



# DOCTORAL DISSERTATION

Faculty of Chemistry

Department of Trace Analysis

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**Interaction problem between the environmentally friendly modern food  
contact materials (FCMs) and food**

**Współczesne naczynia przyjazne środowisku – problem interakcji pomiędzy  
materiałem a żywnością**

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## Abstract

The pursuit of sustainability in all aspects of public life is currently a fundamental global responsibility, due to the constantly deteriorating state of the environment. Numerous regulations have been introduced in the packaging sector (including the Plastics Directive). Based on these, new biodegradable and recyclable food contact materials (FCMs) have appeared on the consumer market, which may raise food safety concerns. The doctoral dissertation carried out a comprehensive characterization of the interactions between newly introduced FCMs and food. For this purpose, 13 FCMs (of plant origin, bio-based plastics) were selected and subjected to migration tests under different time and temperature conditions, using food or food simulants of different nature. A wide spectrum of chemical compounds (untargeted approach) and migration markers (targeted approach) were determined using analytical, sensory and statistical tools. This enabled the identification and quantification of various organic and inorganic contaminants that can easily migrate from FCMs to food and affect its sensory profile and quality.

The obtained results clearly showed that some plant-based FCMs can distort the sensory profile of coffee and tea. Chemical compounds affecting noticeable undesirable changes include saturated and unsaturated carbonyl compounds (e.g., Strecker aldehydes: 3-methylbutanal and 2-methylbutanal), and saturated alcohols (e.g., hexan-1-ol, heptan-2-ol, octan-3-ol). In order to assess the influence of various factors (time and temperature of FCM-food contact, microwave radiation, type of food, chemical composition of food) on the intensity of FCM-food interactions, low-molecular-weight carbonyl compounds were selected as markers of undesirable changes. These compounds are ubiquitous in the environment, are reactive and undergo dynamic changes, and the optimized measurement procedure used allowed their monitoring at low concentration levels (ng/L). Consumer exposure to particularly hazardous compounds migrating (e.g., formaldehyde, bisphenol-A, toxic elements) from new FCMs to food was also estimated using specific migration limits (SML) or tolerable daily intake (TDI). The presented results and discussion provide a basis for deepening knowledge and understanding the nature of currently popular FCMs and their impact on the environment, and especially on food.

**Keywords:** environmental pollution; food contact materials (FCMs); migration studies; food simulants; organic and inorganic contaminants; food safety; markers of changes; analytical tools; sensory analysis.

## Streszczenie

W obliczu nieustannie pogarszającego się stanu środowiska dążenie do zrównoważonego rozwoju w każdym aspekcie życia publicznego stanowi obecnie fundamentalny, globalny obowiązek. W sektorze opakowaniowym wprowadzono liczne regulacje prawne (m.in. Dyrektywę Plastikową), na mocy których na rynku konsumenckim zaczęły pojawiać się nowe, biodegradowalne i zdadne do recyklingu materiały do kontaktu z żywnością (*ang. food contact materials; FCMs*), co może budzić wątpliwości dotyczące bezpieczeństwa żywności. W rozprawie doktorskiej przeprowadzono kompleksową charakterystykę interakcji zachodzących między nowo wprowadzanymi FCMs a żywnością. W tym celu wybrano 13 FCMs (pochodzenia roślinnego i bioplastiki), które poddano badaniom migracji w różnych warunkach czasowych i temperaturowych, z wykorzystaniem żywności lub płynów modelowych imitujących żywność o różnym charakterze. W celu oceny bezpieczeństwa FCMs, oznaczono szerokie spektrum związków chemicznych (podejście nieukierunkowane) oraz markery migracji (podejście ukierunkowane) za pomocą narzędzi analitycznych, sensorycznych i statystycznych. Umożliwiło to zidentyfikowanie oraz skwantyfikowanie różnych zanieczyszczeń organicznych oraz nieorganicznych, które mogą łatwo migrować z FCMs do żywności i wpływać na jej profil sensoryczny i jakość.

Uzyskane wyniki jednoznacznie wykazały, że niektóre FCMs pochodzenia roślinnego mogą zniekształcać profil sensoryczny kawy i herbaty, a do wiodących związków chemicznych wpływających na wyczuwalne, niepożądane zmiany można zaliczyć nasycone i nienasycone związki karbonylowe (m.in. aldehydy Streckera: 3-metylbutanal i 2-metylbutanal) i nasycone alkohole (np. heksan-1-ol, heptan-2-ol, oktan-3-ol). W celu oceny wpływu różnych czynników (m.in. czasu i temperatury kontaktu FCM-żywność, promieniowania mikrofalowego, rodzaju żywności, składu chemicznego żywności) na intensywność interakcji FCMs-żywność, wybrano niskocząsteczkowe związki karbonylowe jako markery zachodzących, niepożądanych zmian. Związki te są wszechobecne w środowisku, są reaktywne i ulegają dynamicznym zmianom, a zastosowana zoptymalizowana procedura pomiarowa pozwoliła na ich monitorowanie na niskich poziomach stężeń (ng/L). Oszacowano również narażenie konsumentów na szczególnie niebezpieczne związki migrujące (np. formaldehyd, bisfenol-A, pierwiastki toksyczne) z nowych FCM do żywności przy użyciu limitów migracji specyficznej (SML) lub tolerowanego dziennego pobrania (TDI). Przedstawione wyniki i dyskusja stanowią podstawę do pogłębienia wiedzy i zrozumienia natury obecnie popularnych FCMs i ich wpływu na środowisko, a zwłaszcza na żywność.

**Słowa kluczowe:** zanieczyszczenie środowiska; materiały do kontaktu z żywnością; badania migracji; płyny modelowe; organiczne i nieorganiczne zanieczyszczenia; bezpieczeństwo żywności; markery zmian; narzędzia analityczne; analizy sensoryczne.

## List of symbols

AD – anaerobic digestion

ANT – anthracene

BAM – bamboo bowl

BET (isotherm) – Brunauer-Emmett-Teller (isotherm)

BIOPP – bio-polypropylene cup

BPA – bisphenol-A

BPS – bisphenol-S

CAGR – compound annual growth rate

CE – circular economy

CRMs - certified reference materials

EDCs – endocrine disrupting compounds

EFSA – European Food Safety Authority

EMAS – eco-management and audit system

EPP – expanded polypropylene bowl

ETVS – environmental technology verification system

EU – European Union

FCMs – food contact materials

FCS – food contact substances

GCxGC-TOF/MS - comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry

GC-ECD – gas chromatography coupled with electron capture detector

GC-O-FID – gas chromatography, olfactometry and flame ionization detector

GC-TOF/MS – gas chromatography time-of-flight mass spectrometry

**GHG** – greenhouse gas

**GMP** – Good Manufacturing Practice

**HA** – Hierarchical analysis of components

**HDPE** – high-density polyethylene

**HPLC-DAD** - high-performance liquid chromatography with diode array detector

**HS-SPME** – headspace solid microextraction

**IAS** – intentionally added substances

**ICP-MS** - inductively coupled plasma mass spectrometry

**IUPAC** – International Union of Pure and Applied Chemistry

**KI** – Kovats Index

**LDPE** – low-density polyethylene

**LLE** – liquid-liquid extraction

**LOD** – limit of detection

**LOQ** – limit of quantification

**MB** – mater-bi material (thermoplastic starch)

**NIAS** – non-intentionally added substances

**NIR** – near infrared

**OAV** – odor activity value

**OECD** – Organization for Economic Cooperation and Development

**OML** – overall migration limit

**OT** – odor threshold

**PAHs** – polycyclic aromatic hydrocarbons

**PBAT** - polybutylene adipate terephthalate

**PC** – paper cup



**PCA** – Principal Component Analysis

**PCL** - Polycaprolactone

**PCW** – paper cup white

**PDLA** – (D)-polylactic acid

**PE** – polyethylene

**PET** – polyethylene terephthalate

**PFBOA** – O-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine

**PHAs** - polyhydroxyalkanoates

**PHE** – phenanthrene

**PLA** – polylactide cup

**PLB** – palm leaf bowl

**PLLA** – (L)-polylactic acid

**PLR** – plant residues bowl

**PP** – polypropylene

**PPB** – black bio-polypropylene cup

**PP/PA** – polypropylene/polyamide blend

**PS** – polystyrene

**PSC** – plate of sugar cane

**PWB** – plate of wheat bran

**ROP** – ring-opening polymerization

**RSD** – relative standard deviation

**SAFE** – solvent-assisted flavor evaporation

**SML** – specific migration limit

**SML(T)** – total specific migration limit

**SUPD** – Single-Use Plastics Directive

**TDI** – tolerable daily intake

**TPO** – diphenyl-(2,4,6-trimethylbenzoyl)phosphine oxide

**TS** – thermoplastic starch cup

**2,4-DHBP** – 2,4-dihydroxybenzophenone

**2-H-4-MBP** – 2-hydroxy-4-methoxybenzophenone

**2,2',4,4'-THBP** – 2,2',4,4'-tetrahydroxybenzophenone

**US EPA** – United States Environmental Protection Agency

**VOCs** – volatile organic compounds

**WB** – wooden bowl

**WTE** – Waste-To-Energy

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## 1. Introduction

In recent years, a variety of pro-environmental regulations have been introduced in the European Union with the overarching goal of protecting and improving the environment (including the Plastics Directive; European Commission, 2019). Therefore, the packaging industry has changed the materials that are popularly used as food contact materials (FCMs) over the past few years. The promotion of the circular economy and the dissemination of environmentally friendly substitutes for fossil-based plastics began (Bhuyar, Muniyasamy & Govindan, 2018; Abu Bakar & Othman, 2019; Di Bartolo, Infurna & Dintcheva, 2021). Plant-based materials (e.g., wheat bran) and bio-based plastic (e.g., polylactide) have become dominant and are treated as “ecological materials”. They are environmentally friendly alternatives to fossil-based plastics due to their susceptibility to rapid biodegradation or reusability (Steven, Octiano & Mardiyati, 2020). Ecological materials focus on creating a more sustainable world with less environmental impact, as they decompose in an optimal time. As a result, they create biomass and environmentally friendly chemical compounds, such as carbon dioxide and water. At the same time, they have similar properties to traditional conventional materials, which largely determines the global demand for these materials (Jabeen, Majid & Nayik, 2015). However, new ecological materials can become a source of food contamination. Some of the contaminants migrating from such packaging/vessels may become from the environment, due to the natural process of sorption of environmental contaminants by plants (phytoremediation). In addition, the limited mechanical strength of ecological materials creates the need for reinforcements, such as synthetic fibers, adhesives and polymeric protective layers in the manufacturing process. They can degrade into different chemical compounds during storage or heating, which may easily migrate into the food. It can often cause undesirable changes in the quality and sensory properties of food.

Therefore, the introduction of new materials on the market can be controversial. Replacing plastics with new FCMs may introduce other toxic substances that are hazardous to health and the environment (Akouesan et al., 2023). New FCMs are of various origins, which means that the number of potential contaminants that can migrate into food is constantly increasing and may still not be fully recognized. Moreover, very often materials from different production batches differ from each other. This requires constant monitoring, especially if detailed information about the material is not available from the manufacturer. Therefore, determining the safety of new, currently popular FCMs on the consumer market is a current, urgent challenge. The impact of FCMs on the amount of particularly dangerous organic and inorganic contaminants that can migrate from FCMs to food of various nature under different contact conditions should be critically assessed. Migration studies will enable a better recognition and understanding of the interactions between FCMs and food.

## 2. Theoretical section

### 2.1 The global problem of fossil-based plastic waste

The invention of bakelite in 1909 by Leo Hedrik Baekeland gave rise to the polymer era (Rangel-Buitrago, Neal & Williams, 2022). The unique and desirable properties of these materials, such as lightness, transparency, ease of shaping, relatively low production cost and convenient transportation, ensured that plastics rapidly gained a global demand that continues to the present day (Nayanathara Thathsarani Pilapitiya & Ratnayake, 2024). According to Plastic Globe (2024) (Plastics Europe, 2024), global plastics production is growing year-on-year, reaching more than 413 million tonnes in 2023. The leader in global plastics production is Asia (53 %), followed by North America (17.1 %) and Europe (12.3 %). The largest sector using plastics is packaging (39.9 %). This sector has recorded accelerated growth by the global shift from reusable to disposable containers. As a result, the share of plastics in municipal solid waste (by weight) has increased from less than 1 % in 1960 to more than 10 % in 2005 in the middle- and high-income countries (Geyer, Jambeck & Law, 2017).

Most used plastics (more than 370 million tonnes) are still fossil fuel-based plastics (based on oil or natural gas), which are resistant to degradation and can easily accumulate in the environment. The combination of the dynamic, uncontrolled production of such materials and the use of poorly developed waste management systems (mainly linear economy, based on actions: take-make-consume-dispose) has led to the dumping of huge amounts of waste into the environment, which can finally lead to irreversible changes (Gucina, 2023; Beghetto et al., 2023). According to Geyer et al. (2017) and Beghetto et al. (2023) over the past 65 years, more than 4,900 Mt of the 8,300 Mt of fossil-based polymers produced have been burned, pyrolyzed or dispersed into the environment, e.g., in the packaging industry about 32 % of all packaging produced has been “disposed of” in this way. Plastic waste still remains in all major ocean basins and can have toxic effects on marine biota as a global result of these activities (Yu & Singh, 2023; Tekman et al., 2023). Marine animals often mistake plastic fragments for food, leading to problems associated with ingestion, such as gastrointestinal blockages or leaching of toxic chemicals into tissues (Simon, 2022).

One of the largest dumping grounds for plastic waste is the Great Pacific Garbage Patch, which was discovered in 1997 by Charles Moore (Rochman, Cook & Koelmans, 2016). The patch is currently estimated to consist of 1.8 trillion pieces of plastic (79,000 Mt) and has an area larger than Italy and Germany combined (about 660,000 km<sup>2</sup>) (Lebreton et al., 2018; Beghetto et al., 2023). Plastic fragments can form microplastics (sizes ranging from 1 µm to 5 mm) and nanoplastics (sizes less than 1 µm) in the

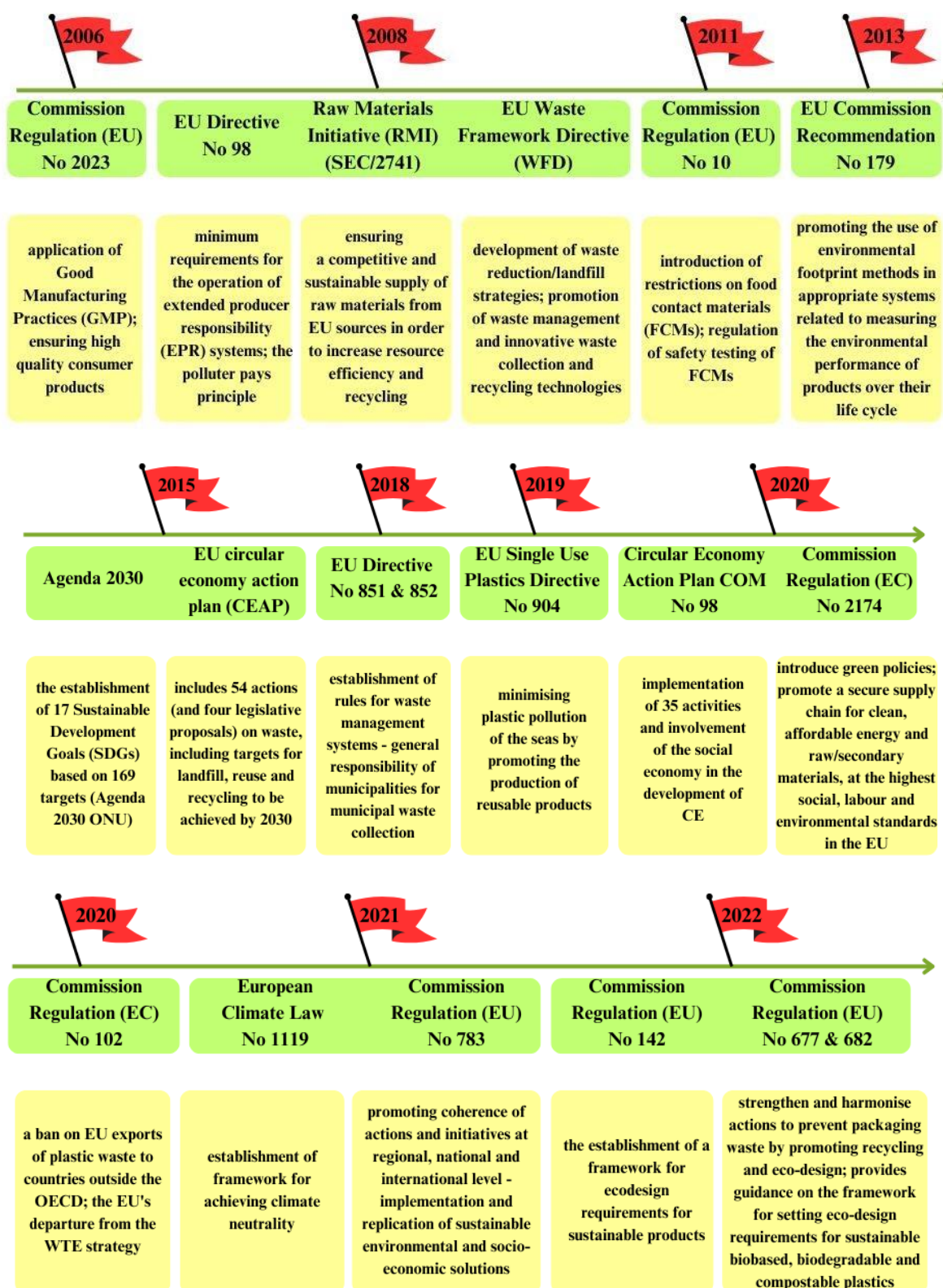
environment, which are harmful to living organisms due to bioaccumulation and possible absorption of hazardous contaminants (i.e., heavy metals, hormone-like molecules, hydrocarbons and dioxins) (Fred-Ahmadu et al., 2020; Gucina, 2023; Mariani et al., 2023).

Contamination of freshwater systems and land habitats is also increasingly reported (Wagner et al., 2014; Dris et al., 2016). Plastic pollution degrades soil quality, disrupts nutrient cycles, plant growth and ecosystem dynamics (Dahiya, Kumar, D., Kumar, S., Pandey & Devi, 2024). The presence of hazardous polymer waste in the environment contributes to noticeable climate change, including global warming and depletion of non-renewable resources (Michelini, Moraes, Cunha, Costa & Ometto, 2017; Mora-Contreras et al., 2023). Waste that is disposed of in landfills can produce methane, a greenhouse gas with a much greater harmful impact on the environment than carbon dioxide (Ncube, Ude, Ogunmuyiwa, Zulkifli & Beas, 2021). The constantly deteriorating state of the environment has led to the recognition of the linear economic model as a driving force of unsustainable development, posing a threat to environmental security and economic development (Islam et al., 2024).

## **2.2. Sustainable development regulations**

The urgent global environmental challenges mean that the search/implementation of innovative, sustainable economic systems that meet the needs of current and future generations is currently required (FAO, 2021). The global threat of the ubiquity of plastics means that European Union (EU) directives and regulations related to the production and disposal of plastics need to address several pressing aspects. These may include product quality, emissions from industrial production, worker and consumer health, food contact requirements, recovery and recycling of post-consumer waste (Beghetto et al., 2023). Sustainability efforts include the implementation of various regulations, as presented in **Fig. 1.**

## *TOWARDS SUSTAINABLE DEVELOPMENT*



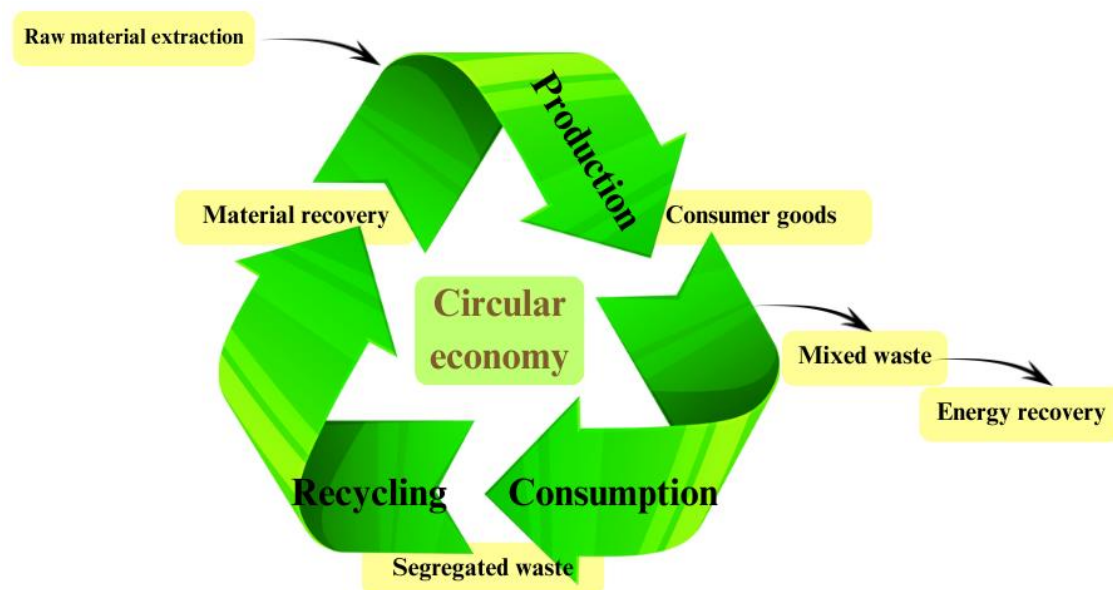
**Fig. 1.** Various regulations of the EU, introducing changes to promote sustainable development over the past two decades



One of the most important regulation was EU Directive 2019/904 (European Parliament and Council, 2019) on reducing the environmental impact of certain plastic products. It was adopted in June 2019 and entered on 3 July 2021. This document, commonly known as the Single-Use Plastics Directive (SUPD), was designed to minimize the global environmental contamination with plastic and to promote the use of reusable, biodegradable or recyclable materials. The main objective is to introduce a more sustainable and environmentally friendly economy (circular economy; CE) (Poluszyńska, Ciesielczuk, Biernacki & Paciorkowski, 2021; Uwalomwa et al., 2025). According to Beghetto et al. (2023), the environment is the basis, the economy is the tool and the well-being of society is the main goal in this economic model.

The CE concept is derived from various ideologies that have evolved over the past decades (Uwalomwa et al., 2025). The first mentions of sustainability and pro-environmental practices appeared in 1966 in the work of Kenneth Boulding (Boulding, 1966), who emphasized the depletion of natural resources in the environment and pointed to the need for sustainable development practices and a circular economy system. The industrial ecology movement of the 1970s and 1980s (Rosenboom, Langer & Traverso, 2022), which launched the term “industrial ecology”, was also an important development in the field. The main motive was to design industrial systems that would reflect the functioning of natural ecosystems (Frosch & Gallopoulos, 1989). The term “circular economy” was officially introduced in 1976 by the European Commission, based on the work of Walter Stahel and Genevieve Reday-Mulvey (Stahel & Reday-Mulvey, 1981).

The global popularity of the CE concept is due to the work of the Ellen MacArthur Foundation since 2010. Its main goal is to accelerate the transition of the global economy to CE. Since its inception, the foundation has become a global leader in CE and collaboration between academia, business and government in this area. CE is a model of sustainability that aims to reduce waste and increase resource use. CE focuses on closed systems that promote the reuse, repair, remanufacturing and recycling of goods, materials and resources (Kirchherr et al., 2018). The basic principles of the closed-loop economy model are based on maximizing the value of resources used, reusing production and consumption waste and pursuing renewable energy sources (Didenko, Klochkov & Skripnuk, 2018; Geissdoerfer, Morioka, Carvalho, Evans, 2018; Moshood et al., 2022). This creates a material-energy cycle in the economic system that considers the closed cycle of goods (**Fig. 2**). The initial 3R principles (reduce, recycle, reuse) have evolved into a more comprehensive 9R framework, including reject (**R0**), rethink (**R1**), reduce (**R2**), reuse (**R3**), repair (**R4**), refurbish (**R5**), remanufacture (**R6**), reuse (**R7**), recycle (**R8**) and recover (**R9**) to enhance corporate responsibility and facilitate a smoother transition to CE (Islam et al., 2024).



**Fig. 2.** *Flow chart of the circular economy*

The formation and functioning of circular economy are supported by various approaches. The first one is the design and production in accordance with the “cradle to cradle” philosophy. This means considering the entire life cycle of products and promoting the use of materials that can be safely reintegrated into the environment or continuously reused in industrial processes (Uwalomwa et al., 2025). The second approach is the concept of the restorative economy, which emphasizes the need to protect and enhance natural resources and encourages economic activities that contribute to environmental regeneration and sustainable development (Stahel, 2016). The third approach concerns natural capital accounting, which integrates the value of natural resources and ecosystem services in financial statements. This helps companies understand their impact on the environment and make informed decisions about the use of resources (Uwalomwa et al., 2025).

According to Jaworski and Grochowska (2017), the product design stage is crucial for meeting the main CE assumptions. The product and its entire life cycle are shaped at this stage. The use of practices and tools such as resource saving, eco-design, life cycle assessment and eco-labelling can ensure compliance with the CE idea. The production stage is associated with the extraction and processing of resources, which requires energy input and generates large amounts of waste, especially in highly developed companies. Fulfilling the CE principle at this stage can be particularly difficult. It is important to meet Good Manufacturing Practice (GMP) principles, strive to improve the efficiency of technological processes and introduce innovative solutions using tools such as the environmental technology

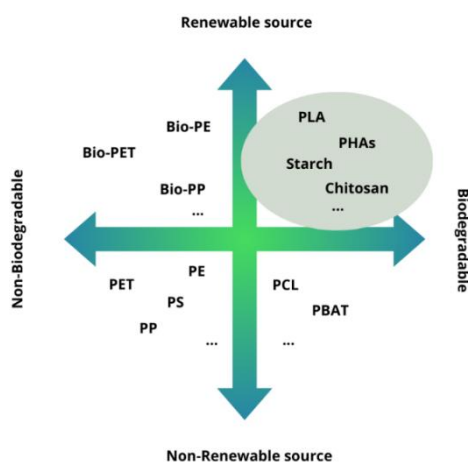
verification system (ETVS), the eco-management and audit system (EMAS) and the environmental footprint.

The product use stage is associated with consumerism. It requires ecological awareness of society and promotion of pro-ecological attitudes. The product should be used in the most effective way, which will contribute to minimizing excessive consumption. The final stage is waste management and activities are focused on waste prevention and promoting recycling (waste can be recovered and reintroduced into circulation and used in the next cycle). Waste that is not suitable for recycling should be subjected to other recovery processes (incineration and co-incineration of waste), which allow for a high level of energy recovery and processing of waste into solid, liquid or gaseous fuels. The least desirable form of waste management is its neutralization (wasting potential), which includes waste storage in landfills and thermal processing of waste without significant energy recovery.

A global popularization of new materials in the packaging sector is currently observed in order to achieve the above-mentioned, main objectives of sustainable development.

## 2.3 New materials used as food contact materials (FCMs)

Sustainable development strategies (mainly the CE approach) and society's concern for the environment makes it necessary to introduce changes in the packaging sector. Research is currently underway to find alternative materials with functional properties similar to fossil-based plastics, but safe for the environment. In general, all materials used in packaging can be divided in terms of renewable resources and biodegradability, as presented in Fig. 3.

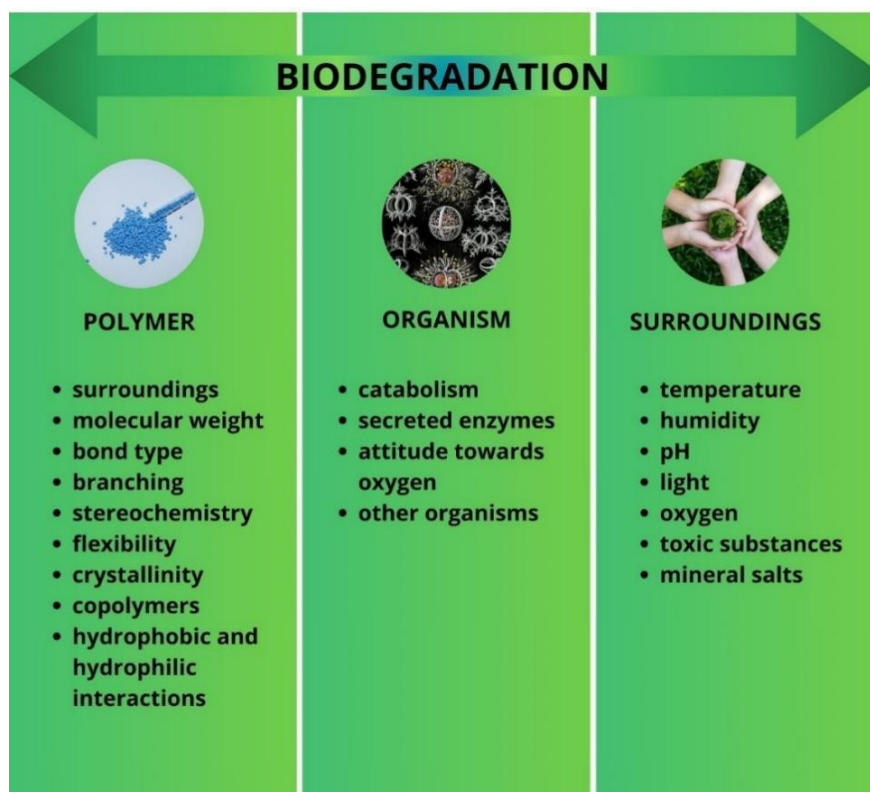


**Fig. 3.** Division of materials based on renewable resources and biodegradability (adapted from European Bioplastics, *Bioplastic Materials*, 2020; (the abbreviations used are explained in the List of Symbols)

The most desirable are “double green” materials, which are produced from renewable resources and are biodegradable (so-called plant-based materials and bio-based plastics) (Barbale et al., 2021). Another important area of research is the search for methods to increase the recycling rate of non-biodegradable polymers obtained from fossil raw materials. These measures will reduce the use of natural resources. Global demand for more environmentally friendly materials has led to an increase in the production of these materials and is expected to continue to grow in the next few years. According to Plastic Globe (Plastics Europe, 2024), global production of “ecological materials” was almost 40 million tons (about 10 % of global plastic production) in 2023. More than 36 million tons include recyclable materials and about 3 million tons were bio-based plastics. Between 2018 and 2023, production of such materials increased by more than 8 million tons.

### **2.3.1 Characteristic of biodegradable/compostable FCMs**

Based on the definition proposed by the International Union of Pure and Applied Chemistry (IUPAC), bio-based plastics are materials derived from “biomass or monomers derived from biomass and which, at some stage in its processing into finished products, can be shaped by flow” (McNaught & Wilkinson, 1997). Such bio-based plastics contain natural polymers or salt mixtures that biodegrade much faster than traditional plastics. Biodegradable plastics are considered environmentally friendly because they are produced from renewable agricultural materials (Lomwongsopon & Varrone, 2022). They contribute to the conservation of limited natural resources. Biodegradation is the process of decomposition of plastics under the activity of microorganisms (bacteria, fungi, algae) under certain environmental conditions into natural chemical compounds (biomass, water and carbon dioxide). This reduces the impact of such materials on ecosystems (especially marine) and human health. Furthermore, the production of bio-based plastics and biomaterials often requires less energy, thus reducing greenhouse gas (GHG) emissions (Mahmoud, Yasien, Swilam, Gamil & Ahmed, 2023). The biodegradation process of plastics depends on many factors, which are summarized in **Fig. 4**.



**Fig. 4.** Factors influencing the rate of the biodegradation process

Plastics that biodegrade quickly and under well-defined conditions are called compostable polymers. This means that under controlled composting conditions, 90 % of the plastic degrades within six months and the compost produced is not harmful to plants. In many countries (e.g., Italy), biodegradable bio-based plastics certified as compostable (based on EN 13432:2000) are collected with biowaste and processed in anaerobic digestion (AD) plants and composting facilities. According to Cucina et al. (2022), the circularity of biosolids is particularly enhanced in AD systems, where they can be converted to biogas, generating a corresponding amount of renewable energy and reducing their release to the environment.

### 2.3.2 Characteristic of recyclable FCMs

The global waste management market was estimated to cost at USD 1,293.70 billion in 2022 and is expected to grow at a compound annual growth rate (CAGR) of 5.4 % from 2023 to 2030 (Report ID: GVR-4-68039-917-8). In Europe, 23 million tons of plastic packaging are produced per year and current forecasts predict 92 million tons by 2050 (Guillard et al., 2018; Ncube et al., 2021). However, recycling rates for single-use plastic packaging are currently low. According to Ncube et al. (2021), only 14 % of

plastic packaging is collected for recycling and 5 % is successfully recycled into new plastic. The planned EU packaging waste targets are related to ensuring that 75 % of packaging is recycled by 2030. Therefore, increasing the efficiency of recycling and upcycling of plastic waste is crucial. Recycling can reduce the consumption of raw materials and reduce waste through a closed loop. Upcycling is the addition of value to plastic waste to produce a higher value product (Jung et al., 2023). The effectiveness of recycling and upcycling depends on the functioning of the several system elements, which can include:

- appropriate legislative policies to promote recycling and the development of waste treatment technologies,
- the design of goods consisting of homogeneous materials sent for recycling, which facilitate waste separation,
- the design of products consisting of different materials that will be easily separable,
- the design of goods allowing waste to be stored and reused without treatment (or with minimal treatment),
- proper labelling of packaging and product components, which facilitates recognition and proper segregation of waste.

### 2.3.3 Production of new FCMs

FCMs made of renewable raw materials (plants) are increasingly appearing on the consumer market, due to environmental concerns. The most commonly used plant-based FCMs include sugar cane fiber (bagasse), wheat bran, palm leaves, wood and others. In general, the production technology of plant-based FCMs is based on the initial cleaning of the raw material, soaking, drying and extrusion of the desired shapes (usually using pressure extrusion). Plants are also used as primary raw materials for obtaining polysaccharides (**Fig. 5**).

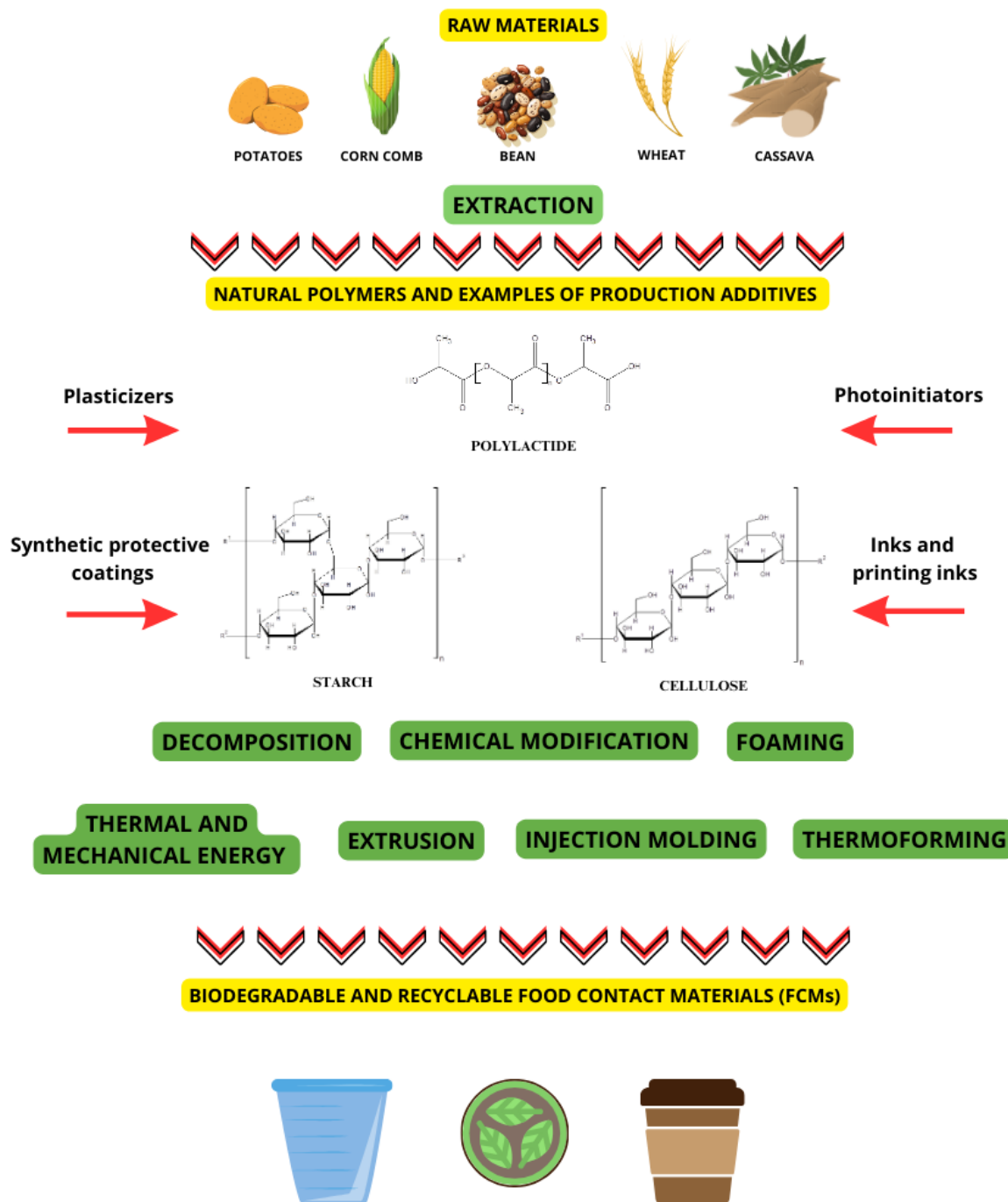


Fig. 5. Main stages of production of plant-based and bio-based plastics FCMs

Starch is a key component in the production of biodegradable (and compostable) plastics due to its cost-effectiveness and ease of processing. This raw material has found wide application in packaging

(Matheus et al., 2023; Garavito, Peña-Venegas & Castellanos, 2024; Haq et al., 2025). Starch can be extracted from cassava, corn, potatoes and beans. It is a natural, crystalline polysaccharide and occurs in the form of grains. The production of starch packaging/vessels involves its decomposition (destructuring) and chemical modification, such as etherification or esterification. These processes aim to improve the mechanical properties, water resistance of starch and compatibility with other polymers (Kim & Jung, 2022). Plasticizers (e.g., sorbitol, glycerol) are also often added at the production stage to improve the mechanical properties of starch-based products (e.g., increase elasticity) (Kshirsagar & Shinde, 2023). The whole is subjected to the action of thermal and mechanical energy, resulting in the formation of thermoplastic starch (TS), which can be considered a substitute for polystyrene (PS). Starch is most often used for the production of films characterized by high tensile and bending strength. The degradation time of starch products in conventional composting plants is 20-45 days (Fazal et al., 2025).

Another natural polymer is polylactide (PLA) composed of many connected 2-hydroxypropanoic acid molecules. This aliphatic polyester is produced by fermentation of starch-rich agricultural by-products (e.g., potatoes, corn, wheat). There are three known routes for the synthesis of PLA: direct condensation polymerization, azeotropic dehydration condensation and ring-opening polymerization (ROP), which is the most commonly used, although it requires purification and the use of heavy metal catalysts (Singhvi, Zinjarde & Gokhale, 2019; Li et al., 2020; Oliver-Cuenca et al., 2024).

Several methods are used to process PLA, including extrusion, injection molding, thermoforming and foaming (Castro-Aguirre, Iñiguez-Franco, Samsudin, Fang & Auras, 2016). Thermoforming is most commonly used in the production of FCMs. The process involves heating PLA to soften it, then using compressed air and pressing the material into the mold. The properties of PLA depend on the ratio between the two optical isomers of the lactic acid monomer (PLLA and PDLA). In order to improve functional properties and flexibility, PLA is often blended with plasticizers (glycerin, polyethylene glycol or vegetable oils) (Carbonell-Verdu et al., 2017). PLA can be considered as an ecological substitute for high-density polyethylene (HDPE), low-density polyethylene (LDPE), polyethylene terephthalate (PET) and polystyrene (PS). PLA is subjected to microbial degradation. In strictly defined environmental conditions, enzymes produced by microorganisms (e.g., lipases, proteases) can catalyze the hydrolysis of PLA chains. PLA, under the right conditions, degrades within 80 days (Oliver-Cuenca et al., 2024).

In turn, cellulose has been widely used in the production of recyclable paper products. Cellulose fibers can be recovered from wastepaper and further processed into new products (Copenhaver et al., 2021; Wang et al., 2021; Fazal et al., 2025). Cellulose is obtained from trees, cotton and sugar cane stalks. It is a tasteless and odorless solid. It has a linear structure formed from  $\beta$ -D-glucopyranose



molecules connected by  $\beta$ -(1,4)-glycosidic bonds. Subsequent layers of the chain overlap, which results in the formation of fibers stabilized by hydrogen bonds. This gives the entire structure a very high durability and creates major problems in polymer processing. High chemical and mechanical strength cause poor solubility in water and organic solvents. Therefore, it is necessary to modify cellulose into water-soluble derivatives to obtain paper. For this purpose, an esterification reaction is carried out, which produces cellulose ethers and esters (i.e., cellulose acetate). Cellulose packaging is often reinforced with synthetic polymer films (e.g., polyethylene (PE)). According to Fazal et al. (2025), the process of producing cellulose vessels is environmentally friendly, as it causes the emission of about 0.2 kg CO<sub>2</sub>/kg of material (for comparison, the production of PS produces 7.4 kg/kg of material, respectively).

