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Determination of pyridine and furfuryl alcohol in breath after coffee consumption

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We aimed to demonstrate that breath analysis can be used as a method for the detection of potentially harmful compounds in food after their ingestion. Development of such a method could be adapted as a tool for detection of food intoxication. To achieve this, we compared the levels of pyridine (Py) and furfuryl alcohol (FFA) found in breath with the quantity of these compounds ingested when drinking coffee. Coffee drink beverages were prepared in the laboratory and consumed by volunteers (n = 5). An aliquot of coffee was analysed using high performance liquid chromatography with diode-array detection (HPLC-DAD) to quantify Py and FFA in the beverage. Breath samples were collected several times over a 45 min period after ingestion of coffee and analysed by thermal desorption coupled to gas chromatography/mass spectrometry (TD/GC-MS). The levels of Py and FFA found in coffee ranged from 0.2 to 3 mg/cup of coffee, and from 7 to 30 mg/cup of coffee, respectively. The levels of these compounds detected in breath ranged from 7 to 1200 ng/l breath for Py and from 1 to 760 ng/l breath for FFA. Several parameters can influence the levels of these chemicals in breath, especially the collection time of the breath sample.

Keywords: coffee, breath, food, toxins, chromatography

Abbreviations:
ADI – Acceptable Daily Intake
Py – Pyridine
FFA – Furfuryl Alcohol
MRPs – Maillard Reaction Products
OSHA – Occupational Safety and Health Administration
PEL – Permissible Exposure Limit
TWA – Time-Weight Average
VOCs – Volatile Organic Compounds
TD/GC-MS – Thermal Desorption coupled to Gas Chromatography/Mass Spectrometry
HS/GC-MS – Head Space coupled to Gas Chromatography/Mass Spectrometry
SPE – Solid Phase Extraction
SPME – Solid Phase Micro-Extraction
HPLC-DAD – High Performance Liquid Chromatography with Diode-Array Detection

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INTRODUCTION

Drinking coffee is a common cultural practice among adult populations across the globe. In 2019/2020, around 168.5 million 60-kilogram bags of coffee were consumed worldwide [1], making coffee one of the most widely consumed beverages. Northern European countries consume the highest quantities of coffee. Finland is the top consumer country with an average of 12 kg of coffee consumed per person per year [2].

Coffee contains over 1500 chemical components, most of which over 800 are volatile organic compounds (VOCs) created after the coffee roasting process, consequently providing the specific taste and smell [3, 4]. Roasting also facilitates chemical reactions between amino acids and reducing sugars leading to the formation of Maillard reaction products (MRPs). Depending on the way the food is being processed, both beneficial and toxic MRPs can be produced. When people cook food at home, they will 'create' new compounds that cannot be controlled by food safety agencies. Pyridine (Py) and furfuryl alcohol (FFA) are two MRPs found in brewed coffee [5, 6]. Even though coffee is not classifiable as carcinogenic to humans, Py and FFA are classified as group 2B (possible carcinogens) [7, 8]. The current Occupational Safety and Health Administration (OSHA) airborne permissible exposure limit (PEL) for Py and FFA is 15 and 50 mg/m^3 TWA (time-weight average), respectively [9, 10]. The Joint Expert Committee on Food Additives (JECFA) [11] has allocated an Acceptable Daily Intake (ADI) of 0.5 mg/kg bw (bodyweight) for FFA and 0.002 mg/kg/day for inhalation exposure for Py [12].

Many studies have been performed studying health implication of drinking coffee, mostly focusing on the benefits of antioxidants content (polyphenols, chlorogenic acids, caffeine and melanoidins) [4, 13]. The studies show an apparently beneficial association of consuming three cups of coffee a day. But, this might depend on the type of beans used, degree of roasting, preparation method, extra addition of ingredients (sugar or milk) and the tolerance from the person [14]. Even though drinking coffee does not seem to have definitive harmful outcomes for health, the presence of toxic MRPs in high levels could raise health concerns [15–17]. Specially, with the presence of MRPs like acrylamide and furan (classified as 2A and 2B carcinogens), which have raised a large concern after their high levels in processed food [18, 19], coffee is one of their important dietary sources [20, 21]. Previously, determination of volatile compounds in coffee has been studied employing the methods of head space coupled to gas chromatography/mass spectrometry (HS/GC-MS) [22], dispersive solid phase extraction (SPE) with gas chromatography/mass spectrometry (GC-MS) [23] and solid phase microextraction with gas chromatography/mass spectrometry (SPME/GC-MS) [24].

A potential method to indicate exposure to toxic foodborne volatile compounds after consumption could be breath analysis using TD/GC-MS. Breath analysis has been widely studied as a non-invasive method to diagnose and monitor various diseases like cancer, tuberculosis, asthma, liver disease and diabetes [25–29]. In relation to toxins, Py has been found in the breath of active smokers [30]. In this study, we aimed to identify and quantify Py and FFA in human breath after coffee ingestion using TD/GC-MS methodology and to compare these to the quantities of the same compounds in the coffee beverage. Development of such a method could be adapted as a tool for detection of food intoxication.

