

EXHALED BREATH ANALYSIS FOR THE DETERMINATION OF FOOD CONTAMINANTS

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Introduction

- In 2019/2020, around **10 million tones of coffee** were consumed worldwide [1].
- Many **compounds** have been identified coming from coffee [2, 3] and most of them come **after the process of roasting**, giving its specific taste and smell.
- Pyridine and furfuryl alcohol (FA)** are two of the most abundant compounds appearing **in breath** after coffee consumption (Fig. 1).
- As those compounds might be **harmful for human health** [4], they can be considered **food contaminants**.
- The aim of the work is to **identify and quantify** food contaminants after ingestion by using **breath analysis**.

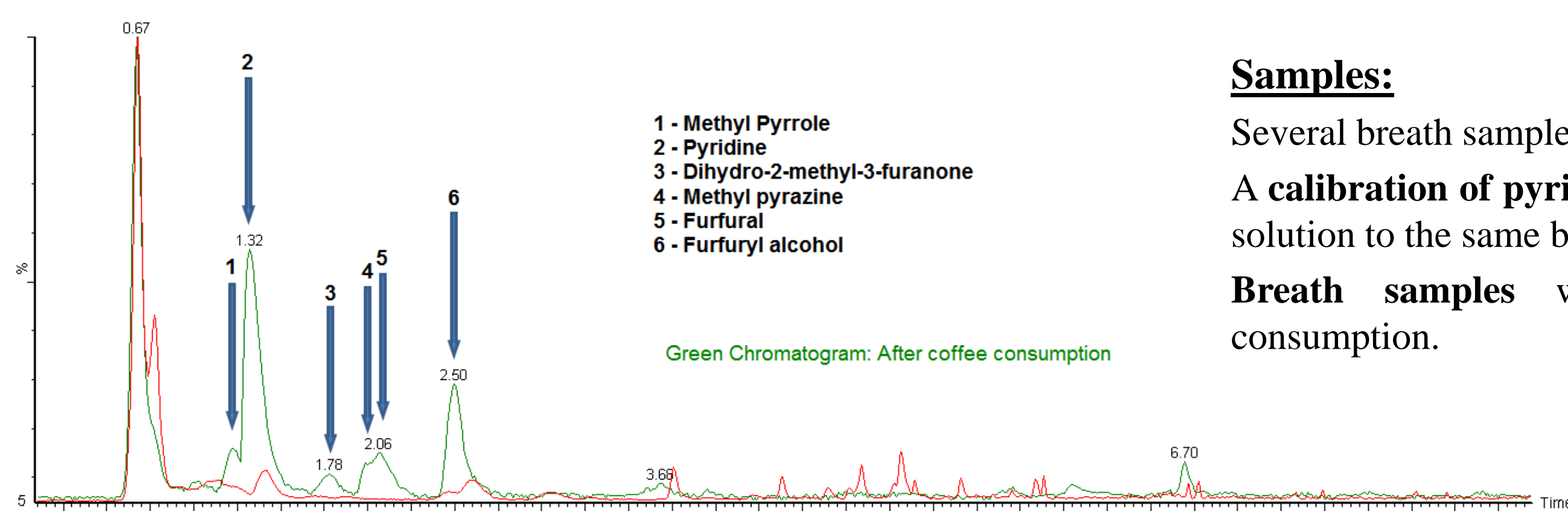


Fig. 1: Chromatogram from breath sample before (red) and after (green) coffee consumption. Column DB-5MS (30x0.25x0.25). Magnet Scan 50-100m/z

Samples:

Several breath samples were collected into a **self-designed collection bag**. A **calibration of pyridine and FA** was performed by adding the standard solution to the same bags and then **filled with nitrogen gas**.

Breath samples were collected from **volunteers** after coffee consumption.

Methods:

- LDPE “Minigrip” plastic bags** were modified and used to collect breath samples.
- Breath samples were collected from volunteers just **after coffee consumption**.
- The bags with collected samples **were connected** to an air sampler (Dupont Alpha-2) through **Desorption tubes** (Markes Tenax TA).
- Breath samples were collected at 250mL/min flow. In total **2L of breath** trapped in the sorbent tubes were run in our **Thermal Desorption** system (ATD 400 Perkin Elmer) **followed by GC-HRMS** (Agilent 6890N coupled with Waters MS AutoSpec Premier) analysis.
- 60 minutes after** coffee consumption, another breath sample was collected from volunteers.
- Standard solution of **pyridine and FA** was added to the bag and **filled with nitrogen**.
- Concentrations from **100 pg to 1000 pg** of each standard was used to make the **calibration**.



Parameters:

Pump		Thermal Desorption		GC-HRMS	
Flow	250 mL/min	Carrier gas	Helium	Oven temperatures	40°C; 3 min
Sampling time	10 min	Desorption flow	60 mL/min		20°C/min; 220°C ; 3 min
		Desorption time	10 min	Total time	15.00 min
		Oven Temp.	280°C	Gas flow	1 mL/min
		Outlet split	6 mL/min	MS range (full scan)	50-100 u

Conclusions and future work:

- Exposure to food contaminants** can be detected in **breath VOCs composition**.
- Both food contaminants can be detected **60 minutes after consumption**.
- Our method could detect **levels as low as 5pg/liter of breath sample**.
- Influence of many parameters on the levels of pyridine and FA in prepared coffee drink, the amount of grounded coffee, the amount of water, the type of coffee beans.
- We will study the **possible correlation** of the **quantity of contaminant ingested** with the levels **detected in breath**.
- Breath VOCs collection can be used for the **detection of food contaminants after consumption**.

