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Lecture Proceedings

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THE ROLE OF CELLULAR REDUCING AGENTS IN THE PROTECTION OF ZINC FINGER PROTEINS AGAINST TOXIC METAL IONS

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In recent years, there has been an increasing use of silver in medicine, especially in the form of silver nanoparticles (AgNPs), which is strengthened by the antimicrobial effect of Ag(I) ions. Today 30% of nanoparticulate products contain AgNPs. Not only medical devices or bone implants, but also products for everyday use, including cosmetics, bedding, sportswear, protective equipment and food containers, are coated with AgNP for their antibacterial properties [1]. The rapid spread of these coatings increases the environment's and also the population's exposure to Ag(I) ions. However, AgNPs and the Ag(I) ions they release intracellularly can also be toxic. The intracellular dissolution of AgNP is followed by the mass formation of Ag-S bonds, therefore thiol groups in proteins have been identified as cellular targets of Ag(I) ions. Similarly, Hg(II) is an extremely toxic metal ion mostly attributed to its interaction with S-donor atoms of biomolecules, thereby altering their structure. In cell culture experiments, inhibition of zinc finger proteins (ZFPs) has been identified as one of the mechanisms of toxicity of these metal ions [2].

The zinc finger (ZF) motifs of ZFPs are responsible for molecular recognition. The structure of the ZF motif is stabilized by the tetrahedral coordination of Zn(II) and the formation of a hydrophobic core. A ZFP can specifically recognize its target sequence in the DNA molecule only if Zn(II) coordinates to the protein and stabilizes its secondary structure. Therefore, potential competition with foreign metal ions may change the DNA-binding property of ZFPs and their original function [3].

At the same time, cysteine-containing peptides or proteins present in the cells may prevent the binding of these metal ions to the ZF motifs through competition due to their high affinity toward the toxic metal ions with a soft character. In our research project, the effect such molecules was investigated. The main goal of this research was to quantify the metal ion interaction with an artificial Cys2His2-type zinc finger protein (1MEY#) in the absence and presence of DNA. We also monitored the DNA recognition ability of 1MEY# in the absence and presence of interfering agents. The results to be presented are promising and suggest that the intracellular environment is well equipped for the defence of the cell against such toxic heavy metal ions.

Acknowledgements

This research work was supported by the bilateral cooperation project of the Polish and Hungarian Academy of Sciences (NKM2023-38). It was also supported by the National Research, Development and Innovation Fund (No.: 150330).

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PRELIMINARY STUDIES ON A NEW SCHIFF BASE AND ITS COPPER(II) COMPLEX: SYNTHESIS, CHARACTERIZATION, AND SINGLE CRYSTAL X-RAY STRUCTURES

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Thiophene-based Schiff bases and their metal complexes have recently attracted considerable interest as potential antimicrobial and anticancer agents, owing to their significant biological activities. [1] Notably, metal complexes often display enhanced efficacy compared to the free ligands. This improvement is attributed to chelation, which lowers the polarity of the metal ion, facilitates membrane penetration, and interferes with microbial enzymatic functions. [2]

In this work, we describe the synthesis of a new thiophene-derived Schiff base ligand, ethyl (E)-2-((2-hydroxy-3-methoxybenzylidene)amino)-6-methyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (HL), together with its copper(II) complex. The compounds were characterized using a combination of spectroscopic methods, including ¹H NMR, FT-IR, UV–Vis, and single-crystal X-ray diffraction. Crystallographic analysis revealed that the ligand crystallizes in the orthorhombic space group and forms an intramolecular hydrogen bond between the phenolic oxygen and the imino nitrogen.

The copper(II) complex features a binuclear unit, [Cu₂LCl₄H₂O]·1.5H₂O, in the asymmetric unit of the crystal lattice. One copper center adopts a distorted square-pyramidal geometry, with the basal plane defined by a tridentate NOO donor set and a coordinated water molecule, while a bridging chloride ion occupies the apical position, linking two Cu(II) centers. The second copper atom is coordinated in a distorted tetrahedral fashion by four chloride ligands. Further studies will be conducted to assess the potential biological properties of the ligand and copper(II) complex.

Acknowledgement

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A NEW APPROACH IN OBTAINING LUMINESCENT ORDERED HYBRID SYSTEMS USING METALLOMESOGENS AND CARBON-BASED MATERIALS

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Abstract

Nowadays, the interest into luminescent hybrid liquid crystalline systems has increased significantly due to their unique properties as electro-optic active materials arising from the combination of the molecular and supramolecular order of liquid crystals (LC) with the emissive properties of carbon-based materials (CDs). Currently, this research area is limited to organic liquid crystals, although the use of liquid crystalline coordination complexes (metallomesogens) would bring additional properties induced by the presence of the metal ion (redox, magnetic, etc.), increasing their applicability. In this respect, our group recently reported the first hybrid materials containing metallomesogens and carbon-based nanomaterials designed for non-enzymatic electrochemical detection of various analytes [1-3].

Herein, two new series of hybrid materials based on room-temperature luminescent/non-luminescent metallomesogens (Zn_MM and Cu_MM, respectively) and optical-active polymeric carbon dots are described. The hybrid systems are obtained by ultrasonically mixing of the counterparts in different weight ratios and studied for their mesomorphic properties by polarized optical microscopy (POM) and differential scanning calorimetry (DSC). The luminescent properties of the final hybrid materials were investigated both in pristine and ordered state by polarized optical microscopy with epifluorescence (POM-EPIFL) (Figure 1) and fluorimetry.

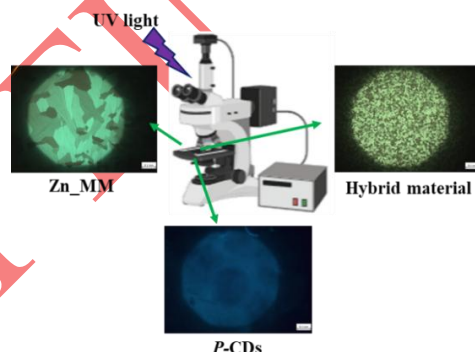


Figure 1. Schematic representation of luminescent hybrid LC system and their precursors

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TOWARD A SUSTAINABLE STRATEGY FOR THE PRODUCTION OF BIOACTIVE FLAVONOLS

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Flavonols, a prominent subclass of flavonoids, have emerged as biomolecules of considerable scientific and clinical interest owing to their wide-ranging bioactivities, including antioxidant, neuroprotective, cardioprotective, anti-aging, and cytotoxic effects [1–3]. Despite their therapeutic promise, the biomedical application of flavonols is often hampered by poor aqueous solubility and limited bioavailability. Glycosylation has been identified as a powerful strategy to overcome these challenges, as it enhances solubility and stability, thereby improving the pharmacological performance of flavonols [4–5]. UDP-glycosyltransferases (UGTs) represent a particularly attractive class of biocatalysts for this purpose, offering high substrate specificity, environmentally benign processes devoid of toxic reagents, and scalable, cost-effective production [6–7]. However, the industrial implementation of UGT-based systems requires further optimization to address issues of enzyme stability, reusability, and cost efficiency. Immobilization of UGTs onto agro-industrial lignocellulosic biomass provides a sustainable and economical solution, as it not only improves operational stability and reduces protein leaching but also enables catalyst recyclability, thereby lowering overall production costs. Within this context, agricultural residues such as rice husk and groundnut husk represent abundant, low-cost, and underutilized resources with potential for high-value applications. Beyond their role in waste management, these by-products offer favorable structural and compositional features that make them promising candidates as immobilization matrices for UGTs. Our preliminary investigations address the morphology, chemical composition, surface area, and porosity of biomass-based materials, since these parameters play a crucial role in defining their performances as supports for biocatalysts, ultimately contributing to the development of a cost-efficient and sustainable route for flavonol glycoside production.

Acknowledgements

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We also acknowledge the Romanian Academy, Program 4 and the project ROOPENSCREEN, MySMIS code: 127952, Contract no. 371/20.07.2020, co-financed by European Regional Development Fund through the Competitiveness Operational Program 2014-2020, for support.

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IDENTIFICATION OF INORGANIC ELEMENTS IN STANDARDIZED BLACK CHOKEBERRY EXTRACTS AND PRIMARY BIOLOGICAL INSIGHTS ON HUMAN PULMONARY ARTERY ENDOTHELIAL CELLS (HPAEC)

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Abstract

Cardiovascular diseases (CVDs) persist as the preeminent cause of mortality on a global scale, accounting for approximately one-third of global deaths and more than half of those reported in Romania [1,2]. A substantial proportion of these outcomes are associated with modifiable behavioral factors, including inadequate diet, physical inactivity, tobacco use, and alcohol consumption. The vascular endothelium plays a pivotal role in blood pressure regulation and vascular homeostasis. Premature endothelial aging, which is triggered by cardiovascular risk factors, is a significant contributor to hypertension and other cardiovascular diseases (CVDs). Given this, tackling changeable risk factors is the primary suggestion for the mitigation and oversight of CVDs and metabolic disorders before taking into account medical treatments.

In recent years, phytotherapy has attracted increasing scientific and clinical attention. Herbal preparations are often regarded as safer, more affordable, and nutritionally advantageous alternatives to conventional treatments. Among plant-derived products, berries have gained widespread recognition due to their high antioxidant, vitamin, and mineral content, combined with low caloric content. The distinctive blue, red, and purple pigmentation exhibited by these plants is attributable to elevated levels of anthocyanins, a subclass of polyphenols that has garnered significant attention due to its documented nutraceutical potential [3].

The black chokeberry (*Aronia melanocarpa* [Michx.] Elliott) has been utilized for a considerable period for both nutritional and therapeutic purposes, including incorporation into functional foods, beverages, natural preservatives, colorants, and cardiovascular or metabolic health products. The present study is the inaugural report on the inorganic element composition of three standardized *Aronia* extracts: frozen berries (FrozArs), dried berries (DryArs), and evaporated juice (EvArJ). Elemental analysis revealed measurable levels of several metals, including aluminum (Al), cadmium (Cd), chromium (Cr), copper (Cu), iron (Fe), manganese (Mn), and zinc (Zn). Cadmium was detected in minimal quantities (0.026 µg/g in FrozArs), while iron was the most prevalent element, particularly in juice (597.665 µg/g).

Furthermore, biological assays employing human pulmonary artery endothelial cells (HPAECs) have demonstrated the antiproliferative effects of all three extracts across the tested concentration range (1–10 µg/mL). Cell cycle analysis revealed a decrease in the proportion of

cells in the G2/M phase, concomitant with the emergence of a sub-G0 population at higher concentrations. Furthermore, the DryAr extract led to a decrease in cells in the G0-G1 phase, accompanied by a modest increase in necrotic cells, as evidenced by Annexin V/PI staining.

These findings underscore the elemental composition and bioactive effects of Aronia extracts, emphasizing their potential relevance for vascular health and suggesting further exploration of their role as dietary supplements with preventive or therapeutic implications in cardiovascular contexts.

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NOT FINALIZED

DRUG LOADING AND RELEASE DISSOLUTION TESTS USING AS CARRIERS, FUNCTIONALIZED MESOPOROUS SILICA

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Abstract

Functionalised mesoporous silica particles were synthesized by sol-gel method, starting from mixed silica precursors, tetraethoxysilane and mercaptopropyltriethoxysilane. Subsequently, they were evaluated as carriers for a drug loading, the clotrimazole, and they demonstrated enhanced drug loading capacity. The loaded carriers were also tested for their release behaviour in different buffered solutions with different pH values, by using a dissolution instrument. The cumulative percent of drug release in hydrochloric acid solution 0.1 N, was 45.07 % after 6 hours of release. The best results concerning the drug release in different buffered solutions were obtained when the same buffer was used for the drug entrapment as well for the drug release, compared with the carriers loaded with drug in ethanol. The percent of drug release in acidic buffered solution of pH= 2 was constantly in the 51-91 % range of release and of pH= 4.5 was constantly in the 11-20 % range of release. The percent of drug release has been evaluated during more then 3 hours.

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MISCIBILITY STUDIES ON Ni(II) AND Co(III) LUMINESCENT METALLOMESOGENS

Evelyn Popa, Carmen Cretu, Ildiko Buta, Elisabeta I. Szerb

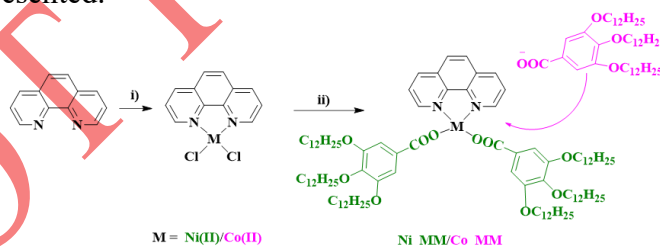
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Abstract

Metallomesogens (MMs), are a class of metal-containing liquid crystals that merge the anisotropic properties of liquid crystals with the unique electronic and magnetic characteristics of coordination complexes [1]. The promise of carefully crafted advanced materials for applications in electro-optics, sensing, and biomedicine [2] depends critically on understanding how molecular structure dictates function, which in turn is influenced by the 'soft' supramolecular order yielding tunable properties of these systems.

Our aim was to synthesize isostructural nickel(II) and cobalt(II) analogues using the same N^N chelating and O-monoanionic gallate ligands following our previous investigation of octahedral, heteroleptic zinc(II) and copper(II) MMs [3]. The key was to explore the formation of heterobimetallic liquid crystalline luminescent ordered blends with synergistic properties. Despite using the same synthetic protocol, the two new complexes exhibited different molecular geometries due to the stereochemical preferences of the metal ions (Scheme 1). The nickel(II) complex adopted an octahedral structure mirroring its counterparts with Zn(II) and Cu(II) [3]. Surprisingly, the cobalt(II) precursor underwent an in-situ oxidation to cobalt(III) during the final step, leading to the formation of a five-coordinate, neutral heteroleptic complex. This finding underscores the profound influence of the metal center on the final molecular geometry, and reveals a rare coordination motif for cobalt.

Miscibility studies in the liquid crystalline state were performed by obtaining blends with different mass ratio of the precursors and the photophysical properties of the MMs precursors and blends will be presented.



Scheme 1. Synthesis of Ni_MM and Co_MM. Conditions: i) MCl_2 , EtOH, r.t., 24 hours; ii) $\text{Ag}[\text{OOCC}_6\text{H}_2(\text{OC}_{12}\text{H}_{25})_3]$, $\text{CHCl}_3/\text{MeOH}$, r.t., 24 hours.

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NOT FINALIZED

RAPID FABRICATION OF UIO-66 USING A MICROWAVE-ASSISTED APPROACH AND ITS PERFORMANCE IN HYDROGEN STORAGE

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Abstract

This study presents a rapid and efficient microwave-assisted synthesis method for the synthesis of the zirconium-based metal-organic framework UiO-66, employing acetic acid as a modulating agent. X-ray diffraction (XRD) analysis confirms the successful formation of pure and crystalline UiO-66 material, with diffraction patterns matching those reported in the literature and showing no signs of structural impurities. Scanning electron microscopy (SEM) images reveal that the materials consist of small, irregularly shaped agglomerated nanoparticles. Energy-dispersive X-ray spectroscopy (EDX) analysis verifies the elemental composition of the framework, confirming the presence of zirconium (Zr), oxygen (O), and carbon (C), corresponding elements for UiO-66. The synthesized samples exhibit relatively high specific surface areas, with the maximum reaching 725 m²/g, and display a mixed porosity profile comprising both micropores and mesopores. Despite a notable deficiency of organic linkers per Zr₆ unit, the materials maintain high thermal stability. A direct correlation was observed between the increase in total specific surface area and the enhancement of microporous surface area, which in turn led to improved hydrogen (H₂) adsorption performance.

SYNTHESIS OF COPPER(II)-COMPLEXES WITH SCHIFF BASES, SEMI- AND THIOSEMICARBAZONES, AND THEIR PHYSICO-CHEMICAL STUDIES

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Abstract

The copper is an essential microelement in the human body. Copper(II)-complexes are used as antimicrobial agents, and moreover, derivatives with aminoacids-, peptides-, chinoxaline-, mono- and bis-semicarbazones ligands gain importance in cancer therapy. Copper compounds also play notable role in the convalescence processes.

In our research work new copper(II) complexes were synthesized with Schiff bases, such as $[\text{Cu}(\text{2-heptanone})_2\text{A}(\text{L}_2)]$, $[\text{Cu}(\text{3-heptanone})_2\text{A}(\text{L}_2)]$, where A = hydrazone, phenyl-hydrazone, L = 3-chloroaniline, $[\text{Cu}(\text{dipivaloyl-methane-(T)SC})_2]$, $[\text{Cu}(\text{3,4-hexanedione-(T)SC})_2]$, (T)SC = semi- or thiosemicarbazone. In syntheses copper(II)-acetate was dissolved in water and mixed with alcoholic solution of the Schiff base, or semi- or thiosemicarbazone. In case of some Schiff base complexes amines were added too. The synthetic reactions were completed after refluxing for 2–3 hours.

The molecular structures of our products were studied using a range of techniques, including IR (middle and far), ESR and UV–VIS spectroscopies, mass spectrometry (MS), elemental analysis and thermoanalytical measurements (TG-DTG-DTA).

Introduction

Azomethine derivatives of 3–6 d transition metals are often studied in a parallel way with the same ligand. The thermal stability of Cu(II) derivatives is often lower than other analogous compounds, and there are also notable differences in their physico-chemical properties. In the literature numerous mono- and polynuclear products are known with 2-, 3- and 4-dentate ligands. The electron configuration of Cu(II) is $[\text{Ar}]3d^9$ with a free, uncompensated “hole electron” that allows to study the fine structure of Cu(II) compounds using electron spin resonance spectroscopy (ESR).

One of the major advantages of using copper complexes as antitumor agents is that they are less toxic to living organisms than the pure organic ligands. Their mechanism of action is based on catalyzing the decomposition of free peroxide radicals in the body, converting them into O_2 molecules [1].

Schiff bases containing N and O atoms usually show biological activity and attract great interest in their research due to the large number of ways in which they can bind to metal ions.

It is known that certain metals, such as Cu^{2+} , increase the efficiency of biologically active compounds, and therefore one of the main goals of their use is in medicine. In fact, Schiff bases are able to stabilize different oxidation states of metal ions, thus enabling a wide range of applications of their complexes in biological, clinical, analytical and industrial fields. They play also significant role in their use as catalysts in organic syntheses [2].

A wide variety of Schiff bases can be prepared by condensation reactions of carbonyl derivatives with various diamines. The resulting Schiff bases usually react in 1:1 molar ratio with the corresponding metal ion to form $[\text{ML}]$ -type complexes.

Thiosemicarbazones and semicarbazones have a wide range of biological applications including their anticancer and antibacterial activities [3].

In this paper we report the synthesis and characterization of novel copper complexes with Schiff bases, semi- and thiosemicarbazone derivatives.

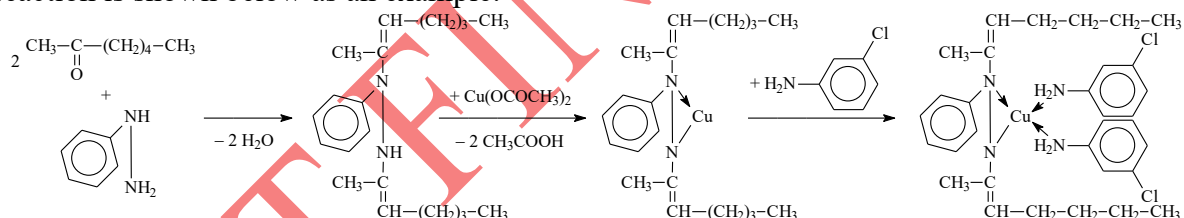
Experimental

Used materials: $\text{Cu}(\text{CH}_3\text{COO})_2$, 2-heptanone, 3-heptanone, hydrazine, phenyl-hydrazine, 3-chloroaniline, dipivaloyl-methane, 3,4-hexanedione, semicarbazone, thiosemicarbazone, MeOH, EtOH.

Methods:

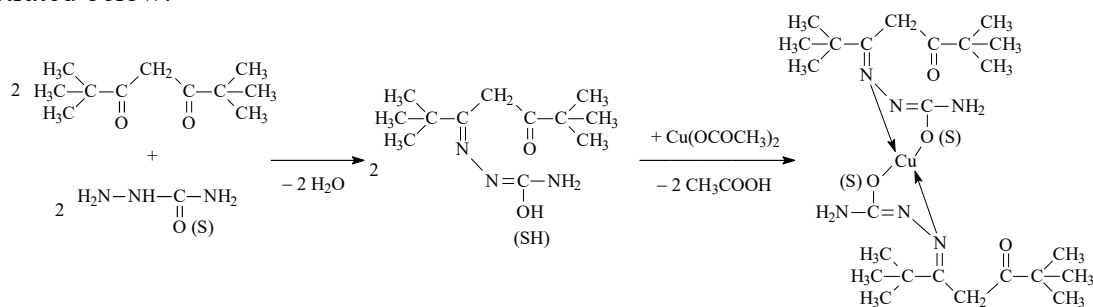
- Synthesis of $[\text{Cu}(\text{ketone})_2\text{A}(\text{L}_2)]$ type complexes

0.01 mol ketone (2-heptanone or 3-heptanone) was mixed with hydrazine or phenyl-hydrazine dissolved in 10 ml EtOH, then refluxed for $\frac{1}{2}$ hour to obtain the Schiff bases. Afterwards 0.005 mol $\text{Cu}(\text{CH}_3\text{COO})_2$ was added dissolved in 20 ml distilled water. The mixture was refluxed on water bath for 2–3 hours. The filtered crystalline complexes were washed with MeOH–water mixture (1:1) and dried on air. In some cases when no precipitation of the complex occurred, 0.01 mol 3-chloroaniline was added to the mixture, and heated for 1 more hour. A typical reaction is shown below as an example:



- Synthesis of $[\text{Cu}(\text{ketone-SC}_2)]$ and $[\text{Cu}(\text{ketone-TSC}_2)]$ type complexes

0.01 mol ketone (dipivaloyl-methane or 3,4-hexanedione) was mixed with 0.01 mol semi- or thiosemicarbazide dissolved in 50 ml EtOH and 10 ml distilled water. In the case of semicarbazide 0.01 mol CH_3COOH was dissolved in 10 ml water for HCl neutralization. The obtained mixture was heated for 1 hour on water bath to obtain the semi- or thiosemicarbazone. Subsequently 0.005 mol $\text{Cu}(\text{CH}_3\text{COO})_2$ in 20 ml distilled water was added, and heating was continued for 2–3 hours on water bath. After cooling the crystalline complexes were filtered off, washed with MeOH–water mixture (1:1) and dried on air. A representative reaction is illustrated below:



Microscopic characterization and yields of the prepared complexes are listed in Table 1.

Table 1. Microscopic characterization, calculated molecular weights and yields of the prepared complexes.

Nr.	Compound	Calc. mol. weight	Yield (%)	Microscopic characterization
1.	[Cu(2-heptanone) ₂ (hydrazone)]	285.91	20	Reddish-brown triangle-based prisms (microcrystals)
2.	[Cu(2-heptanone) ₂ (Ph-hydrazone)]	363.02	20	Reddish-brown triangle-based prisms (microcrystals)
3.	[Cu(3-heptanone) ₂ (hydrazone)]	285.91	20	Reddish-brown triangle-based prisms (microcrystals)
4.	[Cu(3-heptanone) ₂ (Ph- hydrazone)]	363.02	25	Reddish-brown triangle-based prisms (microcrystals)
5.	[Cu(2-heptanone) ₂ (Ph-hydrazone)(3-Cl-aniline) ₂]	618.17	15	Dark brown triangle-based prisms
6.	[Cu(3-heptanone) ₂ (Ph-hydrazone)(3-Cl-aniline) ₂]	618.17	10	Dark brown triangle-based prisms
7.	[Cu(dipivaloyl-methane-SC) ₂]	544.19	55	Violet triangle-based prisms
8.	[Cu(dipivaloyl-methane-TSC) ₂]	576.31	20	Brown triangle-based prisms (microcrystals)
9.	[Cu(3,4-hexanedione-SC) ₂]	403.92	10	Green triangle-based prisms (microcrystals)
10.	[Cu(3,4-hexanedione-TSC) ₂]	436.04	50	Brown triangle-based prisms (microcrystals)

Infrared spectroscopic study

The data of the most characteristic IR bands for some selected complexes are presented in Table 2.

Table 2. IR data of the selected complexes.

Comp. cm ⁻¹	1	2	3	4	5	6	7	8	9	10
VO-H	-	-	-	-	-	-	3381 w	3407 m	3455 s	3447 w
VN-H	3371 m	3261 m	3364 m	3262 m	3351 m	3351 m	3298 w	3277 m	3269 m	3298 m
VC-H	2941 w	2928 m	2941 w	2930 m	2928 m	2969 m	2952 s	2969 m	2971 s	2971 s
VC=C	1649 w	1672 m	1649 w	1672 m	1672 w	1719 w	1656 w	1738 s	1684 vs	1682 s
VC=N	1596 vs	1588 s	1595 vs	1588 vs	1588 s	1588 s	1548 vs	1587 vs	1578 vs	1583 vs
δCH ₂	1419 vs	1466 vs	1418 vs	1467 vs	1468 vs	1481 vs	1497 vs	1474 s	1438 vs	1458 vs
VC-O	-	-	-	-	-	-	1226 s	-	1227 m	-
VC-S	-	-	-	-	-	-	-	1217 s	-	1216 vs
VN-N	1217 w	1293 s	1230w	1213 s	1214 s	1216 s	1148 s	1106 m	1159 s	1150 vs
γC-H	686 vs	683 vs	686 vs	682 vs	688 s	684 s	643 s	763 s	666 s	672 m
VCu-N	515 s	567 s	521 s	592 s	592 s	592 s	515 s	528 vs	553 s	544 m
VCu-O	-	-	-	-	-	-	494 s	-	455 s	-
VCu-S	-	-	-	-	-	-	-	447 s	-	431 w

$\delta_{\text{N-Cu-N}}$	370 s	364 m	368 s	363 m	366 s	365 s	341 s	363 m	326 vs	370 w
$\delta_{\text{O-Cu-O}}$	-		-	-	-	-	285 s	-	253 s	-
$\delta_{\text{S-Cu-S}}$	-		-	-	-	-	-	270 m	-	270 w

(Abbreviations: vs = very strong, s = strong, m = medium, w = weak)

The mid-IR spectra were recorded with a Bruker Alpha FTIR spectrometer (Platinum single reflection diamond ATR), at room temperature, in the wavenumber range of 4000–400 cm^{-1} , and the far-IR range of 500–50 cm^{-1} , respectively, on a Bio Rad – FTS 60A, PIKE Gladi ATR spectrometer, with a resolution of 4 cm^{-1} . The samples were measured in solid state (in powder form).

The most important bands for the characterization of complexes are $\nu_{\text{C=N}}$ (1548 – 1596 cm^{-1}) and $\nu_{\text{Cu-N}}$ (515 – 592 cm^{-1}) [4]. In the far IR region the $\delta_{\text{N-Cu-N}}$ deformation bands appear which demonstrate the stability of complexes. In case of thiosemicarbazone type complexes $\nu_{\text{C-S}}$ valence band is shown with high intensity.

Mass spectrometry

Mass spectra of the samples were recorded on an Agilent 1200/6410B Triple Quad LC-MS/MS system using electrospray ionization (ESI). In the spectra we could detect the molecular ions and some decomposition fragments.

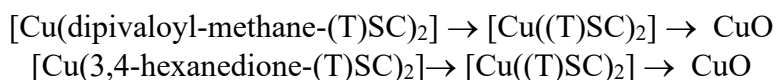
Electron Spin Resonance spectroscopy

The measurements were performed with a Bruker ELEXSYS 500 type device. By comparing the experimental and calculated spectra, and by calculating the characteristic parameters, the Cu–N and Cu–O couplings can be identified. Samples $[\text{Cu}(2\text{-heptanone})_2(\text{hydrazone})]$ and $[\text{Cu}(3\text{-heptanone})_2(\text{hydrazone})]$ exhibited slightly larger linewidths, however, the ligand field was quite small thus suggesting that 1N coordination is probable in these complexes. These spectra show a uniform coordination sphere with nitrogen coordination around the copper. In case of $[\text{Cu}(\text{dipivaloyl-methane-SC})_2]$ and $[\text{Cu}(\text{dipivaloyl-methane-TSC})_2]$ the linewidth is very narrow indicating that oxygen coordination is possible in these complexes.

Thermoanalytical measurements (TG-DTG-DTA)

Thermal measurements were performed with a 951 TG and 910 DSC calorimeter (TA Instruments) in air at a heating rate of 10 $\text{K} \cdot \text{min}^{-1}$ (sample mass of 4–10 mg).

The thermal stability of complexes in the case of $[\text{Cu}(\text{dipivaloyl-methane-SC})_2]$ and $[\text{Cu}(\text{dipivaloyl-methane-TSC})_2]$ is limited within the temperature range of 100–124 °C. The first step of the decomposition is the loss of the dipivaloyl-methane group until 215–350 °C, then the semi- or thiosemicarbazone units leave. The end of the process is between 315–755 °C. The first decomposition step is accompanied by a small endothermic peak, then a big exothermic peak appears at 242 °C, 400 °C respectively. The residue is CuO. In the case of $[\text{Cu}(3,4\text{-hexanedione-SC})_2]$ and $[\text{Cu}(3,4\text{-hexanedione-TSC})_2]$ complexes the thermal stability is limited between 192–197 °C. The first decomposition step belongs to leaving of 3,4-hexanedione group, until 269 °C, 500 °C respectively. The end of the process is between 435–730 °C, and CuO is the residue. Subsequently, the decomposition steps are accompanied by big exothermic peaks at 223 °C and 496 °C respectively. The general mechanism for decomposition is as follows:



UV-VIS spectroscopy

The electronic spectra were recorded with a Jasco V-670 Spectrophotometer in 10% EtOH/water solutions containing the substance in 10^{-4} mol/dm^3 concentration. Using Sørensen buffer solutions the electronic spectra were also recorded as a function of pH, and then the

acidity constants were calculated, too. The obtained values were between $4.836 \cdot 10^{-11}$ – $1.886 \cdot 10^{-9}$.

Powder X-ray diffraction measurements

The crystal structure of the complexes was studied with powder XRD measurements, carried out on a PANalytical X'pert Pro MPD X-ray diffractometer. As being novel compounds their diffractograms can not be found in the Cambridge database. The majority of the complexes exhibits amorphous form, except for $[Cu(dipivaloyl-methane-SC)_2]$ which is crystalline.

Elemental analysis

Elemental analyses were performed with a Vario EL III element analyzer.

In case of $[Cu(dipivaloyl-methane-SC)_2]$ the obtained/calculated values for carbon, hydrogen and nitrogen are: C: 54.54% / 52.97%, H: 8.61% / 8.15, N: 13.68% / 15.44%.

Conclusion

New copper(II) complexes with Schiff-base type ligands were synthesized and characterized using a range of physicochemical methods. The thermal decomposition mechanism was determined by thermoanalytical measurements.

Acknowledgement

The authors wish to express their thankfulness to the “Domus Hungarica Foundation” of Hungary for the several fellowships provided to Csaba Várhelyi jr.

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ULTRAVIOLET PHOTODETECTORS BASED ON TiO₂-COMPOSITE MATERIALS

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Abstract

Lately, sensors have played an important role in various aspects of our daily lives especially chemical sensors which serve as essential tools for capturing real-time chemical data from our environment. Such information can supply control systems with vital feedback across a wide range of chemical processes—including the detection of toxic substances and explosives, activation of safety alerts for gas appliances, protection mechanisms for workers exposed to chemical risks, environmental monitoring, regulation of the food supply chain, and even health monitoring [1]. Photodetectors are gaining increasing attention due to their relevance in everyday life, and lately the metal oxides materials are widely used in the development of UV sensors due to their wide bandgaps, high thermal and chemical stability, and photoconductivity under UV illumination [2]. As materials for sensors, numerous approaches have been used to study metal oxide material nanostructures from the perspectives of synthesis, structure, and properties, and titanium dioxide (TiO₂) is a versatile compound known for its brightening and UV-absorbing properties, non-toxicity, and chemical stability.

In this research, the heterostructures based on *aero*-TiO₂ and TiO₂/CuMnO₂ materials were successfully used for development of ultraviolet photodetectors, and characterization under ultraviolet irradiation was assessed. The as-obtained heterostructures were morpho-structural characterized by X-ray diffraction (XRD), UV-Vis spectroscopy and Scanning Electron Microscopy (SEM), and analysis. To demonstrate the *n*-TiO₂/*p*-CuMnO₂ heterojunction, the Mott-Schottky measurement was performed. The UV sensing measurements were performed at ambient temperature in dark and under UV irradiation at $\lambda = 365$ nm and $\lambda = 395$ nm, using a commercial LED source. The *I-V* measurements of the *n*-TiO₂ nanolayer/*p*-CuMnO₂ thin film heterostructure confirm its diode characteristics under dark state, UV and VIS conditions [3]. In conclusion, the TiO₂-based heterostructures demonstrates the practical viability and application potential of this emerging class of materials in sensing technologies.

Acknowledgements

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EVALUATION OF QUATERNARY PHOSPHONIUM SALTS AS POTENTIAL ANTIMICROBIAL AGENTS

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Abstract

The interest in quaternary phosphonium salts increased due to their alignment with the principles of green chemistry, which aim to reduce harm to the environment and human health, while making chemical processes more efficient and sustainable. This study reports the synthesis and applications as antimicrobial agents of five quaternary phosphonium salts.

Introduction

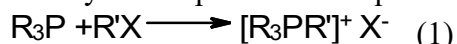
The family of quaternary phosphonium salts explored in this study is particularly appealing due to their unique physicochemical properties, ease of synthesis, and structural versatility. These compounds have broad applicability across multiple fields, including biology, medicine, and industrial processes. The synthesized salts described above were characterized using a combination of one-dimensional and two-dimensional nuclear magnetic resonance (NMR) techniques, which provided detailed information for accurate spectral interpretation. In these compounds, the alkyl chain length, the halide counterions, and the aryl moieties attached to the phosphorus atom were systematically varied. These structural modifications were designed to investigate their influence on the physicochemical properties and potential biological activities of the salts, providing valuable insights into structure–activity relationships and guiding the development of more effective antimicrobial agents [1-3].

Experimental

The quaternary phosphonium salts were evaluated for their antimicrobial activity against two Gram-negative bacterial species (*Escherichia coli* - ATCC 25922 and *Pseudomonas aeruginosa* - ATCC 15692), two Gram-positive bacterial species (*Staphylococcus aureus* - ATCC 25923 and *Bacillus cereus*- ATCC 10878), and one yeast species (*Candida albicans* ATCC 10231). The antimicrobial susceptibility tests were conducted using the disk diffusion method (Kirby-Bauer). Actively growing cultures were used: 24-hour-old cultures for bacteria and 48-hour-old cultures for yeast. Mueller-Hinton broth (Oxoid) was employed for bacterial cultivation, while Sabouraud dextrose agar was used for yeast culture.

Results and discussions

Due to their nucleophilicity, phosphines react with alkyl and aryl halides to form the corresponding phosphonium salts, with reactivity decreasing in the order $R'I > R'Br > R'Cl$. The general synthetic procedure of quaternary phosphonium salt is following reaction 1.



R = alkyl, aryl, H; $R'X$ = alkyl or benzyl halide.

The structural information was further supported by FTIR spectroscopy and elemental analysis. The findings indicate that by increasing the number of 3-furyl groups attached to the

phosphorus atom leads to shifts to higher fields in the ^{31}P -NMR, which means it shows lower chemical shift (ppm) values [4].

The applicative research on this class of compounds has shown that they exhibit effect against both Gram-positive (*Bacillus cereus* and *Staphylococcus aureus*) and Gram-negative (*Pseudomonas aeruginosa*, *Escherichia coli*) strains, and fungus *Candida albicans* [5,6]. To evaluate antimicrobial activity, the diameters of the inhibition zones around each disc were measured using a micrometer, with the total measurement including the 6 mm diameter of the disc itself. The antimicrobial activity of the tested compounds was evaluated in comparison to control sample, which consisted of ethanol solutions (code:1). The most significant antimicrobial activity was observed for samples butyltriphenylphosphonium iodide (4) and pentyltriphenylphosphonium iodide (5), particularly against Gram-positive bacterial strains. As an example, Figure 1 illustrates the results of the antimicrobial testing of these compounds against a culture of *Staphylococcus aureus*. The antibacterial effect observed against *Staphylococcus aureus* was superior to that of the antibiotic used as a positive control (Oxacillin). The preliminary antimicrobial studies conducted on the previously mentioned strains showed promising results, indicating good potential for future applications.

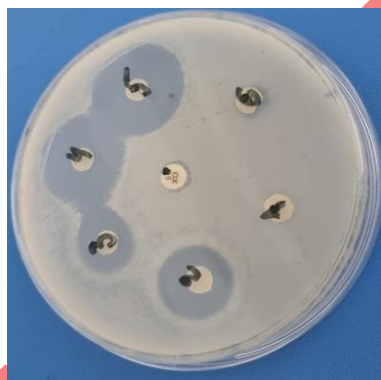


Figure 1. Antibacterial studies on *Staphylococcus aureus*.

Conclusions

This study has demonstrated that these compounds exhibit stronger effects on Gram-positive bacteria (*Bacillus cereus* and *Staphylococcus aureus*), comparing with Gram-negative bacteria (*Pseudomonas aeruginosa* and *Escherichia coli*), and the fungus *Candida albicans*.

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INFLUENCE OF X-RAY IRRADIATION ON SPECTROSCOPIC PROPERTIES OF TmF₃ –DOPED FLUORIDE (CaF₂ AND BaF₂) CRYSTALS

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Abstract

Rare-earth ions-doped fluorides crystals have been extensively investigated due to the possible use in various applications like medicine, energy or laser materials, optical amplifiers, quantum materials or scintillators [1]. In this regard the interaction of X-ray irradiation with fluoride crystals has significant implications for both fundamental materials science and applied radiation technologies.

Introduction

In hosts like CaF₂ (calcium fluoride) and BaF₂ (barium fluoride), some rare-earth ions (RE) are usually introduced in the trivalent state. The fluoride lattice has relatively low phonon energies, which helps reduce non radiative decay of rare earth emissions (good for luminescence). Under certain conditions (irradiation, additive coloration, etc.), some RE³⁺ can be reduced to the divalent state, RE²⁺. This is interesting because RE²⁺ has different energy levels and thus different absorption/emission behavior. This study investigates the optical properties changes induced in various fluoride crystals—such as CaF₂, BaF₂, doped with TmF₃ under controlled X-ray exposure.

Experimental

Through spectroscopic analysis we explore the formation of color centers, and charge conversion of thulium ions. Pure and various concentration TmF₃-doped fluoride (CaF₂ and BaF₂) crystals have been grown using an in-house vertical Bridgman method [2]. Disks cleaved from the obtained single crystals have been irradiated with X-rays (Bruker D8 Advance diffractometer) at room temperature at different intervals up to 4h [3].

Results and discussion

Room temperature optical absorption spectra for the non-irradiated samples demonstrate the distinct absorption features consistent with thulium ions for its divalent and trivalent states [4]. After X-rays irradiation, absorption bands modifications have been observed for the in UV-VIS domain. The magnitude of the intensity absorption bands was studied with the TmF₃ content and demonstrates a variation with time. Also the matrix type (CaF₂ or BaF₂) influence was studied. Not least, the decay optical measurements over a long period of time (days) was analyzed for the evaluation of the long-term stability properties.

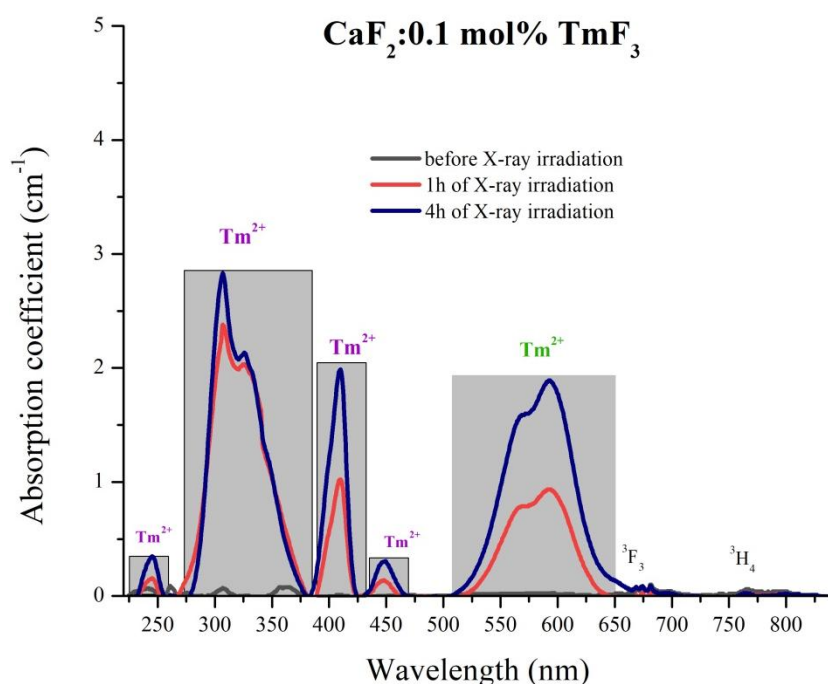


Figure 1. X-ray irradiation influence on the absorption spectra of $\text{CaF}_2: 0.1\text{mol}\% \text{TmF}_3$.

Conclusion

The insights and results of the study demonstrate the importance of continuous research for the development of radiation-resistant optical materials, dosimetry applications, and the advancement of photonic devices operating in high-radiation environments.

Acknowledgements

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EXPLORING THE CHEMICAL SPACE OF BILIRUBIN ANALOGUES: VIRTUAL SCREENING AND EVALUATION OF PHARMACOKINETICS AND DRUG-LIKENESS PROFILES

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Abstract

Bilirubin is widely recognized as an important endogenous molecule, offering significant benefits in the context of chronic diseases, although it may become toxic at high concentrations [1]. Based on this premise, our study aimed to identify novel compounds that reproduce the beneficial effects of bilirubin while potentially exhibiting improved safety profiles. Using the Pharmit [2] platform for pharmacophore virtual screening, we identified nine candidate molecules that were further assessed for their pharmacokinetic behavior and drug-likeness using OSIRIS Property Explorer [3], SwissADME [4], and Molinspiration [5]. From these, five compounds were selected based on ADME/Tox parameters and according to established drug-likeness criteria. This work presents an *in silico* framework for the rational selection of bilirubin-based scaffolds in the design of new, safer analogues. Further experimental investigations will be necessary to verify their *in vivo* effectiveness and safety profile.

Acknowledgements

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METAL–ORGANIC FRAMEWORK COMPOSITES FOR TARGETED PHENOLIC DERIVATIVES REMOVAL FROM WATER

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Abstract

Due to the toxicity and difficult removal of petrochemical-derived phenol derivatives from water, this study focused on creating sustainable and low-cost adsorbents. We synthesized and functionalized metal-organic frameworks (MOFs) with ionic liquids, demonstrating a high adsorption capacity for pollutants like 2,6-dimethylphenol, which is driven by a physical sorption mechanism.

Introduction

In water, pollutants like phenol derivatives, resulting from petrochemical processes, pose a significant risk to both the environment and human health. Their high solubility and the high cost of existing removal methods make them particularly difficult to eliminate. This study focused on developing a more sustainable and cost-effective solution, a new class of solid adsorbent materials.

Experimental

Following the 12 principles of green chemistry, we synthesized phosphonate metal organic frameworks (MOFs) using a hydrothermal synthesis method [1,2] with water as solvent. The MOFs synthesized starting from etidronic acid (HEDP) with various metal salts, including divalent ions such as Co^{2+} , Ni^{2+} , Cu^{2+} as well as the trivalent ion Ce^{3+} . Figure 1 shows the synthesis of the material CeHEDP.

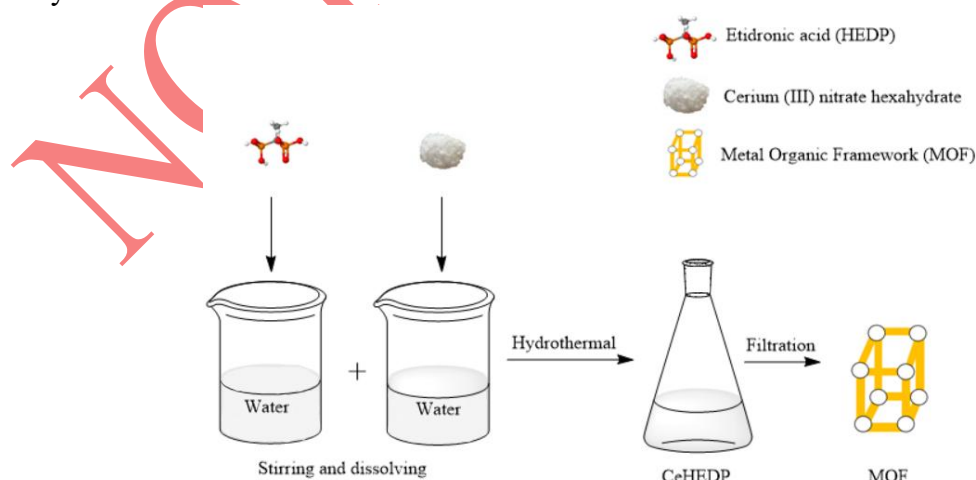


Figure 1. The hydrothermal synthesis of CeHEDP

To increase their adsorption properties, the resulting materials were impregnated with imidazolium-based ionic liquids (IL), specifically 1-ethyl-3-methylimidazolium chloride and 1-hexyl-3-methylimidazolium chloride, obtaining IL@MOFs.

The resulted materials (CoHEDP, NiHEDP, CuHEDP, CeHEDP, IL@MOFs) have been characterized by Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction, and thermogravimetric analysis.

Results and discussion

The ability of metal–organic frameworks (MOFs) synthesized to adsorb phenol derivatives was investigated. The MOFs exhibited the following order of increasing adsorption capacity: CuHEDP < NiHEDP < CoHEDP < CeHEDP.

The highest adsorption capacity was achieved by the materials impregnated with 1-hexyl-3-methylimidazolium chloride. The best result was observed with CeHEDP, which demonstrated an impressive adsorption capacity of 23.1 mg/g for 2,6-dimethylphenol.

The adsorption behavior of phenol derivatives on these MOFs was systematically investigated using multiple isotherm models, including Langmuir, Freundlich, and Redlich–Peterson. The experimental data aligned well with the Langmuir and Redlich–Peterson isotherms, indicating that the adsorption of phenol derivatives by these materials is a physical sorption process [3].

Conclusion

This study successfully demonstrated the synthesis of low-cost and environmentally friendly materials with high potential for removing phenol derivatives from water. The investigations indicates that adsorption occurs predominantly via physical sorption, with the different isotherms providing complementary insights into the surface heterogeneity, adsorption capacity, and interaction mechanisms of the MOF materials.

Acknowledgements

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APPLICATION OF MANGANESE-DOPED IRON OXIDE NANOPARTICLES AS ADSORBENTS FOR DYES REMOVAL: PRELIMINARY STUDIES

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Abstract

The unprecedented development of textile industrial activities has led to the generation of colored polluted waters, which threaten the aquatic environment, but also human health. [1,2]. Among the techniques applied for the removal of colored contaminants from wastewater, adsorption has proven to be a simple and accessible method [1]. In recent years, research on iron oxide nanoparticles has received increased attention due to their high potential as adsorbent materials and their magnetic properties, which ensure easy and efficient separation [3]. In this work, composite materials based on iron oxide and manganese were synthesized and applied as adsorbents for removal of dyes from aqueous solution.

Iron oxide and manganese-doped iron oxide nanoparticles were synthesized by the co-precipitation method, at 80°C, under mechanical stirring 400 rpm, for 30 min. Manganese-doped iron oxide nanoparticles were synthesized by gradually replacing the Fe^{2+} with Mn^{2+} , in different ratio: $\text{Mn}_x\text{Fe}_{1-x}$, where $0 < x < 1$ (0.1, 0.25, 0.5, 0.75, 1). The influence of the dopant content upon adsorption properties of the synthesized nanoparticles was investigated. The synthesized materials were characterized by X-ray diffraction (XRD) analysis, FT-IR spectroscopy, and the specific surface area was evaluated using BET method.

The obtained nanoparticles were applied as adsorbents for the removal of dyes from aqueous solutions. Two cationic dyes: Kresyl Violet (KV) and Blu Metil (BM) were selected as potential pollutants. The concentration of dyes was determined by UV-Vis spectrophotometry at a wavelength set at 553 nm for KV and at 587.5 nm for BM.

The results obtained in adsorption studies indicated that removal percentages reached up to 93% for KV and 97% for BM within 180 minutes, under normal working conditions. The removal efficiencies increase from S1 to S5, in accordance with the increase in the amount of manganese in the material composition. Also, the adsorption capacity of iron oxide nanoparticles increased with the level of Mn doping. Fourier transform infrared spectroscopy (FT-IR) was used to investigate the surface functional groups, before and after adsorption studies. Fitting the data obtained at certain time intervals showed that the pseudo-second-order kinetic model best describes the adsorption process.

Preliminary results obtained working under normal conditions revealed that the obtained manganese-doped iron oxide materials are promising adsorbents for the removal of dyes from aqueous solutions.

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INVESTIGATING THE CORROSION INHIBITION CHARACTERISTICS OF METAL PHOSPHONATES THAT INCORPORATE TRANSITION METALS

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Abstract

For some metals, phosphonates frequently function as corrosion inhibitors by creating protective coatings on the metal's surface and minimizing direct contact with corrosive environments [1]. Phosphonates have the ability to bind metal ions under specific circumstances, halting corrosion or deposit formation. The application of phosphonates in industrial systems helps to lower maintenance costs and increase the lifespan of metal equipment [2].

Organophosphorus compounds are known to be good corrosion inhibitors. As a result, their metal phosphonate derivatives have been investigated as potential candidates for inhibiting iron corrosion in acidic saline solutions [1-3]. The inhibitory action of three metal phosphonates (Ni, Cu, and Ni) was analyzed by electrochemical impedance spectroscopy, polarization curves, FT-IR, optical microscopy, and quantum chemical calculations. The experimental results recorded showed that the Cu network was less effective in preventing corrosion. The HOMO and LUMO energy levels of iron (Fe) were examined and compared with those calculated for each metal phosphonate. According to these calculations, the metal phosphonate supports its function as a cathodic/anodic inhibitor by acting as a Lewis acid and iron as a Lewis base. The HOMO orbital of iron and the LUMO orbital of the metal phosphonate interact during the reaction. These energy gaps should approach zero eV to predict a strong covalent bond and effective corrosion inhibition. CoPA presents the smallest energy gap, which is consistent with the experimental results. Among the metal phosphonates investigated, CoPA exhibits better inhibitory action, especially after prolonged immersion, providing an inhibition efficiency greater than 90% on carbon steel surfaces.

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CORRELATIONS BETWEEN STRUCTURE AND PROPERTIES IN RARE EARTH DOPED FLUORIDE MATERIALS

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Abstract

Fluoride MF₂ (with M = Ca or Ba) materials doped with trivalent Rare-Earth (RE³⁺) cations open up opportunities in many application fields especially for optical devices [1]. The MF₂ fluoride materials crystallize into a cubic structure (Fm-3m space group) characterized by M²⁺ cations surrounded by eight F⁻ ions, F⁻ atoms enclosed by four M²⁺ ions and can accept a wide variety of ions, both bivalent and trivalent, due to the same number of octahedral interstitial sites (positions) as the number of M²⁺ ions. The RE³⁺ doping into the host lattice is made without change in the symmetry and the excess of charge is compensated by interstitial F⁻ ions leading to different isolated site symmetry centers depending on the RE³⁺ concentrations i.e. at low RE³⁺: tetragonal (C_{4v}), trigonal (C_{3v}) or cubic (O_h) or complex clusters for higher RE³⁺ doping [2]. In order to analyse the influence of Rare-Earth doping upon structural and optical properties of MF₂ (M=Ca or Ba) matrix, the following single crystals were grown by using the vertical Bridgman-Stockbarger method [3]: pure MF₂ (M = Ca and Ba) single crystals, and MF₂ crystals doped with 0.1 mol.%, 1 mol.% and 5 mol.% TmF₃ and 0.1% mol and 5 mol% ErF₃.

To gain a deeper understanding of the physics processes of these materials, investigations by RT X-Ray or neutron diffraction on single crystal or crushed single crystals and optical absorption spectroscopy have been performed. The structural refinements revealed the behaviour of thulium or erbium doping upon CaF₂ or BaF₂ lattice and these are correlated with host-specific charge compensation mechanisms and local lattice distortions. Moreover, changes of the host matrix significantly influence the local coordination environment of the RE ions, which in turn could influence their optical properties, such as the position and intensity of absorption bands [4-6].

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MASS SPECTROMETRY-BASED INSIGHTS INTO HUMAN BRAIN GANGLIOSIDE DYNAMICS IN HEALTH AND NEUROLOGICAL DISORDERS

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Abstract

Gangliosides (GGs), glycosphingolipids abundant in the central nervous system (CNS), regulate neural development and signaling, making them valuable as biomarkers and therapeutic targets. Due to their involvement in neural development and signaling, GGs are valuable indicators for the early diagnosis of CNS pathologies. We report a nanoelectrospray ionization (nanoESI) ion mobility spectrometry (IMS) mass spectrometry (MS) and collision-induced dissociation (CID) tandem MS platform for high-resolution CNS glycolipidomics. Applied to brain tissues, tumors, and cerebrospinal fluid [1-3], this method revealed tumor-associated alterations in GG composition, including increased glycoform and ceramide diversity, enhanced sialylation, and novel acetate-modified structures. These alterations underscore GG overexpression in glioblastoma and metastases as promising diagnostic markers and therapeutic targets, establishing a powerful workflow for brain tumor and neurodegenerative disease research.

Introduction

GGs are critical regulators of brain function, and their dysregulation is linked to CNS pathology. Due to their structural complexity and low abundance in fluids, sensitive analytical platforms are required for reliable detection. Our work applies advanced IMS MS and CID MS/MS to characterize GGs, discover biomarkers in glioblastoma and metastatic tumors, and profile GGs in cerebrospinal fluid.

Experimental

Extracted GGs were dissolved in methanol at a concentration of 5 pmol/mL and directly infused into a Synapt G2-S instrument. Data were acquired over two minutes in negative ion mode using a 1.5 kV ESI voltage and a 45 V cone voltage. IMS parameters were set to a wave velocity of 650 m/s, wave height of 40 V, and gas flow of 90 L/min to optimize separation. CID MS/MS was performed following mobility separation, using collision energies between 30–35 eV in the transfer cell.

Results and discussion

Systematic investigations of GGs in brain tumors revealed significant alterations in expression profiles relative to healthy brain matrices. IMS MS provided compelling evidence of the structural complexity of GG patterns in these pathological matrices, identifying: i) an increased number of glycoforms and greater ceramide chain diversity; ii) markedly elevated sialylation levels, ranging from mono- to octasialogangliosides; iii) novel GG structures bearing acetate (CH_3COO^-) modifications, suggesting potential implications in cholinergic signaling. These

findings emphasize the high sensitivity and specificity of IMS MS and CID MS/MS in detecting rare GG species and resolving structural isomers in body fluids, where such molecules occur at considerably lower abundance than in brain tissue. Several of the identified GGs may serve as promising biochemical markers for early disease detection and prognosis, and could potentially be exploited as therapeutic targets. Furthermore, the pronounced overexpression of certain glycolipids in patient biopsies, compared to healthy controls, underscores their diagnostic potential.

Conclusion

Our IMS MS and CID MS/MS workflow enables detailed structural characterization of GGs, revealing tumor-specific alterations with biomarker and therapeutic potential. This high-performance method represents a valuable tool for CNS glycolipidomics, advancing both fundamental neuroscience and clinical applications in brain tumor and neurodegenerative disease research.

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COMPUTATIONAL APPROACH FOR SELECTIVITY INVESTIGATION OF HOMOLOGOUS KINASES

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Abstract

Janus Kinases (JAKs) are tyrosine kinases central to cytokine-mediated signaling pathways and play vital roles in chronic inflammatory diseases such as rheumatoid arthritis and psoriasis [1,2]. Within this family, JAK1 represents an attractive therapeutic target due to its involvement in immune signaling. However, the high structural similarity between JAK1 and JAK2 complicates the design of selective inhibitors, raising the need for refined analytical approaches. In this work, we applied an intricate computational workflow combining molecular docking, interaction fingerprint analysis, and statistical validation to explore subtle structural differences between JAK1 and JAK2. Bioactivity data for about 2000 kinase inhibitors were retrieved from activity databases and filtered into active and inactive subsets. Structural alignments revealed six critical residue differences near the ATP-binding site, including substitutions in the glycine loop and gatekeeper region, which modify binding pocket shape and electrostatic properties. A validation set of known actives and inactives was used to benchmark docking protocols in Schrödinger Maestro[3]. Receiver operating characteristic (ROC) analysis identified the energy scoring of superior enrichment, supporting its use as a decisive ranking metric [4]. Interaction profiling of the resulting data highlighted JAK1-specific hydrogen bonding and side-chain interactions in β -sheet regions, suggesting opportunities for exploiting larger ligand scaffolds. Subsequent virtual screening of an in-house library of bioactive compounds identified the top candidates with preferential JAK1 selectivity. Notably, the set included clinically relevant kinase inhibitors, thereby validating the robustness of the workflow. These results underline that even subtle amino acid differences between homologous kinases can be analytically harnessed to predict selective binding.

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CATALYTIC/PHOTOCTALYTIC ACTIVITY OF MELAMINE-MODIFIED BIOCHAR FOR TRIMETHOPRIM DEGRADATION

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Recalcitrant contaminants like Trimethoprim (TRIM) and other antibiotics in wastewater effluents pose significant ecological risks, including bacterial resistance threatening human and animal health. The EU has mandated advanced treatment processes to address this. Persulfate-based advanced oxidation processes (PS-AOPs) effectively remove these pollutants, with biochar/modified biochar as a robust catalyst for persulfate activation. Modified biochar can offer both catalytic and photocatalytic efficiency. Melamine (M), a nitrogen-rich compound, can enhance biochar's activity by replacing O-species with N-species, and enhance electron density and stability. Further, melamine converts to graphitic carbon nitride (g-C₃N₄, a photocatalyst) at $\approx 550^\circ\text{C}$ and it may combine with biochar that likely boost its catalytic/photocatalytic efficiency, reusability, and stability.

The current research therefore, focuses on the preparation melamine composites using grass-pellet (GP) biomass under the nitrogen atmosphere for TRIM degradation. Firstly, melamine was mixed with grass pellet and pyrolyzed at 700°C (i.e. GP-M) and second, it was mixed with prepared biochar (BC) at 700°C and then reheated at 550°C (i.e. BC-M). Varied ratios of GP/BC: M was used. Both composite sets were investigated under UV source i.e. LED at 398 nm for photocatalytic experiments.

In the GP-M composite set under dark conditions, increasing the melamine ratio in GP enhanced TRIM degradation, with the most effective 1:2 ratio degrading 80% of 5×10^{-5} M TRIM in 20 min using 2 mM PMS and 0.5 g/L catalyst dose; however, 20% adsorption also occurred, accounting for complete TRIM removal. Activity largely depended on the melamine amount mixed with GP. In the BC-M composite set, efficiency was significantly less than GP-M, achieving only 44% degradation at a BC: M ratio of 1:051 under the same TRIM, PMS, and catalyst dose. It was better to treat the grass-pellet with melamine rather than the prepared biochar to achieve higher efficiency in dark conditions. Under UV light, both composites performed better with combined use of PMS, UV and catalysts achieving over 90% TRIM degradation even with the lowest melamine ratio. However, using PMS or UV alone with catalyst did not significantly improve degradation for either composite type. A synergistic effect of PMS, UV, and catalyst likely enhances TRIM degradation when used together compared to individual applications.

It can be concluded that GP-M effectively activated PMS and degraded TRIM in both dark and UV light conditions, while BC-M showed better performance under UV light than in dark. The melamine quantity and its integration method—mixed with raw grass-pellet or biochar—affect degradation efficiency. Ongoing studies explore radical mechanisms, characterization, and reusability.

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THE EFFECT OF THE METAL IONS ON THE CATALYTIC ACTIVITY OF TEM-1 β -LACTAMASE

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Abstract

The kinetic parameters of TEM-1 β -lactamase promoted ampicillin hydrolysis were revisited. The hydrolytic process was described by the kinetic analysis of the set of catalytic progress curves recorded at multiple wavelengths, including various concentrations of the enzyme and substrate. The primary hydrolysis product of ampicillin was converted to a second product, needed also to be considered in the evaluation process. Thus, instead of the usual Michealis-Menten formalism, the full set of the stoichiometric and rate equations were used in the calculations. We showed that the catalytic activity of TEM-1 β -lactamase was slightly decreased by the gradual increase of concentration of Hg(II). These catalytic progress curves could be fitted allowing the change of the active enzyme concentration, yielding the same kinetic parameter values as in the absence of Hg(II). However, we have found that Ni(II) and Cd(II) ions slightly promoted the enzyme activity. We suggest the binding of these metal ions to the β -lactam ring of antibiotics activating the substrate for the nucleophilic attack by the enzyme.

Introduction

Some bacteria are resistant to β -lactam antibiotics due to the expression of enzymes like TEM-1 β -lactamase. The enzyme consists of 286 amino acids, but 24-286 residues were detected by the X-ray diffraction method reflecting the mature form of the enzyme [1,2]. Ser70 is employed as a nucleophile hydrolyzing β -lactams while metallo- β -lactamases utilize a Zn(II)-activated water molecule as a nucleophile. TEM-1 β -lactamase is not a metallo-enzyme, but it contains several putative metal ion binding sites in its amino acid side-chains: three histidine pairs, two cysteines forming disulfide bridge, nine methionine residues, and other negatively charged side chains such as Asp, Glu residues. The success of the purification procedure by immobilized Ni(II) ion affinity chromatography proved that the protein can bind e.g., Ni(II) in its native form. In other words, the three pairs of His residues on the TEM-1 β lactamase surface allowed for binding to the borderline transition metal ion such as Ni(II) [3]. The two Cys residues of the mature TEM-1 β -lactamase close to the active center are involved in a structural disulfide bridge [4] that rarely interacts with metal ions, with the exception of Hg(II) [5]. In addition, TEM-1 β -lactamase the sulfur donor atoms in the thioether groups of Met residues can also bind Hg(II) ion and more weakly Cd(II) and Ni(II) [6-9]. The catalytic activity of the enzyme was assessed in the absence and presence of metal ions like Ni(II), Cd(II), and Hg(II) against the ampicillin substrate. Interaction of TEM-1 β -lactamase with some metal ions Ni(II), Hg(II), and Cd(II) is our target of scientific research due to developing efficient antibiotics, as well as their environmental effects.

Experimental

Two buffers (20 mM Tris-HCl, pH 7.5; and 50 mM phosphate buffer, pH 7.0) were applied in the process of determination of kinetic parameters. The purified TEM-1 β -lactamase or metallized TEM-1 β lactamase catalyzed the hydrolysis of ampicillin in the substrate concentrations range of 230 μ M – 930 μ M. The final concentration of purified enzyme was between 0.24 - 2.4 nM with and without metal ions (HgCl_2 , $\text{Hg}(\text{ClO}_4)_2$, NiCl_2 , CdCl_2) at various protein:metal ion molar ratios. The kinetic reactions were monitored using a Cary 3500 UV-Vis double beam 51 multi-cell and controlled temperature spectrophotometer at two temperatures (25 $^\circ\text{C}$ and 30 $^\circ\text{C}$) at multiple wavelengths between 210 – 235 nm, with 1.0 cm path length quartz cuvette (Hellma). The kinetic calculations were performed using ChemMech program. This program was developed specifically to fit more experimental curves simultaneously in a single run. The absorbance versus time curves can be calculated by the Beer-Lambert equation with an appropriate set of molar absorbance values. The experiments were supplemented by cell culture investigations at various metal ion concentrations.

Results and discussion

Complexation of TEM-1 β -lactamase by a metal ion may cause changes in the catalytic efficiency of the enzyme in the hydrolysis of β -lactam molecules. No significant changes were detected in the absorbance at 235 nm for the ampicillin solution without the enzyme but in the presence or absence metal ions upon incubation for several hours. The primary hydrolysis product was further converted into second product depending on the pH and temperature.

The catalytic activity of TEM-1 β -lactamase was slightly reduced by the gradual increase the $\text{Hg}(\text{II})$ ion concentration. However, this led to the same parameter values as in the absence of $\text{Hg}(\text{II})$ ion. This suggests that only the V_{max} values decreased when molar ratio of the $\text{Hg}(\text{II})$ ion and the enzyme increased, i.e., that $\text{Hg}(\text{II})$ ions did not affect the substrate binding property of the enzyme in a competitive manner, but they affected the concentration of the catalytically effective enzyme, thereby blocking a fraction of the enzyme molecules.

$\text{Ni}(\text{II})$, as a borderline transition metal ion, and $\text{Cd}(\text{II})$, which has a moderately soft character, probably could bind to the His residue pairs that are positioned on the surface of the enzyme. The experiment containing 10 $\times$ excess of $\text{Ni}(\text{II})$, and $\text{Cd}(\text{II})$ as compared to the apo-enzyme itself, revealed that in contrast to the $\text{Hg}(\text{II})$ containing catalytic system, the presence of $\text{Ni}(\text{II})$ or $\text{Cd}(\text{II})$ ions slightly promoted the catalytic activity of TEM-1 β -lactamase (**Fig. 1**).

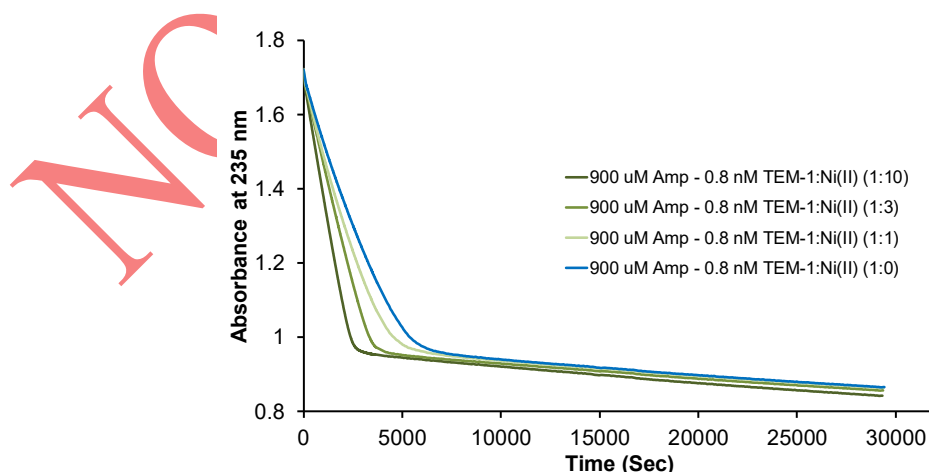


Figure 1. The effect of $\text{Ni}(\text{II})$ on the hydrolytic process of ampicillin catalyzed by TEM-1 β -lactamase in 50 mM phosphate buffer (pH 7.0) at 30 $^\circ\text{C}$.