EXPERIMENTAL

Chemicals

Standards of Py (ReagentPlus, ≥99%, CAS: 110-86-1) and FFA (≥98 %, CAS 98-00-0) were purchased from Sigma-Aldrich. Mobile phase solvents methanol CHROMASOLV™ (gradient grade, for HPLC ≥99.9%, Honeywell) were used when running the HPLC system, and deionized water was obtained using a deionizer system NANOpure Infinity (Barnstead/Thermolyne, USA). Acetic acid glacial (USP, BP, Ph. Eur.) pure, pharma grade (Applichem) was used to acidify the water mobile phase (0.1%).

Coffee drink preparation

Coffee beans (dark roasted, 100% Arabica) were purchased from a local store. Coffee drink samples were obtained using two different brewing methods, CafeRomatica (NIVONA) espresso coffee machine and Italian moka pot. Two different parameters could be adjusted on the CafeRomatica coffee machine when the coffee beverages were prepared. The first parameter was the quantity of coffee beans

used, and the second was the quantity of water used to brew the coffee. Light, normal and strong coffee could be chosen and 3.50, 7.50 and 9.00 g of coffee beans were used, respectively. The most common volumes of brewing water used by our volunteers were analysed (i.e. 30, 100 and 240 ml of water). For Italian moka pot coffee drinks, 12 g of ground coffee and 200 ml of water were used.

HPLC analysis

Coffee drinks were prepared as described above. A sample of 2 ml was collected into a closed 2 ml plastic centrifuge vial to avoid evaporation of the VOCs and left to cool. The samples were then filtered using a 0.45 μm PTFE Captiva Econofilter (Agilent). An aliquot of 100 μl was spiked with Py and FFA standards and taken to a final volume of 1000 μl by adding deionized water with 0.1% acetic acid. An aliquot of 50 μl of each sample was analysed using an Agilent 1100 series HPLC system with a diode array detector and an Agilent Zorbax XDB-CN (3.0 × 150 mm, 3.5 μm) column.

Separation was achieved using a gradient mobile phase of 0.1% acetic acid in water (A) and methanol (B) at 25°C. The gradient started at 95% Phase A, increased to 20% Phase B after 2.5 min, reaching 100% phase B after 10 min, and was held until the end of the run (15 min). The flow rate used for the entire run was 0.5 ml/min. The absorption recorded for the detection of Py was 254 nm, and 217 nm for FFA. HPLC conditions were similar to the proposed [16] where furan derivates were analysed in coffee. As we wanted to analyse both Py and FFA in a single run using the same parameters, different columns and mobile phase gradients were studied until the desired separation of both compounds was obtained.

TD/GC-MS analysis

Once the coffee drink was prepared and an aliquot of 2 ml was collected for HPLC analysis, the rest of the sample was consumed by the volunteer. Five volunteers participated in the study, providing samples during several days. All the volunteers were non-smokers and could drink and eat any time before the study. Because of that, a breath sample was collected from the volunteer just before the coffee was consumed, using a self-modified 2-liter plastic bag [31]. The background signal obtained was subtracted from the breath sample after coffee consumption. This helped to ensure that the concentrations of MRPs obtained were coming only from the coffee ingested for the experiment. Immediately after finishing the drink, another breath sample was collected.

The breath sample was passed through a thermal desorption tube (Markes International, with Tenax TA sorbent) at 250 ml/min (air sampler Dupont Alpha-2). The thermal desorption (TD) tube with the sample was then inserted in the TD system (Perkin Elmer ATD400) and heated to 280°C for 10 min at a desorption flow of 60 ml/min. The compounds were released inside the system using helium gas (purity 5.0) and refocused inside the system's cold trap (–15°C). Fast heating of the trap to 250°C (and hold for 3 min) at 8 ml/min desorption flow released the compounds into the gas chromatographic system where the analytes were separated using a temperature ramp. An outlet split of 6 ml/min was used to allow a flow of 2 ml/ml through the chromatographic system. The initial temperature of 40°C was held for 3 min and then increased to 220°C at a rate of 20°C/min.

An Agilent 6890N gas chromatography system with DB-5MS (30 m × 0.25 mm × 0.25 μm) column was used for the separation of the analytes, followed by a Waters AutoSpec Premier (Waters/MicroMass Technologies) mass spectrometer for detection and identification. The transfer line to the mass spectrometer was maintained at 250°C. Mass spectra were obtained by electronic ionisation at 70 eV, and magnetic scan was performed in the range *m/z* 50–100. For the quantification of the analytes, *m/z* 79 and *m/z* 98 were extracted for Py and FFA, respectively.

Standards preparation

For the HPLC analysis, each coffee sample was spiked with a standard solution of 1, 2 and 4 ppm of Py and 10, 20 and 40 ppm of FFA and injected into the HPLC system. The linearity obtained for this method was satisfactory (Table 1). Each coffee sample was prepared in triplicate to assess repeatability.

