Rapid Detection of TCA Off Flavor in Coffee with the Vocus CI-TOF

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The TCA Taint Problem

Aroma is fundamental to a consumer's perception of coffee quality and critical to their acceptance or disproval of the final product. Aroma complexity is derived from a variety of volatile organic compounds (VOCs) which are perceived directly by the nose before consumption, by ortho-nasal olfaction, and during consumption, by retro-nasal olfaction. Some of these VOCs constitute the coffee "bouquet" while unwanted VOCs, the so-called "off flavors", cause bad aroma and lead to the consumer's reduced appreciation or rejection of the product. 2,4,6-Trichloroanisole (TCA) is a well-known off-flavor VOC. Our perception of TCA is very powerful since humans can perceive extremely low concentrations of this compound. In water, TCA contamination of 1 ng/L – corresponding to one person out of all mammals living on earth – leads to a taint perception.

Similar to coffee, TCA is of utmost importance in wine [1], accounting for more than 80% of off flavoring. In wine, TCA origin is related to tainted cork stoppers. Such taint derives from the microbial conversion of 2,4,6-trichlorophenol into 2,4,6-trichloroanisole in the cork's tree. Being a localized phenomenon, TCA contamination can occur at different levels for cork stoppers belonging to the same batch. Therefore, within the same batch, some cork stoppers have high levels of TCA contamination, while others may be clean. This variation necessitates the need to screen each cork stopper independently in order to ensure TCA levels are below the sensory threshold and avoid unnecessary losses. This screening of every cork is fulfilled by the Vocus Cork Analyzer. This solution was the subject of a recent study, which showed that the analyzer could detect TCA concentrations well below the human sensory limit [2].

TCA presence and its associated taint is a wide-spread problem in several food matrices, not only inducing an unpleasant smell but also inhibiting ciliary transduction channels [3]. The latter finding means that TCA reduces flavor perception. Such effect is proportional to TCA concentration and occurs even for contaminations below the sensory perception of TCA [3]. The plethora of food products where TCA could occur (often at concentrations below the sensory threshold) includes coffee. The origin of TCA in coffee is still unknown. Some coffee beans can be tainted with TCA that survives the roasting process. The resulting problem is twofold. On the one side, TCA

contamination can cause taint perception if the concentration in the coffee is above the consumer's sensory threshold. On the other side, it could suppress coffee flavor perception, even at concentrations not directly perceived.

TCA Detection at Ultra-Low Concentration by the Vocus CI-TOF

The Vocus CI-TOF is the only instrument that detects TCA at concentrations below the sensory threshold in just three seconds. It has been successfully implemented for TCA screening of natural cork stoppers and here we demonstrate the detection of TCA in coffee.

Ground green coffee beans belonging to eight different batches were subject to both sensory analysis and direct injection headspace analysis by the Vocus CI-TOF. In the experiment, 700mg of coffee powder was placed in a small flask at a controlled temperature with a continuous flow of VOC-free, synthetic air purging the flask. The coffee powder headspace was sampled directly via heated transfer line into the Vocus CI-TOF.

Four coffees (A, B, C, D) were described as tainted upon sensory analysis. The other four coffees (E, F, G, H) were described as not tainted. Figure 1 reports the spectra measured by the Vocus CI-TOF, averaged over 3 second measurements for two coffees (A and G). The theoretical isotopic pattern of TCA is reported on the same figure. Coffee A shows the presence of spectral peaks unambiguously related to TCA at m/z 209.9400 (corresponding to the ion $C_7H_5Cl_3O^+$), 211.9371 and 213.9341 (corresponding to $C_7H_5Cl_3O^+$ isotopologues). Contrary to this, the spectrum of Coffee G does not show any presence of TCA. The excellent agreement between sensory assessment and assessment with the Vocus CI-TOF for TCA in all eight coffee batches is evident in Table 1 which reports the peak area of the ion $C_7H_5Cl_3O^+$ as well as the corresponding sensory evaluation.

This work demonstrates the capability of the Vocus CI-TOF for the fast estimation of TCA contamination in green coffee bean batches, in agreement with sensory evaluations.

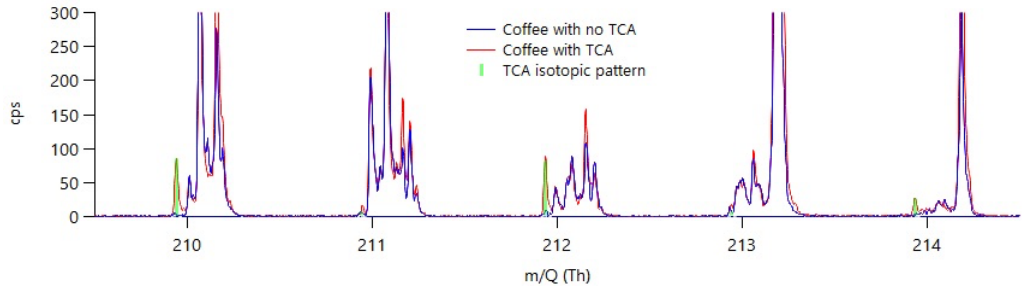

Figure 1. *Vocus CI-MS mass spectra of two green coffee bean powders. 3-s average spectra are reported. Red: Green coffee bean powder described as TCA-tainted by a trained sensory panel. Blue: Green coffee bean powder described as TCA-free by a trained sensory panel. Green: Isotopic pattern of TCA. Unambiguous identification of TCA in the red spectra is made possible upon the excellent agreement between the measured spectra and the theoretical TCA isotopic pattern.*

Batch (ground coffee)	Vocus CI-TOF TCA (cps) mean ± std	Sensory
A	45 ± 3	TCA present
B	127 ± 28	TCA present
C	231 ± 36	TCA present
D	166 ± 13	TCA present
E	0 ± 5	clean
F	4 ± 9	clean
G	2 ± 1	clean
H	5 ± 2	clean

Table 1. *Comparison between TCA assessments by sensory and the Vocus CI-TOF on eight batches of green coffee bean powder. The Vocus signal is reported as mean ± standard deviation over three biological replicates.*

References

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