These His residue pairs are far away from the active center, so this could not account for a direct effect of Ni(II) and Cd(II) on substrate-enzyme complex in the active center. On the other hand, these metal ions are also supposed to bind ampicillin close to the β lactam ring via nitrogen and oxygen donor groups [11;12]. It is well known that the Lewis acid property of metal ions may promote the hydrolysis processes of the β -lactam ring by a different mechanistic pathway [13;14]. Therefore, we suppose that the hydrolytic efficiency may be enhanced by Ni(II) or Cd(II) ions, by binding to the antibiotics with a concomitant deactivation or activation of the substrate for the nucleophilic attack by Ser70 residue of the enzyme [11;15]. At the same time, Hg(II) is supposed to bind to the sulfur donor atom of a soft character (**Fig. 2**)

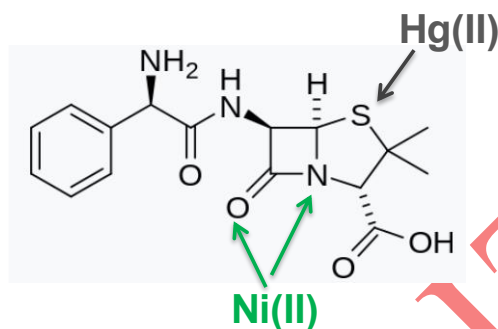


Figure 2. The proposed binding sites of metal ions to ampicillin.

The above results were well supported by the cell culture experiments, which also reflected the activation of the enzyme by Ni(II), and inhibition by Hg(II).

Conclusion

TEM-1 β -lactamase activity was monitored by spectrophotometry via hydrolysis of ampicillin as a substrate. Continuous decrease of the measured values was experienced upon recording the absorbances for an extended period suggesting that the primary hydrolysis product was further converted into different molecules depending on the pH and temperature. Ni(II) and Cd(II) slightly promoted the enzyme activity but it was slightly reduced by the gradual increase of Hg(II). We suggested the coordination of the metal ions to antibiotic donor groups. This coordination in case of Ni(II) and Cd(II) occurs through the β lactam O and N donor atoms, which causes activation of the substrate. Hg(II) shall bind to the S donor atom. The observed changes in the hydrolytic activity in the presence of Hg(II) could not be explained only by the metal ion interaction with the substrate, but complexation with the methionine S atoms close to the active center shall also be considered. Hg(II) in fact, influences the concentration of the catalytically effective enzyme possibly by blocking a fraction of the enzyme molecules.

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EFFECT OF PRINTING TEMPERATURE ON THE MECHANICAL AND THERMAL PROPERTIES OF PRINTED SPECIMENS MADE FROM PACKAGING PLA

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Abstract

Traditional plastic packaging ending up in the environment poses a serious problem, one possible solution to which would be the use of biopolymer packaging materials such as PLA. However, it would be even better if we could recycle the used packaging PLA as printing filament. The popularity of 3D printing and the demand for sustainable raw materials would ensure a steady market for recycled PLA filaments. First, we need to know whether the raw material is printable and how it is affected by various printing parameters, such as printing temperature. The properties of the printed test specimens made from the original Ingeo 7032D PLA for packaging can be changed by increasing the printing temperature. The higher the temperature at which they are printed, the higher the degree of crystallinity of the test specimens. Increasing the printing temperature also affects the mechanical properties, but this is not only due to the increase in crystallinity, but as higher printing temperatures also improve the welding of the filaments, thereby improving the mechanical properties.

Introduction

One of the biggest problems of consumer society is the large amount of waste generated and what we do with it, or rather, what we do not do with it. The issue of responsibility goes beyond the average person; we also need to talk about the responsibility of companies, company managers, countries, and country leaders. Just as the average person can decide whether to throw an empty bottle in the trash or just throw it away, companies and country leaders are also responsible for the decisions they make that affect the environment. More studies and publications are coming to light in which the most polluting companies are collected, and it is sad that less than a hundred companies have been causing the greatest destruction to the environment for a little more than a century. These include large oil companies and large food manufacturing companies that package their products in plastic. [1-3]

The sorting and recycling of selectively collected plastic waste could be solved, the main problem is the lack of proper collection, so a lot of otherwise recyclable plastic ends up in landfills. [4-7] Or, even worse, container ships take the garbage of richer countries to for example Africa, labeling the garbage as a second-hand product, and it is dumped right along the coast, then the lightweight plastic pieces can be washed into the sea and oceans, where garbage islands are formed. [8-14]

One of the possible solutions in an engineer way to reduce the amount of waste is to make plastics degradable or to use biodegradable polymers. One of the most intensively researched biopolymers is PLA (Poly-Lactic Acid). PLA can be produced from natural materials and is a biodegradable polymer under industrial conditions, by composting. PLA is a thermoplastic, semi-crystalline polyester, the basis of its production is lactic acid fermentation. Two isomers occur: L-lactide and D-lactide. Commercially available PLA materials are copolymers that contain L-lactide (PLLA, Poly-L-Lactic Acid) and D,L-lactide (PDLLA, Poly-D,L-Lactic

Acid). Due to their different ratios, they have different properties, different glass transition and melting temperatures.

The good mechanical properties of PLA (60 MPa tensile strength, 3 GPa modulus of elasticity) have also contributed to its widespread use in two areas. One of these areas is the packaging industry, where it is a good alternative to traditional materials. The other area is 3D printing, where its ease of use makes it popular not only with companies but also with average consumers. [15-19]

Due to its brittleness, it has not yet become widespread in the engineering field, but many researchers are working to modify this. However, its popularity as a printing material could be exploited, and the production of printer filaments from packaging waste could be an alternative way of recycling it.

Previous research [20] has shown that Natureworks Ingeo 7032D packaging-optimized PLA raw material is suitable for producing printing filaments. The aim of this study is to examine how the different printing temperatures affect the mechanical and thermal properties of the printed test specimen made from the original material.

Experimental

Natureworks Ingeo 7032D is a PLA used for bottle blowing, so it is suitable for replacing traditional PET bottles in case of storing non-carbonated beverages.

The filament from Ingeo PLA was prepared by Collin Teach-Line E20T extruder using a Collin Teach-Line CSG171T extruder line. Before extrusion, PLA was drying at 60°C and 4 hours. The temperatures of the extruder were 190, 200, 210, 220°C (from hopper to die) and the rate of the screw was 40 rpm. The diameter of the filament was 1.75 mm.

A Craftbot Plus FFF technique 3D printer was used to print test specimens. Two shapes were printed on the measurements, dog bone shaped specimen to tensile test and simple rectangular column shaped specimen for impact test. In both cases 5-5 pieces were measured in every setting, and the investigated cross-section was 4x10 mm.

The printer can create different structures. For the tests, a triangular structure was selected from the standard settings, where a layer of printing is formed from triangular shapes (Figure 1). The infill density was 100%. The printing temperature was set to three different levels: 210, 220, and 230 °C. The tray temperature was 60 °C and the printing speed was 50 mm/s.

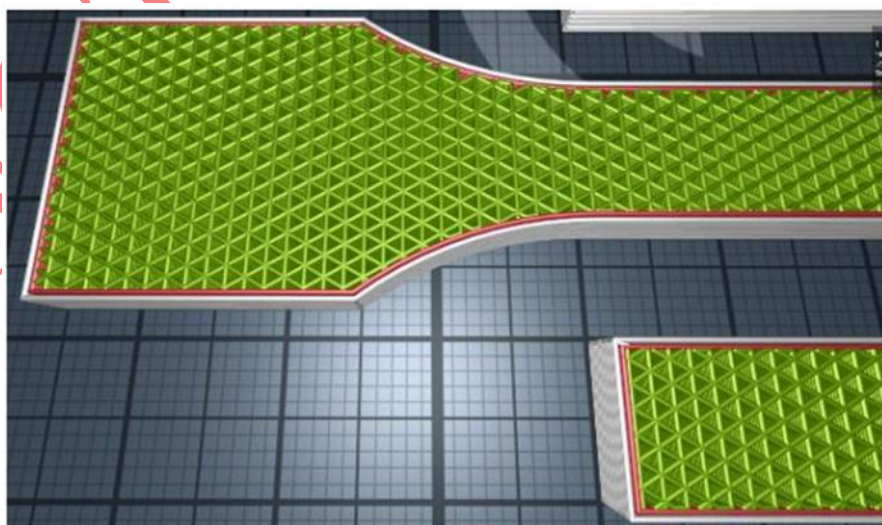


Figure 1. Triangle shape printed structure of the specimens

DSC (Differential Scanning Calorimetry) tests were performed on the specimens by TA Q200 heat-flux DSC instrument. The sample weights were about 5 mg. The applied gas during the DSC scan was nitrogen with 50 mL/min flowing rate. The temperature range was from 30°C to 200°C and the heating rate was 20 °C/min. The DSC measurements were analyzed with the TA Universal Analysis software. Only the first heating was analyzed.

The printing samples were investigated by tensile and Charpy impact tests at room temperature. The tensile test was performed by Instron 3366 universal testing machine with a 10 mm/min measuring rate. Charpy impact test was performed by Ceast Impactor II with 5 J hammer.

Results and discussion

One disadvantage of PLA, similar to PET, is that its crystallization tendency is slow, so with the usual processing technologies and technological settings, it is difficult to achieve the appropriate degree of crystallinity when using pure material and it is more often possible to produce a product with a larger amorphous fraction. [21-26]

The DSC curves of samples printed at different temperatures also confirm this (Figure 2). The cooling conditions of the printing were too intense for PLA, preventing the crystallization process from being completed, resulting in cold crystallization visible at around 120 °C on all three samples. This means that once the glass transition temperature (around 60 °C) is exceeded, the macromolecules begin to move using the heating energy and can create the missing crystalline phases.

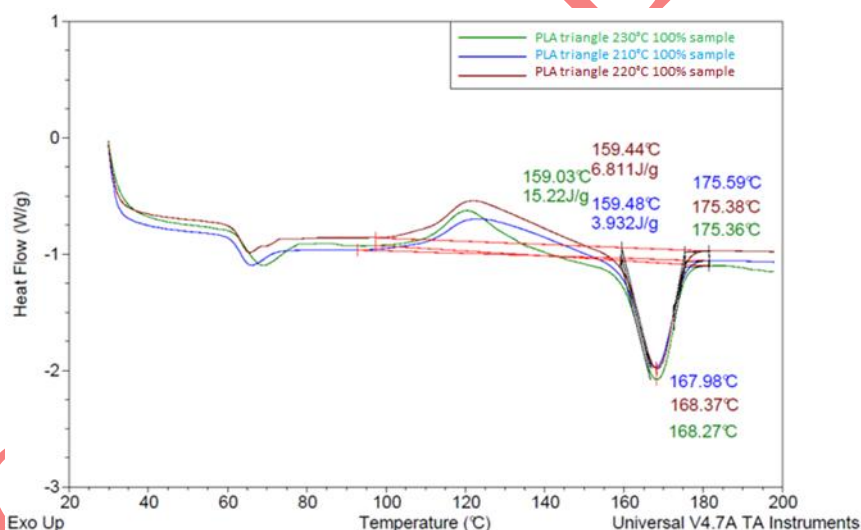


Figure 2. DSC curves of printed specimens

However, Figure 2 also shows that, with increasing printing temperatures, with almost the same melting curves, the shapes of the cold crystallizations differ, appearing smaller as the temperature increases, and the heat of melting values read in J/g also increase. In Figure 2 corrected values are represented that no longer include the J/g values measured during cold crystallization. The enthalpy change of cold crystallization has been subtracted from the enthalpy change of melting. It means that higher printing temperatures result in the formation of more crystalline phases. This is presumably due to the fact that, under the same cooling conditions, the higher printing temperature allows more time for the material to cool, thus allowing more time to create a hierarchically built-up polymer crystal structure.

Since the degree of crystallinity of the printed test specimen increases with rising printing temperature, this predicts a change in strength values.

Table 1 shows the mechanical properties of the examined test specimens. The results prove that increasing the printing temperature causes a slight increase in impact strength and tensile strength, while the tensile modulus decreases slightly accordingly. Due to the brittle behavior of PLA, increasing the printing temperature has practically no effect on tensile strain.

However, the change in mechanical properties cannot be entirely attributed to the increase in crystallinity, as higher printing temperatures also improve filaments welding, which leads to an increase in strength values, too.

At higher temperatures, the viscosity of the material decreases, its flowability improves, allowing the macromolecules of the contacting surfaces to diffuse into each other more easily.

Table 1. Mechanical properties of the printed specimens

Mechanical properties	Printing temperature [°C]		
	210	220	230
Impact strenght, average [kJ/m ²]	9,08	9,95	12,5
Impact strenght, st. dev. [kJ/m ²]	0,82	0,58	0,96
Tensile modulus, average [MPa]	2161	2109	1881
Tensile modulus, st. dev. [MPa]	129	90	130
Tensile strenght, average [MPa]	28,7	30,2	33,9
Tensile strenght, st. dev. [MPa]	2,89	1,94	3,82
Tensile strain, average [%]	2,15	2,17	2,33
Tensile strain, st. dev. [%]	0,2	0,07	0,33

Conclusion

The properties of printed test specimens from Ingeo 7032D packaging PLA can be changed by increasing the printing temperature. The higher the temperature at which they are printed, the higher the degree of crystallinity of the test specimens, because the material has more time to cool down, allowing it to form more crystalline phases.

Increasing the printing temperature also affects the mechanical properties, with an increase in impact strength and tensile strength values. However, these are not only due to the increase in crystallinity; the higher printing temperature also improves the welding of the filaments, thereby improving the mechanical properties.

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LCA OF SEMI-TRANSPARENT PHOTOVOLTAICS UNDER DEVELOPMENT IN THE TRANSMIT PROJECT

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Abstract

Window-integrated solar panels offer a complementary solution to rooftop photovoltaics by converting building facades into energy-harvesting surfaces while improving energy efficiency. The TRANSMIT international research project develops semi-transparent photovoltaic (STPV) windows with a target average visual transparency of 50% and a power conversion efficiency of 8%, using micro-stripped architectures based on CIGS and perovskite materials. Life Cycle Assessments (LCA) of laboratory-scale devices show climate change impacts of 251.69 kg CO₂ eq. per m² for CIGS type STPV, and 136.09 kg CO₂ eq. per m² for the perovskite type. Although these impacts reflect early-stage prototypes, significant reductions are expected with process optimization and scale-up. The project also investigates recycling strategies to support circular economy principles and reduce dependence on critical raw materials, highlighting STPVs' role in advancing net-zero energy buildings.

Introduction

Window-integrated solar panels are valuable supplements to traditional rooftop photovoltaic (PV) panels, primarily by maximizing a building's total energy-generating surface area. While conventional panels are limited to roof space, solar windows convert vertical facades—especially on skyscrapers—into massive, productive solar arrays. This expands the system's capacity without occupying extra land or compromising a building's aesthetic. Furthermore, they contribute to overall energy efficiency by reducing solar heat gain through the glass, which lowers the cooling load on HVAC systems. By combining electricity generation with reduced energy consumption from the building envelope, solar windows and rooftop panels work together to move a structure closer to net-zero energy status.

The TRANSMIT project aims to develop advanced semi-transparent photovoltaic (STPV) technology for energy-harvesting windows. The primary goal is to create devices with a high average visual transparency (AVT) of 50% and a power conversion efficiency (PCE) of 8%. The core innovation is a design based on micro-stripped solar cells, which are indistinguishable to the human eye, separated by transparent gaps. This approach is intended to overcome the aesthetic drawbacks of current building-integrated photovoltaics (BIPV), such as the impeded view of crystalline silicon (c-Si) or the unpleasant orange color of amorphous silicon (a-Si) windows. The project utilizes two high-performing solar cell materials: CIGS (Cu (In,Ga) Se₂) which has been long-known for its stability and high efficiency and Perovskites (PSC) which is a newcomer but has tremendous potential for high performance.

Key objectives of the TRANSMIT project include fabricating STPV mini-modules and advancing the technology from a proof-of-concept stage (TRL3) to a validated prototype in a

relevant environment (TRL5). The consortium of partners will also conduct comprehensive assessments on the devices' performance, durability, environmental impact, and socio-economic acceptance. The project is coordinated by the International Iberian Nanotechnology Laboratory (INL), the participants are: Italian National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy; University of Cyprus (UCY), Cyprus; Middle East Technical University (METU), Türkiye; ODTU Center for Solar Energy Research and Applications, (ODTU-GUNAM), Türkiye and Bay Zoltán Research Centre (BZN), Hungary.

Life Cycle Assessments

The LCA examinations evaluate the environmental impacts of laboratory-scale STPVs to identify production "hotspots" for improvement. The assessment used a declared unit of 1 m² of the solar panel. The system boundary was defined as "cradle-to-gate", meaning it covers the raw material supply and the manufacturing phases but excludes the transport of raw materials, as well as the product's use and end-of-life stages. The life cycle modelling was conducted in accordance with the ISO 14040 and ISO 14044 standards. The model was created using the LCA for Experts software (formerly known as GaBi Professional). Process data was sourced from the Managed LCA content (Sphera) database and the Ecoinvent (v3.10) database. Environmental impacts were calculated using the Environmental Footprint (EF 3.1) method. The analysis focused on four key impact categories: Climate Change, Resource use (fossils), Resource use (minerals and metals), and Water use. This study contains the life cycle models and results of the TRL3 devices.

CIGS

The specific input and output data for the CIGS manufacturing process were provided by the project partner INL. The European average electricity grid mix was used in the model, as the theoretical production is not tied to a single country. Nitrogen gas was excluded from the CIGS model because the amount used was not determined and was considered negligible. The model follows the seven main manufacturing stages: photoresist deposition, photoresist exposure, DC (direct current) sputtering, photoresist removal, selenization, buffer layer deposition and finally window layer deposition.

Results

- The total Climate Change impact was 251.69 kg CO₂ eq. per m², which converts to 0.082 kg CO₂ eq. per kWh for comparison purposes.
- The DC Sputtering manufacturing step was the one with the highest environmental impact in the Climate Change – total and both Resource use impact categories.
- In the Climate Change – total environmental impact category the impact was primarily driven by high electricity consumption due to the unoptimized, repetitive nature of laboratory-scale production.
- For the resource use of minerals and metals, indium and molybdenum were the main contributors for the DC Sputtering manufacturing step.

Perovskite

The data for material and energy flows was determined through allocation by the Italian National Interuniversity Consortium of Materials Science and Technology (INSTM), who developed the perovskite cell. The main stages of fabrication were the following: substrate cleaning, ETL (Electron Transport Layer) deposition, perovskite deposition, HTL (Hole Transport Layer) deposition, TCO (Transparent Conductive Oxide) deposition, laser ablation

and encapsulation. When data for specific precursor materials was not available, a similar, well-documented chemical was substituted as a proxy.

Results

- The total Climate Change impact was 136.09 kg CO₂ eq. per m², which converts to 0.044 kg CO₂ eq. per kWh.
- The most significant contributing steps were Substrate cleaning and TCO deposition in all four chosen environmental impact categories.
- The main drivers for these impacts for Substrate cleaning in the Climate Change – total impact category were the incineration of waste solvents (acetone and isopropanol) and the production of these two solvents.

A critical point which needs to be emphasized is that these results are for TRL3 laboratory prototypes and are not directly comparable to the lower environmental impacts of commercially produced (TRL 9-10), opaque solar cells reported in the literature. The environmental impacts are expected to decrease significantly as the technology matures and scales up to industrial production.

Conclusion

In the TRANSMIT project, early-stage LCA results highlight key environmental hotspots in CIGS and perovskite manufacturing. Future work will expand the system boundary of the studies for the whole life cycle of the STPVs: producing raw materials, PV manufacturing, installation, the use phase and recycling methods after the developed STPV product becomes waste. Supposed recycling procedures will enable applying circular economy principles; thus, the depletion of rare earth metals and other substances necessary to produce STPVs can be diminished.

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CHANGING APPROACH TO CORPORATE SOCIAL RESPONSIBILITY

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Abstract

The responses to environmental and social problems have shown a significant development in recent decades. Achieving sustainability is a challenging goal. The initiatives under the concept of corporate social responsibility represent voluntary contributions. Ultimately, individuals stand behind the solutions and they are the beneficiaries of the results. Understanding their approach to the values and actions is essential. The study presents a survey among higher education students between 2018 and 2024. The results suggest a decline in confidence in corporate social responsibility, which strengthens the need for appropriate education.

Introduction

There has been significant development since the middle of the 20th century, from identifying environmental and social problems, through sustainability and corporate social responsibility (CSR) to recent solutions. Similarly, from waste management to circular economy, or from the rethinking of the SNA (System of National Accounts) indicators [1], through GRI (Global Reporting Initiatives) [2] and Sustainable Development Goals (SDG) [3] to ESG (Environmental, Social and Governance) reporting [4] the efforts and publications suggest remarkable progress. It should be noted that the past few decades seem like a lot for one lifetime; the above-mentioned concepts are essentially trying to answer the same question at a single moment in history.

The UN's SDGs offer a comprehensive framework for individuals, corporations, and nations alike. The top level of the goals is clear and understandable, while the detailed subject areas, with indicators and interrelations between them, make the complex nature of the problems unambiguous.

The concept of Corporate Social Responsibility (CSR) has been continuously evolving, with no single, definitive definition [5]. An early approach by Bowen [6] is still actual, which "refers to the obligations of businessmen to pursue those policies, to make those decisions, or to follow those lines of action which are desirable in terms of the objectives and values of our society" [6]. CSR can be considered a set of initiatives addressing sustainability issues at the corporate level, incorporating stakeholder values and interests into the business [7]. The main criticism against CSR is related to its voluntary nature. ESG takes the discussion of the problem to a new level; the systematic set of indicators offers comparable corporate reports.

However, the high priority of business interests, and especially, the greenwashing actions, may hinder the progress; building trust in CSR is important to effect any change.

In my opinion, the development of tools and methods will not stop in the near future, and former results should not be discarded. The values behind CSR initiatives are rooted in corporate culture, and their successful application depends on personal approaches. Local studies of student opinions in the field may contribute to a deeper understanding of the motivations behind environmentally conscious initiatives.

However, CSR covers corporate decisions, the decision-makers paying are individuals. Their knowledge level and values of the decision-makers are reflected in the design and implementation of such actions, of course, in line with corporate rules [8].

The goal of the study is to present the changes in the approach to CSR among higher education students between 2018 and 2024. The results draw attention to key issues and support the need for further research.

Experimental

A voluntary online survey was designed to explore the opinions of higher education students as future decision-makers about CSR. The questionnaire includes statements about CSR and asks the respondents to mark their level of agreement on a 5-point scale (1: do not agree at all, 5: totally agree). The database allows comparisons in time and space, with the purpose of searching for characteristic patterns and assessing the changes in opinions. The paper shows the analysis of the 2022-2024 data collection, and provides a comparison over time, including data from 2018 (Table 1).

	2018 sample	2022-2024 sample
Number of respondents	355	113
Gender		
female	184 (51.8%)	37 (32.7%)
male	171 (48.2%)	76 (67.3%)
CSR studies		
no CSR knowledge	215 (60.6%)	79 (69.9%)
superficial CSR knowledge	85 (23.9%)	19 (16.8%)
detailed CSR knowledge	55 (15.5%)	15 (13.3%)

Table 1. Sample characteristics

The student opinions are presented with the mean values of their assessment by questions and sub-samples. The statistical analysis used the non-parametric Kruskal-Wallis H test of IBM SPSS software [9] to check the significant differences in the sample. Additionally, a cluster analysis was performed. A limitation of the study is that the representativeness of the sample is not verified or assured; the generalization of the results is not feasible.

Results and discussion

The survey shows a declining confidence in CSR during the period under review (Table 2). Based on the mean values, trust is weakened regarding CSR's ability to help achieve sustainability and its coordinative support for various initiatives.

Survey items	2022-2024		2018	
	Mean	Std. Deviation	Mean	Std. Deviation
Help achieving sustainability	3.37	.990	3.73	.732
Another tool for companies to generate profit	3.13	.990	3.22	.904
Tool of greenwashing	3.10	1.077	2.94	.994
Help companies to coordinate initiatives	3.41	.930	3.55	.834
Successful only in large companies	2.74	1.161	2.66	1.074
Implementation is expensive	3.42	1.050	3.54	1.018

Table 2. Mean values and standard deviations in 2022-204 and 2028 samples

The students tend to think that CSR is available only for large companies and is often used as a greenwashing tool. At the same time, the high standard deviations suggest diverse opinions in both periods.

Figure 1 confirms the changes in opinions, but the slight differences are not decisive due to the sampling method. The Kruskal-Wallis H test revealed significant differences only in the first statement, regarding how CSR helps achieve sustainability ($H = 11.983$, $df = 1$, $p < 0.001$).

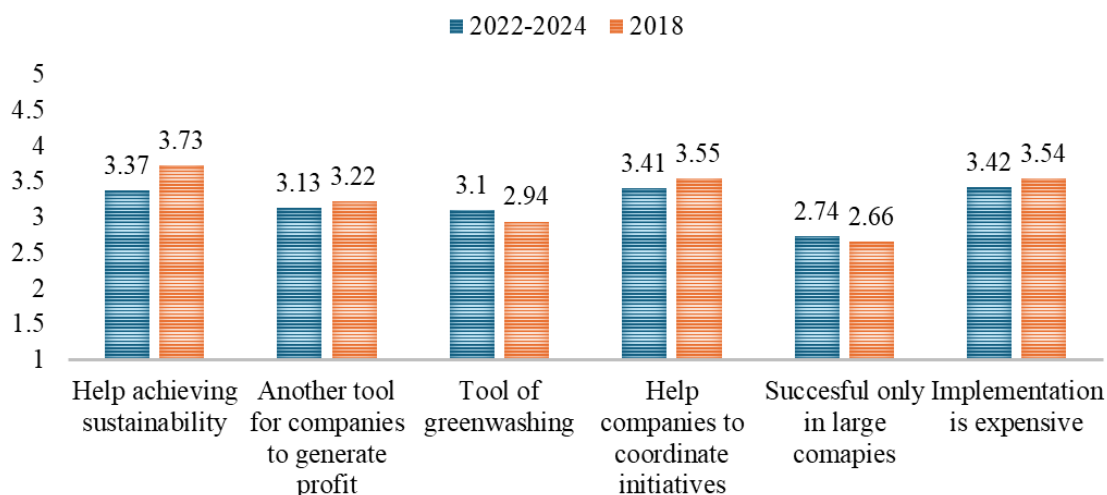


Figure 1. Comparing the mean values between the 2022-2024 and 2018 samples

Table 3 summarizes the results according to the 2022-2024 sample.

	Help achieving sustainability	Another tool for companies to generate profit	Tool of greenwashing	Help companies to coordinate initiatives	Successful only in large companies	Implementation is expensive
female	3.55	3.15	2.92	3.64	2.74	3.57
<i>Std. Deviation</i>	.904	.957	1.048	.913	1.130	1.006
male	3.18	3.11	3.29	3.17	2.73	3.27
<i>Std. Deviation</i>	1.042	1.026	1.078	.888	1.197	1.078
No CSR knowledge	3.43	3.13	3.13	3.42	2.84	3.55
<i>Std. Deviation</i>	.959	.999	1.082	.913	1.118	.993
Superficial knowledge	3.22	3.11	3.11	3.34	2.60	3.19
<i>Std. Deviation</i>	.993	.964	1.080	.933	1.157	1.041
Detailed knowledge	3.36	3.20	2.98	3.49	2.55	3.27
<i>Std. Deviation</i>	1.095	1.007	1.063	.998	1.303	1.209

Table 3. Mean values and standard deviations by questions, 2022-2024 sample

The statistical analysis of the sub-samples in the 2022-2024 sample found significant differences by gender about the role of CSR in achieving sustainability ($H = 13.213$, $df = 1$, $p < 0.001$).

0.001), greenwashing ($H = 9,878$, $df = 1$, $p = 0.002$), coordinative role ($H = 23.137$, $df = 1$, $p < 0.001$), and the expensive nature ($H = 6.308$, $df = 1$, $p = 0.012$). Females have higher confidence in CSR across all survey items.

According to the CSR knowledge level, the costs of implementation show significant differences ($H = 7.429$, $df = 2$, $p = 0.024$). Joining the students with superficial or detailed CSR knowledge, and compared to those without it, beyond the costs of implementation ($H = 7,150$, $df = 1$, $p = 0.007$), a significant difference was found that it can only be in large companies ($H = 4.948$, $df = 1$, $p = 0.026$).

Additionally, an automatic two-step cluster analysis was performed by IBM SPSS software. Three clusters (Figure 2) were identified, characterized by a fair silhouette measure of cohesion and separation (average silhouette = 0.3). There is a high level of agreement in profit generation, while other questions reveal different opinion patterns.

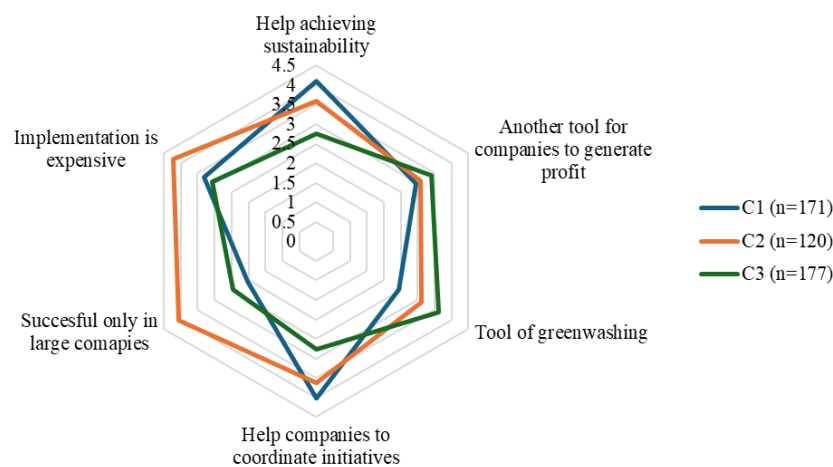


Figure 2. Mean values of the responses by clusters

A crosstabulation analysis between the grouping factors and the cluster membership could show significant differences by the period of data collection (Chi-square = 8.432, $df = 2$, $p = 0.015$). 41.4% of the 2022-2024 sample belongs to the C3 cluster (C1: 33.8%, C2: 24.8%), while 45.1% of the 2018 sample is the member of C1 cluster (C2: 28.4%, C3: 26.5%) which also confirms the unfavorable change in judgment about CSR.

Conclusion

The results indicate a decline in confidence in CSR between 2018 and 2024. The high standard deviations of the responses suggest that there is no ultimate agreement among the students. More respondents believe that CSR is merely a greenwashing tool, applicable only to large companies that justify their endeavors towards ESG measurements. Distrust seems to be general: the students do not believe that the cost implications could be a barrier to success.

The detailed analysis of recent data underlines the higher confidence of female respondents compared to males. In the mirror of the CSR knowledge level, the study confirmed previous results [10] [11]. The highest mean values (trust) are found among students with no prior knowledge of CSR. Superficial knowledge represents the greatest distrust. The results underline the well-known and long-voiced conclusion that establishing a targeted and effective education in the field remains pending. The opportunities of ESG may give a new impulse, and CSR will be rehabilitated as the value system behind the assessment. At the same time, SDGs play a key

role in setting the directions. According to scientific publications and academic initiatives, their relation to the goals is emphasized [12] to promote sustainability.

The data collection was performed before and after the COVID-19 lockdown period, but its direct impacts were not measured. However, the social and organizing changes affected by the pandemic have changed our lives in many areas [13] [14]; but many things have been rearranged. It can be assumed that uncertainty, failures, and concerns about the future left a mark on thinking about the future. Strict measures during the lockdown presented a completely different solution than voluntary and vague initiatives.

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PARAMETERIZED SYNTHESIS OF CSPbI₃ NANOCRYSTALS AND THEIR EFFECTS ON THE LIFECYCLE OF ISOPODS

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Abstract

In this study, the environmental impact of lead-containing perovskite semiconductor nanoparticles, widely used in next-generation solar cells, was evaluated. Perovskite solar cells are known for their outstanding power conversion efficiency (~26%) and relatively low production costs; however, their rapid market expansion raises concerns regarding the potential environmental consequences of future waste and the release of embedded nanomaterials. CsPbI₃ was synthesized via a solvothermal method at different temperatures to examine the influence of crystal size. The resulting perovskites were comprehensively characterized using multiple techniques: X-ray diffraction (XRD) for crystal structure analysis, scanning electron microscopy (SEM) for morphological characterization, and diffuse reflectance spectroscopy (DRS) for optical property assessment. The effects of the synthesized materials were investigated during a 4-week period, in different concentrations: 0,1%, 0,5% and 1,5% of the soil's weight. Each experimental unit contained 10 adult and 5 juvenile *Porcellio laevis* isopods. Throughout the study, a defined amount of fresh soil, controlled humidity, shelters, and minimal protein and calcium sources were provided, while no additional food was introduced to promote soil ingestion. Sampling was performed every four days. The primary objectives were to evaluate the effects of CsPbI₃ on isopod morphology (body length and mass) and mortality, and to determine the compound's half lethal dose (LD₅₀), thereby assessing its broader environmental impact.

DETERMINATION OF TOXICOLOGICALLY SIGNIFICANT IMPURITIES IN THE TECHNICAL SUBSTANCE PROTHIOCONAZOLE

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Abstract

In order to fulfill its potential, a plant protection product must be of satisfactory quality, which, among other things, implies that the active substance has the appropriate characteristics. In the synthesis of the active substance, a technical product is created. Besides the active substance, it could contain various impurities formed during the production process. The quality of technical substance is of great importance since it can contain contaminants that can harm human and animal health. Therefore, it is necessary, before using the technical substance, to determine the content of impurities of toxicological significance. The determination is carried out using appropriate qualitative and quantitative analytical methods. This study aimed to determine prothioconazole-desthio and toluene, impurities of toxicological significance in the technical material of the fungicide prothioconazole, widely applied to protect field crops from various phytopathogenic fungi. To determine the prothioconazole-desthio impurity in the prothioconazole technical substance, the high-performance liquid chromatography (HPLC) method was validated, while the gas chromatography (GC) method was assessed for the determination of toluene. Validation parameters such as linearity of the detector response, precision and accuracy of the method, limit of detection and limit of quantification were tested. The obtained results showed that all tested parameters fully met the requirements, thus confirming the methods' reliability for the determination of impurities prothioconazole-desthio and toluene in technical substance prothioconazole.

Introduction

Plant protection products (PPPs) may be produced, placed on the market, and used only if they are registered and supplied with a declaration and instructions for use, in accordance with the law and regulations [1]. Registration of a PPP includes testing its efficacy on target organisms, testing of the active substance, and physical and chemical properties. The safety assessment of pesticides requires, besides the main compound content, potential impurities that may be produced during synthesis.

The use of a pesticide of inadequate quality can lead to a decrease in its biological efficacy, the occurrence of phytotoxicity on cultivated plants, or a negative effect on the environment and human health. The verification of quality parameters is carried out using standard methods of CIPAC (Collaborative International Pesticides Analytical Council) or AOAC (Association of Official Agriculture Chemists), in laboratories that meet the standards of the ISO/IEC 17025:2017 system.

If there is no standardized procedure, it is necessary to validate the appropriate method. Validation involves testing a set of characteristics of an analytical method with the aim of proving that a given analytical method is suitable for a specific analytical purpose. The use of validated methods is one of the basic requirements of the ISO standard 17025 and the OECD principles of Good Laboratory Practice (GLP) [2].

Providing fast, accurate and reliable analytical data is one of the key factors for a successful production program in many industries. The quality of these data depends greatly on the analytical method used and its validity [3].

Prothioconazole is a broad-spectrum systemic fungicide from the triazole chemical group. Prothioconazole-based preparations are registered for use in field crops to control various fungi. In wheat, they are used to control the causative agents of various diseases of leaves, stems and ears (powdery mildew - *Blumeria graminis*, gray leaf spot - *Septoria tritici*, rust - *Puccinia spp*, fusarium head blight - *Fusarium spp*, head blight - *Tilletia caries*). In barley, they are used to control net leaf spot - *Pyrenophora teres*). They have also found application in oat, rye and corn crops. In oilseed rape, sunflower and soybeans, they are used to control the causative agent of white rot (*Sclerotinia sclerotiorum*) brown leaf spot (*Septoria glycines*) of soybeans and in sugar beet leaf spot (*Cercospora beticola*) [4].

Impurities of toxicological significance in the technical substance of prothioconazole are prothioconazole-desthio (< 0.5 g/kg) and toluene (< 5 g/kg) [5]. Since they occur in trace amounts, it is necessary to apply sufficiently sensitive and reliable analytical methods for their determination.

In this work, methods for the determination of prothioconazole-desthio and toluene, impurities of toxicological significance in the technical material of the fungicide prothioconazole, have been developed and validated.

Experimental

The experimental part of the study was conducted at the Laboratory for Biological Research and Pesticides, Department for Plant and Environmental Protection, Faculty of Agriculture in Novi Sad.

A stock solution with a concentration of 0.5085 mg/ml was prepared by dissolving 5.1 mg of the prothioconazole-desthio standard in a 10 ml standard beaker. A series of working solutions with concentrations of 0.05–0.51 mg/ml were prepared by diluting the stock solution.

An appropriate amount of toluene (105.0 mg) was dissolved in 25 ml of acetone (4.2 mg/ml) and homogenized ultrasonically. A series of standard solutions in the concentration range of 0.01–4.2 mg/ml were prepared from the stock solution.

Verification of chromatographic conditions was performed by examining the linearity of the detector response, the precision and accuracy of the method, the limit of detection and quantification.

Results and discussion

Determination of prothioconazole-desthio in the technical substance prothioconazole

The determination of the content of the prothioconazole-desthio, in the technical substance prothioconazole was performed using liquid chromatography.

For the analysis, LC system an Agilent Technologies 1100 Series with DAD detector was used. The satisfactory result was achieved using a Zorbax Eclipse XDB-C18 column (50 mm × 4.6mm × 1.8µm). The mobile phase was 1% phosphoric acid/acetonitrile 40/60 from 0 to 20 minutes, and changed to ratio of 30:70 after 20 minutes. The flow rate was 0.6 ml/min, and UV detection at 200 nm wavelength. The column temperature was 20 °C, and the injected volume was 10 µl. Retention time of prothioconazole-desthio was 2.823 min.

Figure 1 shows the chromatogram of the analytical standard prothioconazole-desthio (0.1 µg/ml) in acetonitrile, left, and the spectrum at a wavelength of 200 nm, right.

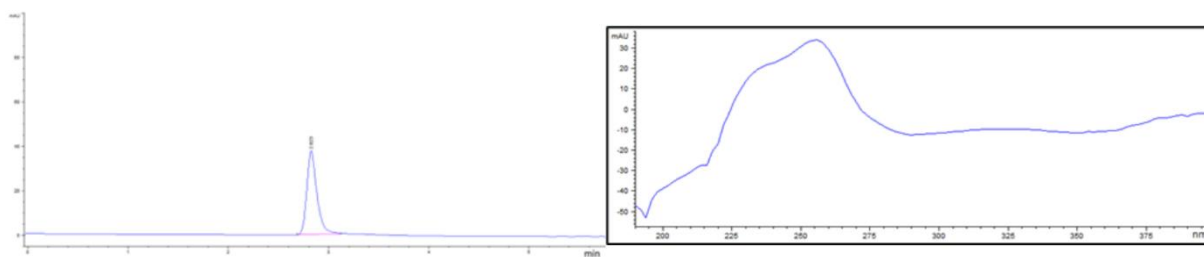


Figure 1 Chromatogram of the analytical standard prothioconazole-desthio (0.1 $\mu\text{g/ml}$) in acetonitrile, left; the spectrum of the analytical standard prothioconazole-desthio (0.1 $\mu\text{g/ml}$) at a wavelength of 200 nm, right

Validation parameters of the method for the determination of prothioconazole-desthio are given in Table 1.

Table 1 Validation parameters of the method for determination of prothioconazole-desthio in the technical substance prothioconazole

Parameter	Concentration interval (mg/ml)	Correlation coefficient	Precision of the method (%)	Recovery (%)	LOD (mg/ml)	LOQ (mg/ml)
Value	0.05–0.51	0.993	1.29	80.1–95.2	0.02	0.05

Linearity of this method was determined at five concentration levels in the range of 0.05–0.51 mg/ml. The correlation coefficient value of 0.993 confirms that the increase in the concentration of the analyte linearly follows the increase in the peak area. The precision was determined by injecting a solution of the analytical standard prothioconazole-desthio in acetonitrile six times. The relative standard deviation (RSD%) value of 1.29% indicates that good reproducibility of the determination of this compound was achieved by the applied method, considering the standard requirement of $\text{RSD} \leq 2$. The method accuracy was tested for three levels of enrichment. The recoveries (Rec, %) were in a range from 80.1% to 95.2%. The high agreement between the values obtained in the procedure and the actual values confirms the accuracy of the applied method. The LOD and LOQ of prothioconazole-desthio by the presented method are 0.02 mg/ml and 0.05 mg/ml.

Determination of toluene in the technical substance prothioconazole

To determine the content of toluene in the technical substance prothioconazole, gas chromatography with a flame ionization detector (GC-FID) was used. The analysis was performed using Shimadzu 2010 Gas Chromatograph equipped with a InterCap 5 column (df 0.25 μm , 0.32mm I.D. $\times$ 30 m), with nitrogen as the carrier gas, a split ratio of 20:3, an initial column temperature of 40 $^{\circ}\text{C}$ (held for 2 min); followed by a ramp of 20 $^{\circ}\text{C}/\text{min}$ to 260 $^{\circ}\text{C}$ (held for 3 min). The injector temperature was set at 230 $^{\circ}\text{C}$, the detector (FID) temperature at 250 $^{\circ}\text{C}$, and the injection volume was 1 μl . The retention time of toluene was 2.852 min, with a total run time of 10 min.

Figure 2 shows the chromatogram of prothioconazole technical substance in acetone with added toluene (0.5 mg/ml).

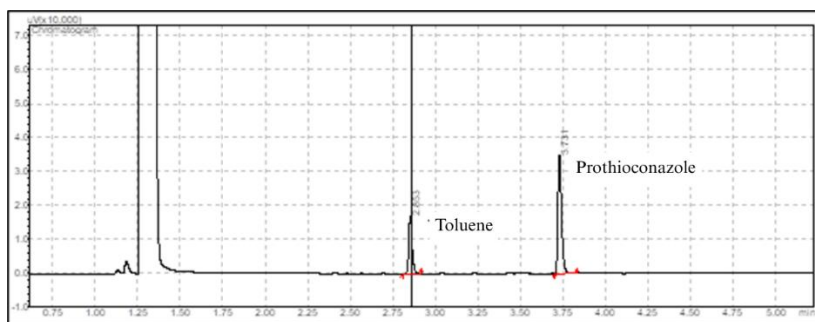


Figure 2 Chromatogram of prothioconazole technical substance in acetone with added toluene (0.5 mg/ml)

Table 2 summarizes the validation parameters of the method for the determination of toluene in the technical substance prothioconazole.

Table 2 Validation parameters of the method for the determination of toluene in the technical substance prothioconazole

Parameter	Concentration interval (mg/ml)	Correlation coefficient	Precision of the method (%)	Recovery (%)	LOD (mg/ml)	LOQ (mg/ml)
Value	0.1–4.0	0.999	1.27	86.3–91.2	0.03	0.1

Linearity was determined at five concentration levels in the range of 0.01–4.0 mg/ml. The correlation coefficient of 0.999 confirms that the increase in the concentration follows the increase in the peak area. The precision of the analysis was determined by injecting a solution of toluene in acetone six times. The value of the relative standard deviation (RSD%) of 1.27% indicates good reproducibility of the determination of this compound. As a parameter of the accuracy, the extraction yield (Rec, %) for three enrichment levels was examined. The average recoveries were 86.3–91.2%. The high agreement between the values obtained in the procedure and the actual values confirms the accuracy of the applied method. The LOD and LOQ for the determination of toluene in the technical substance prothioconazole are 0.03 mg/ml and 0.1 mg/ml.

Conclusion

In this research, reliable and reproducible analytical methods for determining prothioconazole-desthio and toluene impurities in the technical substance prothioconazole were developed. The study confirmed satisfactory linearity of the detectors' responses, the precision and accuracy of the methods, as well as the detection and quantification limits.

The results suggest that the presented methods meet the criteria for determining these impurities of toxicological significance in the technical prothioconazole, which recommends them for use in laboratories.

Acknowledgements

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NOT FINALIZED

ENHANCED SOLUBILIZATION OF KETOPROFEN USING TRITON X-100, TRITON X-165, BRIJ C10, AND THEIR MIXED MICELLE SYSTEMS

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Abstract

Ketoprofen, a Biopharmaceutics Classification System (BCS) class II drug, exhibits poor aqueous solubility, which limits its bioavailability and therapeutic performance. To address this, we investigated micellar systems composed of Triton X-100, Triton X-165, and Brij C10, studied individually and in binary and ternary mixtures, with the aim of enhancing solubilization efficiency. Critical micelle concentrations (*cmc*) were determined by fluorescence spectroscopy using pyrene as a probe, and the thermodynamics of mixed micelle formation were evaluated by Rubingh's model, Regular Solution Theory, and the Margules function to obtain interaction parameters and excess Gibbs free energies. Solubilization of ketoprofen was quantified by HPLC in terms of molar solubilization ratios and partition coefficients. Brij C10 exhibited the lowest *cmc* and the highest solubilization capacity, with molar solubilization ratios exceeding 6, while Triton micelles showed lower efficiency. Binary Brij–Triton mixtures revealed synergistic stabilization but occasional antagonistic solubilization, highlighting a trade-off between stability and drug incorporation. The ternary system, although thermodynamically stable, showed reduced solubilization due to compact packing. Overall, Brij-rich systems proved to be the most effective carriers, combining low *cmc* with high solubilization efficiency. These findings provide a thermodynamic basis for the rational design of surfactant mixtures for the solubilization of poorly water-soluble drugs.

Introduction

Ketoprofen, a widely used NSAID, suffers from low aqueous solubility despite high permeability, placing it in BCS Class II. Improving its solubility is critical for enhancing oral bioavailability. Micellar solubilization is a versatile approach, as surfactants self-assemble above the *cmc* to incorporate hydrophobic drugs. Mixed micelles can outperform single surfactants due to synergistic interactions. TX100 and TX165 are polyoxyethylene-based non-ionic surfactants of varying hydrophilicity, while BC10 is a Brij surfactant with strong hydrophobic contribution. The study aims to clarify how these systems, alone and in mixtures, influence micelle stability and ketoprofen uptake.

Experimental

- ***cmc* determination:** Fluorescence spectroscopy with pyrene probe at 278.15–318.15 K.
- **Thermodynamic analysis:** Rubingh's model, Regular Solution Theory, and Margules equations used to calculate β , ΔG^E , ΔS^E , and ΔH^E .
- **Solubilization studies:** Ketoprofen quantification via HPLC on C18 column, isocratic mobile phase (acetonitrile:acetic acid 65:35 v/v), detection at 330 nm. MSR, Δ MSR, and K_m calculated to assess solubilization efficiency.

Results and Discussion

- **cmc values:** BC10 showed the lowest *cmc* ($0.018\text{--}0.020\text{ mmol}\cdot\text{dm}^{-3}$), consistent with its hydrophobic chain. TX100 and TX165 *cmc* values matched literature ($0.2\text{--}0.6\text{ mmol}\cdot\text{dm}^{-3}$).
- **Binary mixtures:** BC10 + TX165 exhibited the strongest synergism ($\beta \approx -4.8$; $g^E \approx -2300\text{ J}\cdot\text{mol}^{-1}$ at 318 K). TX100 + BC10 showed composition-dependent behaviour, with negative g^E near equimolar ratios but positive values in BC10-rich mixtures.
- **Ternary mixture:** Though g^E was negative at most temperatures, indicating stability, compact micellar packing reduced drug accommodation.
- **Solubilization:** BC10 micelles achieved the highest molar solubilization ratio (MSR) (>6). Triton-only systems had $\text{MSR} < 1$. Binary Brij-Triton micelles improved stability but sometimes showed antagonistic ΔMSR . K_m values followed hydrophobicity: $\text{BC10} > \text{TX165/BC10} > \text{TX100/BC10}$.
- **Temperature effects:** At lower T , micellization was enthalpy-driven ($h^E < 0$), while at higher T entropy became dominant ($s^E > 0$), reflecting hydration changes and chain flexibility.

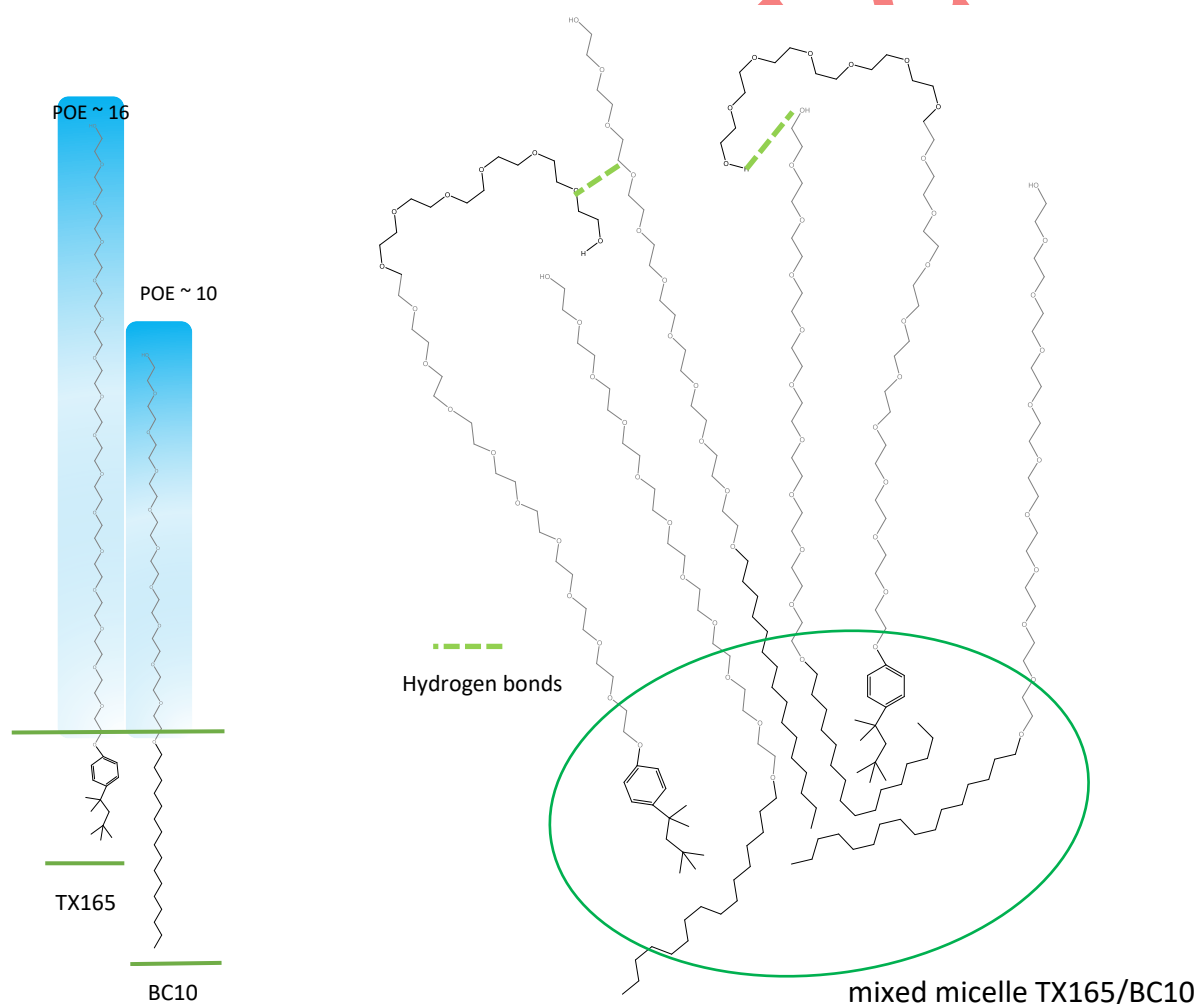


Figure 1. The TX165/BC10 mixed micelle

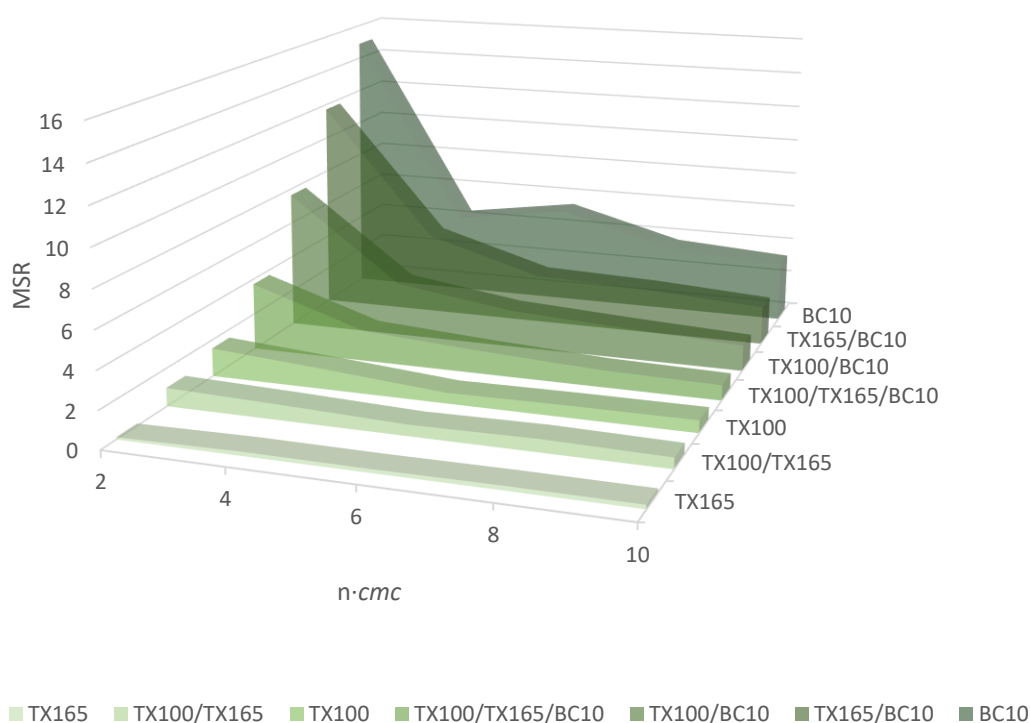


Figure 2. MSR values for single, binary, and ternary systems.

Conclusion

Micellar stability and drug solubilization efficiency are not directly correlated. Brij C10 micelles provide the strongest ketoprofen solubilization, while ternary mixtures highlight that excessive stabilization can reduce drug loading. These findings emphasize the need to balance stability and flexibility in surfactant design. Rational formulation using Brij-containing systems offers a promising strategy for BCS Class II drugs.

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POTENTIAL APPLICATION OF SILVER-DOPED TIN OXIDE THIN FILMS IN CNT GROWTH

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Abstract

Carbon nanotubes (CNTs) have outstanding electronic, thermal, and mechanical properties that have made them very attractive for applications in the field of energy storage, electronics, water treatment, sensors, and composites and structural materials. However, realizing the controlled CNT growth with the required diameter, density and uniformity remains a great challenge. The support layer, which is located between the substrate and the catalyst, has a critically important role in the regulation of the catalyst nanoparticle stability, diffusion and morphology. Also, it strongly influences the shape and productivity of CNTs. In this paper, undoped and silver-doped tin oxide (SnO₂ and Ag-SnO₂) thin films were fabricated by using spray pyrolysis with the moving nozzle (SPMN) technique. Effects of Ag as doped on the structural, optical, and electrical properties of SnO₂ thin films were studied for new recommendations as a support layer to grow the CNTs. The SnO₂ and Ag-SnO₂ thin films were characterized using XRD, IR, and UV-VIS spectrophotometry analysis, as well as four-point probe measurements. Therefore, their properties to control the catalysts and the growth of CNTs will be undertaken in future studies.

Introduction

Since the discovery of carbon nanotubes (CNTs) by Iijima in 1991 [1] which marked the initiation of extensive research on their unique structural, electronic, and mechanistic properties [2,3]. These characteristics make CNTs valuable in a large variety of applications mainly in the field of electronics, storage of energy, nanotechnologies, and bio-medical devices. Nevertheless, being able to effectively control the CNTs growth in terms of alignment, distribution of diameter, density, and purity is still a key hurdle to large-scale applications [4,5]. Among the existing CNTs fabrication methods, chemical vapor deposition (CVD) seems to be the most suitable one for growing CNTs as it provides better control over growth parameters and predefined locations on an etched substrate such as Si, stainless steel, and quartz [6,7]. A critical element in the outcome of CNTs growth based on CVD is the support layer that performs several basic functions, including prevention of catalyst diffusion in the substrate, prevention of Ostwald ripening and catalyst ripening. Different deposition methods were developed to prepare support layers with exact thickness, uniformity, and precise chemical properties. The materials widely used as support layer to overcome this barrier, a diverse range of oxidized metals (for example: Al₂O₃, SiO₂, MgO, TiO₂, and ZrO₂) [3] and metallic as TiN [3] are used for this purpose. It is worth noting that alumina (Al₂O₃) has been occurred as the most effective one due to its capability to yield high-density, thermally stable, and long-life catalytic nanoparticles. Furthermore, the surface energy of the substrate is the main factor controlling the size of the catalyst particles that form on the surface at a given temperature. The analytical characterization of CNTs using techniques such as SEM, TEM, Raman and XRD is focused on, as careful analyses are crucial not only to understanding its properties but also to

evaluate the potential environmental effects [8]. Although, SnO₂ thin films are extensively investigated in the field of materials science and nanotechnology because of their large band gap (approximately over 3.6 eV) and high transparency in the visible spectrum with excellent electrical conductivity. These properties make SnO₂ films suitable for different uses in conductive transparent electrodes, optoelectronic devices and gas sensors [9]. There is no research on using SnO₂ as a support layer for CNT growth, marking a clear unexplored area. A focus on SnO₂/MWCNTs nanocomposite with its usage in different fields such as gas sensors and photocatalysis, and high-performance Li-ion battery anodes [10]. Thus, behavior of SnO₂ as support layer on growth of the CNTs needs to be investigated as recent subject.

The aim of this paper is to exhibit procedures that were employed to deposit undoped SnO₂ and Ag-SnO₂ silver tin oxide (AgTO) thin films, and the finding results of these refined thin films. The structural, optical, and optoelectrical characteristics of undoped SnO₂ and AgTO, which were characterized using XRD, IR, and UV-VIS spectrophotometry analysis, as well as four-point probe measurements. SPMN deposited thin films are the main emphasis of this part of the present work. To establish the appropriate features that make our films as relevant as possible, effects of silver doping on the properties of AgTO films will be examined.

Experimental

Tin (II) chloride dihydrate (SnCl₂·2H₂O), a white crystalline solid, was used as the precursor for tin, while silver nitrate (AgNO₃) served as the dopant source with Ag/Sn concentrations averaged in (0 – 3) % at. Ag/Sn. Solution of tin precursor was prepared by melting 1.1282 g of SnCl₂·2H₂O in 10 mL of a mixture of solvents composed of double-distilled water and methanol in a 2:1 volume ratio. To guarantee complete solubility and clearness, a few drops of hydrochloric acid (HCl) was added. The solution was agitated for 30 minutes at room temperature to produce a transparent and clear solution. This basic solution was utilized directly to deposit SnO₂ thin films without any Ag addition, whereas Ag-doped SnO₂ thin films were achieved by addition to the mother solution the needed quantity of AgNO₃ to reach doping rates of 1, 1.5, 2, 2.5, and 3% at. Ag/Sn. Thin films were deposited by spray pyrolysis with a moving nozzle (SPMN) on 485 °C heated glass substrates having the follow characteristics (76.2 × 25.4 × 1–1.2 mm, TICARE). Such substrates were thoroughly cleaned with alcohol and distilled water, and then dried with a nitrogen gas stream in order to remove dust, oils, and other pollutants, to ensure a clean surface for high-quality thin film growth. Before deposition nozzle-substrate distance was fixed at 1.5 cm for all experiments.

Characterization Techniques

Deposited SnO₂ and Ag-doped SnO₂ thin films were systematically characterized. UV-Vis spectroscopy was utilized to assess the mean optical transparency (T) and estimate the optical band gap (E_g) of the films by using the Tauc's relation. The structural properties were investigated by X-ray diffraction (XRD), which gave insight into the crystalline phase, favored direction (Miller indices hkl), the lattice constants (a , b , and c), and the average crystal size (D) computed from the full width at half maximum (FWHM) of diffraction peaks by using the Scherrer equation. Fourier transform infrared spectroscopy (FT-IR) analysis was used both to confirm the chemical composition and identify characteristic absorption bands of Sn-O, O-Sn-O or Ag-O, and to verify any resulting structural modifications caused by silver addition. Lastly, the electrical performance of the films was evaluated using the four-point probe method to measure sheet resistance (R_{sh}), and the figure of merit ($\Phi = T^{10} / R_{sh}$) was calculated by combining optical and electrical data to assess the suitability of the films as transparent conductive oxides (TCOs).

Results and Discuss of Future Work to Grow CNTs

Impregnating SnO₂ with silver (Ag) doping improves electrical conductivity and optimizes crystallization and increases oxygen vacancy concentration. Such modifications further enhance the functionality of SnO₂ films in various applications [11, 12]. Effect of silver doping (0-3% at. Ag/Sn) on SnO₂ structural, optical, and electrical characteristics was investigated using XRD and IR, UV-VIS spectrophotometry analysis, and four-point probes as seen in Fig 1. Carried out results are as follows:

1. Structural and IR Analysis

- ✓ (0-3% at. Ag/Sn) Ag doped SnO₂ thin films were polycrystalline with a tetragonal rutile structure, according to X-ray diffraction (XRD) patterns. At Ag/Sn doping, a minor additive peak of silver oxide (Ag₂O) was seen at 2θ (29.5 and 31°). The incorporation of silver in the SnO₂ matrix was behaved by a left shift in 2θ degree of the peaks.
- ✓ Grain sizes were estimated to be between 16.071-27.304 nm on average.
- ✓ Before and after silver doped, FT-IR spectra of SnO₂ products revealed a novel Ag-O vibration mode with the well-known Sn-O vibrations which were observed at about 406-495 cm⁻¹.

2. Optical Analysis

- ✓ In the visible spectrum of 0-3% at. Ag/Sn doped SnO₂ thin films demonstrated remarkable transparency of over 70% for all silver doping concentrations, including 1.0, 1.5, 2.0, 2.5, and 3.0% at. Ag/Sn.
- ✓ Optical band gap (E_g) shows a significant drop, going from 3.76 eV for pure SnO₂ to about 3.06 eV for doped ones.

3. Electrical properties

- ✓ According to the electrical analysis, the thin films are n-type electrical conductivity which depends on silver doping concentration. For pure SnO₂ and AgTO with estimated thicknesses of 450 nm, the calculated figure of merit, Φ at $\lambda = 550$ nm showed a maximum value of around 1.427×10^{-2} ($\square/\Omega$) for 2.5% at. Ag/Sn silver doping concentration in thin films.
- ✓ Due to the high value of Φ and the low barrier for electrons to jump, $E_g \sim 3.06$ eV, AgTO may be considered preferred transparent electrodes for solar cells application.

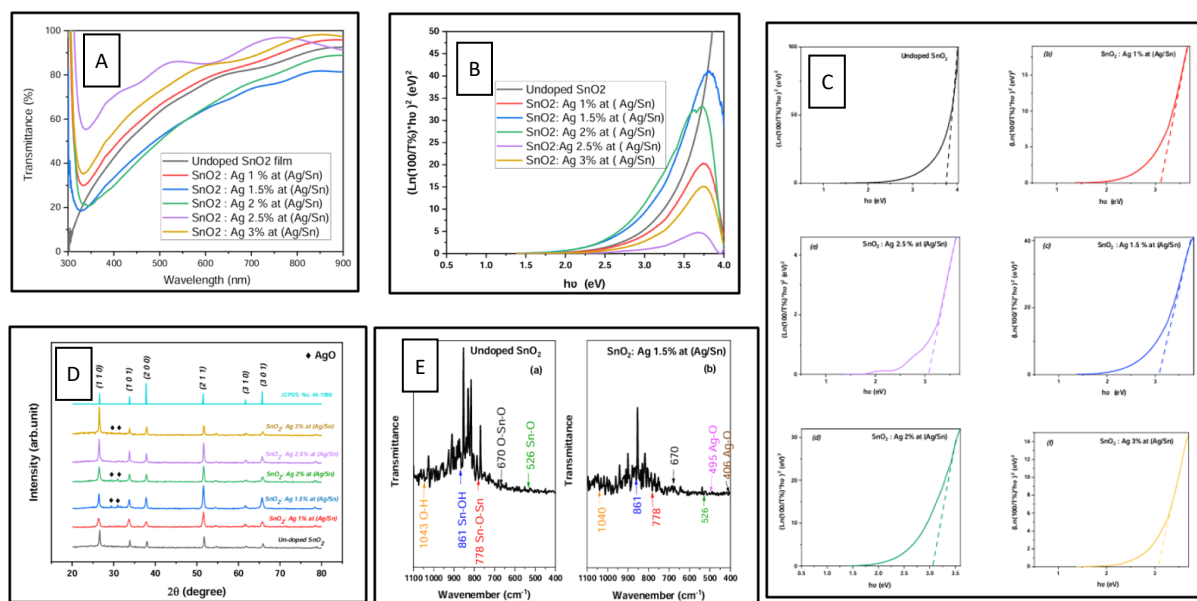


Fig.1: A) Optical transmittance plot of Ag (0–3 % at. Ag/Sn) doped SnO₂ thin films. B) Tauc relation plots gathering the feature of all samples. C) Tauc relation plots for each sample separately: a for undoped sample b, c, d, e, and f for 1, 1.5, 2, 2.5, and 3% at. Ag/Sn respectively. D) XRD patterns of Ag (0-3% at. Ag/Sn) doped SnO₂ thin films. E) FT-IR spectra of undoped and Ag-doped SnO₂ for 1% at. Ag/Sn films.