To calibrate the breath analysis, two water solutions of 5 and 50 ppm of both analytes were prepared. From each solution, 5, 10 and 20 μl were selected to obtain a 6-point calibration curve. As the range of concentrations in breath was very wide, we wanted to obtain the highest possible range of concentration by using the same volume

Table 1. **r^2 values from the standard addition calibration of coffee samples spiked with Py and FFA for 3 different aliquots**

Coffee sample[a]		Py			FFA		
		1st	2nd	3rd	1st	2nd	3rd
Si		0.9977	0.9972	0.9995	0.9832	0.9742	0.9760
N	30	0.9958	0.9963	0.9902	0.9830	0.9872	0.9892
St		0.9974	0.9982	0.9968	0.9636	0.9634	0.9643
Si		0.9998	0.9997	0.9994	0.9923	0.9916	0.9916
N	100	0.9995	0.9998	1.0000	0.9854	0.9859	0.9793
St		0.9995	0.9994	0.9995	0.9924	0.9844	0.9836
Si		0.9995	0.9980	0.9995	0.9846	0.9860	0.9840
N	240	0.9880	0.9913	n/a[b]	0.9978	0.9992	n/a[b]
St		0.9988	0.9984	0.9979	0.9862	0.9848	0.9874
Mk	200	0.9964	0.9999	n/a[b]	0.9852	0.9895	n/a[b]

[a] Si (Light coffee), 3.5 g; N (Normal coffee), 7.5 g; St (Strong coffee), 9 g; Mk (Moka coffee), 12 g and brewing water volume (ml). [b] Not enough sample to perform a third run of samples.

intake for both solutions to avoid errors. Therefore, the calibration points were not equidistant.

A self-made 2-liter plastic bag was partly filled with nitrogen gas and placed into the oven for a few minutes at 40°C. Then, a volume from the standard solution was collected in a gas-tight syringe and quickly injected into the conditioned bag through the plastic valve and closed. The bag was then completely filled with nitrogen gas and a sample was collected for analysis. Before a set of breath samples was analysed, a standard injection was performed to assess reproducibility. When standard levels differed more than 10%, a new calibration was made.

RESULTS AND DISCUSSION

Amount of MRPs in breath does not depend on the amount of ingested MRPs

Regardless of the quantity of coffee beans used, levels of Py and FFA extracted per gram of coffee beans with the CafeRomantica coffee machine were similar (Table 2). Higher quantities of both MRPs

Table 2. **Quantities of pyridine (Py) and furfuryl alcohol (FFA) determined in coffee drink**

Name[a]	Coffee[b], g	Water[c], ml	Sample[d], µg/ml		Cup[e], mg/cup		Beans[f], mg/g	
			FFA	Py	FFA	Py	FFA	Py
Si30	3.5	30	236.7	7.5	7.1	0.23	2.0	0.07
N30	7.5		368.1	18.3	11.0	0.55	1.5	0.07
St30	9		427.9	20.2	12.8	0.61	1.4	0.07
Si100	3.5	100	67.0	3.5	6.7	0.35	1.9	0.10
N100	7.5		126.2	8.7	12.6	0.87	1.7	0.12
St100	9		108.4	8.1	10.8	0.81	1.2	0.09
Si240	3.5	240	40.1	3.1	9.6	0.75	2.7	0.21
N240	7.5		55.5	12.5	13.3	3.0	1.8	0.40
St240	9		67.8	5.1	16.3	1.2	1.8	0.14
Mk200	12	200	151.9	16.3	30.4	3.3	2.5	0.27

[a] Si (Light coffee), N (Normal coffee), St (Strong coffee), Mk (Moka coffee). [b] Grams of coffee used. [c] Millilitres of water used for brewing. [d] Concentration of target compounds in the sample, in micrograms per millilitre. [e] Milligrams of target compounds in the full cup of coffee. [f] Milligrams of target compounds per gram of coffee bean.

Note: standard deviation <10%.

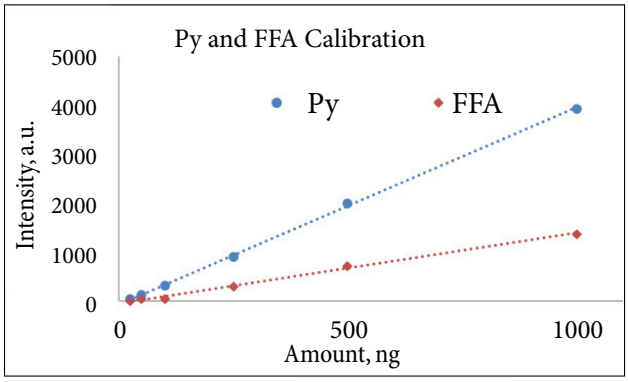

Fig. 1. Pyridine (Py) and furfuryl alcohol (FFA) calibration curves using TD/GC-MS

R^2 (Py) = 0.9996; R^2 (FFA) = 0.9963.

were obtained when preparing the coffee using an Italian moka pot due to higher temperature reached by the steam and longer time to brew the coffee [32, 33]. The quantities of toxic MRPs present in the coffee drinks ranged from 0.2 to 3 mg/cup for Py, and from 7 to 30 mg/cup for FFA both depending on the amount of water used for brewing the coffee.

Similar levels of FFA in espresso coffee (1.6 mg/g) were found in other studies [34], but also lower levels were found in the literature, where maximum levels of 0.41 mg/g were detected (Okaru, 2017). Also, lower levels of Py (0.04 mg/g) were detected [35]. This difference in the concentrations of MRPs in coffee could be due to the different roasting procedures of the coffee beans [16], as well as the different bean growing locations, which might change the composition of the coffee [36].