On the other hand, recycling materials involves several important steps that impact a sustainable approach to waste management. First, the efficiency of the recycling and the final product is highly dependent on the initial collection and sorting stages, as the quality of the input material has a strong influence on the efficiency of the waste management and material recovery process. Therefore, many techniques have found widespread application in this field, such as near infrared (NIR) (Cimpan, Maul, Jansen, Pretz & Wenzel, 2015), Fourier transform infrared, ultrasound, laser-induced breakdown spectroscopy or X-ray fluorescence (Rahimi & García, 2017; Singh et al., 2017). Currently, plastics are recycled mechanically and chemically. The first one (also called secondary recycling) is for homogeneous waste with a low degree of contamination and consists of the following steps:

- I) the recycled plastics have to be separated from the non-plastic components and then the different plastics are collected separately using optical, manual, floating/sinking techniques,
- II) grinding and milling – common polymers and/or additives can be added to the recycled material,
- III) extrusion – the efficiency of polymer recycling depends on the sorption properties and inertness of the polymer and the diffusion behavior of the polymer. FCMs produced from transparent polymers (PET and HDPE) are suitable for recycling in this way, while HDPE is susceptible to sorption of contaminants (Clark, Jung & Lamsal, 2014).

Mechanical recycling is mainly implemented in developing countries because it is a low-cost and efficient process. However, this process has some limitations because with each successive recovery cycle the material loses its quality. Chemical recycling (also called raw material recycling) is the decomposition of polymers in a controlled manner into monomers and oligomers by chemical reactions such as pyrolysis, hydrogenation, hydrolysis and hydrocracking. Chemical recycling is considered as a

complementary strategy to mechanical recycling and allows to increase the percentage of recycled plastic waste (Huang, Veksha, Chan, Giannis & Lisak, 2022).

Another form of recycling is energy recovery, which is based on waste incineration and recovery of heat and electricity. Energy sources are mainly plastics from crude oil, which are characterized by high calorific value, e.g., for polyethylene and polypropylene they are about 45 and 46.5 MJ/kg, respectively, while the calorific value of crude oil is about 42.5 MJ/kg (Panda, Singh & Mishra, 2010). Incineration reduces the volume of waste by about 99 %, but on the other hand it can contribute to the emission of harmful chemical compounds into the environment (this requires air quality control) (Ferronato & Torretta, 2019). Popular methods of waste-to-energy (WTE) used in developed countries are divided into thermal (pyrolysis, incineration and gasification), chemical (esterification) and biochemical (fermentation) (Rafey, Prabhat & Samar, 2020). Currently, the efficiency of electricity generation using WTE technology is about 80 %. Modern incinerators are equipped with state-of-the-art air pollution control technologies to minimize emitted air pollutants (Al Qattan et al., 2018; Hahladakis, Velis, Weber, Iacovidou & Purnell, 2018).

### **2.3.4 Advantages and limitations of new FCMs**

The current poor state of the environment requires major changes in the packaging sector. Regulations promote investment in bio-based plastic, plant-based and recyclable material technologies, which increases market demand (Moshood et al., 2021). Filho et al. (2021) suggest that most consumers are aware of the problem of plastic pollution and are committed to reducing plastic consumption by using sustainable alternatives to fossil-based plastics.

According to Mousavi et al. (2024), Mohery, Mindil and Soliman (2024), Fazal et al. (2025), the implementation of biodegradable and recyclable materials presents challenges and opportunities. Significant opportunities include reducing pollution, promoting sustainable material alternatives and supporting new recycling technologies. However, key challenges are related to high production costs (compared to conventional plastics) and the need to improve waste management infrastructure. It has been estimated that the production of about 1 kg of bio-based plastic requires about 1-2 kg of corn or about 5-10 kg of potatoes, which may result in deforestation of the crops used to produce these materials (Jeremic, Milovanovic, Mojicevic, Bogojevic & Nikodinovic-Runic, 2020).

Moreover, plastics recycling processes are difficult to implement. Most plastics (more than 50 % of waste) are produced from olefins (e.g., LDPE, HDPE, PP) (Vieyra, Molina-Romero, Calderon-Najera &

Santana-Diaz, 2022). Their structure consists of polymer chains with strong covalent C-C bonds. This makes their decomposition require high energy inputs and the use of high-performance catalysts (Jung et al., 2023). Therefore, the recycling rate of olefin-based polymers is currently low at less than 10 % (Chaudhari et al., 2021). Some plastics (e.g., PET) are more given to reuse, as there is an ester bond in their structure that is susceptible to decomposition by hydrolysis. However, PET waste currently accounts for about 10 % of all plastic waste generated. Mixtures of plastics that are combined within a single product are also a major limitation, making the sorting efficiency of such waste low (Roosen et al., 2020; Vogt, Stokes & Kumar, 2021; Jung et al., 2023). Furthermore, the use of a wide range of new materials as food contact materials (FCMs) may raise food safety concerns.

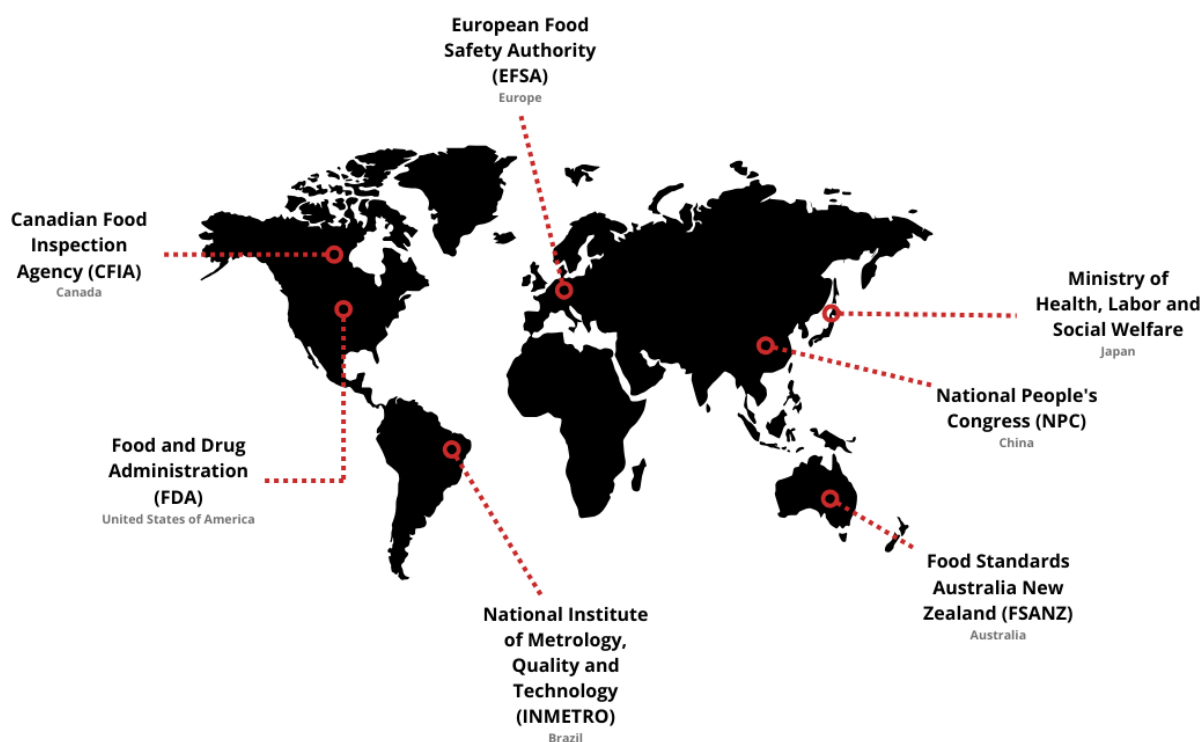
## 2.4 Contamination problems in FCMs

Food contact materials (FCMs) are an important element of packaged/served food because they fulfill various functions, i.e., protection, information, marketing and logistics (Kato & Conte-Junior, 2021). However, not every material can be used as a FCMs, because they must comply with basic food safety requirements (European Commissions, 2011, 2018). This means that FCMs should be manufactured in compliance with GMP principles in order to limit transfer contaminants into food that could adversely affect human health or cause unacceptable changes in the composition or properties of foodstuffs (Commission Regulation, 2006).

However, since the 1970s and 1980s, some researchers have reported that the phenomenon of migration of various contaminants from packaging materials (conventional plastics) can significantly reduce the quality of food and change its sensory profile (Figge & Koch, 1973; Senich, 1982; Taverdet & Vergnaud, 1984; Scriven, Sporns & Wolfe, 1987). The packaging material is often reinforced and enriched on the production line by adding various chemical compounds that improve the final properties of FCMs, such as light, oxidation and impact resistance, appropriate hardness and the others (Rodrigues et al., 2019; Kato & Conte-Junior, 2021; Fengler & Gruber, 2022; Lerch, Fengler, Mbog, Nguyen & Granby, 2023; Phelps, Parkinson, Boucher, Muncke & Geueke, 2024). This means that interactions between FCMs and food require monitoring and control to assess the safety of popular FCMs.

### 2.4.1 Regulations for the served/packed food safety

Interactions that occur between FCMs and food can lead to significant changes in the quality and sensory properties of food. The most undesirable changes may be caused by the bidirectional migrations. This phenomenon occurs mainly with molecularly dispersed low-molecular-weight substances, which can be easily transferred from FCMs to food and conversely (Kato & Conte-Junior, 2021). Based on the Fick's law, it can be assumed that the migration of substances occurs by diffusion between media of different concentrations, until an equilibrium state is established (Kato & Conte-Junior, 2021; Wang, Gao, Liu, Lin & Xia, 2020). In general, the stages of migration can be divided into desorption of dispersed molecules from the surface of FCMs, sorption of compounds at the FCM-food interface and desorption of compounds in food (Bhunja, Sablani, Tang & Rasco, 2013; Schmid & Welle, 2020). Regulating the safety of served/packaged food requires the establishment of appropriate supervisory authorities, which is globally presented in the Fig. 6.



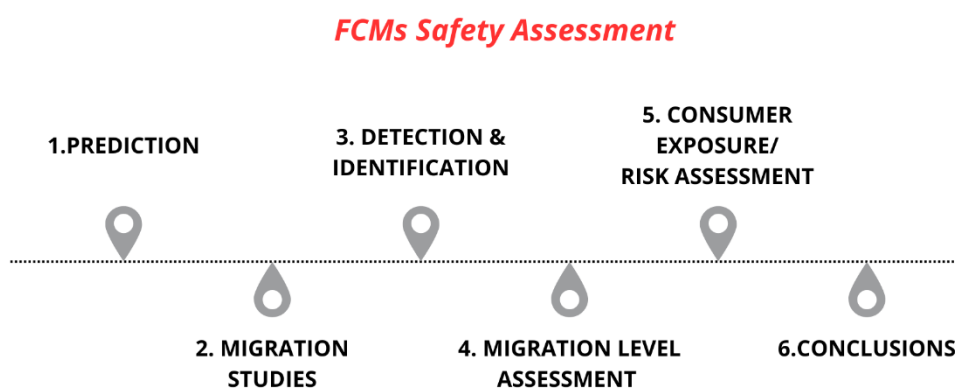
**Fig. 6.** FCM safety regulators around the world

In the EU, the European Food Safety Authority (EFSA) operates, which is an advisory body to the legislator (Commission) in terms of authorizing permitted substances added to plastic products (risk assessment). On the other hand, the European Commission establishes regulations on FCMs. One of the

most important regulations in this area is Regulation (EU) No. 10/2011 (amendment on September 23, 2020), which applies to materials and articles intended for contact with food, made of plastics. Annex I of this regulation contains a positive list (the so-called Union list) of substances (including monomers, auxiliary agents, macromolecules produced by microbiological fermentation and others) that are permitted as intentional additives used in the production process of plastic materials and products. Although no specific regulations have been established for the use of other, currently popular FCMs yet, controlling their safety is subject to the same regulations as plastics.

## 2.4.2 FCMs safety assessment

The safety assessment of FCMs consists of several steps, which are summarized in Fig. 7.



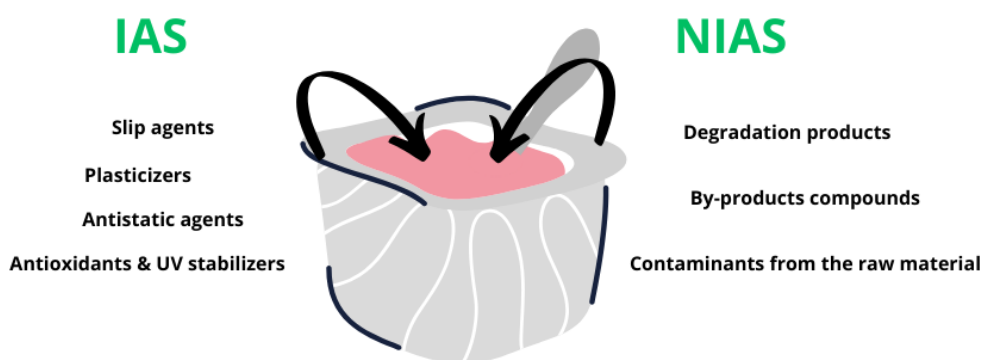
**Fig. 7.** *FCM safety assessment steps*

Prediction and migration tests are conducted to assess the impact of FCMs on the quality and sensory properties of food, in accordance with Commission Regulations (No. 10/2011; No. 213/2018 and No. 1245/2020). The contact time and temperature between the vessel/package material and the food should reflect the worst possible conditions (highest temperature and longest time), e.g., if the FCM is intended for short-term contact with hot food, then the migration test conditions of 2 h and 70°C are used.

The detection and identification methods depend on the substance that can migrate from FCMs to food (so called food contact substances (FCS)). They can be defined as “any substance intended for use as a component of materials used in the production, packaging, transportation or storage of food, where such use of the substance is not intended to have any technical effect on such food.” (Bhunia et

al., 2013; Kato & Conte-Junior, 2021). FCS are divided into intentionally added substances (IAS) or non-intentionally added substances (NIAS). The sources of their migration are several, as presented in the Fig. 8. These may include:

- I) **antioxidants and UV stabilizers** – are added to many FCMs to protect them from photo- or thermo-oxidation,
- II) **antistatic agents** – prevent the accumulation of electric charges on the surface of plastics, which facilitates the packaging process and prevents dusting,
- III) **plasticizers** – ensure the appropriate flexibility and strength of FCMs,
- IV) **slip agents** – facilitate mechanical packaging,
- V) **by-products compound** – production of starting substances, materials, additives and food packaging side reactions can occur, which lead to new, often unknown products,
- VI) **degradation products** – may be formed as a result of thermal decomposition of polymers; decomposition products are the main source of NIAS in FCM. Degradation of polymers and additives leads to the formation of new low molecular weight substances that can easily migrate into food,
- VII) **contaminants from the raw material** – these can be any substances left over from the production process, e.g., residues of catalysts, solvents, paints; in the case of plant raw materials, these can also be contaminants adsorbed by the plant during its growth from a polluted environment (phytoremediation process). The processes of migration of various chemical compounds from FCMs to food can lead to undesirable changes in the physicochemical properties of food (Groh et al., 2019; Kato & Conte-Junior, 2021).



**Fig. 8.** Examples of intentionally and non-intentionally added substances (IAS and NIAS, respectively) in FCMs that can easily migrate into served/packaged foods

IAS are included in the positive list of the European Commission, 2011. The specific migration limit (SML) has been established for each IAS which allows for the assessment of the migration level and consumer exposure. SML determines the maximum concentration of undesirable chemical compounds that can be identified in food (mg/kg food or  $\mu\text{g/g}$  of food). However, the presence of NIAS may pose the greatest concern for food safety, mainly due to the not fully understood and spontaneous mechanisms of formation of such substances (Wrona & Nerín, 2020). Although it is impossible to establish an SML for them, they are subject to an overall migration limit (OML). This parameter represents the general limit of FCM inertness and is established on the basis of gravimetric measurements. The OML determines the sum of all substances migrating from the analyzed FCMs under test conditions (for non-volatile compounds, it must not exceed  $10 \text{ mg/dm}^2$  FCM or  $60 \text{ mg/kg}$  of food). Based on the determined concentrations of migrating organic and inorganic contaminants, the safety of FCMs can be assessed, which is the final conclusion of the FCMs safety assessment.

The increasing popularization of new plant-based FCMs and bio-based plastics FCMs, has raised questions about their safety and impact on food. To date, there are still few literature reports on the safety of new plant-based raw materials, such as wheat bran, palm leaves, bamboo, sugarcane, wood, plant residues and bio-based plastics. This is an important research gap, because these materials can have particularly effect of food quality. Plant raw materials may contain various environmental contaminants. The natural ability of plants to biodegrade, accumulate and inactivate substances from the environment means that dangerous chemical compounds can be stored in their tissues. Moreover, toxic chemical substances may be produced by plants as secondary metabolites in response to environmental stresses, e.g., during shearing. An additional source of contamination is the bio-based plastic FCM production process, in which various NIAS can enter FCMs through cross-contamination. Therefore, the global production of new FCMs may become a serious food contamination problem and cause controversy. This issue is important, especially nowadays, when there are changes in food trends and a clear focus on: smaller packages with larger food contact surfaces, more processed foods with long shelf life and packaged heated products. Additionally, the group of people potentially exposed is also increasing due to the spread of new FCMs in fast food bars, restaurants, schools and hospital canteens.

### 3. Goal and scope of doctoral dissertation

The research objective of the dissertation is to comprehensively characterize the bidirectional interactions occurring between plant-based and bio-based plastics food contact materials (FCMs) and food or food simulants (imitating foods of different nature). The realization of this objective includes conducting migration studies under well-defined conditions (based on current regulations), which will allow assessing the impact of currently popular FCMs on the sensory profile and safety of foods.

In the first part of the study, a wide spectrum of different groups of chemical compounds that can easily migrate from FCMs to food was determined (non-targeted analysis). On this basis, the scale of diversity of the FCMs studied was assessed and targeted analyses presented in the second part of the study were designed. Targeted analyses enabled the assessment of the impact of the FCMs studied on the sensory profile of food, the selection of markers for assessing the impact of various factors on the intensity of migration processes and the assessment of the impact of new, popular FCMs on food quality and safety.

The research assumptions allow to formulate the following research theses:

- the materials analyzed differ in terms of contaminants released into food depending on their origin,
- volatile contaminants of low molecular weight can be easily released from FCMs, therefore they can be successfully used as markers to assess the effect of different factors on the intensity of FCMs-food interaction,
- plant-based FCMs can specifically alter the sensory profile of food,
- some hazardous compounds can migrate from FCMs into food at concentrations exceeding the specific migration limits (SML) or tolerable daily intake (TDI).





## 4. Experimental section



### 4.1 Analyzed FCMs

Commercially available plant- and bio-based plastics FCMs were analyzed. A description of vessel material details with the corresponding photo is presented in **Table 1**. In addition to the presented FCMs, glass (GLA) was used as a reference material in some migration studies.

**Table 1.** *Description of the tested FCMs*

Type of FCM		Abbreviation of the sample name	Average weight of the entire vessel (n=10) [g]
	Plate of wheat bran	PWB	97.3
	Palm leaf bowl	PLB	10.8
	Bamboo bowl	BAM	5.1
	Plate of sugar cane	PSC	10.6

	Wooden bowl	WB	1.5
	Plant residues bowl	PLR	10.3
	Polyethylene coated paper cup	PC	13.2
	Paper cup (white)	PCW	7.5
	Polylactide cup	PLA	4.5
	Bio-polypropylene cup	BIOPP	2.8
	Thermoplastic starch cup	TS	3.0

	Expanded polypropylene bowl	EPP	12.9
	Black bio-polypropylene bowl	PPB	9.8

## 4.2 Solids and chemical reagents

The chemical reagents that were used during the research tasks are presented in **Table 2**.

**Table 2.** *List of solids and solvents*

Solids / Solvents	Company	Product Specification
O-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine hydrochloride	Merck Ltd.	LiChropur™, purity ≥ 99.0 %
Tenax		Matrix Tenax® TA, 60-80 mesh, bottle of 10 g
Standards of analytes (see Tables 6 and 11)	Merck Ltd.	Analytical standards
Multielement Calibration Standard 3-10 mg/L in 5 % HNO <sub>3</sub> (CAS 7697-37-2)	Perkin Elmer Pure Plus	Analytical standards
ICP Standards: Ge and Rh 1000mg/L	Merck Ltd.	CertiPure
Anhydrous Sodium Chloride	Avantor Performance Materials Poland S.A.	Purity ≥ 99.5 %
Anhydrous Magnesium Sulfate	Chempur®	Purity ≥ 99.0 %
Absolute Ethanol	Merck Ltd.	Absolute for analysis EMSURE® ACS, ISO, Reag. Ph Eur
Anhydrous Acetic Acid		Glacial, ReagentPlus®, purity ≥99 %

Hexane		Suitable for HPLC, LiChrosolv <sup>®</sup> , purity $\geq 98\%$ (GC)
Sulphuric acid		Suprapur <sup>®</sup>
Methanol		Gradient grade, suitable for HPLC, LiChrosolv <sup>®</sup> , reagent Ph. Eur., purity $\geq 99.9\%$ (GC)
Dichlorometane		Puriss. p.a., ACS reagent, reagent ISO, purity $\geq 99.9\%$ (GC)
63 % nitric acid Trace Metal Grade		Suprapur <sup>®</sup>
30 % Hydrogen peroxide		(Perhydrol TM) for analysis EMSURE <sup>®</sup> ISO
Acetone	P.P.H. "STANLAB" Sp. j.	Purity $\geq 99.0\%$

### 4.3 Apparatus and small laboratory equipment

Apparatus and small laboratory equipment that were used during the research tasks are presented in Table 3.

**Table 3.** *Summary of apparatus and small laboratory equipment*

Type	Producer
GC-TOF/MS	Agilent 7890&7820
GC-O-FID	Hewlett 5890, Packard Series II, Wilmington, DE, U.S.A.
GCxGC-TOF/MS	Pegasus 4D, LECO, St. Joseph, MI
GC-ECD	Fisons Series 8000 GC
GC-FID	HEWLETT PACKARD 5890 SERIES II
HPLC-DAD	Agilent 1100 Series
ICP-MS	Agilent 7700x
Spring 25 demineralizer	HLP Hydrolab Poland
Laboratory drying oven	POL-EKO-APARATURA, SLW 53, 115, 240, 400, 750, 1000; SLN53, 115, 240. Version 3.0

Magnetic heating stirrers	VWR®, VMS-C4 Advanced
Centrifuge	UNIVERSAL 320, HETTICH Z
IKA KS 130 shaker	Merck Ltd.
SAFE with heating controller (ESM-3711-H) and vacuum (T-Station <sup>85</sup> )	Laboplay; Edwards Lifesciences Poland Sp. z o.o.
Kuderna Danish concentrator	Merck Ltd.
Microwave oven	LG; MS-1042G
Autosorb iQ Station 1 port transducer	Quantachrome® ASiQwin™ Automatic Gas Sorption Data Acquisition and Reduction ©1994-2013, Quantachrome Instruments version 3.01.
Rotary Vacuum Evaporator RVO 200A	INGOS s.r.o.
Ball mill	Mini-Mill Pulverisette 23, Fritsch, Germany
High Performance Microwave Digestion System	ETHOS ONE, Italy
Small laboratory equipment, i.e., cellulose thimbles, reflux condenser, desiccator, SPME fiber, pipettes, volumetric flasks, conical flasks, round-bottomed flasks (100 ml), vials, chromatographic needles (1 µl; 5 µl) and columns, Petri dishes, teflon vessels and others	Merck Ltd.; Alchem Group Ltd.; LaboService

## 4.4 Research methodology

### 4.4.1 Characteristic of food simulants used in migration studies

It is complicated and analytically challenged to conduct IAS and NIAS migration studies from FCMs to real food due to the complex composition of the food. Therefore, food simulants are commonly used in migration studies to simplify control processes. Each of the food simulants represents a different type of food (Regulation (EU) No. 10/2011) (**Table 4**).

Pure water was obtained by distilling tap water in a Spring 25 demineralizer (HLP Hydrolab Poland). Ethanol solutions of appropriate concentrations (10 %, 20 % and 50 % v/v) were obtained by diluting absolute ethanol. Similarly, 3 % acetic acid was obtained by diluting glacial acetic acid. Preparation of Tenax for migration studies was carried out similarly to the procedure described in the works (Rubio, Sarabia & Ortiz, 2018; Rubio, Valverde-Som, Sarabia & Ortiz, 2019) with the following modifications. Five g of Tenax was placed in a cellulose thimble and purified with 70 ml of methanol using a reflux condenser for 6 hours before use. The food simulant was then heated to 160°C for 6 h using laboratory drying oven and stored in a desiccator. Tenax was mixed to homogenize the material before migration studies.

**Table 4.** *List of food simulants commonly used in migration studies (in accordance with Regulation (EU) No. 10/2011)*

Symbol of food simulant	Name of food simulant	Type of simulated foods	Example of simulated foods
A	10 % ethanol / water	Neutral foods	Mineral waters, honey
B	3 % acetic acid	Acidic foods	Vegetable soups, fruit juice
C	20 % ethanol	Alcoholic foods	Wine, beer
D1	50 % ethanol	Lipophilic foods containing more than 20% alcohol and oil-in-water emulsions	Milk and milk-based drinks, whole, partially dehydrated and skimmed or partially skimmed
E	Tenax	Dry and frozen foods	Pasta, groats, rice, ice cream

## 4.4.2 Migration studies

The migration studies were performed depending on the type of food simulant used. The analyzed FCMs were weighed, cut into equal pieces (1 cm × 1 cm) and extracted with 200 ml of properly liquid food simulant (A: 10 % EtOH, distilled water; B: 3 % acetic acid; C: 20 % EtOH and D1: 50 % EtOH) in 70°C for 2 h (in accordance with the recommendations of Commission Regulation (EC) No 10/2011). Temperature stability over time was achieved using magnetic heating stirrers with temperature control function (**Fig. 9 I**). One sample contained half of the original weight of the vessel, assuming that half of the material is in contact with food at meal time. After the migration tests, the material was separated from the simulant (filtered and centrifuged).

Four g of Tenax per 1 dm<sup>2</sup> of surface was used in migration tests, according to the guidelines (Commission Regulation (EU) No 10/2011). The analyzed materials were cut into pieces measuring 5 cm x 5 cm (the surface was 25 cm<sup>2</sup>), placed on watch glasses and covered with one g of Tenax (**Fig. 9 II**). The sample was wrapped in aluminum foil (to eliminate the possibility of evaporation) and placed in an oven heated to 70°C for 2 hours or to 40°C for 10 days, which corresponds to short or long contact conditions between food and the vessel (Commission Regulation (EU) No 10/2011). In next step, Tenax was extracted twice with 25 mL of extractant (acetone or methanol) within 1 h at ambient temperature. The extracts were concentrated to 4 mL by vacuum evaporation ( $p = 850$  hPa) and placed in amber glass vials. Blank samples were prepared for all analysis in the same way as tested samples, but without the use of FCMs. Three replicates were performed for each sample and blanks.



I



II

**Fig. 9.** Migration studies of various contaminants from analyzed FCMs to (I) liquid food simulants and (II) Tenax

#### 4.4.3 Different approaches in assessing the safety of food contact materials (FCMs)

Currently observed global environmental pollution (air, water, soil) may affect the contamination of primary raw materials used for the production of food contact materials. In turn, improving the functional properties of new FCMs requires the use of additives and enhancers on the production line. As a result of FCM-food interactions, food may be contaminated with various groups of chemical compounds (organic and inorganic) that may come from the environment or the production line. Therefore, the evaluation of FCMs-food interactions was carried out on a wide group of different, currently popular FCMs. Due to the large diversity of the FCMs studied (plant materials, paper, bio-based plastics), a non-targeted and a targeted approach were used to qualitatively and quantitatively assess the migrating contaminants (intentionally added substances – IAS and non-intentionally added substances – NIAS). The first approach is intended to group migrating contaminants (e.g., into more-toxic-less-toxic, organic-inorganic, volatile-non-volatile, odor active-odorless, etc.) from FCMs into different food simulants under test conditions. This makes it possible to compare, evaluate and predict the effects of FCMs on food simulant (food). It also allows for selecting FCMs that may pose a particular risk to food and therefore require detailed control. In addition, the non-targeted approach simplifies the selection of markers for targeted analyses.

In turn, the targeted approach enables quantitative assessment of monitored organic and inorganic contaminants (IAS and NIAS) and comprehensive assessment of the impact of various FCMs on the sensory profile and quality of the food simulant, using appropriately selected analytical, statistical



and sensory methods. It enables searching for the causes of differences in the intensity of FCMs-food interactions, depending on the type of FCMs, type of food and other factors.

#### **4.4.3.1 Non-targeted approach in safety assessment of food contact materials (FCMs)**

Intentionally added substances (IAS) and non-intentionally added substances (NIAS) in food samples were detected using GC/TOF-MS (Agilent 7890&7820). Compounds were determined using a capillary column coated with SLB-5MS phase (30 m × 250 µm i.d., 0.25 µm film thickness). One microliter of samples was injected in split/splitless mode. The initial oven temperature was held at 40°C for 2 min, ramped to 280°C at a rate of 9°C /min and held for 4 min. Helium was used as a carrier gas at a constant flow rate of 1 mL/min through the column. The temperatures of the front inlet, transfer line and electron impact ion source were set at 250, 280 and 230°C, respectively. The ionization energy was 70 eV. The mass spectral data was collected in a full scan mode ( $m/z$  33–333) and in selected ion monitoring mode. Acquisition delay was 240 sec, rate was 30 spectra/sec and extraction frequency were 30 kHz.

Principal Component Analysis (PCA) was used to determine the groups of key compounds migrating from currently popular FCMs into food using SIMCA software.

#### **4.4.3.2 Target approach in safety assessment of food contact materials (FCMs)**

Intentionally added substances (IAS) and non-intentionally added substances (NIAS) that may migrate from FCMs to food can include toxic elements, which can be formed in natural (erosion of metallic minerals) and anthropogenic processes (energy production, metal processing and waste management) and polycyclic aromatic hydrocarbons (PAHs), which can be by-products of incomplete combustion processes of organic matter in the environment. Plants can easily sorb toxic elements and PAHs from contaminated environment through roots and tubers. As a result of FCM-food interactions, toxic elements and PAHs can migrate from FCM into food, which is an undesirable phenomenon as they exhibit mutagenic, genotoxic and carcinogenic effects on the health (Bansal & Kim, 2015; Joseph, Jun, Flora, Park & Yoon, 2019; Ghuniem, Khorshed, El-Safty, Souaya & Khalil, 2020; Sampaio et al., 2021).

Some PAHs may be degraded to carbonyl compounds in the environment (William, Pangzhen, Danyang & Zhongxiang, 2023).

Carbonyl compounds (low molecular weight aldehydes and ketones) belong to the group of chemicals ubiquitous in the environment (Szeląg-Wasielewska & Dąbrowska 2020; Aznar, Domeño, Osorio & Nerin, 2020; Sauter et al., 2021; Werner, et al., 2024). Some of them are classified as by-products of polymerization process (Cincotta, Verzera, Tripodi & Condurso, 2018; Dehghani, Farhang & Zarei, 2018; Abe et al., 2021; Cardozo, Pereira dos Anjos, Campos da Rocha & de Andrade, 2021; Dhaka et al., 2022). The presence of low molecular weight carbonyl compounds in food is undesirable and requires constant monitoring. Some aldehydes are considered carcinogenic, mutagenic and allergenic, such as formaldehyde and acetaldehyde (WHO 2011). In addition, the identification of a mixture of carbonyl compounds (saturated C3-C10 aldehydes, ketones) in food may suggest undesirable changes in the sensory profile of food, because aldehydes and ketones with simple structure are characterized by low sensory thresholds. Migration of carbonyl compounds from the surfaces of FCMs to food may be the reason for noticeable changes in the smell and taste of food (Gonzalez, Domenek, Plessis & Ducruet, 2017; Dehghani et al., 2018; Marín-Morocho, Domenek & Salazar, 2021; McGorin, 2019; Osorio, Aznar & Nerin, 2019; Miralles, Yusa, Sanchis & Coscolla, 2021; Aznar et al., 2020).

In addition, some manufacturing additives (e.g., bisphenol-A (BPA), bisphenol-S (BPS), photoinitiators, phthalates) should be used in moderation because they can exhibit proestrogenic effects and are defined as endocrine disrupting compounds (EDCs) (Ma et al., 2019; Dong et al., 2022; Heindel et al., 2022; Sawadogo et al., 2023; Prueitt et al., 2023; Topdas, 2023; Tsochatzis et al., 2023; Zhu et al., 2024). Due to the undesirable properties of many IAS and NIAS, target approach is needed to determine the impact of FCM on food sensory profile and quality.

## **I) Overall migration study of volatile, odor-active contaminants**

Undesirable interactions between FCMs and food can include change the sensory profile of food for two reasons: as a result of migration of odor-active compounds from FCMs into food or sorption of key food odor-active compounds by FCMs. To evaluate the effect of FCMs on the sensory profile of food, a three-stage experiment was conducted, which include:

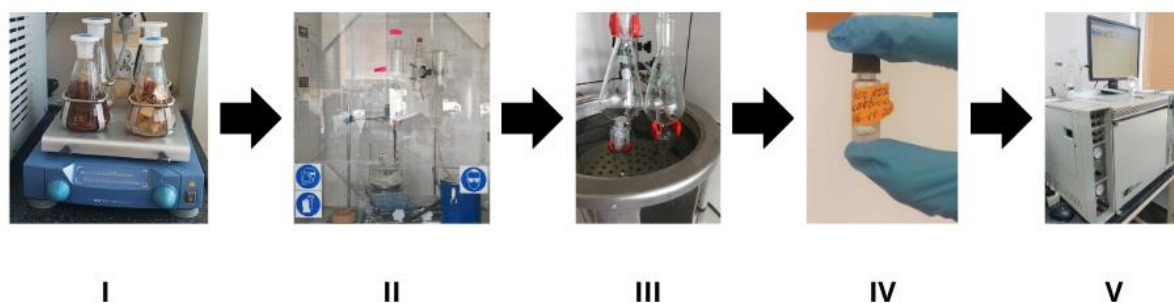
I) determination of odor-active compounds characteristic of FCMs,

- II) determination of odor-active compounds in coffee or tea whose presence was caused by the FCMs-food interactions,
- III) sensory evaluation of coffee and tea brewed in different FCMs.

In all of the above steps, glass was treated as a reference material.

Firstly, gas chromatography-olfactometry (GC-O) analysis was carried out to identify the volatile aroma compounds characteristic of FCMs. GC-O is an analytical technique that combines gas chromatography with human sensory detection to identify and evaluate odor-active compounds in complex mixtures. In GC-O, trained panelists sniff the effluent directly from the capillary column to detect and describe odor-active compounds as they elute from the chromatograph.

Solvent-assisted flavor evaporation (SAFE), described by Engel, Bahr and Schieberle (1999), has found widespread application in the identification of key aroma compounds from various matrices (Majcher, Olszak-Ossowska, Szudera-Kończal & Jeleń, 2020; Gąsior et al., 2021). Prior to SAFE extraction, samples (50 g) were extracted with methylene chloride (100 mL) for 24 h by shaking in the IKA KS 130 shaker (Fig. 10). After the volatiles were isolated, the extract was dried over anhydrous sodium sulfate and concentrated with a Kuderna Danish concentrator to about 500 µL.

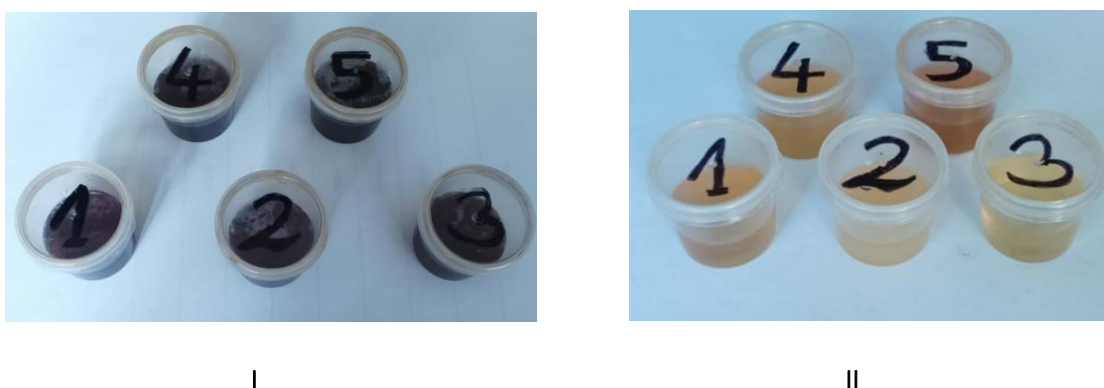


**Fig. 10.** Sample preparation for analysis of odor-active compounds characteristic of FCMs; steps included: (I) - extraction with dichloromethane, (II) - SAFE, (III/IV)- concentration, (V) - GC-O analysis

Odor-active compounds were identified from SAFE extracts by GC-O on a HP 5890 chromatograph (Hewlett-Packard, Wilmington, DE, U.S.A.) using two capillary columns with different polarities: SPB 5 (30 m × 0.53 mm × 1.5 µm) and SUPELCOWAX 10 (30 m × 0.53 mm × 1 µm) (Supelco, Bellefonte, PA, U.S.A.). GC was equipped with a Y splitter dividing the effluent 1:1 between the olfactometry port with humidified air as a makeup gas and a flame ionization detector. The operating

conditions were as follows for the SPB-5 column: initial oven temperature of 40°C (1 min) raised at 6°C/min to 180°C and at 20°C/min to 280°C. Operating conditions for the SUPELCOWAX 10 column were as follows: initial oven temperature of 40°C (2 min), raised to 240°C at 6°C/min rate and held for 2 min isothermally. The flavor extract (2 µL) was injected into a GC column using splitless mode. Odor-active regions were detected by GC-effluent sniffing (GC-O) and three panelists determined the description of the volatiles. For all peaks and flavor notes, Kovats Index (KI) were calculated to compare results obtained by GC-MS to literature data. KI were calculated for each compound using a homologous series of C7–C24 n-alkanes at a concentration 1 mg/mL, which was injected under the same chromatographic conditions. The samples were also identified using GC/TOF-MS (Agilent 7890&7820) to confirmed results obtained.

Secondly, it was examined how FCMs affect the sensory profile of coffee and tea. For this purpose, coffee (10 g) or tea (1 tea bag  $\approx$  2 g) was brewed (250 ml water) and introduced to different FCMs: glass, palm leaf, paper, wood and wheat bran (covered with a lid of the same material). The samples were left for 30 minutes and then presented to the panelists (**Figs. 11 I and 11 II**). Sensory analyses of the coffee and tea samples were evaluated by 8 panel members (6 females and 2 males). Odor descriptors were selected according to the Basic Flavor Descriptive Language from Givaudan Roure Flavor, Ltd. established in preliminary tests and characterized as grassy, coffee-like, bitter, roasted, musty, cereal-like, earthy, woody, cardboard, citrus and fatty and fruity on a scale of 1–5, where 1 means “none” and 5 means “very strong”. The sensory tests were carried out in a conditioned room.



**Fig. 11.** Samples of (I) coffee and (II) tea prepared for sensory evaluation

At the same time, volatile compounds were extracted from the coffee or tea samples using headspace solid microextraction (HS-SPME). SPME fiber (CAR/PDMS/ DVB; 2 cm) was pre-treated in an

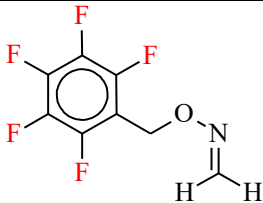
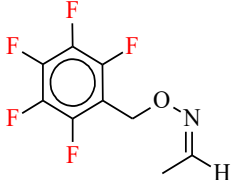
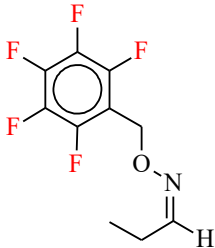
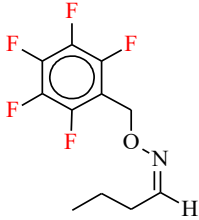
injection port at 270°C for 30 min before analysis. Filtered black coffee or tea extracts (5 mL), were introduced into 20 ml SPME vials and 5 g salt was added. Extraction was carried out at 50°C for 40 min. The fiber compounds were desorbed in the injection port of the GCxGC-TOF/MS apparatus for 5 min (Pegasus 4D, LECO, St. Joseph, MI). The GC system was equipped with a DB-5 primary column (25 m × 0.2 mm × 0.33 µm, Agilent Technologies, Santa Clara, CA) and Supelcowax-10 (1.2 m × 0.1 mm × 0.1 µm, Supelco, Bellefonte, PA) as a secondary column. Injector temperature was set at 240°C and injection was performed in a splitless mode. Gas flow was set at 0.8 mL/min. The primary oven temperature was programmed as follows: 40°C (1 min), 6°C/min to 20°C (0 min), 25°C (1 min) to 235°C (5 min). Secondary oven: 65°C (1 min), 6°C /1 min to 225°C (0 min) 25°C 1 min to 260°C (5 min). The transfer line temperature was 260°C. The modulation time was 4 sec. Time-of-flight mass spectrometer was operating at a mass range of m/z 33-383 and detector voltage – 1700 V at 150 spectra/sec. The data were collected and processed using LECO ChromaTOF v.4.40. The total analysis time was about 34 min. Three replicates were performed for each material. Volatile compounds were identified based on the mass spectra using the NIST library and based on the retention index using Leibniz-LSB@TUM Odorant Database. Semi-quantitative analysis was performed using an internal standard naphthalene (D8) (15.6 mg/25 mL MeOH).