Conclusions

Growth of high-quality CNTs is strongly linked to the support layer design and geometry. The support layer works as much more than just a passive interface; it also controls the stability, diffusion, and crystallinity of the catalytic nanoparticles, which determines the structural and functional properties of the CNTs. So, clean, high-conductivity thin films made of SnO₂ have been optimized by the addition of Ag. Undoped thin films display an optical transmittance of more than 70% in the visible range, whereas the addition of Ag leads to an increase or a decrease depending on the concentration, with better enhancement at 1, 2.5 and 3% at. Ag/Sn. All the films demonstrate a polycrystalline SnO₂ tetragonal rutile structure with crystallite sizes ranging from 16 to 27 nm. FT-IR analysis verified the presence of Sn-O, O-Sn-O and Ag-O bonds. A minimum sheet resistance of 5.93 ($\Omega/\square$) is obtained at 1.5% Ag, and the maximum figure of merit $1.427 \times 10^{-2} \Omega^{-1}$ at 2.5% at. Ag/Sn doping. Thus, these properties of SnO₂ and Ag-SnO₂ will make it more effective and controllable for tailoring CNT growth to specific applications.

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LIFE CYCLE ASSESSMENT OF MATERIALS USED FOR PORTAL FRAME PRODUCTION

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Abstract

The construction sector plays a crucial role in global environmental impacts, making accurate life cycle assessment essential for sustainable decision making. This research evaluates the environmental impacts of timber, steel, and concrete in industrial portal frame structures using life cycle assessment. Timber shows the highest impact on land use but lower contributions to climate change and ecotoxicity. Steel has moderate climate impacts but the highest potential for freshwater ecotoxicity, while concrete is the most carbon-intensive, contributing most to climate change. The results highlight the importance of evaluating multiple impact categories for sustainable material selection.

Introduction

Buildings contribute significantly to environmental impacts, accounting for 35% of global energy use and 19% of energy-related greenhouse gas emissions in 2010, potentially doubling or tripling by 2050 [1]. Assessing the environmental impacts of building designs, particularly their role in climate change and environmental degradation, is a key motivation for this research [2]. Several studies emphasize timber construction's environmental benefits. Liang et al. (2020) [3] found a 12-story mass timber building reduced global warming potential by 18% and eutrophication by 47% compared to concrete. Guo et al. (2017) [4] showed cross laminated timber residential buildings in cold climates used 9.9% less energy and emitted 13.2% less carbon than concrete. Chen et al. (2020) [5] found a 12-story cross laminated timber building used 33% less material and emitted 70% less embodied carbon. Hegeir et al. (2022) [6] confirmed timber's lower environmental impacts in industrial buildings, mainly due to carbon storage.

The starting point of this research was the study by Hegeir et al. (2022) [6] where foreground data was used (Environmental Product Declarations), and in this research background data was used (Ecoinvent 3.7 database) [7]. The aim of this research is to compare the environmental impact of timber, steel, and concrete used in portal frame structures for industrial buildings by conducting a comprehensive LCA.

Experimental

A standardized LCA (ISO 14040:2006; ISO 14044:2006) [8,9] was performed, with environmental impacts calculated using openLCA software (version 2.3), a widely recognized tool for conducting LCA.

Goal and scope

The goal of the LCA is to evaluate potential environmental impacts associated with materials used for portal frame production in industrial buildings. Materials are timber, steel and concrete. The functional unit is kg/m² area. The area of the hall is 250 m², the total quantities of frames are 10 m span and 25 m span. In this research, the calculations refer to a 10 m span. This

research uses cradle to gate system boundaries. The geographic scope of this research is the Global (GLO) region, representing an average worldwide context for data. Fig. 1 presents system boundaries. Fig. 2 presents 3D drawing of the portal frames: (a) timber frames; (b) steel frames; (c) reinforced concrete frames [6]

Figure 1. System boundaries

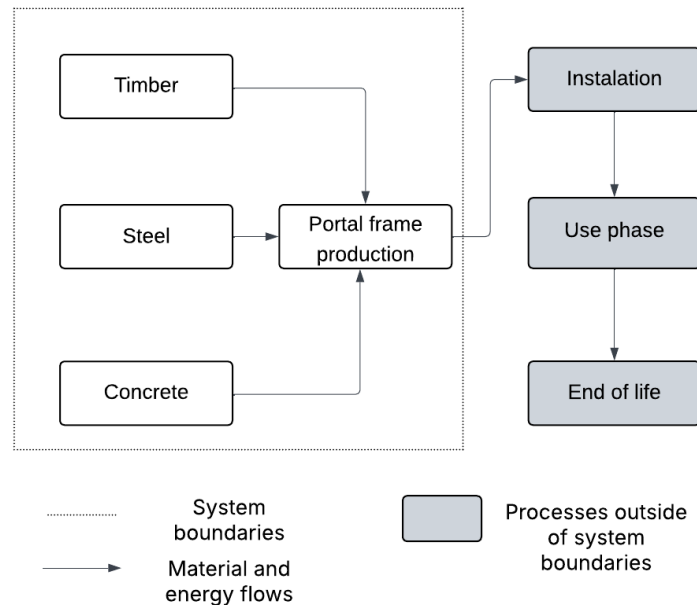
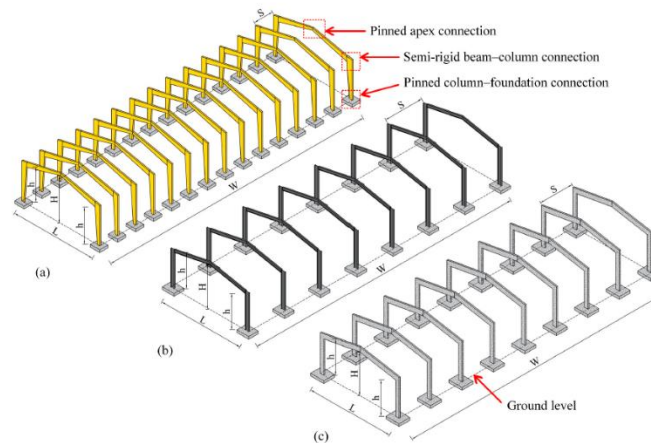


Fig. 2. 3D drawing of the portal frames: (a) timber frames; (b) steel frames; (c) reinforced concrete frames [6]



Assumptions and limitations:

The chosen Life Cycle Impact Assessment (LCIA) method focuses on midpoint indicators. This assumes that assessing impacts at the midpoint level (e.g., climate change, acidification) is sufficient to inform decision-making, even though endpoint assessments (e.g., damage to health or biodiversity) could offer more integrated views.

It is assumed that timber, steel, and concrete serve equivalent structural functions in portal frame applications, allowing for a direct comparison based on environmental impact per unit area. The research does not evaluate how material properties affect design efficiency (e.g., how much material is needed to achieve the same structural performance), potentially biasing results in favor of denser or more structurally efficient materials.

To assess the environmental impacts ReCiPe Midpoint (H) is used. This method is a widely used LCIA approach that translates environmental emissions and resource extractions into 18 impact categories, focusing on specific environmental problems (midpoints) to allow detailed and comparative sustainability assessments. The impact categories considered in this research for ReCiPe Midpoint (H) include: Agricultural land occupation (m^2/year), Climate change ($\text{kg CO}_2 \text{ eq}$), Fossil depletion (kg oil eq), Freshwater ecotoxicity (kg 1,4-DCB eq).

Inventory analysis

Data for used materials were extracted from the Ecoinvent 3.7 database with cut-off system model (Wernet et al., 2016) [7], which provides life cycle inventory data on a wide range of materials and processes. The quantities of material and energy flows are taken from the study by Hegeir et al. (2022) [6] and shown in Table 1.

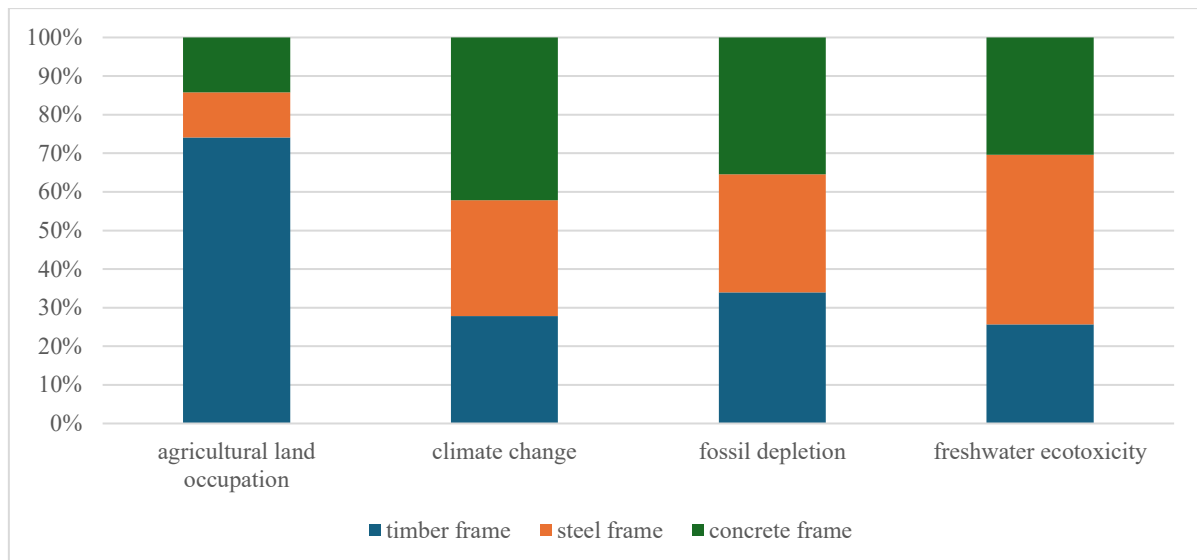
Table 1. Life cycle inventory for portal frame production [6]

Material/energy flow	Activity from Ecoinvent database	Location	Unit	Portal Frame production
timber, cross laminated	market for cross-laminated timber	RER	m^3	37.08
steel dowels	market for steel, low-alloyed	GLO	kg	390.62
steel bolts	market for steel, low-alloyed	GLO	kg	672.23
steel plates	market for steel, low-alloyed, hot rolled	GLO	kg	1180.41
steel low alloyed	market for steel, low-alloyed	GLO	kg	7373.18
concrete 30MPa	market for concrete, 30MPa	RoW	m^3	23.11
reinforcing steel	market for reinforcing steel	GLO	kg	3776.48

Results and discussion

Fig. 3 present comparison of the impact of different materials for frame production on different impact categories.

Fig. 3 Comparison of the impact of different materials for frame production on different impact categories



The timber frame dominates in the agricultural land occupation category, contributing roughly 75% of the impact. Steel and concrete have smaller contributions, around 12% and 13% respectively. This suggests that timber requires more land resources than the other materials. Concrete frames contribute the most in climate change category (around 42%), followed by steel (30%) and timber (28%). This indicates that concrete production is highly carbon-intensive, while timber has a lower contribution. Steel frames have the highest contribution to freshwater ecotoxicity. Steel dominates in freshwater ecotoxicity category (~44%), followed by concrete (~30%) and timber (~26%). Steel production appears to have the highest potential to cause freshwater ecotoxicity. Overall, timber is associated with high land use but lower contributions to climate change and ecotoxicity, steel has moderate climate impact but high ecotoxicity, and concrete has the highest climate change impact while being moderate in other categories. This highlights the trade-offs in environmental impacts depending on the choice of construction material.

Conclusion

This research highlights the diverse environmental impacts of timber, steel, and concrete in industrial portal frame structures. Timber, while often considered sustainable, shows the highest land use but lower contributions to climate change and ecotoxicity. Steel has moderate climate impacts but the highest potential for freshwater ecotoxicity, whereas concrete is the most carbon-intensive, contributing most to climate change while being moderate in other categories. These results emphasize the trade-offs in material choice and the importance of assessing a range of environmental impacts. This comprehensive LCA provides valuable insights for stakeholders to make more informed and sustainable choices in structural design. Future research should focus on refining life cycle inventory data, exploring regional variations in electricity mixes and material sourcing, and evaluating emerging low-impact materials and construction methods to further support sustainable decision-making in the built environment.

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TOWARDS SUSTAINABLE FUELS: ENHANCING EFFICIENCY IN CO₂ HYDROGENATION THROUGH PROCESS INTENSIFICATION

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Abstract

The conversion of carbon dioxide (CO₂) into sustainable fuels via hydrogenation represents a promising pathway for closing the carbon cycle and reducing reliance on fossil fuels. However, the widespread implementation of this technology is hindered by challenges related to process efficiency. This paper explores the application of Process Intensification (PI) as a transformative strategy to overcome these limitations. We examine how advanced PI principles, including the development of process integration, can significantly improve the efficiency of CO₂ hydrogenation processes. The aim of this work is to demonstrate that PI is not merely an incremental improvement but a fundamental redesign essential for advancing CO₂ hydrogenation technologies towards practical and sustainable fuel production.

Introduction

The increasing concentration of atmospheric CO₂ and the urgent need for renewable energy carriers have positioned CO₂ hydrogenation as a critical technology for a sustainable future. This process, which produces hydrocarbons like methanol or synthetic crude, offers a route to store intermittent renewable energy in a chemical form. Despite its potential, conventional CO₂ hydrogenation reactors often operate under suboptimal conditions, facing issues such as inefficient heat removal leading to catalyst deactivation, and limited mass transfer affecting reaction rates. Process Intensification (PI) addresses these core engineering challenges head-on. By rethinking process design, PI aims to dramatically improve efficiency, safety, and sustainability. This paper details the role of PI in advancing CO₂ hydrogenation, moving beyond traditional reactor designs to create more effective and scalable solutions.

Process Intensification and Its Role in CO₂ Hydrogenation Efficiency:

The efficiency of CO₂ hydrogenation is fundamentally governed by reaction kinetics, thermodynamics, and transport phenomena. PI enhances these aspects through innovative equipment and processing methods. Intensified reactors allow for precise temperature control. This isothermal operation not only preserves catalyst longevity but also enables the process to run closer to its optimal thermodynamic window, maximizing yield and selectivity towards the desired fuel products.

Future Outlook

The future of CO₂ hydrogenation is inextricably linked to the advancement of PI technologies. Research directions should focus on the synergistic design of catalysts and reactors, where the catalyst is tailored for the specific transport environment of an intensified system. The integration of PI principles with process control strategies for dynamic operation will also be crucial for aligning fuel production with fluctuating renewable energy inputs. As these technologies mature, PI is poised to enable decentralized fuel synthesis units, transforming CO₂ from a waste product into a valuable feedstock at the point of emission.

Conclusion

Process Intensification offers a paradigm shift in the development of CO₂ hydrogenation technologies. By focusing on fundamental enhancements in heat and mass transfer, PI strategies directly address the key efficiency bottlenecks of conventional systems. This work underscores that embracing PI is essential for unlocking the full potential of CO₂ hydrogenation, accelerating its transition from a promising concept to a cornerstone of a sustainable energy landscape.

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**COMPARING THE EFFECTS OF GREEN SOLVENTS IN HPLC WITH
POLYSACCHARIDE-TYPE CHIRAL STATIONARY PHASES FOR
ENANTIOSEPARATION OF COMPOUNDS OF PHARMACEUTICAL
RELEVANCE**

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The investigation of chiral pharmaceuticals, the synthesis of pure enantiomers, and the separation of racemic mixtures are of the utmost importance in the pharmaceutical industry. Currently, one of the most effective approaches for such separations is the use of chiral stationary phases, applicable to both analytical and preparative scales.

Multimodal polysaccharide-based chiral selectors represent the most widely employed class of chiral stationary phases. Beyond traditional normal-phase separations, reversed-phase, polar-organic, and polar-ionic chromatographic modes utilizing “greener” solvents offer many advantages, such as faster and more efficient separations compared to normal-phase conditions. In this study, immobilized polysaccharide-type chiral stationary phases were employed to separate enantiomeric pairs of pyrimidine derivatives. The influence of mobile phase composition was primarily investigated in the polar-organic mode using various alcohols. The immobilized-type selectors also permitted evaluation of solvents with lower environmental impact, including ethyl acetate and dimethyl carbonate. Structure–retention relationships between the chiral selectors and analytes, along with their effects on chromatographic parameters, were analyzed to investigate the nature of the chiral retention mechanism.

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**SELENIUM NANOPARTICLES CONJUGATED WITH *Scutellaris barbata* D. Don
POLYSACCHARIDES: SYNTHESIS, OPTIMIZATION, STRUCTURAL
CHARACTERIZATION AND
EVALUATION OF ANTI-HEPATOMA ACTIVITY *IN VITRO***

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Introduction

In this study, SBP was conjugated with SeNPs to synthesize SBP selenium nanoparticles (SBP-Se), and response surface methodology (RSM) was employed to optimize the synthesis conditions of SBP-Se. The structural properties of SBP-Se were characterized by multiple analytical techniques, and its anti-hepatoma activity was evaluated both *in vitro*. The results demonstrated that SBP is primarily bound to SeNPs through the adsorption of phenolic hydroxyl groups, forming stable SBP-Se containing elemental selenium. Cell based assays revealed that SBP-Se exhibited significantly enhanced antiproliferative effects against HepG2 cells than SBP or SeNPs alone. These findings suggest that SBP-Se is a promising candidate for the development of antitumor pharmaceuticals, providing a theoretical foundation for the design of novel selenium-based structures and elucidating their anti-liver cancer mechanisms.

Experimental

The SBP was purified by the water extraction and alcohol precipitation method, and SBP-Se was synthesized by chemical synthesis. The synthesis parameters of SBP-Se were optimized through CCD and RSM, and the material structure was characterized by UV-Vis, FTIR, XRD and SEM etc. The anti-liver cancer ability of SBP-Se was verified by CCK8 and clone formation experiments.

Results

Polysaccharides are highly effective stabilizers for SeNPs synthesis due to their abundant hydroxyl groups, complex branching structures, and large surface area, which significantly improve stability. The relatively stable SBP-Se complex is formed through C-O/Se linkages or strong interactions with hydroxyl groups. Although the structure of SBP-Se is predominantly amorphous, certain polysaccharides adopt a microcrystalline during the selenization of SBP. Cellular assays demonstrated that SBP-Se significantly reduced the survival rate of HepG2 cells and inhibited the migration of liver cancer cells *in vitro*. In summary, the conjugation of SBP with SeNPs represents a novel strategy for polysaccharide modification and its application in cancer therapy, demonstrating potential as a promising anticancer therapeutic agent.

OPTIMIZATION AND DEVELOPMENT OF THE RELIABLE HPLC-DAD METHOD FOR THE ANALYSIS OF RESVERATROL IN GRAPES

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Abstract

Secondary metabolites of grapevine, particularly stilbenes such as resveratrol, play a key role in plant defense mechanisms, making their reliable determination essential for a better understanding of the vine's natural resistance to pathogens and other stressors. In this study, a methodology based on solid-phase extraction (SPE) and high-performance liquid chromatography coupled with a diode-array detector (HPLC-DAD) was optimized, developed, and validated for the analysis of this compound in grape samples. The method demonstrated high accuracy and precision, along with the capability of detecting very low concentrations. Furthermore, the use of simple, widely available, and cost-effective techniques enhances the value of the applied methodology, making it well-suited for routine laboratory practices as well as future research on the grapevine immune system and the advancement of viticulture.

Introduction

From the earlier evidence of grape consumption in the Paleolithic era [1] to its current recognition as one of the most significant fruit species, the grapevine has undergone a long process of development and selection. Today, it accounts for more than 95% of the world's vineyard areas, and viticulture, beyond its economic importance, also plays a key role in preserving tradition, national identity, and cultural heritage [2]. The viticulture in the territory of today's Serbia dates back to the Roman Empire and gained strength during the Middle Ages. Despite later challenges, including the devastation caused by the appearance of phylloxera (*Phylloxera vastatrix* Planchon) and the consequences of the numerous wars, this agricultural sector in Serbia was successfully restored, adapted, and developed. Modern approaches to viticulture often combine tradition and innovation, with growing emphasis on sustainability and the vine's capacity to successfully cope with numerous challenges, including the pronounced effects of climate change [3] and increasing adaptability of pathogens and pests through various mechanisms. Under such conditions, the adaptive potential of the grapevine becomes particularly important, with secondary metabolites [4, 5]— especially stilbenes— playing a significant role. Resveratrol is one of the most important members of this chemical group, characterized by well-documented antimicrobial and antioxidant properties [6]. Although naturally present in grapevine tissues, its intensive biosynthesis is induced by diverse stress factors, among which the most notable are infections with phytopathogenic microorganisms [7], particularly fungi such as *Plasmopara viticola*, *Uncinula necator*, and *Botrytis cinerea*. In this context, this compound limits infection spread by establishing an initial barrier that slows down pathogen development [7, 8]. Consequently, resveratrol represents a crucial part of the natural defense system and remains the focus of extensive research directed at enhancing vine resistance through the plant's natural potential and identifying novel strategies in plant protection.

To further examine the grapevine's defensive potential, it is necessary to first isolate the target compound from the plant material and accurately determine its content. This requires the careful selection and optimization of an appropriate extraction method. For the extraction of resveratrol from grapes, both conventional and unconventional approaches are used, including maceration,

Soxhlet extraction [9], solid-phase extraction (SPE) [10], ultrasound-assisted extraction, QuEChERS, enzymatic, and supercritical fluid extraction [11] [12]. The further choice of analytical technique, and ultimately the specific analytical method, depends on the properties of resveratrol, which is primarily a photosensitive and thermolabile compound [13]. To ensure the accuracy, precision, and reproducibility of the analysis results, it is crucial to minimize resveratrol degradation, both before and during the analysis. Therefore, high-performance liquid chromatography (HPLC) with various types of detectors is most commonly used due to its affordability, convenience, and widespread applicability [14]. Considering the above, this research aims to optimize, develop, and validate an efficient extraction and analytical method for the determination of resveratrol, as this process constitutes a crucial step towards advancing scientific knowledge and promoting the development of sustainable viticulture.

Materials and methods

Analytical standard of *trans*-resveratrol (98.37%) from Dr. Ehrenstorfer (Germany). The *trans*-isomer was included in this research due to its commercial availability, greater biological activity, and higher presence in grapes, compared to the *cis*-isomer. Acetonitrile, methanol (HPLC grade), ethanol (99%), and acetic acid (CH_3COOH) (reagent grade) were purchased from Fisher Scientific (SAD). Ultrapure water was purchased from J. T. Baker (Netherlands), while formic acid (HCOOH) and ethyl acetate were from Merck KGaA (Germany).

Standard solution was prepared by dissolving the analytical standard in a mixture of methanol and water (50:50 v/v) with 0.1% HCOOH (v/v), whereby the concentration was 1072.3 $\mu\text{g/ml}$. By its dilution, the series of working solutions was prepared in concentrations of 0.05–107.23 $\mu\text{g/mL}$. The working solutions were kept in the dark, at a temperature of 4°C, until the analysis. For the determination of *trans*-resveratrol in grapes, high-performance liquid chromatography with a diode array detector (HPLC-DAD) was applied. The whole process was optimized by testing different sample preparations and solvent combinations as mobile phases.

The optimal conditions were selected according to the best resolution, after which validation of the chromatographic method was carried out by defining the parameters—linearity, precision, repeatability, accuracy, and limits of detection (LOD) and quantification (LOQ) [15].

All procedures were carried out to determine the *trans*-resveratrol content in grapes precisely.

Results and discussion

Considering the available literature data and our previous experience, this research employed SPE extraction, which enables the selective extraction of stilbenes with minimal losses and degradation. This method was optimized to reliably isolate analytes. The chosen preparation method was based on grinding frozen berries in the presence of the cold solvent, which proved to be the fastest and least invasive approach, while preserving the content of resveratrol. This procedure made it possible to obtain small fractions and a homogeneous consistency, which significantly increased the extraction efficacy. Compared to other procedures such as drying, dehydration at elevated temperatures, and lyophilization, the applied method showed an advantage in preserving thermolabile compounds and avoiding additional technological limitations due to high sugar content. During the optimization of the extraction, different solvents such as ethyl acetate, ethanol, methanol, and acetonitrile were tested, showing different efficiencies in terms of yield and reproducibility. Methanol proved to be superior to its purpose, while the addition of acetonitrile at the final step of extraction improved it. Their combination, therefore, represented an optimal solution.

Also, within this research, the HPLC-DAD method was chosen, considering that it provides reliable quantification of resveratrol and has been widely confirmed for the analysis of stilbenes in grapes [16].

For the development of the method, the first step was to optimize the chromatographic conditions to achieve the best resolution, sensitivity, and accuracy in the determination of *trans*-resveratrol in grapes. Different combinations of mobile phases were examined, such as acetonitrile and 1% CH₃COOH; acetonitrile and water, acetonitrile and 10% methanol (1% CH₃COOH), methanol and water (1% CH₃COOH), as well as acetonitrile and 0.1% HCOOH. The most favorable separation was achieved using the last mobile phase in gradient mode, while isocratic analysis did not show good peak separation in the matrix. The combination that proved most effective for this analysis consisted of a mobile phase of acetonitrile (B) and 0.1% HCOOH in water (A), with a column temperature of 35 °C, a flow rate of 0.32 mL/min, and detection at 306 nm (Figure 1). The gradient elution program was set as follows: B (%) 10 at 0 min, 10 at 4 min, 50 at 18 min, 80 at 18.2 min, 10 at 20.2 min, and 10 at 26 min. The chosen combination enabled clear separation of stilbene peaks and reduced interferences from the sample matrix.

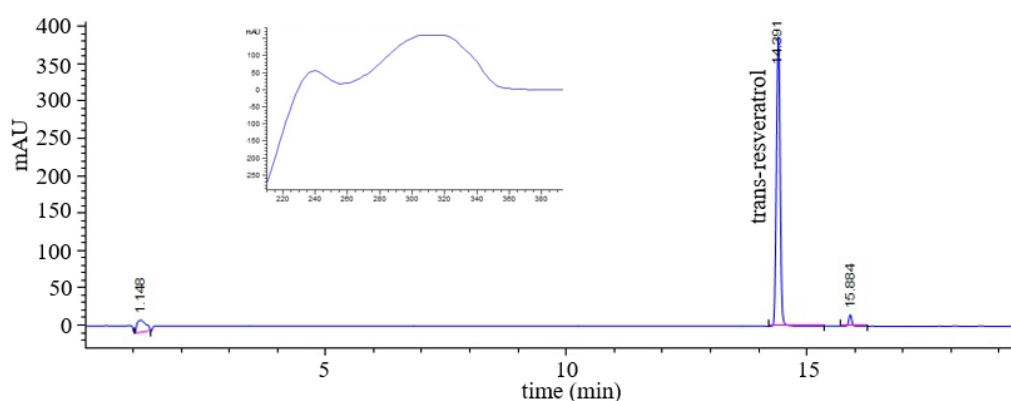


Figure 1. Chromatogram of *trans*-resveratrol (1.07 µg/mL) and its spectrum at a wavelength of 306 nm

For the method validation, linearity was evaluated at seven concentration levels (0.05–107.23 µg/mL), with an obtained R² value of 0.9989, confirming excellent linearity of detector response, in accordance with ICH guidelines [18]. The precision of the method was confirmed by a low value of RSD% (0.19%), while the limits of detection (LOD) and quantification (LOQ) were 0.0053 and 0.0160 µg/mL, indicating a high sensitivity of the method. Recovery values were in the range of 99.21–106.25%, further confirming the satisfactory extraction yield and the suitability of the method for quantitative analysis in grape samples.

Conclusion

The optimized, developed, and validated HPLC-DAD method, with the optimized SPE procedure, proved to be a reliable and efficient combination for the determination of *trans*-resveratrol, with the capability of detecting this compound at very low concentrations. The added value of the applied chromatographic and extraction methods is reflected in their widespread use in laboratories, availability, and economic acceptability, making them suitable for routine laboratory applications.

Acknowledgements

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BINDING AND PARTITIONING BEHAVIOR OF KETOPROFEN WITH SURFACTANTS: INFLUENCE OF POLOXAMER 188 AND 407 IN PREFORMULATION STUDIES

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Abstract

This study explores the interactions between ketoprofen, a poorly water-soluble NSAID, and three surfactants—sodium cholate (SC), dodecyltrimethylammonium bromide (DTAB), and Brij C10 (BC10)—as well as the modulatory effects of Poloxamer 188 (P188) and Poloxamer 407 (P407). Binding constants were determined using Benesi-Hildebrand analysis below the critical micelle concentration (CMC), while micellar partitioning was assessed above the CMC using Kawamura's approach. Job's plots revealed 1:1 complexation in most systems, with an exception in DTAB/P407 mixtures (1.67:1). DTAB showed the highest affinity for ketoprofen ($K_x = 81,386$), particularly in combination with P188, likely due to favorable electrostatic and hydrophobic interactions. SC and BC10 showed moderate and low solubilizing capacities, respectively. Poloxamers modulated micelle formation by altering CMCs and binding behaviors: P407 exhibited synergistic effects with SC and DTAB, while P188 showed antagonistic effects with SC and BC10. All Gibbs free energies of partitioning ($\Delta G_x < 0$) indicated spontaneous solubilization, confirming micellar encapsulation as an effective strategy for enhancing ketoprofen solubility. These findings contribute to the rational design of surfactant-based drug delivery systems.

Introduction

Poor aqueous solubility of ketoprofen limits its bioavailability. Micellar solubilization using surfactants and poloxamers offers a promising strategy for preformulation optimization. This work investigates host-guest interactions at molecular and micellar levels in surfactant-ketoprofen systems, with or without poloxamer modifiers.

Experimental

UV-Vis spectrophotometry was used to monitor absorbance changes at $\lambda = 259$ nm. Job's plots, Benesi-Hildebrand, and Kawamura equations were employed to determine complexation stoichiometry, binding (K_b), and partitioning coefficients (K_x). Fluorescence spectroscopy using pyrene probe was used to determine CMCs.

Results and Discussion

DTAB combined with P188 or P407 enhanced ketoprofen solubilization through favorable electrostatic and hydrophobic interactions (Figure 1). SC showed moderate performance, while BC10 was least effective, likely due to its non-ionic nature. The presence of poloxamers modified CMC values and micelle stability. P407 showed synergistic behavior with SC and DTAB, while P188's effect was more antagonistic, possibly due to hydrogen bonding with surfactants [1, 2]. The spontaneity of solubilization was confirmed by negative ΔG_x values across all systems involving micelles. The highest K_x and most negative ΔG_x values were found in DTAB + P188 systems. At higher poloxamer concentrations, steric hindrance and hydrogen bonding limited drug-surfactant interactions.

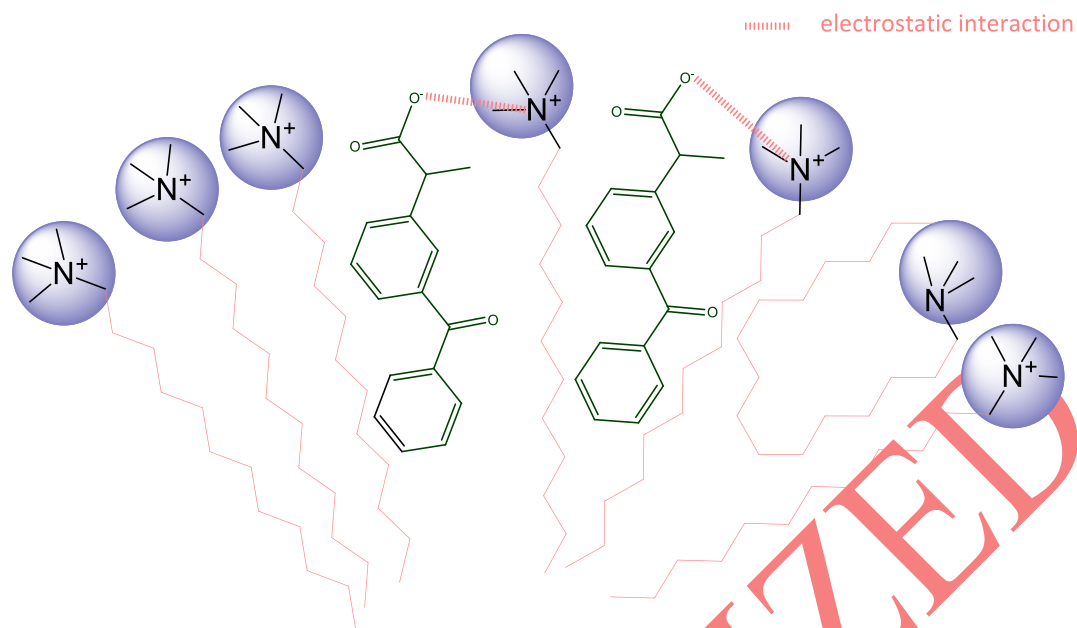


Figure 1. The solubilization of ketoprofen in DTAB micelle

Conclusion

DTAB, particularly in combination with P188 or P407, exhibits the greatest potential for solubilizing ketoprofen. These findings provide a scientific basis for selecting excipients in the development of improved drug formulations.

Acknowledgements

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INVESTIGATING THE ENHANCED THERMAL RESISTANCE OF SUSTAINABLE MICA/PA11 COMPOSITES VIA THERMOGRAVIMETRIC ANALYSIS

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Abstract

Castor-oil derivative polyamide 11 (PA11) is a promising candidate as a sustainable industrial material, where high-performance polymers are required. In this study the effect of a natural clay, muscovite mica, on thermal resistance of PA11 is investigated. Mica/PA11 composites were prepared by melt-compounding to achieve samples with filler contents of up to 5 wt% using two particle sizes. Enhanced thermal stability was evidenced by an enhanced temperature at maximum decomposition rate. Increments by an average of 13 °C were detected, which were higher in case of samples containing larger particles, while surface treatment changed the contribution of the decomposition pathways. Comparing these findings with the results on crystallinity ratio and water uptake, the increased thermal stability was attributed to the barrier effect of the lamellar impermeable fillers.

Introduction

Polyamide 11, derived from castor oil, has been widely studied and applied as a high-performance industrial polymer. In addition to its favorable mechanical properties, it has lower environmental impacts than fossil-based counterparts [1]. On the other hand, as a thermoplastic polymer, it tends to undergo thermal degradation, which is a widely investigated phenomenon [2]. Clays have been reported to improve the thermal stability of polyamides, especially when used as exfoliated fillers [3]. Such effect of lamellar clays are attributed to the barrier effect of the lamellar filler, altered crystallinity and the formation of protective char [4], but in case of polyamide interaction with the hydroxyl groups of the filler also can be taken into account, which changes also the degradation pathway [5].

Present paper investigates the effect of muscovite mica on the thermal decomposition of sustainable PA11 composites through thermogravimetric analysis. To evaluate the results thoroughly, water absorption and results on crystallinity are also presented.

Experimental

Muscovite mica MU 101 ($D_{50}=17.7\ \mu\text{m}$, referred to as ML) and mica MU 2/1 ($D_{50}=6\ \mu\text{m}$, referred to as MS) were obtained from Imerys S.A. (Paris, France), and Rilsan® Roto 11 from Arkema S.A. (Colombes, France). For surface modification of mica Geniosil APTE (Wacker Chemie AG, Munich, Germany) was applied.

Organo-modified mica samples (designated with T, while untreated mica with UNTR) were prepared with the addition of 1 wt% Geniosil APTE, which was mingled with distilled water and mica, then stirred at 70 °C for 4 hours. Mica was then washed with distilled water until pH neutrality.

Raw materials were dried for 4 h at 80 °C before processing. For compounding, a Labtech 26-44 (Labtech Engineering Co. Ltd, Samut Prakan, Thailand) twin screw extruder with a screw diameter of 26 mm and an L/D ratio of 48 was used to prepare composites containing 1, 2 or 5 wt% of filler. Screw speed was 10 rpm, and zone temperatures varied between 180-210 °C.

Differential Scanning Calorimetry (DSC) measurements were carried out on a TA Q200 DSC instrument (TA Instruments Inc., New Castle, DE, USA) in high-purity nitrogen gas. Curves between 30 and 200 °C were evaluated from the second cycle after removing the thermal history. A heating rate of 10 °C min⁻¹ was set after cooling at 20 °C min⁻¹.

Crystallinity ratio (X_c) was calculated by using equation (1):

$$X_c = \frac{\Delta H_m}{(1 - \phi)\Delta H_{m,100}} * 100\% \quad (1)$$

where ΔH_m is the enthalpy absorbed by the test sample during the melting process, ΔH_{100} represents the enthalpy of melting if the polymer were 100% crystalline, ϕ is the mass fraction of the filler. $\Delta H_{m,100}$ of PA11 was taken as 226.4 J g⁻¹ [6].

To determine water absorption, five-five specimens with dimensions of 20*20*2 mm were dried at 80 °C for 48 hours, then weighed and immersed in distilled water at 80 °C for 2 hours. Water uptake was calculated by dividing the weight increase by the initial weight.

Results and discussion

In Figure 1. deconvoluted derivative thermogravimetric (DTG) curves of PA11 and the MS TR5 composite are depicted. PA11 is normally reported to show a single step decomposition, where the temperature of the maximum rate shifts in the presence of fillers [6,7]. However, deep research revealed that polyamides undergo at least two-step thermal decomposition in N₂ in the regime of 350-475 °C, which is followed by another step at 475-600 °C due to the oxidation of char in air [8].

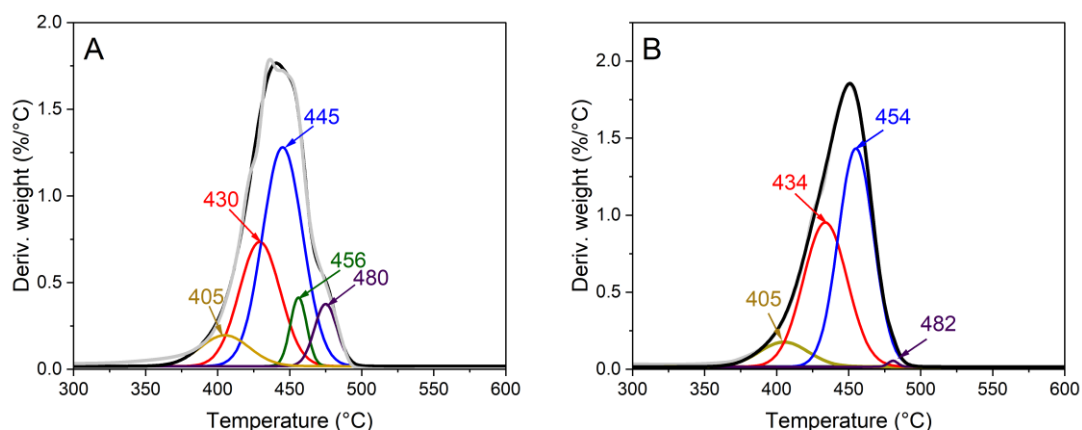


Figure 1. Deconvoluted DTG curves of PA11 (A), and the MS TR5 sample (B).

In Figure 1. and Figure 2. it is demonstrated that a significant shift to the higher temperatures appears mainly in case of the main component in the presence of mica, while the contribution of the side-peaks at higher temperatures decreases. When increasing the filler concentration, the intensity ratio of the main component overbalances that of the feature at around 430-435 °C, and it is more significant at surface-modified samples. Comparing curves in Figure 2A and B, it can be stated that the surface treatment has a more significant effect on the decomposition than the filler size. However, the maximum of the cumulative peaks after deconvolution indicate higher values in case of fillers with larges size (Figure 2.).

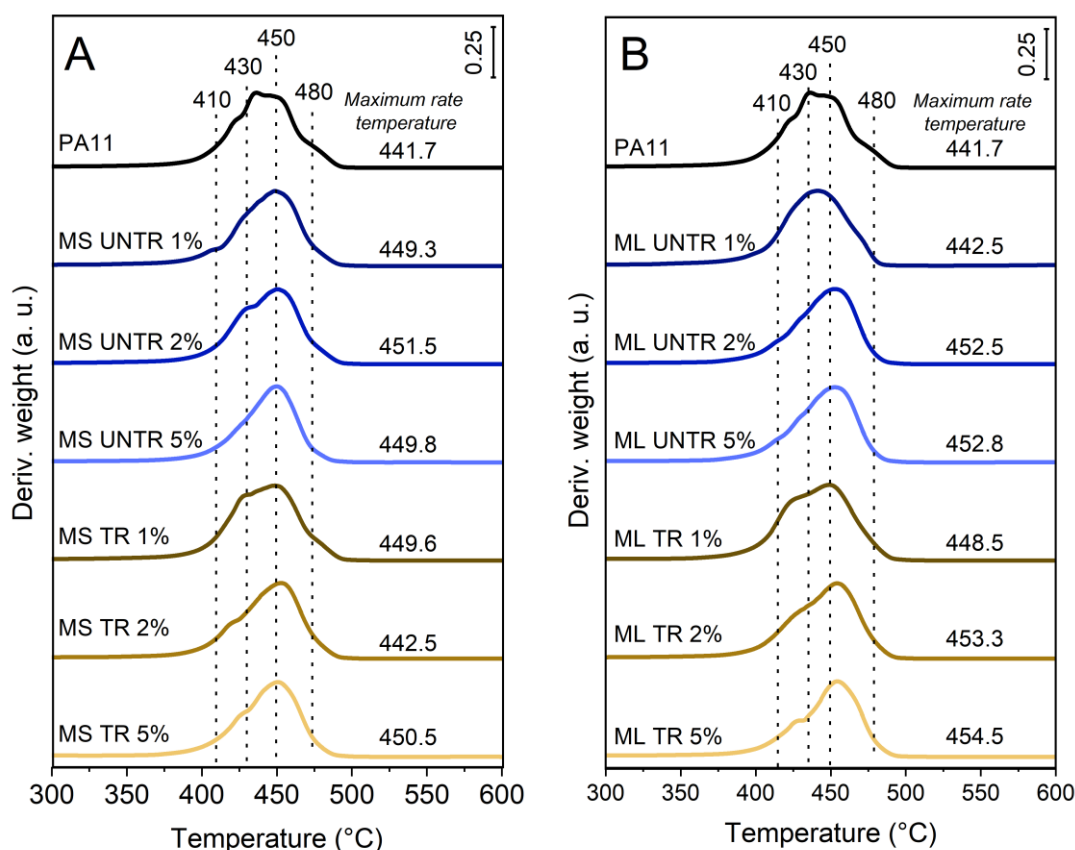


Figure 2. DTG curves of MS (A) and ML (B) composites. Peak maxima of the cumulative signals are added as maximum rate temperature.

Decomposition products at the highest decomposition rate are NH_3 , H_2O , HCN and CO_2 [8]. In our case interestingly a multi-component peak was registered in the case of the neat PA11. The lowest contribution can be attributed to the presence of the different additives, mainly to the plasticizer. Due to the presence of organic molecules on the filler surface, the low-temperature components were more distinguishable in the case of the surface treated samples. Similarly, it was reported previously that the temperature related to the 10% mass loss of graphene/PA11 composites can be attributed to the volatilization of the plasticizer in the matrix, and it shifted to higher temperatures due to the barrier effect of 1% graphene. However, at higher concentration a decrease could be observed, presumably because of agglomeration, but T_{max} increased in all cases thank to the longer pathway of the volatile compounds within the material [9].

Crystallinity degree also can modify the thermal degradation processes either through the free volume among the chains and the diffusion of gases [10], or changing the decomposition kinetics [11]. In our case, crystallinity is higher in case of MS sample compared to that of PA11, while lower after incorporation of ML particles. Except for MS UNTR samples, no clear trends could be observed, which is inconsistent with the decomposition data. On the other hand, water uptake results within a sample type reflect similar trends to what was observed at decomposition tests, proving a barrier effect [12]. Higher values at ML samples might be attributed to the lower specific surface area and to the slightly decreased crystalline phase boundary that decreases the number of defect sites where the degradation initiates. In our case positive influence on the

temperature conductivity can be ruled out as a cause of improved thermal stability, because of the insulation behavior of neat mica [13].

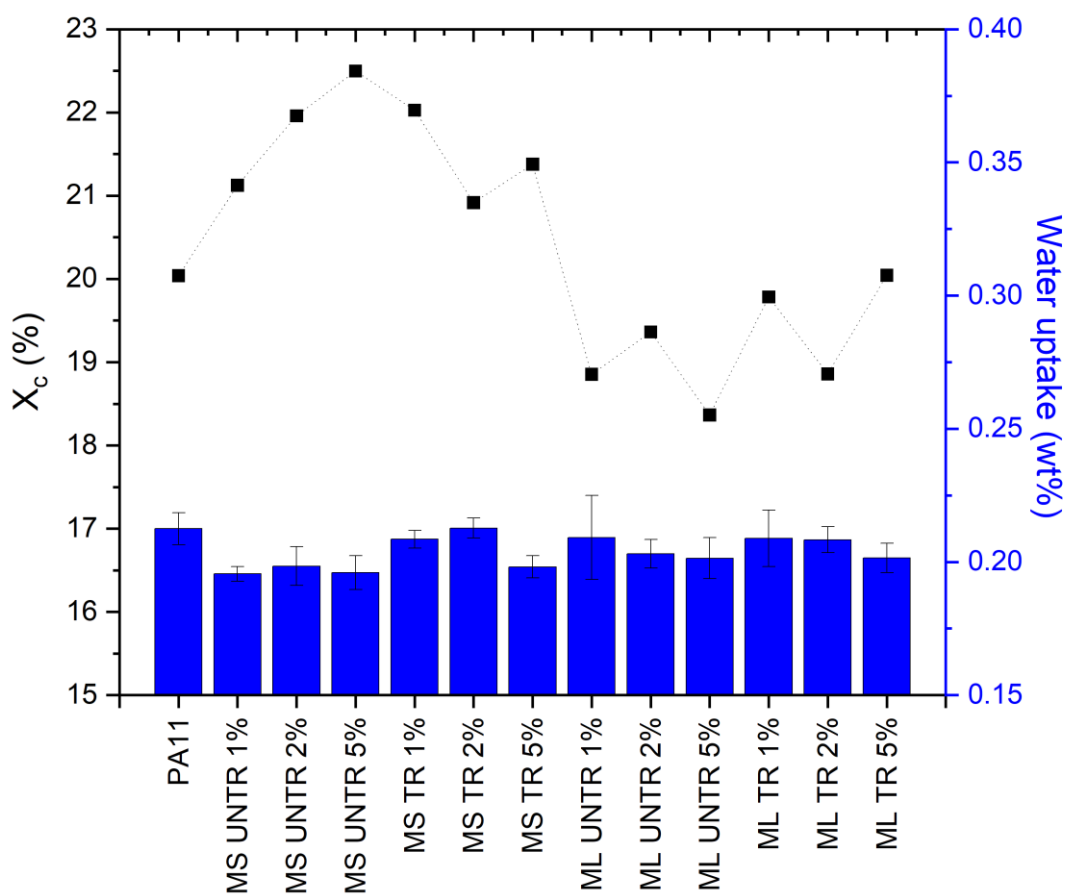


Figure 3. Crystallinity (X_c) and water uptake values at 80 °C after 2 h.

Conclusion

Derivative thermogravimetric curves were analyzed to reveal the effect of mica on the thermal stability of PA11. A positive shift in the decomposition temperature was observed, as well as a concentration and surface chemistry dependent modification in the multi-step decomposition process. After comparing the results with water absorption and the crystallinity ratio, these effects were attributed to the barrier effect of the lamellar mica particles.

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GEOSPATIAL ASSESSMENT OF SOIL DETERMINANTS DRIVING THE DISTRIBUTION AND INVASION RISK OF *ASCLEPIAS SYRIACA* ACROSS HUNGARY

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Abstract

Following habitat loss and fragmentation, biological invasion represents the greatest threat to biodiversity conservation, and in protected areas it poses the most significant conservation challenge. Invasive plant species are generally superior competitors in newly colonized habitats, as they often exploit resources more efficiently, have lower resource requirements, tolerate disturbances better, and lack natural enemies. Nevertheless, their environmental requirements may differ substantially among species. Since the eradication of already established populations and the restoration of the damage they cause are both costly and labor-intensive, the most effective management strategy is to prevent their spread. This requires mapping their current distribution, identifying the environmental factors that determine their occurrence, and predicting areas most at risk of invasion.

Here, we investigated how soil parameters (clay, lime, and sand content; organic matter content; water-holding capacity; groundwater depth; rooting depth) influence the distribution of Common milkweed (*Asclepias syriaca*), one of the most widespread invasive plant species in Hungary. We applied a generalized linear model (GLM) to compare soil parameter values between invaded and non-invaded sites, aiming to identify the factors that influence the species' occurrence. Furthermore, we mapped areas currently non- invaded but potentially at risk of invasion based on the examined soil parameters. We identified the soil parameter values most characteristic of invaded points and examined which currently non- invaded locations share these values. Our results demonstrate that all examined soil parameters significantly affect the occurrence of *A. syriaca*, and that a substantial proportion of non- invaded areas in Hungary show high susceptibility to invasion according to their soil characteristics. These findings provide a valuable basis for targeted monitoring and early detection efforts, enabling more effective prevention of *A. syriaca* invasion in vulnerable habitats.

PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE AND RHODAMINE 6G USING G-C₃N₄/TiO₂ NANOCOMPOSITES SYNTHESIZED BY HYDROTHERMAL METHOD FOR ENVIROMENTAL PROTECTION

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Keywords: Photocatalysis, g-C₃N₄, TiO₂, Hydrothermal synthesis, Methylene Blue, Rhodamine 6G, Wastewater treatment, Enviromental protection

Abstract

Graphitic carbon nitride (g-C₃N₄) and titanium dioxide (TiO₂) composites were synthesized by hydrothermal method and applied as photocatalysts for the degradation of organic dyes for environmental cleanness. The work aims to enhance UV-Visible light-driven photocatalytic activity by combining the advantageous properties of both g-C₃N₄, a with a narrow bandgap, and TiO₂, a well-known but UV-active photocatalyst. The enhanced performance is attributed to the synergistic effect between g-C₃N₄ and TiO₂, where the heterojunction facilitates charge transfer and suppresses electron-hole recombination. It highlights the potential of g-C₃N₄/TiO₂ composites as enhanced, efficient, low-cost photocatalysts for the treatment of dye contaminated wastewater for against the environments and offers insights into the rational design of visible-light-active photocatalytic materials. The rapid growth of industrial activities in the world in turn resulted highly usage of these industrial product of these organic dye pollutants. Industrialization, technologies, and consumption of non-renewable resources have grown at rapidly and polluting the enviroment. The Organic pollutants are series issues due to their effects on the environment including human, air, plants, water as well to all the nature. These major organic pollutants are Methylene Blue (MB), Rhodamine 6G (Rh 6G), Congo Red, Methyl orange and Violin have contributed significant amount different type of chemicals to the pollution of water bodies, air and the environments in different ways. It needs a modern way to get energy from the sun, wind, biofuel, hydropower or other renewable ways for the sake of the environments.

The synthesized g-C₃N₄/TiO₂ composites were characterized using Thermogravimetric analysis (TG), X-ray diffraction (XRD), scanning electron microscopy (SEM), Electron diffraction spectroscopy (EDX), Photoluminescence (PL) and UV-Vis diffuse reflectance spectroscopy (DRS) to investigate their structural, morphological, and optical properties.

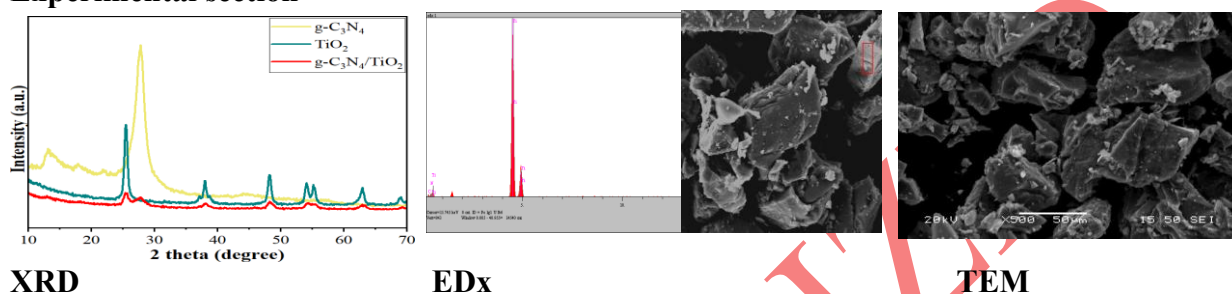
Introduction

The rapid growth of industrial activities in the world in turn resulted highly usage of these industrial product of these organic dye pollutants. Industrialization, different technologies, and consumption of non-renewable resources have grown at rapidly and polluting the enviroment. These Organic pollutants are series issues since they effect the environment in different dimension/side due to their effects on the living organism including human, plants, water as well to all the nature. . Among these organic pollutants, environmental pollutant organic dyes are the major one like synthetic dyes, such as Methylene Blue (MB), Rhodamine 6G (Rh 6G),

Congo Red, Methyl orange and Violin have contributed significant amount different type of chemicals to the pollution of water bodies, air and the environments in different ways.

It needs a modern ways to get energy from the sun, wind or other renewable ways for the sake of the environments. The synthesized $g\text{-C}_3\text{N}_4/\text{TiO}_2$ composites were characterized using Thermogravimetric analysis (TG), X-ray diffraction (XRD), scanning electron microscopy (SEM), Electron diffraction spectroscopy (EDX), Photoluminescence (PL) and UV-Vis diffuse reflectance spectroscopy (DRS) to investigate their structural, morphological, and optical properties.

Experimental section



Results and discussion

TGA analysis covers analysis covered temperatures from room temperature to 700 °C, with a heating rate of 10 °C/min and an air/N₂ flowrate of 130 cm³/min. The surface morphology and composition of the samples SEM and EDX measurements three measurements per sample was done and averaged atomic percentages reported. SEM micrographs was taken using a LEO 1540 XB Scanning Electron Microscope (SEM) under high vacuum. Crystallinity was assessed using a PANalytical X'Pert Pro MPD X-ray diffractometer, employing Cu K- α radiation over a diffraction angle range of 0° to 70°. The Raman spectra 532 nm covering a spectral range from 100 to 1800 cm⁻¹. UV-Vis spectra were obtained with an Avantes AvaSpec-2048 spectrophotometer, using Si wafer as a reference, across a wavelength range of 200–800 nm.

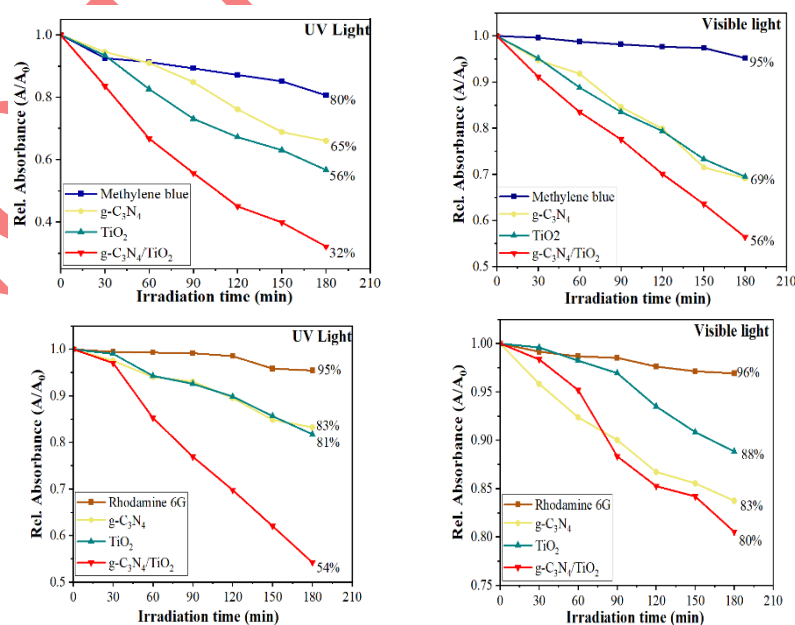


Figure 1. Results of photocatalysis UV-Visible light

Photoluminescence (PL) spectra the excitation wavelength was 260 nm. Notch filters were placed in the emission beam, with nominal wavelengths of 280 nm.

Photocatalytic tests showed that 95% degradation of MB and 96% degradation of Rh 6G in visible and 80% degradation of MB and 96% degradation of Rh 6G

Figure 2. Electropherogram of real sample and results of analysis



Conclusion

The enhanced performance is attributed to the synergistic effect between g-C₃N₄ and TiO₂, where the heterojunction facilitates charge transfer and suppresses electron-hole recombination. This work highlights the potential of g-C₃N₄/TiO₂ composites as enhanced, efficient, low-cost photocatalysts for the treatment of dye-contaminated wastewater and offers insights into the rational design of visible-light-active photocatalytic materials for environmental protection due to degradation. The g-C₃N₄/TiO₂ composite shows promise as a high-performance photocatalyst for the treatment of wastewater containing dyes and other organic pollutants. Its ability to effectively degrade dyes under both UV and visible light makes it a potential candidate for environmental clean-up applications, especially under natural sunlight.

Acknowledgements

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COMPUTATIONAL FLUID DYNAMICS SIMULATION OF MEMBRANE FOULING MITIGATION USING 3D PRINTED TURBULENCE PROMOTERS

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Abstract

Filtration systems are fundamental to water treatment, where achieving an optimal balance between effective contaminant removal and sustainable operation is essential. Computational Fluid Dynamics (CFD) offers a powerful approach for simulating fluid behavior within these systems, allowing researchers to assess and optimize design parameters prior to experimental validation. In this study, CFD simulations were conducted on a laboratory-scale ultrafiltration unit (Millipore), configured to process 100 mL of dairy wastewater. The setup comprised several key components: a plastic mesh, a filter membrane, a 3D-printed flow promoter, and a rotating magnetic stirrer. A static pressure of 2 bar, applied via nitrogen gas at the liquid surface, was used to drive filtration. The primary objective was to characterize the hydrodynamic behavior of the system, with emphasis on flow patterns, pressure distribution, and shear stress profiles. Results revealed that the plastic mesh and Millipore filter were the principal sources of hydraulic resistance, with the greatest pressure drop occurring across these elements. The rotating stirrer improved mixing efficiency, while shear stress analysis identified localized high-stress regions. Notably, the integration of the 3D-printed spacer enhanced permeate flux and reduced overall resistance, highlighting its potential for improving ultrafiltration performance.

Keywords: Computer Fluid Dynamics, Mitigation Membrane Fouling, Turbulence Promoters, Ultrafiltration.

Acknowledgements: This study was supported by the 142414 FK and 2022-1.2.6-TÉT-IPARI-TR-2022-00011 grants from the National Research, Development and Innovation Office (NKFI), Hungary.

FABRICATION AND INVESTIGATION OF $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ PHOTOCATALYST ON THE SURFACE OF CERAMIC PAPER

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Abstract

The study aim on the fabrication and investigation of $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ photocatalyst on the surface of ceramic paper through precipitation method and immobilization of composite onto ceramic paper by in situ and filtration, impregnation method. The integration of magnetite (Fe_3O_4) and silver phosphate (Ag_3PO_4) on ceramic paper results in high performance efficiency of the material due to synergistic effect, improved charge separation, improved light absorption, stability and durability, increased surface area and active site. The ceramic paper supports uniform distribution of catalyst and since it can withstand high temperature, resist corrosion and chemical attack as well as possess excellent heat and electrical barrier, hence fabricated $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ photocatalyst on the surface of ceramic paper leads it to be applied for water treatment, photocatalysis and environmental remediation. Also, it has to be note that immobilization of the $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ photocatalyst on ceramic paper is of great importance due to the fact that ceramic paper prevent photocatalyst bleaching, allow good interaction of pollutants and catalyst surface due to porous structure, enhance durability and allows reuse over multiple cycles, in contrast most photocatalysts are tested on slurry suspension systems in which long term use is limited by particle aggregation, poor recovery and risk of secondary contamination.

Under this study, the photocatalytic activity of the fabricated photocatalyst will be assessed via methylene blue and methyl orange degradation experiment. The fabricated photocatalyst will be characterized by **X-ray diffraction (XRD)**, Scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX) before and after degradation experiments.

Keywords: magnetite, silver phosphate, photocatalyst, ceramic paper, precipitation method, immobilization.

Introduction

The increasing contamination of water sources due to industrial and domestic activities has necessitated the development of efficient wastewater treatment technologies. Among various approaches, photocatalysis has emerged as a promising method for degrading organic pollutants in contrast to conventional treatment methods, are often unable to completely remove organic pollutants especially (POPs) leading to their accumulation in natural waters. Due to the phenomena photocatalysis has gained strong interest as a sustainable and efficient method for degrading persistent organic pollutants (POPs) into harmless end-products of CO_2 and H_2O .

When magnetite (Fe_3O_4) and silver phosphate (Ag_3PO_4) are combined in a Z-scheme heterostructure supported on **ceramic paper** offers an effective solution due to the fact that Fe_3O_4 provides magnetic properties for easy separation and enhances charge transfer, while Ag_3PO_4 provide strong visible-light photocatalytic activity. The ceramic paper serves as a stable, flexible, and heat-resistant substrate, improving the durability and allows reuse over multiple cycles of the photocatalyst. Therefore $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ @ceramic paper composite in this

study is designed to efficiently degrade organic pollutants in wastewater under visible light, offering a practical and sustainable approach to water purification.

Experimental

Catalyst Synthesis

Silver phosphate (Ag_3PO_4) was synthesized via a precipitation method by reacting silver nitrate (AgNO_3) with various phosphate sources. Specifically, 0.2 M aqueous solutions of AgNO_3 and phosphate precursor of $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ were prepared separately and mixed in a 4:3 molar ratio under stirring. Upon mixing, a yellow Ag_3PO_4 precipitate formed rapidly. The mixture was stirred for an additional 10 minutes, then the product was collected by centrifugation, washed three times with Milli-Q water, and dried overnight at 40 °C.

Ceramic Paper Support

As a photocatalyst support, commercial Alsitra KP1250 ceramic paper was used. It consists of thermally stable mullite and polycrystalline alumina fibers, with high porosity and chemical resistance. Circular paper samples with a radius of approximately 22 mm were cut and used for catalyst immobilization.

Immobilization Techniques

Two approaches were explored for immobilizing the catalysts onto the ceramic paper:

1. Filtration based deposition

A total of 50 mg of catalyst powder $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$ was suspended in 100 mL of ethanol and ultrasonicated for uniform dispersion. The suspension was then vacuum-filtered through the ceramic paper discs. After filtration, the paper was dried at 40 °C overnight.

2. In situ synthesis on ceramic paper

The ceramic paper was immersed in precursor solutions, and the synthesis reaction (e.g., Ag_3PO_4 precipitation) was allowed to proceed directly on the paper. For silver phosphate, equimolar solutions of AgNO_3 and phosphate salts (0.2 M) were sequentially added to the support by submersion, allowing the reaction to occur in situ. After synthesis, the papers were washed, dried, and stored under ambient conditions.

Photocatalytic testing of the immobilized catalysts is planned, while the activity of the powdered materials has already been confirmed in previous studies using methyl orange under visible light irradiation.

Results and discussion

We successfully immobilized photocatalytic nanomaterials onto ceramic paper (Alsitra KP1250) using two different approaches: filtration and in-situ synthesis. Scanning Electron Microscopy (SEM) confirmed the presence of the catalysts on the ceramic support as shown in figure 1.

The two immobilization techniques yielded markedly different outcomes:

- **Filtration method** resulted in a thick catalyst layer on the surface of the ceramic paper. The coverage was visually more uniform and continuous; however, the adhesion was weaker. Some material detachment was observed during handling and washing, especially at the edges.
- **In-situ synthesis** led to a more integrated catalyst layer with stronger adherence to the ceramic fibers. Although the coverage appeared less homogeneous and slightly patchy, the catalyst showed improved mechanical stability and resistance to washing.

In both cases, we observed partial leaching of the catalyst material, but the in-situ synthesized samples were noticeably more resistant to bleaching.

Photocatalytic activity of the immobilized catalysts has not yet been evaluated. Initial attempts were hindered by technical challenges: our current lab-scale reactor setup degraded the ceramic paper during testing due to poor physical compatibility. As a result, all photocatalytic performance evaluations so far refer only to the powdered catalysts before immobilization. Despite these limitations, our immobilization strategies proved viable, and future tests using a modified or custom-built reactor (as outlined in our future plans) will focus on optimizing both durability and performance of the immobilized systems.

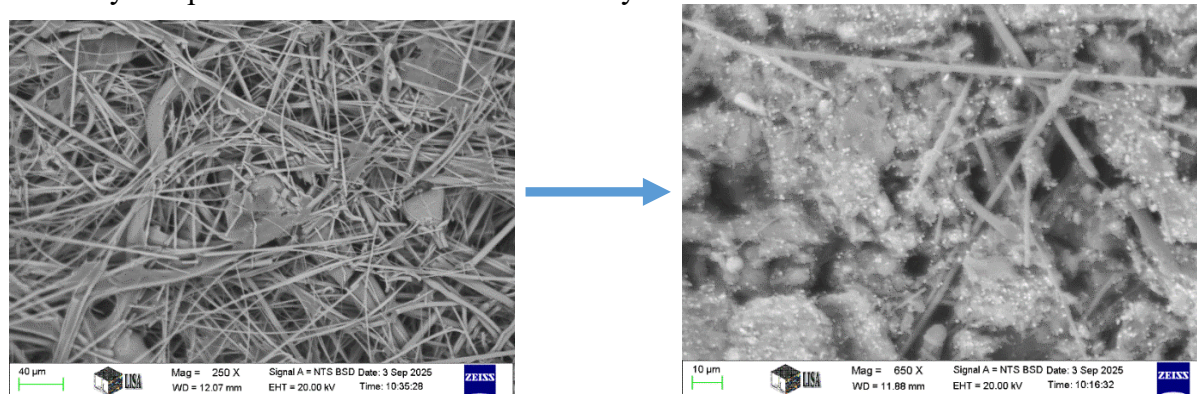


Figure 1: SEM image of ceramic paper before and after immobilized with $\text{Fe}_3\text{O}_4/\text{Ag}_3\text{PO}_4$

Conclusion

This study aims to bridge the gap between fundamental materials science and scalable environmental technologies by integrating catalyst synthesis, ceramic paper immobilization, and system-level design.

Acknowledgements

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NOVEL UHPLC-MS/MS METHOD AND PERMEABILITY STUDY OF THE BRAIN PENETRANT NEUROPROTECTIVE AGENTS: KYNA ANALOGS—A CRITICAL STEP IN DRUG DEVELOPMENT

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Abstract

Kynurenic acid (KYNA) is an endogenous compound produced through the Kynurenine pathway. It exhibits neuromodulator and neuroactive properties by regulating several neurotransmitters such as dopamine, glutamate, γ -aminobutyric acid (GABA), and acetylcholine (ACh). Thus, KYNA is involved in most of CNS disorders including, Huntington's disease, Parkinson's disease, and Alzheimer's Dementia and many others [1,2]. However, when KYNA is administered as a drug externally, it has a limited permeability in the blood-brain barrier (BBB). For that reason, newly synthesized KYNA analogs with better BBB permeability and enhanced pharmacokinetics were presented as an alternative to KYNA. We aimed in this research to determine the concentration of KYNA analogues in an in vitro rat blood-brain barrier model using a highly sensitive and analytical method and determine the Log P and Log D of these analogues as well [3,4,5].