Breath samples from all volunteers showed the concentrations of both toxic MRPs in a range from 1 to 1200 ng/l for pyridine and to 760 ng/l for FFA (Fig. 2). We could observe a big dispersion of the results for each sample replicate. According to the literature, the values of Py in breath from 0.66 to 141 µg/l were found in patients with end-stage renal disease [37], and up to 300 µg/l in active

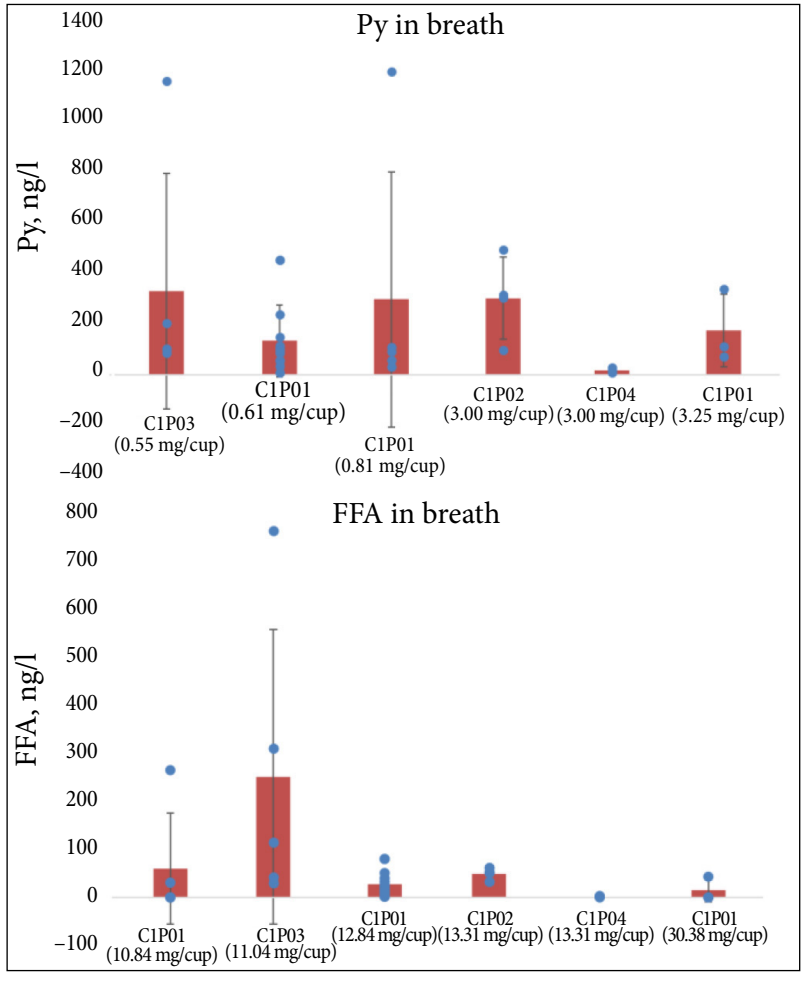

Fig. 2. Levels of Py and FFA (ng/l) found in breath for different volunteers with their quantities ingested by the volunteer in a cup of coffee (in parenthesis)

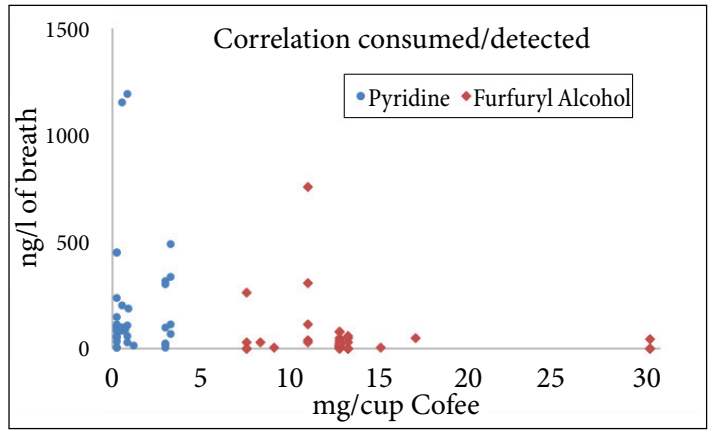

Fig. 3. Correlation of concentrations of the target compounds in the coffee beverage with the levels detected in breath from volunteers

smokers [38]. Regarding FFA, we did not find other studies reporting FFA in breath.

The levels of toxic MRPs in coffee drink were compared with their levels found in breath of each volunteer after drinking the beverage (Fig. 3) using the Pearson test. No correlation between the levels of toxics ingested and their presence in breath was observed (Py = 0.00135 and FFA = –0.168). Furthermore, we observed a big dispersion of the results for each volunteer ingesting the same amount of MRPs. Thus, we studied different factors that could influence the MRP levels in breath when drinking coffee or collecting the sample.

Factors affecting the results

The lack of correlation between the ingested toxic MRPs in coffee and those present in breath, as well as the big dispersion in the results, indicates that there could be other factors influencing their concentration. We looked at 1) the time that one takes to drink the coffee (or collection time after the start of drinking the coffee), and 2) the ingestion of water (or other liquids) after/while drinking coffee.

To check the possible influence of time, our volunteers, before collecting the breath sample, had a small shot of coffee (N30) in a time range between 5 and 10 s. Just after drinking the coffee, a breath sample was collected. Subsequent breath samples were collected after 3, 6, 10, 15, 20, 30 and 45 min. We observed how the levels of both Py and FFA decrease with time obtaining the same results when repeating the experiment for several days (Fig. 4). A power trendline was obtained for each data set that fit the results obtained the best.