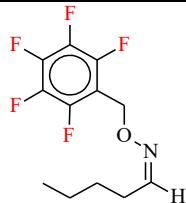
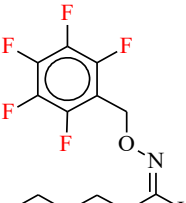
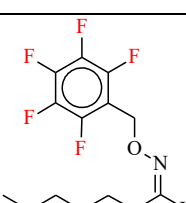
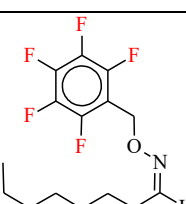
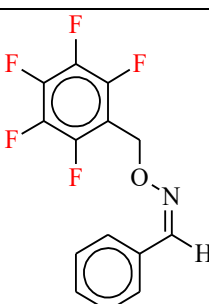
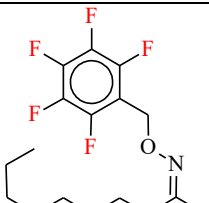
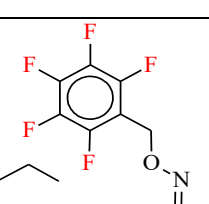
## **II) Migration study of volatile markers - carbonyl compounds**

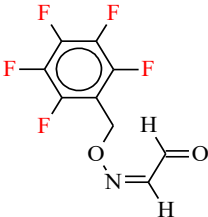
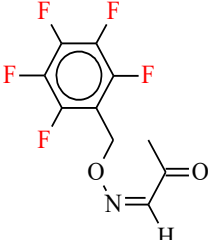
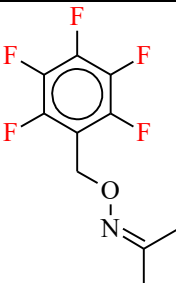
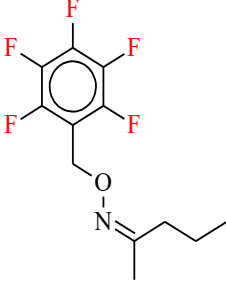
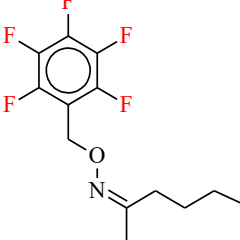
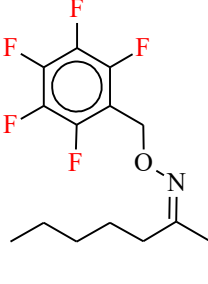
Carbonyl compounds belong to a group of chemical compounds ubiquitous in the surrounding environment, in which they undergo dynamic changes and are highly reactive. The use of suitably sensitive analytical tools that allow monitoring the concentration levels of low-molecular-weight carbonyl compounds makes it possible to observe the changes taking place and establish correlations, even at low concentrations (ng/L). This means that these compounds can be successfully used as environmental markers. The intensity of migration of carbonyl compounds (and other contaminants) from FCMs into food can be determined by various physicochemical factors, e.g., type of FCMs, type of food (i.e., pH value), contact time and temperature between FCMs and food. Therefore, migration studies of carbonyl compounds (as markers) from FCMs into various food simulants at different times (15 min, 30 min, 2h, 5 h and 10 h), temperatures (5°C, 20°C, 60°C and 70°C), pH value (2.75-6.00) were carried out. Additionally, heating the food with popularly 700 W microwave radiation may also be an important factor that can influence the intensity of migration processes. FCMs with distilled water and 3 % acetic acid were stored under refrigeration (4°C) for different times (12 h, 24 h, 192 h), after which the sample was heated in a microwave oven for different times (1-4 min).

Carbonyl compounds dissolve well in polar matrices, therefore the determination of these compounds in polar matrices is difficult. Their isolation requires special preparation of samples for testing. The qualitative and quantitative determination of migrating carbonyl compounds was carried out using the technique proposed by Scilimenti, Krasner, Glaze and Weinberg (1990). The technique is based on the use of pre-derivatization of the sample with the reagent O-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine (PFBOA), which allows the transformation of carbonyl compounds into less polar and more volatile oximes (Table 5). For most aldehydes, two geometric isomers are formed: E- and Z-PFBOA, except for symmetrical carbonyls, such as formaldehyde.

**Table 5.** Formulas of oximes formed by the reaction of carbonyl compounds with the PFBOA reagent, their molecular masses, molar volume and density

Carbonyl compound	Example of derivatization process product with PFBOA reagent	Molecular mass of oxime (Da)*	Molar volume (cm <sup>3</sup> /mol)*	Density (g/cm <sup>3</sup> )*
formaldehyde		225	157.7 ± 7.0	1.42 ± 0.10
acetaldehyde		239	173.8 ± 7.0	1.37 ± 0.10
propanal		253	189.9 ± 7.0	1.33 ± 0.10
butanal		267	206.0 ± 7.0	1.29 ± 0.10

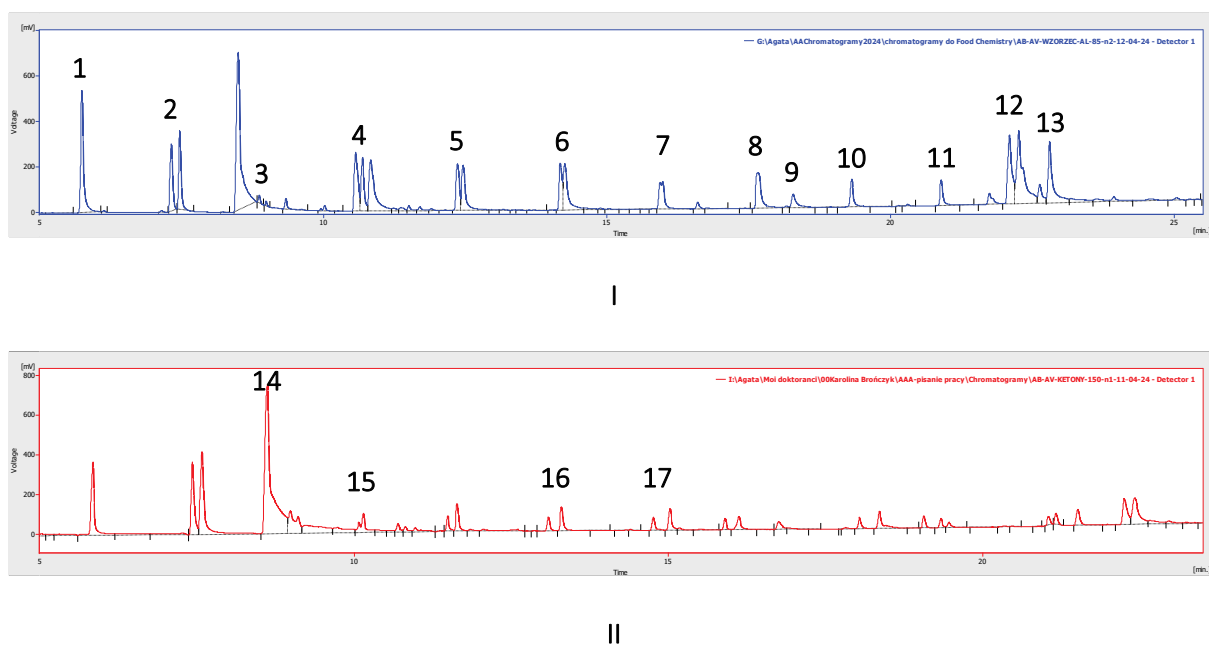
pentanal		281	222.1 ± 7.0	1.26 ± 0.10
hexanal		295	238.2 ± 7.0	1.23 ± 0.10
heptanal		309	254.3 ± 7.0	1.21 ± 0.10
octanal		323	270.4 ± 7.0	1.19 ± 0.10
benzaldehyde		301	226.7 ± 7.0	1.32 ± 0.10
nonanal		337	286.5 ± 7.0	1.17 ± 0.10
decanal		351	302.5 ± 7.0	1.16 ± 0.10

glyoxal		253	172.0 ± 7.0	1.47 ± 0.10
methylglyoxal		267	187.2 ± 7.0	1.42 ± 0.10
acetone		253	189.1 ± 7.0	1.33 ± 0.10
pentan-2-one		281	221.3 ± 7.0	1.27 ± 0.10
hexan-2-one		295	237.4 ± 7.0	1.24 ± 0.10
octan-3-one		323	269.5 ± 7.0	1.19 ± 0.10

\*based on the ChemSketch Programme Database



1 ml of 2 mg/mL PFBOA aqueous solution was added to 50 mL of food simulants and left at room temperature for 1 h. 50  $\mu$ L of concentrated sulfuric acid was added to complete the derivatization reaction. The oximes were extracted by liquid-liquid extraction (LLE) with 1 mL of hexane for 1 min. Then the extract was purified with 2 mL of 0.1 M sulfuric acid solution. The hexane extracts were analyzed by gas chromatography using a Fisons Instruments 8000 equipped with  $^{63}\text{Ni}$  electron capture detectors (GC-ECD). Injections of 0.5  $\mu$ L of the extract were introduced via "on column" injector into chromatographic column. A Rtx-5MS (Restek) fused silica capillary column (30m  $\times$  0.25mm i.d.  $\times$  0.25 $\mu$ m film thickness) was employed for analysis and a Rtx-1301 (Restek) fused silica capillary column (30m  $\times$  0.32mm i.d.  $\times$  0.5 $\mu$ m film thickness) was used as a confirmation column. Injector temperature was set at 80°C. Gas flow was set at 80 kPa. Helium was used as carrier gas and nitrogen was used as make-up gas for the detector. The analysis were carried out in a temperature program starting at 80°C for 4 min, then increasing the temperature to 240°C with an increase of 7°C/min and then to 290°C with an increase of 20°C/min. DataApex, Clarity 6.2, Czech Republic software was used to collect and process chromatographic data. Chromatograms of aldehyde and ketone standards are presented in Fig. 12.



**Fig. 12.** Carbonyl compound standards: (I) aldehydes: (1) formaldehyde; (2) acetaldehyde; (3) propanal; (4) butanal; (5) pentanal; (6) hexanal; (7) heptanal; (8) octanal; (9) benzaldehyde; (10) nonanal; (11) decanal; (12) glyoxal; (13) methylglyoxal and (II) ketones: (14) acetone; (15) 2-pentanone; (16) 2-hexanone; (17) 3-octanone

Quantification for carbonyl compounds was performed using an external standard calibration curve. All standards were prepared gravimetrically in concentration ranges 1-30 µg/L. The linearity of the calibration curve was calculated as the correlation coefficient (R), the value of which is greater than 0.9996 for all analytes. Limit of detection (LOD) and quantification (LOQ) were determined for each analyte using "Regression Statistics". The precision of the method was evaluated in terms of repeatability and expressed as relative standard deviation (RSD %). The RSD% was obtained by analyzing the samples in optimized conditions, using three replicates and three points of calibration curve for each analyte. The analytical parameters of all migrants analyzed are shown in **Table 6**.

### III) Migration study of high-molecular weight contaminants

Polycyclic aromatic hydrocarbons were determined by the GC-FID technique (HP 5890II) with autosampler and flame ionization detector (FID). The injection volume was 1 µL, injector and detector temperature were set at 280°C. The chromatograph was equipped with Rtx 5-W/Integra Guard capillary column (30 m × 0.25 mm × 0.25 µm, Restek, USA). The analysis was performed using helium as carrier gas at a flow rate of 1.75 mL/min. The initial column temperature was 90°C (hold for 3 min) and then ramped at 10°C/min to 270°C. The total analysis time was 21 min.

Bisphenols and benzophenone derivatives were determined by the HPLC-DAD technique (Agilent 1100 Series HPLC System with Diode Array Detector). The injection volume was 1 µL. The chromatograph was equipped with an Ultra AQ C18 column (5 µm, 250 mm × 4.6 mm; Restek, USA). A mixture of acetonitrile and water in a volume ratio of 70:30 was used as the mobile phase in the analysis of BPA and BPS and methanol (100 %) was used in the analysis of 2,4-DHBP, 2,2,4,4'-THBP and 2-H-4-MBP, respectively. The mobile phase flow rate in both analyzes was 1 mL/min in isocratic mode. The total analysis time was 3 min for bisphenols and 4 min for benzophenone derivatives, respectively. Spectra were collected at a wavelength of  $\lambda = 254$  nm.

Quantification for each migrant was performed using an external standard calibration curve. All standards were prepared gravimetrically in concentration ranges: for ANT and PHE, 1-10 µg/L; and for BPA, BPS and benzophenone derivatives, 0.05-10.00 µg/L, respectively. All chromatographic data were obtained analogously to the carbonyl compounds and are presented in **Table 6**.

**Table 6.** List of tested organic contaminants with IAS/NIAS division and SML values (based on the Commission Regulations No. 10/2011 and No. 2018/213) and chromatographic data: retention time (min), standard curve equation (includes measurement errors of parameters  $a$  and  $b$  and expressed in the form  $y=a(\pm SE)x+b(\pm SE)$ ), limit of detection (LOD), limit of quantification (LOQ) and relative standard deviation (RSD)

Analytical tools	Migrants	IAS/NIAS	SML	Retention time (min)	Calibration curve	LOD ( $\mu\text{g/l}$ )	LOQ ( $\mu\text{g/l}$ )	RSD (%)
GC-ECD	formaldehyde	IAS	15	5.68	$y=41(\pm 2)x + 291(\pm 24)$	0.003	0.009	9.8
	acetaldehyde	IAS	6	8.10; 8.24	$y=82(\pm 3)x + 457(\pm 42)$	0.005	0.015	9.1
	acetone	NIAS	-	8,56	$y=184(\pm 10)x + 1217(\pm 158)$	0.020	0.060	6.5
	propanal	NIAS	-	8.94; 9.07	$y=37(\pm 2)x + 502(\pm 65)$	0.015	0.045	9.8
	butanal	NIAS	-	10.65; 10.76	$y=51(\pm 3)x + 893(\pm 25)$	0.020	0.060	9.9
	pentan-2-one	NIAS	-	11.25; 11.40	$y=8(\pm 1)x + 905(\pm 166)$	0.012	0.040	6.4
	pentanal	NIAS	-	12.44; 12.54	$y=57(\pm 3)x + 906(\pm 30)$	0.020	0.080	9.9
	hexan-2-one	NIAS	-	12.84; 13.05	$y=7(\pm 1)x + 787(\pm 31)$	0.020	0.080	6.4
	octan-3-one	NIAS	-	14.51; 14.76	$y=5(\pm 1) + 534(\pm 49)$	0.060	0.190	5.2
	hexanal	NIAS	-	15.15; 15.25	$y=210(\pm 4)x+622(\pm 35)$	0.003	0.009	6.4
	heptanal	NIAS	-	16.95; 17.00	$y=41(\pm 1)x + 148(\pm 4)$	0.003	0.009	6.8
	octanal	NIAS	-	17.76	$y=72(\pm 3)x + 215(\pm 28)$	0.010	0.030	9.9
	benzaldehyde	NIAS	-	20.12	$y=38(\pm 2)x - 60(\pm 8)$	0.010	0.030	8.8
	nonanal	NIAS	-	20.38	$y=26(\pm 1)x + 122(\pm 9)$	0.010	0.030	8.7
	decanal	NIAS	-	21.00	$y=15(\pm 1)x + 148(\pm 6)$	0.020	0.090	9.9

	glyoxal	NIAS	-	23.23; 23.50	$y=48(\pm 2)x + 851(\pm 28)$	0.015	0.045	6.8
	methylglyoxal	NIAS	-	23.84	$y=22(\pm 1)x + 795(\pm 9)$	0.015	0.045	7.5
GC-FID	phenanthrene (PHE)	NIAS	-	14.67	$y=2.70(\pm 0.15)x - 1.60(\pm 0.69)$	0.88	2.70	8.5
	anthracene (ANT)	NIAS	-	14.79	$y = 1.51(\pm 0.07)x - 0.91(\pm 0.34)$	0.77	2.30	9.3
HPLC-DAD	bisphenol-A (BPA)	IAS	0.05	2.89	$y=1.07(\pm 0.02)x + 4.05(\pm 0.57)$	0.12	0.36	1.8
	bisphenol-S (BPS)	IAS	0.05	2.33	$y=1.27(\pm 0.09)x + 2.49(\pm 0.04)$	0.13	0.38	1.7
	2,4-dihydroxybenzophenone (2,4-DHBP)	IAS	6*	3.19	$y=3.55(\pm 0.05)x + 0.14(\pm 0.10)$	0.13	0.38	2.3
	2,2',4,4'-tetrahydroxybenzophenone (2,2',4,4'-THBP)	NIAS	-	2.80	$y=1.84(\pm 0.11)x + 0.09(\pm 0.02)$	0.52	1.60	9.7
	2-hydroxy-4-methoxybenzophenone (2-H-4-MBP)	IAS	6*	3.74	$y=4.02(\pm 0.16)x + 0.33(\pm 0.03)$	0.35	1.10	5.9

\* expressed as total specific migration limit (SML(T)) for 2,4-DHBP and 2-H-4-MBP

Tenax (food simulant E) is a porous organic polymer that has high chemical stability (up to 350°C) (Alfeeli, Taylor & Agah, 2010). However, some studies report disadvantages of Tenax as a food simulant, including the cost of the reagent, the need for long-term regeneration and the difficult management of Tenax due to static electricity from friction (Rubio et al., 2019). The use of Tenax can also lead to inflated IAS and NIAS concentrations compared to actual food samples (Rubio et al., 2019; Baele, Vermeulen, Claes, Ragaert & De Meulenaer, 2020). These reports suggest that interpretation of the results of Tenax migration studies should be cautious. Therefore, it is important to compare the intensity of FCMs-Tenax and FCMs-real food interactions to better understand the factors affecting the migration processes that occur. The Brunauer-Emmett-Teller (BET) gas adsorption method has become the most widely used standard procedure for determining the surface area of fine-grained and porous materials from adsorption data. This method is based on the physical adsorption of a vapour or gas into the surface of a solid. The specific surface area and pore size (BET isotherm) of Tenax and food samples (powdered milk, baby cereal, oat flakes) were examined, to evaluate the influence of the structure of simulated and real foods and the properties of contaminants on the intensity of migration processes. The composition of the food analyzed is summarized in **Table 7**.

**Table 7.** Description of the composition of the food samples (expressed in g/100g of product), according to the manufacturer's data

Food sample	Content of					
	Fat (including saturated fatty acids)	Carbohydrates (including sugars)	Fiber	Protein	Salt	Mineral components
Granulated, non-fat powdered milk	0.80	51.00	NS*	35.00	1.20	Calcium (1.404)  Phosphorus (1.012)
Baby cereal	1.40	87.00	2.10	7.60	0.02	Sodium (6.5)
Whole grain oat flakes	6.90	60.00	9.80	12.00	<0.01	NS*

NS\*: not specified by the manufacturer

High-purity nitrogen (> 99.999 %) was used as adsorbate. The powdered materials were pre-gassed at 100°C for 24 hours. The selection of pre-degassing parameters took into account resistance to elevated temperatures, including susceptibility to changes in pore structure. The sample was then filled with nitrogen and weighed to determine the real (dry) weight of the sample. The pre-gassed sample vial and the weighing vial (empty) were sealed in an Autosorb iQ Station 1 port transducer, Quantachrome® ASiQwin™ Automatic Gas Sorption Data Acquisition and Reduction ©1994-2013, Quantachrome Instruments version 3.01. and then immersed in liquid nitrogen at 77.35 K. Measurement of gas adsorption on the test material consisted of gradually filling the volume of two vials with the same amount of nitrogen in the relative pressure range from 0.01 to 0.99  $p/p_0$ .

In the next experiment, the adsorption capacity of Tenax and food samples (powdered milk; infant cereal and oatmeal) and the influence of the physical properties of migrant compounds on the intensity of migration processes were evaluated, as recovery test. The spiking experiment was conducted as follows: 1 mL of standard solutions of the tested migrating compounds (2,4-DHBP, 2,2',4,4'-THBP; 2-H-4-MBP; PHE and ANT) containing analytes at appropriate concentrations were applied to a glass Petri dish to obtain a final concentration of 3 µg/L for 2,4-DHBP, 2,2',4,4'-THBP and 2-H-4-MBP and 5 µg/L for ANT and PHE. These chemical compounds were chosen because of their similar structure, but different molecular weights.

One g of Tenax or food (powdered milk; baby cereal and oat flakes) was applied to the materials, then wrapped in aluminum foil and placed in an oven heated to 70°C for 2 hours. Samples were then prepared according to migration tests typical of Tenax, i.e., double extraction with 25 mL of solvent (acetone, methanol) within 1 h at ambient temperature and concentration by vacuum evaporation ( $p = 850$  hPa). The amount of adsorbed contaminants was determined by appropriate chromatographic techniques (GC-FID and HPLC-DAD).

#### **IV) Migration study of inorganic contaminants**

Inorganic contaminants pose a particular challenge in food safety control, due to the harmfulness of many elements even at low (trace) concentration levels. In order to assess the risk of migration of various elements, the total content of elements in FCMs and in food simulants after their contact with FCMs (after 30 min and 10h at 60°C) was determined. The steps of the analytical procedure consisted of:

- I) determination of the analytical problem and selection of the appropriate analytical technique,
- II) development of sample preparation for ICP-MS analysis,
- III) optimization of ICP-MS - calibration, interference correction,
- IV) validation of the analytical procedure - determination of validation parameters,
- V) performance of analyses and verification of the analytical method,
- VI) statistical processing of the results and their interpretation.

The sample preparation step is crucial in the analysis. It should be characterized by the highest possible efficiency and reproducibility. Two sample preparation methods were used: mineralization and extraction, in order to evaluate the elemental composition of analyzed FCMs.

Pre-preparation of FCMs samples for mineralization consisted of gentle washing with demineralized water (cleaning the surface of the raw material from dust) and drying at 40 °C in a laboratory dryer. Digestion of the powdered samples of FCMs (homogenous samples) were carried out in the EthosOne (Milestone, Italy) closed microwave mineralization system in the next step. For this purpose,  $0.5000 \pm 0.0001$  g of FCM samples were placed in a Teflon vessel with 8 mL of concentrated (65 %)  $\text{HNO}_3$  (analytical purity, Merck, Darmstadt, Germany) and 1 mL of  $\text{H}_2\text{O}_2$  (Merck, Darmstadt, Germany). The program of digestion included the following stages:

- I) first stage - temperature to 80°C, 10 min, power 600 W;
- II) second stage - temperature 140°C, 12 min, power 1200 W;
- III) third stage - temperature 180°C, 15 min, power 1200 W.

The solutions were and made up to a final volume of 15 mL with deionized water.

Extraction experiment was conducted in the second step. Elements were determined in food simulants: neutral (distilled water) and acidic (3 % acetic acid) after migration studies with FCMs, which were conducted in different conditions: 30 min (short contact) and 10 h (long contact) at 60°C (in accordance with Regulation (EU) No 10/2011). Based on two experiments, the percentage of migration of various elements from FCMs to neutral and acidic food was assessed and the consumer risk associated with the consumption of neutral and acidic food served in currently popular FCMs was estimated. Procedural blanks and reference materials were carried out in the same way as the samples in each digestion run.

The concentration of 20 elements (Na, Mg, Al, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Sr, Cd, Sb, Ba, Pb) in samples was carried out using an inductively coupled plasma mass spectrometer (ICP-MS

7700xAgilent, Santa Clara, CA, USA) equipped with an octopole reaction system (ORS). MicroMist concentric nebulizer and quartz Scott double pass spray chamber, Ni cones and a quadrupole mass spectrometer. The ICP-MS technique allows the determination of multiple elements during a single analysis due to the possibility of setting individual analytical conditions for an analyte. Optimization of the analytical procedure for multi-element analysis, aims to achieve low LOD and LOQ, high precision, good sensitivity and linearity of indications over a wide range of concentrations. Optimization of the ICP-MS spectrometer is a fundamental activity that has a significant impact on the quality of analytical measurement results and the subsequent application of the developed analytical procedure. It is important to obtain the highest possible signal intensity for the determined elements and the lowest possible background signals during optimization. The daily optimized parameters include: the flow of plasma gas, auxiliary gas and sputtering gas, voltage on the focusing lenses. ICP torch settings, mass calibration, and plasma generator power are also monitored periodically. High purity argon (99.999 %) was used as a nebulizer, auxiliary and plasma gas for the ICP-MS (Linde Gas, Poland). The operating conditions for the ICP-MS instrument were daily optimized (using the commercial Tuning Solution, (Agilent, USA)) and shown in **Table 8**.

**Table 8.** *Operating conditions of ICP-MS instrument*

Parameter	Setting
Spectrometrer	ICP-QMS, Agilent 7700x
Nebulizer gas flow (L/min)	1.00
Auxiliary gas flow (L/min)	0.90
Plasma gas flow (L/min)	15
RF power (W)	1550
Perylstatic pump rotation speed [rps]	0.10
Lens voltage [V]	8.50
Sweeps	1
Repetition	3
Integration time [s]	0.10
Reaction gas flow [mL/min]	3
Oxides [%]	<1.0
Double ion charged [%]	<1.2



Calibration process was performed using the matrix-matched standard series method in order to determine the dependence of the analytical signal on the concentration of the analyzed elements. Calibration solutions were prepared by dilution of 10 mg/L of multielement stock solution in 5 % HNO<sub>3</sub> (Multi-Element Calibration Standard 3, PerkinElmer, MA, USA). The calibration curves were determined using the interpolation method and were constructed in the concentration ranges: 0.05–50 µg/L for Al, Ti, V, Cr, Mn, Co, Ni, Cu, Zn, As, Se, Sr, Cd, Sb, Ba, Pb and 5 – 500 µg/L for Na, Mg, Ca and Fe. The calibration curves showed satisfactory linearity with correlation coefficients (R) reaching values >0.90 for macroelements (Ca, Mg, Na) and >0.99 for other elements (Table 9).

**Table 9.** Calibration curves of the determined elements ( $y=ax+b$ )

Mass	Element	R	a	b
23	Na	0.9668	0.1314	1.0546
26	Mg	0.9930	0.0095	0.0473
27	Al	0.9997	0.0505	0.0802
43	Ca	0.9658	0.0009	0.0137
47	Ti	0.9989	0.0116	0.0107
51	V	0.9996	0.1651	0.0044
52	Cr	0.9997	0.1509	0.0239
55	Mn	0.9998	0.1914	0.0202
56	Fe	0.9981	0.1641	4.1977
59	Co	0.9999	0.1714	0.0007
60	Ni	0.9996	0.0370	0.0102
65	Cu	0.9997	0.0405	0.0067
68	Zn	0.9993	0.0199	0.0175
75	As	0.9973	0.0290	0.0004
82	Se	0.9997	0.0021	0.0001
88	Sr	0.9999	0.2590	0.0102
111	Cd	0.9999	0.0260	0.0001
121	Sb	0.9970	0.1037	0.0013
137	Ba	0.9999	0.0374	0.0009
207	Pb	0.9999	0.0471	0.0028

Interference from matrix components and interferences caused by the reagents used, gases and related to the operation of the instrument used should be expected, during the determination of trace elements in the analyzed samples. The selection of appropriate isotopes of elements, helium as a reaction gas, the internal standard (rhodium solution (20 µg/L)) and sample dilution were used to eliminate the adverse effects of factors.

The next step includes the validation of the analytical procedure. Providing meaningful results is the goal of a procedure designed to determine analytes in samples. The precision of the method was determined by analyzing samples of certified reference materials (CRMs) with repeatability and intermediate precision conditions maintained, as well as using the standard addition method. **Table 10** summarizes the analytical results obtained and the values presented in the CRMs used. The working range of a prepared analytical method is the interval bounded by the lowest and highest concentrations that can be determined from it. The lower value of the working range refers to the LOQ, and the top value is the concentration of the highest standard used for calibration. The resulting working range values for the determined elements are also shown in the **Table 10**. Ensuring measurement consistency is a key aspect of analytical procedures. Measurement consistency in the present procedure was established using CRMs: SRM 1570a spinach leaves (NIST, USA). The results obtained from the analyses performed and the recovery values were comparable and satisfactory, demonstrating the validity and reliability of the results obtained (**Table 10**). Based on the present data, the validated elemental determination method was applied to the analysis of real samples.

**Table 10.** *Parameters of analytical procedure for determination of inorganic contaminants by ICP/MS- performance quality*

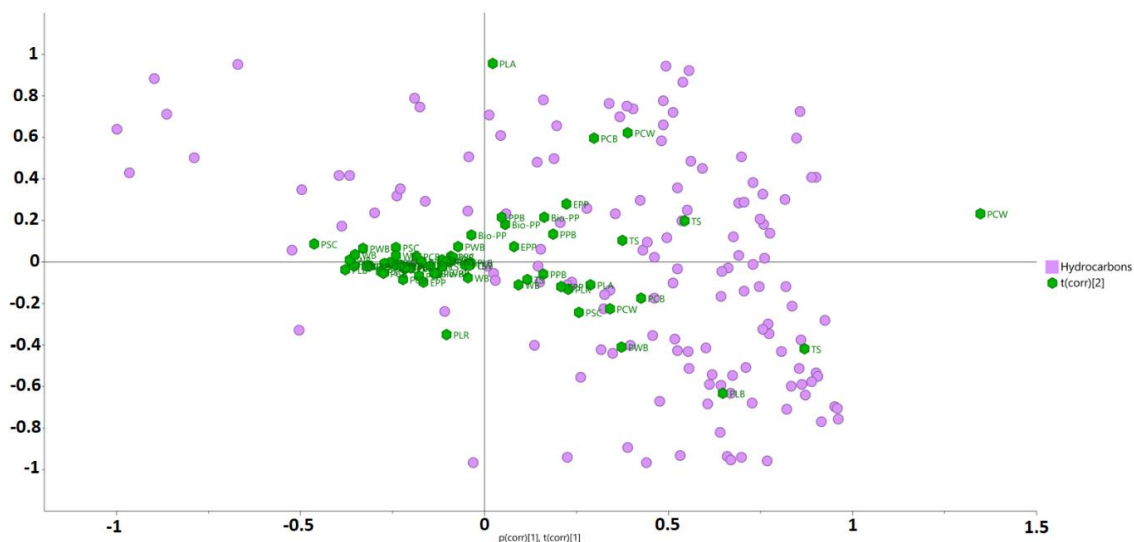
Analyte	Analytical Procedure Parameters					
	MDL [mg/kg] dw	MLQ [mg/kg] dw	Measurement range (µg/L)	Trueness (%)	Precision CV (%)	Traceability
Ca	0.700	2.100	5-500	88	4.7	Provided by certified reference material
Fe	0.200	0.600		95	4.5	
Mg	0.300	0.900		93	4.2	
Na	2.000	6.000		87	5.0	
Al	0.010	0.031	0.05-100.00	91	3.6	

As	0.005	0.015		96	2.7	
Ba	0.007	0.021		92	3.8	
Cd	0.003	0.009		95	2.5	
Co	0.004	0.016		96	2.3	
Cr	0.007	0.021		97	2.6	
Cu	0.008	0.024		92	3.1	
Mn	0.005	0.015		94	3.4	
Ni	0.009	0.027		94	2.8	
Pb	0.004	0.012		95	3.2	
Sb	0.005	0.015		96	3.5	
Se	0.009	0.027		90	3.7	
Sr	0.007	0.021		92	3.5	
Ti	0.010	0.030		90	3.8	
V	0.003	0.009		96	2.7	
Zn	0.009	0.027		92	3.5	

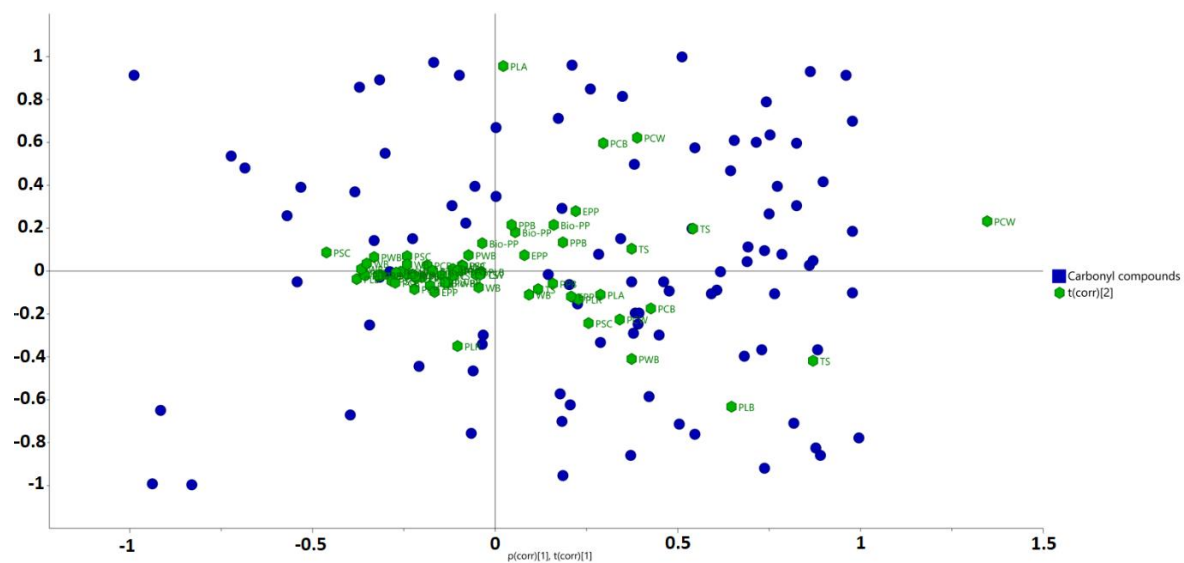
## 5. Results and discussion

### 5.1 Non-targeted approach in safety assessment of food contact materials (FCMs)

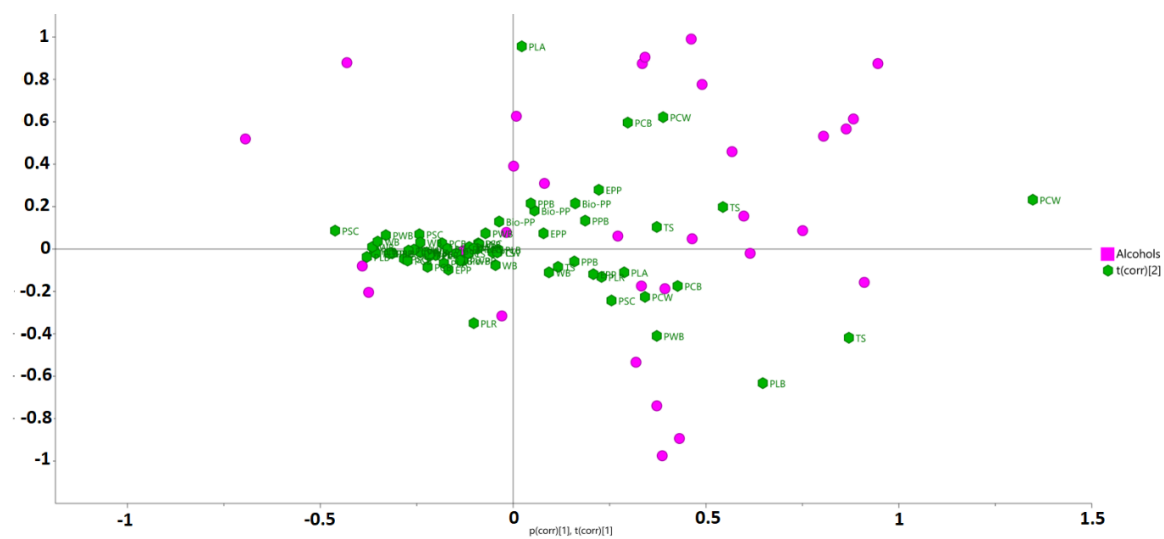
Migration studies of contaminants from FCMs to food of various types (represented by food simulants) were conducted in the initial stage of the FCM safety assessment. Short contact conditions between FCMs and food were used, which were 2h, 70°C (accordingly to Commission Regulation, 2011). In order to evaluate the influence of the type of FCMs on the type of contaminants released into food simulants, an unsupervised PCA was performed (**Fig. 13**). Based on the results, it was determined that the contaminants migrating from the analyzed FCMs into the food simulants mainly belong to the groups of **(I)** hydrocarbons, **(II)** carbonyl compounds, **(III)** alcohols, **(IV)** esters and **(V)** carboxylic acids. In addition, PCA analysis showed that all the FCMs analyzed could be the source of migration of these compounds into food, which means that the FCMs analyzed could affect the sensory profile of food and also its quality. A large variation in the quality of released compounds was observed between FCMs made from paper (PC and PWC samples) and bio-based plastics (PLA, TS, BIOPP, EPP and PPB).



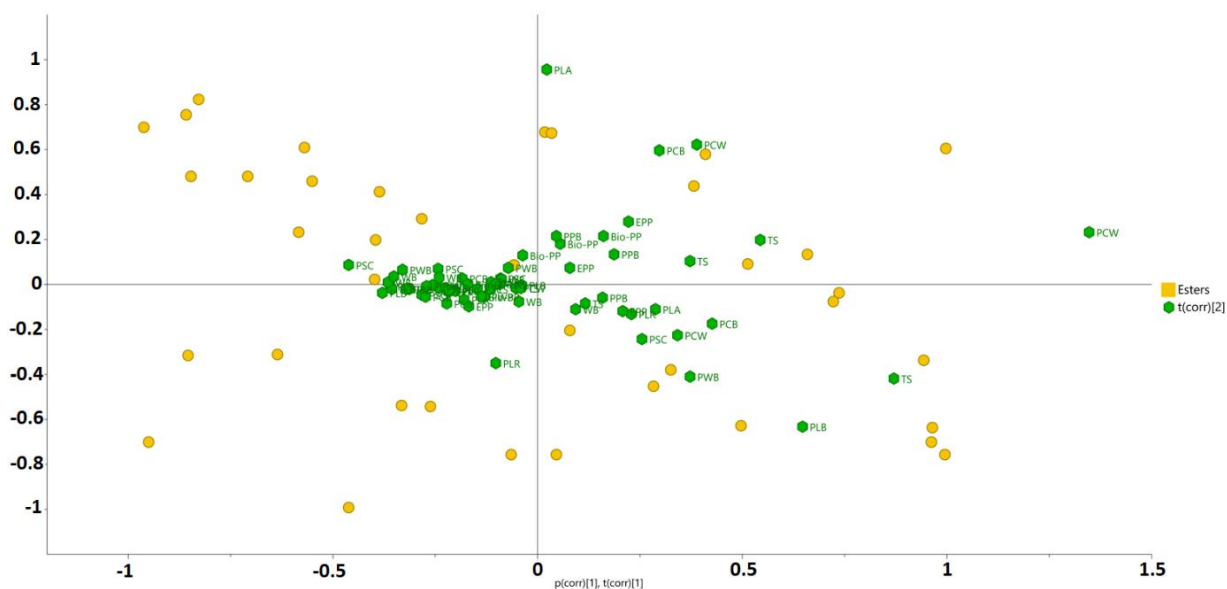
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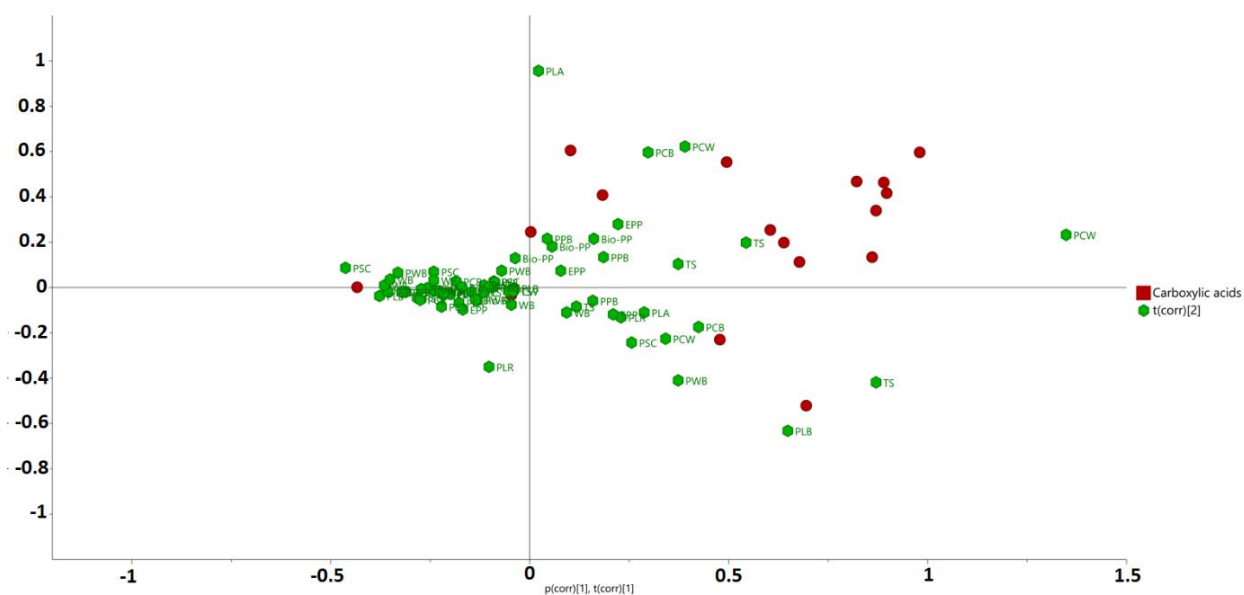
II



III



IV



V

Fig. 13. Biplot from principal component analysis (PCA). PC1 and PC2 explain 40 % of the variance. Green colors represent different FCM samples (for abbreviation see Table 1) and different colors represent different migrating groups of contaminants: (I) hydrocarbons; (II) carbonyl compounds; (III) alcohols; (IV) esters and (V) carboxylic acids

It can be explained that the quality of FCMs used for food packaging and the level of contamination can differ significantly depending on the raw material and industrial procedures (Vera, Canellas & Nerin, 2020; Asensio, Montañés & Nerín, 2020; Guan, Zhong, Wang, Yu & Hu, 2023). For example, Marín-Morocho et al. (2021) classified NIAS migrating from bio-based plastics (PET) into several groups: lubricants (e.g., hexadecanoic and octadecanoic acid), plasticizers (mainly phthalates), antioxidant degradation products (e.g., 2,4-bis(1,1dimethyl)-phenol, 2,6-di-tert-butyl-1,4-benzoquinone and 3,5-di-tert butyl-4-hydroxybenzaldehyde), recycling rates (e.g., limonene) and thermal degradation products (especially BPA and low-molecular carbonyl compounds). Moreover, recycled paper may contain many of the chemicals originally present in recovered paper, including fillers, biocides, inks, pigments, photoinitiators, adhesives, plasticisers, mineral oils and other impurities generated during recovered paper processing. Paper is one of the heterogeneous porous materials, which differs from polymers in terms of sorption, diffusion and partition coefficient values. (Cai et al., 2017). Vápenka et al. (2016) conducted a non-targeted analysis of paper packaging intended for food packaging available on the Czech market. They identified about 100 contaminants, including residues from paper pulp processing (e.g., auxiliaries, wood degradation products), substances from printing inks or adhesives (photoinitiators, plasticizers, solvents), impregnants and coatings (solvents, hydrocarbons), etc. The identified contaminants mainly belonged to the groups of aromatic hydrocarbons, phthalate and non-phthalate plasticizers, photoinitiators and bisphenols. Wrona et al. (2023) studied four different plant-based FCMs and found that one of the compounds migrating from all the FCMs analyzed was diphenyl-(2,4,6-trimethylbenzoyl)-phosphine oxide (TPO), which is commonly used as a UV curing agent for polyesters and resins. In addition, TPO can be used as a component of printing inks and wood coatings and as a coating whitener (Scientific Committee on Consumer Safety SCCS/1528/14). The authors explain that in the case of some FCMs, TPO can be a cross-contamination from the production line. In addition, the authors identified the fatty acids palmitoleic and oleic acids and the monosaccharide D-(+)-glucose, which is characteristic of plant-based FCMs. In addition, oleic acid can be used during production as a surfactant and plasticizer. The authors also identified the presence of photoinitiators and UV absorbers, e.g., 2,2-dihydroxy-4-methoxybenzophenone.