An efficient targeted UHPLC-MS/MS method was developed and validated for the simultaneous determination of KYNA analogues in the brain homogenate. The optimized electrospray ionization (ESI) multiple reaction monitoring (MRM) mode was utilized in the mass spectrometric detection (MS/MS). To determine the quantifier and qualifier of KYNA, and optimize the ESI and MS/MS parameters, a flow injection method was used. The fragmentation behavior of KYNA analogues was studied using the high-resolution tandem mass spectrometry MS/HRMS. Log P and Log D values were determined experimentally using the shake-flask method.

KYNA analogues were separated and measured with a total run time of 10 minutes method. The UHPLC-MS/MS method was fully validated according to ICH guideline M10 bioanalytical method validation. The developed method was successfully applied to quantify KYNA analogues in an in vitro rat blood-brain barrier model and Log D results were correlated with the predicted values.

Keywords: Kynurenic Acid, UHPLC-MS/MS, Log P, Log D, Kynurenic Acid Analogue

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Poster Proceedings

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**MOLECULAR NUTRITION MEETS ENVIRONMENTAL SCIENCE:
A REVIEW OF NOVEL BIOACTIVE COMPOUNDS AND THEIR
ECOTOXICOLOGICAL IMPACT**

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Abstract

Molecular nutrition has introduced a range of novel bioactive compounds, including synthetic micronutrients, bioactive peptides, and nanoformulations, designed to enhance health and metabolic function. However, their fate in the environment remains largely unexplored. These compounds can enter ecosystems through excretions, agricultural runoff, or industrial processes, with potential impacts on soil and aquatic organisms. This review examines the environmental pathways and ecotoxicological risks associated with emerging nutritional molecules. Analytical techniques such as LC-MS/MS and HPLC for detecting these substances in environmental matrices are discussed. Current regulatory frameworks often overlook these compounds, despite evidence of bioaccumulation or endocrine disruption in non-target species. By linking biotechnology, analytical chemistry, and ecotoxicology, this paper highlights the urgent need for environmental risk assessments in the development of future nutritional products. A sustainable approach to molecular nutrition must consider both human health benefits and ecological safety.

Introduction

Molecular nutrition is an interdisciplinary field at the interface of biochemistry, genomics, and nutritional science, exploring how nutrients and bioactive food components influence cellular processes and gene expression. The rise of precision nutrition and biotechnological advancements has led to the development of novel bioactive compounds, including synthetic micronutrients, functional lipids, bioactive peptides, and nanocarriers for targeted delivery. These innovations aim to improve metabolic health, reduce disease risk, and personalize dietary interventions. However, while their physiological benefits are increasingly documented, their environmental fate and potential ecological risks remain largely under-investigated.

Upon ingestion, many of these compounds—or their active metabolites—are excreted via urine and feces, entering wastewater systems or agricultural environments through manure and sludge application. Industrial production also contributes to environmental release. Current wastewater treatment facilities are often not equipped to remove complex bioactive molecules, allowing their persistence and bioaccumulation in ecosystems. Additionally, nanoformulations designed for enhanced delivery may exhibit unexpected mobility, toxicity, or interactions with other environmental contaminants.

This review explores the ecological implications of novel compounds used in molecular nutrition. It addresses their classification, environmental pathways, detection methods, ecotoxicological effects, and the gaps in current regulations and risk assessment strategies. By bridging molecular nutrition and environmental/ecological science, the paper highlights the need for sustainable innovation that considers both human health and ecological integrity.

Novel chemicals in molecular nutrition

The scope of molecular nutrition has rapidly expanded beyond traditional nutrients to include a wide range of engineered bioactive compounds that exert targeted effects at the cellular and molecular level. These compounds can be classified into several categories (figure 1):

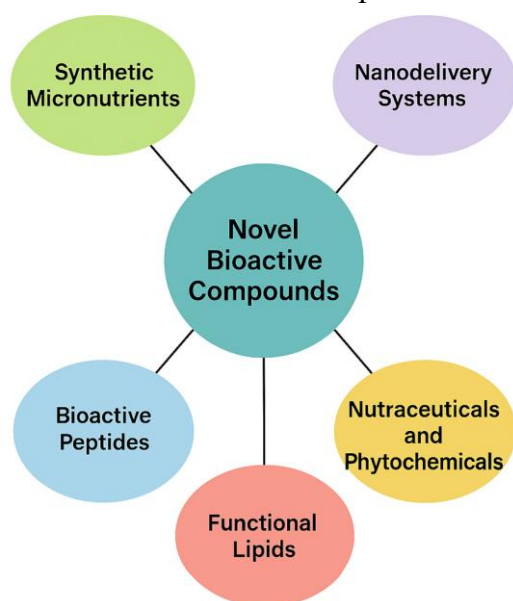


Figure 1. The main classes of novel bioactive compounds involved in molecular nutrition

- **Synthetic micronutrients:** Modified versions of essential vitamins and minerals with enhanced bioavailability or stability (e.g., methylated B vitamins, chelated minerals).
- **Bioactive peptides:** Short amino acid sequences derived from protein hydrolysis, exhibiting antihypertensive, antioxidant, and immunomodulatory activities [1].
- **Functional lipids:** Structured lipids and synthetic omega-3 analogs designed to influence lipid metabolism and inflammation [2].
- **Phytochemicals and nutraceuticals:** Concentrated plant-derived compounds like curcumin, catechins, and resveratrol, often with anti-inflammatory or antioxidant properties [3-5].
- **Nanodelivery systems:** Liposomes, nanoemulsions, and polymeric nanoparticles are employed to improve stability, solubility, and targeted release of active compounds [6].

These substances are increasingly present in functional foods, dietary supplements, and fortified animal feeds. While they are generally regarded as safe for human use, their biochemical complexity may result in environmental persistence and unexpected biological activity in non-target organisms (figure 2). For instance, nanoencapsulated compounds may resist degradation or promote co-transport of other environmental pollutants, increasing their ecological footprint [7].

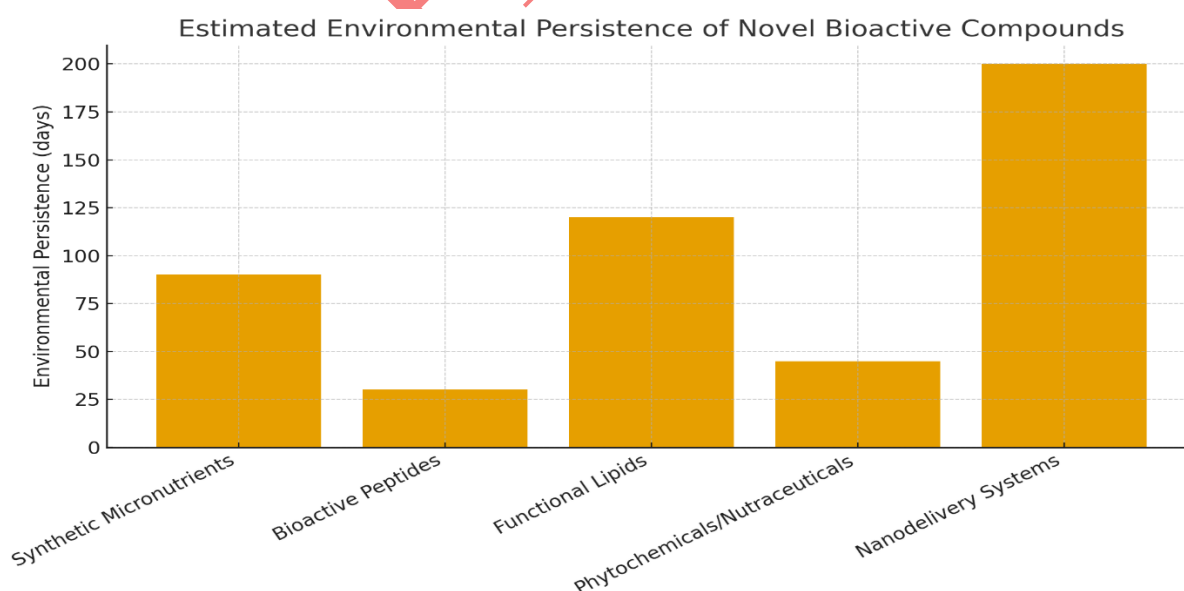


Figure 2. Estimated environmental persistence, bioaccumulation potential, and documented ecotoxicity of different classes of novel bioactive compounds used in molecular nutrition

The continuous development and commercialization of these compounds demand a closer look at their life cycle, particularly post-consumption and disposal. Given the complexity of their structures and the novel formulations involved, it is critical to assess their long-term interactions with environmental matrices, especially aquatic and soil ecosystems.

Environmental pathways and mechanisms

Novel compounds used in molecular nutrition enter the environment through diverse and often overlooked pathways. One primary route is human and animal excretion, where unmetabolized compounds and their transformation products are released into wastewater. Standard sewage treatment plants (STPs) are often not optimized to degrade these complex molecules, allowing them to reach surface waters or accumulate in sludge [8].

Agricultural runoff represents another significant pathway. Nutrient-fortified feeds and veterinary supplements administered to livestock result in manure rich in bioactive residues. When used as fertilizer, these residues can leach into soil and water systems. Furthermore, industrial discharge from nutraceutical manufacturing processes can introduce high concentrations of active compounds directly into aquatic systems.

Nanoformulations pose unique concerns due to their small size and surface reactivity. They can penetrate biological membranes, bind to soil or sediment particles, and persist under environmental conditions that would degrade conventional compounds [9]. Some may facilitate the transport of heavy metals or other contaminants, creating synergistic toxicity effects (figure 2).

Understanding these mechanisms is essential for predicting exposure levels in ecosystems and evaluating the potential for bioaccumulation or ecotoxicological impact.

Analytical techniques for detection

Detecting emerging bioactive compounds in environmental samples requires advanced analytical methods capable of handling complex matrices and low analyte concentrations. The most widely used techniques include:

- Solid-phase extraction (SPE): Used for sample pre-concentration and cleanup.

Emerging technologies such as biosensors and nano-enabled detectors offer potential for real-time, in-situ analysis, though they require further validation. A key challenge remains the lack of standardized protocols and reference materials for many novel compounds, limiting the comparability and reproducibility of results across studies.

- Liquid Chromatography coupled with Tandem Mass Spectrometry (LC-MS/MS): Offers high specificity and sensitivity for quantifying trace levels in water, soil, and sludge [10].

- High-Performance Liquid Chromatography (HPLC): Commonly employed for separating structurally similar compounds, especially plant-derived substances.

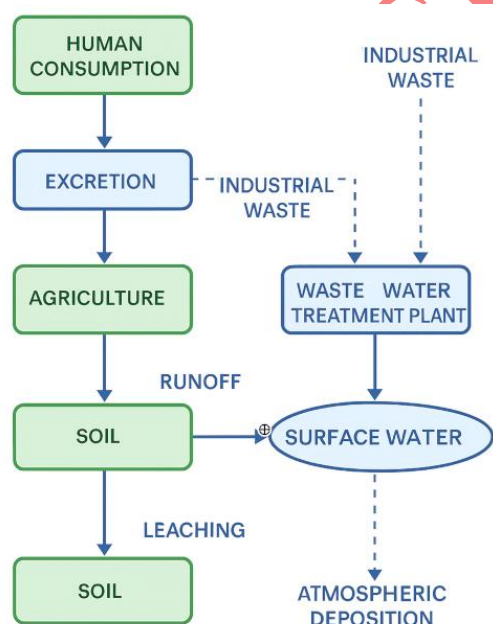


Figure 2. Major pathways through which bioactive nutritional compounds enter and move through

Ecotoxicological evidence

Initial ecotoxicological studies suggest that novel nutritional compounds can pose risks to various environmental organisms. For instance, bioactive

peptides and synthetic antioxidants have been shown to affect the reproductive systems of aquatic invertebrates and fish at sublethal concentrations [11]. Functional lipids and polyunsaturated fatty acids, when accumulated in sediments, may alter microbial community structures and enzyme activities.

Of particular concern are nanoencapsulated compounds, which can exhibit enhanced bioavailability and cellular uptake, leading to oxidative stress, inflammation, or DNA damage in non-target organisms [12]. Studies on *Daphnia magna* and zebrafish embryos exposed to nanoparticle-based formulations of curcumin or resveratrol have reported impaired development and increased mortality [13].

Additionally, phytochemicals like genistein and catechins have demonstrated estrogenic or endocrine-disrupting effects in aquatic species, raising concerns about their release in significant quantities through wastewater [14].

While short-term toxicity is increasingly documented, data on chronic exposure, mixture effects, and long-term ecosystem-level impacts remain scarce. The interaction of these compounds with existing pollutants—such as heavy metals or pharmaceuticals—could produce synergistic or antagonistic effects, further complicating risk assessments.

Critical gaps and opportunities for advancement

Despite the increasing production and consumption of bioactive nutritional compounds, environmental risk assessments remain limited. Regulatory agencies often do not require ecotoxicological evaluations for compounds considered safe for human use, leading to significant regulatory blind spots.

One major gap lies in toxicological data, particularly concerning chronic exposure and sublethal effects. Many compounds are assessed only for acute toxicity, neglecting their potential to bioaccumulate or interfere with hormonal systems. Furthermore, analytical challenges persist due to the lack of validated detection protocols, reference standards, and environmental occurrence data.

Future research should prioritize:

- Standardized testing frameworks for environmental safety of nutritional compounds
- Life cycle assessments that include environmental endpoints
- Development of biodegradable or eco-safe formulations following green chemistry principles

Interdisciplinary collaboration between nutrition scientists, ecotoxicologists, analytical chemists, and policymakers is essential to close these gaps. The integration of environmental considerations early in the product development pipeline will help ensure that advances in molecular nutrition are sustainable and do not compromise ecosystem health.

Conclusion

Molecular nutrition offers exciting health benefits, but its environmental dimension must not be overlooked. As novel bioactive compounds become more prevalent, understanding their pathways, persistence, and ecotoxicological effects is essential. Improved analytical methods, robust environmental assessments, and interdisciplinary collaboration are urgently needed. By integrating environmental safety into the development of nutritional products, we can ensure that innovation supports both human well-being and ecosystem health. Sustainable nutrition must not end at the body—it must extend to the planet.

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PRECURSOR-DRIVEN RAPID SOLID-STATE SYNTHESIS OF YBO_3 : TOWARD EFFICIENT Pr^{3+} -DOPED UPCONVERSION HOSTS

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Abstract

The rise of antibiotic-resistant bacteria over the past decade has increased the need for new materials and methods for disinfecting water and surfaces. Ultraviolet-C (UVC) irradiation is still a strong germicidal agent because there is minimal microbial resistance to this wavelength [1]. However, the low UVC content in ground-level sunlight limits its direct use. Photonic up-conversion materials that can efficiently turn longer-wavelength solar radiation into UVC offer an appealing and cost-effective way to improve disinfection efficiency [2]. At the same time, some yttrium-based compounds have natural antimicrobial properties. These properties come from either the release of Y^{3+} ions or interactions with microbial cell walls, allowing for a dual-mode bactericidal effect [3,4]. In this study, we present the quick solid-state synthesis of YBO_3 as a host material for Pr^{3+} doping, looking at its combined potential for up-conversion emission in the germicidal UVC range and for non-radiative antibacterial effects. We synthesized YBO_3 using two different yttrium precursors: commercial Y_2O_3 and low-temperature polyol-derived Y_2O_3 nanoparticles. We thoroughly characterized the material using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), UV–Vis–NIR spectrophotometry, dynamic light scattering (DLS), and thermogravimetric analysis (TGA). We systematically assessed how the type of precursor affects reaction kinetics, phase purity, and microstructural development. The results show a significant impact of precursor morphology and reactivity on the synthesis results. Using polyol-derived Y_2O_3 nanoparticles allows for the creation of phase-pure YBO_3 at just 800 °C in under 10 minutes. In contrast, the commercial precursor requires temperatures above 900 °C and longer treatment to achieve similar conversion, often leaving some Y_2O_3 behind. This quick synthesis method not only cuts down on energy use and processing time but also produces finer YBO_3 particles than traditional high-temperature, long-duration techniques. These findings suggest that engineering the precursor can greatly improve YBO_3 production efficiency, offering a scalable and energy-saving approach to advanced host materials for Pr^{3+} doping with potential uses in solar-driven disinfection and antimicrobial technologies.

Acknowledgements

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NOT FINALIZED

NEW SILICONE-BASED MEMBRANES WITH FUNCTIONALIZED SILSESQUIOXANES. CHARACTERIZATION AND PERSPECTIVES FOR ENVIRONMENTAL AND BIOLOGICAL APPLICATIONS

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Abstract

A series of three cubic silsesquioxanes, containing either the original organic function (SH) (silsesquioxane **2**, SH_SS), a derivatized one (NH₃Cl) (silsesquioxane **1**, A_SS) or completely chloro derivative (silsesquioxane **3**, Cl_SS) were obtained by acid hydrolysis of three organo-trialkoxysilane (3-aminopropyltriethoxysilane, 3-mercaptopropyltrimethoxysilane and 3-cyanopropyltriethoxysilane). The structures were investigated through X-ray single crystal diffraction, spectral techniques and elemental analysis. Each silsesquioxane compound was incorporated into a polymeric matrix of low molecular weight polydimethylsiloxane. After the incorporation of the silsesquioxanes, the matrix crosslinking was performed resulting in free-standing films. The composite films were investigated by dynamic vapour sorption (DVS) analysis, scanning electron microscopy (SEM), stress-strain measurements and dielectric spectroscopy. Thermal behavior was studied by thermogravimetric analysis and differential scanning calorimetry. The presence of the siloxane moiety in the materials, improves due to its surface energy effect the compatibility between the silsesquioxanes and the silicone matrix, thus ensuring good mechanical properties. The biological compatibility was tested for all the composite films. Investigations on hybrid membranes surface, based on the water vapor sorption data, have demonstrated that on their surface exist nano-sized pores. The values of water vapors sorption capacities increase in the following order: P_Cl_SS < P_SH_SS < P_A_SS. Consequently, in accordance with our results, for obtaining a good membrane with superior characteristics for environmental applications it is necessary to ensure a high pore density and a high permeability of the free-standing film membrane.

Introduction

The main goal of this study implies the development of high-performance systems based on new polymeric-hybrid materials that will be used in the advanced treatment processes for water purification [1-2]. Such new materials include polymer-based hybrid membranes with adsorption properties. The acid hydrolysis of three organo-trialkoxysilane (3-aminopropyltriethoxysilane, 3-mercaptopropyltrimethoxysilane, and 3-cyanopropyltriethoxysilane) resulted in the formation of cubic silsesquioxanes **1**, **2** and **3**, respectively, containing either original organic function (SH) (**2**), derivatized one (NH₃Cl) (**1**) or completely unexpected chloro derivative (**3**) [3-6]. Three different well-determined complex structures containing siloxane moieties were incorporated into a polymeric matrix based on a polydimethylsiloxane of low molecular weight. After the incorporation of the silsesquioxanes, the matrix crosslinking was performed with tetraethylorthosilicate, resulting in free - standing films. The films were investigated by dynamic vapour sorption (DVS) analysis, stress-strain measurements. The presence of the siloxane moiety in the ligand (by its surface effect) improves the compatibility between the components ensuring good mechanical properties.

Experimental

In this study, we report the preparation and characterization of new POSS composite membranes. The structure and chemical composition of the new materials obtained were estimated on the basis of IR spectra, X-ray diffraction and thermogravimetric analysis while morphology was studied by SEM and water permeability, water vapour isotherms for textural properties. Thermal properties of the new membranes were determined by thermogravimetric analyses. The effect of silsesquioxanes introduction in the polymer matrix, on the mechanical properties of the membranes was also studied. Thermal behavior was studied by thermogravimetric analysis and differential scanning calorimetry. Moisture sorption capacity was evaluated by water vapour sorption in dynamic regime. The biological activity was also tested for the three compounds.

Materials

Octakis(3-ammonium chloride-propyl)octasilsesquioxane (1), octakis(3-mercaptopropyl)octasilsesquioxane (2), and octakis(3-chloropropyl)octasilsesquioxane (3) were obtained by the acid hydrolysis of the three organo-trialkoxysilane above mentioned. The low molecular mass ($M_n = 48000$ g/mole) polydimethylsiloxane- α,ω -diol, PDMS, was synthesized according to the already described procedure [4]: cationic ring-opening polymerization of octamethylcyclotetrasiloxane in the presence of a cation exchanger as catalyst.

Equipments

Fourier transform infrared (FT-IR) spectra were registered using a Bruker Vertex 70 FT-IR spectrometer. Analyses were performed in the transmission mode in the $400\text{--}4000\text{ cm}^{-1}$ range, at room temperature, with a resolution of 2 cm^{-1} and accumulation of 32 scans. The samples were incorporated in dry KBr and processed as pellets in order to be analyzed. The NMR spectra were recorded on a Bruker Avance DRX 400 MHz Spectrometer equipped with a 5 mm QNP direct detection probe and z-gradients. Spectra were recorded in CDCl_3 or DMSO-d_6 , at room temperature. The chemical shifts are reported as δ values (ppm) relative to the solvent residual peak. The carbon, hydrogen, and nitrogen contents were determined by standard methods. The thermogravimetric analyses were performed on STA 449F1 Jupiter NETZSCH (Germany) equipment. The measurements were made in the temperature range $20\text{--}700^\circ\text{C}$ under a nitrogen flow (50 mL/min) using a heating rate of 10°C/min . Dynamic water vapor sorption (DVS) capacity of the samples was determined in the relative humidity (RH) range $0\text{--}90\%$ by using the fully automated gravimetric analyzer IGAsorp produced by Hiden Analytical, Warrington (UK). An ultrasensitive microbalance measures the weight change as the humidity is modified in the sample chamber at a constant regulated temperature. The measurement system is controlled by a software package. Stress-strain measurements were performed on dumbbell-shaped cut samples from thin films on a TIRA test 2161 apparatus, Maschinenbau GmbH Ravenstein, Germany. All samples were measured three times and the averages of the obtained values were taken into consideration. Antibacterial and fungicidal activities of silsesquioxanes functionalized with ammonium chloride (1), mercaptopropyl (2), and chloropropyl groups (3) were evaluated by performing "in vitro" tests against pure culture of three fungi species (*Aspergillus niger*, *Penicillium frequentans*, *Alternaria alternata*) and against both Gram-negative (*Pseudomonas aeruginosa*) and Gram-positive (*Bacillus polymyxa*) bacteria.

Results and discussion

Three new membrane materials with three new silsesquioxanes: - original organic function (SH) (silsesquioxane 2, SH_SS), - derivatized one (NH_3Cl) (silsesquioxane 1, A_SS); - completely substituted chloro derivative (silsesquioxane 3, Cl_SS) with a polymeric matrix of low molecular weight polydimethylsiloxane were obtained and characterized. After the

incorporation of the silsesquioxanes, the matrix crosslinking was performed resulting in free-standing films. Thermal behavior was studied by thermogravimetric analysis and differential scanning calorimetry (Figure 2). Moisture sorption capacity was evaluated by water vapour sorption in dynamic regime. The biological activity was also tested for the three compounds. Three different molecular or polymeric well-determined complex structures containing siloxane moieties were incorporated into a polymeric matrix based on a polydimethylsiloxane of low molecular weight. After the incorporation of the silsesquioxanes, the matrix crosslinking was performed, resulting free - standing films. The films were investigated by dynamic vapour sorption (DVS) analysis, stress–strain measurements (Figure 1). The presence of the siloxane moiety in the ligand (by its surface effect) improves the compatibility between the components ensuring good mechanical properties (Figure 3).

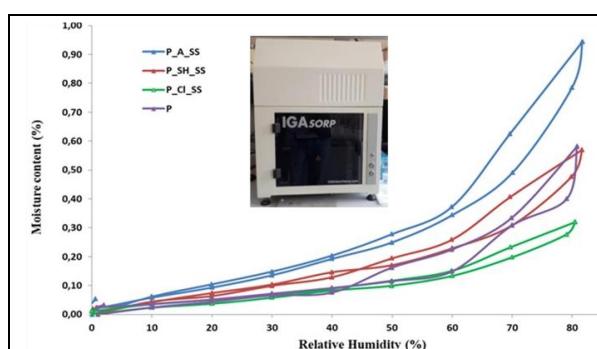


Figure 1. Sorption/desorption isotherms for the membranes

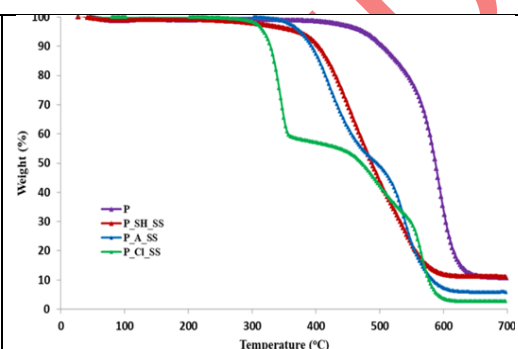


Figure 2. Thermogravimetric curves for the new membranes

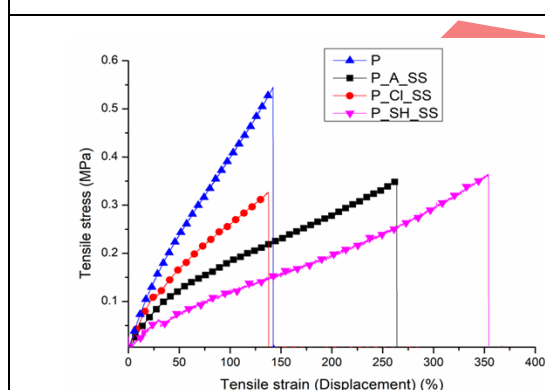


Figure 3. Mechanical measurements for the obtained membranes

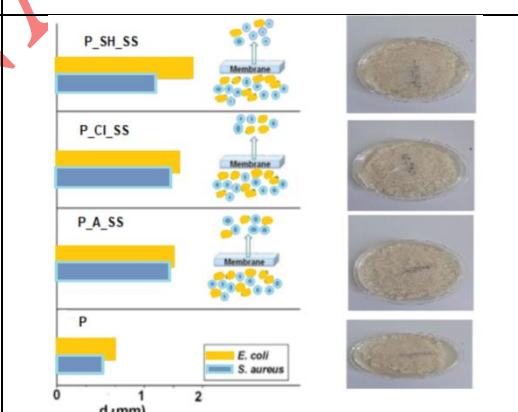


Figure 4. Biological activity for the membranes

$$d_{P\_SH\_SS}^{E.coli} > d_{P\_Cl\_SS}^{E.coli} > d_{P\_A\_SS}^{E.coli}$$

Addition of different type of POSS [3] into the polymeric membranes resulted in the enhancement of pore sizes in longitude compared with pure P membranes. The dense top layer and the separated pore structure of the pure P membranes changed to the finger like interconnected pores after addition of POSS. The bactericidal performance in environmental applications of the new blends with characteristics microarchitecture, controlled porosity, and higher hydrophobicity, is measured by its ability to maintain the balance between the biological selectivity and membranes functionalization as disinfection materials (Figure 4). The inhibition of *E. coli* to P_SH_SS was more pronounced than the inhibition for P_Cl_SS, P_A_SS and P membranes:

Conclusions

Functionalized silsesquioxanes were used for designing new materials with high-performance characteristics in order to apply them in membrane systems for wastewater treatment. The properties of materials generated by the structural properties of the polymeric chains and the history of the films influence the surface morphology indicating that the prepared membranes could be applied in wastewater treatment. Filtration properties of the composite silicone membranes have demonstrated the suitability of these to act as selective barriers, permitting the free transport of water vapor through the pores. Evaluation of the applicative potential of the membranes, tested in terms of antimicrobial activity, confirms their excellent performance as potential candidates in the field of wastewater treatment. New P-POSS membranes with improved adsorption and permeability were prepared and characterized in order to use them in environmental applications, like gas separation or water treatment. The incorporation of the silsesquioxanes nanoparticles at different concentrations to the polymer has a good impact on the morphology, surface characteristics and performance of the obtained membranes. The results showed that the addition of the silsesquioxanes enhance the formation of pores in the principal layer as compared with the principal layer in pure polysiloxane membrane. The silsesquioxanes nanoparticles improve the surface characteristics and the permeability of the membranes making its better candidates for environmental applications. All the P-POSS nanocomposite membranes presented higher porosity in comparison with the pure P membrane.

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UNCOVERING GANGLIOSIDE BIOMARKERS IN HUMAN EPILEPSY BY ION MOBILITY MS/MS

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Abstract

In the present study we introduced ion mobility separation mass spectrometry (IMS MS) for a comprehensive analysis of the changes in ganglioside pattern in human adult hippocampus affected by temporal lobe epilepsy (TLE) vs. normal hippocampus and discovery of disease-associated species.

Introduction

Epilepsy represents a neurological disorder manifested by recurrent seizures caused by damaged brain cells generating abnormal electrical signals. TLE is the most common type of epilepsy and over the years was approached by imaging, electroencephalographic recording, histological and molecular methods, however it still remained poorly understood [1]. Gangliosides (GGs) are implicated in modulation of neuronal excitability via interactions with ion transport systems, which is altered during epileptic seizures [2]. Therefore, here, we comparatively analyze the gangliosidome of normal and epileptic hippocampus using the most advanced MS technique.

Experimental

GG were extracted from the hippocampus of a 28 y.o. female affected by temporal lobe epilepsy (sample 28TLE-HS) and from a normal hippocampus of a 63 y.o. male, used as the control (sample 63CTRL). IMS MS experiments were conducted on a Synapt G2S (Waters) equipped with a nanoESI source at 1.3 kV ESI and 25 V cone potentials, IMS gas flow 90 mL·min⁻¹, IMS wave velocity 650 m·s⁻¹; IMS wave height 40 V. MS/MS experiments were performed by CID using collision energies within (30-50) eV.

Results and discussion

IMS MS analysis conducted under identical parameters for both 28TLE-HS and 63CTRL hippocampal tissue, revealed significant differences in GG profiles between the two samples. A total of 217 ions corresponding to 192 GGs were identified in 28TLE-HS, compared to 156 ions assigned to 137 distinct species in the healthy brain. Most structures were polysialylated and showed variations not only in sialylation degree and glycan core composition but also in ceramide structure. Additional modifications such as fucosylation, O-acetylation, and GalNAc or CH₃COO⁻ attachments were detected. The comparison revealed marked dissimilarities in GG expression and structure between epileptic and normal tissues. Notably, the TLE-associated gangliosidome exhibited higher overall sialylation, with a predominance of penta-, hepta-, and octasialylated species. This could reflect a compensatory mechanism or result from altered neuronal excitability in the diseased hippocampus. Although di- and trisialylated gangliosides

were more present in TLE sample, GT species were more abundant in CTRL (31.8%) than in TLE (28.2%). Another notable finding is the elevated GD3 expression in 28TLE-HS (6.3%) vs. 63CTRL (2.9%), supporting its association with neuronal death in epilepsy and its potential role in TLE-HS pathogenesis and progression. Modified gangliosides also differed in expression pattern, for instance, *O*-acetylated structures were underrepresented in TLE, potentially indicating tissue deterioration as a consequence of this disease. Further, structural characterization was achieved via CID MS/MS analysis under varying collision energies in the transfer cell. These optimized conditions produced relevant fragment ions, crucial for precise structural elucidation and isomer identification.

Conclusion

IMS MS and CID MS/MS discovered a higher number of GG structures associated to TLE than reported before, differences in their expression in the hippocampus affected by epilepsy vs. normal hippocampus and indicated the sialylation and *O*-acetylation of the species as general markers of this pathology of the temporal lobe.

Acknowledgements

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REINTEGRATION OF SEASHELLS WASTE FOR WATER PURIFICATION

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Abstract

Phosphorus released into water bodies in high amount leads to eutrophication, stimulating the over-growth of algae and aquatic plants. Phosphate, extensively used as fertilizer, is carried away from soils and reaches water bodies. Sometimes its removal from wastewaters is a matter of concern since the excess of this ion in nature causes eutrophication phenomena, and it is also present in many industrial processes, which is another source of possible overgrown levels. The natural resources of phosphate (i.e. ores) are being consumed faster than they can regenerate, being a finite supply.

Natural materials and methods are preferred for collecting excess phosphorus from water, offering the possibility of reusing it. The adsorption of ions onto natural materials, such as exoskeletons of marine shells, is a low-cost and efficient method of removing ions from polluted waters. Seashells are abundantly produced all over the world and are considered hazardous in specific circumstances, reason why ways to ecologically integrate them are pursued.

The adsorption process can be enhanced by the use of biomass, grown on an adsorbent. A different way to enhance the efficiency of the adsorption process is the modification of the adsorbent surface. In this study we present the modification of marine exoskeletons in a controlled approach, by simple chemical methods, and the testing of these materials as adsorbents for wastewater treatment. Results have shown that modified exoskeletons offer an increased adsorption compared to raw exoskeletons. This approach also represents a strategy to reintegrate these wastes, which are actually valuable resources.

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SEM STUDY OF CALCIUM PHOSPHATES ELECTRODEPOSITED ON Ti SUPPORT FROM ACIDIC ELECTROLYTE SOLUTION

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Abstract

The global demographic is shifting towards an older population, and this shift is accompanied by an increase in orthopedic and dental clinical interventions involving metallic implants such as Ti- and Ti alloy-based implants [1]. These metals are biocompatible and possess load-bearing properties. By coating their surface with calcium phosphates, they also become bioactive [2]. Calcium phosphates are ceramic materials made of calcium and phosphate ions, identifiable via their Ca:P atomic ratio. The chemical composition of some representatives resembles the inorganic component of human bones. Their stoichiometry influences their solubility in the human body when they are applied as coatings on Ti and Ti alloy supports, and their bioactivity provides long-lasting performance on metallic bone implants [2]. Besides the stoichiometry and solubility of calcium phosphates, the properties of the coatings also depend on the deposition protocol. Several known methods are employed to obtain calcium phosphate coatings on metal supports intended for use as metallic bone implants. While the most widely used deposition method is plasma spraying, the electrochemical deposition approach is simple, cost-effective, and allows the coating of complex or porous structures [3]. The properties of calcium phosphate-based coatings used to obtain metallic bone implants are also influenced by the presence of other reagents employed in the synthesis process. For example, Bucur *et al.* [4,5] have shown that the calcium phosphate known as hydroxyapatite can be synthesized in the presence of tartaric acid using the hydrothermal method. The presence of organic acids affects the morphology and properties of the coatings by diminishing or hindering crystal growth on one or more crystallographic directions. The current work deepens the understanding of the effect of tartaric acid on the formation of calcium phosphates by replacing the standard electrochemical deposition method for coating Ti supports with a more recent and patented one [6]. The standard approach requires both the Ca- and P-based precursors to be present in the electrolysis cell throughout the coating process. The newer method requires that only one of the precursors is present in the cell at the beginning of the process. The other precursor is gradually added to the electrolyte solution until the deposition is complete. For the present study, the patented technique was adapted to include the tartaric acid solution. The samples were morphologically investigated by SEM and the results were compared with data acquired by analyzing specimens obtained via the hydrothermal method. The conclusion is that the calcium phosphates synthesized with the newer electrochemical method exhibit significantly superior morpho-crystalline features.

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PRELIMINARY STUDY OF $\text{TiO}_2@\text{In}_2\text{O}_3$ OBTAINED FROM SOLVOTHERMAL SYNTHESIS AS POTENTIAL RECOMBINATION BARRIER LAYER IN DYE SENSITIZED SOLAR CELLS

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Abstract

In order to successfully commercialize dye-sensitized solar cells (DSSCs) and achieve high conversion efficiency, the technology must be optimized to reduce charge recombination between the electron transport layer and the contact. For such solar cells, undesirable interfacial charge recombination reactions occurs when an electron injected from the dye into the metal oxide photoanode recombines with a hole from an oxidized dye molecule or from a hole-transport material (HTM). It was previously observed that the reduction of oxidized dye molecules by the HTM is relatively fast, hence the recombination with oxidized dye molecules has a smaller impact on charge collection efficiency than does the photoanode-HTM recombination process [1]. In order to reduce this recombination process (photoanode-HTM), many authors have proposed different approaches for thin, passivating, insulating, barrier layers deposited on top the photoanode in a “core-shell” structure prior to dye adsorption [2; 3; 4; 5; 6; 7; 8]

Optimizing the front blocking layer (BL), a crucial part of the DSSC structure, may improve the efficiency of photoelectron transfer from the dye to the semiconductor by reducing charge recombination at the interfaces between the TiO_2 /electrolyte and FTO/electrolyte. The mechanisms by which a barrier layer can enhance DSSC performance was described by O'Regan et al [9], consists of two competitive processes: it can either introduce a surface dipole that increases the photoanode's conduction band or passivate surface defect sites that act as recombination centers or it can also act as an insulating wall between the photoanode and the oxidized dye molecules as well as the HTM, acting as a tunneling barrier to recombination.

In this paper, we are considering using a blocking layer consisting of core-shell $\text{TiO}_2@\text{In}_2\text{O}_3$ structures. The solvothermal synthesis method used for the fabrication of novel core-shell $\text{TiO}_2@\text{In}_2\text{O}_3$ structures is presented. The core of the nano-structures consists of TiO_2 nanoparticles of around 18 nm, obtained through a different solvothermal synthesis [10]. The as-obtained products were characterized by X-ray diffraction and UV-Vis-NIR spectroscopy. Our results show band gaps (calculated from the diffuse reflectance spectra) between 3.31 eV and 3.5 eV for core-shell $\text{TiO}_2@\text{In}_2\text{O}_3$. Since the blocking layer is not intended to absorb light-its main role is to suppress charge/electron recombination, a higher band gap suggests both a optical transparency across the visible spectrum that absorbs only deep UV and does not reduce the light reaching the dye, and also a conduction band offset at the TiO_2 interface, that could improves open-circuit voltage (V_{oc}) and overall charge separation. This preliminary study demonstrate that core-shell $\text{TiO}_2@\text{In}_2\text{O}_3$ structures could be successfully used for DSSC as a layer designed to **block recombination** and **enhance device performance**, while remaining fully transparent to visible light.

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ELECTROCHEMICAL RESPONSE OF METAL OXIDES IN SODIUM HYDROXIDE

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Abstract

This study investigates the electrochemical behavior and surface wettability of Fe₂O₃ and CuO under alkaline conditions, aiming at non-enzymatic glucose sensing. Thermal annealing at 500 °C for Fe₂O₃ and 800 °C in the case of CuO was applied to modify their structural and surface characteristics [1]. Electrochemical behavior, assessed by cyclic voltammetry in sodium hydroxide (NaOH) solutions (pH 7 and 14), revealed pH-dependent redox responses with clearer oxidation–reduction peaks in highly alkaline environments. Contact angle measurements showed that annealing enhanced hydrophilicity, supporting better electrolyte interaction and charge transfer [2]. The importance of morphology control and functionalization in shaping hybrid structures for diverse electrochemical applications has also been highlighted [3,4].

CuO electrodes were further examined for glucose sensing in 0.5 M NaOH. They displayed a concentration-dependent current response with good electrocatalytic activity toward glucose oxidation. A calibration curve confirmed a linear correlation between glucose concentration and peak current, demonstrating reliable quantitative detection across the studied range. Overall, thermally treated CuO emerges as a promising, low-cost, enzyme-free glucose sensor in alkaline media. These findings emphasize how surface modification and electrolyte pH critically govern the electrochemical performance of metal oxide electrodes, offering valuable insights for their future application in biosensing technologies.

Acknowledgements

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ADVANCED HYBRID THIN FILMS BASED ON MONTMORILLONITE FUNCTIONALIZED WITH PEROVSKITE NANOSTRUCTURES

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Abstract

In the field of materials science, the nearly infinite possibility of designing new material combinations with chemical, physical, and mechanical properties distinct from the initial ones has transformed modern society. The miniaturization of electronic devices has become a major challenge for scientists, given their multitude and complexity. Modern technology requires the use of thin films for various applications, such as non-volatile ferroelectric memories, surface acoustic wave devices, pyroelectric devices, and more [1-3].

For the deposition of hybrid materials based on montmorillonite functionalized with perovskite materials obtained through the solid-solid method, as thin films, a paste was prepared for each material in order to achieve an optimal viscosity that would lead to the best possible uniformity. Thus, the paste was made from: 0.15 g of dissolved ethyl cellulose; 15 mL of ethanol; 1 mL of terpineol; 100 mg of powder from each material; 0.1 mL of acetic acid; 0.05 mL of H₂O.

The paste was sonicated for 30 minutes and then mixed with a magnetic stirrer for 1 hour at a speed of 350 rpm and a temperature of 50 °C until an optimal viscosity was achieved. This was deposited onto FTO substrates, which had been previously cleaned with ethanol and acetone for 30 minutes during each process to remove any impurities from their surface. Finally, the plates were exposed to a UV lamp to ensure a perfectly clean surface.

The film deposition was carried out using the spin-coating method at 1500 rpm for 30 seconds, followed by calcination at 450 °C for 60 minutes with a heating rate of 1 °C/min.

From the Mott-Schottky analysis, it can be observed that all the samples exhibit n-type semiconductor behavior. The electron density increases with the introduction of Ag and Pd ions into the LaMnO₃ material. Additionally, as the temperature increases, an increase in current is observed, further confirming the semiconductor nature of the samples.

For the physicochemical analysis of the obtained films, **was used**: Confocal microscopy (type Olympus LEXT OLS4000), Atomic Force Microscopy (type Nanosurf® EasyScan 2 Advanced Research).

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THE INFLUENCE OF CLIMATIC CONDITIONS ON *AMARANTHUS RETROFLEXUS* L. AND *CHENOPODIUM ALBUM* L. PLANTS

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Abstract

The purpose of this research is to investigate how the climatic conditions influence the water content of the species *Amaranthus retroflexus* and *Chenopodium album*. The two species are noxious weeds spread all over the world and which grow rapidly especially in abandoned construction areas, people's gardens but also on agricultural lands among cultivated plants. Plant materials were collected from a single location during three different months of 2025. Humidity was determined by gravimetric method and the values obtained were correlated with the meteorological factors specific to each month. The determinations obtained highlighted the fact that there are considerable differences in humidity between plant parts and between months, indicating a direct link between temperature, precipitation and humidity. The results demonstrate the importance of climatic conditions in the adaptive capacity and the possibility of spreading of these invasive species.

Keywords: moisture content, adaptability, climatic stress, invasive species

Introduction

The ability of plants to adapt to the direct and indirect impacts of climate change will have implications for extinction risks, agricultural and environmental sustainability, and food security. One biological response, driven by shorter winters, earlier growth, and longer droughts is that many species emerge and reproduce considerably earlier in the year [1,2].

Amaranthus retroflexus L. (redroot pigweed) and *Chenopodium album* L. (lambsquarters) are fast-growing, weedy plants belonging to the *Amaranthaceae* family. Both are among the most common weeds in the world and are most commonly found in agricultural areas [3], where they lead to considerable issues. They invade the crops they grow in and, due to their destructive development and allelopathic activity, make them highly competitive and result in reduced crop quality [4].

The two species are adapted to extremely poor and unpredictable environmental conditions, competing with other plants for nutrients, water, light and space [5]. The fact that plants have the ability to oscillate their morphological traits has been established as a favorable survival strategy, which has allowed plants to adapt to changing environmental conditions [6]. The way a plant develops is closely linked to the environment in which it grows [7]. For example, both the root [8] and the stem [9] can significantly modify their shape even in genetically identical plants, when exposed to different conditions. Thus, the same species can survive and thrive in varied habitats, due to its flexibility to adjust its morphology [10].

The aim of the work is to investigate how climatic conditions, air temperature, precipitation levels and humidity, influence the water content of the species *Amaranthus retroflexus* and

Chenopodium album. These two plants can provide important information about the adaptability and resistance of spontaneous vegetation to climatic stress. Analyzing the differences in humidity at the soil level and in the parts of the plant (soil, root, stem, leaves) allows a better understanding of how these species respond to environmental differences. The research contributes to a better understanding of the mechanisms by which plants from the spontaneous flora manage to maintain their competitiveness in agricultural crops, even under stress conditions.

Experimental

The plant samples were collected in 2025, from a single location in Timis County, Romania, Bazosul Nou (forest) for three months: June, August and September. Before analyzing them, the plants were washed very well with tap water and distilled water to remove dust and soil residues. After preparation, the plants were separated into different parts (soil, root, stem, leaves, flowers and seeds).

The water content of the plant parts of *Amaranthus retroflexus* and *Chenopodium album* was determined by thermogravimetric analysis. The samples (≈ 5 g) were weighed and placed in a Sartorius thermobalance. The dehydration process was carried out at increasing temperatures, up to 110°C . The progressive weight loss was monitored in real time, which allowed the precise calculation of moisture and the evaluation of its distribution in the different plant parts.

The weather records (temperature, precipitation, atmospheric humidity) of the studied months were extracted from official meteorological sources specific to the Timisoara region. The values were then processed and interpreted using statistical analysis, with the help of ChatGPT (version GPT-4o, part of OpenAI's GPT-4 family, developer OpenAI, San Francisco, CA, USA) under human supervision ensuring accuracy and consistency throughout the study.

Results and discussion

For a better understanding about the relationship between climate and moisture content in the analyzed plant parts, Table 1 was created and based on this data three graphical representations were constructed.

Table 1. The analyzed plant parts from *Amaranthus retroflexus* and *Chenopodium album* and meteorological conditions.

	ARU%	CAU%	AvDT ($^{\circ}\text{C}$)[11]	PP[mm] [12]
Soil J	28,16	13,09	17,4	8
Root J	64,57	59,69	17,4	8
Steam J	87,53	77,64	17,4	8
Leaves J	84,78	81,67	17,4	8
Soil A	6,16	3,16	23,26	25,5
Root A	73,93	15,69	23,26	25,5
Steam A	82,02	83,02	23,26	25,5
Leaves A	75,96	72,15	23,26	25,5
Soil S	3,21	6,9	17,3	50
Root S	64,27	50,27	17,3	50
Steam S	71,28	53,55	17,3	50
Leaves S	66,87	66,34	17,3	50

Legend: AR-*Amaranthus retroflexus*; CA-*Chenopodium album*; U%-moisture content; AvDT (°C)-Average daily temperature (Celsius degrees); J-june; A-august; S-september; PP[mm]-precipitation [milimeter].

Table 1 shows that in June (J), moisture content were high in both plants, particularly in stems and leaves. In August (A), a noticeable decrease was observed in *Chenopodium album* (CAU%), more noticeable in roots and soil, while *Amaranthus retroflexus* (ARU%) maintained higher values. By September (S), moisture continued to decrease, but the differences between species became smaller, suggesting a possible merging in their adaptation to the climatic conditions specific to late summer.

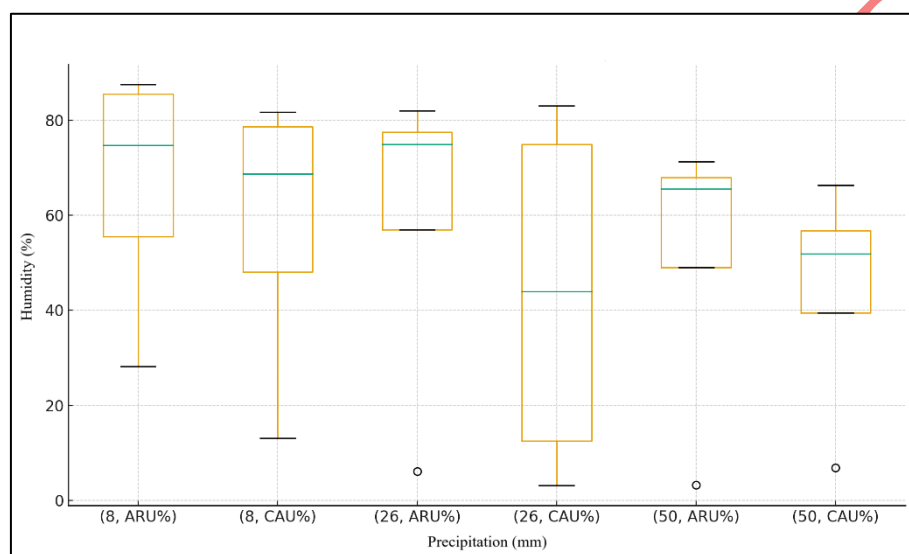


Figure 1. The influence of precipitation on humidity [13].

Legend: AR-*Amaranthus retroflexus*; CA-*Chenopodium album*; U%-moisture content; AvDT (°C)-Average daily temperature (Celsius degrees); J-june; A-august; S-september; PP[mm]-precipitation [milimeter].

In June (8 mm), plants had higher water content due to residual soil moisture. In August (26 mm), levels dropped as high temperatures offset rainfall. By September (50 mm), humidity rose slightly but stayed below June values. Figure 1 illustrates this relationship between rainfall, temperature, and plant water content.

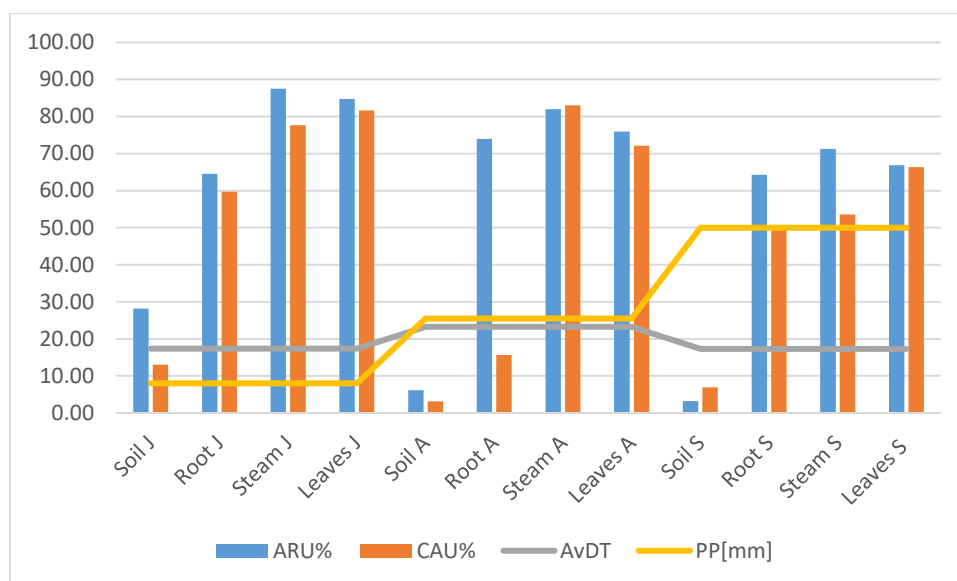


Figure 2. Comparison of water content in different parts of *Amaranthus retroflexus* and *Chenopodium album*.

Legend: AR-*Amaranthus retroflexus*; CA-*Chenopodium album*; U%-moisture content; AvDT (°C)-Average daily temperature (Celsius degrees); J-june; A-august; S-september; PP[mm]-precipitation [milimeter].

In June, both species showed high water content across all plant parts, especially in stems and leaves, with only minor differences between them. Despite the low rainfall, the soil still held enough residual moisture to sustain these levels. By August, the situation had changed: rising temperatures caused a clear drop in water content, more pronounced in *Chenopodium album*, while *Amaranthus retroflexus* managed to keep higher values, particularly in its roots and leaves. While the amount of precipitation was higher than in June, their effect was limited by the heat specific to the month. In September, with the decrease in temperatures and the increase in the rainfall regime, the water level in the plants increased again, but without reaching the values of June. At the same time, the differences between the two species decreased, which suggests a similar adaptation to the end-of-summer conditions.

Conclusion

Temperature, a major factor influencing water content and the increase in average temperature, resulted in a decrease in humidity, especially in August, regardless of the amount of precipitation. Precipitation had a secondary and temperature-dependent effect; in months with more rain but high temperatures (August), water content remained low, suggesting that the beneficial effect of precipitation is canceled by thermal stress. *Amaranthus retroflexus* has a greater capacity to maintain moisture in leaves and stems compared to *Chenopodium album*, which gives it an adaptive advantage in variable climatic conditions. The spread of water in plant parts differs depending on the species and month, indicating differences in physiological strategies in the use of water resources, a perspective that may influence the competitiveness and spread of these invasive species.

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CONDUCTIVITY AND CHARGE TRANSPORT IN SILICONE COMPOSITES CONTAINING PEROVSKITE POWDERS

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Abstract

Silicone rubber (SR) composites with 10–30% perovskite powders were studied for their electrical properties. Conductivity between 0.5 kHz and 2 MHz showed DC values rising from 5.61×10^{-5} to 7.67×10^{-5} S/m. Transport followed Jonscher's law, the correlated barrier hopping model, and the polaron model. Aging reduced conductivity due to microstructural defects.

Introduction

Perovskite-filled SR composites are promising for flexible electronic materials. This work examines how filler concentration affects conductivity and charge transport.

Experimental

SR composites containing 10%, 20%, and 30% perovskite powders were fabricated. Conductivity was measured from 0.5 kHz to 2 MHz and at different temperatures.

Results and discussion

Two regions appeared: a DC plateau and an AC-dependent regime. DC conductivity increased with filler content (5.61×10^{-5} to 7.67×10^{-5} S/m). Temperature studies supported hopping-based transport.

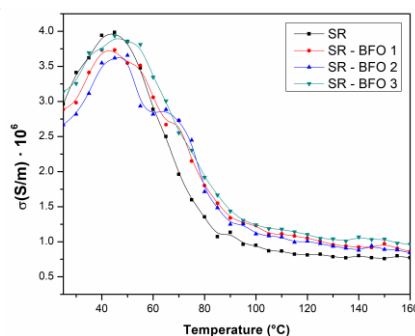


Fig 1. Temperature dependence of the conductivity for SR and SR-BFO samples

Conclusion

Filler concentration controls conductivity and transport behavior in SR–perovskite composites, while aging highlights stability challenges.[1]

Acknowledgements

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STUDIES ON REDUCING ENVIRONMENTAL POLLUTION PRODUCED BY AGRICULTURAL TRACTORS

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Abstract

The purpose of studies on reducing pollution produced by agricultural tractors is to identify, analyze and develop solutions to minimize the negative impact that these machines have on the environment.

The main objectives of such studies include: identifying pollution sources; developing cleaner technologies; optimizing agricultural practices; complying with European standards; analyzing the economic impact.

Energy consumption is a major source of air pollution, contributing to over 90% of sulphur dioxide emissions in the EU. Pollution from internal combustion engines in tractors takes two forms: chemical pollution and dust pollution. Chemical pollution, in turn, is carried out through pollutant emissions, soil pollution and toxicity.

Along with the evolution of technology, pollution regulations have also evolved, becoming increasingly restrictive. Reducing emissions produced by internal combustion engines in vehicles is the most important goal of manufacturers at the moment. The increase in the number of vehicles has led to the need to improve the environmental performance of the engines that equip them, in order not to increase air pollution substantially.

Introduction

Interest in environmental pollution has grown in recent times from a small number of people who dealt with pollution sporadically and randomly to the entire population of the globe and the most diverse institutions and organizations. [1], [3]

Of course, pollution deserves interest, primarily for its current aspects, because it still creates inconveniences and damages that affect health, sometimes involving large masses of people.[2], [4].

This requires its knowledge to be as thorough, urgent and extensive as possible.

The impact of polluting emissions on the environment consists of:

- formation of tropospheric ozone, which is very toxic to organisms;
- damage to flora, especially conifer species and fruit trees. [5], [7].

Effects on the health of the population produced by polluting emissions are:

- respiratory and cardiac diseases due to CO;
- irritation of the respiratory tract due to NOx;
- eye irritation and carcinogenic effects caused by hydrocarbons;
- anemia, diseases of the nervous system due to lead compounds;
- nervous depression due to benzene compounds.

Diesel engine emissions, due to the nature of combustion, consist of a series of pollutants, the most dangerous of which are nitrogen oxides and particulate matter. [6], [9]. The Euro VI emissions regulation, which will apply to all new commercial vehicles and buses produced after 1 January 2014, introduces significant reductions in the levels permitted at the tailpipe. [8].

Thus, nitrogen oxide emissions must be at least 80% lower and particulate emissions reduced by 66% compared to the Euro V standard. Euro VI also introduces a limit on ammonia emissions for the first time [11], [15].

Currently, in diesel engines, injection systems and injection pressure are improved to achieve high pressures when spraying the fuel. This also improves the efficiency of the diesel engine. The combustion process is a very complex one both from a thermodynamic point of view and in terms of heat transfer. [13].

In recent years, internal combustion engines have had and continue to have a spectacular evolution. In addition to mechanical components, electronic control systems have appeared that can implement complex laws to ensure optimal engine operation, achieving a compromise between performance, low emissions and reliability. [10], [14].

The internal combustion engine is also a source of chemical and noise pollution that harms humans and the environment. Chemical pollution is due to the chemical substances and compounds found in the exhaust gases of vehicles. [12].

In recent years, internal combustion engines have had and continue to have a spectacular evolution. In addition to mechanical components, electronic control systems have appeared that can implement complex laws to ensure optimal engine operation, achieving a compromise between performance, low emissions and reliability. [16], [17].

Experimental

Pollution source analysis focuses on identifying how various activities and processes release harmful substances into the environment. The main types of pollutant emissions are exhaust gases and fine particles, which have a significant impact on air quality and human health.

The harmful substances present in the atmosphere fall into two groups, depending on the nature of their origin. Thus, there are primary substances, in gaseous or solid state, which are found directly in the exhaust gases of a vehicle (HC, CO, NO_x and PM) and secondary substances which are represented by photochemical smog and wet smog.

Hydrocarbons (HC)

They are pollutants present in automobile emissions characterized by variable toxicity depending on the chemical composition. The main hydrocarbons in automobile exhaust gases are benzene, toluene and xylenes.

Carbon monoxide (CO)

It is a chemical substance in a gaseous state, colorless and odorless, which is formed due to the incomplete combustion of carbon-rich substances (fuels). Being an asphyxiating gas, it has a toxic effect on the body. The toxic asphyxiating effect of carbon monoxide is due to its combination with hemoglobin.

Nitrogen monoxide (NO)

It is a colorless, toxic gas, with an irritating effect on the respiratory mucosa. Long-term exposure has a carcinogenic effect on the human body. The toxic effect is due to the formation of methemoglobin (a product similar to carbaminohemoglobin), by combination with hemoglobin, which prevents the exchange of oxygen between tissues and respiratory organs.

Nitrogen dioxide (NO₂)

It is a reddish-brown, toxic gas with a pungent odor. It has a harmful effect on the respiratory tract, causing irritation. By combining with water it forms nitric acid (acid rain) which has a devastating effect on the environment.

Particulate matter (PM)

They are made up of carbon molecules that combine with other chemical compounds (hydrocarbons, sulfites, nitrates, metals) and depending on their size form black smoke or soot.

Photochemical smog

It is a smoke-like fog characteristic of cities with heavy traffic and favorable formation conditions. The conditions underlying the formation of photochemical smog are: low humidity, temperature higher than 20°C and sunlight. For the formation of photochemical smog, 13 chain chemical reactions are required, initiated by nitrogen monoxide and dioxide, then ozone (O₃) and hydrocarbons. The effects of photochemical smog on the human body are harmful because it causes irritation of the respiratory tract and eyes.

Wet smog

Unlike photochemical smog, wet smog forms in the atmosphere with high humidity, at relatively low temperatures (4°C). It is formed due to chemical reactions between particles, carbon oxides and sulfur oxides. It has a suffocating effect on the human body.

One of the main directions of research and development in the agricultural industry is the creation of cleaner engines and propulsion systems. These efforts focus on reducing fuel consumption, pollutant emissions and environmental impact, with the ultimate goal of more sustainable agriculture.

To reduce diesel engine emissions, manufacturers are focusing on cleaner combustion and exhaust aftertreatment technologies.

Advanced injection systems, modern engines use high-pressure, electronically controlled injection systems that spray fuel into extremely fine droplets. This ensures more complete combustion and reduces emissions of fine particulate matter (PM) and nitrogen oxides (NO_x).

Diesel Particulate Filters (DPF), these filters capture soot particles from the exhaust gases and periodically burn them, turning them into harmless ash.

Selective Catalytic Reduction (SCR), an SCR system injects a urea-based fluid, known as AdBlue, into the exhaust gas stream. This fluid reacts with nitrogen oxides and converts them into harmless nitrogen and water.

Another important direction is the transition from fossil fuels to cleaner energy sources.

Alternative propulsion systems

Electric propulsion, electric tractors completely eliminate polluting emissions and noise at the point of use. They are ideal for small-scale agricultural operations and offer high torque, essential for field work.

Hybrid systems, hybrid tractors combine an internal combustion engine with an electric motor. This configuration allows the electric motor to take on light loads, reducing fuel consumption and emissions.

Results and discussion

Studies are focusing on developing engines compatible with biofuels (biodiesel) or synthetic fuels, which can reduce the carbon footprint of agriculture.

The use of smart technologies and robotics also contributes to cleaner agriculture:

Autonomous tractors - these machines, guided by GPS and sensors, avoid overlapping work and minimize field passes, reducing fuel consumption and soil compaction.

Route optimization - navigation systems and automatic route planning ensure maximum efficiency in the execution of agricultural tasks, reducing operating time and, implicitly, emissions.

Optimization of agricultural practices is essential to reduce environmental impact and improve sustainability.

Another strategy is the use of machines that exert less pressure on the soil, thus reducing compaction.

Low-pressure tires: Specialized tires with a larger contact patch distribute the tractor's weight over a wider area. This reduces the specific pressure on the soil, protecting its structure and improving water infiltration and root growth.

Lighter equipment: Solutions are being sought to use smaller, lighter equipment for certain tasks, instead of heavy tractors. For example, autonomous agricultural robots can perform operations such as seeding or weeding, with minimal impact on the soil.

These approaches not only protect the environment, but also increase economic efficiency, by reducing fuel costs and improving crop productivity in the long term.

Studies and research are essential to comply with the strict regulations imposed by the European Union on pollutant emissions. These standards change periodically, and the agricultural industry must constantly adapt.

In addition to the environmental benefits, studies also assess the economic efficiency of new technologies. The aim is to provide viable solutions that do not significantly increase costs for farmers.

In short, studies in this field contribute to a more sustainable, more efficient and environmentally friendly agriculture, essential to ensure food security and protect ecosystems.

Conclusion

Internal combustion engines are a major source of atmospheric pollution with toxic emissions. These are the reasons why the effort to reduce the amount of polluting emissions from internal combustion engines is of interest to all countries, and even more so to those that have a vehicle and agricultural tractor manufacturing industry.

The major problem currently posed by the internal combustion engine is the pollution of the atmosphere by combustion gases, a fact that attracts the attention of specialists, especially in order to reduce harmful emissions. Any new type of internal combustion engine, in order to be accepted, must have a type approval certificate in which the measured emissions do not exceed the limits imposed by environmental protection legislation.

The sources of pollutant emissions from an internal combustion engine are caused by the combustion of fuel and the imperfect sealing of the engine cylinders, the fuel tank and the supply pipes. The pollutants generated by combustion are eliminated into the atmosphere through the exhaust gases and partly through the engine crankcase gases. The pollutants determined by the imperfect sealing are discharged directly into the atmosphere through the evaporation of the fuel from the engine fuel system and the fuel tank.

During the periodic technical inspection and traffic checks carried out by representatives of the traffic police and the Romanian Automobile Registry, the first operation consists of checking the tightness of the exhaust gas exhaust. The next operation consists of determining the CO concentration using a gas analyzer.

In Europe, legislation limits the emissions of various polluting gases produced by motor vehicles. All vehicles are built in accordance with this legislation and have an emission control system in their structure that eliminates or considerably reduces these emissions. The car subassemblies that filter exhaust fumes are the catalytic converters and the particulate filters, their action being also controlled by the ECU.

High exhaust emissions occur when the fuel is not burned completely, the engine is not properly adjusted, when starting or stopping the engine, when driving at low speed. Without a catalyst, when the engine is running at a standstill, the CO content in the exhaust gases should not exceed 5%.

Reducing environmental pollution from agricultural tractors is a crucial objective for a more sustainable future.

Air pollution caused by internal combustion engines is a complex problem, and solving it requires an approach that involves both individual-level measures, public policies and technological advances.

Car manufacturers are continuously working to develop more efficient engines that consume less fuel and emit fewer pollutants.

The transition to zero- or low-emission vehicles, such as electric cars (EVs) and hybrids, is seen as a key long-term solution. This transition is supported by innovations in battery technology and the development of charging infrastructure.

By combining these approaches, a significant reduction in air pollution from internal combustion engines can be achieved, contributing to a cleaner environment and better public health.

Research and development of biofuels, green hydrogen or other synthetic fuels, which generate much lower emissions, is another way to reduce pollution.

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ELECTROCHEMICAL BEHAVIOR OF COPPER N,N'-BIS[(2-HYDROXYBENZYLIDENEAMINO)-PROPYL]-PIPERAZINE AS COORDINATION POLYMER IN SALINE SOLUTION

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Abstract

Investigation of the electrochemical behavior of the copper coordination polymer N,N'-bis[(2-hydroxybenzylideneamino)-propyl]-piperazine in saline solution at a pH of 2.5 was carried out to organic compounds containing N, S and O heteroatoms, and/or aromatic or other π -electronic systems, exhibit excellent potential for corrosive protection. [1,2]

The CP molecule, by its extended aromatic structure double bonds heteroatoms is promises to be a potential corrosion inhibitor due to its strong binding ability to metal surfaces. The CP molecule satisfies the theoretical criteria necessary to form a protective layer on metal surface (cover properly the active centers of the metal surface) avoiding the aggressive species to reach to the metal surface. Practically the inhibition efficiency determined is lower than 81%. The electrochemical impedance spectroscopy (EIS) reveals that in the first hour of immersion the adsorption of inductive species is important. With the increase of immersion time the CP shows good anticorrosive protection at lower concentration. The polarization resistance increases from 193.8 Ohm (iron in acid saline media) to 1806.4 Ohm in the presence of 50 ppm CP. The corrosion rate is 1.099 mm/year for iron in saline acid solution and less than 0.214 mm/year for CP. The anti-corrosion protection capacity is related to the CP concentration. In the acidic saline environment, as a result of the cleavage of the CP ligand-metal bond in the system, fractions of the ligand and copper ions are generated. Iron is more reactive than copper, so it "places" higher in the metal activity series, allowing it to reduce copper ions. At concentrations higher than 50 ppm, it is observed that CP does not provide adequate anti-corrosion protection due to the porous and incomplete copper layer that is deposited on the iron surface, the binding capacity of the ligand is limited, and the protective layer formed at concentrations higher than 50 ppm is porous and of poor quality. This results in increased susceptibility to corrosion, undermining the effectiveness of the coating. Therefore, optimizing the concentration of CP is crucial for enhancing the durability and protection of the iron surface against corrosive environments.

