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Non-Target Screening Approaches in Coffee Research–Opportunities and Challenges †

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Abstract: Mass spectrometric non-target screening (NTS) is a powerful analytical strategy applied, among others, in environmental analysis, metabolomics, and foodomics. It is well suitable for the analysis of complex sample sets and can be used to compare, evaluate, and assess these. For the analysis of coffee, NTS provides new insights into the chemical composition of coffee samples, the formation, and degradation of compounds during fermentation processes, and eventually helps to find marker compounds, specific for certain processes and qualities.

Keywords: non-target screening; polarity-extended chromatography; metabolomics; foodomics; fermentation; mass spectrometry

1. Introduction

This study will explain new approaches to mass spectrometric data acquisition from highly complex sample matrices, such as orthogonal serial HILIC-RPLC coupling hyphenated with a modern high-resolution mass spectrometry (HRMS) system (see Figure 1) and data processing using robust and retrospective useable data.

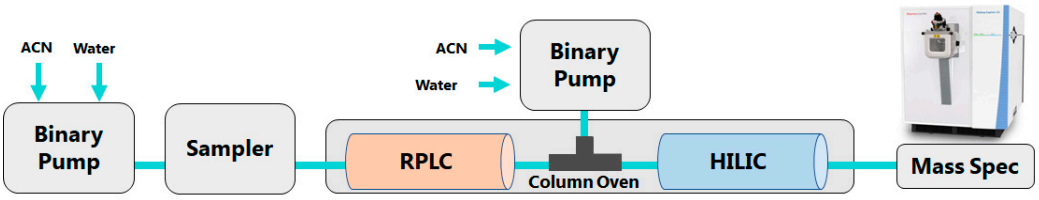

Figure 1. Scheme of the applied NTS analysis technique (reproduced with permission from Bieber and Letzel [1]).

2. Materials and Methods

Various sets of coffee beans (green and roasted) were extracted with a mixture of methanol:water (H_2O) 80:20 (v:v) and filtrated each. The injection volume was 10 µL. The chromatographic setup consisted of an LC system (Thermo Fisher Scientific, Germering, Germany) with two binary pumps, an autosampler, and one column oven, which contained a HILIC and a RPLC column coupled in series via a T-piece (Thermo Fisher Scientific, Germering, Germany). The RP separation was carried out on a ThermoFisher Accucore C18, (50 × 2.1 mm, 2.6 µm) and the HILIC separation on a ThermoFisher Synchronis HILIC (100 × 2.1 mm, 1.7 µm), respectively. The mobile phase of the RP separation pump was a gradient using for solvent A: H_2O/acetonitrile (ACN) 95/5 (*v*/*v*) with 5 mM ammonium acetate (NH_4Ac) and for B: ACN/H_2O 95/5 (*v*/*v*) with 5 mM NH_4Ac and was a gradient using solution A: ACN and solution B: H_2O/ACN 95/5 (*v*/*v*) for the HILIC separation pumps, respectively. Detailed information on the gradients and the mass spectrometric

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hyphenation with an Orbitrap Exploris 120 mass spectrometer (Thermo Fisher Scientific GmbH, Dreieich, Germany) can be found elsewhere [1].

3. Results and Discussion

To enhance the analytical performance in this study, cutting-edge data evaluation strategies are applied, and data interpretation concepts are used and discussed. The presentation will especially describe an exemplary workflow for finding so-called "features" in coffee samples obtained from different fermentation processes. Such "features" reflect the retention time (i.e., polarity) of unknown molecules, their accurate mass (i.e., empirical formula), their intensity, and their fragmentation spectra (i.e., structural information). See an example of an exemplary retention time–mass plot in Figure 2.

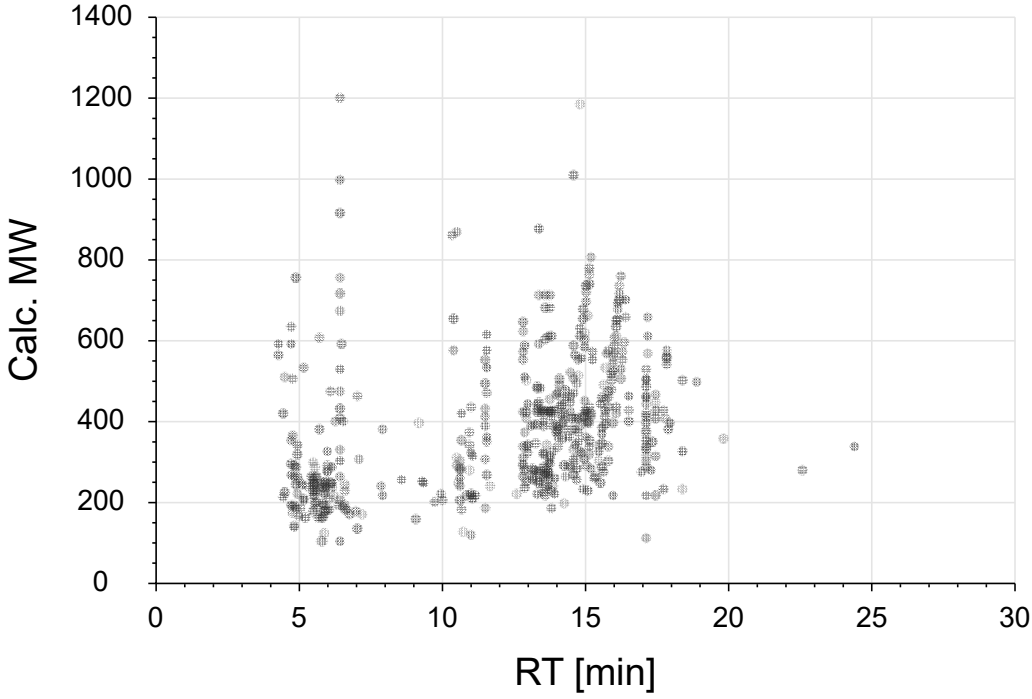

Figure 2. Exemplarily retention time–mass plot presenting various but specific "features".

The statistical comparison of "features" from different samples can be used to gain insight into fermentation processes and track compound formation processes during coffee bean roasting. Combined with meta-data from samples, these comparisons can help to monitor sample authenticity and to find potential (process) markers for such "fingerprints", as shown in Figure 2. Ultimately, this can provide new insights into the basic processes of coffee fermentation and roasting.

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Conflicts of Interest: Authors Letzel and Bieber are employed by the company Afin-TS GmbH. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Reference

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