In general, a large proportion of the identified compounds migrating from FCMs into food simulants belong to sensory-active compounds, which means that their effects on the sensory profile of foods must be determined accordingly.

## 5.2 Targeted approach in safety assessment of food contact materials (FCMs)

### 5.2.1 Migration study of odor-active contaminants

According to Parker (2015), aroma is an important food attribute influencing consumer acceptability and appetite (Parker, 2015). FCMs-food interactions can lead to undesirable changes in the sensory profile of food (Aznar et al., 2020; Vera et al., 2020; Ashraf, Pati, Fatchurrahman, Amodio & Colelli, 2023; Wolf, Hoyer & Simat, 2023). In this area, bio-based plastic FCMs have been widely reported in the literature, i.e., Vera et al. (2020) identified forty-six compounds with a characteristic odor that were released from various materials: PP, PE used as FCM. The most strongly identified odors migrating from PP and PE included acetic, propane, buttery, rancid and fatty odors, which were responsible for carbonyl compounds (mainly aldehydes) and low molecular weight carboxylic acids. Similarly, Ashraf et al. (2023) showed the impact of packaging made of PP, a polypropylene/polyamide blend (PP/PA) and PLA on the migration of volatile organic compounds (VOCs) to artichokes. The VOCs emitted vary depending on the FCMs; in particular, PP/PA emitted the highest number of VOCs, most of which belonged to the class of branched alkanes and alkenes, such as 4-methylheptane, 2,4-dimethylheptane, 4-methyl-octane and 2,4-dimethylheptene; PP released acetate, aldehydes and 1-methoxy 2-propanol; PLA releases aldehydes and propanoic acid. In turn, Song, Wrona, Nerín, Qin-Bao and Huai-Ning (2019) identified a total of 99 volatile and semi-volatile compounds in virgin and recycled expanded polystyrene containers and selected 17 compounds as markers of the degree of material processing, including o-xylene, acetophenone, ethylbenzene,  $\alpha$ -ethylstyrene, 2-phenylpropenal, propylbenzene, 2-phenyl-1-propene, undecanal, benzoic acid ethyl ester, 2-ethyl-1-hexanol, decanal, benzylcarboxylic aldehyde, isopropylbenzene, 2,4-diphenyl-1-butene, dodecanal, benzaldehyde and nonanal.

In turn, plant-based FCMs have not yet been thoroughly investigated for their odor profile and they may have a particular impact on the sensory properties of foods. In order to comprehensively understand the aroma profile of the this FCMs, GC-O-FID and GC-MS techniques were used to characterize the key odor compounds characteristic of each FCM. **Table 11** summarizes the identified odor-active compounds with the retention time, CAS number, Kovats Index (experimental and literature), odor description and odor threshold for water. The intensity of the perceived odors (low, medium, high) was determined based on the odor perception at successive dilutions of the extract, i.e., low without diluting, medium (1:1 v/v) and high (1:4 v/v). In total, 72 odor-active compounds belong to the group of saturated and unsaturated alcohols, aldehydes, ketones, carboxylic acids and esters with different odor intensities were identified. Particular attention was paid to compounds with a high intensity index and low odor threshold (OT) (for water). OT indicates the minimum concentration at which a compound's smell becomes noticeable. A low OT means the compound is very potent and can



be smelled at very low concentrations, while a high OT means it takes a larger amount of the compound before it can be detected by the nose. This is important for understanding which compounds significantly impact a product's aroma.

The highest number of odor-active compounds with high OT was identified for wheat bran (10 compounds), followed by wood (8 compounds), paper (7 compounds) and palm leaf (6 compounds). In general, the dominant odors characteristic of the analyzed FCMs include butter (butane-2,3-dione), vinegar (acetic acid), fruit (pentan-1-ol), fat ((E)-non-2-enal, (E,E)-nona-2,4-dienal), grass (hexanal), anise (unknown), mushrooms (oct-1-en-3-ol), fish ((Z)-hept-4-enal), citrus (decanal), musty (octanoic acid), deep frying ((E,E)-deca-2,4-dienal) and metallic (cis-4,5-epoxy-(E)-dec-2-enal). They may be crucial in the case of interactions occurring between FCMs and food and may lead to changes in the sensory properties of food.

**Table 11.** Identified volatile organic compounds (VOCs) characteristic for plant-based food contact materials (FCMs). Retention time ( $t_R$ ), bibliographic and experimental Kovats indexes ( $Kl_{bib}$  and  $Kl_{exp}$ ), odor description, odor threshold (in water) and compounds odor intensity marked as: **Low** = the noticeable odor without diluting the extract, **Medium** = the noticeable odor after diluting the extract twice (1:1 v/v) and **High** = the noticeable odor after diluting the extract four times (1:4 v/v)

No	$t_R$ (min)	Compound	CAS number	$Kl_{bib}$	$Kl_{exp}$	Odor description	OT mg/kg* (in water)	Odor intensity			
								Wheat bran	Wood	Palm leaf	Paper
1	1.90	acetaldehyde	75-07-0	456	443	Fresh, Green	0.016000 <sup>a</sup>	-	-	Low	Low
2	2.10	acetone	67-64-1	503	498	Solvent-like, Pungent	0.832000 <sup>b</sup>	Low	-	Low	Low
3	2.25	butane-2,3-dione	431-03-8	513	525	Butter-like	0.003000 <sup>a</sup>	High	High	High	High
4	2.50	2-methylpropanal	78-84-2	563	575	Malty	0.000490 <sup>a</sup>	Low	Low	-	-
5	2.80	acetic acid	64-19-7	634	627	Vinegar-like	5.600000 <sup>a</sup>	Low	Low	Medium	High
6	3.00	3-methylbutanal	590-86-3	656	643	Malty	0.000400 <sup>a</sup>	-	Low	Low	Low
7	3.20	2-methylbutanal	96-17-3	661	686	Malty	0.001500 <sup>a</sup>	Low	Low	Low	Low
8	3.25	pentan-2-one	107-87-9	687	697	Fruity, Banana- like	2.300000 <sup>a</sup>	Low	Low	Low	Low
9	3.45	pentanal	110-62-3	717	705	Green, Fatty, Moldy	0.012000 <sup>b</sup>	Low	Low	Low	Low
10	4.32	pentan-1-ol	71-41-0	765	755	Fruity, Etheral	0.150200 <sup>b</sup>	Low	Low	High	Low

11	4.80	hex-1-en-3-one	1629-60-3	775	782	Rubber-like, Pungent	0.000001 <sup>a</sup>	-	-	Low	-
12	5.00	pent-1-en-3-one	616-25-1	800	801	Pungent, Milk- like	0.000940 <sup>a</sup>	-	-	Low	-
13	5.20	hexanal	66-25-1	803	804	Green, Grassy	0.002400 <sup>a</sup>	High	Medium	Low	Low
14	5.60	butanoic acid	107-92-6	820	819	Sweaty	1.000000 <sup>a</sup>	Low	Low	Medium	Low
15	6.50	furfural	98-01-1	835	855	Sweet, Cereal- like	0.282000 <sup>b</sup>	Low	Low	Low	Low
16	6.60	(E)-hex-2-enal	6728-26-3	854	855	green apple- like, bitter almond-like	0.110000 <sup>a</sup>	Low	-	-	-
17	6.90	3-methylbutanoic acid	503-74-2	869	872	Sweaty	0.490000 <sup>a</sup>	Medium	Low	Low	Low
18	7.00	2-methylbutanoic acid	116-53-0	869	876	Malty, Fruity, Sweaty	3.100000 <sup>a</sup>	Medium	-	Medium	Low
19	7.24	hexan-1-ol	111-27-3	872	878	Grassy, Marzipan-like	0.0056000 <sup>b</sup>	Low	Low	Low	Low
20	7.40	heptan-2-one	110-43-0	892	892	Fruity, Soapy	0.140000 <sup>b</sup>	Low	Low	Low	Low
21	7.55	γ-butyrolactone	96-48-0	900	898	Sweet, Aromatic	1.000000 <sup>b</sup>	Medium	Low	Low	Low

22	7.70	(Z)-hept-4-enal	6728-31-0	901	904	Fish-like, train oil-like	0.000060 <sup>a</sup>	High	Low	Low	-
23	7.80	heptanal	111-71-7	903	908	Citrus-like, Fatty	0.006100 <sup>a</sup>	Low	Low	Low	-
24	8.30	pentanoic acid	109-52-4	911	910	Sweaty, fruity	11.000000 <sup>a</sup>	Low	-	Low	-
25	8.35	pentyl acetate	628-63-7	916	920	Fruity	0.0430000 <sup>b</sup>	-	-	-	Low
26	8.40	methyl hexanoate	106-70-7	923	932	Fruity, Musty	0.090000 <sup>a</sup>	Low	Low	Medium	-
27	8.52	$\alpha$ -pinene	7785-70-8	934	933	Fir needle-like	0.041000 <sup>b</sup>	-	Low	-	-
28	8.85	camphene	79-92-5	951	950	Terpene-like	1.860000 <sup>b</sup>	-	Low	-	Low
29	8.90	unknown	-	952	-	Aniseed-like, Licorice-like	-	-	-	High	-
30	9.10	3-methylpentanoic acid	105-43-1	958	953	Cheesy, Sweet	0.046000 <sup>b</sup>	-	Medium	-	Low
31	9.83	benzaldehyde	100-52-7	968	981	Bitter almond- like	0.150000 <sup>a</sup>	Low	Low	Low	Low
32	10.06	oct-1-en-3-ol	3391-86-4	983	988	Mushroom-like	0.045000 <sup>a</sup>	High	High	Low	Low
33	10.10	octan-3-ol	589-98-0	986	989	Citrus-like, soapy	0.078000 <sup>b</sup>	-	-	-	Low
34	10.20	octan-2-one	111-13-7	991	990	Soapy, Fruity	0.150000 <sup>a</sup>	Medium	Low	Low	Low
35	10.45	octanal	124-13-0	1006	1006	Citrus-like, Green	0.003400 <sup>a</sup>	Low	Low	Low	Low

36	10.65	hexanoic acid	142-62-1	1015	1016	Sweaty	3.000000 <sup>a</sup>	Low	Low	Low	Low
37	10.90	(E,E)-hepta-2,4-dienal	4313-03-5	1015	1026	Fatty, Floral	0.015400 <sup>b</sup>	Low	-	-	Low
38	11.10	limonene	138-86-3	1028	1026	Citrus-like	0.013000 <sup>a</sup>	-	Low	-	High
39	11.15	1,8-cineole (eucalyptol)	470-82-6	1031	1029	Eucalyptus-like	0.001100 <sup>b</sup>	-	Low	-	Low
40	11.20	benzyl alcohol	100-51-6	1037	1035	Bitter almond-like, Fruity	2.546210 <sup>b</sup>	-	Low	Low	Low
41	11.52	oct-3-en-2-one	1669-44-9	1041	1040	Floral, Spicy	0.250000 <sup>b</sup>	Low	Low	Medium	Low
42	11.76	(E)-oct-2-enal	2548-87-0	1059	1049	Fatty, Nutty	0.004000 <sup>a</sup>	Low	-	-	Low
43	11.80	(E,E)-octa-3,5-dien-2-one	30086-02-3	1059	1051	Musty, Fatty	0.1000000 <sup>b</sup>	Medium	Low	Low	Medium
44	12.90	heptanoic acid	111-14-8	1086	1081	Rancid, Sweaty	0.640000 <sup>b</sup>	Low	-	Low	Low
45	13.10	nonan-2-one	821-55-6	1095	1099	Fruity, Musty	0.041000 <sup>b</sup>	Medium	High	-	-
46	13.10	methyl benzoate	93-58-3	1097	1099	Starfruit-like, Sweet	0.073000 <sup>a</sup>	-	-	Low	Medium
47	13.25	nonanal	124-19-6	1104	1103	Citrus-like, Soapy	0.002800 <sup>a</sup>	Low	Low	Medium	Low
48	13.40	maltol	118-71-8	1108	1110	Caramel-like, Burned	5.000000 <sup>a</sup>	-	-	Low	-
49	13.53	(E,E)-octa-2,4-dienal	30361-28-5	1111	1115	Fatty	0.010000 <sup>b</sup>	-	-	Low	Low

50	13.80	unknown	-	1125	-	Fatty	-	High	High	High	High
51	13.90	methyl octanoate	111-11-5	1131	1130	Fruity, Musty	0.200000 <sup>b</sup>	-	-	Low	Low
52	14.00	(E)-non-3-en-2-one	18402-83-0	1138	1136	Green, Fatty	0.800000 <sup>b</sup>	Low	-	-	-
53	14.40	(Z)-non-2-enal	60784-31-8	1147	1146	Green, Fatty	0.000020 <sup>b</sup>	-	-	High	High
54	14.45	camphor	76-22-2	1154	1148	Camphor-like	0.250000 <sup>b</sup>	-	-	Low	Low
55	14.50	(E,Z)-nona-2,6-dienal	557-48-2	1155	1150	Cucumber-like	0.000010 <sup>b</sup>	-	-	-	High
56	14.60	(E)-non-2-enal	18829-56-6	1160	1154	Fatty, Green	0.000080 <sup>b</sup>	High	High	High	High
57	14.70	isoborneol	124-76-5	1162	1162	Earthy, Moldy	0.002500 <sup>b</sup>	-	Low	-	Low
58	14.85	borneol	507-70-0	1173	1173		0.014000 <sup>a</sup>	-	Low	-	Low
59	15.30	dec-1-en-3-one	56606-79-2	1182	1180	mushroom-like	0.080000 <sup>a</sup>	-	-	-	Medium
60	15.40	decan-2-one	693-54-9	1185	1184	Fruity, Floral	0.003000 <sup>b</sup>	Low	-	Medium	-
61	15.60	$\alpha$ -terpineol	98-55-5	1191	1189	Floral, Citrus-like	1.200000 <sup>a</sup>	-	Low	-	-
62	15.80	decanal	112-31-2	1204	1199	Soapy, Citrus-like	0.009300 <sup>a</sup>	High	-	-	-
63	16.35	(E,E)-nona-2,4-dienal	5910-87-2	1216	1222	Fatty, Green	0.000062 <sup>a</sup>	High	High	Low	Low
64	16.50	3-carene	13466-78-9	1220	1224	Terpene-like	0.770000 <sup>b</sup>	-	-	-	Low
65	16.60	benzothiazole	95-16-9	1224	1226	Rubber-like, Cabbage-like	0.080000 <sup>b</sup>	Low	-	-	-

66	17.30	octanoic acid	124-07-2	1263	1260	Carrot-like, Musty	0.190000 <sup>a</sup>	High	-	-	-
67	17.40	(E)-dec-2-enal	3913-81-3	1265	1265	Fatty, Green	0.250000 <sup>b</sup>	-	-	-	Low
68	18.50	acetophenone	98-86-2	1312	1308	Foxy, Bitter almond-like,	0.170000 <sup>b</sup>	Low	Low	Low	Low
69	18.60	(E,E)-deca-2,4-dienal	25152-84-5	1318	1310	Fatty, Deep- fried	0.000070 <sup>b</sup>	High	High	-	-
70	20.30	cis-4,5-epoxy-(E)- dec-2-enal	134454-31-2	1369	1369	Metallic	0.000220 <sup>b</sup>	-	High	-	-
71	20.40	(Z)-2-butyloct-2-enal	99915-14-7	1374	1380	Citrus-like, Soapy, Green	0.020000 <sup>b</sup>	Low	Low	-	-
72	20.50	indole	120-72-9	1391	1391	Fecal, Mothball-like	0.011000 <sup>a</sup>	-	-	-	Low

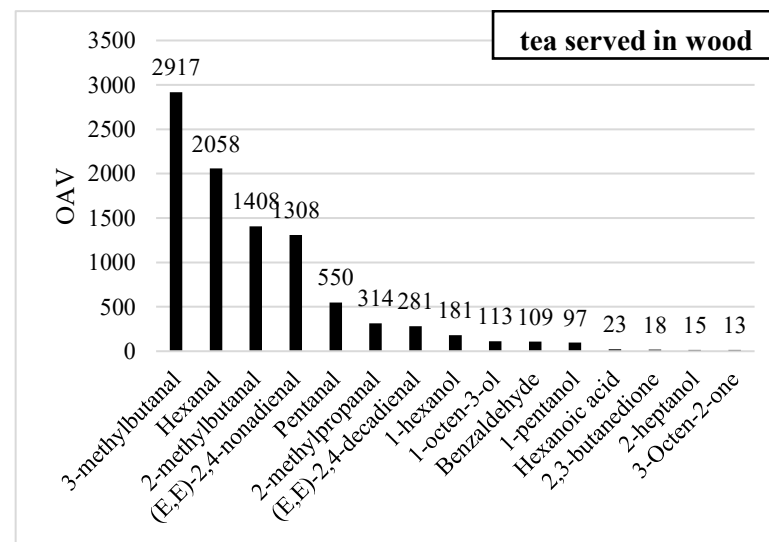
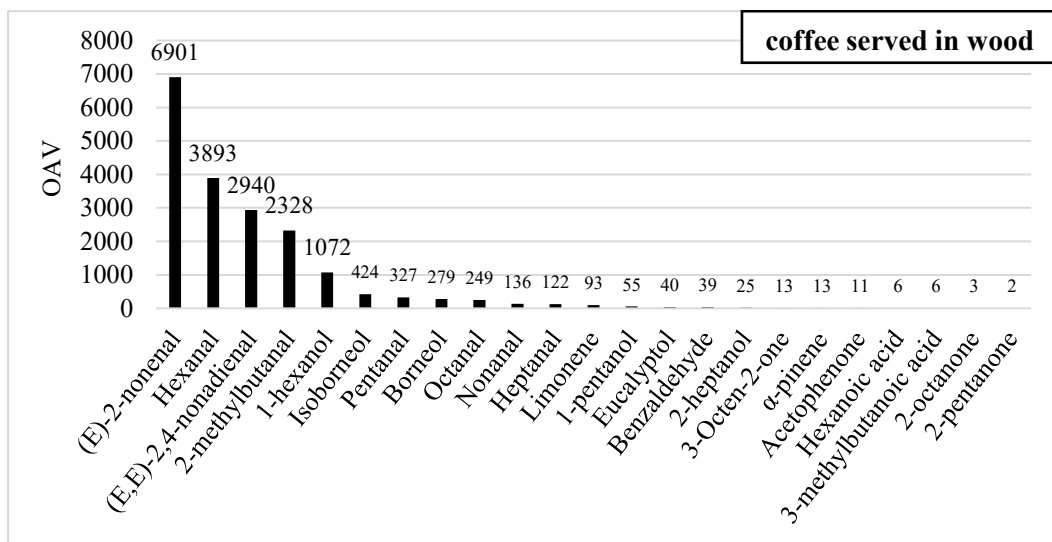
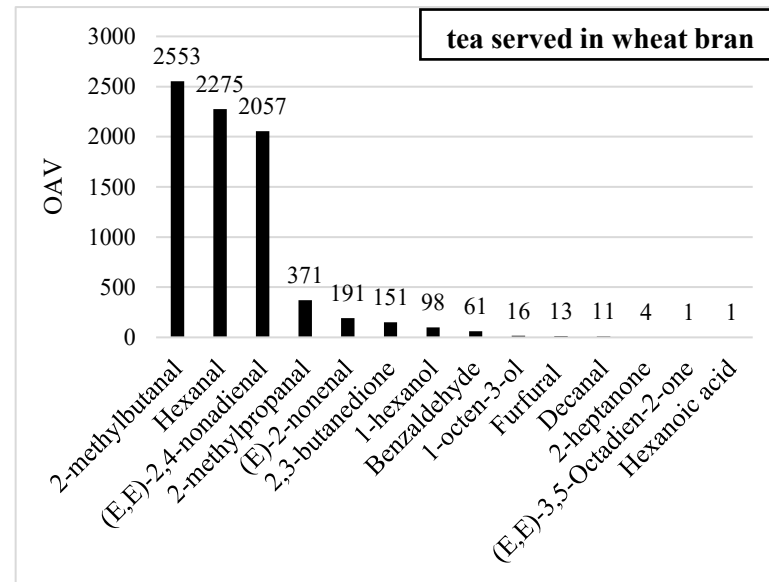
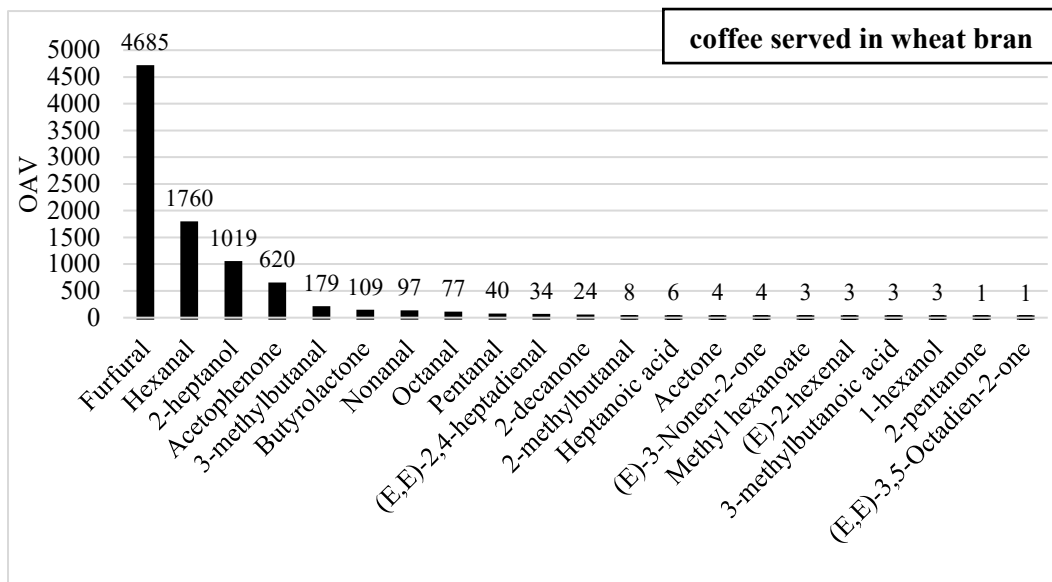
\*OT expressed based on the: <sup>a</sup> Leibniz-LSB@TUM Odorant Database or <sup>b</sup>van Gemert, L.J. Odor thresholds. Compilations of odor threshold values in air, water and other media (Edition 2011).

The uniquely complex aroma of black coffee and green tea is due to the presence of many aromatically active ingredients in these extracts. Changes in the amount of odor active compounds in coffee and tea samples served in various FCMs can cause aroma differences between them. Aroma-active compounds that migrate from FCMs into roasted black coffee and green tea were identified and quantified to evaluate the effect of FCMs on the sensory profile of beverages.

Odor Activity Value (OAV) is measured by dividing the concentration of an odor-active compound in a sample by its odor threshold ( $\text{OAV} = \text{concentration} / \text{odor threshold}$ ). A high OAV (greater than 1) means the compound is present at a concentration above its odor threshold and likely contributes to the overall aroma, while an OAV below 1 suggests the compound is present at a concentration too low to be perceived and is unlikely to influence the odor. OAV was determined for the identified compounds, which is a measure of the importance of a specific compound to the overall odor of a sample (including coffee and tea). Odor-active compounds with OAVs that were identified in the beverages (coffee and tea) as FCM-derived compounds (after removed the blank samples) are presented in **Fig. 14**. The results clearly indicate that the FCMs analyzed can affect the sensory properties of the beverages served. The dominant aroma-active compounds (with  $\text{OAV} > 1000$ ) mainly include compounds from the group of saturated and unsaturated aldehydes, such as. 3-methylbutanal, 2-methylbutanal (Strecker aldehydes; Maillard reaction products), (E)-non-2-enal, hexanal, nonanal, acetaldehyde, (E)-oct-2-enal, furfural, (E,E)-nona-2,4-dienal, (E,E)-octa-2,4-dienal and saturated alcohols, e.g., hexan-1-ol, heptan-2-ol, octan-3-ol. These compounds are mainly responsible for malty, fatty, cereal, green, grassy, citrus and fruity notes (according to the Leibniz-LSB@TUM Odorant Database), which can shape the undesirable, foreign aroma bouquet of coffee and tea.

Comparing the OAV values of compounds migrating from FCMs to beverages, it can be concluded that the sensory profile of coffee can change more than the sensory profile of tea. The OAVs of compounds migrating into coffee are much higher, which can be observed in particular by comparing the OAVs of compounds migrating into coffee and tea from palm leaves and paper (**Fig. 14**). Black coffee has an acidic pH, while green tea has a slightly alkaline pH. The reason for the observed differences in the migration intensity of aroma-active compounds may therefore be the higher stability of volatile compounds at acidic pH. Similar correlations in the migration intensity of IAS and NIAS from PET bottles were observed for carbonated (acidic pH) and non-carbonated (neutral pH) water (Dehghani et al, 2018; Cardozo et al., 2021; Abe et al 2021).





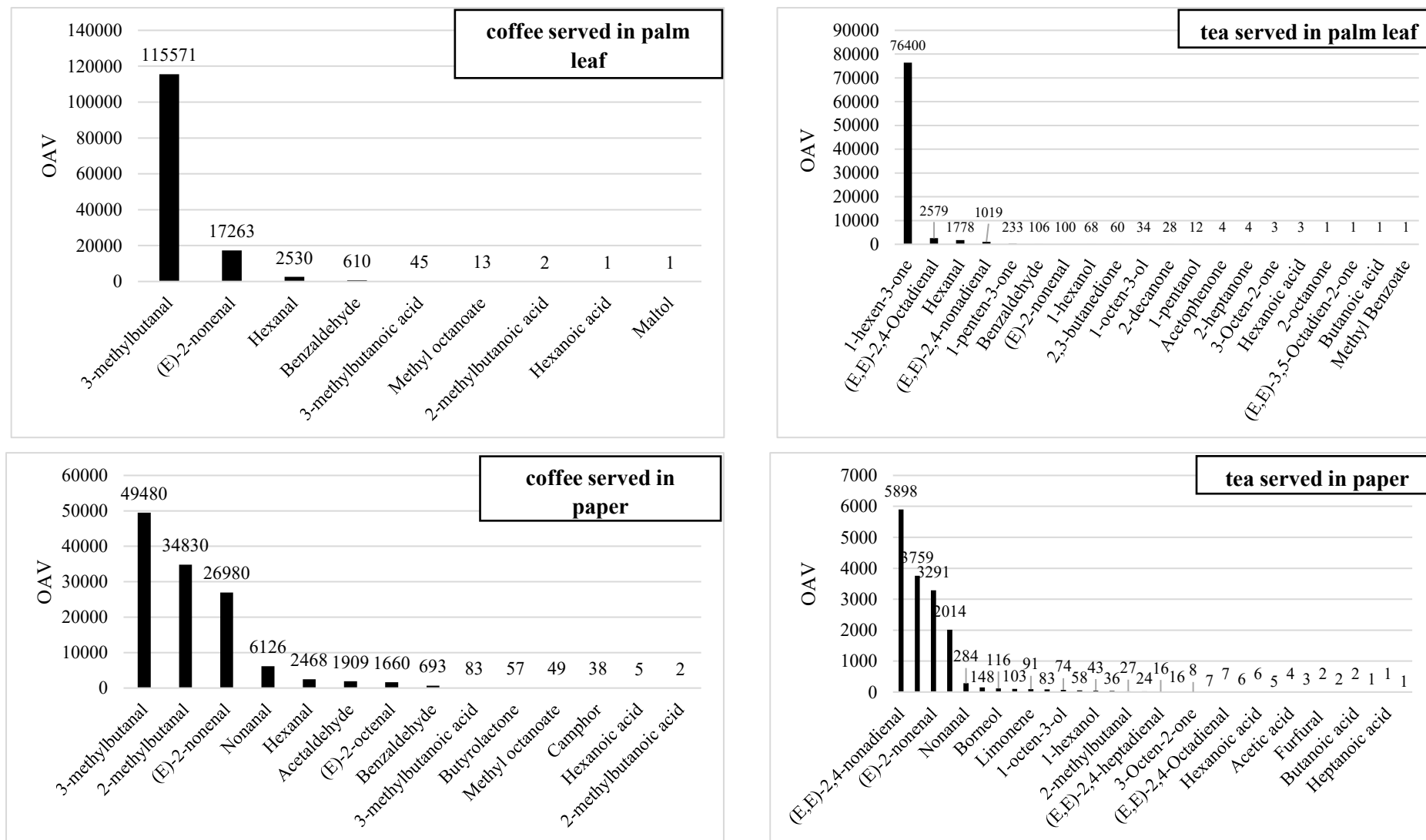


Fig. 14. Odor active compounds with OAV values that were identified in beverages (coffee and tea) as FCM-derived compounds

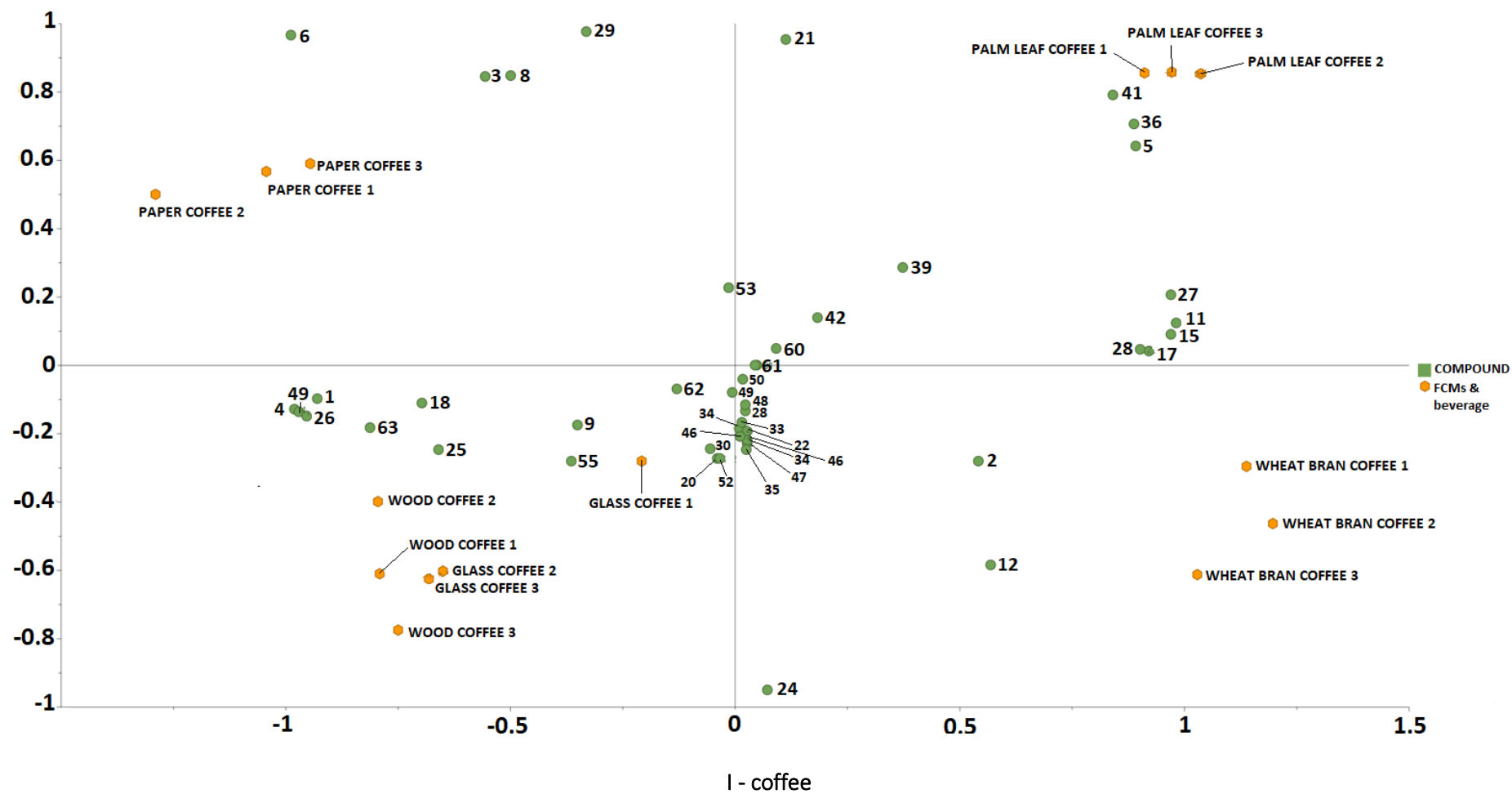
Based on the results, it is clear that the FCMs analyzed can affect the sensory properties of the beverages served. In the case of coffee, the presence of aroma-active compounds was noted, mainly responsible for malty, fatty, green, grassy, citrus and fruity notes, which can shape the undesirable final aroma bouquet of coffee.

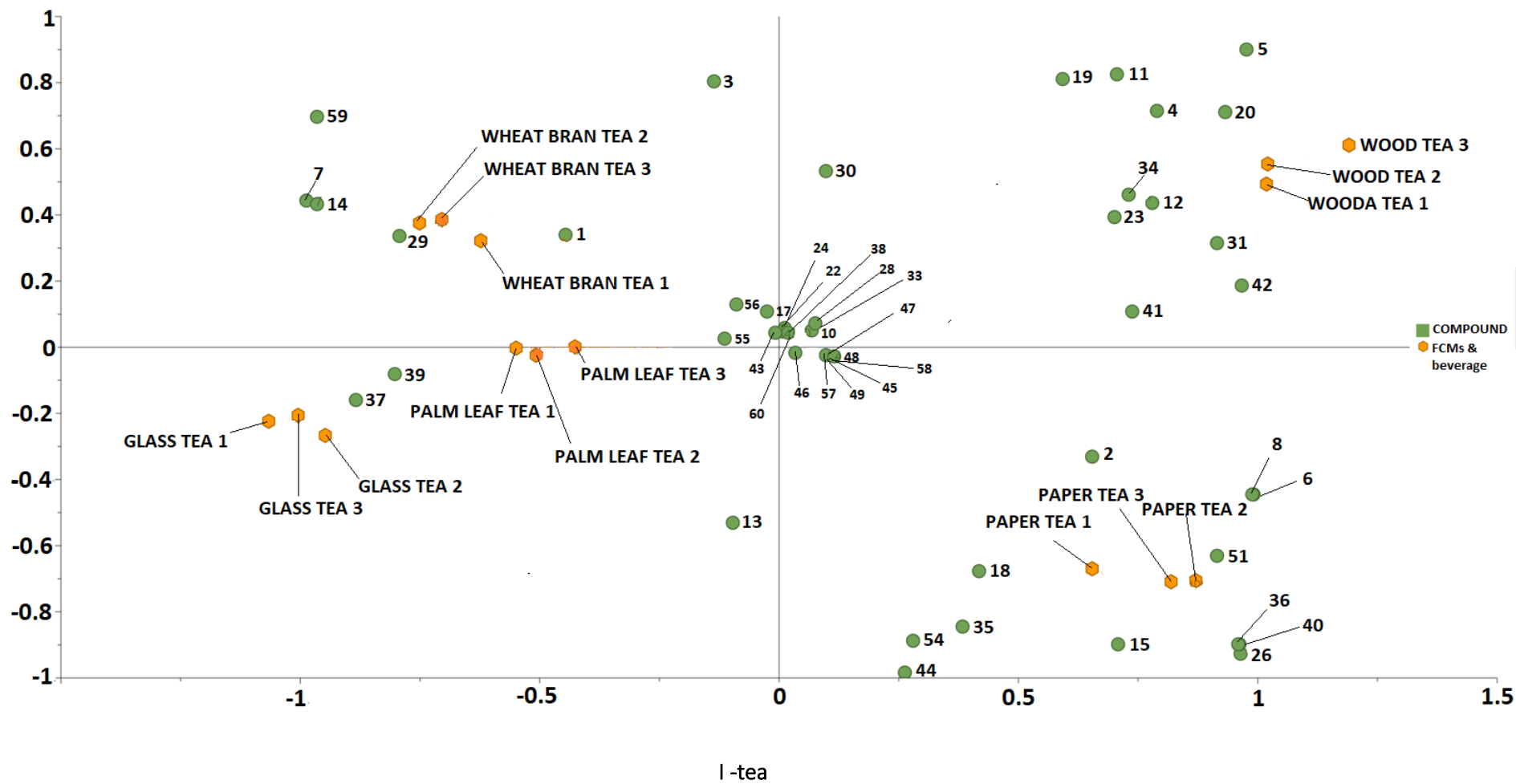
It has been observed that most of the aroma-active compounds (characterized by OAV >1000) can migrate from the paper and the key compounds include saturated and unsaturated aldehydes: 3-methylbutanal and 2-methylbutanal (malt aroma), (E)-non-2-enal (oily, green aroma), nonanal (citrus, soapy aroma), hexanal (grassy aroma), acetaldehyde (green, fresh aroma) and (E)-oct-2-enal (oily, nutty aroma). This may be due to the effect of the degree of moisture in the paper on the amount of aroma-active compounds released. Similarly, Wolf et al. (2023) presented a proportional correlation between the degree of material moisture and the intensity of VOCs released. Authors showed that the paper's odor profile at 33 and 58 % relative humidity was described as cardboard-like, sweet and smoky. The substances influencing these olfactory sensations were (E)-non-2-enal, vanillin and 2-methoxyphenol. Increasing relative humidity to 75 and 100 % resulted in additional astringency/stain and fatty/rancid sensations, which were mainly caused by short-chain fatty acids and unsaturated aldehydes (Wolf et al., 2023). It has been observed that (E)-non-2-enal, hexanal and (E,E)-nona-2,4-dienal (oily, green aroma), 2-methylbutanal (malt aroma) and hexan-1-ol (grassy aroma) can migrate into coffee from wood. In addition, furfural (grain aroma), hexanal and heptan-1-ol (fruit aroma) were identified in coffee served in wheat bran, while 3-methylbutanal (malt aroma), (E)-non-2-enal and hexanal were identified in coffee served in palm leaves.