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EVALUATION OF THE NUTRITIONAL PROFILE OF RED ONION (*ALLIUM CEPA* L.) – PRELIMINARY RESULTS

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Abstract

Onion (*Allium cepa* L.) is one of the most important vegetables plants cultivated and consumed worldwide, being appreciated both for its culinary role and for its health benefits. The specialized literature shows that onion has a high nutritional value, being a source of vitamins, minerals, dietary fiber, simple carbohydrates and bioactive compounds (flavonoids, polyphenols, sulfur compounds). The red variety is distinguished by a higher content of anthocyanin pigments and flavonoids, which give it superior antioxidant properties and a sweeter taste than white onion. The aim of this work is to evaluate the basic nutritional composition (proximate composition) of a red onion assortment sold in local agri-food markets. Preliminary determinations of moisture, ash, protein, lipid, fiber and carbohydrate content revealed a significant contribution of carbohydrates and fiber, complemented by a reduced amount of protein and lipid. The results obtained: 10.12-11.06% moisture, 3.38-3.87% ash, 2.62-3.47% protein, 1.51-2.04% fat, 6.49- 7.22% fibers, and 72.48-75.31% carbohydrates propose the use of red onion powder as a natural additive in food with added value or as an alternative source in animal feed ingredients. The results confirm that red onion is a valuable food due to its basic composition and can contribute to maintaining a balanced and healthy diet.

Introduction

Onion (*Allium cepa* L.) is a very important agricultural economic crop that is widely planted around the world. Onion is a bulbous vegetable and spicy plant, being appreciated for its distinct flavor, health benefits, and active ingredients. Onion (*Allium cepa* L.), one of the most cultivated and consumed vegetables worldwide, has been cultivated for over 5000 years in the ancient world due to its unique pharmacological, medicinal, and culinary qualities [1, 2]. As a food, onions are used fresh, for salads as well as processed for pickles, chutneys, sauces and dehydrated powder for seasoning. Its medicinal uses are found in diuretic, digestive, heart, eye and joint conditions [3,4]. Studies suggest that onions contribute to heart health by potentially lowering blood pressure and cholesterol levels, helping to reduce the risk of cardiovascular disease, and their consumption is associated with the prevention of liver, gastrointestinal, lung, stomach and colorectal cancer [5,6]. Onions are a perfect blend of diverse and valuable nutritional compounds and phytochemicals such as allicin, quercetin, organosulfur compounds, antioxidants, phenolic compounds, flavonoids and fructo-oligosaccharides. Fresh onion bulbs contain approximately 89.11% water, 1.10% protein, 0.10% lipids, 0.35% ash, 0.34% carbohydrates, 1.70% dietary fiber, and 4.24% total sugar (0.99% sucrose, 1.97% dextrose, 1.29% fructose), as well as 0.21% minerals (potassium, phosphorus, calcium, magnesium, sodium, iron) and a significant amount of vitamins B, C, and E [2, 7].

Red onions are a variety of onions that generally contain the same nutritional compounds as white or yellow onions. Red onions, in contrast to white or green onions, due to the red pigment that gives them their color, quercetin, provide the body with a greater amount of antioxidants. Rich in flavonoids, sulfur compounds and vitamin C, red onions also prevent the occurrence of certain neurodegenerative and cardiovascular diseases, if consumed correctly, in moderate quantities. Red onions contain calcium, manganese, copper, magnesium, iron, zinc, phosphorus, potassium, cellulose and organic acids. Also, the pulp of an onion contains vitamin K, B5, B6 and beta-carotene along with ascorbic acid.

Experimental

Plant material consisted of red onion bulbs were commercialized from local agri-food markets. Red onion bulbs without physical defects were collected from different local vegetable producers, and three distinct groups of about 1 kg each were formed and marked G1, G2, and G3. The red onion bulbs, previously cleaned of the dry outer skin (the papery tunic protecting the edible part), root residues, and other adhering impurities, were used for the determination of nutritional parameters. The nutritional parameters of red onion were performed on dried material. For this purpose, the red onion bulbs were sliced and dried in an oven at 60 °C until constant mass. After drying, the slices were ground using a kitchen blender and stored in an airtight container in the refrigerator (approximately 4 °C) until further analyses were carried out. The determination of the nutritional composition of red onions (*Allium cepa* L.) was performed according to the AOAC Official Methods of Analysis, 2000 (AOAC, 2000) and following the recommendations of Velcirov et al [8]. Mineral substances (ash) were determined by the calcination method at 550 °C. Protein content was determined by the Kjeldahl method, using a nitrogen conversion factor of 6.25. Crude fat was determined using the Soxhlet method with hexane as solvent. Crude fiber was determined using the acid–base digestion method. Carbohydrate content was obtained by difference.

Results and discussion

The results obtained for the determination of the nutritional parameters in the analysis of the red bulbs of red onion are shown in table 1.

Table 1. The nutritional parameters of analyzed red onion

Specification	Nutritional parameter values, g/100 g dried matter (DM)					
	Moisture	Ash	Protein	Fat	Fiber	Carbohydrate
Limits	10.12 - 11.06	3.38- 3.87	2.62 - 3.47	1.51 - 2.04	6.49- 7.22	72.48 – 75.31
Average values	10.51± 0.47	3.51± 0.25	3.05± 0.42	1.87± 0.27	6.81± 0.36	73.86± 1.42

As can be seen from the data presented in table 1, and figure 1, the determined nutritional parameters show different values that vary depending on the origin of the red onion bulbs and the analyzed parameter.

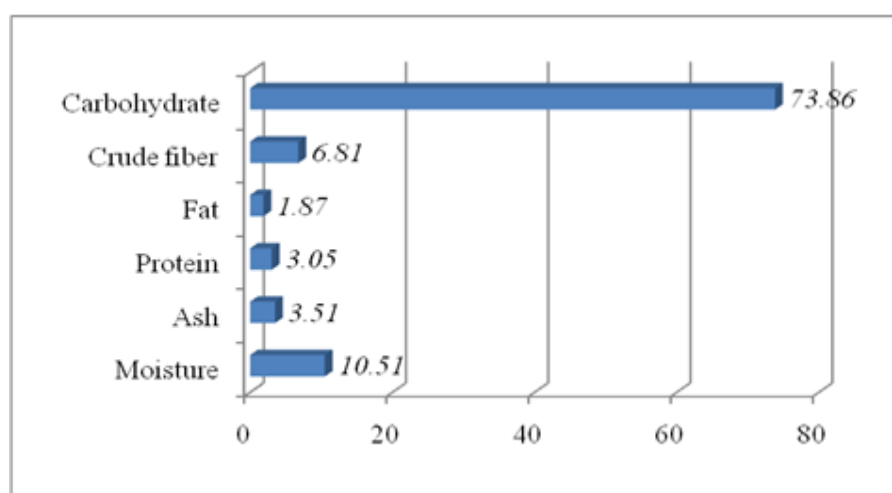


Figure 1. Nutritional values of red onion bulbs

Humidity is the parameter that provides information on the amount of water contained in a certain product, respectively the amount of dry matter of that product. In addition, this parameter provides indications related to the storage and processing of food [9]. Foods with low moisture content (especially those with less than 10%) have a longer shelf life, with limited deterioration in quality due to microbial activities; while foods with moisture content major than 10% cannot be stored for long periods of time. Considering the high value of raw red onion reported by Ani et al. (2021) and Czech et al. (2022): 84.60, respectively 88.57%, it can be notice that this vegetable has a limited shelf life. In contrast, the powder obtained from the red onion taken in the experiment, with a moisture content between 10.12 - 11.06 g/100g DM, has a higher content of nutritional compounds and can be stored for a longer period of time [10,11].

The ash content is an indicator of the total concentrations of mineral elements present in the analyzed samples [9]. The values obtained for the determination of the ash content of the analyzed samples show values ranging from 3.38- 3.87 g/100g DM. These values, as well as the average value of the ash content (3.51g/100g DM) reveal that red onion bulbs analyzed can be considered as a potential source of mineral elements in the form of essential macro and micro elements.

Proteins are essential component of the diet needed for the survival of animals and human being important biomolecules for the body's homeostasis [9]. Protein deficiency is closely related to a number of diseases such as Kwashiorkor, Marasmus (energy deficiency), mental disorders, insufficiency of different organs, edema and immune system weakness [8]. The concentration of these essential macronutrients determined in the analyzed red onions shows values ranging between 2.62 - 3.47 g/100g DM. These limits, and also the average concentration (3.05) show that the analyzed samples contain moderate amounts of protein, these having a relatively low protein intake. However, these values show that dried red onions cannot be considered an important source of protein.

Fats are essential macronutrients that play an important physiological and biochemical role in the functioning of the human body and can also be used as ingredients to improve the texture, taste and aroma of foods [9]. The fat concentration in the analyzed red onion samples shows values between 1.51 - 2.04 g/100g. These values show that the analyzed red onion bulbs are a poor source of calories.

The term **crude fibre** refers to the insoluble dietary fibre fractions and comprises the constituents of the cell walls found in plant tissues, including lignin, cellulose and hemicellulose. The crude fiber content of the analyzed red onion samples shows values ranging

between 6.49 - 7.22 g/100g DM. These values show that the analyzed red onion contains modest amounts of crude fiber. Since crude fiber represents only a part of the total fiber, it can be seen that the analyzed red onion samples cannot be considered as potential sources of dietary fiber. **Carbohydrates** are the body's main source of energy, being necessary for the normal functioning of muscles and the brain and helping to use fats, protecting cells against external harmful effects. The major metabolic role of carbohydrates in diets is energy production [9]. Although there are different types of carbohydrates, only total carbohydrates are taken into consideration in food and remains when the protein, fat, moisture and ash of the food have been removed [8]. Carbohydrates are one of the three macronutrients in the human diet, along with protein and fat. As can be seen from Table 1 and Figure 1, the analyzed red onion samples contain high amounts of carbohydrates, their concentration being between 72.48 - 75.31 g/100g DM. These values show that the analyzed red onion samples are rich in carbohydrates, and can be considered as sources of carbohydrates.

From those presented, it can be stated that the analyzed red onion bulbs contain increased amounts of carbohydrates and minerals (ash), moderate amounts of proteins and fibers and reduced contents of moisture and fats.

Conclusion

The study revealed the quality of proximate nutritive value for moisture content, ash, protein, fat, fiber, carbohydrate of red onions commercialized from local agri-food markets from different local vegetable producers. The results obtained: 10.12-11.06% moisture, 3.38-3.87% ash, 2.62-3.47% protein, 1.51-2.04% fat, 6.49- 7.22% fibers, and 72.48-75.31% carbohydrates propose the use of red onion powder as a natural additive in food with added value or as an alternative source in animal feed ingredients. The results obtained regarding nutritional values contribute to drawing a better perspective on the benefits of onions, which could be developed as functional foods favorable for human health. The analyzed red onion bulbs contain increased amounts of carbohydrates and minerals (ash), moderate amounts of proteins and fibers and reduced contents of moisture and fats.

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CHEMISTRY WITH IMPACT IN EDUCATION FOR A HEALTHY LIFESTYLE

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Abstract

Modern lifestyles offer numerous benefits, yet population health is increasingly challenged by environmental factors and a lack of awareness about determinants of well-being. Involving researchers in pre-university education ensures that students receive scientifically grounded knowledge, enabling them to distinguish between valid and misleading information related to both health and environmental impact. Through school-based activities, researchers can share their passion for science, emphasizing the connection between informed lifestyle choices, sustainable practices, and overall health.

The general objective of the *CHemistry with IMPACT in Education for a Healthy Lifestyle (CHIMPACT)* project is to provide high school and middle school students with quality scientific education that highlights the interdependence of human health and environmental well-being. Through experimental activities, students learn to appreciate science in a practical way while understanding how daily choices regarding food, personal care products, and environmental practices affect both individual and planetary health. High school and middle school students actively explore balanced behaviors and learn to make conscious, responsible decisions that promote well-being while respecting the environment. They gain insight into molecules and chemical processes that support health and sustainability and discover how to integrate eco-friendly practices into everyday life. By connecting scientific knowledge with real-world environmental and health issues, the project also introduces students to potential careers in science and technology focused on sustainable solutions.

CHIMPACT stimulates interest in Science (S), Technology (T), Engineering (E), Arts (A), and Mathematics (M) - STEAM subjects through non-formal educational activities, motivates experiential learning, and fosters collaboration among high school and middle school students, teachers, and researchers. This approach not only promotes personal and environmental health awareness, but also encourages curiosity, critical thinking and system thinking, together with a long-term commitment to sustainable and healthy living.

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GLYCOLIPIDOMIC CHARACTERIZATION OF ASTROCYTOMA AND ADJACENT TISSUE: A MASS SPECTROMETRY APPROACH TO GANGLIOSIDE PROFILING

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Abstract

This study highlights the use of ion mobility mass spectrometry to characterize gangliosides in peritumoral tissue of diffuse astrocytoma. The identification of specific species, such as GT1b and Fuc-GD1 variants, suggests their potential as biomarkers and contributors to tumor progression. These findings open new avenues for diagnostic and therapeutic strategies.

Introduction

Diffuse astrocytoma is a primary brain tumor marked by the subtle infiltration of cancer cells into adjacent brain tissue. Due to this invasive nature, studying the peritumoral region is crucial for understanding tumor progression [1]. The present study introduces ion mobility mass spectrometry (IMS MS) as a novel tool for analyzing gangliosides in this region. Using high-resolution nanoESI IMS MS and tandem MS, a diverse array of ganglioside species was identified. Several species, including GT1b and Fuc-GD1 variants, may serve as biomarkers or contribute to tumor infiltration. These findings create new opportunities for diagnostic and therapeutic targeting in diffuse astrocytoma.

Experimental

Peritumoral brain tissue from a 30-year-old male with WHO grade II diffuse astrocytoma was collected with informed consent and ethical approval. Gangliosides were extracted using a modified Svennerholm and Fredman method, purified by protein precipitation, Sephadex G-25 filtration, and dialysis, then reconstituted in methanol and diluted to 5 pmol/μl. Samples were ionized via nanoESI in negative ion mode and analyzed by IMS MS and MS/MS on a Synapt G2-S system (Waters, UK). Instrument settings included 1.4 kV capillary voltage, 40 V cone voltage, and source/desolvation temperatures of 100/150 °C. Collision-induced dissociation (CID) was conducted following IMS, with energies ranging from 20 to 45 eV.

Results

IMS MS profiling of gangliosides in the peritumoral tissue revealed a significantly higher diversity of structures compared to previous reports. Several species were found prominently expressed, including GT1(d18:1/18:0), GT1(d18:1/20:0), GM2(d18:1/16:2), GD1(d18:1/16:0), GD2(d18:1/20:0), Fuc-GT3(d18:1/24:4), and Fuc-GD1(d18:1/18:2). These gangliosides may contribute to the creation of a tumor-supportive microenvironment, promoting cell–cell interactions, immune modulation, and tumor invasion. Structural characterization by tandem

MS confirmed GT1(d18:1/20:0) as the GT1b isomer, highlighting the resolving power of IMS MS for isomer differentiation. Overall, the results suggest that specific ganglioside patterns in peritumoral tissue could serve as biomarkers and play functional roles in diffuse astrocytoma progression.

Conclusions

The study demonstrates that ion mobility mass spectrometry allows for detailed characterization of the complex ganglioside composition in peritumoral tissue. The identification of specific ganglioside species suggests their potential as biomarkers and their possible role in tumor progression. These results offer new insights into the aberrant molecular landscape that triggers and even facilitates diffuse astrocytoma invasion.

Acknowledgement

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DETERMINATION OF THE SUPRAMOLECULAR ARCHITECTURE OF SOME *N*-(2-BROMO-PHENYL)-2-HYDROXY-BENZAMIDE INCLUSION COMPLEXES

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Abstract

Three structures of the *N*-(2-bromo-phenyl)-2-hydroxy-benzamide derivatives (ethyl ester EE, hydrazide HD, hydrazone HN) were optimized at B3LYP/6-311+G level of theory [1]. The graphical representation of the frontier molecular orbitals HOMO/LUMO has been performed and the energy difference between the orbitals was employed for the evaluation of the stability of the compounds. The results suggest a higher stability for both the EE and HD, the HOMO orbitals are located on the 2-bromo-phenyl moiety, while the LUMO orbitals are delocalized over the two aromatic cycles. For hydrazone, where a decrease in the HOMO energy and an increase in the LUMO energy was observed, the HOMO orbitals are present over the benzaldehyde moiety, not on the 2-bromo-phenyl moiety. Also, the LUMO orbitals of the HN are located on the two aromatic rings of the salicylanilide structure.

The logP, polarizability, polar surface area and steric parameters like ovality, molecular area and volume were computed [2]. Similarities of properties like ovality, molecular area and volume for the EE and the HD were observed. Larger values of the polar surface area were obtained for HD and HN, compounds with free amine and hydroxyl groups. All compounds are hydrophobic, a larger logP value being obtained for HN with three phenyl rings.

The molecular docking and visualization of the ligand–receptor (β -cyclodextrin β -CD) interactions have been performed with AutoDock Vina [3]. To calculate the variation in energy associated with the formation of the β -cyclodextrin–ligand inclusion complexes, single-point energy calculation was performed for the inclusion complexes of β -CD with the best conformation of the ligands, and for the ligands and receptor alone, at the B3LYP/6-31G level of theory. The size of β -CD cavity allows the partial inclusion of the compounds. The best binding affinities were obtained for HN (–5.59 kcal/mol). Regarding the interaction between the compounds and β -CD, atoms in close contact were present, and only in case of HN, one hydrogen bond is formed. These results suggest the partial inclusion of the compounds within the β -CD cavity. Molecular docking computations also suggested that hydrazone, characterized by the largest area, volume and polarizability within the series, has the highest binding affinity towards β -CD.

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THE CHARACTERIZATION AND VALUATION OF THE POTENTIAL OF THE AGRICULTURAL LAND FUND IN THE MUNICIPALITY OF SACALAZ, TIMIȘ COUNTY

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Abstract

The pedological and credit assessment study carried out on the territory of Săcălaz commune (Timiș county) aims at the scientific basis of effective measures for the use and conservation of the functional agricultural fund. The analysis highlighted the diversity of soil types (chernozoms, eutricambosols, faeozoms, alluviosols, vertosols, solonets, etc.), with different degrees of fertility, productive potential and limitations. The results show that more than 60% of the agricultural area is occupied by soils with high fertility (chernozims and eutricambosols), capable of supporting large agricultural productions, while problematic solutions (pelosols, solonets, gleosols) require ameliorative measures. Dewatering-drainage works, combating salinization, adapted technologies and rational crop rotations are recommended for the sustainable exploitation of pedological resources.

Introduction

Fondul funciar agricol reprezintă o resursă strategică, a cărei utilizare durabilă este condiționată de calitatea solurilor și de aplicarea unor tehnologii adaptate condițiilor locale. Numeroase cercetări internaționale subliniază presiunea asupra resurselor pedologice și necesitatea unor sisteme de monitorizare și conservare [1–3]. La nivel european, politicile agricole și de mediu pun accent pe reducerea degradării solurilor și pe adaptarea practicilor agricole la schimbările climatice [4,5]. În România, lucrările de cartare pedologică și bonitare au furnizat date esențiale pentru organizarea teritoriului agricol și fundamentarea deciziilor privind asolamentele și lucrările de ameliorare [6–8]. În Câmpia Banatului, solurile sunt în general fertile, dar expuse excesului de umiditate, salinizării și compactării, necesitând măsuri specifice [9,10]. Scopul prezentei lucrări este de a caracteriza resursele pedologice din comuna Săcălaz, de a evalua bonitatea și fertilitatea solurilor și de a propune direcții pentru valorificarea durabilă a acestora.

Experimental

Săcălaz commune is located west of Timișoara municipality and includes the villages of Săcălaz, Beregsăul Mare and Beregsăul Mic. The relief is specific to the low plain, with beams, roofs, abandoned beds and micro depressions. The climate is temperate-continental, with hot summers and average annual precipitation of 550–600 mm.

The study was based on data provided by OSPA Timiș (2004), supplemented with recent pedological and agrochemical observations. The analysis focused on: identification and delimitation of soil units; determination of agrochemical parameters (pH, humus, phosphorus, potassium); establishing credit ratings for the main crops; productivity analysis based on production data (2018–2021).

Results and discussion

The main types of soil.

In Săcălaz commune, chernozoms predominate, with 3446.36 ha (36.2%) and eutricambosols, with 2594.08 ha (27.3%), followed by pelosols, with 1159.45 ha (13.5%), faeozoms (5.7%), alluviosols (9.1%), vertosols (4.5%), gleosols (2.3%) and rattlesnakes (2.8%) (fig. 1).

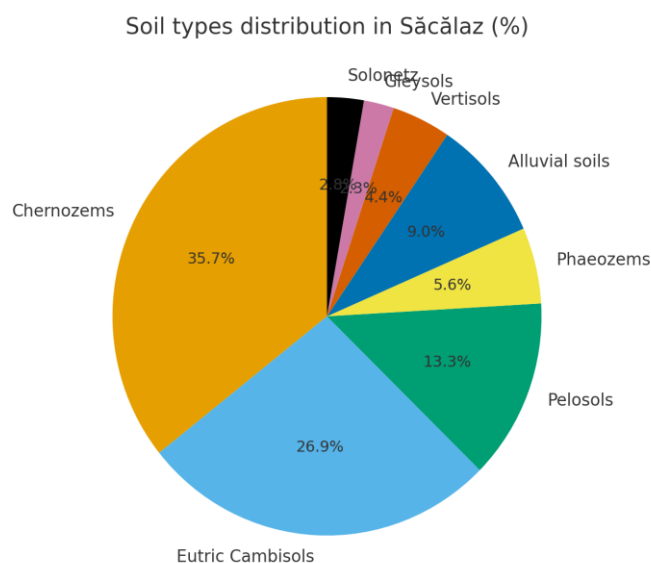


Fig 1. Distribution of soil types in Săcălaz

The chernozems are the most fertile, with credit scores between 99-33 points. They are rich in humus and phosphorus, favorable for wheat, corn and sunflower, ensuring high yields (over 10 t/ha corn, 7–8 t/ha wheat).

The Eutricambosols show average fertility, credit scores 35–70 points. They are suitable for various crops, but with lower productivity than chernozoms.

Phaeozomes and pelosols have important limitations (excess moisture, compactness), requiring specific drainage works and adapted technologies.

Solonets and gleosols have low fertility, with credit scores below 40 points, requiring improvement through salt washing, landfill leveling and drying works.

Land use.

Over 50% of the surface is arable, the rest being occupied by pastures, hayfields and orchards.



Fig. 3. Bonitation classes of main crops by soil type

The quality class is between I-IV, credit scores between 99-33 points. Soils with a rich humus content ensuring an increased quality of these soils. The total porosity is high and the aeration is medium. Weakly alkaline soil reaction in the upper horizons. The phosphorus content is high, while the potassium content is medium, which indicates a medium humus content

Agricultural products.

Data from the period 2018–2021 show the stability of productions on chernozems (wheat 6–7 t/ha, corn 9–10 t/ha, sunflower 3.5–4 t/ha, rapeseed 3.6–4 t/ha) (fig. 2)

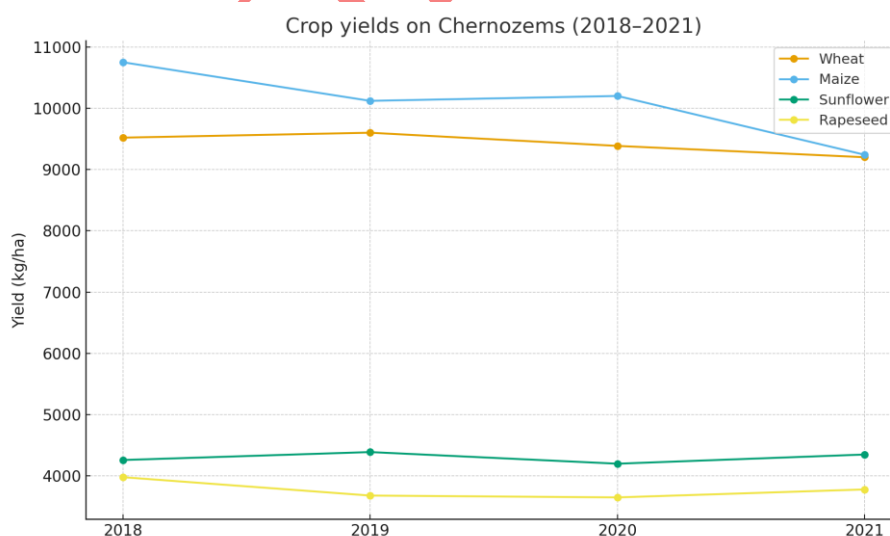


Fig 2. Productions on typical chernozem from Săcălaz

It can be seen that the chernozem encounters favorable conditions to realize the maximum production potential in the area of the commune. In order to preserve these soils, it is necessary to apply appropriate technology, both for fertilizers and for works adjacent to crops in the rotation.

On phaeozoums and eutricambosols, yields are lower by 10–20%.

The results confirm the particularly fertile character of the soils of Banat, in accordance with previous studies [6,9,11]. However, the glazing, salinization and compaction processes can significantly reduce productivity, an aspect also reported by other authors [12,13]. In relation to other agricultural areas in Romania, Săcălaz commune has a higher potential, but sustainable exploitation depends on the application of ameliorative measures and the adaptation of technologies to local conditions [14-21].

Conclusions

1. Săcălaz commune has a valuable agricultural land fund, dominated by soils with high fertility.
2. Chernosiomas and eutricambosols provide the best conditions for field crops, ensuring high yields.
3. Soils with low fertility (pelosols, solonets, gleosols) require ameliorative measures (drainage, leveling, combating salinity).
4. For sustainable exploitation it is recommended: the application of rational crop rotations, balanced fertilization, water conservation technologies and improvement works.

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CORROSION TEST IN 0.1 M HCl OF THE PSEUDO-BINARY OXIDES UNDOPED AND DOPED WITH Er^{3+} IONS

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Abstract

This study presents the realization of new type materials based on $\text{Zn}_3\text{Nb}_2\text{O}_8$ undoped and doped with Er^{3+} ions designed to improve corrosion inhibition of steel in aggressive media. The thin films structures were obtained on carbon steel through the spin-coating technique. Morphological investigations of thin films were carried out by atomic force microscopy (AFM). The inhibition of a steel corrosion process was evaluated in an aggressive environment of 0.1 M HCl by performing electrochemical investigations such as open circuit potential (OCP) and the potentiodynamic polarization technique. The influence of variations in the cathodic Tafel slopes β_c and anodic Tafel slopes β_a over the corrosion rates was discussed. The best corrosion inhibition efficiency of 93.3% was realized by the steel electrode covered with spin coating techniques were obtained when the layer was made for the $\text{Zn}_3\text{Nb}_2\text{O}_8:\text{Er}^{3+}$ type structure obtained first by the solid-state method using $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$, Nb_2O_5 and $\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$.

Introduction

Nowadays corrosion is a natural process and also a universal phenomenon of metals and is one of the main problems faced by almost all industries and can lead to safety issues and destroy the integrity of equipment and consumables. Corrosion of metals is a natural and inevitable process that imposes considerable costs on many industries and can also have irreparable consequences. Corrosion is the deterioration of metal in the presence of the environment by chemical or electrochemical means [1–5]. Corrosion of metals leads to a huge economic loss worldwide [6–8]. There are various methods of reducing or preventing corrosion. The use of corrosion inhibitors is one of the ways to protect metal surfaces against corrosion [9–13]. There are several methods, such as: cathodic protection, galvanizing, painting and coatings, to prevent metal corrosion. Choosing the best corrosion prevention method depends on many factors, including cost, effectiveness, metal type, and corrosive environment, but it can be said that coatings are probably the most convenient method of preventing metal corrosion due to their low cost, availability of raw materials, flexibility, and simplicity. In this study, we have developed new knowledge in the field of advanced materials that provide efficient anticorrosion protection, through the design of new nanostructured films based on pseudo-binary oxides of the type $\text{Zn}_3\text{Nb}_2\text{O}_8$ undoped and doped with Er^{3+} ions. The new materials were obtained by solid-state synthesis and were applied to inhibit the corrosion of the carbon steels (OL) by using technologies for the production of thin films by spin-coating in an acidic environment (0.1 M HCl).

Experimental

Nanomaterials of the type $\text{Zn}_3\text{Nb}_2\text{O}_8$ undoped and doped with Er^{3+} were obtained by the solid-state method at a temperature of 1100 °C for 4 hours at a heating/cooling rate of 5 °C/min in a

SNOL calcination furnace. The precursors used in the solid-state synthesis are presented in Table 1.

Table 1. Precursors used in solid-state synthesis

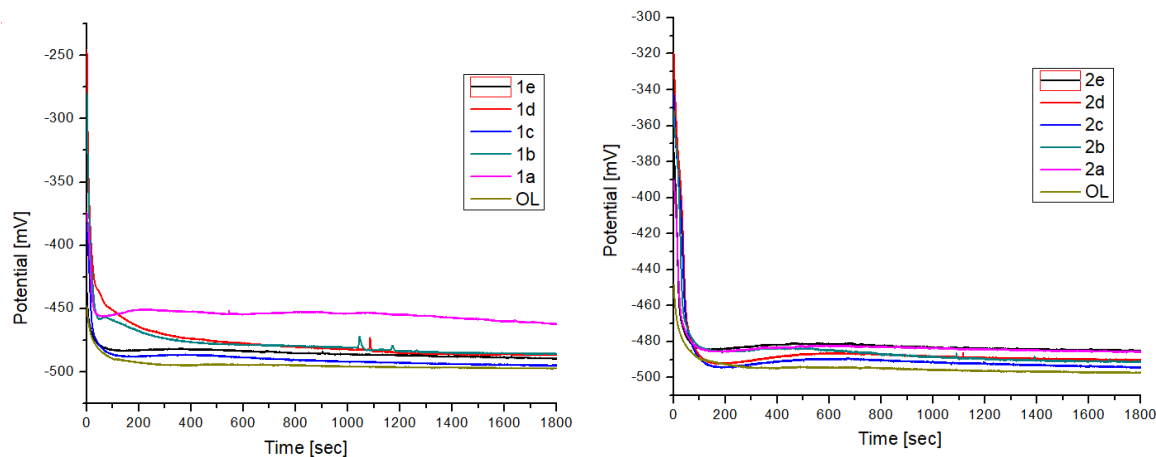
Sample	Precursor 1	Precursor 2	Precursor 3	Molar ratio
1a	Nb ₂ O ₅	Zn(NO ₃) ₂ ·4H ₂ O	-	1:3
1b	Nb ₂ O ₅	Zn(NO ₃) ₂ ·4H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.01
1c	Nb ₂ O ₅	Zn(NO ₃) ₂ ·4H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.02
1d	Nb ₂ O ₅	Zn(NO ₃) ₂ ·4H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.1
1e	Nb ₂ O ₅	Zn(NO ₃) ₂ ·4H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.2
2a	Nb ₂ O ₅	Zn(CH ₃ COO) ₂ ·2H ₂ O	-	1:3
2b	Nb ₂ O ₅	Zn(CH ₃ COO) ₂ ·2H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.01
2c	Nb ₂ O ₅	Zn(CH ₃ COO) ₂ ·2H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.02
2d	Nb ₂ O ₅	Zn(CH ₃ COO) ₂ ·2H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.1
2e	Nb ₂ O ₅	Zn(CH ₃ COO) ₂ ·2H ₂ O	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.2
3a	Nb ₂ O ₅	ZnO	-	1:3
3b	Nb ₂ O ₅	ZnO	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.01
3c	Nb ₂ O ₅	ZnO	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.02
3d	Nb ₂ O ₅	ZnO	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.1
3e	Nb ₂ O ₅	ZnO	Er(NO ₃) ₃ ·5H ₂ O	1:3:0.2

Thin film depositions were performed by spin-coating technique on steel disks with a diameter of 10 mm and a thickness of 2 mm. Before the deposits were made, these discs were polished with sandpaper of various degrees of roughness, washed with double distilled water and then degreased with ethanol.

After the thin films were made, they were subjected to corrosion tests by electrochemical methods in order to validate them as corrosion inhibitors. The open circuit potential (OCP) of the modified electrodes was monitored for 30 minutes before polarization. The corrosive environment in which the corrosion tests were performed consisted of 0.1 M HCl acidic solution.

Results and discussion

The open circuit potential (OCP) measurements in Figure 1 showed that the coated electrodes stabilize at approximately 400-500 s. This result provides preliminary information about the nature of the processes occurring at the interfaces between the metal/thin film and the electrolyte. The OCP is a qualitative indicator of the corrosion state of the steel substrate in an acidic environment and helps to determine the immersion time required to reach the equilibrium state.



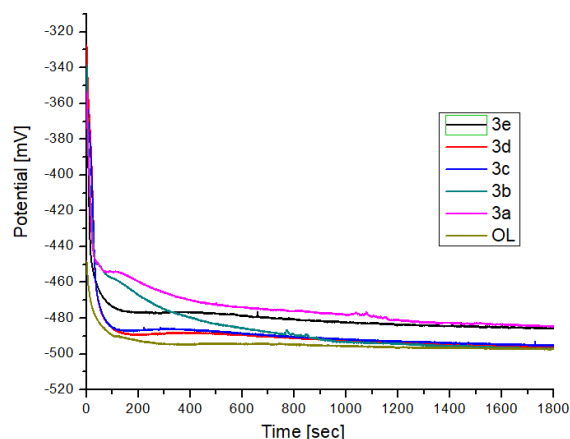


Figure 1. The OCP for electrodes modified by spin coating technique for 30 minutes immersed in 0.1 M HCl: steel electrode, $\text{Zn}_3\text{Nb}_2\text{O}_8$ and $\text{Zn}_3\text{Nb}_2\text{O}_8 \cdot \text{Er}^{3+}$ (notations according to table 1) The polarization curves were analyzed using VoltaMaster 4 v.7.09 software and the Tafel parameters were determined: corrosion potential (E_{corr}), polarization resistance (R_p), corrosion current density (i_{corr}), anodic (β_a) and cathodic (β_c) Tafel curves as well as corrosion rate (v_{corr}). The degree of corrosion inhibition (IE) [7] was calculated for each drop casting deposit.

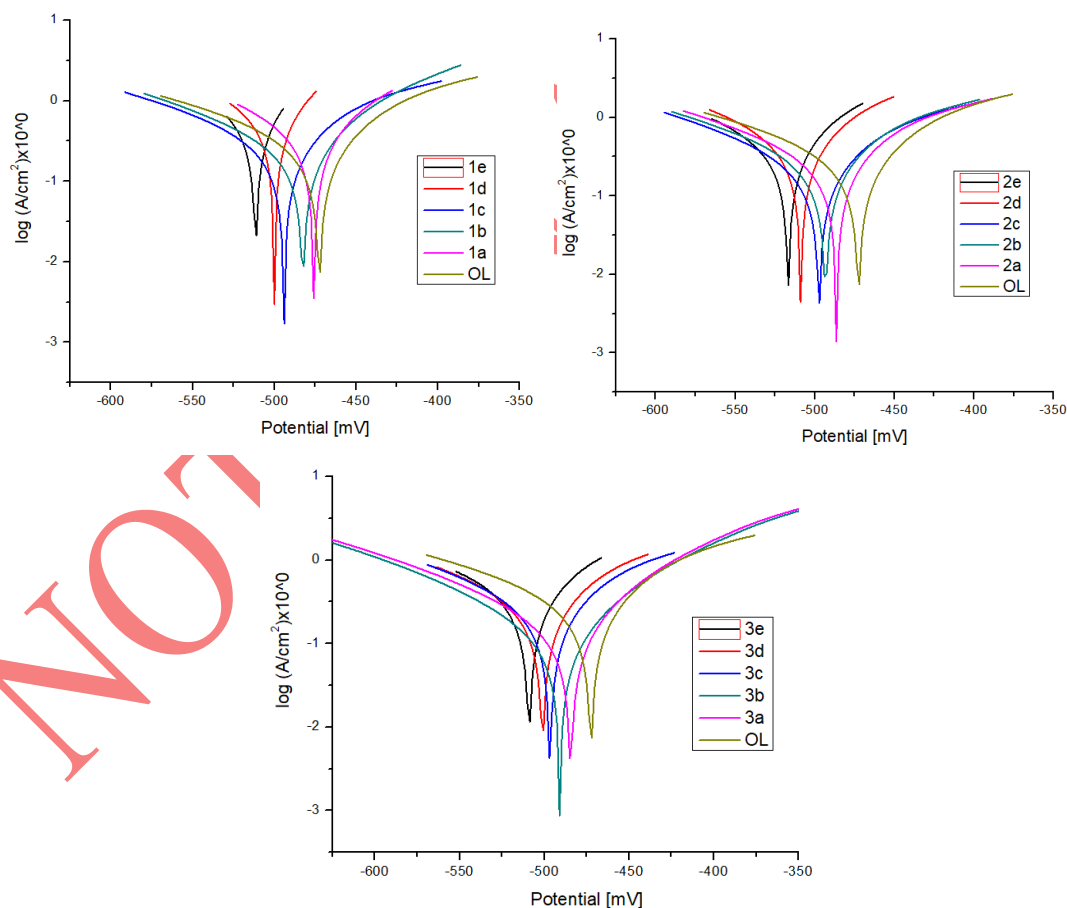


Figure 2. Tafel polarization curves for electrodes modified by spin coating technique after immersion in 0.1 M HCl media of: steel electrode, $\text{Zn}_3\text{Nb}_2\text{O}_8$ and $\text{Zn}_3\text{Nb}_2\text{O}_8 \cdot \text{Er}^{3+}$ (notations according to table 1)

Table 2. Tafel parameters for electrodes deposited by spin coating technique analyzed after 30 minutes immersion in 0.1 M HCl medium.

Electrodes	E (I = 0) (mV)	R _p (Ωxcm ²)	i _{corr} (mA/cm ²)	β _a (mV)	β _c (mV)	v _{corr} (mm/Y)	IE (%)
OL	-471.07	96.95	0.9501	207.2	-220.2	5.265	-
1a	-475.9	129.21	0.1314	70.8	-123.3	1.536	86.16
1b	-482.7	183.37	0.1216	86.6	-133.3	1.422	87.20
1c	-485.1	175.14	0.1096	79.1	-122.5	1.282	88.46
1d	-488.5	179.66	0.0864	70.7	-99.6	1.010	90.90
1e	-494.1	164.13	0.0639	49.7	-74.9	0.748	93.3
2a	-486.8	112.3	0.2727	111	-178.9	3.190	71.3
2b	-486.4	152.7	0.1977	110.9	-164.1	2.311	79.19
2c	-493.8	146.49	0.1527	91	-149.0	1.785	83.92
2d	-493.8	210.35	0.1350	133	-107.8	1.579	85.79
2e	-497.4	188.88	0.0971	76.6	-116.9	1.135	89.78
3a	-484.6	123.69	0.2601	97.44	-169.5	3.042	72.62
3b	-488.8	147.44	0.2421	98.5	-163.9	2.831	74.51
3c	-496.1	177.14	0.2323	89.9	-124.5	2.716	75.54
3d	-496.7	167.47	0.2153	76.4	-106.4	2.518	77.33
3e	-504.8	162.55	0.2046	67.5	-134.7	2.393	78.46

In all cases analyzed of steel electrodes modified by spin coating of thin films made of pseudo-binary oxides, an improvement in their corrosion inhibition was found between 71% and 93%.

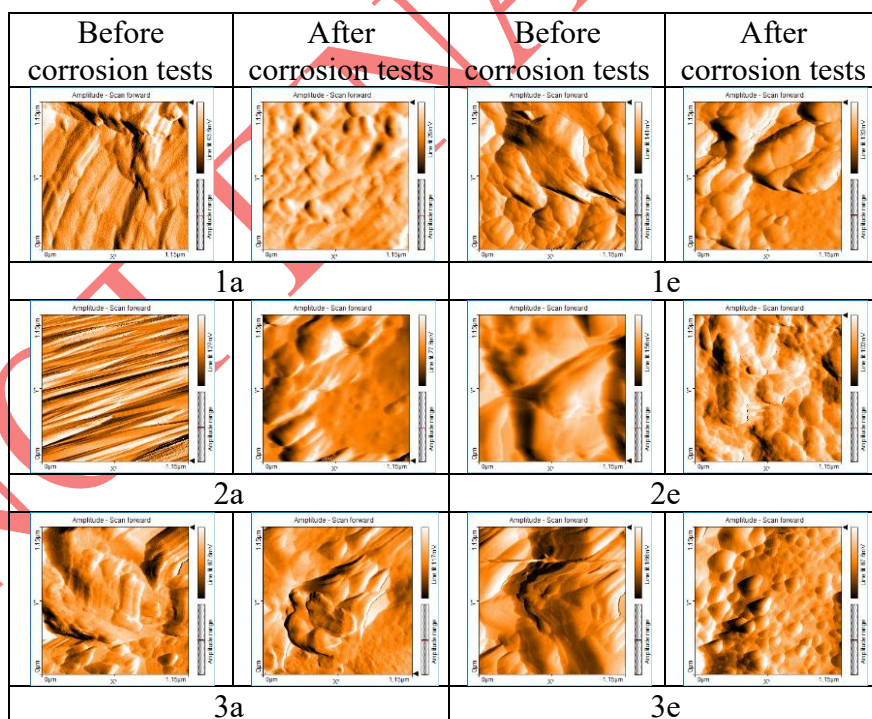


Figure 3. AFM images before and after corrosion tests for samples deposited by spin-coating technique according to table 1

Analyzing the variation of the corrosion potential and corrosion current as the inhibition efficiency increases (Tables 2), it can be observed that the corrosion current decreases proportionally to the corrosion rate, and the corrosion potential moves towards cathodic values. For all deposits with materials obtained by the solid-state method and tested in acidic media,

the polarization resistance (R_p) of the modified OL steel electrode increases. From the AFM (Figure 3) investigations it can be observed that after contact with acidic medium, the thin films retain the structure of the material that comes into direct contact with the corrosion medium, but the morphology is different and the size of the agglomerates is larger.

Conclusion

It was found that the best corrosion inhibition values $IE = 93.3\%$ for spin coating were obtained when the layer was made for the $Zn_3Nb_2O_8:Er^{3+}$ type structure obtained first by the solid-state method using $Zn(NO_3)_2 \cdot 4H_2O$, Nb_2O_5 and $Er(NO_3)_3 \cdot 5H_2O$ as precursors in an acidic medium, which managed to provide a smooth, non-porous and uniformly coated surface. From the AFM measurements it can be seen that the corrosion inhibition mechanism of carbon steel is based on the physical protection caused by the compact and adherent layers made by the pseudo-binary oxide at the interface with the steel.

Acknowledgements

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THE IMPACT OF PEDOCLIMATIC CONDITIONS AND TECHNOLOGICAL ADAPTATION ON WINE PRODUCTION IN THE RECAȘ VINEYARD CENTER (2023–2024)

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Abstract

The study analyzes the interaction between pedological resources, climate variability and technological measures applied in the Recaș Viticulture Center, Timiș County, Romania, in the period 2023–2024. The research aimed at the physico-chemical characterization of the main types of soil (typical leached Eutricambisol, typical Preluvosol and mollic Gleiosol), highlighting the climatic conditions in the two years and their impact on the productions of the Cabernet Sauvignon, Merlot, Pinot Noir, Fetească Neagră and Chardonnay varieties. The results show that the typical Preluvosol has a slightly acidic reaction (pH 5.6 in the Ao horizon) and a low humus content (2.55%), which limits the availability of nutrients, and the Gleiosol is characterized by loamy-clay texture and excess moisture. At the climatic level, the year 2024 was marked by severe drought and maximum temperatures of up to 45°C, which led to average production decreases of approximately 24.8% compared to 2023. The adaptive measures implemented (drip irrigation, night harvesting, advanced mechanization) partially mitigated the effects of water and thermal stress. The conclusions emphasize the importance of an integrated pedological and technological management strategy to increase the resilience of viticulture to climate change.

Introduction

Viticulture is one of the agricultural branches most strongly influenced by pedoclimatic conditions [1,2]. The soil provides the nutritional and water base of the vine, and the climate determines the rate of vegetation, the quality and quantity of the harvest [3,4,5]. In the last two decades, climate change has led to an increase in the frequency of heat waves and droughts, affecting the wine-growing regions of southeastern Europe [6,7,8,9].

At the European level, numerous studies have shown that viticulture in the south of the continent is exposed to the risk of significant production losses, but also of changes in the organoleptic profile of wines [10,11]. In Romania, the western wine-growing regions, including the Banat, are characterized by fertile soils, but with high variability of the chemical reaction and the water regime [12,13].

The Recaș Wine Center is one of the most important wine-growing areas in Romania, recognized for the annual production of over 30 million bottles and significant exports [14]. In the context of recent years, marked by the alternation between favorable and extreme climatic conditions, the integrated analysis of soil resources, climatic conditions and technological

measures becomes essential to assess the sustainability and resilience of viticulture [15,16,17,18].

The aim of the paper is to highlight the relationship between pedological characteristics, climate variability (2023–2024) and technological adaptation, through a case study applied in the Recea Viticulture Center.

Experimental

The research was carried out in the Recea Viticulture Center (45°48' N, 21°31' E), located in western Romania. This Wine Center is part of Timiș county and is located in the center of the county, as can be seen from figure 1, at a distance of 23 Km from the Municipality of Timișoara.

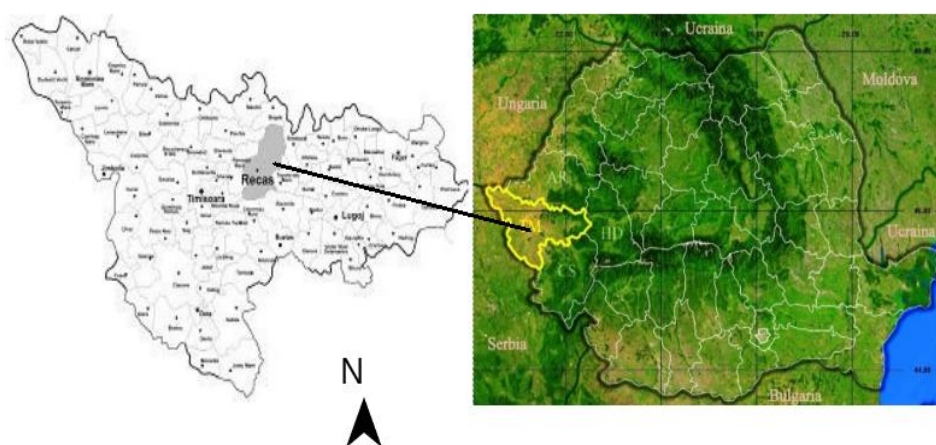


Figure 1. Geographical location of the Recea Viticulture Center within Timiș County, respectively Romania

The soils were characterized based on the samples collected on genetic horizons (0–20 cm, 20–40 cm). Physico-chemical analyzes included granulometry (pipetting method), apparent density (metal cylinders), pH (potentiometric method, ratio 1:2.5), humus (Tiurin), total nitrogen (Kjeldahl), phosphorus and mobile potassium (Egner-Riehm-Domingo).

Climatic data were taken from local meteorological observations (Timișoara Meteorological Station) for the years 2023 and 2024, including average monthly (absolute maximum) and annual temperatures and precipitation.

The productions of the main grape varieties (Cabernet Sauvignon, Merlot, Pinot Noir, Fetească Neagră, Chardonnay) were centralized based on the data provided by the farm, reported in kg/ha.

Results and discussion

1. Soil characterization

Three types of soil were identified: eutricambosol, preluvosol and gleiosol, within which the texture was analyzed (textural class was determined), soil reaction (pH values), humus content, NPK. Based on soil analyzes and interpretations, the fertility of each soil was determined Table 1.

Table 1. Texture of the soils of the Recas Winery Center

Soil type	Depth (cm)	Coarse sand (%)	Fine sand (%)	Dust (%)	Clay (%)	Textural class name
Eutricambosol typical leached	0-20	6.9	39.2	32.7	21.2	LP
	20-40	7.3	36.1	34.1	22.5	LP
Typical Preluvosol	0-20	0.6	38.0	33.2	28.2	LP
	20-40	0.5	38.8	31.7	29.0	LL
Gleiosol molic	0-20	0.3	30.6	34.8	34.3	TT
	20-40	0.4	32.5	32.5	34.6	TT

Typical leached Eutricambosol – has a clayey-dusty texture.

Typical Preluvosol – it has a loamy-dusty texture on the surface (ad. 0-20 cm) and loamy at a depth of 20-40 cm.

Molic Gleyosol – loamy-clay texture.

Regarding the analyzed chemical properties (table 2), the situation is different from one soil to another, which tells us the availability of nutrients for the vine culture and the fertility that each type of soil has.

Table 2. The chemical properties of the soils of the Recas Viticulture Center

Tipul de sol	Depth (cm)	pH in H ₂ O	Humus (%)	Total nitrogen (%)	Mobile phosphorus (ppm)	Mobile potassium (ppm)
Eutricambosol tipic levigat	0-20	6.45	2.43	0.14	25	350
	20-40	6.05	1.37	0.07	13	90
Preluvosol tipic	0-20	5.6	2.55	0.108	28	100
	20-40	6.25	2.13	0.094	26	90
Gleiosol molic	0-20	6.82	5.75	0.258	40	131
	20-40	6.8	3.02	0.148	13	101

Typical leached Eutricambosol – slightly acidic reaction (pH of 6.05-6.45), reduced humus content at 20-40 cm and sub-middle, at 0-20 cm, respectively a moderate fertility.

Typical Preluvosol – slightly acidic reaction (pH 5.6-6.25), humus 2.55-2.13%, total N 0.108%, mobile P 28 ppm, mobile K 100 ppm; low to average fertility; requires organic amendments and pH corrections.

Molic Gleiosol – neutral reaction, medium humus on the surface and very high (>5.7%), at ad. 20-40 cm, high fertility, but has as a limiting factor, excess moisture and glaze.

2. Climate conditions 2023–2024

The climate is temperate-continental, with slight Mediterranean influences. The winters are mild, the summers very warm and the autumns prolonged [14]. The transitions between seasons (especially from spring to summer) are rapid. This affects the vine in certain years. However, the climatic and soil conditions are favorable for vine cultivation.

The year 2023 was distinguished by moderate precipitation in the spring, balanced summer; maximum temperatures up to 34–35°C; high productions.

The year 2024 was a year with severe drought (in the period May–August), low precipitation, heat waves with maximums of 38–45°C, accentuated water stress.

3. Productions

Table 3 shows the productions obtained over the two years, for the main vine varieties [15].

Variety	2023 (kg/ha)	2024 (kg/ha)	Diference	% change
Cabernet Sauvignon	13,000	10,000	-3 000	-23.1%
Merlot	12,000	9000	-3 000	-25.0%
Pinot Noir	11,000	8 000	-3 000	-27.3%
Fetească Neagră	10,500	7 500	-3 000	-28.6%
Chardonnay	12,500	10 000	-2 500	-20.0%

The productions obtained were high (10500-13000 kg/ha) in 2023 and lower (7500-10000 kg/ha) in 2024, with production differences of 2500-3000 kg/ha. The average decrease in production was -24.8%.

4. Technological adaptation

Compared to other wine centers in Romania, Centru Viticol Receaș through the investments made in recent years in technology and infrastructure, has adapted the technology to the new climate challenges:

- digitized drip irrigation;
- night harvesting (for the protection of aromatic compounds and the reduction of thermal stress on the fruits);
- mechanized harvesting >95% of the surface;
- investments in the bottling line (13,000 bottles/hour).

Discussions

The results obtained confirm that climate variability has a direct impact on viticultural productivity, in agreement with similar studies carried out in southern Europe [9,18,19]. Production declines in 2024, between 20 and 28%, align with values reported by Moriondo et al. (2021) for vineyards in Spain and Italy, where heat waves in recent years have affected yields by 15–30%.

From a pedological perspective, the moderate acidity and low humus content of the Preluvosol confirm the need to apply some ameliorative measures (organic amendments, cover crops), as pointed out by Dumitru et al. (2019) in studies on wine-growing soils in western Romania.

The adaptive measures implemented at Receaș (drip irrigation, night harvesting) comply with international recommendations for sustainable viticulture [4,6,20,21] and contribute to maintaining the quality of the wines even in unfavorable climatic conditions.

Conclusion

The soils in the Receaș vineyard area show great variability, from fertile Eutricambosols to Gleiosols with excess moisture, which requires a differentiated management.

The year 2024 was characterized by extreme climatic conditions (drought and temperatures >40°C), which reduced average production by ~25% compared to 2023.

The varieties most sensitive to water stress were Pinot Noir and Fetească Neagră (-27–29%), and the most resistant Chardonnay and Cabernet (-20–23%).

The measures taken (drip irrigation, night harvesting, mechanization) have contributed to reducing the climate impact, but it is necessary to diversify the portfolio of varieties and apply water conservation technologies.

The integration of pedological management with climate adaptation strategies is the key to the resilience of viticulture in the Banat area.

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CHARACTERIZATION OF THE RAINFALL AND WIND REGIME AT THE TIMISOARA AND SANNICOLAU MARE METEOROLOGICAL STATIONS OVER A FIVE-YEAR PERIOD

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Abstract

The paper analyzes the wind regime and the rainfall regime over a period of five years, at two representative stations in western Romania, more precisely in Timiș County, at the stations in Timișoara and Sannicolau Mare. Also, with the help of data provided by the Banat Crisana Regional Meteorological Center, the rainfall regime was interpreted at the two representative stations in Banat. After analyzing the data from the two stations, we found that in Timișoara the predominant wind direction among the 8 main directions is the NW sector with a frequency of 13.1% in April, the average speed being 3.9 m/s, also from the NW. At the Timișoara meteorological station, the annual amount of precipitation was only 296.3 l/m², in the driest year analyzed, 2000, with a minus of 321.5 l/m² compared to the multi-annual average value.

Introduction

The southwest of Romania benefits from a moderate continental temperate climate with oceanic and Mediterranean influences, the result of the action of genetic climate factors. Under the action of the atmospheric circulation that transports maritime air masses from the west to the southwest of Europe, of the orographic barrier of the Carpathians, the continental influences from the east, characterized by special contrasts, are felt very little at the studied stations [1,2,3]. For this reason, an increase in precipitation amounts is noted from west to east, from the low plain regions, to the hilly ones and then to the mountainous ones [4,5,6].

The average annual precipitation amounts can vary in relation to the altitude from less than 540 mm, at the Sannicolau Mare meteorological station, at the Jimbolia meteorological station the average annual precipitation amounts are 556 mm, at the Timișoara meteorological station the average annual amounts reach 617 mm, up to 1150 mm in the Semenic Mountains and over 940 mm on the mountain peaks at 2000 m altitude in the Țarcului Mountains [4,7,8].

Experimental

Here we analyzed the frequency and speed of the wind in the eight main directions, exemplifying through the wind rose graph in the months of the warm season: April, May, June, July, August and September, over a period of five years. Also, with the help of data provided by the Banat Crisana Regional Meteorological Center, the rainfall regime was interpreted at the

two representative stations in Banat. The Timișoara meteorological station is part of the category of plain stations, being located in the Banat Plain. It is a County meteorological station, from an administrative point of view it belongs to Timiș County and Timișoara Municipality. The station has the following coordinates - latitude 45° 46', longitude 25° 15', platform altitude 85.5 m, barometer altitude: 87.7 m.

The Sânnicolau Mare meteorological station falls into the category of plain stations, being located in the Torontal Plain at an altitude of 85 m. From an administrative point of view, the station belongs to Timiș County and the city of Sânnicolau Mare. The station coordinates are the following - latitude: 46° 04', longitude 20° 37', platform altitude 84.5 m and barometer altitude 85.8 m.

The Sânnicolau Mare meteorological station is located in the low Mureș Plain, in its non-floodable part, at an altitude of 86 m. The most striking feature is the smoothing of the relief interrupted only by some forms that appeared as a result of the unfolding, meandering and changing of the riverbeds.

Results and discussion

In the paper, we analyzed the frequency and speed of the wind in the eight main directions, exemplifying it through the wind rose graph in the warm months: April, May, June, July, August and September, over the course of five years. Also, with the help of data provided by the Banat Crisana Regional Meteorological Center, the rainfall regime at the two representative stations in Banat was interpreted. The wind rose is illustrated for the months analyzed in the following representative figures for the Timișoara station and the Sannicolau Mare station [9,10].

Multiannual averages at the Timișoara Meteorological Station in April									
direction	N	NE	E	SE	S	SV	V	NV	Calm
Frequency (%)	9.1	5.5	7.3	4.7	10.3	8.5	11.7	13.1	36.0
speed (m/s)	3.8	2.5	2.6	3.1	3.9	3.5	3.7	3.9	---

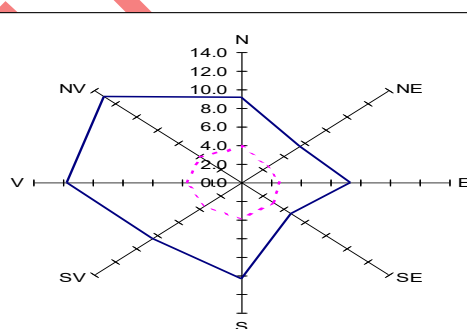


Fig.1 Multiannual averages at the Timișoara Meteorological Station in April

Multiannual averages at the Timișoara Meteorological Station in May									
direction	N	NE	E	SE	S	SV	V	NV	Calm
Frequency (%)	9.1	5.3	7.0	5.4	10.5	5.8	8.8	15.0	38.2
speed (m/s)	4.1	3.1	2.4	3.4	3.7	3.4	3.4	3.5	---

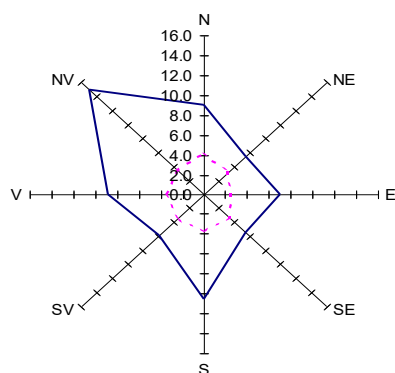


Fig.2 Multiannual averages at the Timișoara Meteorological Station in May

Multiannual averages at the Sannicolau Mare Meteorological Station in May									
direction	N	NE	E	SE	S	SV	V	NV	Calm
frequency(%)	15.5	4.7	7.6	12.6	15.0	8.0	12.3	10.0	19.3
speed (m/s)	4.3	3.0	2.8	3.5	4.0	3.6	4.4	4.4	---

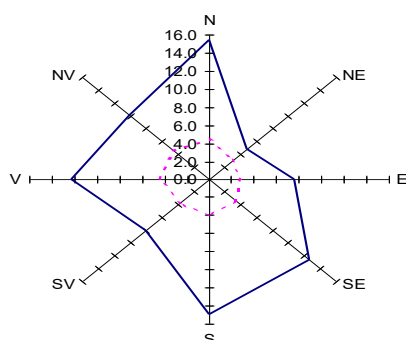


Fig.3 Multiannual averages at the Sannicolau Mare Meteorological Station in May

Multiannual averages at the Sannicolau Mare Meteorological Station in Jun									
direction	N	NE	E	SE	S	SV	V	NV	Calm
Frequency (%)	12.2	4.0	4.2	8.6	11.7	8.0	16.5	14.2	25.5
speed (m/s)	3.8	3.0	3.0	3.2	3.4	3.3	3.8	4.2	---

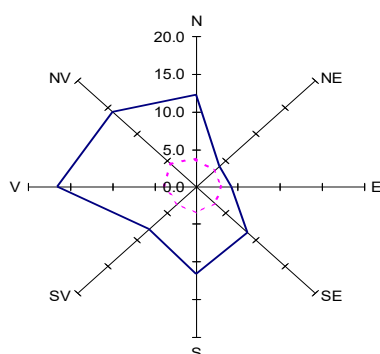


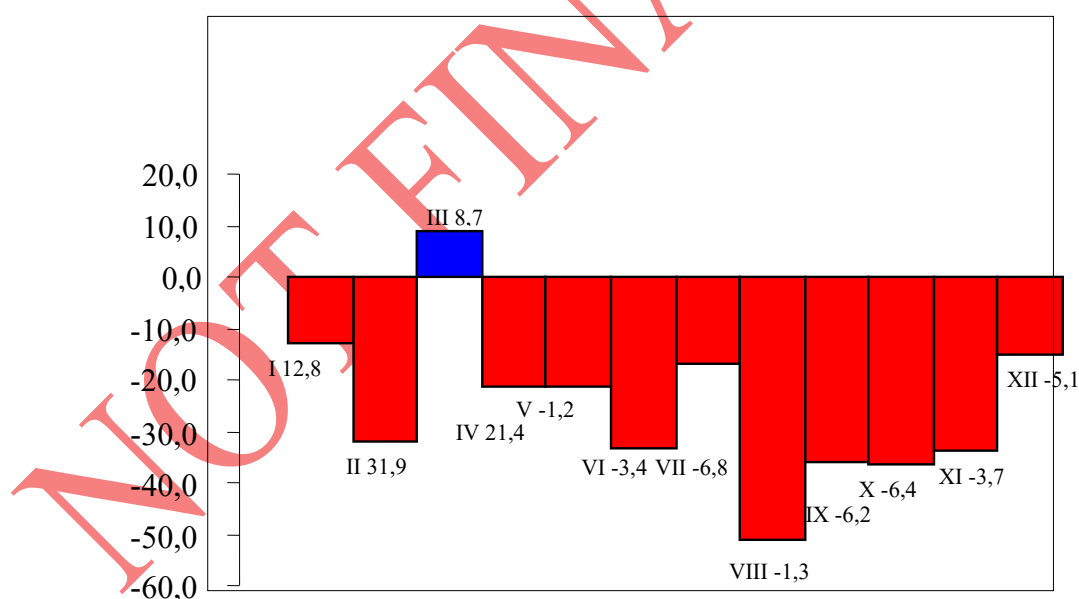
Fig.4 Multiannual averages at the Sannicolau Mare Meteorological Station in May

The table below presents the monthly values of the rainfall regime recorded at the Timisoara station, during the period 1999-2003.

Table 1. Rainfall regime recorded at the Timisoara station during 1999-2003

Year/Month	1999	2000	2001	2002	2003
I	37,9	21,5	35,4	8,7	69,0
II	88,7	8,5	18,6	10,5	26,7
III	11,3	45,1	58,8	7,6	10,2
IV	50,6	34,3	79,6	4,7	46,3
V	74,6	31,5	31,8	53,1	51,4
VI	38,3	40,9	130,2	74,8	80,5
VII	187,1	25,3	58,6	62,0	55,4
VIII	49,7	8,6	30,6	98,6	4,2
IX	35,5	23,7	146,6	48,2	66,3
X	22,6	1,8	15,4	52,6	113,2
XI	64,5	20,6	66,1	42,7	31,3
XII	110,3	34,5	14,0	66,7	22,5
Annual amount	771,1	296,3	685,7	530,2	577,0

At the Timișoara meteorological station, the annual amount of precipitation was only 296.3 l/m², in the driest year analyzed, the year 2000, with a minus of 321.5 l/m² compared to the multiannual average value of 617.8 l/m² in percentage minus 52%[9,10]. In Timișoara, unlike Sânnicolau Mare and Jimbolia, the month with the richest precipitation was March with a precipitation amount of 45.1 l/m² and even with a plus of 8.7 l/m², which in percentage represents an plus of 23.9%. The rainiest decade of the year 2000 was the first decade of April with 32.0 l/m².

**Fig.5 Evolution of precipitation compared to normal in 2000 in Timisoara**

Conclusion

After analyzing the wind regime and the pluviometric regime at the meteorological stations in Timisoara and Sânnicolau Mare, we found that in Timisoara the predominant wind direction among the 8 main directions is the NW sector with a frequency of 13.1% in April, the average speed being 3.9 m/s also from the NW. The predominant wind direction in May is from the NW sector with a frequency of 15%, the average wind speed being 4.1 m/s from the N sector.

The predominant wind direction in June is from the NW sector with a frequency of 16.4%, the average wind speed being 4.0 m/s from the NW sector.

For the Sannicolau Mare station, the predominant wind direction in July is from the V sector with a frequency of 15.1%, the average wind speed being 4.2 m/s from the NW sector. The predominant wind direction in August for Sannicolau Mare is from the V sector with a frequency of 12.3%, the average wind speed being 4.0 m/s from the V sector.

In 1999, the annual amount of rainfall reached 771.1 l/m², an increase of 153.3 l/m² compared to the multi-annual average of 617.8 l/m². In 2001, Timisoara received 685.7 l/m² of rain, and the driest year in the analyzed period was by far 2000, with only 296.3 l/m².

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OXIDATIVE STABILITY OF FORTIFIED SESAME OIL WITH SPICES

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Abstract

In the context of an increasingly heightened concern for health and healthy eating, vegetable oils play an important role in modern diets. In this regard, cold-pressed oil is an excellent source of lipids and bioactive compounds, which have beneficial health potential. Sesame (*Sesamum indicum* L.) is cultivated in several countries and plays an important role in human nutrition. The plant's seeds are used both as a spice and a source of oil. Sesame oil is a common ingredient in Asian cuisine, used to add flavour to a variety of dishes but never used as a cooking oil. Sesame oil is characterized by a strong and dominant aroma. Similarly, the spices add aroma and flavor to food. The aim of the study was to monitor the oxidative stability of four sesame oil samples fortified with some spices: garlic (*Allium sativum*), basil (*Ocimum basilicum*), cumin (*Cuminum cyminum*) and cinnamon (*Cinnamomum zeylanicum*) during storage for 9 month in room conditions.

Introduction

The process of foods fortification has been a fundamental aspect of global nutrition policy, with the objective of reducing the problem of nutrient deficiencies on a worldwide scale. The most commonly fortified foods are: cereals and bakery products, milk and dairy products, fats and oils, tea and other beverages, infant formulas and accessory food items [12].

Sesame oil obtained from sesame (*Sesamum indicum* L) seeds and is a high-quality edible oil that is traditionally used in Asian cuisine, renowned for its distinctive flavour and aroma [5]. It is recommended that its use in food be in small quantities [9]. The chemical composition of sesame indicates that the seed constitutes an important source of oil (44–58%), protein (18–25%), carbohydrate (13.5%) and ash (5%). In general, it seems that room temperature preserves the nutritional value of sesame due to the increase in omega-6 and vitamin content, and can be the optimal storage conditions for sesame for use in food industry [1, 7]. Spices are known to be the fundamental components of flavour in foods. Spices have many functions in foods: the enhancement of flavour in food products (condiment) and the preservation of food items [10]. Spices have their aromatic properties distributed in different organs of plants, so: in roots (ginger and turmeric), bulbs (garlic and onion), twigs or bark of trees (cinnamon), leaves (basil, rosemary, marjoram, oregano, mint), flowers (lavender, clove and orange), fruits (peppers, star anise and tamarind), seeds and grains (coriander, cumin, fennel, nutmeg, and sesame), etc [6]. Has been demonstrated to offer significant nutritional benefits, contributing to a good human health [10]. The factors that affect the oxidation of vegetable oils are numerous and include temperature, production-related processes, heating techniques, light, fatty acid composition of the oil, antioxidants compounds, oxygen concentration, thermal oxidizable compounds and transition metal ions [4].