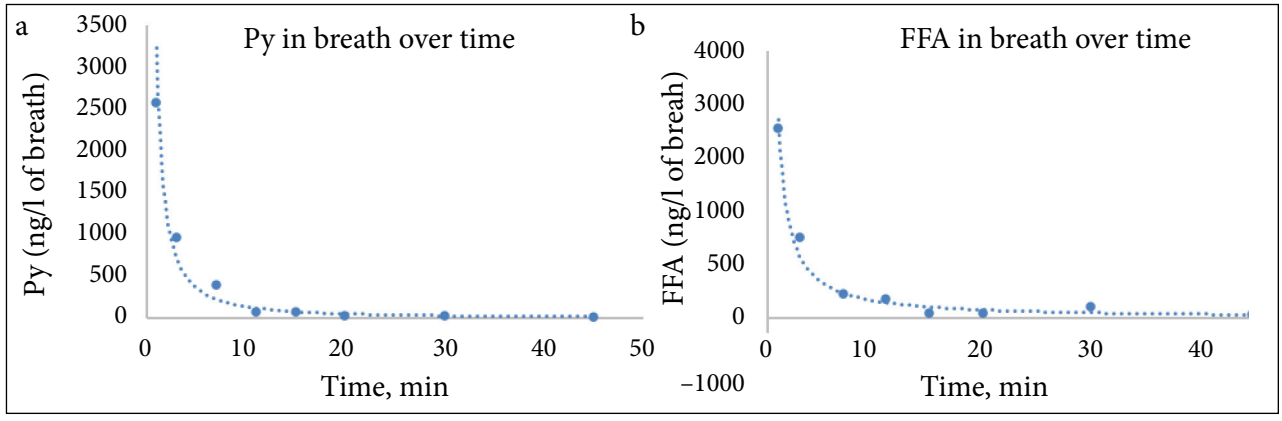

Fig. 4. Quantity of (a) pyridine (Py) and (b) furfuryl alcohol (FFA) detected in breath depending on the time of collecting the sample after coffee ingestion

Equations for (a) Py: $y = 3317.1x^{-1.369}$ and $R^2 = 0.9608$;

Equations for (b) FFA: $y = 2970.4x^{-1.06}$ and $R^2 = 0.9043$.

The results show a consistent drop in the levels of both MRPs. A high deviation of the results (30% for Py and more than 100 % for FFA) in the first seconds of breath sampling might be due to the fast drop in the concentration. The results could be different if the sampling is delayed just for a few seconds. The deviation of the results gets much lower with time. The most probable cause for the drop in the concentration is the high volatility of both of the compounds.

In the next experiment, our volunteers had the same amount of coffee (30 ml of Normal coffee) but consumed it more slowly, taking about 1 min to finish the coffee. The breath sample was collected straight after finishing the drink. The second experiment indicates that levels of both toxic MRPs are decreasing before the total amount of coffee is consumed (Fig. 5). This makes it difficult to relate the levels of toxic MRPs in a volunteer drinking a small espresso (30 ml) with the other drinking a long coffee (240 ml), as they will need different times to finish the drink. Therefore, it is recommended to set the initial time when the person starts to drink the coffee, and not when the sample is collected after finishing the drink.

The second possible factor that we studied was the ingestion of other liquids while drinking coffee as other liquids might dilute the toxic MRPs. We checked the influence of drinking the same coffee (30 ml, normal) with milk (100 ml), and the influence of drinking a glass of water after drinking the coffee. As the drink volume with milk is higher we counted the time from the start of ingesting the coffee, taking 2 min longer than drinking an espresso. There was no change on the concentration curve for Py when analysing the breath after drinking coffee with milk. However, we observed a drop in the signal for FFA (Fig. 6). A possible explanation for this behaviour

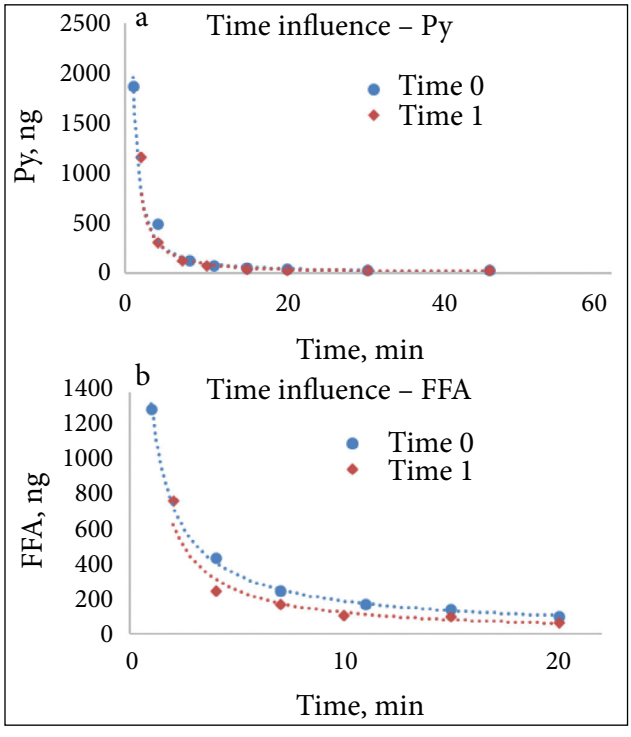

Fig. 5. Quantity of pyridine (Py) (a) and furfuryl alcohol (FFA) (b) detected in breath depending on the time of collecting the sample, finishing drinking the coffee within seconds (Time 0) and slowly for 1 min (Time 1)

Equations for (a) Py:

Time 0: $y = 1953.7x^{-1.303}$ and $R^2 = 0.9742$,

Time 1: $y = 1995.9x^{-1.357}$ and $R^2 = 0.9489$.

