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Programme and Abstracts

MONITORING VOLATILE COMPOUND RELEASE IN COFFEE WITH PTR-TOF-MS: FROM SINGLE BEAN ROASTING TO BREWED COFFEE

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In this study proton transfer reaction-time of flight-mass spectrometry (PTR-ToF-MS) was used for the analysis of volatile compounds released from coffee in different aspects of technological and fundamental relevance. Firstly, the applicability of PTR-ToF-MS to discriminate three ground coffee samples from three different countries was tested [1]. The methodology is then applied on increased number of coffee origins by testing both coffee powder and coffee brew [2]. PTR-ToF-MS was operated in three different ionization modes (H_3O^+ , NO^+ , O_2^+) and the classification efficiency of each ionization agent was tested by supervised classification methods. Lastly, a methodological approach was developed on offline headspace volatile profiling of individual coffee beans during roasting. A single coffee bean was roasted up to 25 minutes and the volatiles were analyzed after every minute.

Direct analysis of the headspace of coffee (both powder and brew) allowed origin discrimination with low classification error. Merging the information obtained by the three different ionization agents increased the overall classification efficiency. Monitoring the volatile emissions of single-coffee beans roasted for different times allowed the investigation of roasting dynamics and also its relation with raw material characteristics.

In conclusion, direct, fast and rapid volatile detection with PTR-ToF-MS allows the characterization of coffees in different conditions (single bean, powder, brew) and the identification of volatile markers of origin.

REFERENCES

[1] Yener, S. et al., *Journal of Mass Spectrometry* 49, 929-935 (2014)

[2] Yener, S. et al., *Food Research International* 69, 235-243 (2015)