Experimental

The oil samples and the dry spices were acquired from local supermarkets from Timisoara (Romania). The dry spices were introduced in four dark bottle and covered with cold - pressed sesame oil, in a ratio of 1:10 at room temperature (20°C) during 21 days and were stirred periodically during maceration. After this time, the macerates were filtered, analyzed and stored in the refrigerator until consumption. The primary and secondary oxidation products – the peroxide value and the p-anisidine value – were periodically determined every three months during 9 months. The oil samples have been kept away from light in dark colored bottles. Oxidative stability was made on non-oxidized sesame oil samples (initial point) for sesame oil (C) and four fortified sesame oil samples with spices: garlic (FSeO1), basil (FSeO2), cumin (FSeO3) and cinnamon (FSeO4) after storage at room temperature condition.

Physico-chemical analysis

The peroxide value (PV) was determined according to standard iodometric methods for the edible oil and the results were expressed in milliequivalents O₂/kg (mEq O₂/kg). According to AOCS [3], the p-anisidine value (p-AV) standard method is based on the reactivity of the aldehyde carbonyl bond on the p-anisidine amine group and the formation of a Schiff base that absorbs at 350 nm. Thus, 2 g (w) of fortified sesame oil sample were dissolved in 25 mL isooctane and the absorbance (A₁) were measured at 350 nm. A blank was prepared with isooctane. An aliquot (5 mL) of this solution, respectively 5 mL of isooctane (as blank) was transferred to each of two test tubes of 10 mL and was added, to each, 1 mL anisidine solution (0.25% g/v glacial acetic acid). The absorbance (A₂) has been read, after 10 minutes, also at the same wavelength, against isooctane containing p-anisidine. p-AV was calculated to the formula (1):

$$p-AV = 25 \times \frac{1.2 \times A_2 - A_1}{w} \quad (1)$$

In order to estimate the oxidative deterioration of lipids was used *TOTOX value* (total oxidation value) and was calculated according to the formula (2) [11]:

$$TOTOX \text{ value} = 2PV + p-AV \quad (2)$$

All determinations were carried out in triplicates. All reagents and solvents used in this study were of analytical reagent grade.

Results and discussion

The oxidative stability of oils is one of the most important indicators of shelf life [8]. Sesame oil is characterized by a low oxidation rate, due to its low content of unsaturated fatty acids. These acids react readily with oxygen to form peroxides [9]. The oxidative stability of fortified sesame oil is determined by the monitoring of chemical quality indicators. The oxidation degree of sesame oil samples, both without and with the fortified of spices, is presented for comparison in Table 1.

Table 1. Oxidation degree of fortified sesame oil samples

Sample	PV (mEq O ₂ /kg)				p-AV				TOTOX			
	Time (months)				Time (months)				Time (months)			
	0	3	6	9	0	3	6	9	0	3	6	9
C	1.49	1.49	1.49	1.54	1.64	1.87	1.86	2.09	4.62	4.85	4.84	5.16
FSeO1	2.76	2.77	2.80	2.77	1.78	1.78	1.80	1.80	7.30	7.32	7.40	7.34
FSeO2	3.28	3.28	3.30	3.36	1.88	1.88	1.92	1.96	8.44	8.44	8.52	8.68
FSeO3	2.38	2.38	2.39	2.38	1.59	1.59	1.64	1.61	6.35	6.35	6.42	6.37
FSeO4	2.54	2.56	2.64	2.60	1.74	1.76	1.80	1.86	6.82	6.84	7.08	7.06

The initial peroxide value range of the fortified oils was found to be relatively low, ranging from 1.49 to 3.28 meq/kg, thereby indicating a high degree of stability against oxidation. The PV increases slightly from one month to the next. After 9 months, the PV values decreased for samples FSeO1 and FSeO3 - corresponding to the garlic and cinnamon fortified oils. This decline occurred concurrently with the appearance of secondary oxidation compounds [10]. According by AOCS [3] standard methods, PV of fresh oils should be less than 10 mEq O₂/kg oil, while the PV above 30 mEq O₂/kg indicate a rancid oil.

The p-anisidine value was used to assess the secondary oxidation of the oil or fat, which is mainly due to aldehydes and ketones; represent an indicator of oxidative rancidity in oils and fatty foods. The p-anisidine value for sesame oil samples ranged from 1.64 to 2.09. There were no significant differences in the p-anisidine value between the flavored sesame oil samples. Since the sesame oil samples obtained in this study have p-anisidine values less than 1, it means that the oils are of good quality. The control sample was found to have the highest value, indicating that the addition of spices has an inhibitory effect on the secondary oxidation products. It has been demonstrated that an oil's TOTOX value is an important indicator of its quality. The lower the TOTOX value, the better the quality of the oil [2].

Conclusion

It is evident that the all spices utilized in the study ensure the oxidative stability of the fortified oil samples. Among these, sesame oil samples containing garlic and cinnamon demonstrated the most significant resistance to oxidation. Chemical analysis of spices fortified cold-pressed sesame oils did not show a clear pattern related to changes during storage. However, the most significant changes were observed after 6 months of conditions specified in this study.

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ANTICORROSIVE NANOMATERIALS OF THE TYPE $\text{Zn}_3\text{Nb}_2\text{O}_8$ UNDOPED AND DOPED WITH TRIVALENT Er^{3+} IONS IN SALINE ENVIRONMENT

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Abstract

This study involves the depositions of metal-oxide films via the spin-coating method, using pseudo-binary $\text{Zn}_3\text{Nb}_2\text{O}_8$ oxides, both undoped and doped with Er^{3+} ions, synthesized hydrothermally on metallic substrates. Following the preparation of the thin films, electrochemical method were employed to evaluate their corrosion resistance and to validate their potential as corrosion inhibitors.

The tests were carried out using a Voltalab PGZ 402 potentiostat connected to a three-electrode electrochemical cell, with the working electrodes consisting of steels discs coated with the thin films. The working parameters included a potential range set between -1.3V and -0.6V and a scan rate of 1mV/s. The measurements were performed at a temperature of 23°C. The open circuit potential (OCP) of the modified electrodes was monitored for 30 minutes prior to polarization. The corrosive medium used for the tests was a 0.3 M NaCl saline solution.

Introduction

Over time, zinc alloys like Zn-Ni and Zn-Co were developed to improve corrosion resistance, thanks to densely packed crystallographic planes and a more stable ionization environment. Additional improvements were achieved using protective porphyrin layers, amorphous oxide compounds, or pseudo-binary oxide nanomaterials [1].

Experimental

In order to obtain nanomaterials via hydrothermal synthesis, the following precursors were used, as follows:

Sample	Precursor 1	Precursor 2	Precursor 3	Molar ratio
1e	Nb_2O_5	$\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$	Er_2O_3	1:3:0.2
2e	Nb_2O_5	$\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$	Er_2O_3	1:3:0.2
3e	Nb_2O_5	ZnO	Er_2O_3	1:3:0.2
4a	Nb_2O_5	$\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$	-	1:3
4e	Nb_2O_5	$\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$	$\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$	1:3:0.2
5a	Nb_2O_5	$\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$	-	1:3
5e	Nb_2O_5	$\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$	$\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$	1:3:0.2
6a	Nb_2O_5	ZnO	-	1:3
6e	Nb_2O_5	ZnO	$\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$	1:3:0.2

Table 1. Precursors used in the hydrothermal synthesis

Experimental condition using the hydrothermal method depended on temperature (240°C), time (12h) and pH (7). Thin films depositions were carried out on steel

discs(OL) with a diameter of 10 mm and a thickness of 2mm. The chemical compositions of OL used was as follows(wt.%):

Fe	Al	Cu	Si	Mn	Cr
98	0.0309	0.311	0.339	0.219	0.18
C	Ni	Mo	Pb	Nb	Ti
0.165	0.179	0.339	0.05	0.0023	0.005
Zn	V	W	P	S	Co
0.005	0.005	0.05	0.005	0.005	0.0138

Table 2. Chemical compositions of OL

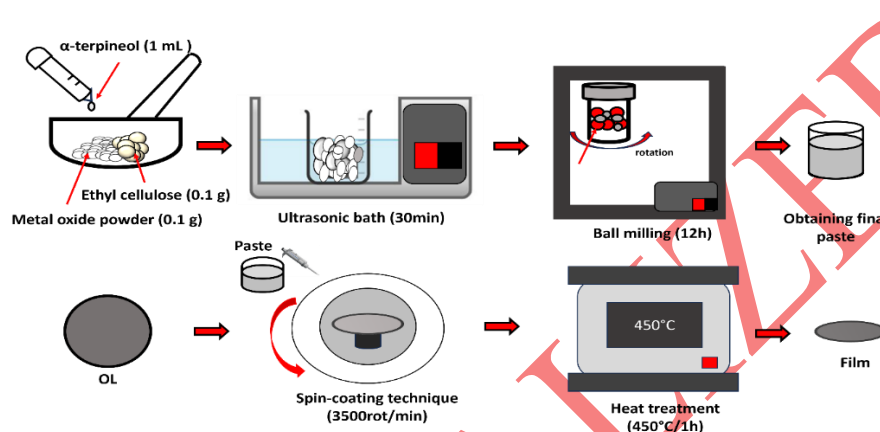


Figure 1. Schematic diagram of the thin film deposition process using the spin coating method

In the first stage, a paste was prepared by mixing 0.1g of metal oxide power with a matrix solution composed of 0.1g of ethyl cellulose and 1 mL of a α -terpineol in an agate mortar. To achieve proper homogenization of the mixture, the resulting solution was ultrasonicated for 30 minutes., followed by further processing in a planetary ball mill (Lab Mills 1 x QM) at a constant frequency of 40kHz for 12 hours.

In the second stage the films of undoped metal oxide ($\text{Zn}_3\text{Nb}_2\text{O}_8$) and doped (Er^{3+}) were then deposited onto low carbon steel substrates using the spin-coating technique. A homogeneous diluted paste of the metal oxide in ethanol was prepared and deposited onto the steel substrate at a rotation speed of 3500 rpm for 30 seconds. In order to remove the organic compounds used in the homogeneous solution (metal oxide- polymeric matrix) and to ensure proper adhesion of the oxide films to the steel substrates, a thermal treatment was applied at 450° C for 1 hour, with a heating rate of 2°C per minute.

Results and discussion

The OCP measurements presented in figure 2 (0.3NaCl) show that the coated electrodes stabilize with difficulty, reaching a quasi-stable state around 1500 seconds and displaying a non-uniform behavior, whereas the uncoated electrode stabilizes at approximately 1700 seconds. This results provides preliminary insights into the nature of the processes occurring at the metal/thin film-electrolyte interfaces.

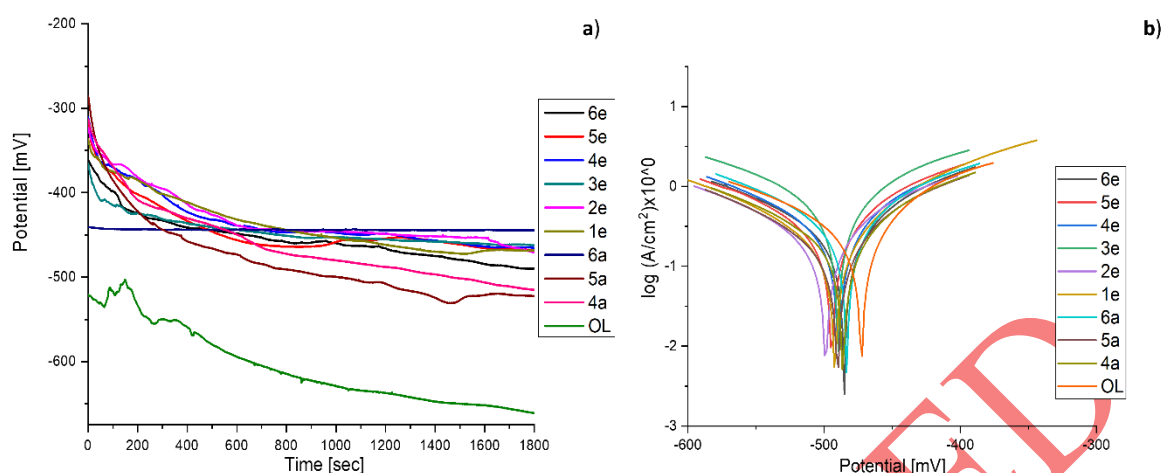


Figure 2. a) OCP measurements for the modified electrodes over 30 minutes: steel electrode, $Zn_3Nb_2O_8$, and $Zn_3Nb_2O_8:Er^{3+}$ in 0.3 M NaCl and b) Tafel curves for the modified electrodes after immersion of the steel electrode, $Zn_3Nb_2O_8$ and $Zn_3Nb_2O_8:Er^{3+}$ in 0.3 M NaCl for 30 minutes (notations according to Table 1)

Electrode	E (I = 0) (mV)	R _p (Ωcm^2)	i _{corr} (mA/cm ²)	β_a (mV)	β_c (mV)	v _{corr} (mm/Y)	IE (%)
OL	-389.14	68.20	3.8190	240.8	-251.5	21.27	-
1e	-553.2	15.75	1.8031	173.5	-189.8	15.049	52.79
2e	-577.0	8.81	1.6106	153	-139.7	11.879	57.82
3e	-433.2	27.74	1.1780	152.9	-122.2	9.393	69.15
4a	-426.9	5.33	2.0680	175	-128.9	18.831	45.84
4e	-563.0	14.51	1.6300	54.5	-61	10.591	61.34
5a	-512.2	9.95	1.9145	172.6	201.3	16.728	49.86
5e	-549.1	9.13	1.7328	155.3	-188.3	12.624	54.62
6a	-693.6	5.48	1.8068	223.9	-107.9	15.368	52.69
6e	-442.7	14.67	1.0841	109.6	-154.7	8.570	71.61

Tabel 3. Tafel parameters for electrodes analyzed after 30 minutes immersion in 0.3 M saline medium

In all analyzed cases of steel electrodes modified by spin coating deposition of thin films made from pseudo-binary oxides, an improvement in corrosion inhibition was observed. Moreover, it was found that the best IE value (71.61) was obtained when the layer was formed using the $Zn_3Nb_2O_8:Er^{3+}$ structure, synthesized by the hydrothermal method using: ZnO , Nb_2O_5 and $Er(NO_3)_3 \cdot 5H_2O$ as precursors in a saline medium. By analyzing the variation of corrosion potential and corrosion current as the inhibition efficiency increases (Table 3), it can be observed that the corrosion current decreases proportionally with the corrosion rate, while the corrosion potential shifts toward more cathodic values.

For all the deposits with materials obtained by the hydrothermal method and tested in saline environment, the polarization resistance (R_p) of the modified OL steel electrode increases. The best value recorded for the same test (6e).

The shift of the corrosion potential (E_{corr}) toward more negative values in the presence of undoped and Er^{3+} -doped $Zn_3Nb_2O_8$ is caused by the different nature of the electrochemically active species on the metallic surface (Zn, Nb, Er), in addition to Fe. The presence of Nb ions

together with Zn ions shifts the corrosion potential to more negative values (-389.14 mV), and the corrosion current density decreases from 3.8190 mA/cm² (bare steel) to 1.0841 mA/cm² in saline medium.

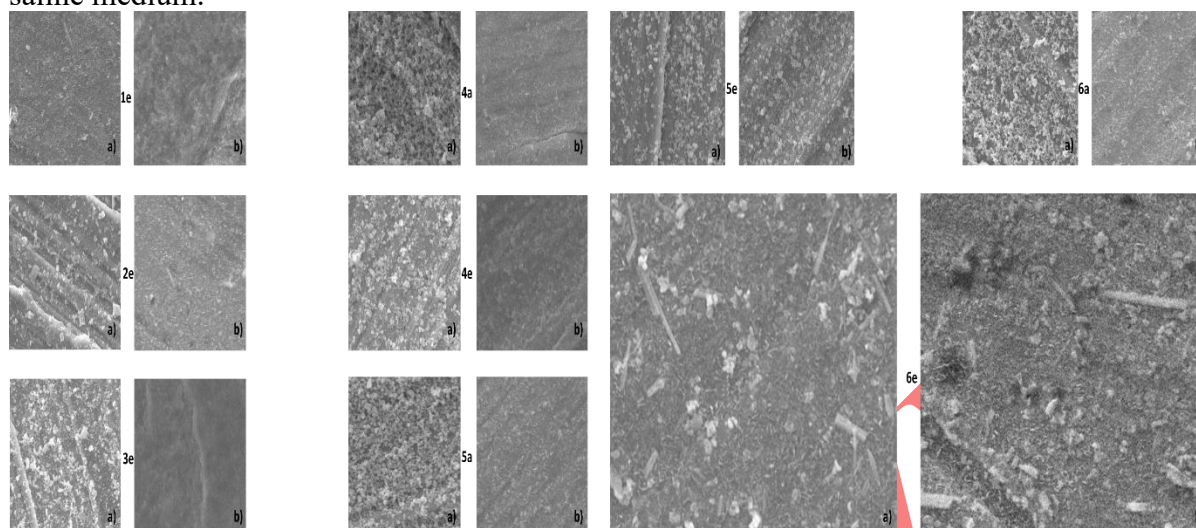


Figure 4. SEM images for the spin coated samples according to table 1 before (a) and after (b) corrosion tests in saline environment.

From the SEM images (Figure 4), it can be observed that doping the material with Er^{3+} ions leads to crystallization in the form of rod-like structures. SEM images of the doped and undoped oxides obtained by the hydrothermal method were taken at 12000x analysis magnification in medium vacuum.

Figure 5. shows the AFM images of the surfaces for each of the thin films deposited on the OL electrodes, measured before and after the corrosion tests, using the non-contact working mode. The measurements were performed in aggressive environments, namely 0.3 M NaCl.

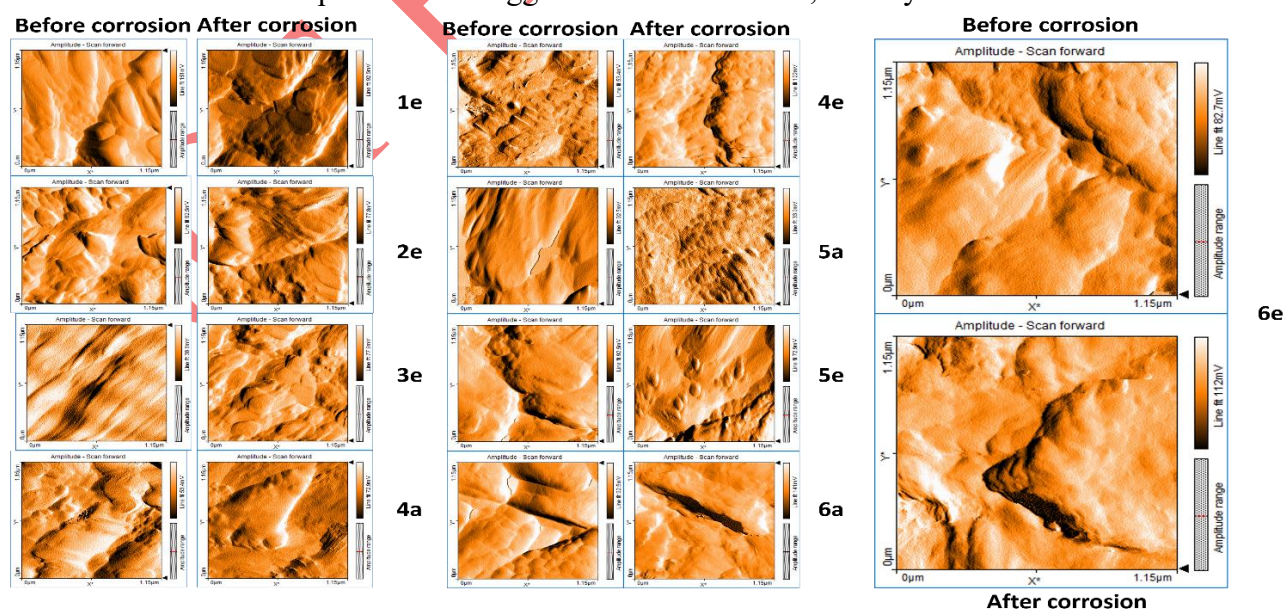


Figure 5. AFM images before and after corrosion tests for the samples deposited by spin coating according to table 1 before and after corrosion tests in saline environment

Electrode	Area (pm ²)	S_a before/ after 0.3 M NaCl (nm)	S_q before/ after 0.3 M NaCl (nm)	S_y before/ after 0.3 M NaCl (nm)
OL	1.326	11.281 / 46.154	16.405 / 56.855	-
1e		9.7957 / 35.209	12.368 / 44.446	750.43 / 265.12
2e		10.346 / 32.275	13.485 / 43.673	80.548 / 278.57
3e		14.307 / 21.176	18.6 / 26.795	132.59 / 161.51
4a		16.518 / 19.66	20.76 / 24.261	113.93 / 181.42
4e		16.867 / 40.598	20.20 / 47.235	120.15 / 222.63
5a		9.073 / 28.01	11.511 / 32.492	59.184 / 207.84
5e		19.384 / 30.724	24.772 / 38.124	150.18 / 236.23
6a		16.857 / 42.171	20.509 / 51.864	113.9 / 280.74
6e		22.186 / 33.844	27.499 / 251.94	156.57 / 251.94

Table 4. Nanoroughness of thin films obtained by spin coating technique

Using the Nanosurf®EasyScan 2 software, the nanoroughness of the monolayer thin films was calculated before and after the corrosion tests (Table 4).

Conclusion

Table 3 shows that the oxid corrosion inhibitor forms a barrier on the metal surface, reducing contact between the steel and saline environment, which ultimately decreases the corrosion rate. If a cathodic reaction occurs in the corrosion process, the corrosion potential becomes more negative (our case). The Tafel curves show that all thin films deposited as monolayer structures on electrodes exhibit lower corrosion current densities compared to the OL disk.

AFM microscopy reveals that after exposure to the saline environment, the thin films retain their material structure at the corrosion interface, though the morphology changes and aggregate size increases. This suggests that the corrosion inhibition mechanism in carbon steel relies on the physical protection provided by the compact and adherent pseudo-binary oxide layers at the steel interface.

The most distinct morphology (shown in Figure 4) was observed in sample 6e, synthesized using $\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$, ZnO , and Nb_2O_5 as precursors. Notably, this sample also exhibited the highest corrosion protection efficiency in the tested environments

The corrosion protection mechanism of steel can be attributed to a physical/mechanical barrier effect. Correlating microscopic observations with electrochemical measurements, it is evident that $\text{Zn}_3\text{Nb}_2\text{O}_8\text{:Er}^{3+}$ layers obtained via the hydrothermal method act as an effective barrier against salt ion penetration, thereby protecting the steel surface.

Acknowledgements

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BLUE-TO-UVC UPCONVERSION PHOSPHOR-POLYMER HYBRIDS FOR LIGHT-DRIVEN ANTIMICROBIAL APPLICATIONS

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Abstract

Ultraviolet C (UVC) radiation is a well-known antimicrobial agent. It is widely used to inactivate microorganisms because it can cause irreversible DNA damage, which stops replication and survival. Even though UVC disinfection is essential for cleaning water, food, and surfaces, its widespread use is limited by high energy needs, costs, and material challenges associated with traditional UVC light sources [1,2]. To tackle these issues, blue-to-UVC upconversion (UC) materials have become an appealing alternative. They allow for the local production of germicidal UVC photons from common and cheap blue light sources. Rare-earth-doped inorganic phosphors work particularly well in these applications due to their unique optical traits, chemical stability, and adjustable emission profiles [3,4].

Our study looks into the synthesis, structural and optical characterization, and antimicrobial performance of two Pr³⁺-doped inorganic compounds, Y₂SiO₅:Pr³⁺ and La(PO₃)₃:Pr³⁺, along with hybrid materials made from them. We prepared the powders and analyzed them using Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), and photoluminescence (PL) spectroscopy. Emission spectra indicated that these materials can produce germicidal UVC radiation when exposed to blue light, showing promise as low-energy disinfection tools.

For the microbiological evaluation, we used *Escherichia coli* ATCC 8739 as a model organism and performed two complementary experiments. In the first experiment, we mixed the powders directly with bacterial suspensions without light exposure to check their intrinsic toxicity. In the second experiment, we embedded Y₂SiO₅:Pr³⁺ in a polydimethylsiloxane (PDMS) matrix and formed a thin film on glass substrates. This setup allowed us to irradiate bacterial cultures through the composite under blue light. We included two control conditions: exposure through bare borosilicate glass and bacterial suspension without irradiation. We compared colony-forming units (CFU) to measure the antimicrobial effect.

The results show that La(PO₃)₃:Pr³⁺ has much higher intrinsic toxicity toward *E. coli* than Y₂SiO₅:Pr³⁺. On the other hand, Y₂SiO₅:Pr³⁺/PDMS composites are non-toxic without light but do show some antimicrobial activity under blue-light exposure. We observed an about 25% reduction in viable CFU counts in cultures irradiated through the PDMS/Y₂SiO₅:Pr³⁺ membrane, while the control exposed only through borosilicate glass showed an 11% increase in CFU. These findings highlight the important role of upconversion-driven UVC emission in bolstering light-based bacterial inhibition and support the idea of polymer-phosphor hybrid coatings as functional disinfection materials.

Overall, the study provides a solid basis for developing Pr³⁺-doped inorganic phosphors and integrating them into polymer matrices for antimicrobial technologies. By combining structural, optical, and microbiological studies, it emphasizes both the potential and current challenges of blue-to-UVC upconversion systems for sustainable, low-energy water and surface cleaning applications.

Acknowledgements

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NOT FINAL VERSION

REMOVAL OF DYES FROM TERNARY SYSTEM BY ADSORPTION

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Abstract

Wastewater from the textile industry typically contains several types of dyes, as well as other compounds considered contaminants, which interact in ways that can significantly influence the efficiency of the removal process. Therefore, investigating dye removal from multiple systems provides a more realistic assessment of the effectiveness of the wastewater treatment process [1]. Factorial design and Response Surface Methodology (RSM) are powerful tools in optimizing dye removal conditions [2], allowing the simultaneous exploration of multiple factors (pH, adsorbent dosage, temperature, dyes concentration) to identify the most effective combination that ensures the best removal efficiency. This approach not only reduces experimental time and saves resources, but also provides a comprehensive understanding of the process, crucial for the development of sustainable and efficient solutions in wastewater treatment and environmental remediation.

This paper presents experimental and theoretical studies for the simultaneous removal of three dyes from aqueous solutions using a magnetite/carbon nanocomposite (NC) as an adsorbent. The NC was synthesized by combustion method, and characterized by XRD, FTIR spectroscopy, SEM, thermal analysis, and N₂ adsorption-desorption techniques.

For the experimental studies, the optimal working conditions established for the adsorption of dyes (Acid Orange 7, Methylene Blue, Basic Red 1) from single-component systems were selected as initial conditions for the simultaneous adsorption of dyes from the ternary system.

The efficiency of removing all dyes from the ternary system decreased compared to individual removal, due to the competitive effect. However, the removal yield is more than 72%, for all selected dyes, which is important for application on polluted industrial waters.

A series of factorial design experiments using selected dyes was conducted. To further explore the system's behaviour, a central composite design (CCD) was implemented for the ternary mixture, aiming to determine whether optimal removal conditions shift with the presence of more additional dyes in the system. The results obtained highlighted that, for efficient removal in a ternary mixture of dyes, it is essential to maintain pH and dye concentrations within optimal ranges, to leverage synergistic effects, while minimizing cross-inhibition. Predicted data obtained for the removal efficiency were in good agreement with the experimental determinations (98%).

The obtained results demonstrated that NC is a promising adsorbent for removal of dyes from ternary system, and response surface optimization can be successfully used to optimize the adsorption process parameters.

Acknowledgements

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THE CHARACTERIZATION OF RECYCLED ACRYLONITRILE-DIVINYLBENZENE POLYMER FOR POSSIBLE ANTIMICROBIAL TESTS

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Abstract

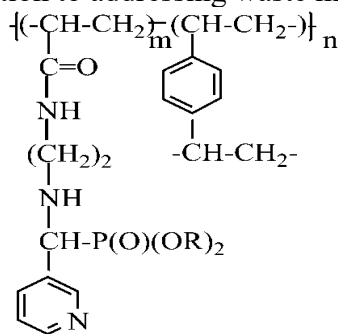
This work presented the analysis of acrylonitrile-divinylbenzene copolymers with functional groups (by aminophosphonate type) recovered from a biological medium for possible future use in an antimicrobial test study. Their stability was confirmed by Fourier transform infrared spectroscopy, energy dispersive X-ray analysis (EDX) and scanning electron microscopy (SEM).

Introduction

Bacteria play an important part in our lives. They are found in soil, water, and the air. They could lead to a variety of health issues. Certain materials were used as antimicrobial agents to stop bacterial infections. It is clear that new materials with antibacterial properties are needed. The creation of polymers with antibacterial properties, or polymeric biocides, is a topic of great contemporary interest in polymer research, which has not received sufficient attention. The problem of creating polymeric biocides can often be solved if the bactericide is covalently grafted onto polymeric carriers or other insoluble support materials [1].

The potential antibacterial properties of acrylonitrile-divinylbenzene (AN-DVB) polymers with aminophosphonate groups (see Figure 1) [2] make them worthy of study, as they can improve water purification and other biological applications. The biological activity of these polymers, especially their antibacterial properties, can be enhanced by the addition of aminophosphonate groups [3-5]. Aminophosphonates not only directly inhibit bacterial growth, but also enhance the immune response, making them valuable in fighting infections.

One area that is expanding to reduce their environmental impact is the use of recycled materials. Recycling acrylonitrile-divinylbenzene offers a sustainable source for the synthesis of antimicrobial compounds, in addition to addressing waste management concerns.



where: R= Bz or Et

Figure 1. The structure of the functionalized copolymers: Bz-DVB-AN and Et-DVB-AN.

In water treatment, the most usual treatment method to disinfect and sterilize water is to use chlorine and other related chemicals. But their residues can grow to be concentrated in the food chain and in the environment as well as the possible formation of halomethane analogues that are suspected of being carcinogenic should lead to the prevention of their use [6]. Due to the associated problems result from the use of conventional antimicrobial agents, the idea for using of polymeric antimicrobial agents appeared to be an attractive choice.

This study concerns the characterization of recycled AN-DVB grafted with aminophosphonate groups (see Figure 1) [2] for possible future use in an antimicrobial assay. The efficacy of the copolymers was investigated by Fourier transform infrared spectroscopy (FTIR), Optical image, energy dispersive X-ray analysis (EDX) and scanning electron microscopy (SEM).

Experimental

Instruments

Fourier transform infrared spectroscopy (FTIR) using a JASCO-FT/IR-4200 spectrophotometer, ZEISS Stemi 508 Stereo Microscope, Energy dispersive X-ray (EDX) analysis and scanning electron microscopy (SEM) were performed using an Energy-Dispersive X-ray (EDX) analyzer (Octane Elect Super SDD detector, Ametek, Berwyn, PA, USA) equipped on a Verios G4 UC (Thermo Scientific, Brno, Czech Republic) SEM device.

Working method

All four samples (Bz-AN-DVB-*S. aureus*, Et-AN-DVB-*S. aureus*, Bz-AN-DVB-*E. coli* and Et-AN-DVB-*E. coli*) were recovered from antibacterial solutions where they were tested against a Gram-positive bacterial species (*Staphylococcus aureus*) (code: Bz-AN-DVB-*S. aureus* and Et-AN-DVB-*S. aureus*) and a Gram-negative bacterial species (*Escherichia coli*) (code: Bz-AN-DVB-*E. coli* and Et-AN-DVB-*E. coli*). Then, the samples were filtered, autoclaved at a pressure of 1 atm and a temperature of 120 °C for 30 minutes. These recovered samples were characterized by FTIR, Optical Image, SEM and EDX.

Results and discussion

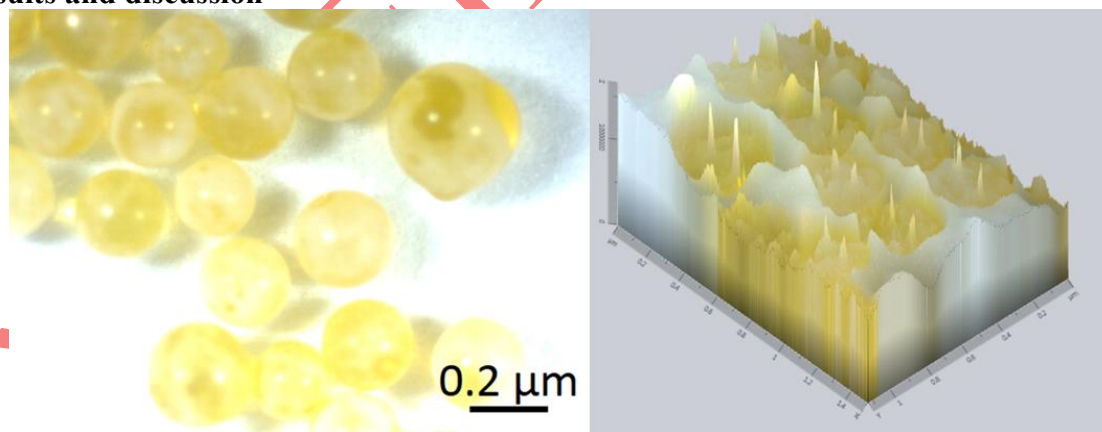


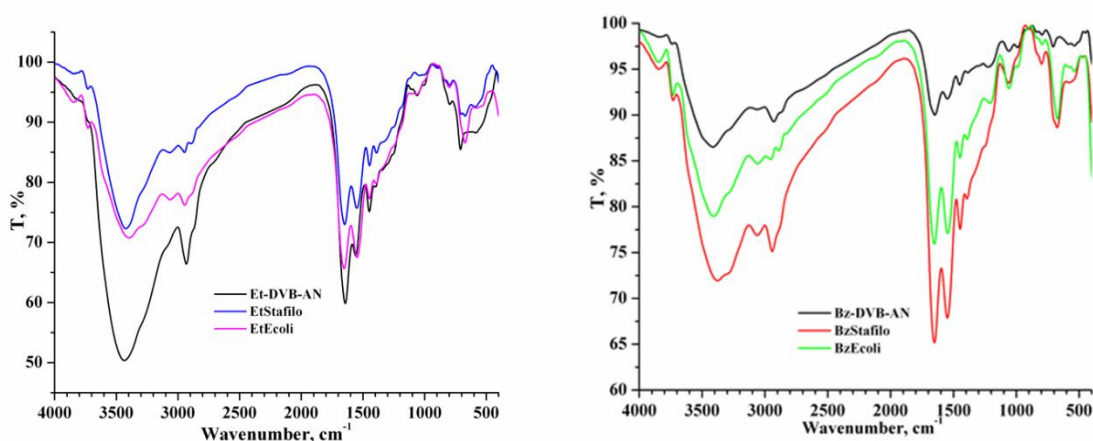
Figure 1. Optical Image of Et-AN-DVB *S.aureus* sample after autoclaved and sterilized.

The variation regarding the number of total germs (CFU/mL) and percentage of microbial reduction at contact times with the two antimicrobial materials are presented in Table 1 [2].

We considered that the antibacterial activity is the result of hydrogen bonding between the organic phosphorus groups (P=O) from aminophosphonate groups and the OH groups in the cell walls of the bacteria, as we described in our previous study [2]. Because of this, it is thought that the copolymers' antibacterial action occurred more quickly for gram-positive bacteria than gram-negative bacteria.

Table 1. The antimicrobial activity of functionalized copolymers [2].

Sample	in the start moment (0 h)	after 18 h of contact	
	CFU/mL	CFU/mL	Percentage of microbial reduction, %
<i>Escherichia coli</i>			
BzDVB-AN	1.337.216	371.475	72.2
EtDVB-AN	1.269.800	196.850	84.4
<i>Staphylococcus aureus</i>			
BzDVB-AN	2.952.770	726.381	75.4
EtDVB-AN	2.572.250	133.757	94.8

**Figure 2. FTIR spectrum for samples obtained after their recovered.**

The graphic (see Fig. 2) highlights the characteristic bands of both the phosphonate groups and the amino group, observed at 1170 cm^{-1} and 1570 cm^{-1} , respectively, in the spectra.

The phosphorus content of the recovered copolymers, presented in Tables 2 and 3, is an indication that they can be used in subsequent antibacterial testing.

Table 2. Semi-quantitative EDX-analysis of Bz-DVB-AN- recovered.

Type of analysis/Element	Wt, %			
	C	N	O	P
Bz-AN-DVB- it was recovered after testing with <i>S. aureus</i>				
EDX	78.08	14.05	2.85	5.01
Bz-AN-DVB- it was recovered after testing with <i>E. coli</i>				
EDX	73.05	14.76	5.81	5.34

Table 3. Semi-quantitative EDX-analysis of Et-DVB-AN- recovered.

Type of analysis/Element	Wt, %			
	C	N	O	P
Et-AN-DVB- it was recovered after testing with <i>S. aureus</i>				
EDX	68.21	20.85	7.79	3.14
Et-AN-DVB- it was recovered after testing with <i>E. coli</i>				
EDX	67.18	20.64	6.63	4.31

As illustrated in Figure 3 and detailed in Tables 2 and 3, the EDX spectra of the recovered samples confirm that their functionalization is fully preserved.

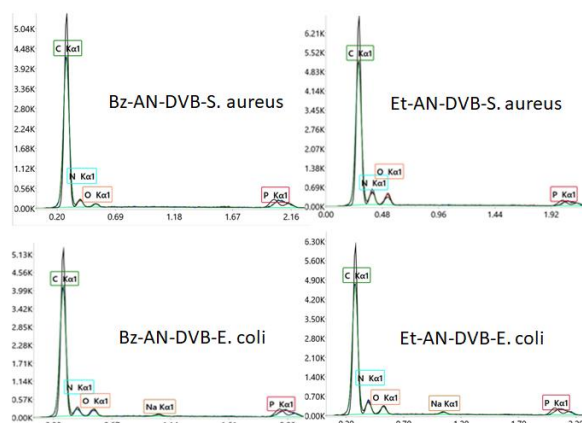


Figure 3. EDX image for samples obtained after their recovered.

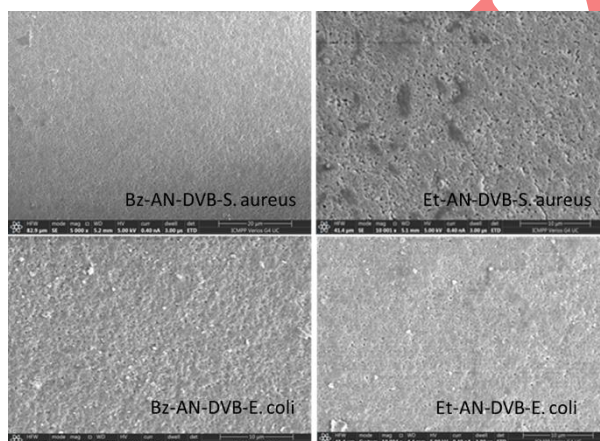


Figure 4. SEM image for samples were obtained after their recovered.

Figure 4 presents SEM images of the recovered samples, revealing that the copolymers exhibit a uniform surface morphology.

Conclusion

The analysis of recycled acrylonitrile-divinylbenzene polymers functionalized with aminophosphonate groups presents a promising approach for developing antimicrobial materials with practical applications.

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INTEGRATION OF AEROTITANIA MICROTUBES IN UV PHOTODETECTORS

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Abstract

In the past years, a new class of porous materials known as aero-materials has gained attention for their unique properties. Similar to aerogels in structure but obtained by different methods, aero-materials are typically synthesized by growing materials on sacrificial templates, avoiding the liquid phase. After removing the template, the material retains the shape of the substrate, resulting in an extremely porous and ultra-lightweight structure with special properties [1,2].

Aerotitania represent a 3D nanoarchitecture based on interconnected hollow microtetrapods based on Titanium dioxide (TiO₂). The material was synthesized using the Atomic Layer Deposition technique, by depositing ultrathin TiO₂ layers onto a sacrificial template consisting of an interconnected network of ZnO microtetrapods [3].

In this research, it is demonstrate a simple method to integrate aerotitania on a sensor platform based on interconnected electrodes by using spin coating technique. The sensitivity of the aerotitania sensor was measured through dynamic current and resistance responses to the alternation of UV illumination. The responsivity value was calculated, showing that it is directly influenced by the optical power and the thickness of aero-TiO₂ layer.

Acknowledgements

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THE COURSE AND EVOLUTION OF AGRICULTURE IN THE BERLIȘTE AREA, CARAȘ SEVERIN COUNTY

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Abstract

Agriculture is one of the oldest human activities, forming the basis of food security and economic development in many regions of the world (FAO, 2020). Currently, the transition from subsistence to commercial agriculture poses major challenges in terms of sustainability, resource use and adaptation to climate change (Tilman et al., 2011). This study analyzes the evolution and characteristics of agriculture in Berliște commune, Caraș-Severin county, Romania, over the period 2022–2024, based on data provided by local authorities and farmers in the area. The methodology included the collection of data on cultivated areas, agricultural yields, fertilizer use and crop rotation. The results show a predominance of wheat and corn crops, complemented by oilseeds (sunflower, soybean) and vegetables, with moderate fluctuations in areas and yields. Organic fertilizers had a significant share, supported by animal husbandry, while the use of chemical fertilizers remained low. The conclusions point to a subsistence agricultural system, with low inputs, but with a potential for improvement through the application of modern technologies and the exploitation of local resources. The study contributes to the understanding of the particularities of agriculture in southwestern Romania and provides benchmarks for adapting agricultural practices to the requirements of sustainable development.

Introduction

Agriculture is one of the main branches of the world economy, providing food, raw materials and jobs for a significant part of the population [1,2]. Globally, current challenges are related to population growth, increased use of natural resources and the effects of climate change on agricultural production [3,4,15] .

In the European area, agriculture is marked by the Common Agricultural Policy (CAP), which promotes sustainability, environmental protection and diversification of production [5,6,7]. At the same time, there are considerable differences between Member States, depending on natural conditions, technological infrastructure and farm structure [8].

In Romania, agriculture has played a fundamental role in history, being recognized in the nineteenth and early twentieth centuries as the "breadbasket of Europe" [9]. After the period of collectivization and the post-1990 transition, the Romanian agricultural sector faces problems of fragmentation of farms, reduced use of modern inputs and limited adaptation to European standards [10] . Pedological studies have highlighted the variable fertility of Romanian soils, from high-productivity mollisols to clay and cambisols with medium potential [11,12].

In southwestern Romania, Caraş-Severin County has a predominantly mixed agricultural structure, in which vegetable crops are combined with animal husbandry [13]. Berlişte is a relevant example of subsistence agriculture, where cereal crops (wheat, corn) and oilseeds (sunflowers) predominate, complemented by vegetables and fodder. The present study aims to analyze the dynamics of cultivated areas, agricultural productions and fertilization in the period 2022–2024, in order to highlight the particularities of the local agricultural system and the prospects for sustainable development.

Experimental

The data used in this study were collected from official sources and through direct consultation with local farmers. The main information comes from the Berlişte Town Hall (2022–2024), which provided statistics on agricultural areas, the yields obtained and the quantities of fertilizers used. The information was supplemented by interviews with farmers, in order to capture the particularities of traditional agricultural practices and the way farms are organized. Methodology included:

- centralization of cultivated areas on basic crops (wheat, corn, barley, triticale, oats, sunflowers, soybeans, vegetables);
- calculation of total yields and average yields (kg/ha) for each crop category;
- analysis of the use of fertilizers, both organic and chemical, to highlight the degree of intensification of agriculture;
- comparing data for the period 2022–2024, in order to capture trends and variations.

The working method was mainly descriptive and comparative, without applying complex statistical models, given the character of a local case study. In interpreting the results, specialized works in the field of agriculture and pedology [11, 12, 13, 14] were taken into account, which allowed the correlation of local data with existing knowledge at regional and national level.

Results and discussions

Agriculture of the Year 2022

Table 1. Cereal crop areas

Culture	Area ha	ProTon Production
Autumn wheat	344	1444
Barley	27	140.7
Corn kernels	170	850
Triticale	13	50.7
Autumn oats	5	12.5
Spring wheat	26	101.4
Spring oats	11	30.8
Sunflower	34	74.8
Soy	4	11.4

In 2022, it is observed that the area cultivated with wheat increased to 344 ha, with a total amount of 1444 tons, reaching an average production of 4200kg/ha. The area occupied by maize decreased by 10 ha, reaching 170 ha, with a total of 850 tons, reaching an average production of 5 tons/ha. The other cereal categories fluctuated very little in terms of area and production. In oilseed crops, in 2022, rapeseed was replaced by soybeans on an area of 4 ha with an average production of 2500 kg/ha. The sunflower crop has expanded by 4 hectares, reaching a total of 34 ha with a production of 2100kg/ha. The production is close to that achieved in 2021.

Table 2. Areas in vegetable crops

Culture	Area ha	Tonne production
Autumn potatoes	14	120.4
Tomato	3	6
Dried onion	1.5	4.5
Dried garlic	2	3.6
Cabbage	3	138
Pepper	1.5	4.5
Cucumbers	2	5.4
Carrots	1.5	5.1
Pea pods	1.5	3
Bean pods	1	1.6
Eggplant	0.7	2.8

As for the vegetable crop, the cultivated areas increased compared to the previous year, the largest area being recorded for cabbage by 3 ha and a production of 45 t/ha, followed by tomatoes by 3 ha and a production of 2 tons/ha.

Table 3. Surfaces applied with fertilizers

Chemical fertilizers	Area ha
Nitrogen	53.4
Phosphate	18
Potassium	18
Natural fertilizers	600
Changes	52

Agriculture of the Year 2023

Table 4. Cereal crop areas

Culture	Area ha	Tonne production
Autumn wheat	290	1276
Barley	25	140
Corn kernels	160	770
Triticale	10	38
Autumn oats	4	8.8
Spring wheat	29	109.2
Spring oats	9	22.6
Sunflower	31	71.4
Soy	3	8.7

In 2023, it is observed that the area cultivated with wheat decreased to 290 ha, with a total amount of 1276 tons, reaching an average production of 4300kg/ha. The area occupied by corn decreased by 10 ha, reaching 160 ha, with a total of 770 tons, reaching an average production of 4800 tons/ha. The other cereal categories fluctuated very little in terms of area and production. In oilseed plants, the same trend as in 2022 was maintained, with no notable changes in terms of both area and production.

Table 5. Areas in vegetable crops

Culture	Area ha	Tonne production
Autumn potatoes	12	108
Tomato	2.2	4.4
Dried onion	1.3	3.9
Dried garlic	1	1.8
Cabbage	3	145.5
Pepper	1	2.9
Cucumbers	1	2.8
Carrots	0.5	1.6
Pea pods	0.5	1.1
Bean pods	1.2	2
Eggplant	0.5	2

As for the vegetable crop, the cultivated areas remained at the level of 2022, the largest area is recorded for cabbage with 3 ha and a production of 48 t/ha, followed by tomatoes with 2.2 ha and a production of 2.1 tons/ha. Potatoes also keep the cultivated area constant of about 12 ha, with a total production of 108 tons/ha.

Table 6. Surfaces applied with fertilizers

Chemical fertilizers	Area ha
Nitrogen	43.7
Phosphate	16
Potassium	16
Natural fertilizers	580
Changes	50

Agriculture of the Year 2024

Table 7. Cereal crop areas

Culture	Area ha	Tonne production
Autumn wheat	300	1260
Barley	25	135
Corn kernels	150	720
Triticale	10	40
Autumn oats	4	9
Spring wheat	29	113
Spring oats	9	24
Sunflower	32	70
Soy	2	5

In 2023, it is observed that the area cultivated with wheat increased to 300 ha, with a total amount of 1260 tons, reaching an average production of 4200kg/ha. The area occupied by corn decreased by 10 ha, reaching 150 ha, with a total of 720 tons, reaching an average production of 4700 tons/ha. The other cereal categories fluctuated very little in terms of area and production, due to crop rotation. For oilseeds, the situation in terms of production and cultivated areas is similar to that of 2023.

Table 8. Areas in vegetable crops

Culture	Area ha	Tonne production
Autumn potatoes	12	103
Tomato	2	4
Dried onion	1	3
Dried garlic	1	2
Cabbage	2	98
Pepper	1	3
Cucumbers	1	3
Carrots	0.5	1.7
Pea pods	0.5	1
Bean pods	1	1.8
Eggplant	0.5	2

As for the vegetable crop, the cultivated areas remained at the level of 2022, the largest area is recorded for cabbage with 2 ha and a production of 47 t/ha, followed by tomatoes with 2 ha and a production of 2 tons/ha.

Table 9. Surfaces applied with fertilizers

Chemical fertilizers	Area ha
Nitrogen	42.8
Phosphate	15
Potassium	15
Natural fertilizers	450
Changes	48

Conclusions

The analysis of the evolution of agriculture in Berliște commune in the period 2022–2024 highlighted some essential features:

The crop structure remained relatively constant, being dominated by cereals (wheat and corn), followed by oilseeds (sunflower, soybeans) and vegetable crops on smaller areas.

Average yields varied slightly from year to year, with values between 4–5 t/ha for the main cereals, depending on climatic conditions and crop rotation.

Organic fertilizers were the main source of fertilization (450–600 ha annually), suggesting a traditional agricultural system based on the integration of livestock farming with agriculture.

Chemical fertilisers were used on limited areas (approx. 10% of the total), which explains the low level of productivity compared to commercial farms in other regions.

The general trend confirms the character of subsistence agriculture, where limited resources and low inputs keep production at moderate levels, but ensure a certain stability and adaptability to local conditions.

It can be concluded that, in order to increase agricultural performance, a moderate intensification of technologies is necessary, through balanced fertilization, diversification of crop rotation and the introduction of modern agricultural practices, without affecting the local ecological balance.

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THE COURSE AND EVOLUTION OF AGRICULTURE IN CUJMIR, MEHEDINTI COUNTY

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Abstract

Agriculture is the foundation of civilization and remains one of the key areas for food security and sustainable development. This study analyzes the evolution of agriculture in Cujmir commune (Mehedinti County, Romania), based on data collected from the local administration and through interviews with farmers. The research follows the dynamics of cultivated areas, the structure of the predominant crops and the level of productions obtained in the period 2023–2024. The results show a high share of cereals (wheat, corn, barley), complemented by technical crops (sunflower, rapeseed) and vegetables (tomatoes, onions, cabbage, cucumbers). Yields vary significantly depending on climatic conditions and low fertilisation, reflecting predominantly conventional agriculture with subsistence influences. The study contributes to the understanding of local agricultural particularities and provides a useful database for the development of rural and sustainable development strategies in southwestern Romania.

Introduction

Agriculture has been, throughout history, one of the main pillars of social and economic development, being indispensable for ensuring food and basic resources for the population [1,2]. Globally, transformations in agriculture have been driven by factors such as climate change, population growth and pressure on natural resources [3,4,5]. In Europe, common agricultural policies have aimed to adapt to new economic and technological realities, with a focus on productivity and environmental protection [6,7].

In Romania, the transition from collectivized agriculture to private structures has generated a sharp fragmentation of land, with small-scale farms, which limits competitiveness on the European market [8,9]. Studies show that medium-sized family farms are the most efficient in terms of production-cost ratio [10,11]. At the same time, soil fertility and the application of modern agricultural technologies remain key factors for increasing yields [3,9].

At the regional level, in southwestern Romania, pedoclimatic conditions favor a diversity of crops, but climatic instability and low input levels affect yields [12,13,14,15]. In Mehedinti County, agriculture is characterized by a combination of cereal and technical crops, complemented by vegetable growing, melons and subsistence crops, which play an important role in the local economy and in farmers' incomes [2,13].

The purpose of this paper is to highlight the evolution of agriculture in Cujmir commune in the period 2023–2024, by analyzing the cultivated areas, the productions achieved and the technologies used, in order to formulate directions to improve local agricultural sustainability.

Material and methods

The research was based on statistical data and direct observations made in Cujmir commune, Mehedinti County, in the period 2023–2024. The primary data were provided by the Cujmir City Hall and the local Agricultural Chamber, and the qualitative information was obtained through discussions with farmers in the area.

The analysis included:

- record of cultivated areas by types of crops (cereals, technical plants, vegetables, melons);
- recording of total productions and average yields per hectare;
- evaluation of the use of chemical and organic fertilizers;
- comparison between agricultural years 2023 and 2024.

The data were processed into tables and graphs to highlight variations in production in relation to climatic and technological factors. The methodology follows the approaches recommended in the literature on the monitoring of agricultural productions and the analysis of soil and climatic resources [3,8,9,11,16].

Results and discussions

Agriculture in 2023

Table 1. Cereal crop areas

Culture	Area ha	Tonne production
Autumn wheat	1300	5460
Spring barley	70	266
Corn kernels	1328	5046
Autumn barley	200	800
Spring oats	8	0
Sunflower	550	880
Dried peas	250	375
Bean	5	1

As can be seen from the table and figures above, the main cereal plants cultivated in 2023 are winter wheat with 1300 ha and a total production of 5460 tons, which represents an average production per hectare of 4200 kg/ha, a lower production than in 2022. Maize ranks 1st with a cultivated area of 1328 ha with a total production of 5046 tons, which represents an average production of 3.8 tons/ha, a lower production than in previous years. This is due to adverse weather conditions. This is followed by sunflower on an area of 550 ha and a total production of 880 tons, which translates into an average production of 1600 kg/ha, then we find oats, barley and barley in different areas. In relation to pea and bean crops, along with early and summer potatoes, the cultivated areas occupy a fairly large area, peas occupy an area of 250 ha with an average production of 1.5 tons/ha, beans occupy 5 hectares with an average production of 0.250 t/ha, and potatoes are found on 4 hectares with an average production of 4t/ha. The yields of these crops are lower than in 2022, due to the lack of rainfall.

Table 2. Areas in vegetable crops

Culture	Area ha	Tonne production
Early and semi-early potatoes	1	4
Summer potatoes	3	11
Tomato	30	120
Dried onion	5	13
Dried garlic	5	12
Cabbage	6	60
Pepper	6	72
Cucumbers	1	12
Carrots	2	20
Other vegetables	28	180
Bean pods	1	9
Eggplant	2	18
Cauliflower	2	20

Vegetable crops occupy an area of 88 ha with different areas for vegetable species, this fact being due to the crop rotation with diversified productions according to the species and the care work that has been carried out, offering producers an alternative source of income.

Table 3. Areas in melon crops

Culture	Area ha	Tonne production
Melons	60	480
Melons	10	60

Watermelon and melons, occupying an area of 70 ha, due to the climate and favorable soil conditions, offer an average production of 7.7 tons/ha.

Table 4. Surfaces applied with fertilizers

Chemical fertilizers	Area ha	Tonne Quantity
Nitrogen	3178	165
Phosphate	3178	165
Potassium	3178	48
Natural fertilizers	15	300

The natural and chemical fertilizers applied, as can be seen from the table and graphs above, are quantitatively well below the needs of crop plants, resulting in an average of 50 kg s.c./ha according to the statistical data provided by the agricultural chamber of Cujmir.

3.4. Agriculture in 2024

Table 5. Cultivated areas and cereal crop yields

Culture	Area ha	Tonne production
Autumn wheat	1560	9360
Barley	40	200
Corn kernels	1000	8000
Autumn barley	70	420
Spring oats	8	0
Sunflower	70	175
Rape	300	1200
Dried peas	260	390

As can be seen from the table and figures above, the main cereal crops cultivated in 2024 are winter wheat with 1560 ha and a total production of 9360 tons, which represents an average production per hectare of 6000 kg/ha, a higher production than in 2023. Corn is in 2nd place with a cultivated area of 1000 ha with a total production of 8000 tons, which represents an average production of 8 tons/ha, a lower production than in previous years. This is due to adverse weather conditions. This is followed by sunflower on an area of 70 ha and a total production of 175 tons, which translates into an average production of 2500 kg/ha, then we find oats, barley and barley in different areas, and this year rapeseed enters cultivation on an area of 300 ha, with a total production of 1200 tons, which means an average production of 4 t/ha. In relation to pea crops, along with early and summer potatoes, the cultivated areas occupy a fairly large area, peas occupy an area of 260 ha with an average production of 1.5 tons/ha, and potatoes are found on 4 hectares with an average production of 4t/ha. The productions of these crops are close to 2023, due to the lack of rainfall

Table 6. Areas in vegetable crops

Culture	Area ha	Tonne production
Early and semi-early potatoes	1	4
Summer potatoes	3	11
Tomato	40	160
Dried onion	5	13
Dried garlic	5	10
Cabbage	5	50
Pepper	5	50
Cucumbers	3	36
Carrots	2	20
Other vegetables	25	150
Bean pods	1	8
Eggplant	2	18
Cauliflower	1	10
Pea pods	1	7
Courgette	1	5
Sugar corn	1	3

Vegetable crops occupy an area of 97 ha, with different areas for vegetable species, this is due to the rotation of crops with diversified productions, in 2024 there will also be sugar corn per 1 ha, with an average production of 3t/ha. Depending on the species and the care work that has been carried out, it provides producers with a complementary source of income.

Table 7. Areas in melon crops

Culture	Area ha	Tonne production
Melons	50	500
Melons	10	60

Watermelon occupying an area of 60 ha, due to the climate and favorable soil conditions, offers an average production of 9.3 tons/ha.

Table 8. Surfaces applied with fertilizers

Chemical fertilizers	Area ha	Tonne Quantity
Nitrogen	3178	165
Phosphate	3178	165
Potassium	3178	48
Natural fertilizers	15	300

The natural and chemical fertilizers applied, as can be seen from the table and graphs above, are quantitatively well below the needs of crop plants, resulting in an average of 50 kg s.c./ha according to the statistical data provided by the agricultural chamber of Cujmir.

Conclusions

The study on agriculture in Cujmir commune highlights several major aspects:

1. The crop structure is dominated by wheat, corn and rapeseed, which are the main field crops of the area.
2. Yields vary significantly between years, influenced by adverse climatic conditions and insufficient fertilisation.
3. Agricultural diversity is supported by the presence of vegetable crops and melons, which provide farmers with complementary sources of income.
4. The level of fertilization (on average 50 kg s.a./ha) is below the optimal requirement, which limits the production potential.
5. Local agriculture is characterised by a combination of subsistence farms and commercial family farms, and sustainable development involves investing in modern technologies, increasing fertilisation and adapting crops to climate change.

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NOT FINALIZED

CHARACTERIZATION OF NEW PEPTAIBIOTICS IN MONGOLIAN *TRICHODERMA* ISOLATES

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Abstract

Members of the genus *Trichoderma* are commonly found in soil, promoting plants by enhancing their growth. Many species of *Trichoderma* are considered beneficial for plants and are extensively applied in agriculture as important biological agents. *Trichoderma* species are the main producers of peptaibiotics, a group of bioactive secondary metabolites. This study revealed the peptaibiotic production of *T. citrinoviride* isolates from Mongolian natural litter sources. Using an optimized HPLC coupled with a high-resolution mass spectrometry, we identified 19- and 20-residue peptaibols, as well as 7-residue lipopeptaibols. Certain detected compounds showed strong similarity to previously reported peptaibols, including newly found compounds, while all 19-residue peptaibols appear to represent novel compounds. These were named as brevilongibrachins, differing from longibrachins by a missing Gln residue at the C-terminus. The lipopeptaibols were similar to the previously reported Trichobrachin III B a, however, the masses of N-termini are $\Delta m/z$ 182, 196, 208, 210, 22, and 224 Da, pointing to branched or hydroxylated acyl chains. This indicates that these lipopeptaibols belong to a new group or subgroup of peptaibiotics. These findings highlight the metabolic potential of Mongolian *Trichoderma* isolates and expand the current knowledge of fungal peptaibiotic diversity. This study also enables future research activities to be conducted for specific bioactivity tests with purified peptaibiotic compounds.

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CHARACTERIZATION AND APPLICATION OF STARCH/CHITOSAN-BASED FILM INCORPORATED WITH VANILLIN FOR ACTIVE FOOD PACKAGING

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Abstract

Starch-based films are increasingly recognized as an environmentally sustainable substitute for petroleum-based packaging materials, owing to their biodegradable nature, renewability. This research aimed to characterize the starch/chitosan-based film incorporated with vanillin compound through their biological activity and physical-mechanical properties and application for fruit preservation. The antimicrobial activity of starch/vanillin film effectively showed inhibition against *Escherichia coli*, *Staphylococcus aureus*, *Salmonella enterica*, *Bacillus subtilis* and *Listeria monocytogenes* between 12% and 44%. The physical-mechanical-chemical analysis demonstrated that chitosan can increase the film hardness and time of elongation. Moreover, differential scanning calorimetry, thermogravimetry, and X-ray powder diffraction indicated that starch/chitosan/vanillin films were thermally stable at elevated temperatures up to 250 °C and the vanillin became amorphous during the casting process. Scanning electron microscopy revealed that the vanillin-incorporated films exhibited a smoother and denser surface relative to the control. Furthermore, the application of starch/chitosan/vanillin films as strawberry coatings and packaging materials significantly reduced the total bacterial load after 8 and 16 days of storage, respectively. The bioactive films developed in this study present a promising basis for the advancement of consumer-oriented food preservation technologies. This research was supported by the projects HUN-REN 2001007, TKP2021-EGA-28 and EU Horizon 2020 739593.

SYNTHESIS AND CHARACTERIZATION OF PROMOTED Fe_3O_4 CATALYSTS FOR CO_2 REDUCTION

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Abstract

Anthropogenic carbon dioxide (CO_2) released into the atmosphere can both be considered a wasted raw material and a greenhouse gas. CO_2 is very stable, which means it accumulates in the atmosphere. It can be chemically converted, making it a useful raw material for the chemical industry. One such solution is the reaction of carbon dioxide with hydrogen, which produces carbon monoxide and methane, as well as liquid hydrocarbons. Due to the stability of CO_2 , we must utilise catalysts to activate it chemically. Iron-based catalysts, which have been modified to have high carbon dioxide conversion and good selectivity, can provide an effective and inexpensive solution.

Our research group has previously demonstrated in publications that modified iron oxide catalysts are well suited for CO_2 hydrogenation reactions [1,2]. In this study, we characterized mixed iron oxide catalysts impregnated with various metals (K, Mg, Mn, Na, Zn) and examined their catalytic performance. The prepared samples were characterized using XRD, TEM, H_2 -TPR, and CO_2 -TPD technologies. The reaction was carried out in a high-pressure (30 bar) tubular reactor. Gas chromatography was used to analyze the products of the catalytic reactions. The K- Fe_3O_4 sample gave the highest CO_2 conversion value (40.03%) and the highest C_{5+} hydrocarbon selectivity (36.61%), while the Zn- Fe_3O_4 sample had the lowest CO selectivity (2.01%). *In situ* DRIFTS measurements showed, that in case of all five catalysts the reaction pathway were identical. 'Quasi' *in situ* XPS was utilised in order to gain insight regarding the oxidation states of the surface metals. The samples were measured in pretreated state and after reaction. Following reduction all samples showed to consist of metallic iron. After reaction the composition of surface metals were dependant on the promoter used [3,4].

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FORMULATION OF FUNCTIONAL ORANGE JELLIES ENRICHED WITH ROSEHIP POWDER

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Abstract

The contemporary food industry increasingly focuses on developing functional products that meet consumer demand for a healthy and balanced diet. This study aimed to develop healthier orange jelly formulations by incorporating rosehip powder (RP), a valuable unconventional ingredient rich in bioactive compounds. In this study, RP was incorporated into a conventional orange juice jelly recipe at concentrations of 0% (control), 2%, 4%, and 6% (w/w). Both the rosehip powder and the resulting jelly formulations were analyzed for total phenolic content (TPC), total flavonoid content (TFC), vitamin C, and antioxidant capacity, expressed as ferric reducing antioxidant power (FRAP), as key indicators of their functional properties. The rosehip powder exhibited high levels of total phenolic content (TPC: 2015.89 mg GAE/100 g d.w.), total flavonoids (TFC: 1280.42 mg QE/100 g d.w.), vitamin C (992.71 mg/100 g d.w.), and antioxidant capacity measured as FRAP (469.38 μ M Fe²⁺/g d.w.). By supplementing orange jelly with RP at levels of 2%, 4%, and 6%, increases of 8.93%, 17.19%, and 25.81% in TPC, 9.73%, 20.48%, and 28.91% in TFC, 15.88%, 32.34%, and 46.51% in FRAP, and 31.73%, 61.70%, and 87.05% in vitamin C were observed compared to the control. These results indicate that RP is a rich source of polyphenols and vitamin C, substantially contributing to the antioxidant activity and functional properties of food products. In the RP-enriched jelly formulations, levels of bioactive compounds and antioxidant activity increased progressively, reaching their highest values in the 6% RP sample. Overall, the study demonstrates that RP represents a promising functional ingredient for jelly fortification. Its incorporation enhances the antioxidant profile, offering a promising strategy for developing value-added, health-supporting foods.

Key words: rosehip powder; fortified orange jellies; bioactive compounds; functional profile

Introduction

The food industry is increasingly focused on developing functional products that meet consumer demand for healthy nutrition. Gelatin-based confectionery products, such as jellies, are characterized by a soft, translucent, and elastic texture, combined with a sweet and slightly tart taste. Typically made from sugar, glucose syrup, and gelling agents, along with colors, flavors, and acids, jellies offer a unique texture and visual appeal and are enjoyed across all age groups. The color, flavor, and overall sensory quality largely depend on the choice of fruit ingredients, while the firm yet elastic texture is achieved through gelling agents such as agar-agar, pectin, gelatin, gum arabic, or starch [1, 2]. Growing consumer interest in healthy foods has prompted the development of enriched jellies through the incorporation of plant-based ingredients rich in bioactive compounds [2]. Rosehip powder, derived from various *Rosa* species, has attracted attention as a functional ingredient due to its high content of vitamin C, carotenoids, polyphenols, and dietary fiber, which provide antioxidant and anti-inflammatory

benefits [3–6]. It provides both nutritional and technological benefits, enhancing the functional properties of food products [7–9]. Despite its widespread use in bakery products, the application of rosehip powder in jelly formulations remains limited. Jellies can serve as an excellent vehicle for functional ingredients without compromising sensory attributes. Therefore, this study aims to evaluate the effects of incorporating rosehip powder at 0%, 2%, 4%, and 6% (w/w) into an orange juice jelly, focusing on its potential to enhance bioactive compounds, antioxidant capacity, and overall functional properties of the resulting formulations.