Equations for (b) FFA:

Time 0: $y = 1333.1x^{-0.846}$ and $R^2 = 0.9970$,

Time 1: $y = 1283.5x^{-1.014}$ and $R^2 = 0.9592$.

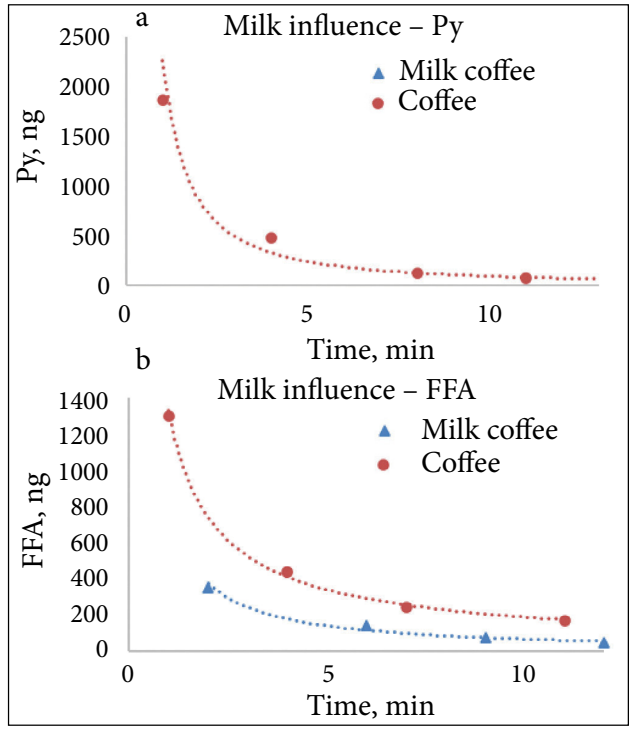

Fig. 6. Quantity of pyridine (Py) (a) and furfuryl alcohol (FFA) (b) detected in breath depending on the time of collecting the sample after coffee ingestion, comparing drinking espresso 30 ml (Coffee) with coffee 30 ml with milk 100 ml (Milk coffee)

Equations for (a) Py:

Milk coffee: $y = 2261.8x^{-1.404}$ and $R^2 = 0.9756$,

Coffee: $y = 3028.3x^{-1.613}$ and $R^2 = 0.9869$.

Equations for (b) FFA:

Milk coffee: $y = 1329.2x^{-0.846}$ and $R^2 = 0.9973$,

Coffee: $y = 779.05x^{-1.058}$ and $R^2 = 0.9794$.

could be from the case in the milk complexing the alcohol group of FFA.

To analyse the effect of drinking water after coffee, we collected the breath sample just after having the coffee, then the volunteer had a glass of water, and then we collected another breath sample.

We observe (Fig. 7) that drinking water after having a cup of coffee does not affect the levels of toxic MRPs in breath, and we detected the same drop in concentration as when drinking only coffee.

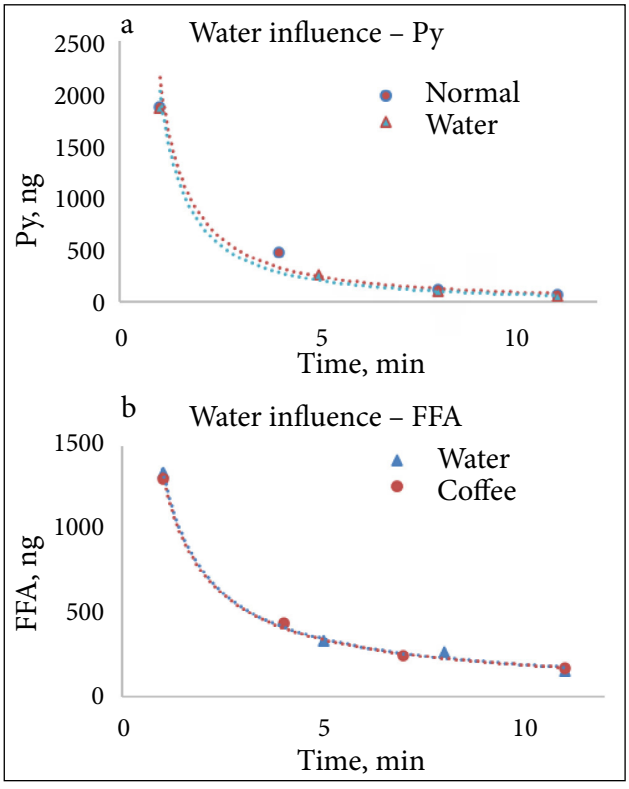

Fig. 7. Quantity of pyridine (Py) (a) and furfuryl alcohol (FFA) (b) detected in breath depending on the time of collecting the sample after coffee ingestion, drinking water after finishing the coffee (Water) compared with a shot of coffee (Normal)

Equations for (a) Py:

Normal: $y = 2150.1x^{-1.34}$ and $R^2 = 0.9721$,

Water: $y = 2018.5x^{-1.404}$ and $R^2 = 0.9868$.

Equations for (b) FFA:

Normal: $y = 1329.2x^{-0.846}$ and $R^2 = 0.9973$,

Water: $y = 1360.5x^{-0.853}$ and $R^2 = 0.9880$.