References:

- [1] International Coffee Organization (www.ico.org).
- [2] A.N. Gloess, C. Yeretziyan, R. Knochenmuss, M. Groessl / International Journal of Mass Spectrometry Volume 424, January 2018, Pages 49-57.
- [3] F. Cincotta et al. / LWT - Food Science and Technology 118 (2020) 108718.
- [4] A. O. Okaru and D. W. Lachenmeier / Toxics 2017, 5, 9.

Results:

- ✓ **Good repeatability** was obtained when doing the standard calibration.
- ✓ **LoD of 5 pg/liter** of breath sample was obtained for both Pyridine and FA.
- ✓ Different levels of **contaminants** were **quantified** from volunteers (Fig.2).
- ✓ Small quantities of **pyridine and FA** was still found in breath **after 60 minutes**.
- ✓ **Higher levels** of both compounds were detected when **roasting level** of coffee was higher.

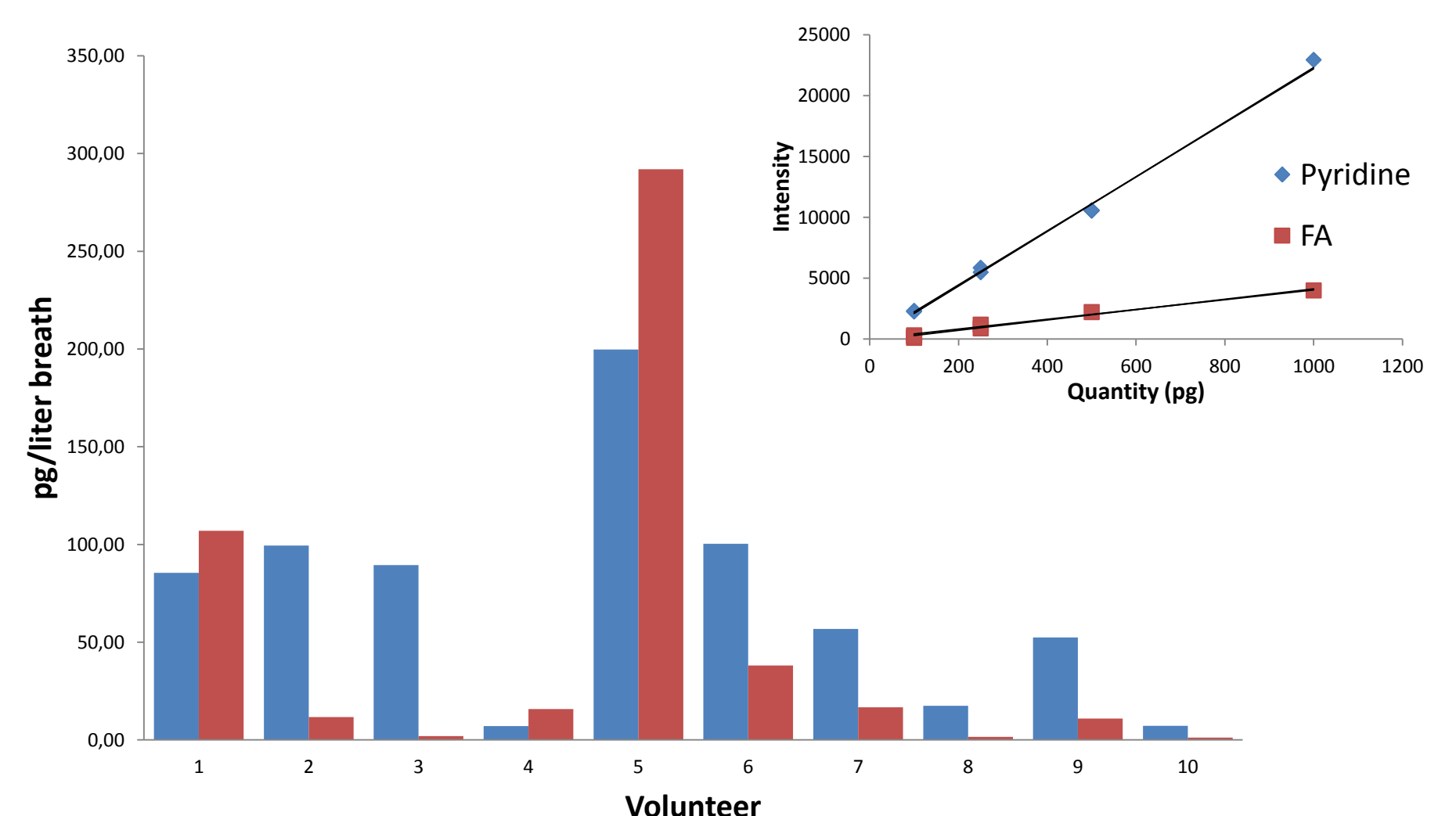


Fig. 2: Quantification results of pyridine and furfuryl alcohol (FA).