Experimental

Preparation of rosehip-enriched jellies

Control jellies were made with 400 mL of orange juice, 20 g of gelatin, and 10 g of sugar. Three formulations of enriched jellies were prepared from the base recipe by adding rosehip powder at 2, 4, or 6% (w/w). Gelatin was hydrated in the juice for 10 minutes, then sugar was added. Each mixture was gently heated to 55 °C to dissolve the gelatin and initiate gelation, then poured into molds and allowed to set at room temperature. Once fully gelled, jellies were removed from the molds and cooled completely. The final products were coded as J (control), J+2%RP, J+4%RP, and J+6%RP. Both RP and jellies were analyzed for total phenolic content (TPC), total flavonoid content (TFC), vitamin C, and antioxidant capacity (FRAP) to assess their functional properties.

Analytical procedures

Preparation of alcoholic extracts for phytochemical and antioxidant analysis. RP and jellies were extracted with 70% ethanol by mixing 0.5 g of sample with 10 mL solvent. The mixture was stirred at room temperature for 2 h and centrifuged at 10,000 rpm for 10 minutes. The residue was re-extracted under the same conditions for an additional 60 minutes [10]. Supernatants from both steps were combined, adjusted to 20 mL with ethanol, and stored at –20 °C in the dark until further analysis of total phenolic and flavonoid contents, as well as antioxidant activity. All extractions were performed in triplicate.

Determination of total phenolic content (TPC). The total phenolic content was assessed using the Folin–Ciocalteu method [11]. Diluted extracts (1:10, v/v) were mixed with Folin–Ciocalteu reagent and sodium carbonate solution, then incubated at 50 °C for 30 minutes. Absorbance was recorded at 750 nm, and TFC was calculated from a gallic acid calibration curve. Results were expressed as mg gallic acid equivalents (GAE) per gram of dry weight.

Evaluation of total flavonoid content (TFC). Flavonoid concentration was assessed using a colorimetric method described by Al-Farsi et al. [12]. Extracts were treated with sodium nitrite, aluminum nitrate, and sodium hydroxide, then diluted to volume with 70% ethanol. After incubation at room temperature, absorbance was measured at 510 nm. Quantification was based on a quercetin calibration curve, and results were expressed as mg quercetin equivalents (QE) per 100 g dry weight of sample.

Determination of vitamin C content. Vitamin C content was determined by titration with 2,6-dichlorophenol-indophenol solution. 1 g of fruit powder was extracted with oxalic acid, filtered, treated with kaolin, and re-filtered to obtain a clear solution. An aliquot was titrated until a persistent pink endpoint appeared. The results were calculated and expressed as mg/100 g dry weight of sample, according to Žlabur et al. [13] with slight modifications.

Antioxidant activity by FRAP assay. The antioxidant capacity of samples was evaluated using the FRAP method, which measures the reduction of ferric (Fe^{3+}) to ferrous (Fe^{2+}) ions, forming a blue Fe^{2+} –TPTZ complex with absorption at 593 nm [14]. Diluted extracts were mixed with FRAP reagent and incubated at 37 °C for 30 minutes. Absorbance was recorded at 593 nm, and

antioxidant activity was calculated from a FeSO_4 calibration curve. Results were expressed as $\mu\text{M Fe}^{2+}$ equivalents per gram dry weight of sample.

Statistical analysis

All results were expressed as mean $\pm$ standard deviation (SD). Differences between jelly samples were evaluated using one-way analysis of variance (ANOVA).

Results and discussion

The characteristics of the rosehip powder used as a functional food ingredient to enhance the antioxidant properties and bioactive compound content of the jellies are presented in Table 1.

Table 1. Bioactive compound content and total antioxidant capacity of rosehip powder

Investigated parameter	Value
TPC (mg GAE/100 g d.w.)	2015.89 ± 3.47
TFC (mg GAE/100 g d.w.)	1280.42 ± 3.12
FRAP ($\mu\text{M Fe}^{2+}/\text{g d.w.}$)	469.38 ± 1.32
Vitamin C (mg/100 g d.w.)	992.71 ± 3.69

The rosehip powder was characterized by a high TPC (2015.89 mg gallic acid equivalents, GAE/100 g d.w.), TFC (1280.42 mg quercetin equivalents, QE/100 g d.w.), vitamin C content (992.71 mg/100 g d.w.), and ferric reducing antioxidant power (FRAP: 469.38 $\mu\text{M Fe}^{2+}/\text{g d.w.}$). These results indicate that RP is a valuable source of polyphenolic compounds in addition to its high vitamin C content. These bioactive compounds contribute significantly to the antioxidant properties of the powder, as reflected by the elevated FRAP value. Thus, RP represents a valuable non-conventional ingredient that can be used to enhance the functional properties of food products. The functional potential of rosehip powder was utilized by incorporating it into an orange juice jelly formulation. The resulting jelly formulations were analyzed for total phenolic content, vitamin C, and antioxidant capacity, as key indicators of their functional profile. The characteristics of the RP-enriched jellies are presented in Figures 1 (TPC, TFC) and Figure 2 (vitamin C and FRAP value).

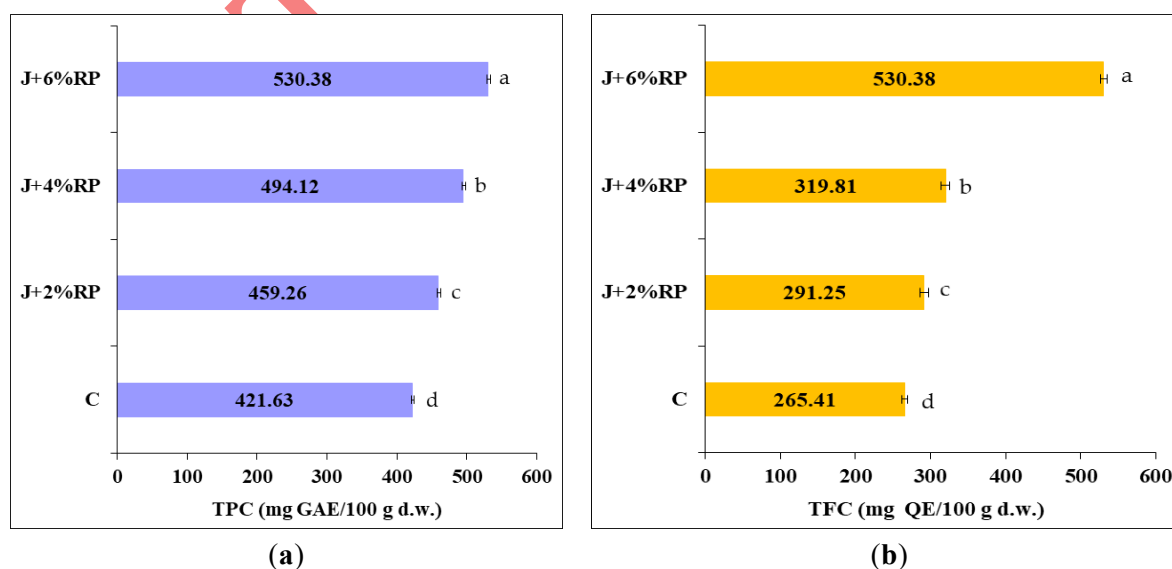


Figure 1. Total phenolic content (a) and total flavonoid content (b) of rosehip powder-enriched jellies compared to the control

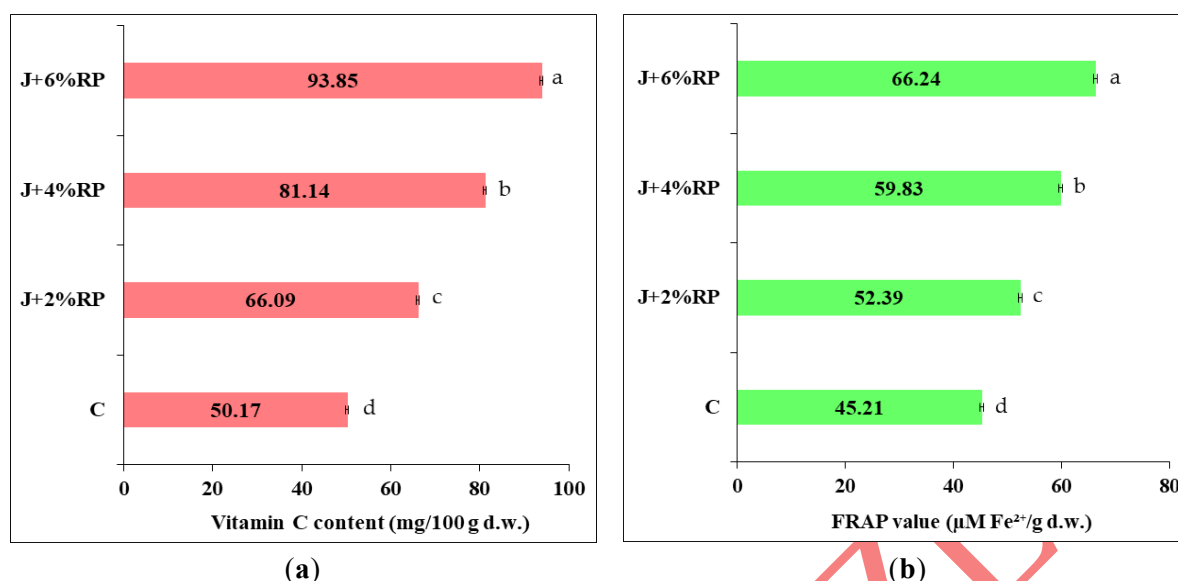


Figure 2. Vitamin C content (a) and total antioxidant capacity (b) of rosehip powder-enriched jellies compared to the control

The results clearly demonstrate that incorporating RP into the orange juice jelly formulation positively influenced its functional properties. The total polyphenol content (TPC) increased progressively with the level of RP: 459.26, 487.32, and 530.38 mg GAE/100 g d.w. for 2%, 4%, and 6% RP, respectively, representing increases of 8.93%, 17.19%, and 25.81% compared to the control (421.63 mg GAE/100 g d.w.). Similarly, the total flavonoid content (TFC) increased from 265.45 mg QE/100 g d.w. in the control to 291.25, 319.83, and 342.19 mg QE/100 g d.w., corresponding to enhancements of 9.73%, 20.48%, and 28.91%. The vitamin C content showed substantial improvements, increasing from 50.17 mg/100 g d.w. in the control to 66.09, 81.14, and 93.85 mg/100 g d.w. in the 2%, 4%, and 6% RP-enriched jellies, respectively, reflecting increases of 31.73%, 61.70%, and 87.05%. The antioxidant capacity also improved significantly with increasing RP levels. FRAP values increased from 45.21 μM Fe²⁺/g d.w. in the control to 52.39, 59.83, and 66.24 μM Fe²⁺/g d.w. in the 2%, 4%, and 6% RP jellies, corresponding to improvements of 15.88%, 32.34%, and 46.51%, highlighting a clear dose-dependent effect. The results indicate that higher RP levels boosted bioactive compounds and antioxidant capacity in the jellies, confirming its role as a valuable functional ingredient.

Conclusion

Rosehips are an accessible and rich source of bioactive compounds, including vitamin C, polyphenols, and antioxidants, making them an ideal functional ingredient for food products. Rosehip powder, due to its pronounced bioactive properties, represents a valuable non-conventional material for enhancing the functional quality of foods. Incorporation of 2%, 4%, and 6% rosehip powder into an orange juice jelly formulation improved its functional profile, with the highest levels of total phenolic content (TPC), total flavonoid content (TFC), vitamin C, and ferric reducing antioxidant power (FRAP) observed at 6% enrichment. Overall, the results confirm that rosehip powder is a promising functional food ingredient for jelly fortification, with potential health benefits through its antioxidant activity.

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CHEMICAL PROPERTIES AND NUTRITIONAL RELEVANCE OF ROMANIAN EDIBLE FOREST FRUITS

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Abstract

A diet rich in fruits and vegetables has long been associated with a reduced risk of degenerative disorders, including cardiovascular diseases and certain types of cancer. Recent research has increasingly focused on the biochemical variability of phenolic compounds and antioxidants naturally present in fruits and vegetables. This variability is influenced by species diversity, applied cultivation or processing technologies, and environmental conditions.

Wild forest fruits are valuable sources of antioxidants and polyphenols, exhibiting multiple biological activities such as antioxidant, anticancer, and anti-inflammatory effects.

The present study aimed to assess the chemical and nutritional parameters of wild raspberry (*Rubus idaeus*) and blackberry (*Rubus discolor*) genotypes collected from native populations in unpolluted areas of Romania.

Keywords: Rubus, forest fruit, blackberry, raspberry, chemical properties,

Introduction

Romania ranks among the richest European countries in plant diversity, owing to its geographical position in South-Eastern Europe and its distinctive ecological, climatic, and geomorphological conditions. Numerous wild-growing species of the genus *Rubus* can also be found in vineyards, large orchards, hedgerows, pastures, as well as in abandoned meadows and other ruderal habitats [1, 2].

Berry fruits are small, fleshy fruits widely consumed both fresh and in processed forms. This category includes red raspberry (*Rubus idaeus*), blackberry (*Rubus spp.*), black raspberry (*Rubus occidentalis*), blueberry (*Vaccinium corymbosum*), and strawberry (*Fragaria × ananassa*). Berries are an excellent source of natural antioxidants and bioactive phenolic compounds, including flavonoids, stilbenes, phenolic acids, and tannins [3], which, individually or in synergy, may contribute to the prevention of cardiovascular disease, cancer, inflammation, obesity, diabetes, and other chronic disorders [1,4,5].

Raspberry (*Rubus idaeus* L.) and blackberry (*Rubus fruticosus* L.) are berry fruits valued for their nutritional content and bioactive properties [6,7]. The fruits are rich in phenolic compounds, flavonoids, and anthocyanins, which provide antioxidant and anti-inflammatory properties, as well as in vitamin C, fiber, and minerals [8, 9].

This paper aims to provide a synthesis of the chemical and nutritional composition of raspberries and blackberries, while also presenting the analytical methods used to determine

these parameters. The main objective is to highlight the potential of these fruits as a source of nutrients, with applications in nutrition and the food industry.

Experimental

In this study all reagents were of analytical grade and were purchased from Merck (Germany), Sigma–Aldrich (Germany) and Fluka.

The sweet berry fruits were collected randomly from the Sibiu county in summer of 2024. The fruits were collected from the forests of Mounts Cindrel area.

The following basic nutritional parameters of harvested fruits were determined: dry matter (total and soluble), moisture, and macronutrients composition (fat, proteins, ash and carbohydrates). Fruit weight has been measured by using a digital balance with a sensitivity of 0.001 g. The moisture of samples has been determined by Sartorius thermobalance. Total solid content can be determined from moisture content as below:

$$\text{Total solids / Dry matter} = 100 - \% \text{ Moisture}$$

Ash content was determined by placing 5-10 g of fruit sample in a crucible in an oven and heating at 500 ± 15 °C.

Total soluble solid contents (TSS) were determined by extracting and mixing one drop of juice from each fruit into a digital refractometer (Model KRÜSS) at 22 °C.

Twenty fruits from each clone (10 fruit per brambles) of each species were used for analysis.

The fruits were examined through standard procedures, for their nutritional chemical composition (fat, proteins, ash and carbohydrates) [10, 11].

Average fruit weight (g) was measured by using a digital balance with a sensitivity of 0.001 g. For moisture content determination, fruit samples were accurately weighed and kept by drying at 103 ± 2 °C until they reached constant weight [11].

The crude protein content ($N \times 6.25$) found in the samples was estimated by the macro-Kjeldahl method. The crude fats were determined by extraction with petroleum ether from a known weight of dried and chopped/grinded fruit, using a Soxhlet extractor. Total carbohydrates were calculated by difference.

Results and discussion

The results of the nutritional characterization of raspberry (*Rubus idaeus*) and blackberry (*Rubus discolor*) fruits are shown in Table 1.

Table 1. Characterization of raspberry and blackberry genotypes fruits in macronutrients

Species		Glucid (g/100g FW)	Lipids (g/100g FW)	Protein (g/100g FW)	Ash (g/100g FW)
<i>Rubus discolor</i>	MBb	13.94 ± 0.89	0.48 ± 0.11	1.19 ± 0.23	0.4 ± 0.12
<i>Rubus idaeus</i>	ZRb	12.07 ± 0.59	0.59 ± 0.13	1.32 ± 0.3	0.37 ± 0.11

ZRb: raspberry genotypes and (*Rubus idaeus*) MBb: blackberry (*Rubus discolor*) genotypes, FW- fresh weight

The most abundant macronutrients found in berry fruits were carbohydrates, followed by proteins. The glucid (carbohydrate) content ranged from 10 % to 15.5%.; *Rubus idaeus* has an average content of 12.07, while *Rubus discolor* shows an average content of 13.5.

Rubus idaeus (ZRb-raspberry variety) has an average content of 12.07%, while *Rubus discolor* (MBb –blackberry variety) shows an average content of 13.94%. The total lipids contents of the berry species were low. The lower fat content was found in *Rubus discolor*. The protein content ranged from 0.76 % (blackberry) to 1.5 % (raspberry). *Raspberry* has an average content proteins of 1.32 %, while blackberry shows an average protein content of 119%. The data obtained in this study are comparable to those in the literature [13, 14]

The physical–chemical characteristics of blackberry and raspberry fruits: fruit weight, moisture, total soluble solids (TSS) and total dry weight (TDW) contents of berry species are given in table 2.

Table 2. Fruit moisture, TDW (total dry weight), weight and TSS (total soluble solids) contents of berry species

Species		Fruit weight (g)	TSS (%)	TDW (%)	Moisture (g/100g FW)
<i>Rubus discolor</i>	MBb	2.31 ± 0.5	12.5 ± 0.78	19.96 ± 2.77	80.04 ± 2.77
<i>Rubus idaeus</i>	ZRb	2.54 ± 0.56	10.6 ± 0.67	22.3 ± 2.43	77.7 ± 2.43

ZRb: raspberry (*Rubus idaeus*) genotypes and MBb: blackberry (*Rubus discolor*) genotypes, TSS: total soluble solids, TDW: total dry matter content weight; FW- fresh weight

The fruit weight of berry species ranged between 1.04 g and 3.3 g, with *Rubus discolor* having the biggest fruit. For the analyzed wild berries, the average weight was 2.31 g for wild blackberries and 2.54 g for wild raspberries. The obtained data are consistent with those reported in the literature [14]. Fruit weight is dependent on the species and the soil. The tested blackberries had a lower weight compared to the tested raspberries, the blackberry dimensions being smaller than those of raspberry fruits.

The average moisture contents of berry fruit species were of 77.7 g/100g raspberry up to 80.04 g/100g blackberry. The results obtained are in close agreement with previously reported data [12, 13, 14].

TSS average values were of 10.6 % (*Rubus idaeus*) to 12.5 % (*Rubus discolor*). With respect to total soluble solids (TSS). The data obtained in this study are comparable to those in the literature [13, 14]. According to these results, raspberry and blackberry fruits may be recommended for fresh fruit production, since they have attractive fruit, and also may be recommended for processing, due to higher TSS and TDW contents.

Conclusion

In the present study, physicochemical investigations have been undertaken in order to reveal the chemical composition, nutritional values of the two *Rubus* species in Romania.

In terms of the physicochemical characteristics of two berry species grown in Romania, inter-species variability was generally greater than intra-species difference. The inter-species differences were found in the fruit weight, and macronutrients content. The *Rubus idaeus* and *Rubus discolor* cultivars showed good characteristics for fresh-eating, since it has attractive fruit, and also may be suitable for processing.

The present indications lead us to the conclusion that this fruit is a potential candidate for bioactivity study as well as functional fruit development.

The results indicate that the studied berry fruits are a valuable horticultural product, based on their rich and beneficial nutrient composition and may be useful in a balanced diet. In addition, this study brings numerous arguments towards the standardization of these fruits as potential healthy foods and their use in food and pharmaceutical industries. For these fruits, determinations of antioxidant content and other bioactive compounds were also carried out; however, these results are not included in the present paper and will be reported in subsequent studies.

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IMPACT OF ESSENTIAL OILS FROM ROMANIAN AROMATIC PLANTS ON MICROBIOLOGICAL QUALITY OF SOFT GOAT CHEESE

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Abstract

Cheeses are traditionally affected by microbiological damage that produces large economic losses. On the one hand, bacteria such as coliforms or butyric bacteria are one of the causes of early and late bloating of cheese. On the other hand, molds are another source of defects in cheese production. They could affect the appearance, flavor, and texture of the cheese, and could even be involved in the development of diseases due to the production of mycotoxins. Available raw milk cheese microbiological control methods are currently expensive, such as bacteriophage or ultrafiltration. This paper set out to provide a natural and alternative way to control these important microbiological defects in cheese through the use of herbal extracts, which are well known for their antimicrobial properties. In order to achieve this objective, it was necessary to analyze the *in vitro* activity of a collection of 5 aromatic plants (*Lavandula officinalis* L., *Ocimum basilicum* L., *Rosmarinus officinalis* L., *Salvia officinalis* L. and *Thymus vulgaris*) in the form of their essential oil (EO) against 8 microorganisms. After evaluating the antimicrobial activity, the plant EOs were added to the milk (2% concentration) intended for the manufacture of soft goat cheese. The processed cheese samples, previously stored at 4° C for 12 days, were analysed for total viable count (TVC), lactic acid bacteria (LAB), enterococci, yeasts and molds.

Introduction

Cheese, a dairy product, resulting as a method of preserving raw milk, many thousands of years ago, is still today one of the most popular foods worldwide, with an estimated production of 19 million tons annually [1]. From a technological point of view, the transformation of milk into cheese is achieved both by a lactic fermentation by the starter cultures, and by the precipitation of casein under the action of rennet, followed then, in the case of many assortments, by the addition of salt and/or maturation of the curd. The contribution of goat's milk production to the economic and nutritional well-being of humanity is undeniable in many developing countries, especially in the Mediterranean countries, the Middle East, Eastern Europe and South America. In developed countries belonging to Europe, Oceania and North America, goat's milk production is gaining increasing economic relevance, especially due to the production of goat cheeses that are properly selected as gourmet foods and receive the highest prices among cheeses on the French and Italian market.

Milk and dairy products, as foods of animal origin, can cause diseases transmissible to humans by consuming them [2]. The microbiological quality of cheese is conditioned by the microbial composition of the milk. The presence of pathogenic microorganisms in milk can be caused by the health status of animals, feed, as well as unsanitized environment and equipment [3,4]. Milk can contain harmful microorganisms, such as fecal coliform bacteria (*Escherichia coli* O157:H7), coagulase-positive staphylococci (*Staphylococcus aureus*), bacteria of the genus

Salmonella, *Listeria monocytogenes*, enterococci (*Yersinia enterocolitica*), anaerobic sporulated bacteria (*Clostridium botulinum*, *Bacillus cereus*), yeasts (*Candida famata*, *C. diffluens*) and molds (*Penicillium* and *Cladosporium*) [5,6,7]. Microbiological contamination of cheeses is a major food safety concern for dairy producers, as milk is an ideal medium for the growth of bacteria and other microorganisms. More recent data from the European Food Safety Authority (EFSA) (2022) indicate that 5.1% of food outbreaks could be attributed to the consumption of contaminated cheese, resulting in 3.4% of cases of food poisoning and 1.5% of hospitalisations [8]. These figures show that, regardless of the technological improvements applied to milk intended for cheese production, the risk of microbial contamination still remains an important problem in both developing and industrialised countries. On the other hand, today's consumers, much more focused on health and well-being, demand foods that are as natural and as unprocessed as possible, without synthetic preservatives, which are often considered harmful and carcinogenic substances [9]. In this sense, medicinal and aromatic plants, long known but partially forgotten, are becoming popular again. Aromatic medicinal plants are defined as plant species whose importance lies in the presence of secondary metabolites (compounds of the terpene class, respectively polyphenols), with specific antioxidant and antimicrobial properties. Romania, due to its geographical position and pedoclimatic conditions, has a diversified flora, containing over 3600 species of superior plants, spontaneous and cultivated, of which 10-12% are used by the local food industry. The purpose of this study was to evaluate the antibacterial activity of five plant extracts (HAE and EO) added to goat cheese. These plants are traditionally used in Romanian gastronomy and have been selected based on literature studies on antimicrobial activity tested *in vitro*.

Experimental

Plant material. Five dried aromatic plants from the western region of Romania (Arad, Caraş-Severin and Timiş counties) were used to test antimicrobial properties in goat cheese production: basil (*Ocimum basilicum* L.), sage (*Salvia officinalis* L.), lavender (*Lavandula officinalis* L.), rosemary (*Rosemarinus officinalis* L.) and thyme (*Thymus vulgaris*). The plants were supplied by commercial producers in October 2024 and stored in dark conditions at room temperature for 1 month before extraction and analysis. The aerial parts were used in all extractions (hydroalcoholic, respectively essential oil).

Extraction of essential oils. The essential oils were obtained by the method of hydrodistillation using a Clevenger apparatus, according to the description of the European Pharmacopoeia (1996). One hundred grams of plant material cut into small fragments were placed in a balloon together with 500 ml of double-distilled water. The mixture was boiled for 3 hours, and the essential oils were separated from the water. After being collected, the oils were dried with sodium sulphate anhydrous and stored in dark vials at 4 °C until use.

GC-MS analysis of essential oils. The chemical composition of the volatile oil samples was performed by gas chromatography analysis coupled with mass spectrometry (GC/MS). The system used was GC/MS QP2010 Plus Shimadzu equipped with AT5MS fused capillary column (30 m x 0.23 mm, 0.15 µm film thickness), with ionization energy of 70 eV, EI detector and supply ionization temperature of 220°C. Temperature gradient was from 50°-250°C (3°C/min). Gas vector Helium at 1 mL/min. Identification was achieved by comparison with published mass spectra and retention indices.

Preparation of goat cheese samples. The goat's milk was purchased from a goat farm in Bihor County, Romania. For milk acidification, freeze-dried mesophilic starter cultures of *Lactococcus lactis* subsp. *lactis* and *Lactococcus lactis* subsp. *Cremoris* were used in proportion of 2% compared to the amount of milk, and for incuration dehydrated calf rennet in the form of tablets purchased on the market. The milk was pasteurized at 65°C for 25 minutes, after which

it was quickly cooled on an ice bath at the inoculation temperature (35°C). Before the addition of the starter culture, a solution of CaCl₂ (0.02 g/L) was added to the milk to achieve a constant clot firmness and to facilitate coagulation. At this point the whole quantity of milk was divided into equal volumes (5L) in 6 sterile valves. Then the rennet solution was added to each container at the same time as the essential oil solutions (3% in sunflower oil). After 90 minutes the clot pieces were cut, dehydrated and salted in 18% sterile brine solution for 6 hours. The ripening period last for 12 days and after that the samples were stored at 4°C in polyethylene bags, for further analysis.

In vitro testing of the antimicrobial activity of plant EOs. The antimicrobial potential of the plant extracts taken in the study was evaluated by a disc diffusion test against 8 bacterial strains of the species: *Salmonella enterica* ser. *Infantis*, *Staphylococcus aureus*, *Listeria monocytogenes*, *Enterococcus faecalis*, *Enterococcus faecium*, *Escherichia coli*, *Clostridium tyrobutiricum*. Lyophilized bacteria were transferred to BHI broth medium (Merck company, Germany) and incubated for 24 h at 37°C and recultured for at least 2 times consecutively.

Microbiological Analyses of goat cheese samples. Cheese samples in the form of serial decimal dilutions were subjected for the determination of total viable count (TVC) [11], lactic acid bacteria (LAB) [12], enterococci [13], yeasts and moulds [14].

Results and discussion

The chemical composition of the 5 volatile oils showed a high heterogeneity, with a total of 121 volatile components (an average of 24 compounds per plant) being identified and classified as monoterpenes (linear, cyclical, aromatic and derivatives), sesquiterpenes and aromatic compounds derived from phenylpropane (Table 1).

Table 1. Distribution of volatile compound groups and relative abundance calculated from GC/MS chromatograms for 5 EO^a

Plant species	N ^b	M (%)					S (%) total	A (%) total	Total (%)
		Linear	Cyclic	Aromatic	Derivate	Total%			
Basil	20	1.4	21.2	72.8	0.2	95.8	2.5	NI	98.1
Sage	23	2.8	73.2	0.1	3.1	79.2	19.7	NI	98.9
Tyme	33	0.5	9.4	63.7	7.9	81.5	13.7	1.6	96.8
Lavender	17	2.8	87.3	2.6	1.2	93.9	4.3	NI	98.2
Rosemary	28	39.7	20.0	3.1	20.7	83.5	8.7	NI	92.2

Note: ^aIdentification by comparison of mass spectra with NIST/ADAMS library data. M, the monoterpene group; S, sesquiterpene group; A, aromatic compound group or phenylpropanoid; NI, unidentified. ^bThe number of compounds identified in each EO.

T. vulgaricus EO had the highest number of identified compounds (33 constituents), accounting for 96.8% of its total composition. L. officinalis EO contained the lowest number of identified compounds, 17 constituents, accounting for 98.2% of the total oil composition. On the other hand, R. Officinalis EO, with 28 volatile compounds, showed the lowest total abundance identified (92.2%), as the number of compounds detected was much higher than the number of identified compounds. Given the chemical structure of the identified volatiles, as expected, the monoterpene group formed most of the EO content, with an average value close to 87%. The main monoterpene subgroups in EO were linear, cyclic and aromatic compounds and derivatives, with cyclic monoterpenes generally predominant over linear and aromatic monoterpenes. The highest level of aromatic monoterpenes (72.8%) was found in O. Basilicum. This subgroup of monoterpenes

represents an important part of the total oil composition of some plant species, such as carvacrol in *O. Basilicum* EO (43.2%) and thymol from *T. vulgaris extract* (58.7%). In the case of derived monoterpenes, only *R. officinalis* oil (20.7%) showed values of more than 20% of the total oil content, being mainly represented by linalyl acetate. Overall, sesquiterpene concentrations were much lower than those of monoterpenes. *S. Officinalis* EO had the highest level of sesquiterpene compounds (19.7%), represented mainly by α -humulene and (*E*)- β -caryophyllene. In relation to the above, the most common compounds in the analyzed EOs were α -pinene, camphene, β -pinene and γ -terpinene belonging to the group of linear monoterpene compounds, with three or even more occurrences.

The *in vitro* antimicrobial properties of the essential oils studied are presented in Table 2.

Table 2. The *in vitro* inhibitory activity of EOs on pathogenic bacteria

	Basil	Sage	Lavender	Rosemary	Thyme
<i>Salmonella Infantis</i> 78	-	26.7 $\pm$ 0.57	-	18.7 $\pm$ 0.5	46.7 $\pm$ 0.33
<i>ermA</i> + <i>S. haemolyticus</i> 422	8.75 $\pm$ 0.5	15.34 $\pm$ 0.54	-	18.2 $\pm$ 0.33	18.72 $\pm$ 0.15
<i>ermC</i> + <i>S. haemolyticus</i> 231	8.12 $\pm$ 0.3	14.71 $\pm$ 0.84	7.7 $\pm$ 0.5	18.7 $\pm$ 0.24	27.12 $\pm$ 0.63
<i>Staphylococcus aureus</i>	15.67 $\pm$ 0.4	30.0 $\pm$ 1.1	12.5 $\pm$ 1.4	14.3 $\pm$ 1.23	30.65 $\pm$ 1.4
<i>Listeria monocytogenes</i>	-	9 $\pm$ 0.8	11 $\pm$ 0.0	14 $\pm$ 0.00	43.30 $\pm$ 1.3
<i>Enterococcus faecalis</i>	9.7 $\pm$ 0.4	25.34 $\pm$ 0.5	11 $\pm$ 0.0	15.6 $\pm$ 0.41	30.62 $\pm$ 1.74
<i>Enterococcus faecium</i>	10.72 $\pm$ 0.6	19.12 $\pm$ 0.5	9.3 $\pm$ 0.3	16.1 $\pm$ 0.33	36.00 $\pm$ 1.53
<i>VR Enterococcus faecium</i>	-	19.00 $\pm$ 0.0	-	11.8 $\pm$ 0.87	-
<i>Escherichia coli</i>	-	24.6 $\pm$ 0.8	15.3 $\pm$ 0.2	12.0 $\pm$ 0.43	28.56 $\pm$ 0.34
<i>C. tyrobutyricum</i>	16.44 $\pm$ 0.7	33.2 $\pm$ 1.6	-	13.0 $\pm$ 0.00	44.75 $\pm$ 0.7

A wide variation was observed in the antimicrobial properties of the analyzed EOs. However, it should be noted that in general, the organisms tested were sensitive to most essential oils and that all of the essential oils tested showed antimicrobial activity against three or more strains of bacteria. Of all the strains used in this study, *S. aureus* was the most sensitive bacterium, being sensitive to all essential oils analyzed, followed by *E. faecium* and *E. faecalis*. Among the essential oils evaluated, the highest efficacy was achieved by thyme oil, which showed activity against all bacterial strains tested. The weaker antimicrobial activity against Gram-negative bacteria compared to Gram-positive bacteria is attributed to the structure of their cell walls, mainly in terms of the presence of lipoproteins and lipopolysaccharides in Gram-negative bacteria that form a barrier against hydrophobic compounds [6,8].

The microbiological quality of soft goat cheese on day 12 is shown in table 3. The results present total viable count (TVC), lactic acid bacteria (LAB), enterococci, and the number of yeasts and molds. Samples of goat cheese supplemented with essential oil were microbiologically safe at the end of the process. Moreover, the addition of essential oils significantly improved the microbiological quality of the cheese compared to the control samples.

Table 3. Values of microorganism populations in goat cheese samples supplemented with essential oils

Parameter (log ₁₀ CFU/g)	Basil	Sage	Lavender	Rosemary	Thyme	Control
TVC	7.06 ± 0.71	7.23 ± 0.19	6.95 ± 0.66	7.08 ± 0.05	7.36 ± 0.28	7.81 ± 0.25
LAB	6.98 ± 0.16	7.18 ± 0.40	6.40 ± 0.47	7.87 ± 0.03	7.45 ± 0.20	7.59 ± 0.22
Enterococi	1.63 ± 0.22	2.45 ± 0.14	1.85 ± 0.45	1.62 ± 0.21 ^c	1.42 ± 0.76	2.53 ± 0.11
Yeasts & Molds	1.23 ± 0.12	1.74 ± 1.19	2.21 ± 1.47	3.00 ± 0.00	3.09 ± 0.58	3.43 ± 0.10

Although the differences are small, the addition of lavender essential oil showed the best antibacterial activity ($p < 0.05$) when taken into account TVC and LAB count. On the other hand, the use of thyme EO showed the opposite effect on these populations, but significantly reduced the number of enterococci compared to others.

Conclusion

Incorporating aromatic plants EOs directly into the milk (2% concentration) intended for the manufacture of soft goat cheese may prove beneficial for enhancing its self life. Our study demonstrated the antimicrobial potential of basil (*Ocimum basilicum* L.), sage (*Salvia officinalis* L.) lavender (*Lavandula officinalis* L.), rosemary (*Rosmarinus officinalis* L.), and thyme (*Thymus vulgaris*) when added to goat cheese as EOs.

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EXOTIC FRUIT JAM – SENSORY AND PHYSICOCHEMICAL CHARACTERIZATION

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Abstract

The present study aims to highlight the sensory and physicochemical characteristics of three different types of jam made from exotic fruits: mango jam, pineapple jam, and mango–pineapple jam with added ginger, thus emphasizing the properties and qualities of these products. The preparation method for each jam variety is described, focusing on the development of natural and healthy products with distinct flavors imparted by the selected ingredients. The mango jam, pineapple jam, and the mango–pineapple jam with added ginger were subjected to sensory evaluation by a panel of 10 assessors. The evaluated attributes included appearance, color, consistency, aroma, and taste. The results of the evaluation showed that the mango–pineapple jam enriched with ginger was the most appreciated variety, due to the harmonious balance between flavor and texture. The physicochemical analyses focused on determining acidity, vitamin C content, and sugar content. Among the three samples, the mango–pineapple jam with added ginger exhibited the highest acidity (0.48%) and the highest vitamin C content (1338.85 mg/L), while the mango jam stood out for having the highest sugar content (74.6 °Brix).

Keywords: exotic fruit jam, fruit preserves, functional food, vitamin C content, ginger additive

Introduction

Jam is a traditional product obtained by preserving fruits in sugar and is appreciated for its pleasant taste and nutritional values [1,2]. In recent years, interest in jams made from exotic fruits has significantly increased due to their unique flavors and nutritional benefits [3]. From a nutritional perspective, jam provides energy because of its high sugar content, and by adding certain ingredients such as spices or exotic fruits, it can offer additional benefits owing to its bioactive compounds and antioxidants [4]. Ripe mango fruit is highly aromatic and sweet, with an orange-reddish color, providing an exceptionally high content of vitamins (A, C, E, B6, K), antioxidants, fibers, pectins, starch, Omega-3 and Omega-6 fatty acids, as well as copper (Cu) and zinc (Zn). Moreover, mango contains 17 amino acids, including essential ones involved in protein synthesis and various metabolic processes [5]. Pineapple is a tropical fruit valued for its sweet and sour flavor and juicy texture. It is an important source of vitamin C, manganese, dietary fibers, and the enzyme bromelain, which has anti-inflammatory properties and aids digestion. Additionally, pineapple is rich in antioxidants and bioactive compounds that contribute to overall health [6,7]. Ginger is an aromatic root widely used in both cuisine and traditional medicine, known for its anti-inflammatory, antioxidant, and digestive properties. This rhizome is rich in bioactive compounds such as gingerols, which provide beneficial effects

on the immune system, help reduce nausea symptoms, and support digestive health [8]. These innovations introduced to traditional jam recipes respond to current consumer preferences for tasty and distinct products that are also functional from a nutritional standpoint.

Experimental

2.1 Materials

The raw and auxiliary materials used for the preparation of the jams were purchased from supermarkets and included mango, pineapple, lemons, ginger, and still (non-carbonated) water. Three types of jams were produced as follows: mango jam, pineapple jam, and mango–pineapple jam with added ginger. The recipes for each variety were adapted to ensure a balanced combination of fruits, sugar, lemon juice, and ginger, following traditional boiling and preservation methods.

2.2 Methods

The sensory analysis of the samples was performed using a scoring method by a panel of 10 evaluators. The sensory attributes assessed included appearance, consistency and shape retention, taste, and aroma. A maximum score of 5 points was assigned for each attribute. Physicochemical analyses were conducted to determine acidity (by titration with 0.1 N NaOH solution), vitamin C content (using the iodometric method), and sugar content (measured in degrees Brix with a refractometer). All determinations were performed in triplicate to ensure the accuracy and reliability of the results.

Results and discussion

The sensory analysis conducted with a panel of 10 evaluators highlighted the preferences for the three tested jam variants. Mango jam and the combined mango–pineapple jam with ginger were the most appreciated by the panelists, especially for taste (4.6 and 4.8, respectively) and aroma (4.4 and 4.6), receiving average scores above 4.5 points. Mango jam received a slightly lower score for consistency (4.2) compared to the combined jam variant (4.4), while pineapple jam was less uniformly appreciated, particularly for taste (4.1) and aroma (4.0). Overall, the jam with added ginger stood out as the highest rated, due to its fine balance between flavor and texture.

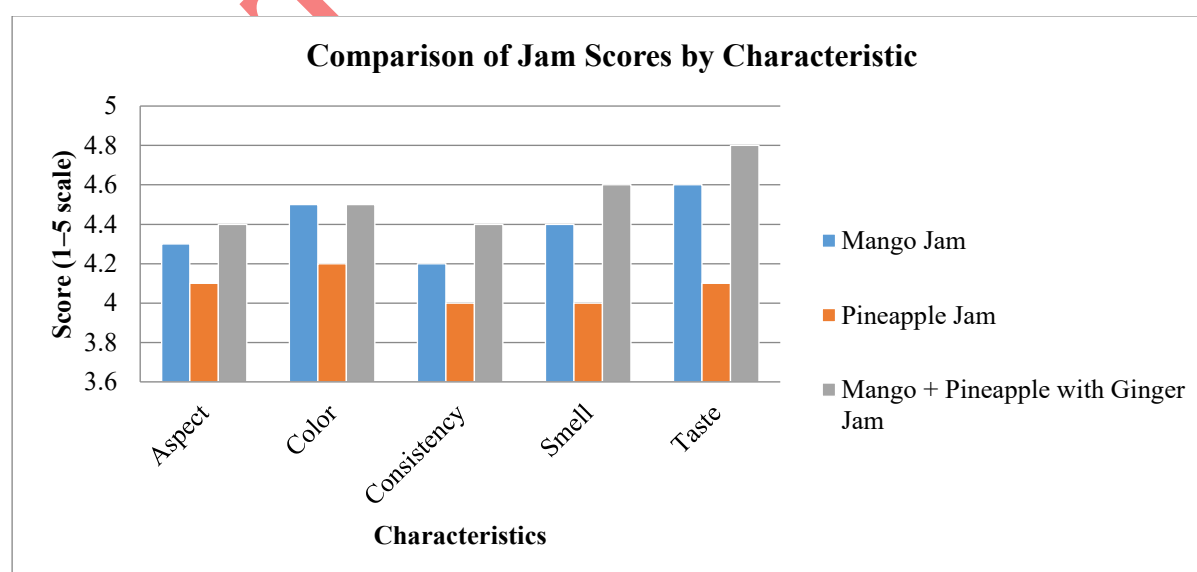


Figure 1. Sensory characterization of mango, pineapple, mango and pineapple with ginger jams

The results of the physicochemical analyses performed on the three jam variants—mango, pineapple, and mango and pineapple with added ginger—are presented in the table below, highlighting key parameters such as total acidity, refractive index, vitamin C content, and sugar concentration.

Table 1. The results of the physicochemical analyses for the three jam variants

Characteristics	Mango Jam	Pineapple Jam	Mango + Pineapple + Ginger Jam
Total acidity (%)	0,32	0,37	0,49
Refractive index	1,4672	1,4595	1,4575
Vitamin C (mg/L)	903,67	832,16	1339,73
Sugar content (°Brix)	74,9	71,8	71,2

Conclusion

Products in the jam category are appreciated for their pleasant taste and extended shelf life, but their sensory and nutritional qualities can vary significantly depending on the fruit composition as well as the additional ingredients used. This study aimed to characterize the sensory and physicochemical properties of three types of jam with different recipes and compositions: mango jam, pineapple jam, and a mixed variant with added ginger. The sensory analysis highlighted that the most appreciated variant was the mango–pineapple jam with added ginger, which recorded the highest overall average score of 4.74 points. This variant was particularly distinguished by its taste (4.8 points) and aroma (4.6 points), followed by the mango jam, which achieved a general score of 4.4 points. The pineapple jam was less favored, obtaining an average total score of 4.08 points, mainly due to lower ratings for taste (4.1) and aroma (4.0). Comparison of the physicochemical parameters of the three jam types revealed significant differences, although all samples fell within accepted limits. Total acidity ranged between 0.32% (mango jam) and 0.49% (ginger-added variant), while sugar content ranged from 71.2 °Brix to 74.9 °Brix, with the highest sugar content recorded in mango jam. Vitamin C content was significantly higher in the ginger-containing jam (1339.73 mg/L), suggesting an increased nutritional value due to the addition of ginger. The results indicate that among the three varieties, the jam with added ginger was the most appreciated sensorially and exhibited a higher concentration of vitamin C, an important bioactive compound, which suggests the potential of this variant as a functional food product.

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NOT FINALIZED

FROM LABORATORY TO SEMI-PILOT SCALE: FISCHER-TROPSCH SYNTHESIS OVER A Na-Fe₃O₄ CATALYST FOR E-FUEL APPLICATIONS

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Abstract

The net-zero commitments adopted by many countries require decisive steps to reduce reliance on fossil fuels. While electrification offers a pathway for several sectors, “hard-to-abate” areas such as aviation, international shipping, and heavy industry will continue to rely on liquid fuels, which must be produced from renewable or low-carbon sources. Among the emerging solutions, e-fuels produced from green hydrogen and captured carbon dioxide are considered a promising alternative.

At the Energy Innovation Test Station of the University of Szeged, renewable energy is used to generate hydrogen, which is subsequently converted into synthetic fuels via Fischer-Tropsch Synthesis (FTS). In this context, we scaled up a 1 wt% Na-Fe₃O₄ catalyst, shown to operate well at the laboratory scale, and tested it under semi-pilot conditions more representative of industrial implementation. The catalyst showed high activity, selectivity toward C₅₊ hydrocarbons, and stable performance across multiple regeneration cycles, confirming both its scalability and sustainability for future e-fuel production.

Introduction

Global demand for aviation fuels continues to rise in line with air travel growth. According to the International Energy Outlook 2023, jet-fuel consumption is projected to increase significantly even as demand for gasoline declines [1]. At the same time, aviation sector accounted for approximately 2.5 % of global CO₂ emissions in 2023, highlighting its non-negligible contribution to climate change [2]. Today, most jet fuels are derived from crude oil, and the corresponding CO₂ emissions greatly contribute to the global carbon footprint. Given the urgency of limiting greenhouse gas emissions and the finite nature of fossil reserves, there is a growing imperative to explore sustainable, low-carbon alternatives. While road transportation can gradually shift toward electrification or biofuels, aviation faces stricter constraints: jet fuels must meet precise compositional and performance standards (e.g. Jet A-1), which limits the feasible substitution pathways.

FTS is a promising gas-to-liquid (GTL) technology for producing synthetic hydrocarbon fuels via syngas (CO + H₂) conversion. When combined with a downstream reverse water gas shift (RWGS) reaction to generate CO, and supplied with green hydrogen, FTS can function as a carbon-recycling platform. In this configuration, synthetic fuel production is effectively decoupled from fossil feedstocks, offering a viable route to reduce the net carbon footprint of the transport and energy sectors.

Fe and Co catalysts are most commonly used in industrial FTS. Among Fe catalysts, Na-promoted Fe₃O₄ (Na-Fe₃O₄) has been extensively studied: the alkali promotion enhances CO dissociation preserving the carbide phase which is active for both FTS and water-gas-shift (WGS) reactions, thus increasing activity and selectivity toward longer-chain hydrocarbons [3] However, most performance studies of the Na-Fe₃O₄ have been confined to lab scale; scaling such catalysts toward industrially relevant scales remains a critical challenge.

Within the framework of the RRF-2.3.1-21-2022-00009 project *National Laboratory for Renewable Energy*, supported by the EU Recovery and Resilience Facility, we successfully scaled up a 1 wt % Na-Fe₃O₄ catalyst by a factor of 20 and tested it at semi-pilot plant level (TRL 4). The scaled-up experiments were conducted in a five-reactor test station capable of producing 1-2 kg of liquid hydrocarbons per day, using hydrogen supplied from solar-powered electrolysis.

Experimental

Catalyst preparation

Pure Fe₃O₄ catalysts were synthesized by the coprecipitation method [4]. The iron salts were dissolved in dilute HCl, and precipitation was carried out by adding aqueous NH₄OH under vigorous stirring until alkaline conditions were reached. The suspension was aged at elevated temperature, then the solid was separated, washed, and dried. Na-promoted catalysts (1 wt%) were obtained by the wet impregnation using an aqueous NaNO₃ solution, followed by sonication, solvent removal, drying, and calcination under inert atmosphere. The product was pressed, crushed, and sieved to the desired particle size for testing. For the larger-scale (90 g) batch, the same procedure was applied with adjusted reagent amounts, and the pellet size was increased accordingly for up-scale experiments.

Characterization

XRD studies of the samples were performed on a Rigaku MiniFlex II instrument with a Ni-filtered CuK_α source in the range of $2\theta = 20-100^\circ$.

The specific surface area (BET method) was determined by the BJH method using a Quantachrome NOVA 2200 gas sorption analyzer by N₂ gas adsorption/desorption at 77 K. Before the measurements, the samples were stored in vacuum (<0.1 mbar) at 473 K for 2 hours. To assess the Na content of the prepared catalysts, a Thermo Scientific Apreo 2 scanning electron microscope was used. Prior to the study, the samples were mounted on electrically conductive carbon tape, and then a thin layer of gold was evaporated onto their surface to prevent charge accumulation due to electron irradiation.

Catalytic activity tests

The catalysts were tested at two different scales: laboratory scale (TRL1) and semi-pilot plant scale (TRL4). The Fischer-Tropsch reactions were performed in a steel, fixed-bed, continuous-flow reactor. Prior to each reaction, the catalysts were first heated to 400 °C under an inert atmosphere and subsequently pretreated in pure hydrogen for 16 h. After the pretreatment, the reactors were cooled to 300 °C, and the feed gas mixture consisting of CO and H₂ was introduced under the following common conditions: pressure 30 bar, temperature 300 °C, H₂/CO ratio of 2, and a gas hourly space velocity (GHSV) of 2700 mL g⁻¹ h⁻¹.

At the TRL1, the reactor parameters were as following: outer diameter was 2 cm and length was 36 cm. The temperature of the reactor was maintained by a digital temperature controller and an electric heating stove. A total of 2 g of catalyst was loaded into the reactor, positioned between quartz wool plugs, while the remaining void space was filled with quartz beads. The reaction time was 5 h.

At the TRL4, the reactor had a length of 115 cm and an outer diameter of 3.5 cm, equipped with five heating zones and monitored by six external and six internal thermocouples. A total of 70 g of catalyst mixed with SiC in different ratios was loaded into the reactor to account for the heat dissipation. The reaction was carried out for 76 h under otherwise identical conditions.

Results and discussion

Both the small-scale (TRL1) and the up-scaled (TRL4) Na-Fe₃O₄ catalyst batches were successfully synthesized and characterized by XRD, BET, and SEM-EDS measurements. The up-scaled sample preserved the structural and textural properties of the small batch, confirming the scalability of the synthesis method (**Fig. 1a**).

XRD patterns showed only reflections corresponding to Fe₃O₄, indicating phase purity and the absence of undesirable crystalline by-products (**Fig. 1b**). SEM-EDS mapping revealed a homogeneous distribution of Na across the catalyst surface, with a loading close to the nominal 1 wt% in both cases (*data not shown*).

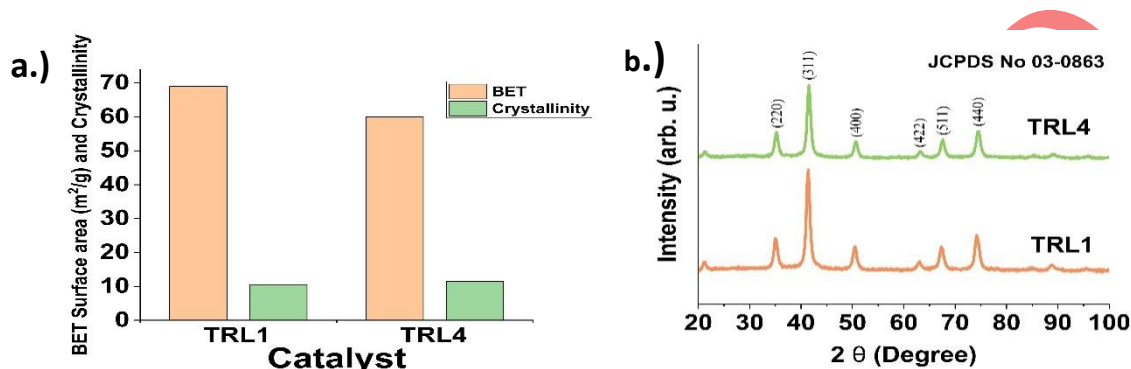


Figure 1. Structural and textural properties of TRL1 and TRL4 batches of Na-Fe₃O₄ catalyst: a) BET surface area and crystallinity (calculated from XRD); b) XRD patterns of freshly-prepared samples

The FTS catalytic activity of both batches was assessed under identical reaction conditions with 2 g of catalyst and 5 h reaction time at the lab-scale and 70 g of catalyst and 76 h reaction time at the up-scale.

In both cases the CO conversion was very high (> 90%) indicative of the catalyst efficiency. In the up-scaled system, the concentration of undesired gases (CO₂ and CH₄) was slightly lower, which can be attributed to the stabilization of the active iron carbide phase during long-term operation and possibly more uniform Na promoter effect.

The collected in a cold trap liquid hydrocarbon product was analyzed offline with the GC-MS (**Fig. 2**). In contrast to the lab-scale, the TRL4 batch produced predominantly linear-chain hydrocarbons dominated by olefins. The longer reaction time and the larger catalyst bed most probably promote steady-state operation and favor chain-growth mechanisms over secondary transformations, which can account for the observed differences. Due to the presence of Na, the catalyst surface was rich in C* species and poor in H* species. The lower surface ratio of H*/C* is also favorable for the growing chain termination via β -hydride abstraction rather than hydrogenation, which explains high selectivity towards olefins. [5]

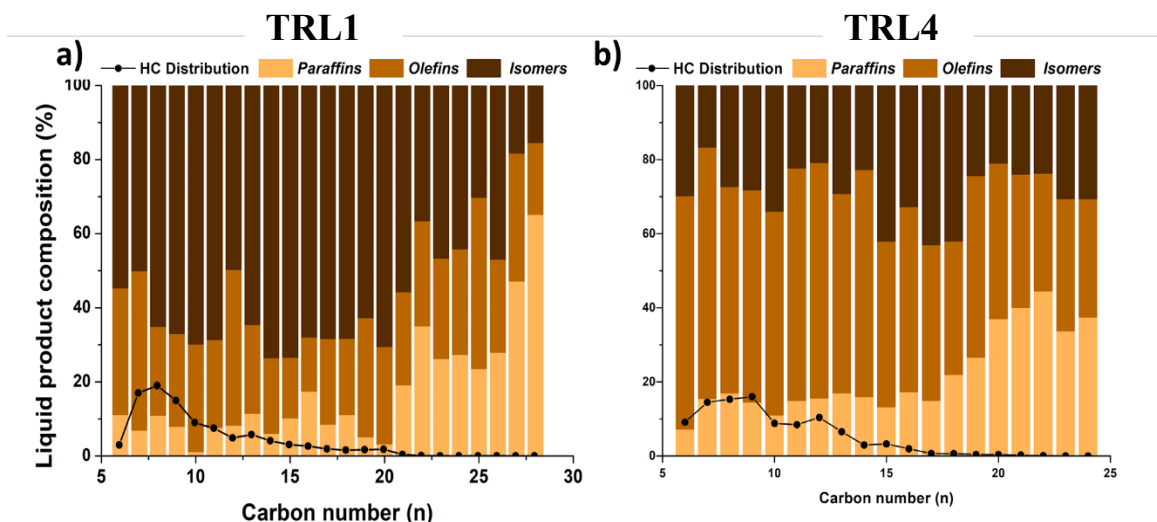


Figure 2. Hydrocarbon distribution for a) TRL1 batch; b) TRL4 batch

After verifying the proof of concept at TRL 4, the long-term stability and reusability of the Na-Fe₃O₄ catalyst were also investigated. Following the initial run (76 h), the catalyst was regenerated by reactivation in H₂ (16 h at 400 °C) and subjected to a second catalytic cycle (74 h). The procedure was repeated once more for a third run (68 h).

The space-time yield (STY) of collected liquid hydrocarbons, expressed as grams of product per gram of catalyst per hour, was determined after each cycle to directly assess and compare the catalyst performance. The calculated values were 148, 129, and 132 mg g⁻¹ cat h⁻¹ for runs I-III, respectively.

Conclusion

Overall, the catalytic results demonstrate that up-scaling the Na-Fe₃O₄ catalyst from TRL1 to TRL4 preserved both high activity and C₅₊ product selectivity. Moreover, the catalyst exhibited stable efficiency over three regeneration cycles, during which a total of ~1 L of liquid hydrocarbons was collected. These findings underline the scalability and sustainability of the system. Future work will focus on optimizing reaction parameters and catalyst loading, and on further scale-up toward production capacities of 5 L and 20 L.

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NOT FINALIZED

PERFORMANCE COMPARISON OF TWO SUBSTRATE-BASED APPROACHES FOR LIQUID LIBS ANALYSIS: NANOPOROUS GLASS vs. Si-WAFER

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Laser-induced breakdown spectroscopy (LIBS) is a powerful and increasingly popular analytical technique in the field of atomic spectroscopy due to its straight-forward, yet versatile operation. In principle, LIBS is capable of analyzing gas, liquid and solid samples, as well as aerosols. In practice, however, the analysis of bulk liquid samples is rather challenging due to their mechanical, thermal, and optical properties which result in unreliable laser coupling, problematic light collection, and the of formation cold, faint plasmas. To bypass these issues, several methodologies have been proposed in the literature. Some of them – among many – involve transforming the bulk liquid sample into different shapes such as liquid jets, aerosols, while others rely on liquid-to-solid transformation e.g. freezing or drying [1].

One of the simplest and widely used techniques is when a small droplet of the aqueous sample is dried onto a chemically pure, nonporous, plane substrate (e.g. Si-wafer), creating a solid residue on the surface which then serves as the target for the LIBS measurements. This approach is low-cost, easy to execute and facilitates a highly sensitive detection, resulting in ppb-level LODs. However, it has a few drawbacks as well, such as the high sensitivity to matrix effects, limited dynamic range, and low reproducibility due to the random distribution of residue caused by the coffee-ring effect [2]. Recently, our group has proposed a simple and effective alternative to tackle the very same problem, relying on the use of nanoporous glass (NPG) substrates. In this approach, a small droplet of the sample solution is placed on a piece of NPG that rapidly absorbs the sample, creating a homogeneous analyte distribution inside the pores near the top surface of the glass. The NPG is then dried and serves as the laser target [3].

In this study, we compare the analytical performance of the two approaches in several regards such as precision, reproducibility, dynamic range, sensitivity (LOD), compatibility, and practicality.

Acknowledgements

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STAINLESS STEEL-BASED ELECTROCATALYSTS FOR SULFITE OXIDATION IN ALKALINE MEDIA

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Sulfites are a secondary product resulting from a lot of industrial processes, such as the combustion of fossil fuels, especially solid fuels. These processes lead to increasing level of pollution. Due to their very strong reducing character, the elimination of sulfites in the environment profoundly affects the fauna and flora of the environment, which is why it is necessary to "neutralize" this category of pollutants. The simplest method of eliminating the negative effects of sulphite ions is their oxidation to sulfate, a process that can be carried out chemically or electrochemically. To reduce the costs related to the oxidation of sulfites, their use as an anodic depolarizer in sulfite/air fuel cells has been proposed. In such a fuel cell, the oxidation of sulfite to sulfate (1) takes place at the anode, while the reduction of oxygen takes place at the cathode.

The electrochemical oxidation of tetravalent sulfur compounds, S(IV), containing oxygen, such as $\text{SO}_2(\text{aq})$, HSO_3^- and SO_3^{2-} , has attracted attention in the development of hydrogen production and fuel cell technologies. In the anodic reaction, the most attractive catalysts are precious metals due to their electrocatalytic properties for the oxidation of these sulfur compounds. Given the high price of these metals, some non-precious metal and carbon-based catalysts have been investigated to reduce costs. Over time, several reaction mechanisms have been proposed, but the oxidation process of these compounds is currently unclear, being considered a complex transformation. Studies on this process have shown that the electrochemical oxidation mechanism of sulfite depends on the anode material, the pH and composition of the solution, and the current density.

In our experimental studies a cell connected to the potentiostat/galvanostat SP 150 Bio-Logic was used during all experiments. The working electrode was a bar of different stainless steel with an active surface of minimum 0.2 cm^2 . Two graphite bars were used as counter electrodes and Ag/AgCl as the reference electrode. Hydroxide de sodium NaOH and sodium sulfite Na_2SO_3 were used to prepare the electrolyte solution.

Cyclic voltammograms, plotted on stainless steel, in 1 mol L^{-1} NaOH solution, at different sulfite concentrations between 10^{-3}M and 1M , highlighted the peaks characteristic of sulfite ion oxidation. At higher anodic potentials, oxygen evolution occurs. The kinetic parameters (exchange current i_o and anodic transfer coefficient α) were determined by the potentiodynamic polarization method. The obtained values were comparable to those reported in the literature on noble metals, which opens the possibility of stainless steel being used as an anode in a sulfite/air fuel cell. The results obtained by potentiodynamic polarization were confirmed by electrochemical impedance spectroscopy.

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OBTAINING AND CHARACTERIZATION OF TiO₂ BY DIP COATING FOR UV-BLOCKING APPLICATIONS

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Abstract

This study reports on the synthesis and characterization of thin films of titanium dioxide (TiO₂) with a focus on their ultraviolet (UV) blocking properties. The thin films were obtained through a sol-gel method, deposited by dip-coating, and subsequently annealed to enhance structural and optical properties. Various precursor solutions, solvents, and deposition speeds were investigated to optimize film quality. The films were analyzed using X-ray diffraction (XRD), Raman spectroscopy, and UV-Vis-NIR spectroscopy. Results showed that the deposited films were well-crystallized, highly transparent in the visible range, and had efficient UV-blocking properties. The results suggest that these thin films are promising candidates for applications in protective coatings and UV filters for high-temperature working materials, combining effective UV shielding with favorable optical transparency in the visible spectrum at high temperatures.

Introduction

Historically, quartz glass envelopes have been doped with cerium to block harmful ultraviolet (UV) radiation. However, this method has significant drawbacks: it lowers the annealing point of the quartz, reducing the lamp's lifespan and efficiency. The cerium dopant also absorbs, rather than reflects, the UV energy, which leads to wasted light and further degradation of the material. A solution to these problems is to use a high-temperature coating that effectively reflects UV emissions while maintaining the transmission of visible light [1].

This study explores a promising alternative: the synthesis and characterisation of thin films of titanium dioxide (TiO₂). These films were produced using a sol-gel method and are designed to provide efficient UV shielding with high transparency in the visible spectrum. The materials were analysed to confirm their well-crystallised structures and excellent UV-blocking properties. The results suggest these thin films are promising candidates for protective coatings and UV filters on high-temperature materials, offering a superior alternative to traditional cerium-doped quartz [2,3].

Experimental

Synthesis of Thin Films

Titanium dioxide, TiO₂, was prepared by the sol-gel method using the hydrolysis of titanium tetra-isopropoxide (Ti(OCH(CH₃)₂)₄ – TTiP; 98+%; Thermo Scientific) with deionised water. The solvents used for the synthesis were isopropanol ((CH₃)₂CH₂OH – iPOH; ACS; Carlo Erba Reagents) and absolute anhydrous ethanol (CH₃CH₂OH – EtOH; HPLC Plus;

Carlo Erba Reagents), while acetylacetone ($\text{CH}_3\text{COCH}_2\text{COCH}_3$ – AcAc; >99.0%; TCI Europe N.V.) was used as a stabiliser. Two TiO_2 solutions were prepared, with concentrations of 3% and 10%, respectively. The code of samples represented the deposition rate (s1, s2, and s4), the solvent (iP and Et being isopropanol and ethanol), and the concentration of TiO_2 in the solution (3 and 10 g TiO_2 per 100 ml of colloidal solution).

Table 1. The sample's parameters.

Sample Name	Deposition speed (mm/s)	TiO_2 Concentration (g/100 ml)	Solvent
s1iP3	s1	3	iP (isopropanol)
s2iP3	s2	3	iP (isopropanol)
s2Et3	s2	3	Et (ethanol)
s2iP10	s2	10	iP (isopropanol)
s4iP3	s4	3	iP (isopropanol)
s4Et3	s4	3	Et (ethanol)

Film Deposition and Characterisation

The thin films were deposited onto quartz glass slides using a dip-coating technique, **Solgelway** dip coater (Model ACedip 2.0). The slides were cleaned, immersed in the precursor solutions, and withdrawn at controlled speeds of 1, 2, or 4 mm/s. After deposition, the samples were dried at 100 °C for 30 minutes, followed by a final annealing step at 800 °C for 15 minutes. The films were then thoroughly characterised. **UV-Vis-NIR spectroscopy** was used to measure their transparency and UV-blocking ability. **X-ray diffraction (XRD)** and **Raman spectroscopy** confirmed their crystalline phases of anatase (TiO_2). The surface structure was examined using **optical microscopy**.

Results and discussion

X-ray diffraction (XRD) analysis confirmed the formation of pure, crystalline phases (fig. 1).

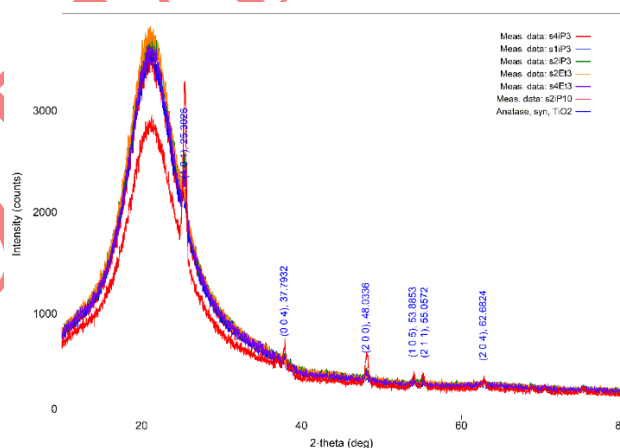


Figure 1. RX spectra for coatings of all TiO_2 samples.

The crystalline phase in the heat-treated TiO_2 films was identified as the **anatase** phase with no impurities detected. The peaks in the XRD patterns for TiO_2 matched those of the anatase structure. **Rietveld refinement** of the XRD data showed that the lattice parameters and crystallite sizes were consistent with those found in the literature, confirming the high structural quality of the films.

The Raman spectra (fig. 2) for the TiO_2 films also confirmed the presence of the anatase phase through characteristic vibration modes at 144, 197, 399, and 513-519 cm^{-1} , indicating high crystallinity.

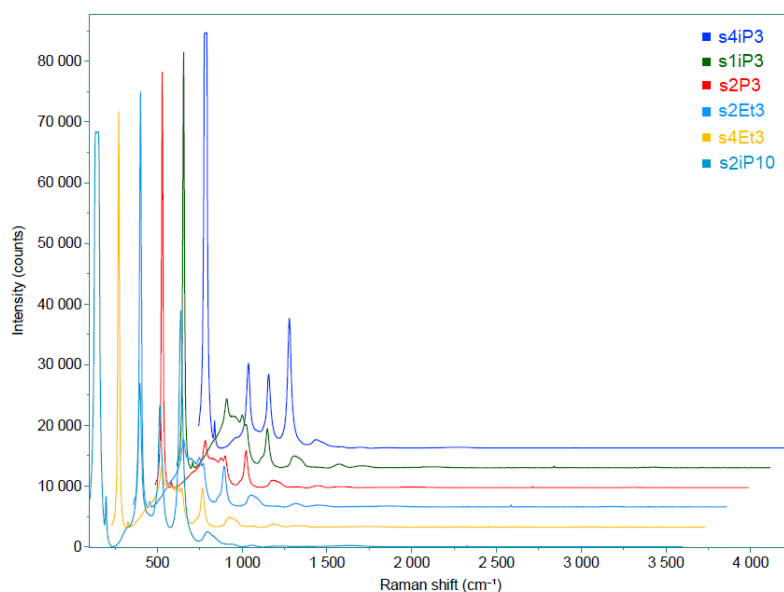


Figure 2. Raman spectra of the quartz glass with TiO₂ thin films.

