of these compounds for quality control of wine is of interest to producers and consumers, alike.

This work demonstrates use of a TOFWERK Vocus 2R PTR-TOF (proton transfer reaction time-of-flight mass spectrometer) for rapid quantification of 4-EP in wine samples. The automated method, which can be used for simultaneous characterization of various flavor compounds, directly analyzes the headspace of wine with no sample preparation. A fast gas-chromatographic (GC) separation isolates compounds of interest from the high-concentration ethanol,

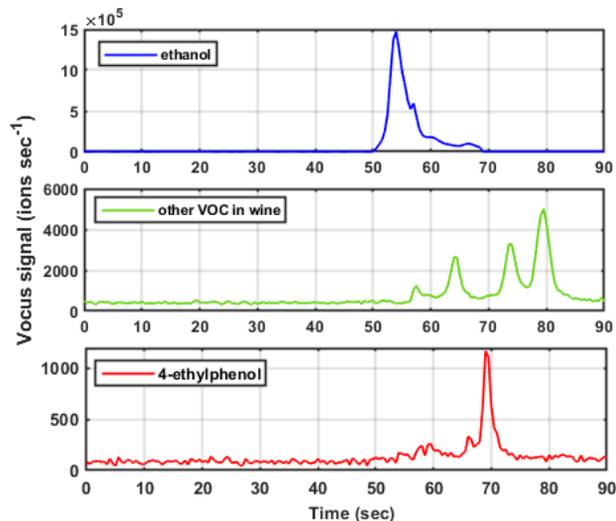


Figure 1 Stacked gas chromatogram of a wine sample spiked with 10 ug/L of 4-ethylphenol, detected with a Vocus 2R PTR-TOF. The fast separation is employed primarily to exclude high-concentration ethanol, which is known to prevent online PTR-MS analysis of VOCs in alcohol-containing beverages. It further contributes to analysis by partially resolving the detected VOCs before the mass spectral measurements.

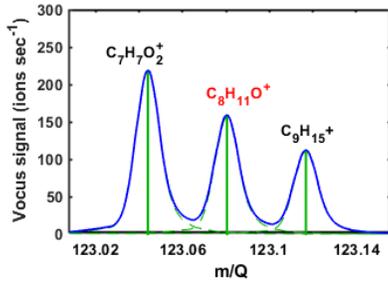


Figure 2 Portion of the Vocus 2R mass spectrum recorded at GC retention time of ~68 sec. The 4-ethylphenol peak ($C_8H_{11}O^+$, 123.0804 Th) is resolved from isobaric VOCs, allowing identification and quantification.

which is known to saturate PTR mass spectrometers and thereby limit online analysis of other compounds in alcoholic beverages. The Vocus 2R serves as the detector, acquiring a complete mass spectrum at each time point in the gas chromatogram. Compounds are then identified using a combination of retention time and exact mass and quantified based on the intensities of mass spectral signals. Analysis of a single sample is complete in 90 seconds, enabling high-throughput quality control measurements.

Figure 1 shows an example fast gas chromatogram for a wine sample

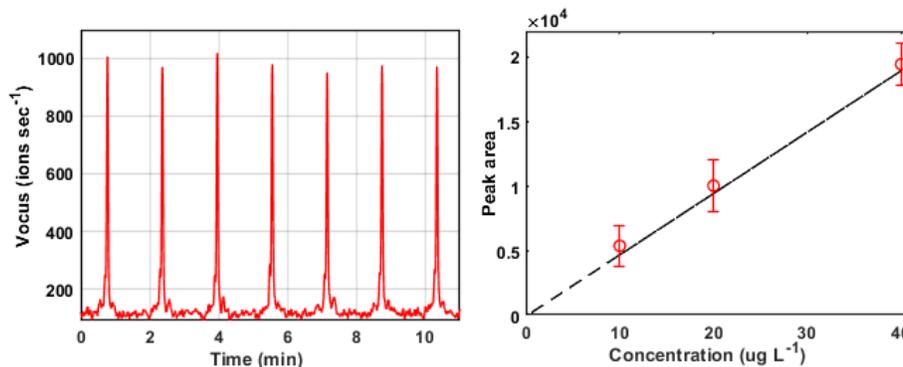


Figure 3 Left) Repeated measurements of a wine sample spiked with 20 ug/L of 4-ethylphenol, demonstrating the throughput and repeatability of the method. Right) Integrated signal of 4-EP in wine samples with controlled concentration of 4-ethylphenol. Error bars correspond to three standard deviations.

spiked with 4-EP. The separation excludes ethanol and partially resolves the numerous volatile organic compounds (VOCs) present in wine. The signal for 4-EP (red) peaks at a retention time of ~68 seconds. The relevant portion of the mass spectrum recorded at this retention time is presented in Figure 2. The Vocus 2R clearly separates the 4-EP from isobaric compounds that have the same retention time, enabling confident identification and quantification of the compound.

Figure 3 presents results for repeated, automated measurements of wine samples spiked with different concentrations of 4-EP, demonstrating the reproducibility and linearity of the technique. The limit of detection for 4-EP was determined to be 3 $\mu\text{g/L}$, well below the human sensory threshold (≈ 140 $\mu\text{g/L}$).

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