CONCLUSIONS

Our study showed that levels of both pyridine (Py) and furfuryl alcohol (FFA) present in coffee can be detected from human breath emissions in concentrations as low as 7 ng/l of breath for Py and 1 ng/l of breath for FFA. Even though the levels of both compounds before coffee intake were below the limit of detection (LOD), the background signal was subtracted from the results. The intake of both compounds reached 3 and 30 mg per cup of coffee for Py and FFA, respectively. Those levels are above the recommended levels established by JECFA (ADI of 0.002 mg/kg/day for Py and 0.5 mg/kg bw for FFA), and the consumption of large amounts of coffee (as found in European Nordic countries) might be concerning for health outcomes. Because we did not find a direct correlation between the quantity of ingested coffee and levels of specific chemicals in a person's breath, we checked for possible factors affecting the results. The results show a very strong drop in the quantities of Py and FFA found in breath with time after finishing the coffee drink, probably due to the fast evaporation of the compounds. Nevertheless, the breath analysis has proven to be effective on detecting Py and FFA after their ingestion; even 45 min after the intake of 1 cup of coffee, the levels of both MRPs could be still detected. The presence of very high levels of MRPs in breath might be due to food intoxication sources and could provide with a proper medical help. This suggests the possible application of breath analysis for the detection of food intoxication by volatile compounds like MRPs.

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References

1. International Coffee Organization, *Coffee Trade Statistics Tables* (2020) [http://www.ico.org/trade_statistics.asp?section=Statistics].
2. World Atlas, *The Top Coffee-consuming Countries* (August 2020) [https://www.worldatlas.com/articles/top-10-coffee-consuming-nations.html].
3. G. V. de Melo Pereira, D. P. de Carvalho Neto, A. I. Magalhães Júnior, et al., *Adv. Food Nutr. Res.*, **91**, 65 (2020). DOI: 10.1016/bs.afnr.2019.10.002.
4. K. Nieber, *Planta Med.*, **83**, 1256 (2017). DOI: 10.1055/s-0043-115007.
5. M. Akiyama, K. Murakami, M. Ikeda, et al., *J. Food Sci.*, **72**, 7, 388 (2007). DOI: 10.1111/j.1750-3841.2007.00447.x.
6. L. Maeztu, C. Sanz, S. Andueza, M. P. de Peña, J. Bello, C. Cid, *J. Agric. Food Chem.*, **49**, 11 (2001). DOI: 10.1021/jf0107959.