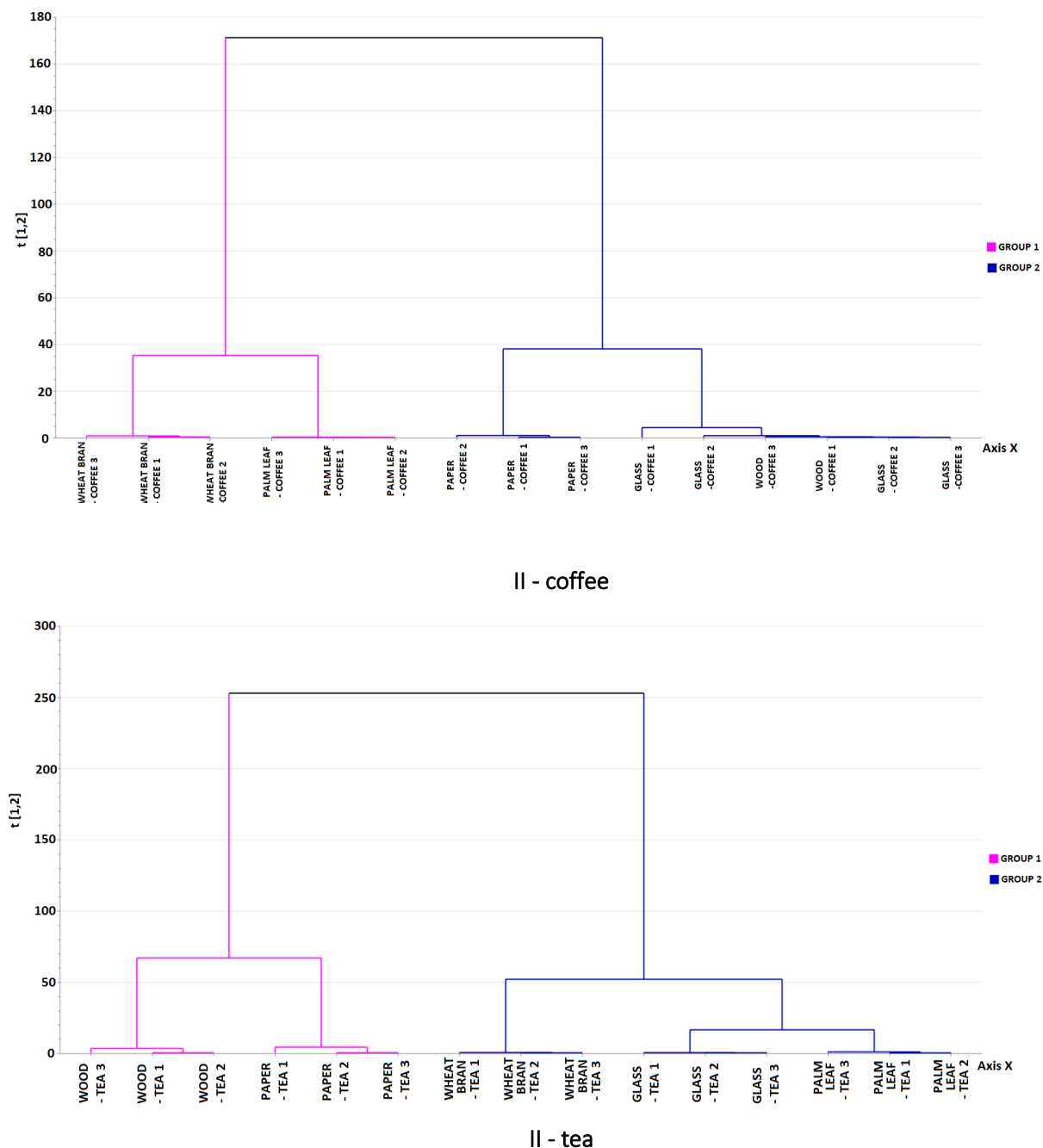
A significant factor influencing the intensity of migration process is the type of FCMs. The most active aroma compounds (characterized by OAV >1000) can migrate to coffee from paper and the key compounds include saturated and unsaturated aldehydes: 3-methylbutanal (OAV=49480) and 2-methylbutanal (OAV=34830) (malty aroma), (E)-non-2-enal (OAV=26980) (fatty, green aroma), nonanal (OAV=6126) (citrus, soapy aroma), hexanal (OAV=2468) (grassy aroma), acetaldehyde (OAV=1909) (green, fresh aroma) and (E)-oct-2-enal (OAV=1660) (fatty, nutty aroma). In the case of wood, it may migrate to coffee (E)-non-2-enal (OAV=6901), hexanal (OAV=3893) and (E,E)-nona-2,4-dienal (OAV=2940) (fatty, green aroma), 2-methylbutanal (OAV=2328) (malty aroma) and hexan-1-ol (OAV=1072) (grassy aroma). Moreover, furfural (OAV=4685) (cereal aroma), hexanal (OAV=1760) and heptan-1-ol (OAV=1019) (fruit aroma) were identified in coffee served in wheat bran. Additionally, a strong influence of palm leaf on the aroma of coffee was noted, in which malty, fatty, green and grassy notes can be detected due to the presence of 3-methylbutanal (OAV=115571), (E)-non-2-enal (OAV=17263) and hexanal (OAV=2530).

PCA was used to determine the influence of the type of FCMs on the sensory characteristics and important aroma compounds of black coffee and green tea. Multivariate analysis confirmed that the type of FCMs has a significant impact on the sensory profile of these beverages. The clear clustering was achieved for the analyzed data (**Figs. 15 I - coffee and 15 I - tea**). It is visible that the sensory profile of coffee brewed in paper, wheat bran, palm leaf and wood are completely different (**Fig. 15 I -coffee**). Interestingly, PCA showed that coffee brewed in wood had the most similar sensory profile to coffee brewed in glass (blank sample). Most of the identified aroma-active compounds were similar in all brews, but some were specific to selected samples. Hierarchical analysis of components (HA) confirmed the clustering of the FCMs analyzed into two main groups: the first FCMs from wheat bran and palm leaves and the second FCMs from paper, glass and wood (**Fig. 15 II - coffee**).

The effect of the type of FCMs on the sensory profile of the tea was also confirmed (**Fig. 15 I - tea**). All of the FCMs analyzed differ from each other in their effects on the sensory profile of tea and none of them is similar to tea served in glass (blank sample). HA confirmed the clustering of the FCMs analyzed into two main groups. In the first are FCMs from paper and wood and in the second are FCMs from wheat bran, palm leaves and glass (**Fig. 15 II – tea**).





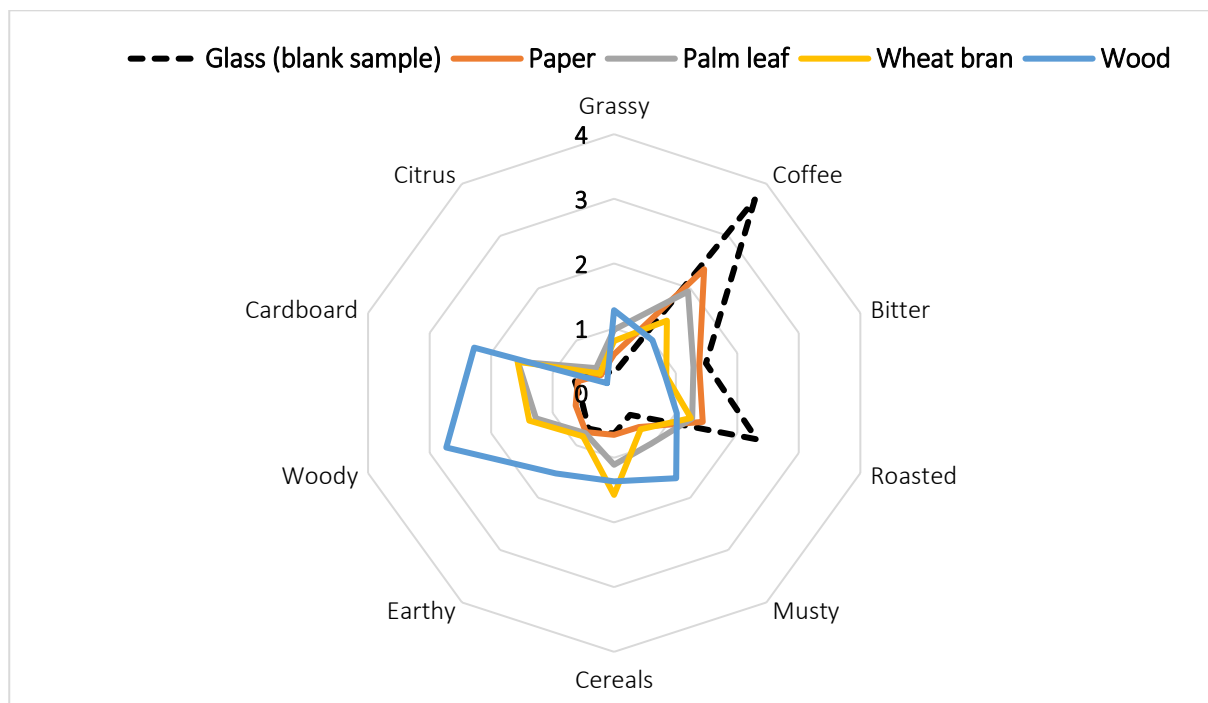


**Fig. 15.** Multivariate analysis of odorant concentrations and sensory attributes of coffee or tea brewed in different FCMs. Results of multivariate analysis of concentrations of important odorants and sensory attributes of beverages obtained using different technologies. (I) Biplot from principal component analysis (PCA). PC1 and PC2 explain 64% (for coffee) and 82 % (for tea) of the variance. Different colors represent different FCM samples (grey) and migrating odor-active compounds (green), according to: (1) furfural, (2) hexanal, (3) 2-methylbutanal, (4) pentan-1-ol, (5) 3-methylbutanal, (6) (E)-oct-2-enal, (7) octanal, (8) nonanal, (9) heptanal, (10) heptan-2-ol, (11) pentanal, (12) hexanoic acid, (13) hex-1-

*en-3-one, (14) (E,E)-hepta-2,4-dienal, (15) octan-2-one, (16) heptanoic acid, (17) acetone, (18) acetophenone, (19) hexan-1-ol, (20) methyl hexanoate, (21) 3-methylbutanoic acid, (22) (E)-hex-2-enal, (23) pentan-2-one, (24) pentanoic acid, (25) benzothiazole, (26) butanoic acid, (27) 2-methylbutanoic acid, (28) (Z)-2-butyl oct-2-enal, (29) butyrolactone, (30) decan-2-one, (31) (E,E)-octa-3,5-dien-2-one, (32) (E)-non-3-en-2-one, (33) nonan-2-one, (34) oct-3-en-2-one, (35) (E,E)-nona-2,4-dienal, (36) (E)-non-2-enal, (37) 2-methylpropanal, (38) (E,E)-deca-2,4-dienal, (39) butane-2,3-dione, (40) heptan-2-one, (41) benzaldehyde, (42) oct-1-en-3-ol, (43) decanal, (44) acetic acid, (45) (E)-dec-2-enal, (46) isoborneol, (47) borneol, (48) limonene, (49) eucalyptol, (50)  $\alpha$ -pinene, (51) methyl benzoate, (52) camphene, (53) *cis*- $\alpha$ -terpineol, (54) benzyl alcohol, (55) octan-3-ol, (56) pent-1-en-3-one, (57) pentyl acetate, (58) 3-carene, (59) (E,E)-octa-2,4-dienal, (60) acetaldehyde, (61) maltol, (62) camphor and (63) methyl octanoate*

(II) Dendrogram from hierarchical analysis. Different colors represent different clusters

In order to confirm the influence of FCMs on the sensory properties of black coffee and green tea, a sensory evaluation was carried out. The results are summarized in Figs. 16 I and 16 II.



I



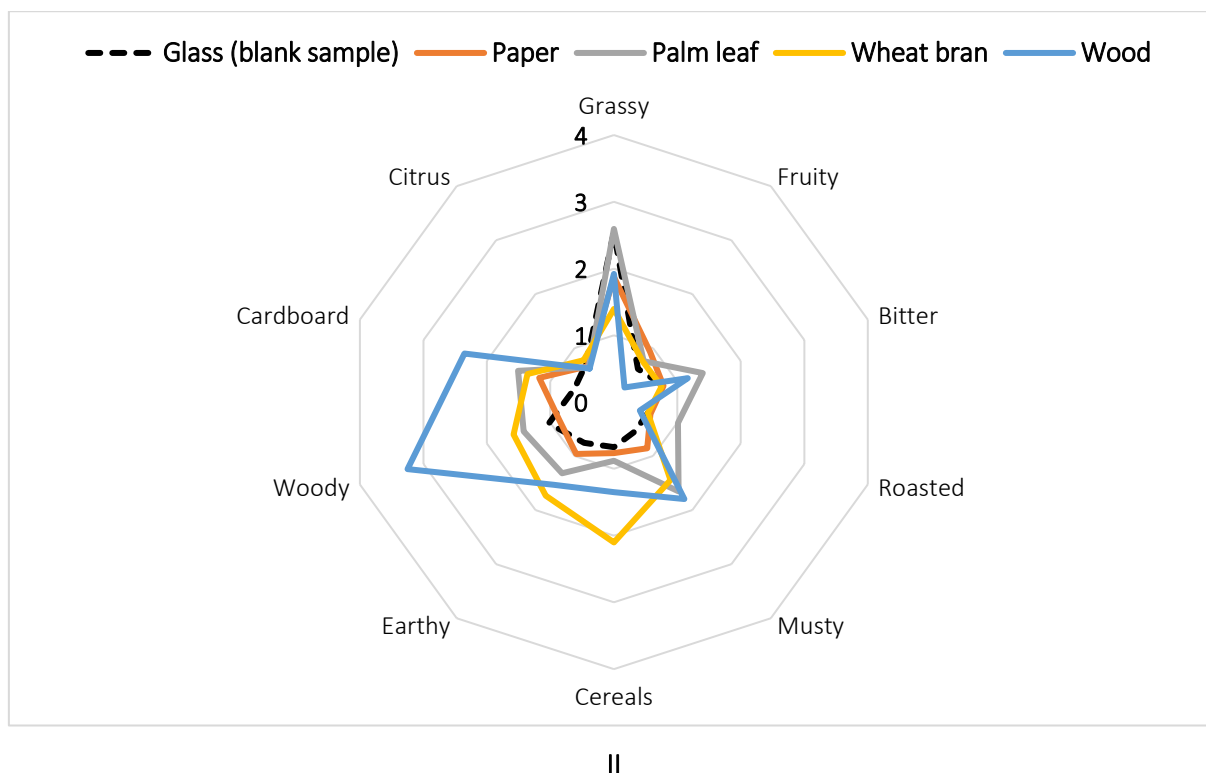


Fig. 16. Sensory profile of (I) coffee and (II) tea served in different FCMs

Based on the obtained aromagrams, it is clear that all the analyzed FCMs affect the sensory profile of black coffee and green tea (compared to glass). This indicates that the overall aroma of coffee and tea depends on the FCMs in which it is served. In the case of black coffee served in a glass vessel, the desired coffee notes (4) are strongly felt, while the roasted (1), bitter (1), cereal (1), earthy (1) and woody (1) notes are less intense, which is caused by the presence of natural aroma-active compounds present in the beverage. In general, coffee brewed in the analyzed FCMs was characterized by a reduced coffee aroma (intensity 2 or 1), which may be caused by the FCMs absorbing key aroma-active compounds characteristic of this beverage. In addition, the sensory profiles of coffee brewed in different FCMs differ significantly. The most undesirable effect on the aroma of coffee is exerted by wood FCMs, from which compounds that shape woody (3), cardboard (2), earthy (2), musty (2), grassy (1) and cereal (1) aromas can migrate. Similarly, in coffee brewed in wheat bran FCMs, cereal (2), cardboard (2), grassy (1) and musty (1) notes were noticeable. In the case of coffee brewed in paper and palm leaf, foreign cardboard, grassy and musty notes were noticeable. Similar observations were noted for green tea, which, served in a glass, was characterized by the desired grassy (2), fruity (1) and citrus (1) notes. On the other hand, other FCMs reduced the desired grassy note (1) for this infusion and the appearance of foreign musty, cereal and woody notes.

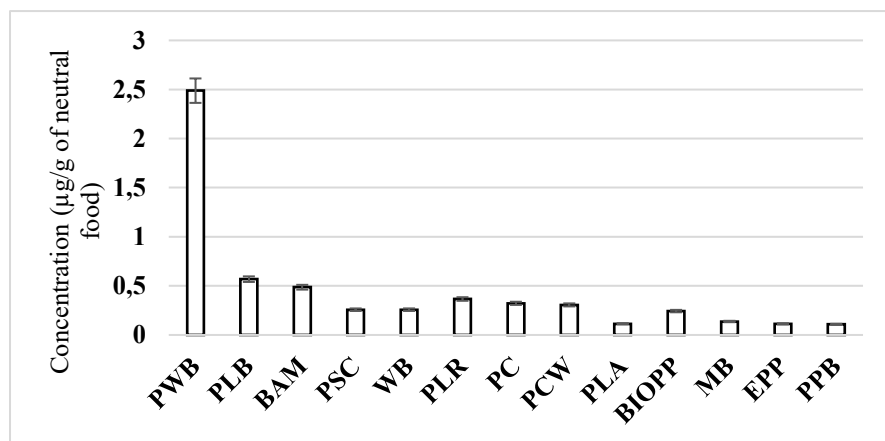
The sensory analysis shows that glass is the most desirable material, which does not affect the sensory profile of black coffee and green tea to as great an extent as the analyzed FCMs. Moreover, as the research shows, one of the most frequently identified active sensory compounds characteristic of FCMs are carbonyl compounds. They include a large group of reactive chemical compounds, among which there are also toxic compound. It means that their concentration levels in food must be controlled.

### 5.2.2 Migration study of carbonyl compounds

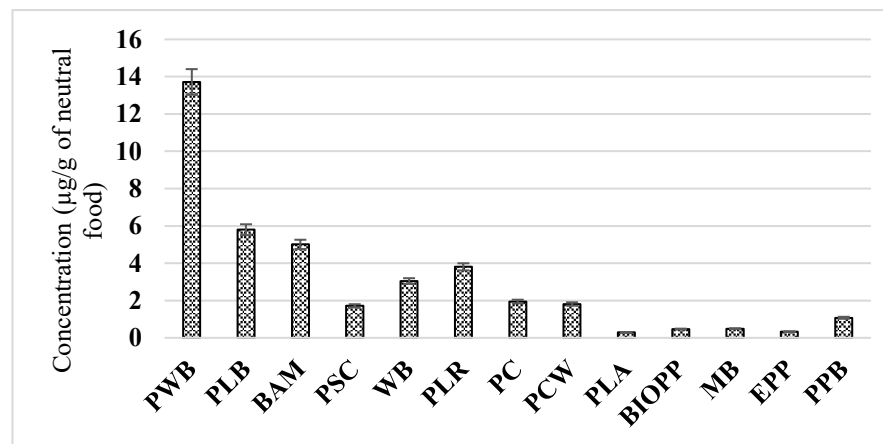
Low-molecular weight carbonyl compounds can be easily released from the FCMs into food. Many previous works have described the contamination with carbonyl compounds of mineral waters stored in PET bottles (Cincotta et al., 2018; Dehghani et al., 2018; Abe et al., 2021; Cardozo et al., 2021; Dhaka et al., 2022). For example, Abe et al. (2021) identified formaldehyde in 61 of 105 tested samples of PET packaged mineral waters on the Japanese market, with average concentrations of the compound ranging from 2.6 to 31.4 µg/L. Similarly, Cardozo et al. (2021) identified formaldehyde in all of the 17 sparkling and still mineral water samples analyzed in the Brazilian market, with an average concentration of 10.4 125.5 µg/L. In turn, Dehghani et al. (2018) determined formaldehyde in the Iranian market in the concentration range of 12-45 µg/L. The presence of aldehydes can affect the uncontrolled growth of bacteria in mineral water and change its sensory properties. The number of aldehydes migrating from plastic bottles depends on the quality of the material and can differ significantly from one production batch to another. The type of resins used has a significant impact on the release of unwanted organic compounds from packaging. Bottle material can be contaminated with recycled pellets, which adversely affects water quality. In addition, the aldehyde content of carbonated waters has been found to be significantly higher than that of non-carbonated waters (Nawrocki, Dąbrowska & Borcz, 2002). The reasons for this phenomenon can be explained by the greater biological stability of carbonated waters, as the carbon dioxide introduced into the water lowers the pH of the water, sometimes even to pH=5. Aldehydes migrating from the bottle material, which are readily bioavailable compounds, are consumed by bacteria that naturally inhabit and reproduce in the aquatic environment. In CO<sub>2</sub>-saturated water, at lower pH, bacterial growth is limited, so the demand for available organic carbon is also reduced. In still water, autochthonous bacteria consume aldehydes and have good conditions for growth. Therefore, there is a paradox: bottled carbonated waters are biologically stable, but may contain increased amounts aldehydes undesirable for health, while still waters contain smaller amounts of aldehydes, but these are waters with an increased number of autochthonous bacteria.

New FCMs can be also a source of food contamination with carbonyl compounds. The analyzed FCMs were divided into plant-based materials (including wheat bran, palm leaf, bamboo, sugar cane, wood, plant residues and recycled and bleached paper) and bio-based plastics (including polylactide, bio-polypropylene (transparent and colored), thermoplastic starch and expanded polypropylene) (abbreviations for FCMs are summarized in the **Table 1**).

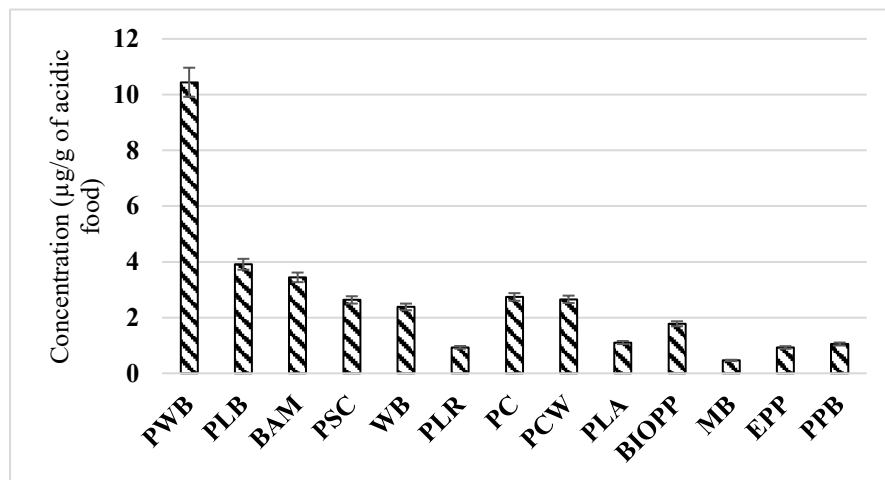
Based on the conducted migration studies (**Fig. 17**), it can be observed that currently popular FCMs can be a source of food contamination with carbonyl compounds, especially low weight aldehydes and ketones. The intensity of migration process depends evidently on the type of FCMs and food. **Figs. 17 I-17 VI** present the total concentrations of carbonyl compounds (aldehydes and ketones) that were identified in food simulants after a short contact time with FCMs, i.e., 2h, 70°C (conditions recommended by the Commission Regulation (EU) No 10/2011). The food simulants used included distilled water (**Fig. 17 I**), 10 % ethanol (**Fig. 17 II**), 3 % acetic acid (**Fig. 17 III**), 20 % ethanol (**Fig. 17 IV**), 50 % ethanol (**Fig. 17 V**) and Tenax (**Fig. 17 VI**).



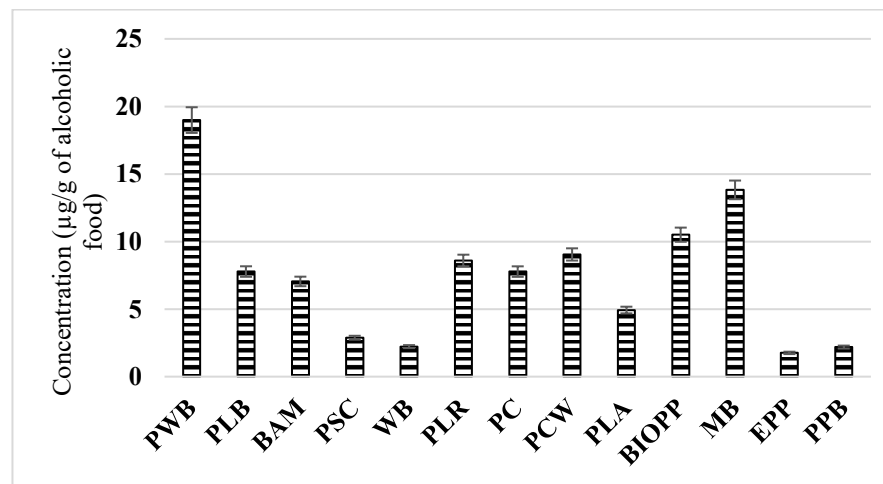
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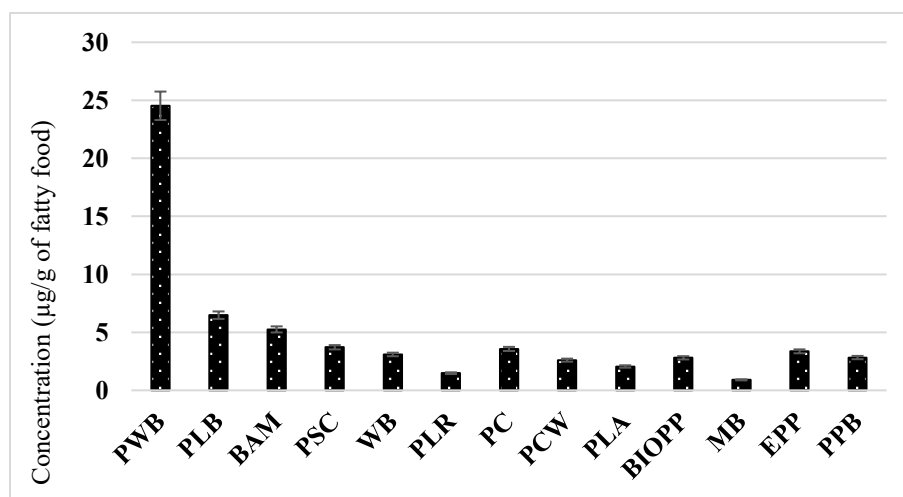
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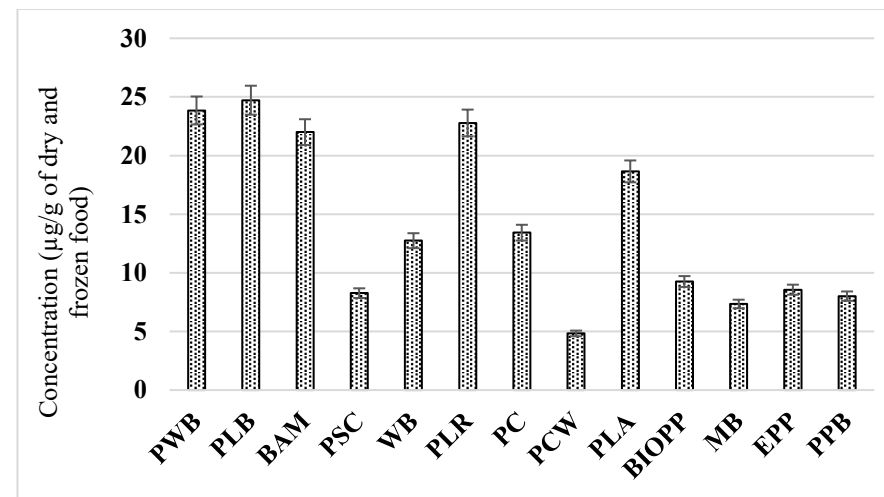
III



IV



V



VI

Fig. 17. Total carbonyl compounds concentration determined in various food simulants (I) distilled water, (II) 10 % ethanol, (III) 3 % acetic acid, (IV) 20 % ethanol, (V) 50 % ethanol and (VI) Tenax from FCMs under contact conditions: 2 h, 70°C (average values from three repetitions per sample; for abbreviations of FCMs see Table 1)

The obtained results clearly show that the type of FCMs (plant-based, bio-based plastic) has a significant impact on the amount of carbonyl compounds released into food. Particularly high amounts of these compounds can be released from plant-based FCMs, especially from wheat bran (PWB), palm leaf (PLB), bamboo (BAM), plant residues (PLR) and wood (WB) into food simulants. This is particularly visible in **Fig. 17 II**. The predominant carbonyl compounds can include acetaldehyde, propanal, pentanal, hexanal, heptanal, benzaldehyde, methylglyoxal and pentan-2-one. Migration of these compounds from plant-based FCMs can be caused by the process of plant vegetation (allelopathy), carbonyl compounds are also the part of essential oils, giving plants a pleasant taste and smell. The presence of certain volatile organic compounds in plants and their emission during environmental stress creates a defense system against pests, bacterial infections and is also a way to deter competition (Dabrowska & Nawrocki, 2013). On the other hand, carbonyl compounds can also be formed as by-products of thermal processing (Marín-Morocho et al., 2021). Most of them can be treated as NIAS (Cincotta et al., 2018; Kato & Conte-Junior, 2021). Carbonyls can be residues from the manufacturing process of recyclable vessels, especially those conducted at elevated temperatures. They can also be components of inks or paints and polymeric protective coatings applied to the surface of the vessel (Aznar et al., 2020). Aznar et al. (2020) showed the influence of the heating method on VOC emissions from kitchen bags. Bags heated in a conventional oven had a greater impact on the increase in odor emission from the packaging than bags heated in a microwave oven. The main causes of odors detected were aldehydes and ketones. In turn, Wrona et al (2024) identified aldehydes (e.g., undecanal, dodecanal, hexadecanal and octadecanal) as compounds migrating from various silicone FCMs to 50 % EtOH. The authors found that the presence of the aldehydes were fragrances or degradation products.

The obtained results also clearly show that the nature of food (i.e., neutral, acidic, alcoholic, fatty and dry) is important in migration intensity (**Figs. 17 I-VI**). The highest concentrations of carbonyl compounds were observed in Tenax, which represents dry food. The total concentrations of these contaminants ranged from 7.342 µg/g of food (from TPS) to even 24.720 µg/g of food (from PLB). However, high concentrations of migrating aldehydes and ketones may be due to the nature of Tenax. Some studies report disadvantages of Tenax as a food simulant, because may lead to overestimated IAS and NIAS concentrations compared to real food samples (Rubio et al., 2019; Baele et al., 2020; Elizalde et al., 2020; Almeida Soares et al., 2023). These reports suggest that the interpretation of migration studies results with Tenax should be cautious. However, it should be noted that the results of such studies can provide an understanding of contaminants that may not necessarily migrate from FCMs into real food. They can be a warning sign for taking early preventive measures.

Comparing the intensity of carbonyl compound migration from FCMs to other simulants, the following trend can be observed: fatty food > alcoholic food > acidic food > neutral food. In the case of fatty and alcoholic food, the highest total concentrations of migrating carbonyl compounds were recorded for PWB (24.527 µg/g and 18.990 µg/g, respectively). The most frequently identified carbonyl compounds include: benzaldehyde, pentan-2-one, hexan-2-one, acetaldehyde, acetone and propanal. It can be expected that acidic foods (e. g. vegetable soups, fruit juices, pickled vegetables and etc.) can be more contaminated with carbonyl compounds than products with neutral pH. It should be noted that acidic foods is more often preferred by consumers due to the desired taste and dietary properties.

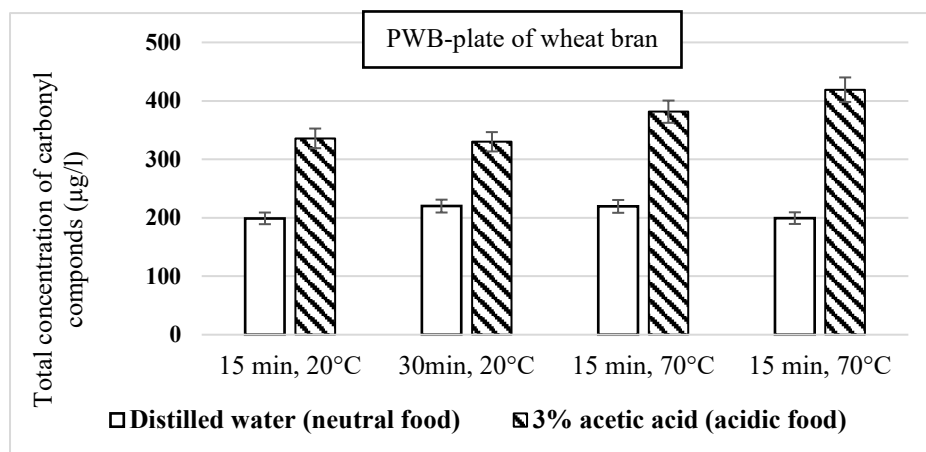
Some carbonyl compounds are suspected of having carcinogenic, mutagenic and cancerogenic properties (WHO, 2011). These include formaldehyde and acetaldehyde and their migration from FCMs to food may be considered particularly undesirable. These carbonyl compounds are classified as IAS, therefore the SML for formaldehyde was set at 15 µg/g of food and for acetaldehyde 6 µg/g of food, respectively (**Table 6**). The conducted studies on the migration of carbonyl compounds from currently popular FCMs to food of various types have shown that none of the FCMs exceeds the permitted SML for formaldehyde and acetaldehyde, although the most formaldehyde can migrate to dry food and acetaldehyde to fatty food. This means that short contact of heated food (2h, 70°C) with plant-based and bio-based plastic FCMs does not pose a risk of formaldehyde and acetaldehyde migration, which have a potential, undesirable carcinogenic effect.

However, the contact of FCMs with food and the temperature of the food consumed are often different, i.e., in the case of fast-food bars, the contact of food with FCMs is short (15 min/30 min), including the meal time. FCMs are also often used for short-term storage of food (5 h/10 h). In addition, food can be served at room temperature (20°C) or hot (70°C). In order to illustrate the intensity of migration of carbonyl compounds under different contact conditions (temperature and time) of FCMs with food, migration studies were carried out using distilled water and 3% acetic acid as food simulants (**Fig. 18**).

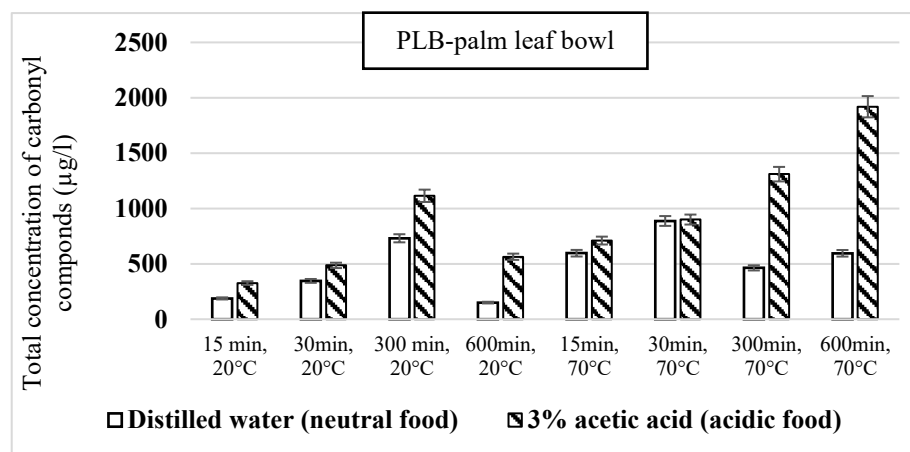
Based on the obtained results, contact time and temperature can have huge impact factor on the migration intensity (**Figs. 18 I-18 XIII**) which is in accordance with the other studies (Aznar et al., 2020; Kato & Conte-Junior, 2021). Thermal degradation reactions of FCMs can occur during contact with food, especially hot food. Carbonyl compounds can be easily released from FCMs as degradation products of coatings, paints and varnishes that are added to FCMs. Therefore, carbonyl compounds can be identified in food even after short contact of FCMs with food (after 15 min/30 min) at ambient temperature (20°C). In these conditions, the most carbonyl compounds can be released from palm leaf (PLB), paper (PC and PCW), plant residues (PLR), especially to acidic food. For most of the analyzed FCMs, a

proportional increase in the total concentration of carbonyl compounds was observed with increasing temperature (from 20 to 70°C) and contact time (from 15 min to 300 min) between the FCMs and the food simulant, e.g., an almost fourfold increase in the concentration of carbonyl compounds was noted, both in distilled water and 3 % acetic acid after extended contact with PLB (from 15 min to 300 min) (**Fig. 18 II**). However, volatile, simple organic compounds (including carbonyl compounds) are thermally unstable and can decompose at elevated temperatures, especially over a long period (600 min).

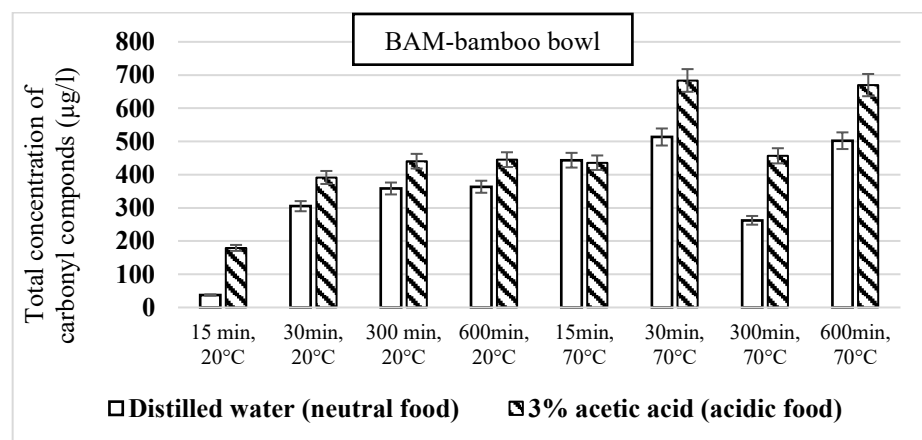




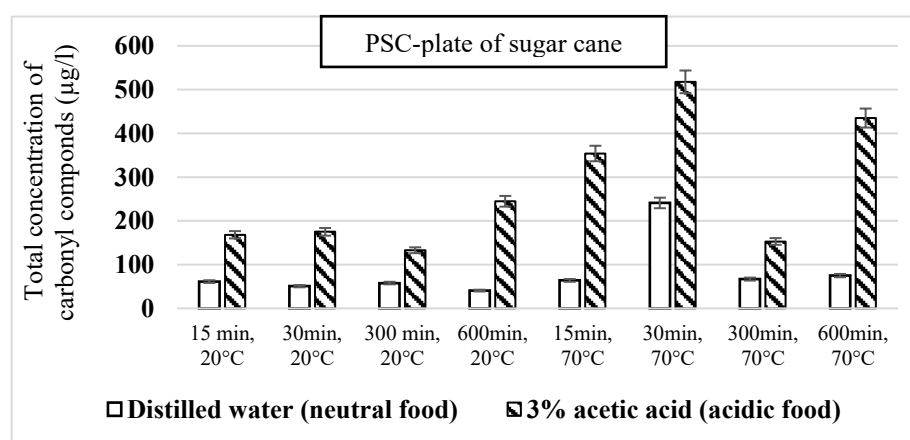
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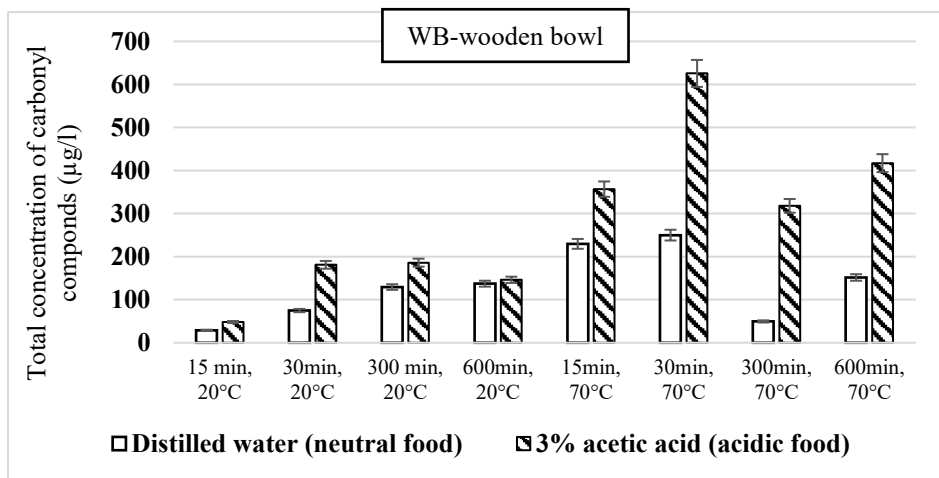
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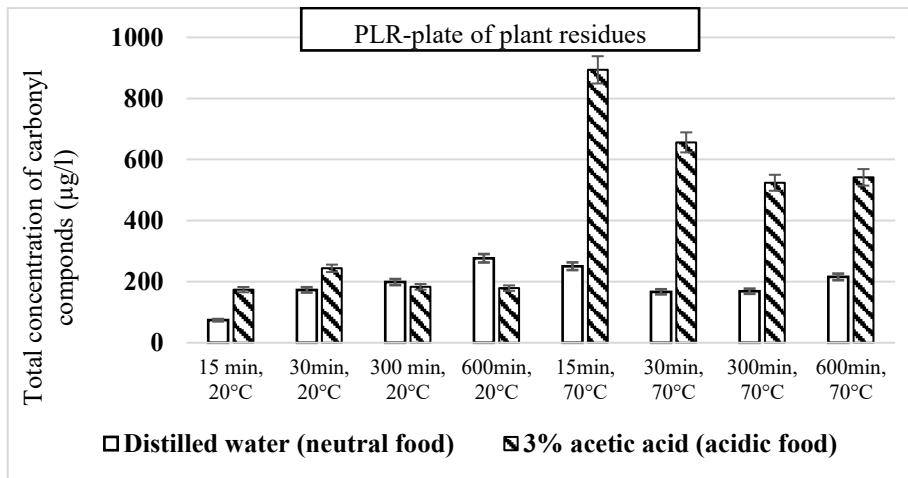
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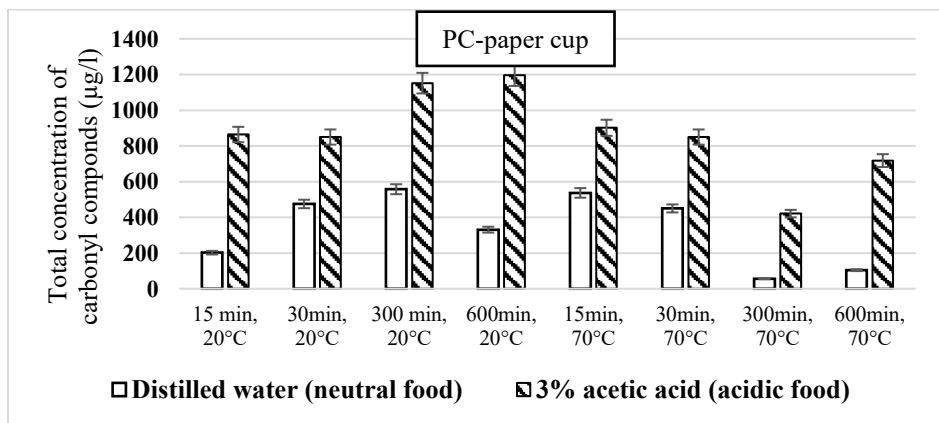
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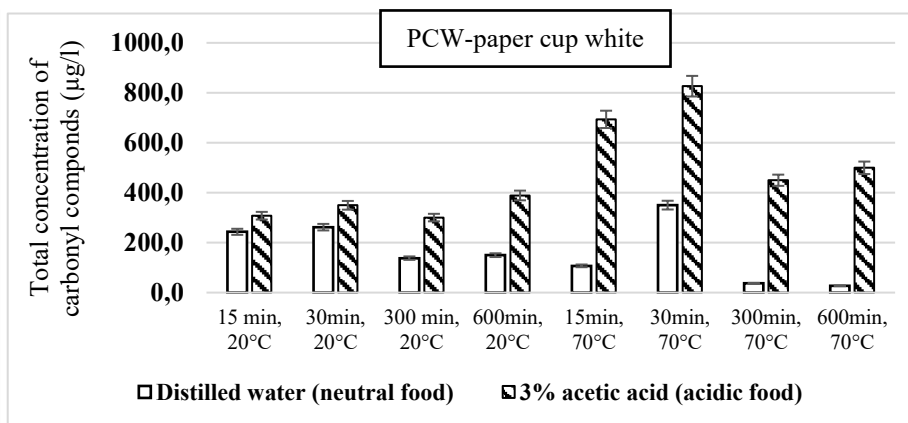
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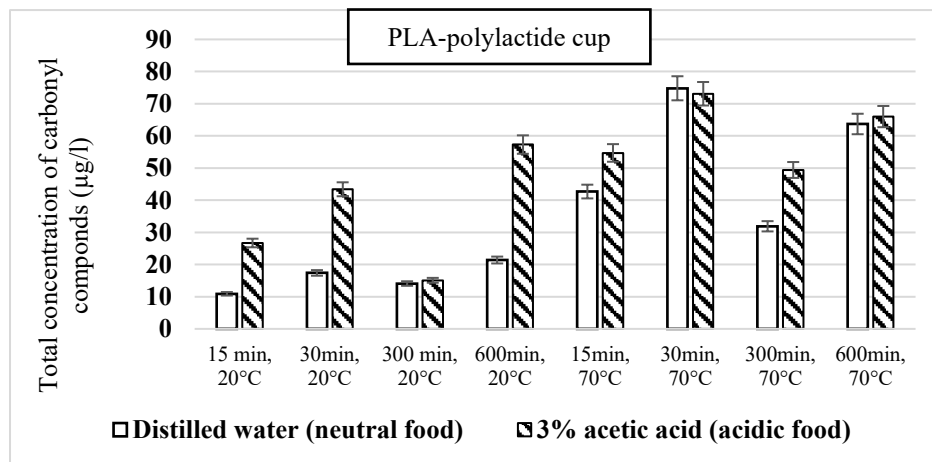
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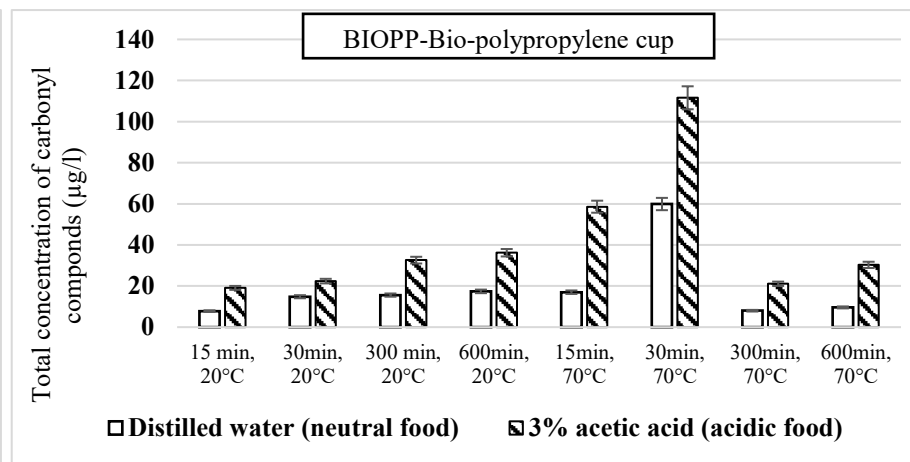
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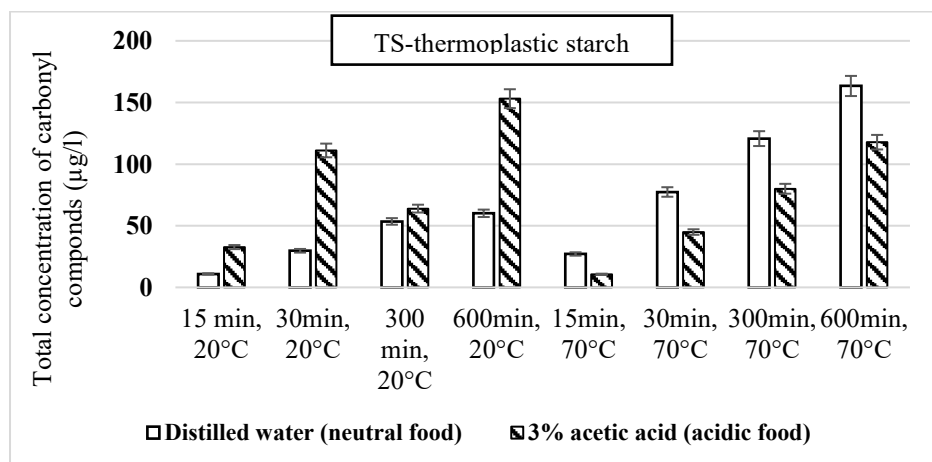
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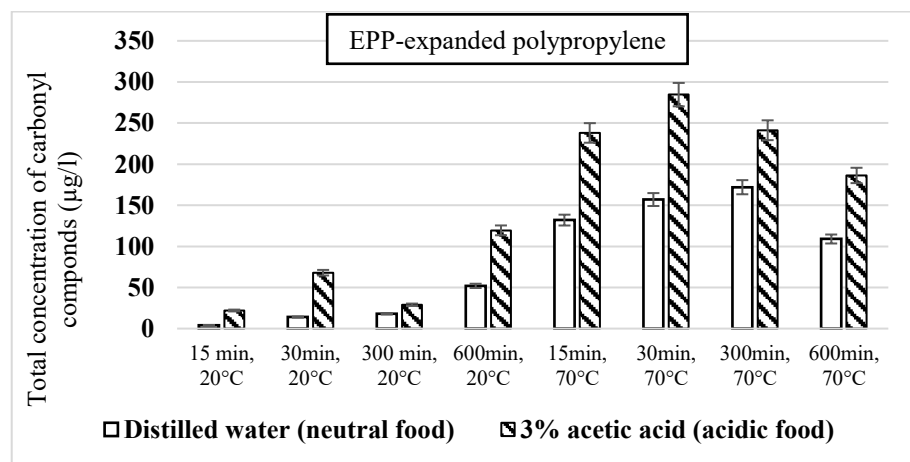
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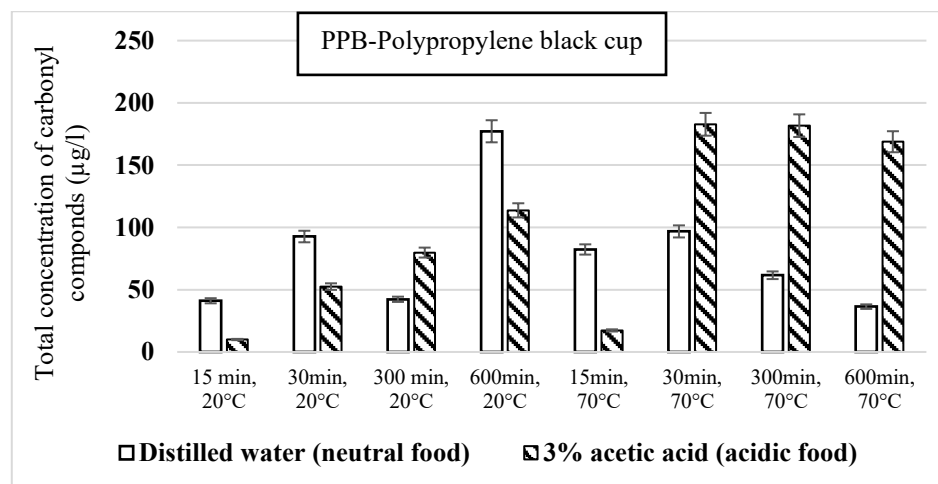
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XI



XII

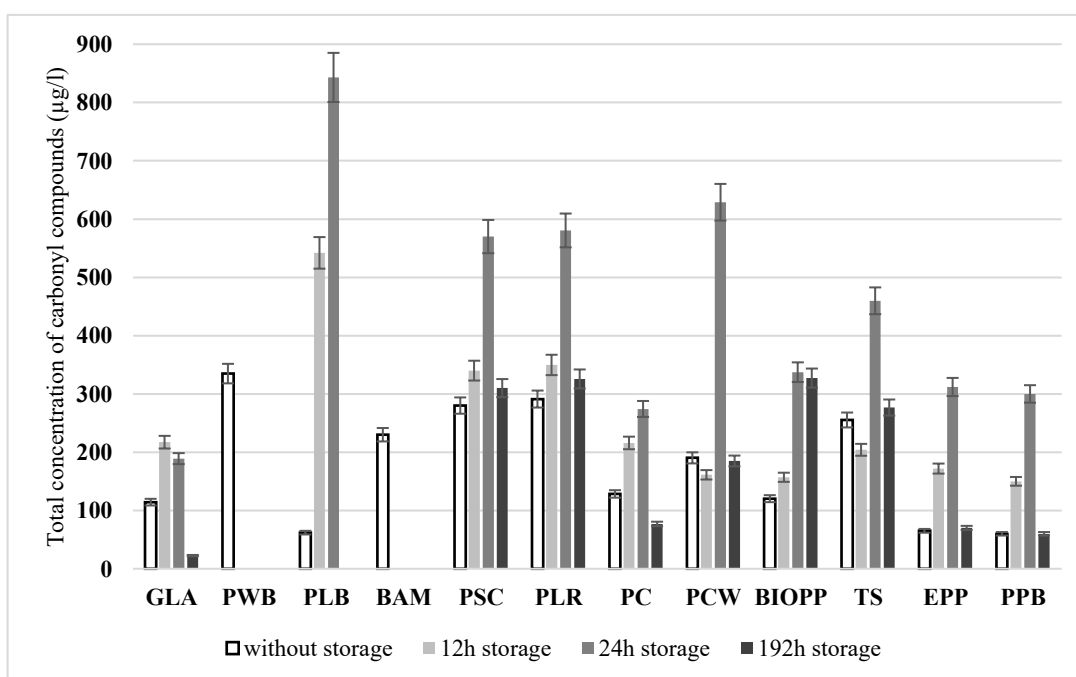


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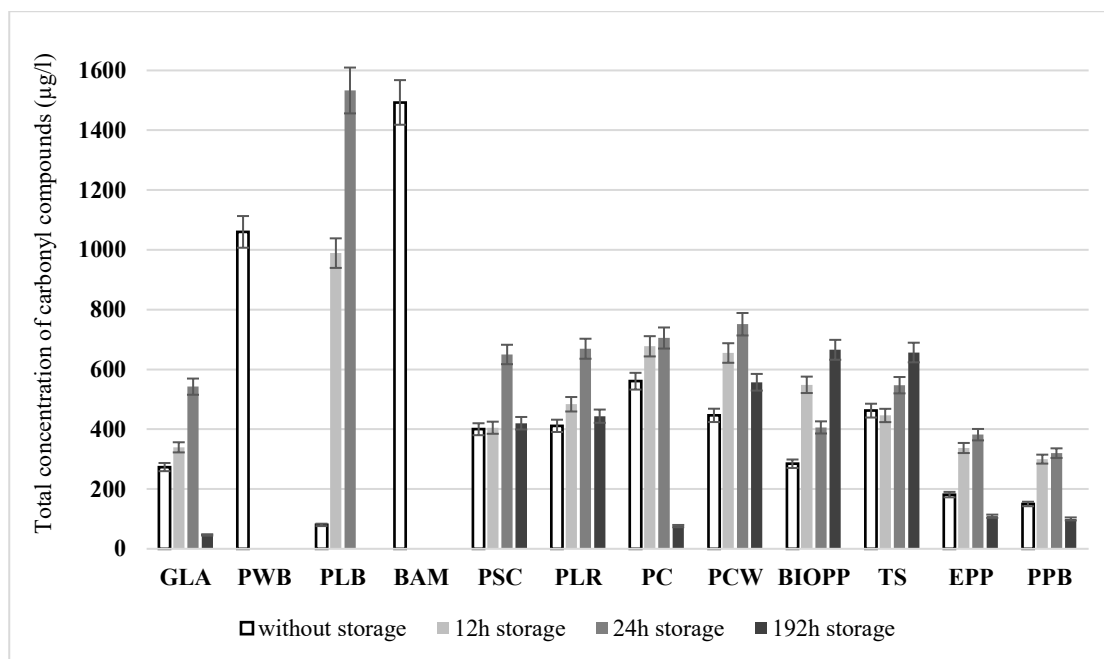
Fig. 18. Total carbonyl compound concentrations determined in distilled water and 3 % acetic acid after contact with different FCMs under different temperature and time conditions

Another factor that may determine the intensity of migration of carbonyl compounds may be heating by microwave radiation (usually at 700 W). Currently, it is one of the most popular method of quick and easy meal preparation (Chandrasekaran, Ramanathan & Basak, 2013; Guzik, Szymkowiak, Kulawik, Zając & Migdał, 2022). Additionally, the amount of water used is reduced, which means that microwaves can be considered as an ecological way of cooking (Krongworakul, Naivikul, Boonsupthip & Wang, 2020).

On the other hand, the heat generated in a microwave oven can be distributed unevenly (Tepnatim et al., 2021) and can also affect the FCMs. As a result, various chemical compounds can migrate into the heated food (Kim et al., 2023; Conchione, Lucci & Moret, 2020; Whitt et al., 2016; Sapozhnikova, Nunez & Johnston, 2021), including carbonyl compounds. The targeted study clearly showed that the key factors influencing the intensity of migration include: the length of time the food was stored in the refrigerator and the length of time it was heated with electromagnetic radiation. Total concentration of carbonyl compounds that were identified in the neutral food simulant and acidic food simulant after different storage periods in the refrigerator (without storage, 12 h, 24 h, 192 h of storage) and heating with microwave radiation (1 min) are presented in **Figs. 19 I and 19 II**.



I



II

**Fig. 19.** Total concentrations of carbonyl compounds identified in (I) distilled water or (II) 3 % acetic acid after different times of storage of samples in a refrigerator and heating by microwave radiation at 700W

Some materials currently available on the market (e.g., wheat bran (PWB), bamboo (BAM)) are not suitable for long-term storage of food in the refrigerator due to their susceptibility to deformation and low tightness. Therefore, tests with longer storage in the refrigerator were not performed for these samples. Palm leaf (PLB) is also subject to deformation, therefore, a test with long storage (192 h) was not performed for this material. However, the contact of the vessel with food is often short, i.e., the vessel is used for quick heating of food in the microwave oven without prior storage in the refrigerator. As presented in **Figs. 19 I and 19 II**, the analyzed FCMs, even without long-term contact with food, can cause its contamination with carbonyl compounds. It is visible that the type of material has a significant effect.

The study clearly showed that plant-based FCMs can particularly contaminate food with carbonyl compounds when food is heated quickly with microwave radiation. The highest amount of carbonyl compounds under these conditions can migrate from wheat bran (PWB) (in the test samples it was 335 µg/L to neutral food and 1060 µg/L to acidic food, respectively), bamboo (BAM) (230 µg/L to neutral food and 1493 µg/L to acidic food), plant residues (PLR) (291 µg/L to neutral food and 411 µg/L to acidic

food), sugar cane (280 µg/L to neutral food and 400 µg/L to acidic food), thermoplastic starch (TS) (255 µg/L to neutral food and 462 µg/L to acidic food), white paper (PCW) (190 µg/L to neutral food and 446 µg/L to acidic food) and brown paper (PC) (128 µg/L to neutral food and 561 µg/L to acidic food). Predominant carbonyl compounds include formaldehyde, acetone, pentanal, hexanal, decanal, glyoxal, methylglyoxal and pentan-2-one.

Migration of carbonyl compounds from glass (GLA) and bio-based plastics (BIOPP and EPP) occurs at lower concentration levels under these conditions. Total concentration of carbonyl compounds, which can migrate from glass (GLA) is 114 µg/L for neutral food and 273 µg/L for acidic food, from polypropylene (PP) is 120 µg/L for neutral food and 285 µg/L for acidic food and from expanded polypropylene (EPP) is 65 µg/L for neutral food and 181 µg/L for acidic food. Glass is a material still used globally. It is produced at high temperatures, so it is considered a safe material for food. Soda-lime glass, popularly used for the production of FCMs, was tested in this study. Chemically pure glass (borosilicate) showed twice lower migration of carbonyl compounds. On the other hand, EPP is a foam material (obtained using the Steam Chest Molding method) and BIOPP is a thermoplastic. Both materials are resistant to high temperatures, therefore the smallest amount of carbonyl compounds are released from these materials when rapidly heated with microwave radiation. The predominant carbonyl compounds identified for this group of materials include formaldehyde, acetaldehyde, acetone, propanal, butanal and pentanal.

However, the migration of carbonyl compounds changes during sample storage (12 h, 24 h, or 192 h) in the refrigerator (**Figs. 19 I and 19 II**). A significant increase in the amount of migrating carbonyl compounds was observed for all analyzed FCMs. The highest concentrations of carbonyls were noted in neutral food after 24 hours of storage. A particular increase in the total concentration of carbonyl compounds was observed for palm leaf (PLB) in these conditions (from 62 µg/L to 843 µg/L) (**Fig. 19 I**). On the other hand, a significant increase in the concentration of carbonyl compounds was noted after just 12 hours of storage for acidic food (**Fig. 19 II**). Only for glass (GLA) there was an increase in the concentration of carbonyls after 24 hours of storage.

In addition, it has been observed that longer storage of neutral food in the refrigerator (up to about a week) reduces the concentration of carbonyl compounds by about 40 % (for TS and PLR), about 70 % (for PC and PCW), about 80 % (for EPP) and about 95 % (for GLA). This means that carbonyl compounds can biodegrade over time. These low-molecular compounds can be a source of easily available organic carbon for the microflora present in the neutral food simulant. It is clear that the biodegradation of carbonyl compounds in acidic food is difficult. Even after storing food in the refrigerator for a week, high concentrations of these compounds were identified in acidic food. Some

materials (e.g., BIOPP and TS) showed an increase in concentration. This means that the contact time of the materials with food and pH of the food have a significant impact on the amount of migrated carbonyl compounds.

The effect of heating time (1-4 min) on the intensity of migration processes of carbonyl compounds from the FCMs into the food simulants was also investigated. As shown in **Fig. 20**, the highest total concentrations of carbonyl compounds were observed after 1 min of heating the analyzed samples with electromagnetic microwave radiation (food temperature was about 60°C), both for neutral and acidic food. However, the pH of food may affect the changes in carbonyl compound concentrations under the influence of heating time. Longer heating of neutral food (2, 3, or 4 min) causes a decrease in the concentration of carbonyl compounds, probably due to their thermal degradation. For some samples (e.g., TS and PLR), degradation of carbonyl compounds was noted only after 4 min of heating. It may be related to the gradual release of carbonyl compounds from the material to food under the influence of the electromagnetic radiation. On the other hand, for acidic food, stabilization of the concentration of carbonyl compounds was observed from 1 min to 3 min of heating for majority of the analyzed samples. This suggests that low pH of food affects the stability of carbonyl compounds, so that acidic food may be more exposed to carbonyl compounds than neutral food.



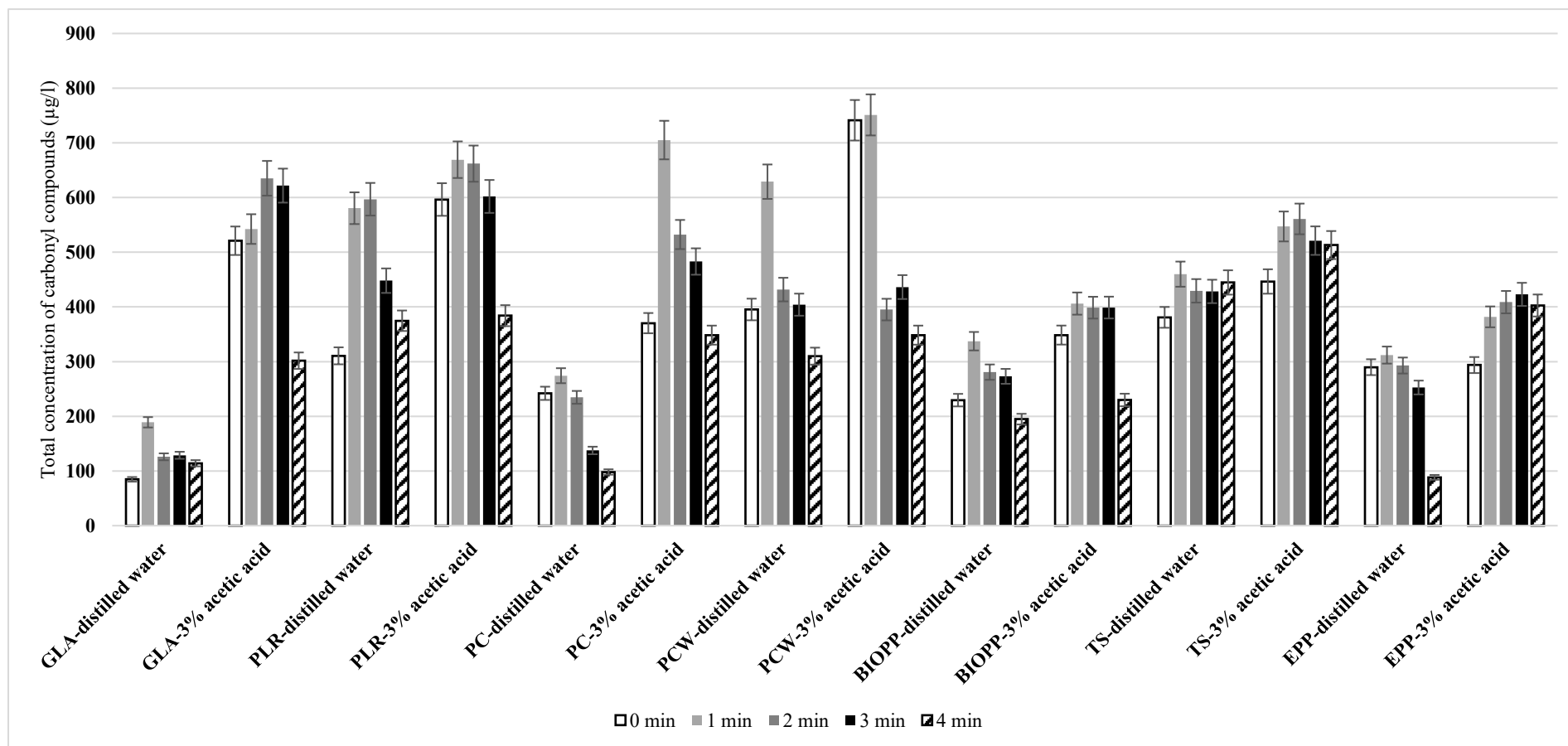


Fig. 20. The total concentration of carbonyl compounds identified in the distilled water and 3 % acetic acid after storage in 24 h in the refrigerator and heating with microwave radiation in different times (1-4 min)

The presence of formaldehyde in food heated in a microwave oven can be dangerous. The tolerable daily intake (TDI) of this compound was set at 150 µg/kg body weight per day (EFSA 2007) to estimate the risk of formaldehyde exposure through food. The largest group exposed to this cancerogenic carbonyl compound are children, based on their relatively low body weight. The level of consumer exposure to undesirable formaldehyde was evaluated during heating of food with microwave radiation for 1 min after 24 h of storage in the refrigerator. It was assumed that the heated neutral or acidic food had a total volume of 250 mL. Tested materials differ in the amount of formaldehyde released into the food, as presented in **Fig. 21**. Most of this undesirable compound can migrate from FCMs made of expanded polypropylene (EPP) or plant residues (PLR). The concentration of migrating formaldehyde can exceed 100 µg for acidic food. Assuming an average child weight of 10 kg, a child can consume more than 10 µg/kg of formaldehyde with a microwave-heated meal. Although this value is significantly lower than the recommended TDI for formaldehyde (150 µg/kg), it should be considered that formaldehyde is a ubiquitous compound in the environment. There are many sources of exposure (e.g., children are exposed to formaldehyde through synthetic toys). Safer materials used for microwave radiation heating include glass or paper in these terms.

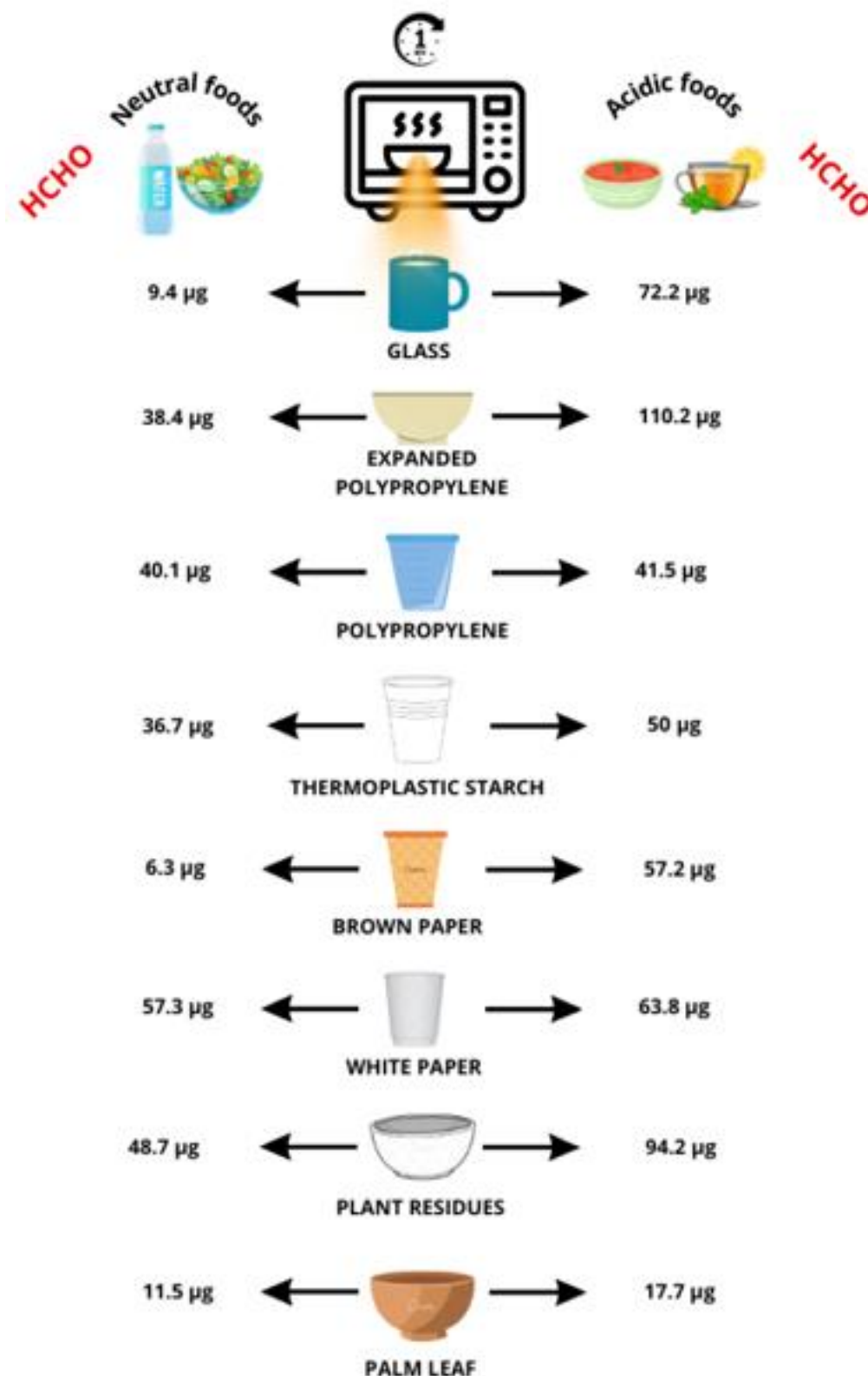


Fig. 21. Simulated assessment of consumer exposure to formaldehyde after storing neutral or acidic foods in different FCMs in the refrigerator for 24 h and heating with a 700 W microwave oven for 1 min; estimated volume of food 250 mL

### 5.2.3 Migration study of high-molecular weight contaminants

Dry and frozen foods (represented in this study by Tenax) can be particularly exposed to contamination due to their long shelf life. PAHs can easily adsorb to the surface of solids due to their poor solubility in water, low vapor pressure and aromatic nature. Plastic waste, especially polystyrene, can be a source of PAHs pollution in the aquatic environment (Si-Qu, Hong-Gang & Hui, 2017). Although the study showed that polyaromatic hydrocarbons do not migrate from the analyzed plant materials under the conditions tested, it is possible that Tenax may be contaminated with EDCs (**Table 12**).

BPA and BPS are commonly used as epoxy resins and polycarbonate precursors to improve the strength, hardness, thermal stability, grease and oil resistance of packaging materials and vessels during manufacturing process (Ma et al., 2019). Moreover, benzophenones are UV stabilizers and ingredients of inks, paints and printed FCMs. In turn, phthalates are added to packaging and vessel materials to improve their functional properties (flexibility, softness and elasticity). They are also used in the production of varnishes and prints and as additives that improve adhesion to surfaces (Moraes da Costa et al., 2023). All of these material additives should be used in moderation. Some of them (e.g., BPA/BPS) exhibit pro-estrogenic effects and are defined as EDCs (Ma et al., 2019; Sawadogo et al., 2023; Prueitt et al., 2023). Substitutes, including BPS, are often used to reduce BPA content. However, *in vivo* and *in vitro* studies have shown the effect of BPS on endocrine disorders, which means that commonly used BPA analogues may also be hazardous food contaminants (Heindel et al., 2022). Benzophenone derivatives, as EDCs, may have a toxic effect on hormonally controlled processes, including fertility, development of the nervous system and sexual differentiation. They can interact with enzymes, leading to digestive disorders and also adversely affect the proliferation and migration of cancer cells (Ma et al., 2023). Moreover, exposure to phthalates (DBP, DiBP and DEHP) and their metabolites, are particularly dangerous for pregnant women and teenagers (Topdas, 2023; Tsochatzis et al., 2023). These compounds can cause oxidative stress, which leads to premature birth (Ferguson et al., 2016) and pancreatic  $\beta$ -cell dysfunction. Phthalates as EDCs may lead to the development of obesity and asthma, especially in adolescents (Hu et al., 2017; Dong et al., 2022; Zhu et al., 2024).

**Table 12.** Determined concentrations ( $\mu\text{g/g}$  material) of environmental and production contaminants (x) in Tenax after contact with different materials under different time and temperature conditions: I (2 h, 70°C) and II (10 days, 40°C), respectively

Migrants	PWB		BAM		PLR		WB		TS		PLA		EPP		PC	
Conditions	I	II	I	II	I	II	I	II	I	II	I	II	I	II	I	II
BPA	<LOD	0.016	<LOD	0.019	<LOD	0.019	0.115	0.014	<LOD	0.011	<LOD	0.030	0.086	0.007	<LOD	0.009
BPS	<LOD	0.004	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.018	<LOD	<LOD	<LOD	<LOD
2,4-DHBP	<LOD	<LOD	0.033	0.024	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.034	0.014
2,2,4,4'-THBP	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
2-H-4-MBP	<LOD	<LOD	0.028	0.005	0.017	0.003	0.115	0.005	0.015	0.002	0.028	0.004	0.032	0.004	0.011	0.005

**Table 12.** continued

Migrants	PLB		PCW		PSC		BIO-PP	
Conditions	I	II	I	II	I	II	I	II
BPA	0.086	<LOD	<LOD	<LOD	<LOD	0.049	<LOD	<LOD
BPS	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
2,4-DHBP	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
2,2,4,4'-THBP	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
2-H-4-MBP	0.028	<LOD	<LOD	0.007	0.014	0.007	0.018	<LOD

Migration studies showed that BPA can migrate from wood (WB) (0.115 µg/g food) and expanded polypropylene (EPP) (0.086 µg/g food) at 2 h, 70°C into food. Both values exceed the SML for BPA (0.050 µg/g food). The cause of BPA migration from bio-based plastic FCMs into food may be due to protective coatings based on polycarbonates and peroxide resins, which can be thermally degraded at elevated temperatures and form monomers, including BPA. Similarly, Sawadogo et al. (2023) found that the intensity of BPA migration is influenced by the contact temperature between the packaging and the food. This means that exposure of bottled water to sunlight can accelerate the migration of BPA into water by up to 55 times. Scientists attribute the causes of these phenomena to possible thermal degradation (fragmentation and depolymerization) of polycarbonate coatings and peroxide resins contained in plastics, which leads to the production of monomers, including: BPA. Additionally, it was found that depolymerization did not occur suddenly, but rather as a function of time, as BPA was identified even after 35 days of storage. However, longer storage (up to 8 weeks) may cause the degradation of BPA, which oxidizes and decomposes in contact with oxygen, especially in the presence of water. Dissolved oxygen plays a major role in the degradation of BPA and is one of many factors that can also act in this way in packaged water.

BPA migration from some plant-based FCMs to food may seem surprising. However, there have been many reports on the serious problem of BPA contamination in the environment recently (Datta et al., 2024). The reason for this phenomenon may be the highly developed plastic industry and thermal paper recycling, which inevitably led to the leaching of BPA into the environment in large quantities, polluting the soil, air and aquatic environment (Ramakrishna, Girigoswami, Chakraborty & Girigoswami, 2022). Moreover, uncontrolled open burning of household waste containers may contribute to high BPA emission rates (Vasiljevic & Harner, 2021). Significant BPA environmental contamination may have a significant impact on the occurrence of this compound in trace amounts in plant- and bio-based plastics FCMs as residues/contaminants in the environment.

In contrast, increasing the contact time of the vessel with food (10 days, 40°C) results in an approximately ten-fold decrease in the concentration of BPA migrating from wood (WB) and expanded polypropylene (EPP), which is likely related to the degradation of BPA over time in the presence of oxygen (aerobic degradation). Guart, Bono-Blay, Borell and Lacorte (2011) identified BPA as a compound migrating into fresh bottled water and after one year of aging from various packaging materials (glass, PP, PC, PET, HDPE, LDPE). They reported lower concentrations of BPA in older samples, which confirmed the possibility of BPA degradation over time. Based on the results, temperature has a greater effect on BPA migration than contact time. This means that food served hot (e.g., pasta) may be more contaminated with BPA than food served cold (e.g., ice cream). In some FCMs (e.g., wheat bran (PWB),

bamboo (BAM), plant residues (PLR), thermoplastic starch (TS), polylactide (PLA), paper (PC)) BPA was identified in foods after a longer period, but at concentrations that do not exceed the SML.

It was also observed that BPS can only migrate into food after prolonged contact with wheat bran (PWB), bamboo (BAM), plant residues (PLR) and polylactide (PLA), but the concentrations do not exceed the SML. BPA contamination of food can be much higher than BPS. The European Food Safety Authority (EFSA) has set the TDI for BPA at 0.20 ng/kg body weight per day (EFSA, 2023). Based on the BPA concentrations determined for WB and EPP at 2h, 70°C and assuming a child's weight of 40 kg and a meal weight of 150 g, it can be estimated that the child will consume about 431.3 ng/kg body weight of BPA from WB and about 320.6 ng/kg body weight of BPA from EP. These values significantly exceed the recommended TDI for BPA.

Migration of benzophenone derivatives into food is also an undesirable phenomenon. Studies have shown the presence of 2,4-DHBP and 2-H-4-MBP in Tenax (**Table 12**). The migration of these compounds is mainly favored by the elevated contact temperature of the food with the vessel (70°C). 2,4-DHBP can migrate from bamboo (BAM) (0.033 µg/g food) and paper (PC) (0.034 µg/g food). In contrast, 2-H-4-MBP was identified as a migrating contaminant from all materials analyzed, except wheat bran (PWB). These compounds, similar to BPA, are susceptible to degradation over time. In addition, 2,2,4,4'-THBP was not identified as a compound migrating to Tenax from the analyzed materials.

Another group of food contaminants are phthalates. The presence of DBP, DiBP and DEHP was confirmed in most of the analyzed samples (**Table 13**). Only thermoplastic starch (TS), polylactide (PLA) and brown paper (PC) do not cause the migration of these compounds into dry and frozen foods. However, they can release 2,4-ditertbutylphenol (2,4-DTBP), which is a commonly used antioxidant food additive. This compound has anti-inflammatory, cytotoxic, insecticidal, antibacterial, antiviral and antifungal properties and is therefore used as an environmentally friendly herbicide (Zhao, Wang, Lucardi, Su & Li, 2020). Squalene, a natural bioactive compound from the triterpenoid group, commonly found as a component of vegetable oils (amaranth oil, olive oil), can migrate from wood (WB) and plant residues (PLR). It occurs as a bioactive component of plants, such as papyrus (*Cyperus Papyrus L.*) (Rosado et al., 2022) and apples (Scortichini et al., 2022). Prolonged contact between the vessel and food can cause migration of octocrylene from wood (WB), wheat bran (PWB), bamboo (BAM) and polylactide (PLA).

**Table 13.** Presence of environmental and production contaminants (x) in Tenax after contact with different materials under different time and temperature conditions: I (2 h, 70°C) and II (10 days, 40°C), respectively

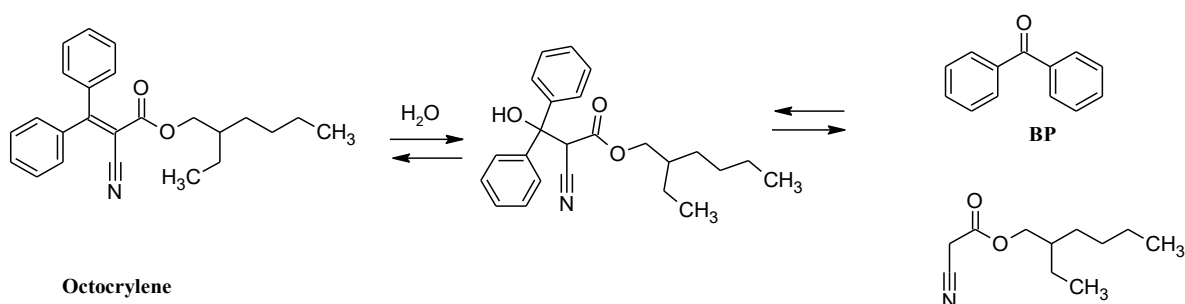
Migrants	PWB		BAM		PLR		WB		TS		PLA		EPP		PC	
Conditions	I	II	I	II	I	II	I	II	I	II	I	II	I	II	I	II
DBP	x	x	x	x	x	x		x					x			
DiBP	x	x	x	x	x	x		x					x			
DEHP		x	x	x			x	x								
2,4-DTBP									x	x		x				
Octocrylene		x		x				x				x				
Squalene					x	x	x	x								

**Table 13.** continued

Migrants	PCW		PSC		BIO-PP	
Conditions	I	II	I	II	I	II
DBP	x	x				
DiBP		x			x	
DEHP		x	x		x	
2,4-DTBP						
Octocrylene						
Squalene						



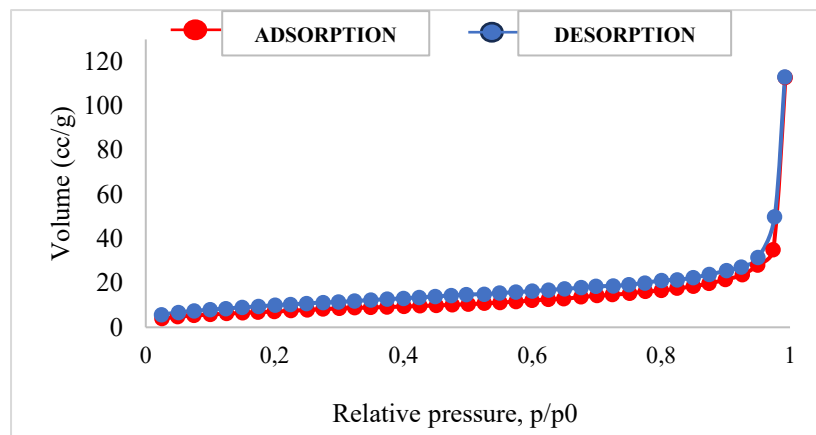
Octocrylene is a ubiquitous and persistent substance in the environment because it is not biodegradable. This compound has found many applications in the industrial sector, e.g., it is used as a common UV stabilizer in various materials. It is often considered a precursor to benzophenone (BP) in the retroaldol condensation (**Fig. 22**) (Downs, DiNardo, Stien, Rodrigues & Lebaron, 2021). For this reason, it is considered an undesirable compound in foods (Lestido-Cardama et al., 2020; Su, Vera, Nerin, Lin & Zhong, 2021). Moreover, octocrylene is one of the global environmental pollutants, since it has been identified in sewage, surface waters and bottom sediments (Kameda, Kimura & Miyazaki, 2011). For these reasons plant-based FCMs, e.g., wheat bran, bamboo or wood, may contain octocrylene at trace levels.