7. International Agency for Research on Cancer, Furfuryl Alcohol, in: *IARC Monographs on the Evaluation of Carcinogenic Risks of Chemicals to Humans*, 63 (1995) [http://monographs.iarc.fr/ENG/Classification/latest_classif.php].
8. International Agency for Research on Cancer, Pyridine, in: *IARC Monographs on the Evaluation of Carcinogenic Risks of Chemicals to Humans*, 63 (1995) [http://monographs.iarc.fr/ENG/Classification/latest_classif.php].
9. Occupational Safety and Health Administration (OSHA), United States Department of Labor, *Pyridine*, Occupational Safety and Health Administration (2021) [https://www.osha.gov/chemicaldata/119].
10. Occupational Safety and Health Administration (OSHA), United States Department of Labor, *Furfuryl Alcohol*, Occupational Safety and Health Administration (2021) [https://www.osha.gov/chemicaldata/771].
11. *Who Food Additives Series 46: Furfuryl Alcohol and Related Substances* [https://inchem.org/documents/jecfa/jecmono/v46je08.htm].
12. U.S. EPA, *Health and Environmental Effects Profile for Pyridine*, EPA/600/X-86/168 (NTIS PB89123384), U.S. Environmental Protection Agency, Washington, D.C. (1986).
13. A. Yesil, Y. Yilmaz, *Aliment. Pharmacol. Ther.*, **38**, 9 (2013). DOI: 10.1111/apt.12489.
14. R. Poole, *BMJ*, **359**, j5024 (2017). DOI: 10.1136/bmj.j5024.
15. A. O. Okaru, D. W. Lachenmeier, *Toxics*, **5**, 9 (2017). DOI: 10.3390/toxics5010009.
16. A. Albouchi, J. Rus, M. Murkovic, *Food Chem. Toxicol.*, **118**, 473 (2018). DOI: 10.1016/j.fct.2018.05.055.
17. F. Cincotta, G. Tripodi, M. Merlino, A. Verzera, C. Condurso, *LWT – Food Sci. Technol.*, **118**, 108718 (2020). DOI: 10.1016/j.lwt.2019.108718.
18. European Food Safety Authority (EFSA), *EFSA J.*, **137** (2004). DOI: 10.2903/j.efsa.2004.137.
19. European Food Safety Authority (EFSA), *EFSA J.*, **13**, 6 (2015). DOI: 10.2903/j.efsa.2015.4104.
20. R. C. Alves, C. Soares, S. Casal, J. O. Fernandes, M. Beatriz, P. P. Oliveira, *Food Chem.*, **119(3)**, 929 (2010). DOI: 10.1016/j.foodchem.2009.07.051.
21. M. S. Altaki, F. J. Santos, M. T. Galceran, *Food Chem.* **126(4)**, 1527 (2010). DOI: 10.1016/j.foodchem.2010.11.134.
22. H.-J. Kim, D.-L. Hong, J.-W. Yu, S.-M. Li, Y.-B. Lee, *Prev. Nutr. Food Sci.*, **24(2)**, 217 (2019). DOI: 10.3746/pnf.2019.24.2.217.
23. A. Sadowska-Rociek, M. Surma, E. Cieślik, *Food Anal. Methods*, **8(1)**, 109 (2015). DOI: 10.1007/s12161-014-9876-9.
24. N. Caporaso, M. B. Whitworth, C. Cui, I. D. Fisk, *Food Res. Int.*, **108**, 628 (2018). DOI: 10.1016/j.foodres.2018.03.077.
25. R. P. Arasaradnam, M. McFarlane, E. Daulton, et al., *J. Gastrointestin. Liver Dis.*, **24(2)**, 197 (2015). DOI: 10.15403/jgld.2014.1121.242.ury.
26. G. Lubes, M. Goodarzi, *J. Pharm. Biomed. Anal.*, **5**, 147 (2018). DOI: 10.1016/j.jpba.2017.07.013.
27. H. Tong, Y. Wang, Y. Li, et al., *Cancer Cell Int.*, **17**, 108 (2017). DOI: 10.1186/s12935-017-0475-x.
28. J. Zhou, Z. A. Huang, U. Kumar, D. D. Y. Chen, *Anal. Chim. Acta*, **15**, 996 (2017). DOI: 10.1016/j.aca.2017.09.021.
29. Q. Zhou, Q. Wang, B. Chen, et al., *J. Breath Res.*, **13(4)**, 046012 (2019). DOI: 10.1088/1752-7163/ab285a.
30. V. Chagovets, A. Kononikhin, N. Starodubtseva, J. Ding, H. Chen, V. Frankevich, *Eur. J. Mass Spectrom.*, **21(6)**, 829 (2015). DOI: 10.1255/ejms.1397.
31. A. Vicent-Claramunt, E. Naujalis, *Methodsx*, **8**, 101386 (2021). DOI: 10.1016/j.mex.2021.101386.
32. L. Navarini, E. Nobile, F. Pinto, A. Scheri, E. Suggi-Liverani, *Appl. Therm. Eng.*, **29**, 998 (2009). DOI: 10.1016/j.applthermaleng.2008.05.014.
33. N. Caporaso, A. Genovese, M. D. Canela, A. Civitella, R. Sacchi, *Food Res. Int.*, **61**, 152 (2014). DOI: 10.1016/j.foodres.2014.01.020.
34. A. Albouchi, M. Murkovic, *J. Sep. Sci.*, **42(9)**, 1695 (2019). DOI: 10.1002/jssc.201900061.
35. A. Amanpour, S. Selli, *J. Food Process. Preserv.*, **40(5)**, 1116 (2016). DOI: 10.1111/jfpp.12692.
36. N. Yang, C. Liu, X. Liu, T. K. Degn, M. Munchow, I. Fisk, *Food Chem.*, **211**, 206 (2016). DOI: 10.1016/j.foodchem.2016.04.124.
37. P. Mochalski, J. King, M. Haas, K. Unterkofler, A. Aman, G. Mayer, *BMC Nephrol.*, **15**, 43 (2014). DOI: 10.1186/1471-2369-15-43.
38. Y. H. Cho, H. Y. Kim, J. K. Lee, S. H. Kim, *J. Korean Soc. Res. Nicotine Tob.*, **12(1)**, 24 (2021). DOI: 10.25055/JKSRNT.2021.12.1.24.

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PIRIDINO IR FURFURILO ALKOHOLIO NUSTATYMAS IŠKVĖPTAME ORE PO KAVOS VARTOJIMO

S a n t r a u k a

Šio tyrimo tikslas buvo parodyti, kad iškvepiamo oro analizė gali būti naudojama kaip metodas potencialiai kenksmingiems junginiams maiste aptikti po jų suvartojimo. Sukurtas toks metodas galėtų būti pritaikytas kaip priemonė apsinuodijimui maistu nustatyti. Tam pasiekti buvo palyginti piridino (Py) ir furfurilo alkoholio (FFA) kiekiai iškvėptame ore su šių junginių kiekiu, suvartojamu geriant kavą. Kavos gėrimai buvo ruošiami laboratorijoje ir juos vartojo savanoriai (n = 5). Siekiant kiekybiškai įvertinti Py ir FFA gėrime, kavos alikvotinė dalis buvo analizuojama naudojant didelio efektyvumo skysčių chromatografiją su diodų matricos detektoriumi (HPLC-DAD). Žmogaus iškvepiamo oro mėginiai buvo paimti kelis kartus per 45 minutes po kavos išgėrimo ir analizuojami naudojant terminę desorbciją, sujungtą su dujų chromatografija-masės spektrometrija (TD / GC-MS). Py ir FFA kiekis kavoje svyravo atitinkamai nuo 0,2 iki 3 mg kavos puodelyje ir nuo 7 iki 30 mg kavos puodelyje. Šių junginių koncentracija iškvėptame ore svyravo nuo 7 iki 1 200 ng/l Py ir nuo 1 iki 760 ng/l FFA. Nustatyta, kad šių medžiagų kiekis iškvėptame ore priklauso nuo keleto parametrų, iš kurių didžiausią įtaką turėjo laiko trukmė nuo kavos suvartojimo iki mėginio paėmimo.