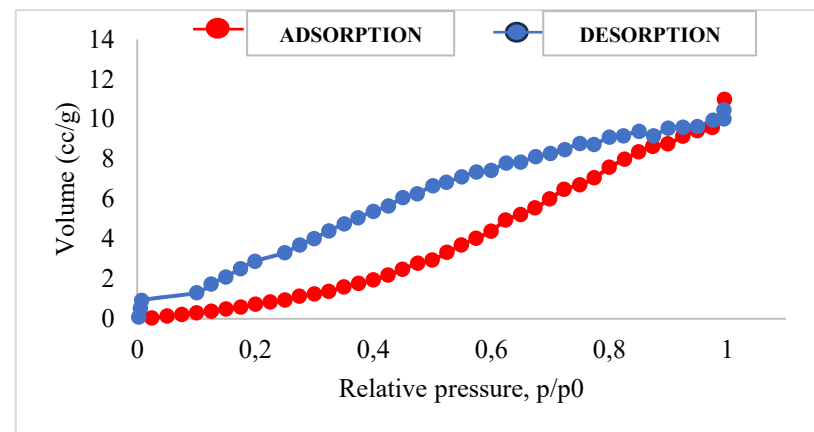
**Fig. 22.** An example mechanism leading to the preparation of BP from octocrylene (based on Downs et al., 2021)

In order to compare the migration intensity of contaminants from FCMs to Tenax and real food samples, the physical properties of solid samples were characterized and a spiking experiment was conducted.

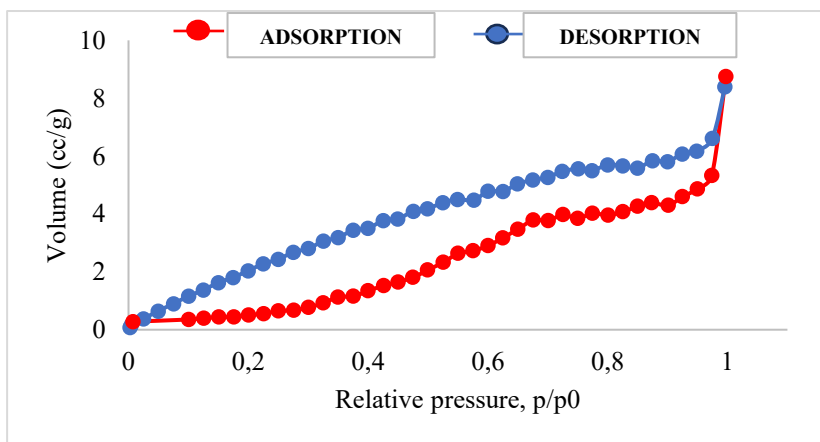
The parameters characterizing the porous structure of the materials tested were determined from the BET isotherms (**Fig. 23**). According to the IUPAC classification, the tested materials demonstrate a type IV isotherm. It is characterized by a hysteresis loop, which is related to capillary condensation occurring in mesopores and limited absorption in the high  $p/p_0$  range (Sing et al., 1985). The specific surface area, total pore volume and average pore diameter were determined from these isotherms (**Table 14**). Their specific surface area and pore volume can be ranked from largest to smallest for Tenax > powdered milk > baby cereal > oat flakes. Based on the average pore diameter, all analyzed samples can be classified as mesoporous materials ( $50 \text{ nm} > d > 2 \text{ nm}$ ).



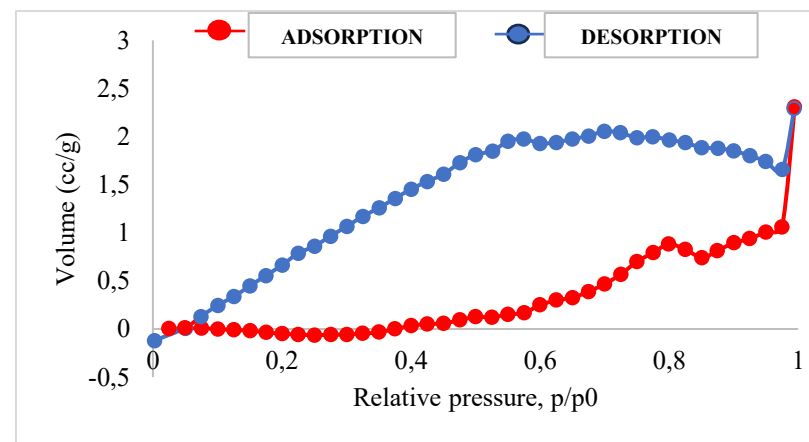
I



II



III



IV

Fig. 23. BET isotherms of the tested materials: (I) Tenax, (II) powdered milk, (III) baby cereal and (IV) oat flakes

**Table 14.** Specific surface area ( $\text{m}^2/\text{g}$ ), pore volume ( $\text{cc}/\text{g}$ ) and average pore diameter (nm) determined for the tested materials

Material	Surface area ( $\text{m}^2/\text{g}$ )	Pore volume ( $\text{cc}/\text{g}$ )	Average pore diameter (nm)
Tenax	27.325	<sup>a</sup> $1.748\text{e}^{-1}$	25.590
Powdered milk	25.218	<sup>b</sup> $1.705\text{e}^{-2}$	2.704
Baby cereal	3.016	<sup>c</sup> $1.357\text{e}^{-2}$	17.990
Oat flakes	0.047	<sup>d</sup> $3.578\text{e}^{-3}$	302.400

<sup>a</sup> Total pore volume for pores with diameter less than 273.12 nm at  $p/p_0 = 0.992919$

<sup>b</sup> Total pore volume for pores with diameter less than 428.32 nm at  $p/p_0 = 0.995502$

<sup>c</sup> Total pore volume for pores with diameter less than 699.28 nm at  $p/p_0 = 0.997252$

<sup>d</sup> Total pore volume for pores with diameter less than 346.89 nm at  $p/p_0 = 0.994437$

The migration of contaminants including 2,4-DHBP, 2,2,4',4'-THBP, 2-H-4-MBP, PHE and ANT to Tenax and real foods such as powdered milk, baby cereal and oat flakes were compared. Percentage of migration of each contaminant identified in Tenax and food is presented in **Fig. 24**. Based on the results, the highest percentage of contaminant migration was observed for Tenax (t-test at  $p < 0.05$  level), which is in accordance with previous reports (López, Batlle, Salafranca & Nerín, 2008; Rubio et al., 2019; Cai et al., 2017; Ji et al., 2019; Otoukesh, Vera, Wrona, Nerin & Es'haghi, 2020; Baele et al, 2020; Elizalde et al., 2020). This means that studies conducted with Tenax as a simulant may lead to overestimated results of contaminant migration, but at the same time constitute a warning signal about hazardous FCMs. Although even half as many contaminants may get into food, studies checking the safety of new FCMs should be conducted using Tenax. In addition, Tenax does not contain any additional ingredients that could contribute to the intensity of contaminant migration. Therefore, comparing the intensity of contaminant migration to Tenax allows for a clear assessment of the influence of the physicochemical properties of migrants and their structure on the migration intensity. The migration sequence for Tenax was as follows:  $\text{ANT} \approx \text{PHE} > 2,4\text{-DHBP} \approx 2\text{-H-4-MBP} > 2,2,4,4'\text{-THBP}$ . In the presented series of pollutants analyzed, their hydrophobicity decreases, which may be an important factor determining the intensity of migration (all pollutants are classified as compounds that are rather poorly soluble in water). The high migration of ANT and PHE to Tenax may be due to the high values of the octanol-water partition coefficient (for ANT 4.5 and for PHE 4.65, respectively) (Vera, Aznar, Mercea & Nerín, 2011; Elizalde et

al., 2020). Additionally, it is clearly seen that 2,4-DHBP and 2-H-4-MBP show similar migration to Tenax, despite the large difference in molecular weight (182.22 and 228.24 Da, respectively). This means that the structure of the molecule and the size of the substituents have a greater impact on migration efficiency than the molecular weight. The lowest migration to Tenax was recorded for 2,2',4,4'-THBP, probably due to the lowest hydrophobicity among the pollutants studied and large branching of this molecule. Similar conclusions were reached by Cai et al. (2017), who showed that the low migration of 2-methylbenzophenone compared to 3-methylbenzophenone and 4-methylbenzophenone may result from steric barriers between the functional groups of the molecule.

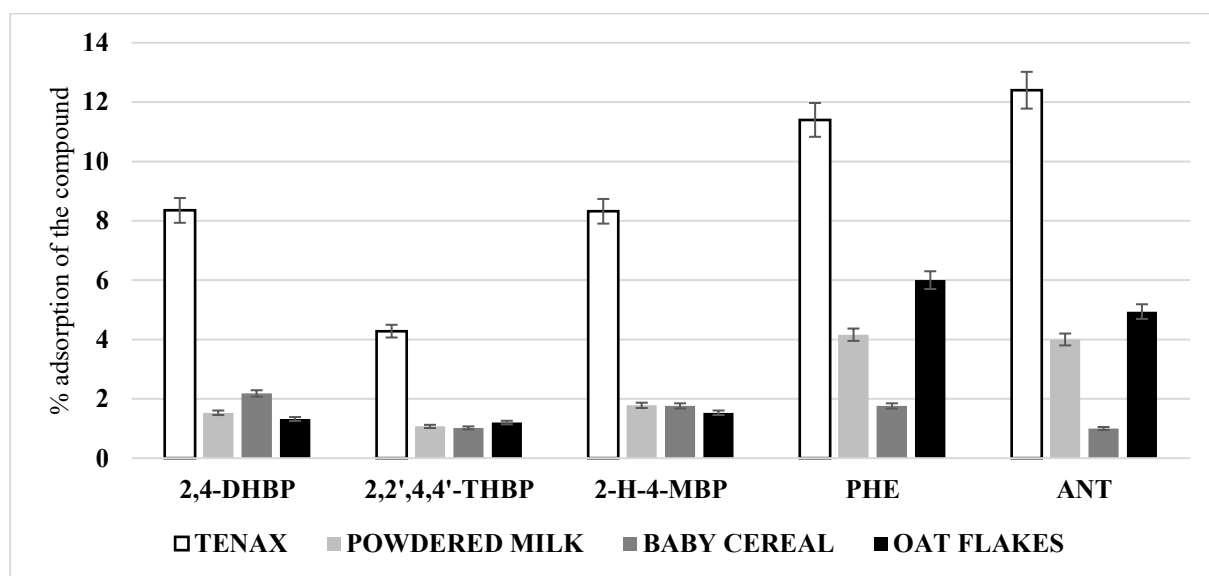


Fig. 24. Migration percentage of the contaminants into the Tenax and real food samples: powdered milk, baby cereal and oat flakes at 2h, 70°C (average values from three repetitions per sample)

On the other hand, the influence of the type of food and its components can be clearly observed for molecules that have similar physicochemical properties and structures, such as PHE and ANT (Fig. 24). The highest migration of these contaminants can be observed for oat flakes, followed by powdered milk and baby cereal. This means that the composition of the food can have a greater influence on the migration of contaminants than the specific surface area, structure and pore distribution of the food for the migration of ANT and PHE. According to Table 14, powdered milk has a specific surface area most similar to Tenax (for powdered milk is 25.218 m<sup>2</sup>/g and for Tenax is 27.325 m<sup>2</sup>/g, respectively). The powdered milk contains the lowest amount of fat (0.8 g/100 g of product) of all the food samples tested, according to the product label (Table 7). The significant difference in migration of ANT and PHE into these two sorbents (to Tenax 12.4 % for PHE and 11.4 % for

ANT and to powdered milk 4 % for PHE and 4.2 % for ANT, respectively) may suggest that the fat content has a large impact on the intensity of migration (López et al., 2008; Baele et al., 2020). Baele et al. (2020) observed clear differences in the migration of 1,2,5-tri-*t*-butylbenzene and other contaminants. It shows that fat content can be an important determinant of the intensity of migration processes.

## 5.2.4 Migration study of inorganic contaminants

Environmental pollution with toxic and potential toxic elements is an increasing challenge on a global scale (Cakaj et al., 2023). Accumulated toxic elements can negatively affect every element of the environment and cause a decrease in the quality of air, water, soil and food. The treatments used during the FCMs production process and the ability of plants to absorb contaminants from the environment means that new FCMs can be one of the links in the chain of elements entering packaged/served foods.

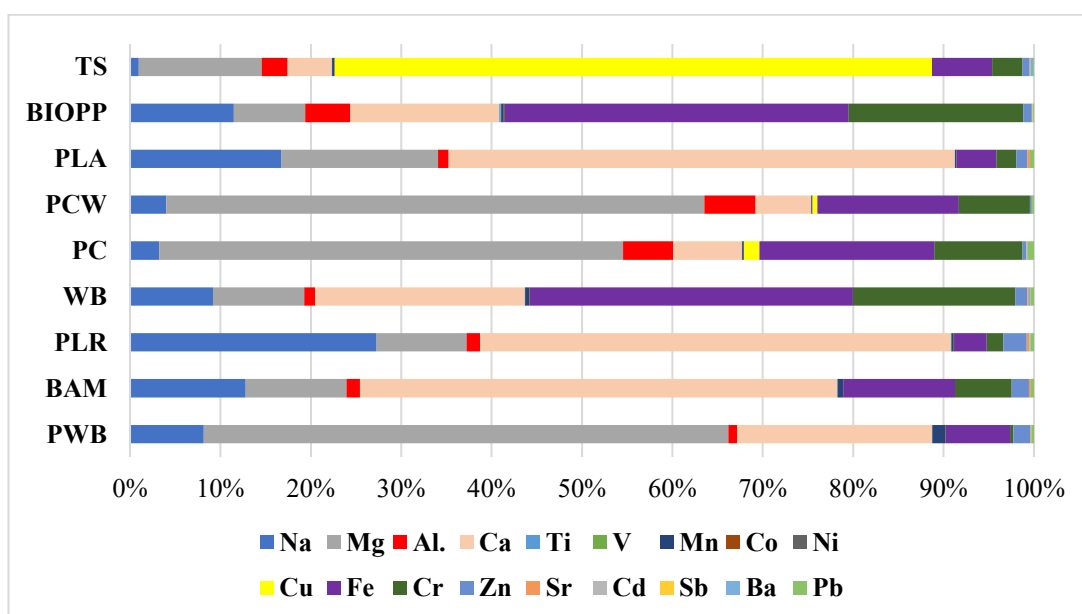


Fig. 25. Percentage content of individual elements in the analyzed FCMs

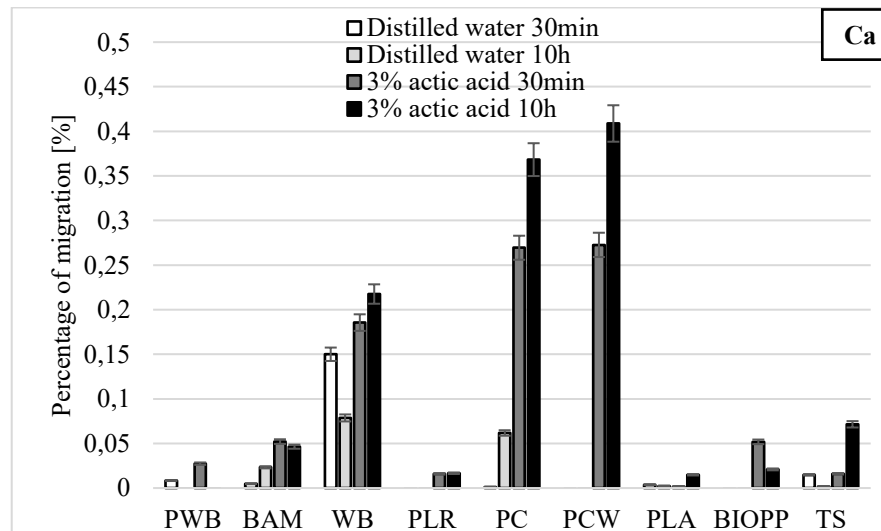
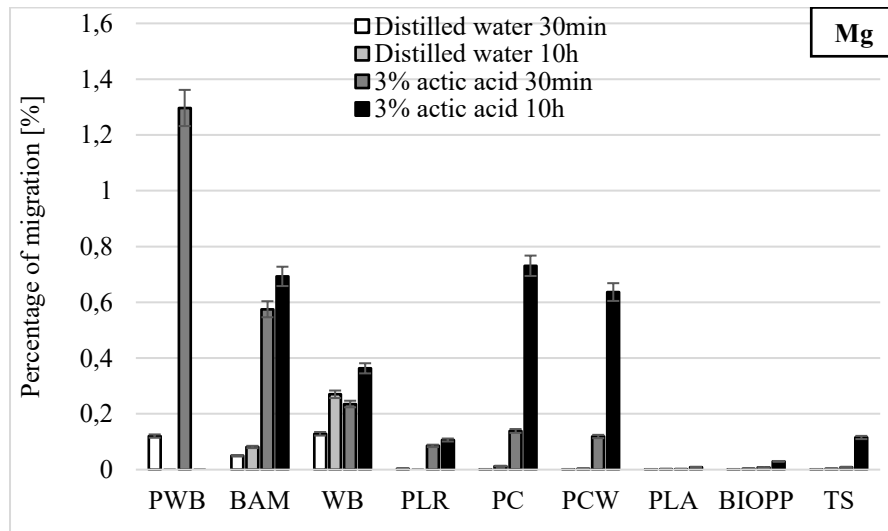
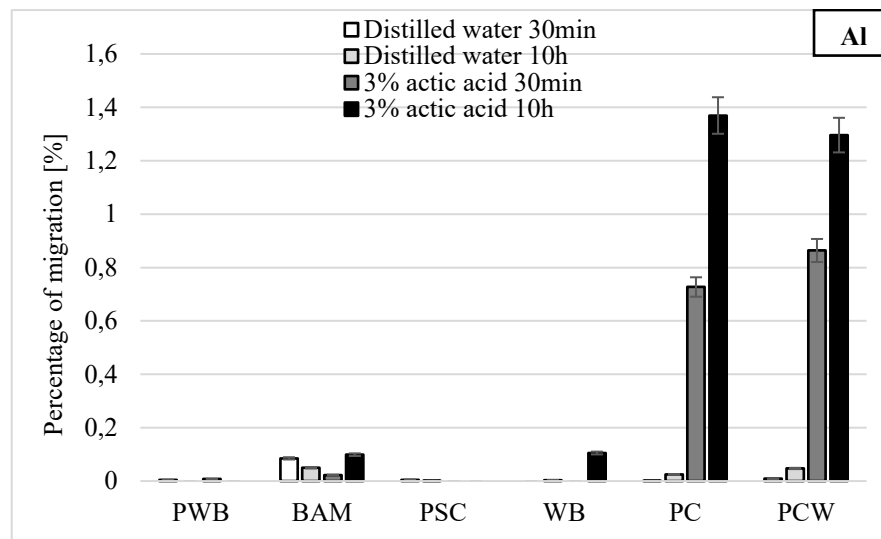
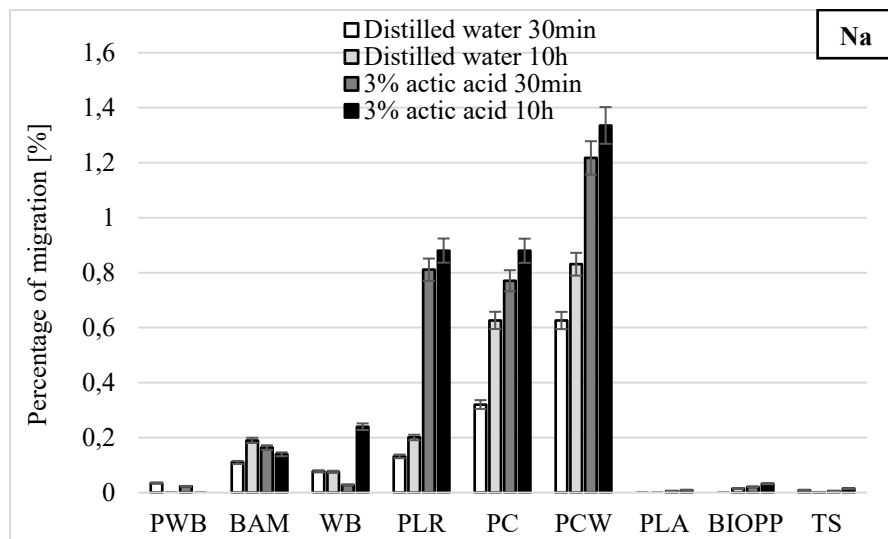
The percentage content of each element in the FCMs analyzed is presented in Fig. 25. It can be clearly seen that FCMs differ in elemental composition. The presence of elements such as Mg, Al, Ca and Fe in FCMs may be related to the use of inorganic fillers during the manufacturing process, e.g.,  $\text{CaCO}_3$ , kaolin, talc, commonly used to improve processing, stiffness and dimensional stability (Klockner, Reemtsma & Wagner, 2021). In addition, high concentrations of Cu, Ba and Sr may be associated with the use of inorganic pigments (Crema et al., 2024). Moreover, Al is a widely distributed component in

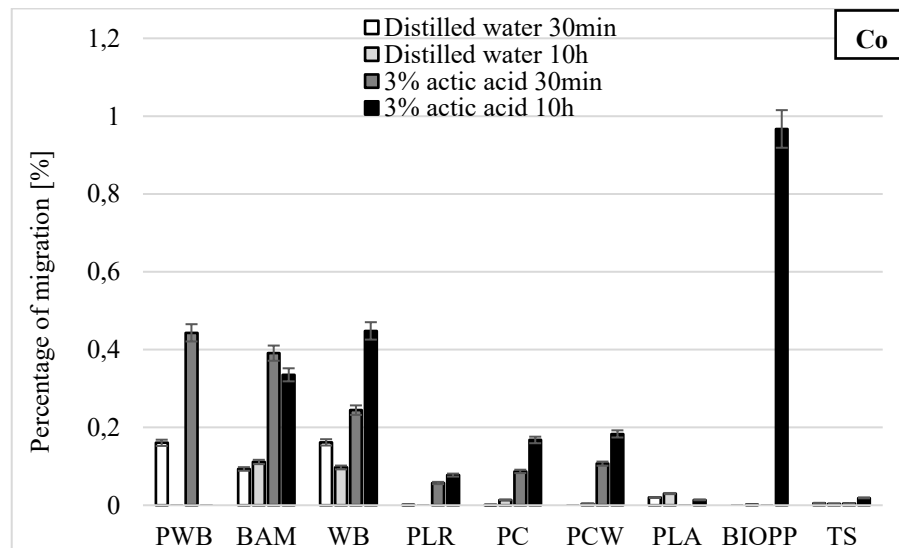
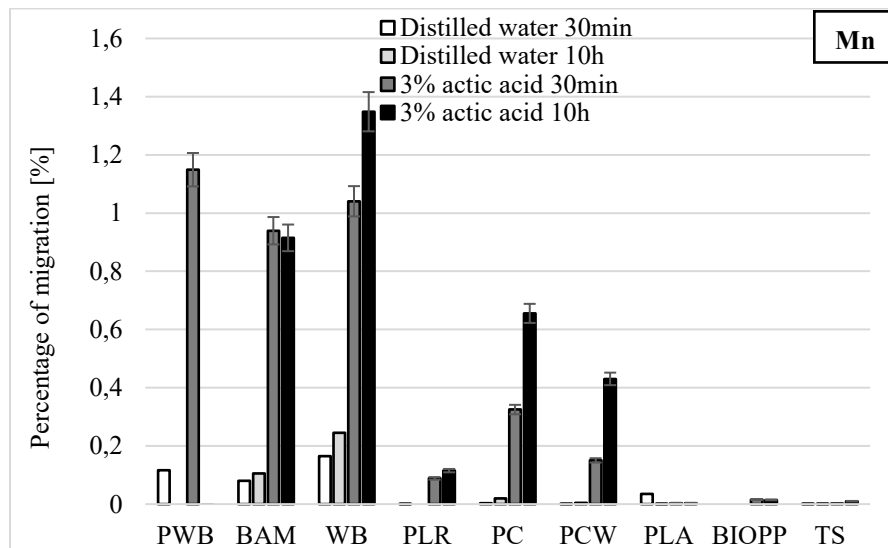
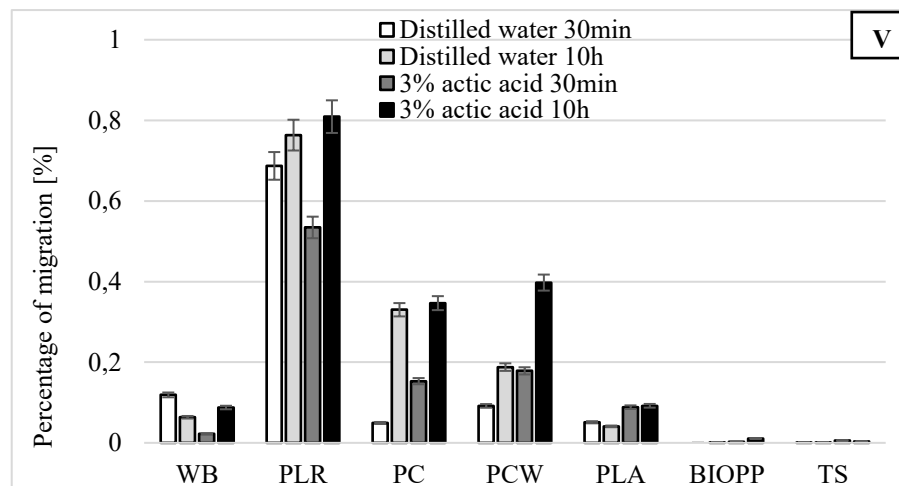
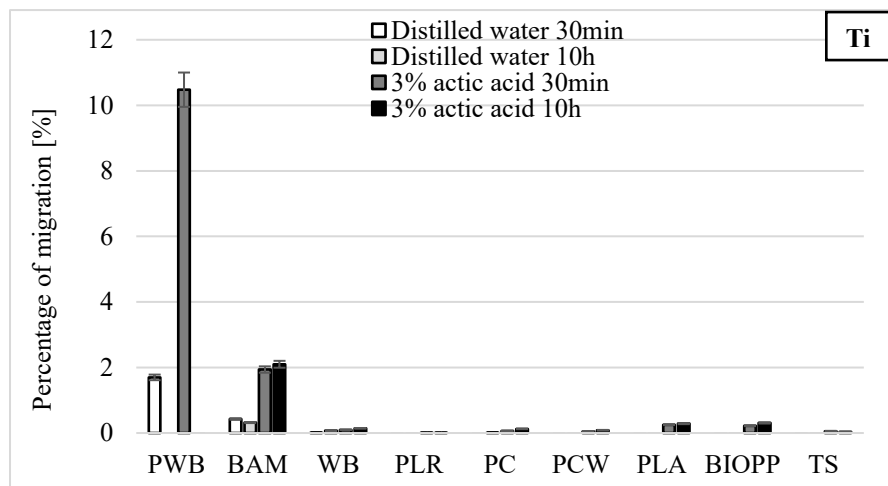
the environment (it is found in the earth's crust) and can be taken up from the environment by plants, especially from acidic soils. Al is often identified in drinking water, due to the widespread use of  $\text{Al}_2(\text{SO}_4)_3$  as a coagulant in physical particulate water purification processes (Stahl, Falk, Taschan, Boschek & Brunn, 2018).

Other elements (Ti, V, Mn, Co, Ni, Zn, Sr, Cd, Sb, Ba and Pb) accounted for about 1% of the content of all FCMs analyzed. The highest Ti content was recorded in TS (2362.8  $\mu\text{g/g}$  of material), which may be due to the use of titanium white ( $\text{TiO}_2$ ) in the manufacturing process.  $\text{TiO}_2$  is a natural inorganic compound and was considered a food additive (E171) - according to Annex II of Regulation (EC) No. 1333/2008. However, in 2022 EFSA issued a ban on the use of  $\text{TiO}_2$  in food, due to suspected genotoxic properties (Commission Regulation (EU) 2022/63; Dand, Bajaj & Wairkar, 2025). Although the direct addition of  $\text{TiO}_2$  to food as a colorant has been banned, its presence in FCMs can affect the quality of packaged foods, where  $\text{TiO}_2$  can enter as a result of FCM-food interactions. On the other hand, in plant-based FCMs, Ti may come from the growth environment, as a result of the cultivation treatments used. Pérez-Zavala et al. (2022) indicate that Ti and its compounds are used as fertilizers due to the improvement of crop yields, as a result of increased plant nutrient uptake and photosynthetic efficiency. This paradoxical effect (hormesis) is related to the positive effects of low doses of toxic elements on plants, which secrete increased amounts of organic acids and phytochelatin in response to the presence of the toxic agent. These compounds increase the availability of nutrients in the soil (such as P and Fe) and facilitate their uptake by the plant. However, plants can also readily accumulate Ti in their roots and stems, resulting in the presence of this element in plant-based FCMs. A hormetic effect was also observed when Zn was excessively added to two different wheat varieties (Chang et al., 2022).

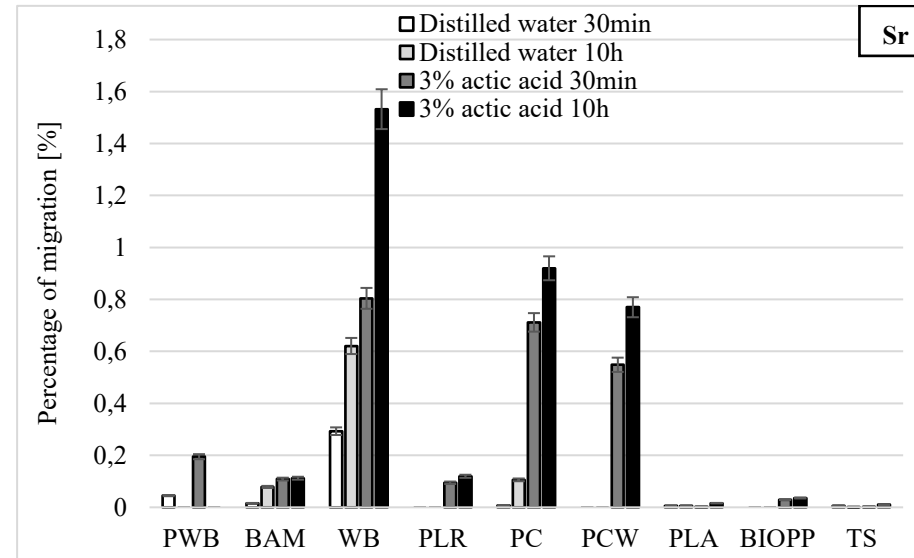
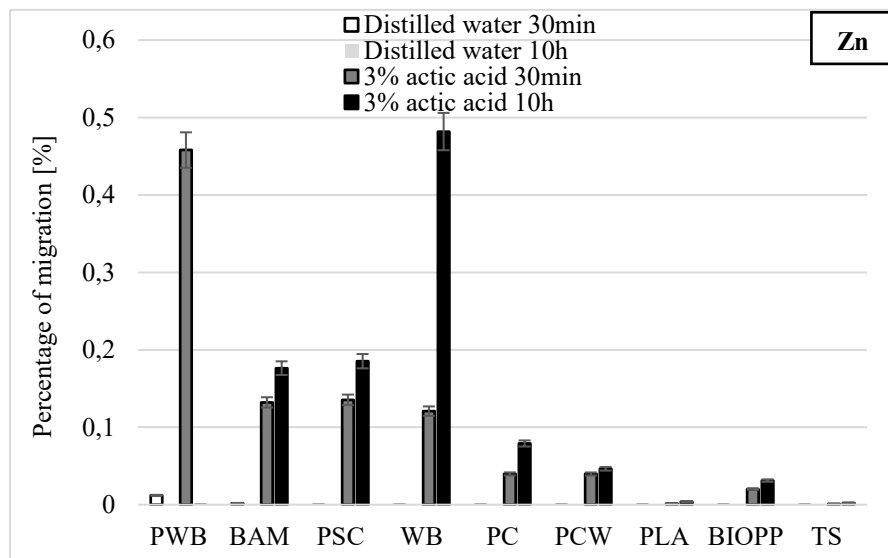
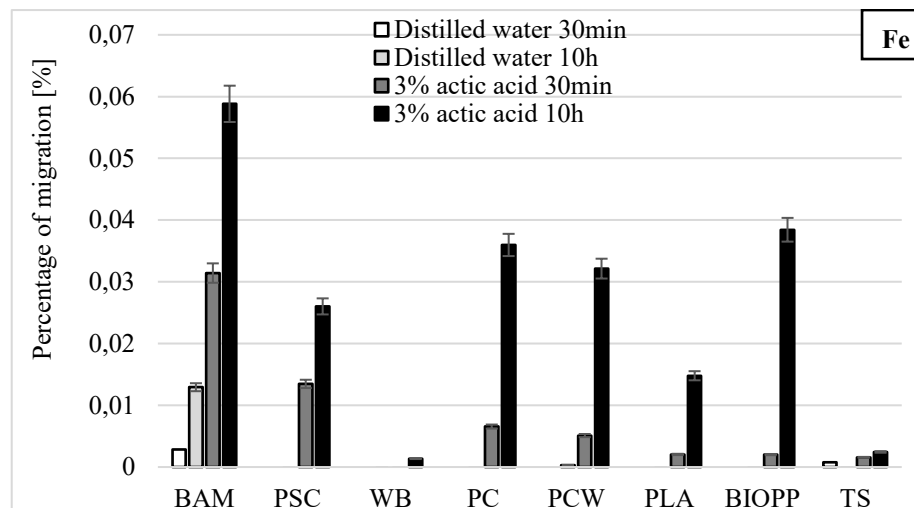
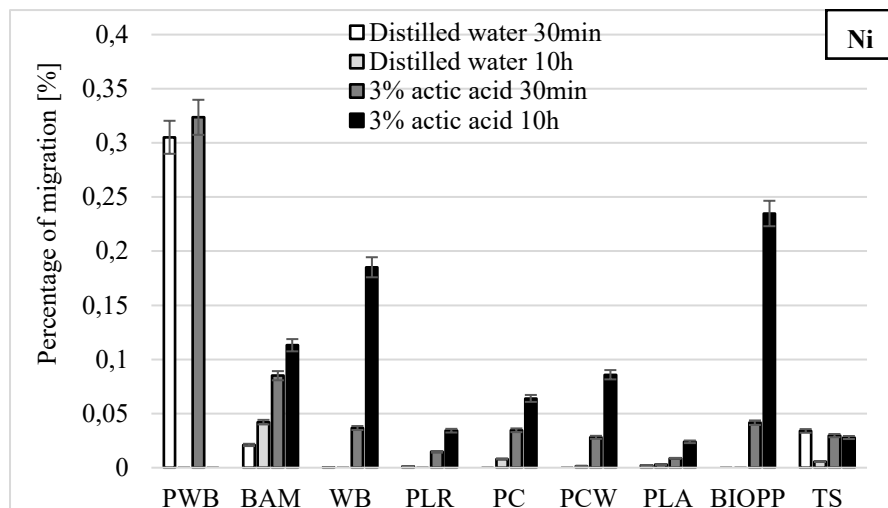
The presence of a numerous group of elements in FCMs means that they can migrate into food and affect its quality (Terbeche et al., 2022). For this purpose, it is necessary to check the migration level and concentrations of individual elements from FCMs into different foods (neutral and acidic), replaced by food simulants (distilled water and 3 % acetic acid). Distilled water can be used to replace 10% EtOH in studies on the migration of elements from FCMs, which facilitates the analytical procedure (Corona, Iglesias & Antico, 2014).

The percentage migration of individual elements from the analyzed FCMs to neutral (distilled water) or acidic (3 % acetic acid) food, after different contact times (30 min, 10 h) is presented in **Fig. 26**. Migration studies were conducted at elevated temperature (60°C), in accordance with the assumption that the intensity of element migration increases linearly with the increase in the temperature of contact of FCMs with food (Dong, Lu, Liu, Tang & Wang, 2014).









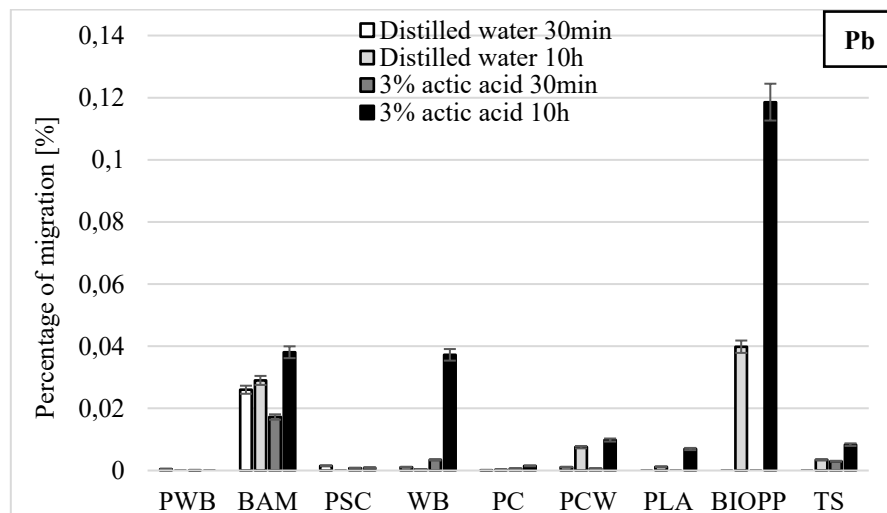
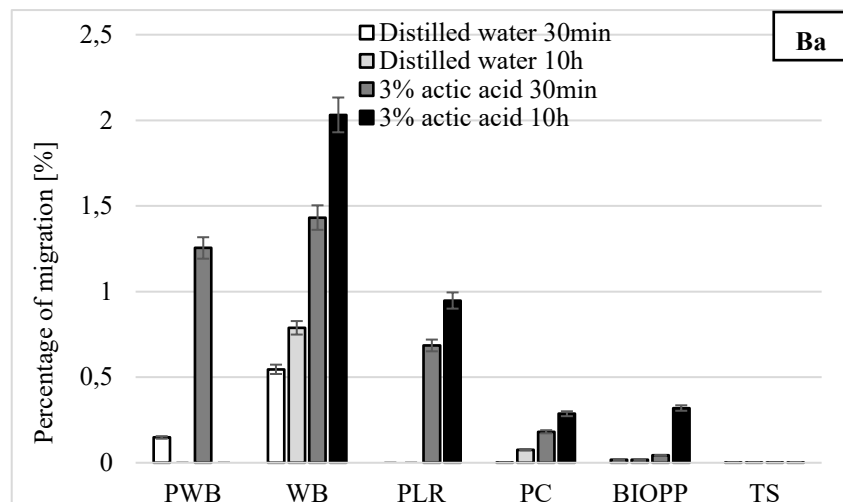
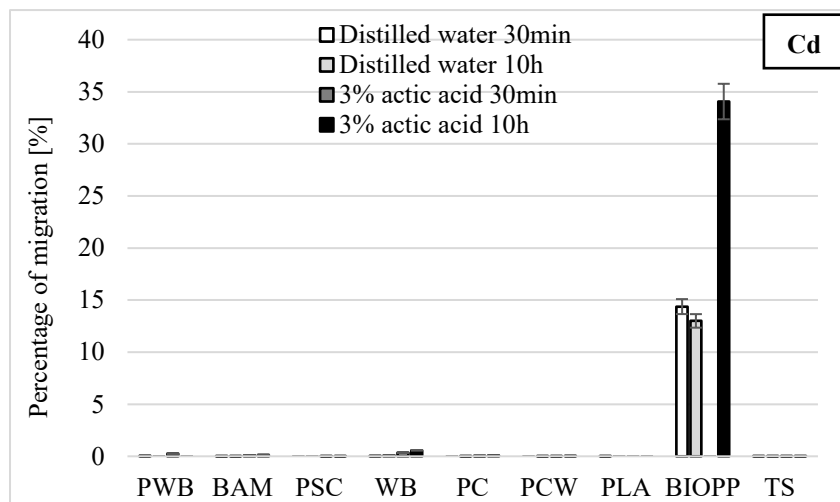


Fig. 26. The percentage migration of individual elements from the analyzed FCMs to neutral (distilled water) or acidic (3 % acetic acid) food, after different contact times (30 min, 10 h) at 60°C

The results presented in **Fig. 26** clearly show that the migration of most elements to neutral and acidic food does not exceed 1.5 % of the total content of elements in FCM. However, a high migration of Ti from PWB (> 10%) was observed, corresponding to the migration of Ti from PWB in the amount of 1.05 µg/g of neutral food and 7.66 µg/g of acidic food, respectively. Moreover, it is clearly seen that low pH of food promotes the migration of elements from FCM. These observations are in agreement with the observations of Ghuniem (2024), who analyzed thirty samples of plastic food packaging for the migration of metals, such as Al, As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Sb and Zn into distilled water, 2% HNO<sub>3</sub> and 3% acetic acid after different contact times of FCM with simulant (24h, 48h, 72h and 96h) at room temperature (23 ± 3°C). The author found that the intensity of element migration from FCM decreases in the sequence: 3% acetic acid > 2% HNO<sub>3</sub> > distilled water and increases up to 72 h of contact of FCM with simulant, after which it stabilizes. Similarly, Forooghi, Ahmadi, Farhoodi and Mortazavian (2022) studied the release kinetics of TiO<sub>2</sub> from laminated packaging for Doogh (famous Iranian drink) and observed a proportional relationship between the contact time and migration intensity of TiO<sub>2</sub> from FCMs to food, which was released even after 60 days of contact between FCMs and 3 % acetic acid.

In general, it was observed that Na, Mg, Ca, Ti, V, Mn, Zn, Sr and Ba are more easily released into food from plant-based FCMs than bio-based plastics FCMs. This is in accordance with Bouma et al. (2024), who included Al, Mn, Fe, Zn and Ba as the main elements migrating from plant-based FCMs. Al is most easily released from paper (PC and PCW), probably due to the printing inks and paints found on these FCMs. Sb is primarily released from bio-based plastics FCMs (e.g., PLA). Antimony trioxide (Sb<sub>2</sub>O<sub>3</sub>) is commonly used as a catalyst in the polycondensation step in polymer production. The recovery of this catalyst in the production process is not complete, which means that some Sb may be retained in the FCMs (Ozaki et al., 2022; Kiyataka, Dantas, Brito, Júnior & Pallone, 2025). Van-Trong, Truong, The-Ky, Quoc-Hung and Thanh-Khue (2023) identified Zn (8.38 %), Al (0.41 %) and Pb (0.19 %) as the main elements migrating from plastics to 3 % acetic acid after 30 min of contact at 60°C. The authors did not detect any migration of Co, As, Cd and Sb under these conditions. The remaining elements (Co, Ni, Fe, Pb) migrated to food in comparable amounts from plant-based FCM and plastic-based FCM.

Inorganic contaminants that have potential carcinogenic properties or other undesirable effects on human health have a particular impact on food quality. The comparison between concentration of elements determined in water or 3% acetic acid as migrants from FCMs in the worst contact condition (10h, 60°C) during migration studies and specific migration limit (SML) for elements is presented in **Table 15**. Based on the results obtained, it can be concluded that most FCMs meet the regulatory requirements for the migration of inorganic contaminants.

Table 15. Comparison between concentration of elements determined in water or 3% acetic acid as migrants from FCMs in the worst contact condition (10h, 60°C) during migration studies and specific migration limit (SML) for elements

FCMs	Food simulant	Elements											
		Al	Mn	Fe	Co	Ni	Cu	Zn	As	Cd	Sb	Ba	Pb
SML (µg/g of food)*		1.000 <sup>b</sup>	0.600 <sup>b</sup>	48.000 <sup>b</sup>	0.050 <sup>b</sup>	0.020 <sup>b</sup>	5.000 <sup>b</sup>	5.000 <sup>b</sup>	0.002 <sup>a</sup>	0.002 <sup>a</sup>	0.040 <sup>b</sup>	1.000 <sup>b</sup>	0.010 <sup>a</sup>
PWB**	Distilled water	0.048	1.903	<LOD	0.001	0.067	<LOD	0.255	<LOD	0.002	<LOD	0.071	0.002
	3 % acetic acid	0.101	22.282	7.610	0.002	0.084	<LOD	11.479	<LOD	0.011	<LOD	0.716	<LOD
BAM	Distilled water	0.032	0.027	0.070	<LOD	0.001	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.004
	3 % acetic acid	0.069	0.250	0.345	<LOD	0.003	<LOD	0.162	<LOD	<LOD	<LOD	<LOD	0.006
WB	Distilled water	0.001	0.018	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.022	<LOD
	3 % acetic acid	0.023	0.108	0.009	<LOD	0.002	<LOD	0.115	<LOD	0.001	<LOD	0.062	0.003
PLR	Distilled water	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
	3 % acetic acid	<LOD	0.015	0.072	<LOD	0.003	<LOD	0.363	<LOD	<LOD	<LOD	0.077	<LOD
PC	Distilled water	0.544	0.014	<LOD	<LOD	0.001	<LOD	<LOD	<LOD	<LOD	<LOD	0.017	0.001
	3 % acetic acid	22.084	0.345	2.016	0.001	0.005	0.014	0.098	<LOD	0.001	<LOD	0.048	0.003
PCW	Distilled water	0.566	0.001	0.011	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.003
	3 % acetic acid	15.630	0.105	1.069	0.001	0.005	0.003	0.018	<LOD	<LOD	<LOD	<LOD	0.004
PLA	Distilled water	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
	3 % acetic acid	<LOD	<LOD	0.023	<LOD	0.001	<LOD	0.002	<LOD	<LOD	<LOD	<LOD	0.001
BIOPP	Distilled water	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.001

	3 % acetic acid	0.029	<LOD	0.173	0.002	0.004	<LOD	0.003	<LOD	<LOD	<LOD	0.002	0.001
TS	Distilled water	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.001	0.001
	3 % acetic acid	<LOD	0.012	0.071	<LOD	0.001	0.008	0.008	<LOD	<LOD	<LOD	0.002	0.003

\*SML in according to Appendix II, Commission Regulations: <sup>a</sup>(EU) No 10/2011 and <sup>b</sup>(EU) No 2020/1245

\*\* the results of element migration tests after 30 minutes and 60 °C are presented for PWB sample

LOD for Al 0.0002573; Mn 0.0000178; Fe 0.0036472; Co 0.0000031; Ni 0.0000474; Cu 0.0000208; Zn 0.0000983; As 0.0000051; Cd 0.0000011; Sb 0.0000070;  
Ba 0.0000074; Pb 0.0000139 µg/g of food simulant, respectively.

However, it has been observed that paper FCMs can contaminate acidic food with Al at concentrations significantly exceeding the SML for this element (more than 22 µg/g of food can migrate from PC and more than 15 µg/g of food can migrate from PCW, respectively). Al is considered a neurotoxic agent that disrupts Ca and Fe metabolism in nervous tissue and can also alter neurotransmission, affecting the synthesis and transport of neurotransmitters (e.g., acetylcholine, serotonin, dopamine and others) (Huat et al., 2019; Przybysz et al., 2024). Some researchers presented that Al may be responsible for the development of Alzheimer's disease (Exley, 2017; Klotz et al., 2017) and respiratory tract and bladder cancers (IARC, 2012; McClure et al., 2020). The tolerable intake defined by EFSA is 1 mg aluminum/kg body weight/week for all groups of people. Assuming consumption of acidic food (250 g) by an average 70 kg person, in paper FCMs, it can be estimated that the weekly exposure to Al is 550 µg from PC and 375 µg from PCW, respectively. However, assuming an average child weight (15 kg), the weekly exposure is more than 2.5 mg from PC and 1.75 mg from PCW, respectively. Therefore, children and the elderly are particularly exposed to Al. Similarly, Zhang et al. (2022) conducted studies on Al migration from aluminum FCMs to 4 % acetic acid and 5 g/L citric acid and found that Al exposure could exceed the TDI in some cases and ranged from 0.65 to 51.21 mg/(kg body weight/week), depending on the FCM. Additionally, Stahl et al. (2017a) showed that regular consumption of 500 ml of tea or apple juice with aluminium FCMs can exceed the TDI for a 15 kg child and in another study (Stahl et al. (2017b)) observed that Al can migrate from aluminium FCMs to fish in acidic marinade at concentrations exceeding the TDI for adults by more than 180 % (assuming a meal weight of 250 g and a person weight of 70 kg). The same study noted that for a 15 kg child, the migrated Al value from this sample exceeded the weekly TDI by almost nine times. Furthermore, Windisch, Keppler and Jirsa (2020) compared the amount of migrated Al to coffee prepared in different FCMs, e.g., aluminum and steel. The authors found that the highest Al was released into coffee from aluminum FCMs. Additionally, they observed a higher concentration of Al in pure water prepared in aluminum FCMs than in coffee, which may be related to the sorption of contaminants by ground coffee beans. The authors estimated that daily consumption of 500 mL of coffee prepared in aluminum FCMs would provide less than 0.50 % of the weekly TDI for Al. In turn, Alabi and Adeoluwa (2021) showed a proportional relationship between the amount of Al released from FCMs into food and the duration of FCMs use and the quality of the internal coating of FCMs.

Moreover, high migration of Mn, Ni, Cd and Zn was observed from the PWB. 1.903 µg/g of food Mn, 0.067 µg/g of food Ni and 0.002 µg/g of food Cd can migrate to distilled water, while 22.282 µg/g of Mn food, 22.282 µg/g of food of food Ni, 0.011 µg/g of food of Cd and 11.479 µg/g of food of Zn can

migrate to 3 % acetic acid. All these values exceed the SMLs for Mn (0.600 µg/g), Ni (0.020 µg/g) and Cd (0.002 µg/g), respectively.

The high Mn content in PWB (9220 µg/g of FCMs) and the high migration of Mn into neutral and acidic foods may be due to the fact that Mn is one of the essential elements for plant growth and is involved in photosynthesis and seed germination (Li, Santos, Butler, Herndon, 2021). Mn accumulates mainly in leaves in the form of hydrated or organic Mn(II), which can be readily oxidized to insoluble Mn(III/IV) oxides, facilitating its accumulation in surface soils and thus its absorption by plants (Herndon, Martínez & Brantley, 2014). Consequently, Mn concentrations in plant leaves often exceed the nutrient requirements of the resulting in oxidative stress and impaired photosynthesis in various plant species. Moreover, Wang, Li, Zhang, Zhao and Dong, (2022) stated that the combined climate warming and drought stress may have unequal effects on the dynamic accumulation and distribution of i.e., Mn in wheat seedlings at different levels, which may ultimately threaten the food supply balance.

High Ni content in PWB (123.514 µg/g of FCM) was also recorded. Ni is a widespread element in plants, it is involved in signal transduction and catalyzes biochemical reactions at active sites of metalloenzymes (Yang & Ma, 2021). However, excess Ni can affect the activity of nonmetalloenzymes, resulting in oxidative stress. In addition, an important carcinogenic mechanism caused by Ni may be direct DNA binding and stimulation of reactive oxygen species (ROS), which leads to DNA damage (Guo et al., 2019). Ni may also be an estrogenic active factor that affects the hormonal balance.

In turn, Cd is considered one of the most toxic heavy metals in soil. The concentration of Cd in soil is on average 0.1-10 mg/kg. Anthropogenic activities have caused excessive release of Cd into the environment, including transport, industrial, mining and agricultural activities (Liang, Ye & Shi, 2024). In particular, the use of Cd found in phosphate rocks in the production of fertilizers has contributed to the widespread problem of Cd presence in soil (Adams, 2016). Moreover, Cd could be derived from natural sources in deep soil of conventional farmland (Jifu et al., 2022). As a result, Cd can be easily absorbed from the soil by plants (e.g., wheat) and accumulate in their tissues (Rizwan et al., 2016; Xiao et al., 2024). The appearance of Cd in particular in packaged/served food is an undesirable phenomenon, due to its small biological function and high problem with excretion from the human body. Even low concentrations of Cd in the body can negatively affect human fertility and increase the risk of osteoporosis - Cd can lead to bone decalcification, because it competes with Ca and blocks the action of vitamin D3. In addition, increased consumption and accumulation of Cd can increase the carcinogenic risk for susceptible organs, e.g., lungs and kidneys.

In addition, based on the obtained results (**Table 15**), it can also be concluded that the analyzed FCMs do not cause the migration of Sb and As to neutral and acidic food under the test conditions.

In order to determine the correlation of the element's migration from FCM to neutral and acidic food, a statistical analysis was performed – first, the selected variables were checked for normal distribution. As a result of the tests, it was found that they did not meet the conditions of normal distribution according to the Shapiro-Wilk and Kolmogorov-Smirnov criteria. Therefore, a nonparametric test was used - Spearman's R rank correlation. For this purpose, the analyzed FCMs were divided into two groups: plant-based FCMs (PWB, PLB, PSC, BAM, WB, PLR, PC, PCW) and bio-based plastics FCMs (PLA, BIOPP, TS, EPP, PPB,). The analysis carried out for all analyzed FCM groups showed a number of strong positive and negative relationships, at the significance level of  $p < 0.001$ ,  $p < 0.01$  and  $p < 0.05$  between the concentrations of individual elements (**Tables 16 I and 16 II**). In the case of all tested plant-based FCMs, strong positive correlations ( $p < 0.001$ ) were demonstrated, e.g., between Mg-Ti (distilled water, 30 min, 60°C); Mg-Ca (distilled water, 10 h, 60°C); Al-Mg (3% acetic acid, 30 min, 60°C), Ca-Sr (distilled water, 30 min, 10 h, 60°C), Ti-Sr (distilled water, 30min, 10 h, 60°C), Ti-Mn (3% acetic acid, 30 min, 60°C), V-Cr (3% acetic acid, 30min, 60st.), Mn-Cr (distilled water, 30 min, 60 °C), Cu-Zn-As (distilled water, 30 min, 10h, 60°C) and Cu-As (3 % acetic acid, 30 min, 10 h, 60°C). No strong negative correlations ( $p < 0.001$ ) were noted.

In turn, in the case of all tested bio-based plastics FCMs, no strong positive and negative correlations were noted at the significance level of  $p < 0.001$ , but positive correlations appeared at the significance level of  $p < 0.01$ , e.g., between Mg-Ti (distilled water, 30 min, 10 h, 60°C), Al-Ti (distilled water, 30 min, 10 h, 60°C), Ti-Mg-Al-Fe-Sr (distilled water, 30 min, 10 h, 60°C), Sr-Ti-Ba (distilled water, 30 min, 10 h, 60°C) and negative correlations, e.g., Cu-Cd (3 % acetic acid, 30 min, 10 h, 60°C).

**Table 16.** Spearman's R rank correlation analysis ((+) (-)) for the concentrations of individual elements migrating into neutral or acidic food from (I) plant-based FCMs and (II) bio-based plastics FCMs at different significance levels (<sup>a</sup> $p < 0.05$ ; <sup>b</sup> $p < 0.01$ ; <sup>c</sup> $p < 0.001$ )

I

Element	Migration studies condition	Distilled water	3 % acetic acid
Na	30 min, 60°C	(+)Cu <sup>a</sup> ,(+)Sb <sup>a</sup> ,(-)Cd <sup>a</sup>	(+)Cu <sup>a</sup> , (+)Sb <sup>a</sup> , (-)Cd <sup>a</sup>
	10 h, 60°C	(+)Cu <sup>a</sup> ,(+)Sb <sup>a</sup> ,(-)Cd <sup>a</sup>	(+)Cu <sup>a</sup> , (+)Sb <sup>a</sup> , (-)Cd <sup>a</sup>



Mg	30 min, 60°C	(+)Ti <sup>c</sup> , (+)Mn <sup>b</sup> , (+)Ni <sup>a</sup> , (-)As <sup>a</sup> (+)Cr <sup>b</sup>	(+)Ti <sup>b</sup> , (+)Mn <sup>a</sup> , (+)Ni <sup>a</sup> , (+)Zn <sup>b</sup> , (+)Fe <sup>a</sup> , (+)Cr <sup>a</sup>
	10 h, 60°C	(+)Ca <sup>c</sup> , (-)Zn <sup>a</sup> , (-)As <sup>a</sup>	(+)Ca <sup>a</sup> , (+)Fe <sup>b</sup>
Al	30 min, 60°C	-	(+)Mg <sup>c</sup> (+)Cu <sup>a</sup> , (+)Ca <sup>a</sup> , (+)Fe <sup>b</sup>
	10 h, 60°C	-	(+)Ca <sup>a</sup> , (+)Fe <sup>b</sup> , (+)Cu <sup>a</sup>
Ca	30 min, 60°C	(+)Sr <sup>c</sup> , (+)Co <sup>b</sup>	(+)Al <sup>a</sup>
	10 h, 60°C	(+)Sr <sup>c</sup> , (+)Mg <sup>a</sup> , (+)Co <sup>a</sup> , (-)As <sup>a</sup>	(+)Mg <sup>a</sup> , (+)Al <sup>a</sup> , (-)As <sup>a</sup>
Ti	30 min, 60°C	(+)Mn <sup>b</sup> , (+)Sr <sup>c</sup>	(+)Mg <sup>b</sup> , (+)Mn <sup>c</sup> , (+)Ni <sup>a</sup> , (+)Zn <sup>a</sup>
	10 h, 60°C	(+)Sr <sup>c</sup>	-
V	30 min, 60°C	-	(+)Cr <sup>c</sup>
	10 h, 60°C	-	(+)Cr <sup>c</sup>
Mn	30 min, 60°C	(+)Mg <sup>b</sup> , (+)Ti <sup>b</sup> , (+)Co <sup>b</sup> , (+)Ni <sup>b</sup> , (+)Zn <sup>b</sup> , (+)Cd <sup>a</sup> , (+)Cr <sup>c</sup> (-)As <sup>a</sup>	(+)Mg <sup>a</sup> , (+)Ti <sup>c</sup> , (+)Ni <sup>b</sup> , (+)Zn <sup>a</sup> , (-)As <sup>a</sup>
	10 h, 60°C	(+)Co <sup>b</sup> , (+)Cr <sup>a</sup> , (-)As <sup>a</sup>	(-)As <sup>a</sup>
Fe	30 min, 60°C	(+)Ni <sup>b</sup>	(+)Mg <sup>a</sup> , (+)Ni <sup>a</sup>
	10 h, 60°C	(+)Ni <sup>b</sup> , (+)Pb <sup>a</sup>	(+)Mg <sup>b</sup>
Co	30 min, 60°C	(+)Ca <sup>b</sup> , (+)Mn <sup>b</sup> , (+)Sr <sup>b</sup> , (+)Cd <sup>b</sup> , (+)Ba <sup>a</sup> , (-)As <sup>a</sup>	(-)As <sup>a</sup> , (-)Sb <sup>a</sup> ,
	10 h, 60°C	(+)Ca <sup>a</sup> , (+)Mn <sup>b</sup> , (+)Sr <sup>b</sup> , (+)Cd <sup>b</sup> , (+)Ba <sup>a</sup> , (-)As <sup>a</sup>	(-)As <sup>a</sup> , (-)Sb <sup>a</sup>
Ni	30 min, 60°C	(+)Mn <sup>b</sup> , (+)Fe <sup>b</sup> (+)Pb <sup>b</sup>	(+)Mg <sup>a</sup> , (+)Ti <sup>a</sup> , (+)Mn <sup>b</sup> , (+)Fe <sup>a</sup> , (+)Zn <sup>a</sup> , (+)Cr <sup>b</sup>
	10 h, 60°C	(+)Fe <sup>b</sup> , (+)Pb <sup>a</sup> ,	-
Cu	30 min, 60°C	(+)Zn <sup>c</sup> (+)As <sup>c</sup> ,	(+)Al <sup>a</sup> , (+)As <sup>c</sup>
	10 h, 60°C	(+)Zn <sup>c</sup> , (+)As <sup>c</sup> ,	(+)Al <sup>a</sup> , (+)As <sup>c</sup>
Zn	30 min, 60°C	(+)Ti <sup>c</sup> , (+)Mn <sup>b</sup> , (+)Cu <sup>c</sup> . (+) Ni <sup>c</sup> , (+)As <sup>c</sup>	(+)Ti <sup>a</sup> , (+)Mn <sup>a</sup> , (+)Ni <sup>a</sup> , (+)As <sup>c</sup>
	10 h, 60°C	(+)Cu <sup>c</sup> , (+)As <sup>c</sup>	(+)As <sup>c</sup>

As	30 min, 60°C	(-)Mg <sup>a</sup> , (-)Co <sup>a</sup> , <b>(+)Cu<sup>c</sup></b> , (+)Sb <sup>b</sup> ,	(-)Mn <sup>a</sup> , (-)Co <sup>a</sup> , <b>(+)Cu<sup>c</sup></b> , <b>(+)Sb<sup>c</sup></b>
	10 h, 60°C	(-)Mg <sup>a</sup> , (-)Ca <sup>a</sup> , (-)Mn <sup>a</sup> , (-)Co <sup>a</sup> , <b>(+)Cu<sup>c</sup></b> , (+)Sb <sup>b</sup> ,	(-)Ca <sup>a</sup> , (-)Mn <sup>a</sup> , (-)Co <sup>a</sup> , <b>(+)Cu<sup>c</sup></b> , (+)Sb <sup>b</sup> ,
Sr	30 min, 60°C	<b>(+)Ti<sup>c</sup></b> , (+)Co <sup>b</sup> , (+)Cd <sup>a</sup> ,	-
	10 h, 60°C	<b>(+)Ti<sup>c</sup></b> , (+)Co <sup>b</sup> , (+)Cd <sup>a</sup> , <b>(+)Ba<sup>c</sup></b>	-
Cd	30 min, 60°C	(-)Na <sup>a</sup> , (+)Mn <sup>a</sup> , (+)Co <sup>b</sup> , (+)Sr <sup>a</sup>	(-)Na <sup>a</sup>
	10 h, 60°C	(-)Na <sup>a</sup> , (+)Co <sup>b</sup> , (+)Sr <sup>a</sup>	(-)Na <sup>a</sup>
Sb	30 min, 60°C	(+)Na <sup>a</sup> , (+)As <sup>b</sup>	(+)Na <sup>a</sup> , (-)Co <sup>a</sup> , <b>(+)As<sup>c</sup></b>
	10 h, 60°C	(+)Na <sup>a</sup> , (+)As <sup>b</sup>	(+)Na <sup>a</sup> , (-)Co <sup>a</sup> , (+)As <sup>b</sup> ,
Ba	30 min, 60°C	(+)Co <sup>a</sup>	-
	10 h, 60°C	(+)Co <sup>a</sup> , <b>(+)Sr<sup>c</sup></b>	-
Pb	30 min, 60°C	(+)Ni <sup>b</sup>	-
	10 h, 60°C	(+)Fe <sup>a</sup> , (+)Ni <sup>a</sup> ,	-
Cr	30 min, 60°C	<b>(+)Mn<sup>c</sup></b> , <b>(+)Ni<sup>c</sup></b>	<b>(+)V<sup>c</sup></b> , (+)Ni <sup>b</sup>
	10 h, 60°C	(+)Mn <sup>a</sup> ,	<b>(+)V<sup>c</sup></b>

## II

Element	Migration studies condition	Distilled water	3 % acetic acid
Mg	30 min, 60°C	(+)Ba <sup>a</sup> , <b>(+)Ti<sup>b</sup></b>	(+)Al <sup>a</sup>
	10 h, 60°C	(+)Ba <sup>a</sup> , <b>(+)Ti<sup>b</sup></b>	(+)Al <sup>a</sup>
Al	30 min, 60°C	<b>(+)Ti<sup>b</sup></b> , (+)Ba <sup>a</sup> , (+)Mn <sup>a</sup>	(+)Mg <sup>a</sup> , (+)Ba <sup>a</sup> , (+)Mn <sup>a</sup>
	10 h, 60°C	<b>(+)Ti<sup>b</sup></b> , (+)Ba <sup>a</sup> , (+)Mn <sup>a</sup> ,	(+)Mg <sup>a</sup> , (+)Mn <sup>a</sup> , (+)Ba <sup>a</sup>
Ca	30 min, 60°C	-	(-)Sb <sup>a</sup>
	10 h, 60°C	-	(-)Sb <sup>a</sup>
Ti	30 min, 60°C	<b>(+)Mg<sup>b</sup></b> , <b>(+)Al<sup>b</sup></b> , <b>(+)Fe<sup>b</sup></b> , <b>(+)Sr<sup>b</sup></b> , (+)Ba <sup>a</sup>	(+)Cr <sup>a</sup>
	10 h, 60°C	<b>(+)Mg<sup>b</sup></b> , <b>(+)Al<sup>b</sup></b> , <b>(+)Fe<sup>b</sup></b> , <b>(+)Sr<sup>b</sup></b> , (+)Ba <sup>a</sup>	(+)Sr <sup>a</sup> , (+)Cr <sup>a</sup>

V	30 min, 60°C	(+)Ba <sup>a</sup>	-
	10 h, 60°C	(+)Ba <sup>a</sup>	-
Mn	30 min, 60°C	(+)Al <sup>a</sup> , (+)Cr <sup>a</sup>	(+)Al <sup>a</sup>
	10 h, 60°C	(+)Al <sup>a</sup> , (+)Cr <sup>a</sup>	(+)Al <sup>a</sup>
Fe	30 min, 60°C	<b>(+)Ti<sup>b</sup></b> , (+)Ba <sup>a</sup>	(-)Cr <sup>a</sup>
	10 h, 60°C	<b>(+)Ti<sup>b</sup></b> , (+)Ba <sup>a</sup>	(-)Cr <sup>a</sup>
Co	30 min, 60°C	-	(-)Sb <sup>a</sup>
	10 h, 60°C	-	(-)Sb <sup>a</sup>
Cu	30 min, 60°C	(+)Ba <sup>a</sup>	<b>(-)Cd<sup>b</sup></b>
	10 h, 60°C	(+)Ba <sup>a</sup>	<b>(-)Cd<sup>b</sup></b>
Sr	30 min, 60°C	(+)Ba <sup>a</sup>	(+)Cr <sup>a</sup>
	10 h, 60°C	<b>(+)Ti<sup>b</sup>, (+)Ba<sup>b</sup></b> , (+)Cr <sup>a</sup>	(+)Ti <sup>a</sup> , (+)Cr <sup>a</sup>
Sb	30 min, 60°C	(+)Cd <sup>a</sup>	(-)Ca <sup>a</sup> , (-)Co <sup>a</sup>
	10 h, 60°C	-	(-)Ca <sup>a</sup> , (-)Co <sup>a</sup>
Ba	30 min, 60°C	(+)Mg <sup>a</sup> , (+)Al <sup>a</sup> , (+)Ti <sup>a</sup> , (+)V <sup>a</sup> , (+)Cu <sup>a</sup> , (+)Fe <sup>a</sup> , (+)Sr <sup>a</sup>	(+)Al <sup>a</sup>
	10 h, 60°C	(+)Mg <sup>a</sup> , (+)Al <sup>a</sup> , (+)Ti <sup>a</sup> , (+)V <sup>a</sup> , (+)Fe <sup>a</sup> , (+)Cu <sup>a</sup> , <b>(+)Sr<sup>b</sup></b>	(+)Al <sup>a</sup>
Cr	30 min, 60°C	(+)Mn <sup>a</sup> ,	(+)Ti <sup>a</sup> , (+)Sr <sup>a</sup> , (-)Fe <sup>a</sup>
	10 h, 60°C	(+)Mn <sup>a</sup> ,	(+)Ti <sup>a</sup> , (+)Sr <sup>a</sup> , (-)Fe <sup>a</sup>

## 6. Summary and conclusions

In summary, the migration studies presented in the doctoral thesis constitute a comprehensive characterization of interactions occurring between FCMs and food of various nature. Plant-based FCMs and bio-based plastic FCMs can be a source of migration of odor-active compounds and organic and inorganic contaminants exhibiting toxic properties to food. Some FCMs (especially wheat bran, palm leaves, wood, paper) can change the sensory profile of roasted black coffee and green tea and the compounds responsible for the identified and perceptible changes include saturated and unsaturated carbonyl compounds. Migration studies have clearly shown that carbonyl compounds can be treated as markers of FCM-food interactions, because monitoring their concentration levels in simulants allowed to determine a number of factors determining the intensity of migration processes. These include: the type of FCMs, food pH, contact time and temperature, refrigerator storage time and microwave heating time. In addition, migration studies have shown that Tenax (as a simulant) can lead to falsely elevated results of migrating contaminant concentrations in relation to real food (e.g., milk powder, infant porridge, oat flakes), which may be due to the influence of food components (e.g., fat) and physicochemical properties of migrating particles on the intensity of migration processes. Furthermore, some plant-based FCMs can contaminate food with elements (e.g., Mn, Ni, Cd, Zn) in concentrations exceeding the SML. It has also been reported that paper FCMs can be a source of migration of high concentrations of Al to food. Pearson correlation analysis showed a number of strong positive and negative relationships, at the significance level of  $p < 0.001$ ,  $p < 0.01$  and  $p < 0.05$  between the concentrations of individual elements migrating to neutral/acidic food from plant-based FCMs and bio-based plastic FCMs.

Based on the above conclusions, it can be stated that the main theses of the doctoral dissertation have been confirmed. The presented results provide a basis for better knowledge and understanding of the characteristics of interactions between new FCMs and food and the environment. Plant-based FCMs can be especially a link in the chain of movement of toxic organic and inorganic contaminants between the environment and humans. Research conducted by EFSA (European Food Safety Authority) emphasizes the need for scientific support in assessing the safety of food chain innovations and sustainable food systems. Research conducted as part of the dissertation can play a key role in the development of safety regulations for packaged/served foods by identifying risks, improving assessment methods, and supporting innovation. In addition, research helps improve methods for evaluating the socioeconomic impacts of regulations, ensuring their efficiency and effectiveness. These research findings can help policymakers create regulations that protect public health with a balanced approach to meeting industry needs.

An important and urgent challenge in food safety assessment is also the search for and development of rapid, screening methods to estimate the safety of various materials commonly used as FCMs. In this approach, low-cost, commercially available electrochemical sensors to monitor the levels of contaminants released from FCMs may be a promising solution. I am currently conducting research within the National Science Centre project Preludium 23 “Fast method for pre-testing the safety of new ecological materials used for food packaging” (2024/53/N/ST4/02325), which focuses on the multi-stage calibration process of electrochemical sensor readings based on reference chromatographic methods. The research goals included in the Preludium project are a continuation of the research and discussions presented in this doctoral dissertation.

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## 10. Scientific achievements

### Publications:

**Bronczyk, K.,** Dabrowska, A. & Majcher, M. (2023). Carbonyl compounds as contaminants migrating from the ecological vessels to food. *Food Packag. Shelf Life*, 39, Article 101139. <https://doi.org/10.1016/j.fpsl.2023.101139>

**Brończyk, K.,** Dąbrowska, A. & Dąbrowski, A. (2023). Wykorzystanie detekcji wychwytu elektronów do badania migracji związków karbonylowych z naczyń ekologicznych do żywności., *Elektronika - konstrukcje, technologie, zastosowania*. Nr 10. <https://doi.org/10.15199/13.2023.10.4>

Konieczka, A., **Brończyk, K.,** Adamski, M., Dąbrowska, A. & Dąbrowski, A. (2024). Urządzenie do szybkiego oznaczania formaldehydu uwalnianego z naczyń ekologicznych do żywności. *Przegląd Elektrotechniczny*, 10, 199-203. <https://doi.org/10.15199/48.2024.10.40>.

Konieczka, A., **Brończyk, K.,** Dąbrowska, A. & Dąbrowski, A. (2025). Electrochemical determination of volatile markers of bio-based plastics contaminants. *Metrol. Meas. Syst.*, 32. <https://doi.org/10.24425/mms.2025.154335>.

**Bronczyk, K.,** Dąbrowska, A., Bielicka-Daszkiwicz, K. & Milczewska, K. (2025). Safety of new food contact materials: migration and sorption studies based on Tenax, powdered milk, baby cereal and oat flakes. *Food Chem.*, Article 144148. <https://doi.org/10.1016/j.foodchem.2025.144148>.

Konieczka, A., **Brończyk, K.,** Dąbrowska, A. & Dąbrowski, A. (2025). Correlation coefficients of electrochemical sensor readings in food contact materials control. (in review)

**Brończyk, K.,** Konieczka, A., Dąbrowska, A. & Dąbrowski, A. (2025). The role of electrochemical sensors in assessing the safety of plant-based vessels. (in review)

### Conference materials:

**Brończyk, K.,** Adamski, M., Dąbrowska, A., Konieczka, A. & Dąbrowski, A. (2023). Two approaches (GC-ECD and electrochemical sensors signals processing) to the determination of carbonyl compounds as markers of air pollution. SPA 2023 Signal Processing: Algorithms, Architectures, Arrangements, and Applications, Conference Proceedings, Poznan, 20<sup>th</sup>-22<sup>nd</sup> September 2023/IEEE, 2023, pp. 66-70. <https://doi.org/10.23919/SPA59660.2023.10274453>.

**Brończyk, K. & Dąbrowska, A. (2023).** Problem migracji niebezpiecznych związków chemicznych z ekologicznych materiałów do żywności suchej i mrożonej. *Na pograniczu chemii, biologii i fizyki - rozwój nauk. Tom 5. Kopernikańskie Seminarium Doktoranckie*, ISBN 978-83-231-5259-0, str. 39-56, <https://doi.org/10.12775/978-83-231-5260-6>.

**Brończyk, K., Adamski, M., Dąbrowska, A., Konieczka, A. & Dąbrowski, A. (2024).** Accuracy and cross-sensitivity analysis of the PMS5003 formaldehyde sensor. SPA 2024 Signal Processing: Algorithms, Architectures, Arrangements, and Applications, Conference Proceedings, Poznan, 25<sup>th</sup>-27<sup>th</sup> September 2024/IEEE, 2023, pp. 200-204. <https://doi.org/10.23919/SPA61993.2024.10715610>.

**Brończyk, K., Adamski, M., Dąbrowska, A., Konieczka, A. & Dąbrowski, A. (2024).** Electrochemical determination of pollutants from various passenger car engines. SPA 2024 Signal Processing: Algorithms, Architectures, Arrangements, and Applications, Conference Proceedings, Poznan, 25<sup>th</sup>-27<sup>th</sup> September 2024/IEEE, 2023, pp. 194-199. <https://doi.org/10.23919/SPA61993.2024.10715606>.

## Lectures and presentations

**2021**, oral presentation entitled: *“Aldehydes as an example of compounds entering food products from packaging.”* at the national conference 25th National Symposium of the Scientific Circle of Chemists;

**2022**, oral presentation entitled: *“Sophisticated analytical method for analysis of aldehydes in environmental waters”* at the international conference ACS Spring 2022;

**2022**, oral presentation entitled: *“Qualitative and quantitative determination of low molecular weight volatile carbonyl compounds as contaminants migrating from the surface of biovessels into model fluids using GC-ECD”* at the international conference Challenges in food flavor and volatile compounds analysis;

**2023**, oral presentation entitled: *“The impact of eco-materials on the quality and sensory profile of food”* at the national conference 28th National Symposium of the Scientific Circle of Chemists;

**2023**, oral presentation entitled: *“The influence of electromagnetic microwaves on the migration of undesirable compounds into food”* at the national conference 22nd National Electronics Conference;

**2023**, oral presentation entitled: *“Using electron capture detection to study the migration of carbonyl compounds from ecological vessels to food”* at the national conference 22nd National Electronics Conference;

**2023**, oral presentation entitled: *“The problem of migration of dangerous chemical compounds from ecological materials to dry and frozen food”* at the national conference 16th Copernicus Doctoral Seminar;

**2023**, oral presentation entitled: *“Two approaches (GC-ECD and electrochemical sensors signals processing) to the determination of carbonyl compounds as markers of air pollution”* at the international conference 26th Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA);

**2024**, presentation of a poster entitled: *“Migration of chemical compounds and toxic elements from vessels to food of various nature”* at the national conference 4th National Conference of Doctoral Students of Exact and Natural Sciences “Bio-Idea 4.0”;

**2024**, oral presentation entitled: *“Testing of inorganic and organic contaminants migrating from ecological vessels into food”* at the national conference 9th Chemometrics and Metrology in Analytics;

**2024**, presentation of a poster entitled: *“A device for quick determination of formaldehyde released from ecological vessels into food”* at the national conference 23rd National Electronics Conference;

**2024**, presentation of a poster entitled: *“Electrochemical determination of a volatile marker of bioplastic contamination. at the national conference 23rd National Electronics Conference.*

**2024**, presentation of a poster entitled: *“The influence of plant-based materials on the quality and sensory profile of food”* at the national conference 66th Congress of the Polish Chemical Society

**2024**, oral presentation entitled: *“Accuracy and cross-sensitivity analysis of the PMS5003 formaldehyde sensor”* at the international conference 27th Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA);

**2024**, oral presentation entitled: *“Electrochemical determination of pollutants from various passenger car engines”* at the international conference 27th Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA);

**2024**, oral presentation entitled: *“Environmental protection for young people challenge”* at the meeting of IEEE Poland Section LMAG.

## Prizes and awards

**2021-2022**, Laureate of the “European PhD in Flavor Research Awards” organized by Giract S.à.r.l., Geneva, Switzerland (contractor). Title of the awarded project: *“Migration of chemical compounds in contemporary food vessels - characteristics and main causes”*;

**2023**, Honorable mention in the “Young Scientists” competition at the national conference 22nd National Electronics Conference. Title of the awarded presentation: *“Using electron capture detection to study the migration of carbonyl compounds from ecological vessels to food”*;

**2023**, second place in the competition for The Best Scientific Communication in the section of Chemical Sciences presented at the national conference 16th Copernicus Doctoral Seminar. Title of the awarded presentation: *“The problem of migration of dangerous chemical compounds from ecological materials to dry and frozen food”*;

**2023-2024**, Laureate of IDUB competition #102 “Minigranty doktoranckie” (Contractor). Title of the awarded project: *“Research on the migration of undesirable chemical compounds from ecological vessels to various types of food”* (No. 102/13/SNŚ/0014);

**2023**; distinction of the article “Carbonyl compounds as contaminants migrating from the ecological vessels to food.” published in Food Packag. Shelf Life in IDUB competition #111 “Wsparcie publikowania w prestiżowych czasopismach naukowych.”;

**2024**, Honorable mention in the “Young Scientists” competition at the national conference 23rd National Electronics Conference. Title of the awarded presentation: *“A device for quick determination of formaldehyde released from ecological vessels into food”*;

**2025-2027**, Project Investigator of the Preludium 23 grant *“Fast method for pre-testing the safety of new ecological materials used for food packaging”* organized by the National Science Centre (No. 2024/53/N/ST4/02325);

**2025**, Laureate of IDUB competition #158 “Badania doktoranckie - badania oraz szkolenia i warsztaty międzynarodowe” (Contractor). Title of the awarded project: *“Estimation of environmental contamination by chemicals of concern (CECs) in Poznań using wastewater-based epidemiology (WBE)”* (No. 158/13/UAM/0048).

**2025**, Laureate of IDUB competition #166 “Open access”. (No. 166/08/POB3/0004).

## Domestic and foreign research internships

**2023, Poland**, Faculty of Chemical Technology, Poznań University of Technology, Research Internship. As part of the research internship, the specific surface area of Tenax, a commonly used food simulant, was characterized (BET isotherm). The intensity of the adsorption-desorption processes of pollutants to Tenax and real food (wheat bran, milk powder, porridge) was compared. Studies were also carried out on the migration of various pollutants (e.g., bisphenols, benzophenones and carbonyl compounds) from various ecological vessels to Tenax;

**2023, Poland**, Faculty of Control, Robotics and Electrical Engineering, Poznań University of Technology, Research Internship. As part of the research internship, preliminary interdisciplinary research was carried out related to the use of electronic devices for rapid analysis of the quality of food packaging and vessels;

**2025, Great Britain**, Faculty of Chemistry, University of Bath. The main issue of research intership was estimation of environmental contamination by chemicals of concern (CECs) using wastewater-based epidemiology (WBE). CECs identified in wastewater may indicate the degree of environmental contamination and can be used as markers in research.

## Other achievements

**2022-2023**, Member of the Scholarship Committee for Doctoral Students, Doctoral School of Science, UAM, Poznan;

**2022**, Member of the Conference Organizing Committee (Challenges in food flavor and volatile compounds analysis);

**2023**, Active participation in the 26th Poznań Festival of Science and Art. Delivering a lecture and leading a workshop entitled: *“Let's protect the environment from littering with plastic, let's learn more about dishes made of ecological materials”*;

**2023**, Member of the Conference Organizing Committee (26th Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA));

**2024**, Member of the Conference Organizing Committee (9th Chemometrics and Metrology in Analytics);

**2024**, participant of *“Workshops on the principles of using metrology in chemical measurements”* (organized as part of the 9th Chemometrics and Metrology in Analytics conference);

**2024-2025**, Teaching postgraduate students *“Calibration curve and detector response factor in gas chromatography”*;

**2024**, Active participation in the 27th Poznań Festival of Science and Art. Delivering a lecture with a demonstration entitled: *“The use of artificial intelligence (AI) in monitoring environmental pollution”*;

**2024**, Member of the Service of the 66th Congress of the Polish Chemical Society;

**2024**, Member of the Conference Organizing Committee (27th Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA));

**2024-2025**, Member of the Scholarship Committee for Doctoral Students, Doctoral School of Science, UAM, Poznań.