Fig. 2 shows the Raman spectra of titanium dioxide, which highlight several distinct peaks characteristic of the anatase phase, a crystalline form of TiO₂. These peaks correspond to the vibration modes of the crystal lattice: 144 cm⁻¹ (E_g), a strong and sharp peak frequently used as a reference for identifying anatase; 197 cm⁻¹ (E_g), of lower intensity; 399 cm⁻¹ (B_{1g}), relatively weak; and 513 cm⁻¹ and 519 cm⁻¹ (B_{1g} and A_{1g}), which usually appear as a single broad peak due to their proximity. The presence of these well-defined peaks confirms the high crystallinity of the analysed samples.

The UV blocking properties depend on the band gap value of TiO₂, which is around 3.2–3.3 eV, corresponding to a wavelength of 387–366 nm. In this range, the energy of UV radiation absorbed by atoms in TiO₂ is high enough to excite electrons from the valence band to the conduction band. The analysis of the spectra in Fig. 3 shows that, in the TiO₂ series, the highest transmittance values in the visible range are obtained for films deposited from ethanolic solutions at a speed of 2 mm/s, but these films also have a relatively high transmittance in the UV range, which makes them less favourable for UV-block applications.

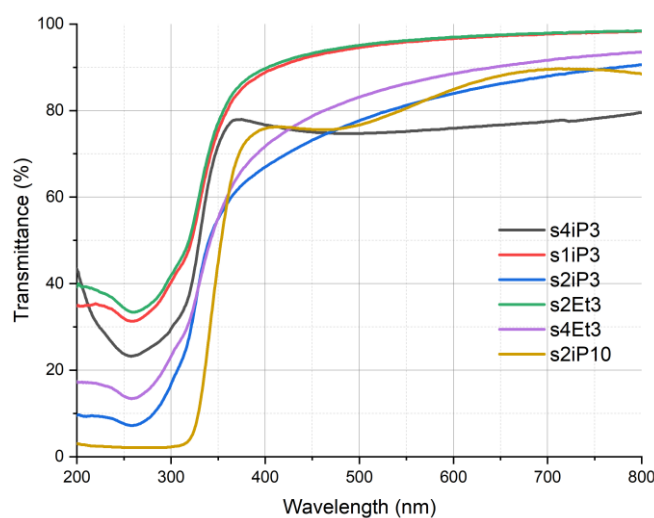


Figure 3. UV-Vis spectra for coatings of all TiO₂ samples.

Fig. 4 shows optical micrographs of thin films, taken at low (20×) magnification, highlighting the influence of deposition parameters on surface morphology and uniformity.

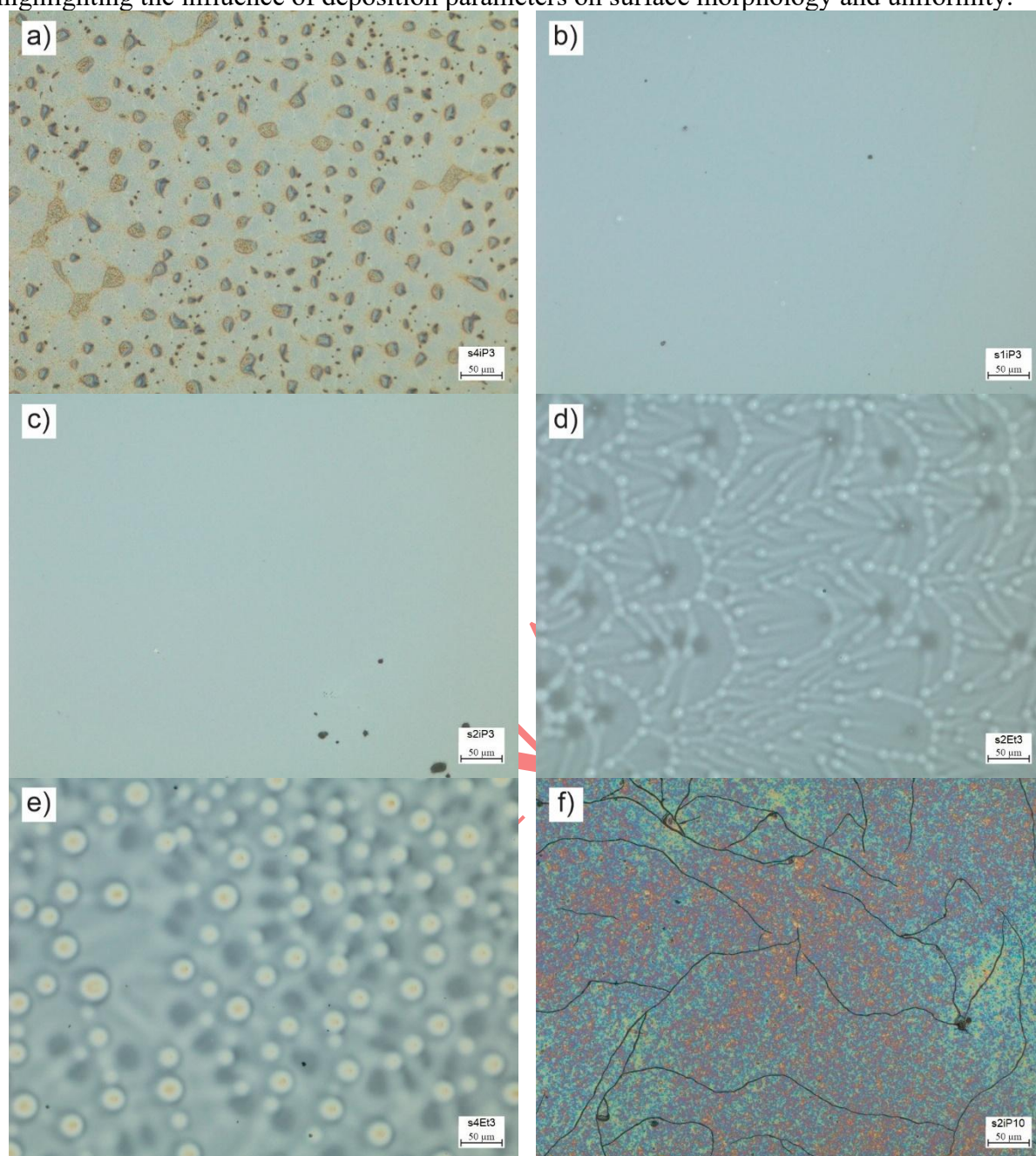


Figure 4. Optical micrographs of the samples

(s4iP3): This image shows a **non-uniform** film with distinct droplet-like structures and agglomerates. This morphology suggests a fast deposition speed or a high concentration of the precursor solution, which led to the formation of separate islands of material rather than a continuous, smooth film.

(s1iP3): This film appears **highly uniform and smooth**, with very few visible defects. This is a sign of an excellent and well-controlled deposition process. This kind of film would be ideal for applications that require optical clarity and a defect-free surface, like anti-reflective coatings.

(s2iP3): Similar to the top-right image, this film is also **very smooth and uniform**. There are some small defects, but overall, the quality is high, indicating optimised deposition parameters that resulted in a homogeneous film.

(s2Et3): This micrograph reveals a unique **"dendritic" or "spider-web" pattern**. This structure is likely the result of a specific deposition parameter, possibly a fast solvent evaporation rate, which caused the TiO_2 particles to self-assemble into this interconnected network. Films with this porous morphology are valuable for applications where a large surface area is beneficial, such as in catalysis or gas sensing.

(s4Et3): This image shows a film with numerous **spherical agglomerates** or "beads." This could be a result of the precursor solution's properties, like surface tension or viscosity, and the interaction with the substrate during the deposition process. This film is less uniform than others.

(s2iP10): This film displays a **complex, porous, and highly interconnected network** with distinct colours. The pattern suggests a rapid, non-equilibrium growth process. The colours are likely due to thin-film interference, which indicates variations in the film's thickness across the surface.

This type of morphology is often used in applications like solar cells or sensors.

Conclusion

This study successfully demonstrated the synthesis of highly crystalline titanium dioxide (TiO_2) thin films using a simple and effective sol-gel dip-coating method. The annealing process at 800 °C yielded pure **anatase** phase TiO_2 films, as confirmed by both **X-ray diffraction (XRD)** and **Raman spectroscopy**. The high structural quality was further validated by Rietveld refinement, which showed that the films' lattice parameters and crystallite sizes were consistent with published literature.

The films exhibit strong **UV-blocking properties**, which are directly linked to the material's band gap. While all films absorb UV radiation, those deposited from ethanolic solutions at 2 mm/s demonstrated the highest transparency in the visible spectrum. However, this highly visible transparency came with a compromise: relatively high UV transmittance, making these specific films less effective for UV-blocking applications. Overall, the results confirm that these TiO_2 thin films are a promising alternative to traditional UV-filtering methods, offering a combination of high crystallinity, good optical transparency, and effective UV absorption for use in high-temperature protective coatings.

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DETERMINATION OF BIOMETRIC AND CHEMICAL PARAMETERS IN THE FRUITS OF SOME QUINCE VARIETIES

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Abstract

Quince (*Cydonia oblonga* Miller) is a commonly cultivated plant throughout the world, known for centuries for its valuable nutritional and curative properties. Although quince fruits are extremely aromatic, due to their high hardness and sour, astringent [10] and bitter taste, they are not suitable for direct consumption in unprocessed form. However, they are an important raw material in fruit processing, for example, in the production of jams, jellies and juices. Quince fruits fall into the category of temperate fruits, so their shelf life can be predicted. Considering that technological processing affects not only the organoleptic properties and shelf life, but also the functional properties of the fruits,

For this study, 20 fruits from 4 quince varieties (Bereczki_RO; Champion_HU; De Portugalia_TR; Constantinopol_RO) that were purchased from the supermarket, in 2024, were analyzed, the fruits were studied from a biometric and qualitative point of view, tracking the following parameters: large diameter (mm), small diameter (mm), height (mm), weight (g), soluble dry matter (°Brix), sugar percentage (%) and fruit firmness.

From the results obtained for the physical (biometric)-chemical parameters, the following results can be observed: for the Bereczki_RO quinces: the average of the large diameter values is 80.42 mm, the highest value was recorded by the Constantinopol_RO variety, with a value of 88.65 mm, with an average of the experiment of 82.48 mm. Regarding the soluble dry matter (°Brix)% and the percentage of sugars, it can be observed that the Bereczki_RO variety recorded the highest value for these parameters, these being 14.01(°Brix), respectively 12.39% [11].

Introduction

The common quince (*Cydonia oblonga* Miller) is the only representative of the genus quince and belongs to the Rosaceae family, which also includes the apple and pear [1]. Its place of origin is considered to be western Asia, although it has now spread to other continents, where it occurs both as a wild plant, planted in domestic gardens and parks as an ornamental plant, and is cultivated for its edible fruit [2]. The largest global producer and distributor is Turkey (supplying 25% of global production), followed by China, Iran, Argentina and Morocco (supplying 10% of global production) [3,4]. Turkey's quince fruit production increased by approximately 66% between 2006 and 2020 [5].

Quince fruits are increasingly attracting the interest of scientists and consumers due to their broad health effects, associated with hypoglycemic, anti-inflammatory, anticancer, antibacterial, antiallergic and antiulcer properties [7,10,11,12].

The annual global production of quince in 2022 was 700,479.34 tonnes, 0.1% less than in 2021, when a total quantity of 701,204.4 tonnes was recorded.

Turkey was the largest producer worldwide, accounting for over a quarter (28.2%) of total global production[1].

In 2023, global production was 687,036 tonnes, 1.92% less than the previous year. The largest global producer remained Turkey, accounting for 27.98% of total global production[1].

In 2017 (the most recent year for which data were reported to FAO), the area covered by quince orchards in Romania was 883 hectares, 13th worldwide and 3rd in the European Union, after Spain and Belgium. The production achieved was 2nd in the European Union, after Spain and 12th globally. Productivity in Romania was 7,407.9 kg/ha, 5th in the European Union, after Greece, Italy, Hungary and Portugal, and 26th worldwide, lower than the global average of 8,583.5 kg/ha[1]. Data comes from the FAOSTAT database of the Food and Agriculture Organization of the United Nations (FAO)[1].

Experimental

Regarding biometric aspects, fruit samples were taken (20 fruits for each variety) and the following were studied: large diameter, small diameter, height.

The external characteristics of the fruits from the varieties studied were determined with a caliper, and the value of soluble dry matter was read with a digital refractometer. The weight of the fruits was determined by weighing on a digital analytical balance [16].



Figure 1. Analytical balance (original photo) (original photo)

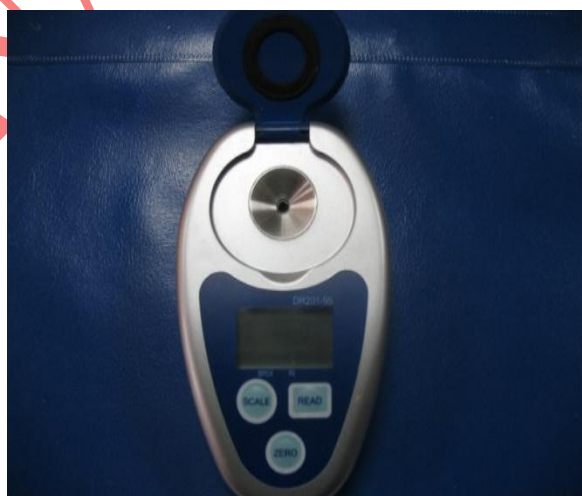


Figure 2. Digital refractometer

The soluble sugar content (0Brix) was measured with a digital refractometer (Fig.2.). The quinces were scraped, after which the juice was squeezed onto the lens, without letting the pulp fall onto the lens. Carefully lower the plastic cover over the juice and take the readings. Testing the refractometer with plain water should indicate zero.

The percentage of sugar in the juice obtained from the sampled fruits was determined based on the formula:

$\% = (N \cdot 4.25) / 4 - 2.5$, where: N= the figure on the refractometer; 4.25= the density of the juice (must); 4 = established coefficient; 2.5=% of unsweetened d.u.. The firmness was determined

with the PCE-PTR 200N Penetrometer, unlike the analog penetrometer, this digital penetrometer offers greater precision and a higher resolution in the measurement.

Results and discussion

From the data obtained, we can see that, in terms of large diameter (mm), the highest value was recorded by the Constantinopol_RO variety, with a value of 88.65 mm, followed by the De Portugalia_TR variety, with an average of 82.45 mm, at the opposite pole we have the Champion_HU variety (78.38 mm) (table 1.); for the small diameter parameter, it is observed that the Constantinopol_RO variety also recorded the highest value (83.35 mm), with an average of the experiment of 76.19 mm; in terms of fruit height and weight, we observe that the Constantinopol_RO variety also recorded the highest values, these being 90.58 mm and 303.93 g.

Table1. Results obtained on the fruits of the quince varieties studied

No. crt.	Variety	Large diameter (mm)	Small diameter (mm)	Height (mm)	Weight (g)
1	Bereczki RO	80.42	74.68	87.56	247.21
2	Champion HU	78.38	68.89	88.31	211.65
3	De Portugalia TR	82.45	77.82	89.15	258.94
4	Constantinopol_R O	88.65	83.35	90.58	303.93
	Average experience	82.48	76.19	88.90	255.43

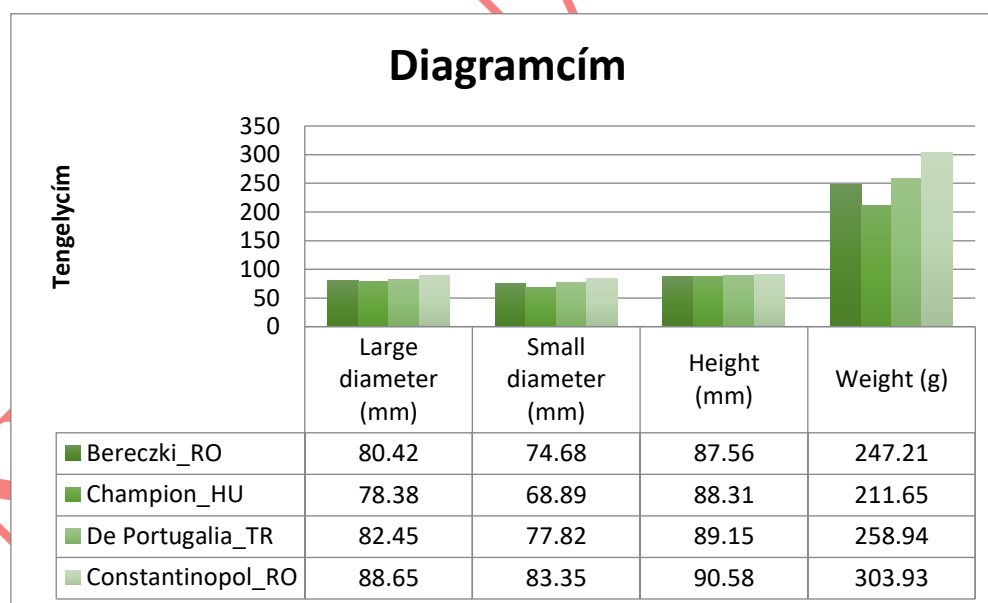


Figure 3. Graphical representation of the data obtained from biometric parameters

From the data obtained regarding soluble dry matter (0Brix)% and sugar percentage. it can be observed that the Bereczki_RO variety recorded the highest value for these parameters. which were 14.01(0Brix) and 12.39%. respectively (table 2). Regarding firmness. we can observe from the data obtained that the Bereczki_RO variety had the highest value. which was 10.87 lb. followed by the Constantinopol_RO variety with a hardness of 8.29 lb.

Table 2. Results obtained on the fruits of the quince varieties studied

No. crt.	Variety	Soluble dry matter (⁰ Brix)%	Sugar percentage (%)	Firmness lb (livre)
1	Bereczki RO	14.01	12.39	10.87
2	Champion HU	13.20	11.52	8.08
3	De Portugalia TR	13.15	11.46	7.99
4	Constantinopol RO	12.53	10.81	8.29
	Average experience	13.22	11.55	8.81

Conclusion

From the results obtained for the quince fruits of the varieties studied. it can be observed that:

- the basic indicators of the large diameter for the Bereczki_RO quinces: the average of the large diameter values is 80.42 mm. for the Champion_HU quinces: the average of the large diameter values is 78.38 mm. for the De Portugalia_TR quinces: the average of the large diameter values is 82.45 mm and for the Constantinopol_RO quinces: the average of the large diameter values is 88.65 mm; with an average of the experience of 82.48 mm.
- the basic indicators of the small diameter for the Bereczki_RO quinces: the average of the large diameter values is 74.68 mm. for the Champion_HU quinces: the average of the large diameter values is 68.89 mm. for the De Portugalia_TR quinces: the average of the large diameter values is 77.82 mm and for the Constantinopol_RO quinces: the average of the large diameter values is 83.35 mm; with an average experience of 76.19 mm.
- basic indicators of fruit height for Bereczki_RO quinces: the average of the large diameter values is 87.56 mm. for Champion_HU quinces: the average of the large diameter values is 88.31 mm. for De Portugalia_TR quinces: the average of the large diameter values is 89.15 mm and for Constantinopol_RO quinces: the average of the large diameter values is 90.58 mm; with an average of the experience of 88.90 mm.
- basic indicators of fruit weight for Bereczki_RO quinces: the average of the large diameter values is 247.21 g. for Champion_HU quinces: the average of the large diameter values is 211.65 g. for De Portugalia_TR quinces: the average of the large diameter values is 258.94 g and for Constantinopol_RO quinces: the average of the large diameter values is 303.93 g; with an average of experience of 255.43 g.
- basic indicators of sugar percentages in fruits of quince varieties Bereczki_RO: the average of large diameter values is 12.39%. for Champion_HU quinces: the average of large diameter values is 11.52%. for De Portugalia_TR quinces: the average of large diameter values is 11.46% and for Constantinopol_RO quinces: the average of large diameter values is 10.81%; with an average of experience of 11.55%.

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FABA BEAN FLOUR: AN ALTERNATIVE SOURCE FOR DEVELOPING GLUTEN-FREE PASTA WITH FUNCTIONAL PROPERTIES

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Abstract

This study aimed to develop a gluten-free pasta formulation enriched with bioactive compounds, proteins, fibers, and minerals through the incorporation of faba bean flour (FBF) at varying substitution levels. Four pasta samples were prepared using rice flour (RF) and FBF in ratios of 100:0, 90:10, 80:20, and 70:30. Standard laboratory analyses were conducted to assess proximate composition, cooking properties, sensory attributes, total phenolic content (TPC), total flavonoid content (TFC), and antioxidant activity (AA). The incorporation of FBF significantly enhanced the nutritional profile of the pasta, with protein, fiber, and ash contents progressively increasing across formulations, while carbohydrate levels decreased. Functional properties also improved: both TPC and TFC showed substantial increases, resulting in a notable rise in antioxidant activity relative to the control. However, higher FBF levels led to technological limitations, such as increased cooking time and higher cooking losses, which negatively impacted overall sensory acceptability. Despite these challenges, the addition of 20% FBF provided the most favorable balance, yielding gluten-free pasta with superior nutritional and functional quality while still maintaining acceptable sensory attributes.

Keywords: *fava bean flour, gluten-free pasta, high nutritional value, food application*

Introduction

In recent years, the rising prevalence of metabolic and cardiovascular disorders associated with obesity and nutritional imbalances has highlighted the importance of balanced diets rich in protein, fiber, phytochemicals, and antioxidants. Functional foods, through the inclusion of nutraceutical ingredients, may help mitigate health risks and enhance overall well-being [1]. A key recommendation is to address both macro- and micronutrient deficiencies through nutrition education programs that promote healthier dietary choices [2, 3]. In this context, growing interest has been directed toward the replacement of wheat flour with alternative flours in bakery and pasta products, particularly starchy roots and tubers, protein-rich legumes, and cereals [4]. Currently, a wide variety of gluten-free (GF) products (e.g., bread, cakes, muffins, pasta, noodles) are available for individuals with coeliac disease. However, many of these products are deficient in minerals and bioactive compounds, rendering them nutritionally inferior to the wheat-based foods they are intended to replace [5, 6]. Therefore, greater attention and continued research are needed to enhance their nutritional quality. In this context, pasta can serve as a complete protein source when complemented with other plant-based foods, such as legumes, which offset its lysine deficiency [5–7]. Moreover, legume-derived proteins and fibers have been shown to exert multiple beneficial health effects [5–7]. In this study, rice flour (RF) and faba bean flour (FBF) were selected for the formulation of gluten-free pasta with functional

potential. The choice of FBF as a partial substitute for RF is based on its complex chemical composition, which underpins the high nutritional value and bioactive potential of legumes. Owing to its low cost and high protein and carbohydrate content, the faba bean is considered to be of substantial nutritional and economic importance [8]. Previous studies have highlighted the nutritional composition and polyphenolic content of FBF, suggesting its potential in the development of functional food products due to its beneficial health effects. Polyphenols from FBF exhibit antioxidant activity and the ability to inhibit enzymes involved in carbohydrate digestion, as demonstrated in vitro [9]. However, to date, only limited studies have reported on the impact of incorporating FBF on the antioxidant and nutritional properties of durum wheat pasta [8, 9]. This study aims to evaluate the potential of fava bean flour (FBF) as an affordable and protein-rich ingredient for the fortification of rice flour (RF) in gluten-free pasta production. The effects of different replacement levels were assessed with respect to nutritional composition, functional properties, cooking quality, and sensory characteristics. The overarching objective was to determine the quality attributes and consumer acceptability of pasta fortified with FBF.

Experimental

Materials

RF, FBF and the other ingredients used in this study were purchased from local market in Timisoara town, Romania.

Technological process for the production of pasta samples

Gluten-free pasta samples were prepared according to Chepkosgei et al. (2021) [4], with slight modifications. In the formulations, RF was partially substituted with FBF, while the control used only RF. The dough, prepared using water, salt, and egg, was kneaded, allowed to rest for 1 h, and then shaped into 6 mm strips with a hand-operated pasta machine. The strips were hung on glass rods and dried in a cabinet dehydrator at 70 °C for 12 h. Finally, the samples were cooled to room temperature, sealed in polyethylene bags, and stored until further analysis.

Analytical procedures

The proximate composition, cooking properties, total phenolic content (TPC), total flavonoid content (TFC), and antioxidant activity (AA) of the gluten-free pasta samples were determined using standard procedures [10–15]. All analyses were performed in triplicate, and the results were expressed as mean values. Statistical evaluation was conducted using Microsoft Excel.

Sensory evaluation

Cooked, coded pasta samples were evaluated by a panel of twenty assessors, who scored color, appearance, odor, flavor, and overall acceptability using a 9-point hedonic scale, where 1 corresponded to “dislike extremely” and 9 to “like extremely.” Pasta made with 100% RF served as the control [12, 14].

Results and discussion

Proximate composition of pasta samples

Table 1 presents the proximate analysis of the pasta samples. Moisture content decreased significantly with increasing FBF levels, ranging from 12.25% in the 100% RF control to 10.84% in the formulation containing 30% FBF.

Table 1. Proximate composition of gluten-free pasta samples

Proximate composition (%)	Gluten-free pasta samples			
	PC	P10FBF	P20FBF	P30FBF
Moisture	12.25 ± 0.07	11.84 ± 0.22	11.24 ± 0.09	10.84 ± 0.24
Fat	2.04 ± 0.24	2.36 ± 0.45	2.92 ± 0.14	3.54 ± 0.11
Protein	8.64 ± 0.09	12.22 ± 0.32	16.46 ± 0.22	18.20 ± 0.04
Crude fiber	1.74 ± 0.12	2.25 ± 0.33	4.22 ± 0.09	6.44 ± 0.54
Ash	1.44 ± 0.21	2.60 ± 0.15	3.24 ± 0.22	3.68 ± 0.07
Carbohydrates	73.89 ± 0.08	68.73 ± 0.42	61.92 ± 0.25	57.30 ± 0.33

All determinations were done in triplicate and the results were reported as average value ± standard deviation (SD). **PC** – control pasta sample prepared with 100% rice flour (RF); **P10FBF** – pasta prepared with 90% RF and 10% FBF; **P20FBF** – pasta prepared with 80% RF and 20% FBF; **P30FBF** – pasta prepared with 70% RF and 30% FBF.

The addition of FBF led to a marked improvement in the nutritional profile of the pasta samples (P10FBF, P20FBF, P30FBF) compared with the control (PC). Protein content increased proportionally with the substitution level, ranging from 12.22% in P10FBF to 18.20% in P30FBF. A similar trend was recorded for fiber and ash contents, which rose from 2.25% to 6.44% and from 2.60% to 3.68%, respectively, compared with 1.74% and 1.44% in PC. These results demonstrate that pasta fortified with FBF can be considered a valuable source of proteins, dietary fiber, and minerals, thereby offering high functional potential. The findings are consistent with previous reports by Rady et al. (2020) [7], Betrouche et al. (2022) [9], and Stoin et al. (2022) [13], reinforcing the suitability of bean flour as a nutritional fortifier in various food products.

Table 2. Cooking properties of gluten-free pasta samples

Treatments	Gluten-free pasta samples			
	PC	P10FBF	P20FBF	P30FBF
Cooking time (min)	5.5 ± 0.11	9.5 ± 0.08	10 ± 0.21	10.5 ± 0.22
Cooked weight (%)	3.46 ± 0.08	3.77 ± 0.38	4.42 ± 0.22	4.88 ± 0.09
Cooking loss (%)	6.42 ± 0.86	9.34 ± 0.44	10.62 ± 0.05	11.87 ± 0.44

With respect to cooking time, a progressive increase was observed as the proportion of FBF increased. The shortest cooking time was recorded in the control sample (5.5 min), whereas the longest was observed in the formulation containing 30% FBF (10.5 min). These differences can be attributed to the distinct gelatinization temperatures of starches from the different flours [12, 14]. Regarding cooking weight, an increasing trend was also observed with higher FBF levels. The lowest value was recorded in the control sample (3.46%), gradually rising to 4.88% in the formulation with 30% FBF. Similarly, cooking loss increased with higher FBF levels and lower RF content. The lowest cooking loss was 6.42% in the control, while the highest was 11.87% in the pasta sample with 30% FBF. These findings are consistent with previous studies, such as Betrouche et al. (2022) [9] and Stoin et al. (2022) [13].

Color scores showed no major differences among samples, although higher values were associated with increased FBF content, with the 20% FBF sample scoring the highest (6.85) and the 100% RF control the lowest (6.33). Panelists displayed a clear preference for the control pasta made from 100% RF, as increasing the proportion of FBF resulted in progressively lower scores for appearance, odor, flavor, and overall acceptability. Appearance scores declined from 4.68 in the control to 4.08 in the 30% FBF sample; odor from 4.48 to 3.86; flavor from 4.66 to 3.84; and overall acceptability from 4.45 to 4.19 [12, 13].

Table 3. Sensory evaluation of gluten-free pasta samples

Sensory evaluation	Gluten-free pasta samples			
	PC	P10FBF	P20FBF	P30FBF
Color	6.33 ± 0.87	6.52 ± 1.22	6.85 ± 0.11	5.88 ± 0.08
Appearance	5.49 ± 0.14	4.68 ± 0.12	4.86 ± 0.04	4.08 ± 0.14
Odor	5.22 ± 0.17	4.48 ± 0.36	4.62 ± 0.11	3.86 ± 0.33
Flavor	5.55 ± 0.47	4.66 ± 0.13	4.78 ± 0.25	3.84 ± 0.18
Overall acceptance	5.34 ± 0.33	4.45 ± 0.14	4.62 ± 0.26	4.19 ± 0.41

The lowest scores were consistently observed in the pasta containing 30% FBF, whereas the highest were recorded in the control sample. These results indicate that higher FBF levels negatively affected sensory properties, in agreement with earlier reports on pasta fortified with other vegetable and legume flours [12 - 14].

Table 4. Phytochemical content and antioxidant activity of pasta samples

Gluten-free pasta samples	Phytochemical parameters		
	TPC (mg GAE/100g DW)	TFC (mg QE/100 g DW)	AA (μ M TE/100g DW)
PC	20.62 ± 0.22	21.36 ± 0.33	24.21 ± 0.14
P10FBF	38.33 ± 0.33	28.45 ± 0.09	35.44 ± 0.03
P20FBF	49.55 ± 0.22	37.36 ± 0.04	45.74 ± 0.08
P30FBF	62.02 ± 0.04	49.78 ± 0.08	54.98 ± 0.04

The results showed that the levels of TPC, TFC, and AA increased with the proportion of FBF added to the pasta samples. The highest TPC and TFC contents were observed in the P30FBF sample (62.02 mg GAE/100 g DW and 49.78 mg QE/100 g DW, respectively), whereas the lowest values were recorded in the control sample (20.62 mg GAE/100 g DW and 21.36 mg QE/100 g DW). A similar trend was observed for antioxidant activity (AA), with the highest level found in P30FBF (54.98 μ M TE/100 g DW) and the lowest in the control (24.21 μ M TE/100 g DW) [8, 9, 13, 16]. This study demonstrates that incorporation of FBF into egg pasta increases protein and fiber contents compared with RF pasta. Moreover, pasta represents a source of polyphenols and antioxidants, whose levels are strongly influenced by the type of ingredients and processing conditions [16, 17].

Conclusions

The results of this study demonstrate that the incorporation of FBF in pasta formulations leads to products with enhanced functional properties. Sensory evaluation indicated that substitution levels of up to 20% FBF yielded higher consumer acceptance compared with the control. Furthermore, the addition of FBF markedly increased the phenolic compound content, total flavonoid content, and antioxidant activity of the gluten-free pasta. Overall, the nutritional, physicochemical, phytochemical, and sensory assessments confirmed that FBF represents a valuable plant-based ingredient for the development of innovative food products with improved functionality.

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NOT FINALIZED

IMPACT OF PEDOGENETIC FACTORS ON THE MORPHOLOGICAL AND CHEMICAL PROPERTIES OF REPRESENTATIVE SOILS IN PECICA, WESTERN ROMANIA

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Abstract

This study aims to characterize the morphological and chemical properties of representative soils in the Pecica area, Arad County, western Romania, and to evaluate the influence of pedogenetic factors on soil formation. The investigated area, part of the Western Plain, is characterized by loess and clay deposits, low altitudes (90–120 m), and a temperate-continental climate with moderate precipitation (580–600 mm/year). Three soil types were analyzed: vertic gleic Chernozem, vertic Phaeozem, and amfogleic Eutric Cambisol. Morphological descriptions and laboratory analyses (pH, humus content, cation exchange capacity, base saturation, and carbonate content) revealed significant differences among soils. Chernozem exhibited high fertility but moderate gleization and localized sodicity. Phaeozem had superior humus content and cation exchange capacity, while Eutric Cambisol was limited by acidity and low phosphorus availability. The study confirms that climate, parent material, topography, groundwater, vegetation, biological activity, and anthropic interventions collectively shape soil properties. The results underline the need for site-specific management practices, including pH correction, organic and mineral fertilization, controlled drainage, and irrigation, to ensure sustainable utilization of the pedological resources in Pecica.

Introduction

Soil is an essential component of terrestrial ecosystems, playing a crucial role in supporting agriculture, regulating the water and nutrient cycles, and maintaining ecological balance [1]. In the context of agricultural intensification and climate change, assessing soil properties and the factors influencing them has become imperative for the sustainable management of agricultural lands [2,3]. The main pedogenetic factors-climate, parent rock, relief, vegetation, organisms, water, and human activity-interact in a complex manner, leading to the formation of soils with distinct characteristics [4,5,6].

At the European level, studies in the Pannonian Plain have highlighted the diversity of soils and their vulnerability to processes such as gleying, erosion, and salinization [7,8]. In Romania, pedological research in the Western Plain has shown that loess and clay soils exhibit high fertility, yet they are sensitive to compaction, excess moisture, and loss of organic matter [9,10]. Several studies have emphasized that agricultural management profoundly affects soil structure and chemical properties, thereby modifying pedogenetic processes over time [11,12].

The Pecica area, Arad County, located in western Romania, is characterized by predominantly flat relief, low altitudes (90–120 m), and a loess-clay substrate. The temperate-continental climate, with annual precipitation of 580–600 mm and mean temperatures of 10.8°C, favors humification processes but also promotes vertisolization during dry years [13,14,15]. The

dominant soils include vertic gleyic chernozems, vertic faeozems, and amphigleyic eutric cambisols, each differently influenced by the groundwater level, parent material, and human activity [16,17]. The aim of this study is the comparative characterization of the three soil types in Pecica through morphological description and chemical analysis, and the interpretation of the results in relation to pedogenetic factors. The main objectives include identifying the morphological and physicochemical properties of the soils, analyzing their differences, and evaluating the implications for soil fertility and the sustainable management of agricultural lands.

Experimental

The study was conducted within the administrative territory of the town of Pecica, located in western Romania, Arad County, approximately 25 km west of the city of Arad, on the right bank of the Mureș River (46°08'N, 21°04'E). Geographically, the area belongs to the Mureș Plain, part of the Western Plain, characterized by low altitudes (90–120 m), flat or gently fragmented relief, and loess or clay deposits that constitute the parent material of the soils. The climate is moderately temperate-continental, with oceanic and sub-Mediterranean influences. The multi-annual mean temperature is 10.8°C, and the average annual precipitation is 580–600 mm, unevenly distributed, with the highest amounts recorded in spring and at the end of summer. The natural vegetation belongs to the forest-steppe zone; however, most of the area is currently used for agriculture, predominantly for field crops such as wheat, maize, and sunflower. For soil characterization, three representative profiles were excavated and described: vertic gleyic chernozem, vertic faeozem, and amphigleyic eutric cambisol. Morphological description was carried out following standard methodologies [1,3,4], analyzing horizon depth and thickness, color (Munsell), texture, structure, consistency, porosity, presence of concretions and coatings, signs of gleying, and carbonatation. The obtained data were compiled and compared among the analyzed soils to identify pedogenetic differences and their implications for fertility and agricultural use.

Results and Discussion

1. Distribution and Characteristics of Soils

The administrative area of the town of Pecica covers 23,717 ha, of which 19,471 ha are agricultural land. Among the agricultural lands, the predominant soils are: chernozems (9,147 ha), faeozems (5,831 ha), and alluviosols (1,217 ha).

In this study, three of the identified soil types are described: vertic gleyic chernozem, vertic faeozem, and amphigleyic eutric cambisol. The three studied soils develop on loess and clay deposits and exhibit significant differences in morphological and chemical properties.

2. Analysis of Pedogenetic Factors

Moderate precipitation and a mean temperature of 10.8°C favor the humification of organic matter, while drought induces large cracks in chernozems and vertisolization in faeozems and eutric cambisols.

Slightly higher interfluvial areas allow better drainage and promote the development of chernozems and faeozems, whereas micro-depressions favor water stagnation and gleying in eutric cambisols.

Loess and heavy clays influence texture, water retention, and cation exchange capacity.

The groundwater level determines gleying and the formation of carbonate coatings in chernozems; permanent water stagnation affects eutric cambisols.

Humus content is higher in chernozems and faeozems due to the original forest-steppe vegetation and intense biological activity, whereas eutric cambisols exhibit lower humification.

The analyzed soils are mature, having formed during the Holocene; however, pedogenetic processes are still active. Vertisolization, gleying, and carbonation demonstrate continuous pedogenetic activity influenced by climate changes and human activity.

Mechanical soil work and intensive agriculture modify horizon structure, reduce porosity, and promote compaction. Intensive plowing and mechanical interventions have altered the structure of the Ap horizons, decreasing porosity and increasing compaction. Additionally, the lack of irrigation during drought years reduces the productive potential of faeozems, while inappropriate exploitation of eutric cambisols aggravates water stagnation.

Table 1. Morphological Properties and Pedogenetic Factors of Soils in Pecica

Characteristic	Vertic Gleyic Chernozem	Vertic Faeozem	Amphigleyic Eutric Cambisol	General Comparison
Horizons	Well-developed (Ap, Am, ABy, Bvy, Ccay), with wide cracks and deep gleying	Deep (Ap, Am, ABy, By, BCyk, Cca), spheroidal structure, slickensides	Shorter profile (Ap, Ao, AByw, Btyw, BC, Cg), evident stagnogleying	Chernozem: deep and stable profile; Faeozem: more clayey and deep; Eutric Cambisol: least developed
pH	Slightly acidic at surface (6.1), alkaline in depth (>8)	Slightly acidic at surface (6.5), neutral down to 125 cm, then slightly alkaline (8.4)	Acidic at surface (5.8), neutral toward base (7.3)	Chernozem and faeozem tend to alkalization; eutric cambisol tends toward acidification
Humus (%)	2.6 in Ap → 1.7 in Bvy (rapid decrease with depth)	3.3 in Ap → 2.3 in ABy (better supplied)	1.9 in Ap → 0.6 in AByw (low)	Fertility higher in faeozem, medium in chernozem, low in eutric cambisol
Carbonation (CaCO₃)	Strong, from 63 cm (13–16%)	Moderate, from 125 cm (3.6–14.2%)	Weak, only in BC and Cg	Chernozem strongly carbonated; faeozem shows delayed carbonation; eutric cambisol almost uncarbonated
Cation Exchange Capacity (T)	28–31 (high)	29.5–31.5 (high)	18–26 (medium)	Chernozem and faeozem – high fertility; eutric cambisol – lower fertility
Base Saturation (V%)	84–85% (eubasic)	92–96% (highly eubasic)	70–86% (medium to high)	Faeozem best base-saturated; eutric cambisol the lowest
Morphological Observations	Large cracks, gleying, local sodicity	Stable structure, cracks and slickensides, high fertility	Gleying and stagnogleying, low porosity, excess moisture	Soils differ in structure stability and water regime
Dominant Pedogenetic Factor	Groundwater and gleying processes; loess deposits	Clayey parent rock, vertisolization processes; water deficit	Excess stagnant water, secondary compaction, fluvio-lacustrine clays	Climate influences all, but hydric and lithologic factors clearly differentiate the three soil types

The results confirm the combined influence of all pedogenetic factors on soil properties, with direct implications for sustainable agricultural management.

Based on morphological description and chemical analyses, the three studied soils exhibit significant differences (Table 2).

Table 2. Comparative Characterization of Soils in Pecica According to Main Properties and Pedogenetic Factors

Factor / Property	Vertic Gleyic Chernozem	Vertic Faeozem	Amphigleyic Eutric Cambisol
Climate	Favors humification, but drought induces cracking	Favorable for humus accumulation, but sensitive to water deficit	Excess stagnant water limits fertility
Relief	Low interfluvies, partial drainage	Slightly higher plain, better drainage	Micro-depressions with evident stagnation
Parent Material	Loess-clay deposits	Heavy clays, vertisolization	Fluvio-lacustrine clays, stagnogleying
Water	Moderate gleying, local sodicity	Oscillating regime, frequent drought	Permanent stagnation, strong gleying
Vegetation	Forest-steppe, moderate humus input	Forest-steppe, high humus input	Hydrophilic vegetation, low humification
Organisms	Intense biological activity	Intense, promotes stable structure	Limited due to excess water
pH	Slightly acidic at surface, alkaline in depth	Slightly acidic-neutral-slightly alkaline	Slightly acidic, neutral
Humus (%)	2.6–1.7, medium fertility	3.3–2.3, high fertility	1.9–0.6, low fertility
CaCO₃	Strongly carbonated (>63 cm)	Moderate–strong (>125 cm)	Very weakly carbonated
CEC (me/100 g)	28–31 (high)	29.5–31.5 (high)	18–26 (medium)
Base Saturation (V%)	84–85 (eubasic)	92–96 (highly eubasic)	70–86 (medium–high)
Anthropic Influence	Compaction due to plowing	Requires irrigation	Difficult management, weed infestation

The results show that vertic faeozem has the most favorable natural fertility conditions, with high humus content and very high base saturation, although irrigation is needed to counteract water deficit. Vertic gleyic chernozem exhibits high fertility but is affected by gleying and local sodicity, which limits its use in wet years. In contrast, amphigleyic eutric cambisol is the least suitable for agriculture, with major limitations related to acidity, low phosphorus availability, and water excess.

Thus, the differences among the three soils confirm the importance of pedogenetic factors (climate, relief, parent material, water, and human activity) in determining their morphological and chemical properties. From a sustainable agriculture perspective, amelioration measures should be adapted to each soil type: correction of acidic reaction and phosphate fertilization for eutric cambisols, irrigation for faeozems, and controlled drainage for chernozems.

Conclusions

The three soils analyzed in Pecica exhibit significant differences in morphological and chemical properties, determined by local pedogenetic factors.

Vertic gleyic chernozem has high fertility, with a tendency toward gleying and local sodicity, requiring controlled drainage and specific fertilization measures.

Vertic faeozem is distinguished by high humus content and superior cation exchange capacity; however, water deficit can limit productivity without adequate irrigation.

Amphigleyic eutric cambisol is the most vulnerable, with acidity and low phosphorus availability, necessitating pH correction and phosphate fertilization.

The comparative analysis highlights the combined importance of all pedogenetic factors—climate, relief, parent material, water, vegetation, organisms, and human activity—on soil properties.

The results support the implementation of differentiated agricultural practices, tailored to each soil type, to ensure sustainable utilization of pedological resources in the Western Plain of Romania.

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ANALYSIS OF THE AMOUNT AND ENVIRONMENTAL IMPACT OF FOOD WASTE IN THE FOOD INDUSTRY

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Abstract

Food waste represents a global challenge and mitigating it requires taking responsibility from the food industry and supply chains at an individual level. The aim of our study is to assess the causes and magnitude of food waste, examine related attitudes within the food industry, and explore potential solutions to address this issue. In my previous work, I examined food waste in households and in a kindergarten catering service. Currently, we aim to explore the food industry environment, which also plays a significant role in the generation of food losses. The objective of our research is to identify the methods applied in handling and valorising industrial by-products, as well as to investigate how food industry actors perceive the issue of food loss. According to Eurostat data from 2022, the total amount of food waste generated in the European Union (EU) exceeded 59 million tonnes, of which one of the largest shares (19%) originated from the food processing and manufacturing sector [1]. In our study, special attention will be given to by-products and food waste arising during the production of food industry products. According to Food and Agriculture Organization (FAO) 13% of the world's food is already lost along the supply chain [2]. This represents not only a considerable environmental burden but also a pressing social issue. Reducing food loss offers multiple benefits, contributing to sustainability while simultaneously helping to alleviate hunger worldwide. Furthermore, we aim to explore potential utilization and recycling solutions. An example is the research conducted by [3], in which brewers spent grain (previously used mainly as animal feed due to its excellent nutritional value) was successfully incorporated into various bakery products, thereby enhancing their quality and nutritional value. An important Hungarian initiative in this context is the Hungarian Food Bank Association, which has been operating since 2005. While in the period between 2010 and 2013 most of the food surplus originated from the processing industry, in recent years the retail sector has become the primary contributor [4]. This continuous growth in donations highlights two key points: on one hand, the persistent issue of overproduction; on the other hand, the increasing awareness and participation of companies in donation schemes, which is a positive development, as it contributes to reducing food waste. In Hungary, 20.7% of food waste is generated during processing and manufacturing, making it the second leading source after households [5]. Based on this data, we consider our research well-founded, as it highlights the importance of addressing food waste at the industrial level. As part of our study, we plan to conduct a questionnaire survey among companies in food processing plants, to assess current practices and attitudes related to food loss and by-product management.

Conclusion

Our findings underline the need for further research and practical solutions to reduce industrial food losses and valorise by-products. Expanding such studies in the future could not only help

mitigate environmental impacts but also promote more sustainable food systems and contribute to reducing global food insecurity.

Acknowledgements

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AEROBIC FERMENTATION OF SORGHUM BY *LACTOBACILLUS ACIDOPHILUS*: IMPACT ON BACTERIAL GROWTH, PHENOLIC COMPOSITION, AND ENZYMATIC ACTIVITY

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Sorghum (*Sorghum bicolor* L. Moench) grain is a gluten-free cereal with a rich phenolic profile, including flavonoids and tannins. Fermentation with lactic acid bacteria (LAB) is a traditional method to adjust the nutritional and functional properties of various grains. Our aim was the characterization of extracts obtained after LAB fermentation of sorghum samples. In this study, we investigated the growth of *Lactobacillus acidophilus* in finely ground sorghum material under aerobic fermentation at 37 °C. Sprouted and non-sprouted sorghum samples were inoculated with *L. acidophilus* and compared to control media (MRS broth and distilled water). The bacterial viability and pH were monitored during the 24-h fermentation, and the total phenolic and flavonoid content, antioxidant activity, reducing sugars, soluble protein content, and cellulolytic and esterolytic activities were analyzed from the extracted cell-free supernatant (CFS).

Sprouted sorghum supported the highest bacterial growth, with CFU increasing from 5.5 to 8.4 log CFU/ml up to the 24-h incubation. However, no significant increase in phenolic or flavonoid content was observed post-fermentation. A decrease in soluble protein content was noted after fermentation for both sorghum samples. Reducing sugar content was highest in sprouted sorghum, particularly in the unfermented samples. Notably, fermented non-sprouted sorghum showed elevated cellobiohydrolase and lipase activities, while sprouted sorghum fermentation led to a marked reduction in all tested enzymes.

These findings highlight the complex biochemical interactions during LAB fermentation, warranting further investigation to elucidate the underlying mechanisms. The probiotic-enriched sorghum ferment obtained can be used as a bioactive additive in functional food developments as it significantly supports the growth of lactic acid bacteria.

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MONITORING OF CARBAMAZEPINE PHARMACEUTICAL ACTIVE INGREDIENT IN RIVER DANUBE AND LAKE BALATON

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Carbamazepine (CBZ), a pharmaceutical active ingredient is extensively prescribed for the treatment of neurological disorders such as epilepsy, nerve pain, trigeminal neuralgia, and acute maniac or mixed episodes in bipolar disorder. As a result of its widespread use and environmental persistence, CBZ has been detected as a contaminant in aquatic environments, including rivers, ponds, and lakes. CBZ is almost entirely metabolized in humans, it is mainly excreted as hydroxylated and conjugated metabolites, with minimal (less than 2%) amounts eliminated unchanged. However, the continuous release to the environment, the low removal rate of wastewater (<45%) and sludge (<10%) treatment process resulted in a continuous pollution in surface water bodies [1–4].

In this study a systematic monitoring study was performed in 2024. To determine the concentration of CBZ in surface water bodies in Hungary, samples were collected at 10 and 8 sampling sites from River Danube and Lake Balaton were collected, respectively in 2024. Concentrations of the active ingredient were measured by an enzyme-linked fluorescent immunoassay (ELFIA) technique. In Lake Balaton, concentration of CBZ was above both the LOD value (0.02 ng/mL) and the LOQ value (0.03 ng/mL) for all samples (frequency of occurrence: 100%). The highest concentration was determined at the Révfülöp sampling site (4.77 ± 0.20 ng/mL), while the lowest concentration was measured at Zamárdi (0.03 ± 0.00 ng/mL). For the Danube River, average concentrations of CBZ on the first sampling date (2nd October 2024) during the flood period were determined mostly around the LOQ value (0.03 ng/mL). Only CBZ content of a sample from Dunaújváros was below the LOD value (0.02 ng/mL). The second sampling date (9th October 2024) was intentionally scheduled for after the flood period. Although, on that date, CBZ concentrations were below the LOD value at 3 sampling sites (Nagybajcs, Komárom, Baja), the concentrations at the remaining sites were 1.59–29.37 times higher than on the first sampling date. The results clearly demonstrated the beneficial effect of the flood on River Danube mostly diluting CBZ concentrations out.

Acknowledgements

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ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY STUDY OF ZINC METAL PHOSPHONATES IN SALINE SOLUTION

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Organic phosphonates such as diphosphonic acids, aminophosphonic acid, and hydroxyphosphonic acid have been the subject of more extensive studies. The structure of phosphonates affects corrosion inhibition efficiency (IE). The concentration of 1-hydroxyethane-1,1-diphosphonic acid (HEDP) influences IE. Therefore, a reduced concentration of HEDP is beneficial. In contrast, if the concentration of HEDP exceeds the optimal value, the protective efficiency decreases because the protective oxide layer dissolves. The primary mechanism that makes corrosion inhibitors effective lies in their ability to adsorb onto the metal surface or react with metal cations to form insoluble compounds. This process results in the formation of a protective layer that shields the metal from the surrounding corrosive environment, thereby blocking aggressive ions from reacting with the metal surface. In addition, phosphonic acids can react with metal cations to form stable, sparingly soluble compounds, further reducing the corrosion rate. These mechanisms are crucial for extending the lifespan of materials and improving the durability of metals exposed to harsh environments [1].

Electrochemical impedance spectroscopy spectra (EIS) (figure 1 and figure 2) were performed to evaluate the corrosive effect of chloride ion on iron in the absence and presence of organic phosphorus compounds. Before each determination, metal phosphonates were dissolved in 3% NaCl solution acidified to pH~2.5 adjusted with HNO₃. The examined metal phosphonates, ZnHEDP and ZnPA were hydrothermally synthesized at 80°C from Zn and HEDP and PA [2]. The impedance measurements were made using the FRA module of the Autolab 302N device, in the frequency range between 0.1-106 Hz and an AC amplitude of 10 mV. For each recorded spectrum, 60 points were collected, with a logarithmic distribution of 10 points per decade. Experimental EIS data were modeled with an electric equivalent circuit (ECE), using the modeling procedure of ZView 3.0 software (Scribner Associates, Inc.) to determine electrochemical parameters for this study.

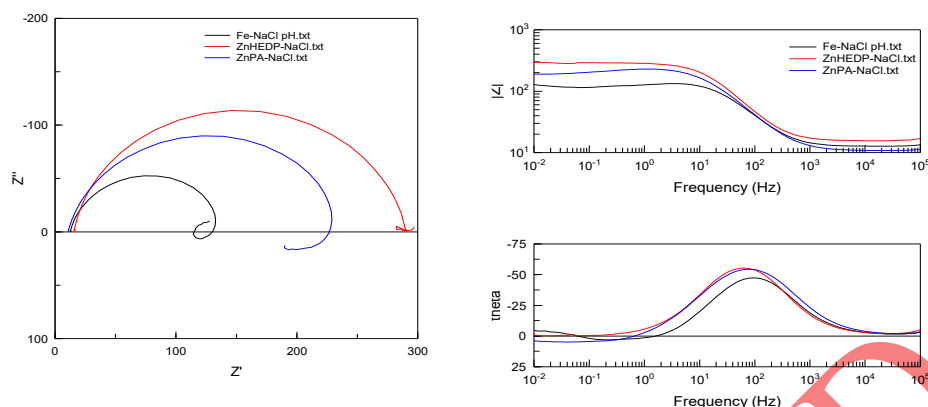


Figure 1. a) Nyquist plot, b) Bode representation (logarithm of the impedance modulus $|Z|$ and phase angle as a function of the logarithm of frequency f , recorded after 60 minutes immersion in 3% NaCl solution at pH 2.5, with and without inhibitor addition.

The values obtained for electrochemical parameters for iron immersed in ZnHEDP indicate the formation of a thicker and more compact layer in the presence of this metal-phosphonate during the first 60 minutes of immersion.

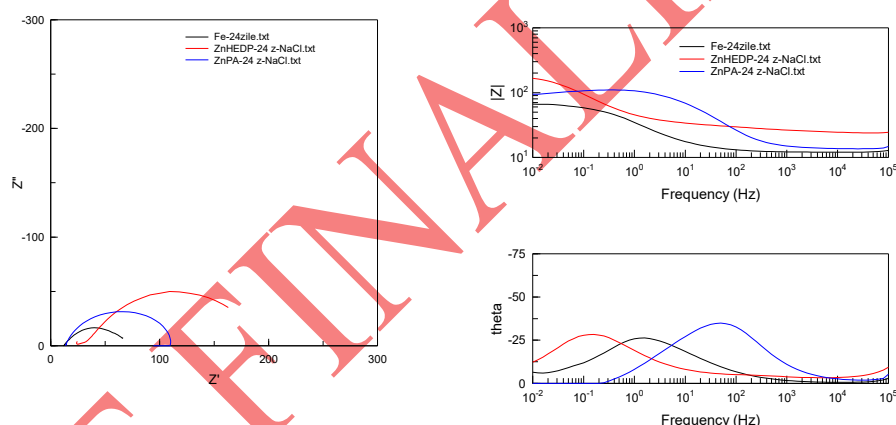


Figure 2. a) Nyquist plot, b) Bode representation (logarithm of the impedance modulus $|Z|$ and phase angle as a function of the logarithm of frequency f , recorded after 24 days immersion in 3% NaCl solution at pH 2.5, with and without inhibitor addition.

Analyzing the EIS data after 24 days of immersion, it was observed that the stability of the metal-phosphonates and the amount of phosphonic acid released and reaching the metal surface determine the effectiveness of the inhibitor. The released phosphonic acid has the ability to form Fe–O–P bonds.

The polarization resistance (R_p) values decrease in the order ZnHEDP > ZnPA > Fe. The lower R_p values for ZnPA are the result of the smaller amount of phosphonic acid released through hydrolytic attack, which leads to the formation of an incomplete layer on the iron surface. It is also possible that the ZnPA inhibitor is significantly more stable than the ZnHEDP compound.

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AN OVERVIEW OF SPECIFIC PORPHYRIN DERIVATIVE-INVOLVING STUDIES
REPORTED IN A TEN YEAR PERIOD AT THE INTERNATIONAL SYMPOSIUM
ON ANALYTICAL AND ENVIRONMENTAL PROBLEMS (ISAEP)

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Abstract

Between 2014 and 2024 Taranu *et al.* presented a total of nine studies relevant to porphyrin chemistry at ISAEP. Four of these were reported in 2014 and describe: a) an electrochemical corrosion protection investigation in acidic medium using pseudo-binary oxides and free-base porphyrins deposited on carbon steel substrate that outlined a maximum inhibition efficiency of 90.66 % for 5-(4-pyridyl)-10,15,20-tris(3,4-dimethoxy-phenyl)porphyrin [1]; b) the evaluation of the fluorescent properties of (5,10,15,20-tetraphenylporphinato) dichlorophosphorus(V) chloride in the presence of the toxic Pb^{2+} which led to an acceptable signal intensity–cation concentration correlation in the 10^{-2} - 10^{-6} M $\text{Pb}(\text{NO}_3)_2$ range [2]; c) the electrochemical study in acidic medium of the corrosion properties of 5,10,15,20-tetratolyl-21H,23H-porphyrin on carbon steel substrate which evidenced an inhibition efficiency of 50% [3] and d) the voltammetric and morphological characterization of glassy carbon electrodes modified with 5,10,15,20-tetra(allyloxy-phenyl)porphyrin [4]. The study published in 2018 concerns the applicability of a hybrid material containing Mn(III)-tetratolylporphyrin chloride and gold nanoparticles as sensor for the determination of 4-aminosalicylic acid [5]. A linear dependence between the hybrid material's absorption intensity and the analyte's concentration was found, with a correlation coefficient of 99.31% in the 2.88×10^{-5} M - 8.89×10^{-4} M range. The obtaining of 5,10,15,20-tetrakis(4-methoxyphenyl)porphyrin-modified graphite electrodes and the determination of their double-layer capacitance is described in a paper published in 2022 [6]. A highest value of 14.017 mF/cm^2 was determined. A similar study was published in 2023 [7]. It focuses on a graphite electrode modified with a mixture of $\text{Ni}_{11}(\text{HPO}_3)_8(\text{OH})_6$ and 5,10,15,20-tetrakis(4-methoxyphenyl)porphyrin and results in a double-layer capacitance value of 7.475 mF/cm^2 . In the same year, the aggregation behavior of 5,10,15,20-tetrakis(N-methyl-4-pyridyl)porphyrin-Zn(II) tetrachloride drop-casted from different organic solvents was analyzed *via* TEM and a variety of porphyrin aggregates was revealed and reported [8]. Lastly, a paper published in 2024 describes the TEM analysis of an organic-inorganic hybrid nanomaterial with 5-(4-carboxyphenyl)-5,10,15-tris(4-phenoxyphenyl)-porphyrin [9]. All these studies supplement the knowledge relevant to porphyrin chemistry and outline the contemporary scientific importance of porphyrins.

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HPLC-MS/MS-BASED METABOLOMIC ANALYSIS OF *PSEUDOMONAS* ISOLATES

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Field damage by phytopathogenic fungi can lead to significant crop losses, and their secondary metabolites can cause health risks in agricultural products. In plant protection, in addition to crop rotation, breeding resistant varieties, and using synthetic chemicals, biocontrol microorganisms such as *Bacillus*, *Streptomyces*, and *Pseudomonas* strains can also be used. However, their use is still limited due to variable efficiency, low market availability, and farmers' distrust.

In our study, the objective was to identify the metabolites responsible for the observed biocontrol effect in *Pseudomonas* isolates that had previously shown antagonistic activity against a selected *Aspergillus flavus* strain. To achieve this, we created a mass spectrometry database based on bioactive compounds previously reported in the literature to be produced by *Pseudomonas* species. Then we analysed the metabolite profiles of 50 isolates by HPLC-ESI-HRMS, and six of these strains showed antagonistic activity in previous experiments.

By analysing the databases and metabolite profiles, we identified known bioactive compounds produced by the isolates, including various biocontrol metabolites, siderophores, cyclic lipopeptides, quorum-sensing molecules, and structurally related compounds. On the basis of our comparative analyses, the presence of these compounds could not be responsible for the observed antagonistic effect. However, we detected seven compounds that could not be identified on the basis of the database and were produced exclusively by the isolates showing antagonistic activity. These compounds were characterised by mass spectrometry, and on the basis of the available experimental data, we proposed a structure for one of the metabolites.

3D-PRINTED DYNAMIC PROMOTER EFFICIENCY TESTING IN A LOW-PRESSURE MIXING CELL

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Abstract

The global population exceeding 8 billion places increasing pressure on natural resources, with the dairy industry emerging as a major consumer of water and generator of high strength wastewater. Owing to their elevated organic, protein, carbohydrate, and lipid content, dairy effluents pose serious environmental risks, including eutrophication and biodiversity loss. Sustainable management therefore requires advanced wastewater treatment strategies and the valorization of organic rich by products.

Membrane separation processes, particularly low-pressure ultrafiltration (UF), offer a promising approach. Literature indicates that turbulence promoting elements often 3D-printed and integrated into filtration cells enhance permeate flux and mitigate fouling. In this study, conducted in collaboration with the Membrane and Environmental Technology Research Group at the University of Szeged, we evaluated the performance of 3D-printed polylactic acid (PLA) promoters in UF treatment of model dairy wastewater.

Three custom designed promoters were tested, two fitting tightly (64.85 mm diameter) into the filtration cell and one (64 mm) rotating dynamically due to a looser fit. Our results aim to elucidate the impact of dynamic promoter motion on permeate flux, solute retention, and fouling behavior, thereby contributing to the development of more sustainable membrane-based wastewater treatment technologies.

Introduction

Currently, the global population has exceeded 8 billion, making it increasingly urgent to address whether our planet can provide sufficient food, drinking water, and energy for future generations while coping with emerging environmental challenges. Due to population growth and the economic development of emerging countries, global food demand is rising rapidly, which in turn significantly increases water consumption in food production. As one of the largest water consuming sectors, the food industry is also a major source of wastewater.

Among food industry effluents, dairy wastewater poses the greatest environmental risk. It's high protein, carbohydrate, lipid, and dry matter content often exceeds that of municipal wastewater several times over [1]. The elevated organic content of dairy effluents primarily originates from by products such as whey, cheese, butter, and curd residues generated during production [2]. If left untreated and discharged directly into the environment, these wastewaters can cause various ecological problems, including eutrophication and, consequently, a decline in biodiversity. Considering these impacts, it is crucial to adopt sustainable practices, modernize wastewater treatment, and effectively recycle high organic content by products.

Membrane separation processes offer a promising alternative for wastewater treatment due to their low energy requirements and ease of operation. Among these methods, ultrafiltration (UF), a pressure driven separation technique (including microfiltration, ultrafiltration, nanofiltration, and reverse osmosis), is particularly noteworthy. UF is capable of significantly reducing the organic content of dairy wastewater at relatively low pressures while maintaining

reasonably high permeate fluxes [3]. In this process, small molecular weight compounds, such as amino acids and disaccharides, pass through the membrane, whereas polymers, macromolecules, and whey proteins are retained. This makes *UF* particularly suitable for concentrating and recovering whey protein fractions, enabling the valorization of low-value by products into higher-value products [4].

Recent literature has increasingly focused on improving *UF* efficiency by enhancing membrane surface shear forces. One promising approach involves the use of flow modifying, turbulence enhancing elements known as promoters. These elements, which can be produced via 3D-printing, induce local turbulence when integrated into filtration cells or modules, thereby increasing permeate flux and reducing membrane fouling [5,6].

At the Membrane and Environmental Technology Research Group (*MEKÖKUT*) at the Department of Biosystems Engineering, Faculty of Engineering, University of Szeged, I applied 3D-printed turbulence promoting elements in my experiments. The aim was to achieve improved ultrafiltration performance of model dairy wastewater using purely physical methods, without adding chemicals, through low cost *PLA* and *PET* 3D-printed promoters. Building on the results obtained with the research group and under the guidance of my supervisor, we are developing solutions to modernize dairy wastewater treatment and enhance its sustainability[7,8].

Experimental

In my research, I aim to investigate the filtration efficiency of three identically designed, custom made *PLA* promoters. Preliminary results from our research group indicated that a “wagon wheel” like configuration, supplemented with columnar elements, improved filtration performance. Two of the three promoters have a diameter of 64.85 mm, perfectly fitting the O-ring in the filtration cell. However, due to a printing variation, one of the 3D-printed turbulence promoting elements was produced with a diameter of only 64 mm. This is particularly interesting because, despite the identical design, this element does not fit tightly in the cell and begins to rotate at 500 rpm. The primary objective of my study is to determine the effect of dynamic promoter motion on the efficiency of ultrafiltration membranes treating model dairy wastewater, as well as its influence on permeate flux, membrane retention (primarily regarding organic matter), and fouling behavior.



Figure 1. The tested 3D printed promoters.

Results and discussion

As my research is still in its early stages, I can provide precise results at a later time, however, my hypotheses are as follows: based on previous findings, in all cases, using a 400 rpm mixing speed and 3D-printed promoters led to a drastic improvement in the filtration performance of the 150 kDa *PES* membrane. The use of turbulence enhancing elements disrupts the laminar

flow profile of the boundary layer and induces local turbulence in the flow field, which increases permeate flux while significantly reducing fouling.

In the current study, experiments will be conducted at a 500 rpm mixing speed using the previously described promoters. I anticipate that the “wagon wheel” like configuration will allow the promoter to make minimal contact with the membrane, resulting in a greater improvement in filtration performance compared to previously tested configurations. The dynamic motion is expected to further delay membrane fouling, as the combination of mixing and additional flow phenomena will act on the system.

The promoters also feature small columnar patterns, which are expected to play an important role during filtration. Particles colliding with these structures can break into smaller fragments, facilitating filtration and helping to prevent potential irreversible membrane fouling.

Conclusion

Dynamic, 3D-printed promoters show significant potential for enhancing ultrafiltration efficiency in dairy wastewater treatment. By generating local turbulence and disrupting the laminar boundary layer, these promoters increase permeate flux and reduce membrane fouling. Promoters that are slightly smaller or loosely fitted introduce additional rotational motion, further improving mixing and delaying fouling. The “wagon wheel” like design, with small columnar features, minimizes direct membrane contact while promoting particle break-up, facilitating filtration and preventing irreversible blockages. This combination of effects not only enhances the reliability and performance of the ultrafiltration process but also enables selective retention and recovery of valuable components, such as whey proteins.

Beyond dairy wastewater treatment, dynamic promoters have broader applications in food processing, biotechnology, and chemical industries where high organic loads and fouling risks are common. By improving filtration efficiency, extending membrane lifespan, and supporting the valorization of organic by-products, dynamic promoters offer both environmental and economic benefits, contributing to more sustainable industrial practices.

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THE INFLUENCE OF WATER CONTENT ON THE MINERAL CONTENT OF *URTICA DIOICA* PLANT

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Abstract

Urtica dioica is a perennial species valued for its medicinal and nutritional potential. Its development is strongly influenced by water status, both in the soil and in the plant itself. Minerals play a crucial role in plant development, supporting key processes such as photosynthesis, protein synthesis, and stress resistance. The aim of this study was to investigate the influence of water content on the development and mineral content of *Urtica dioica* under natural conditions. Moisture and mineral contents were determined through thermogravimetric methods and portable spectrophotometric analysis. The results indicate that maximum hydration was recorded in spring, when moderate temperatures and balanced air humidity created favorable conditions for plant growth. In contrast, during summer, tissue water content declined while mineral concentration increased, even though rainfall and soil moisture were higher. This pattern highlights the decisive role of atmospheric conditions, particularly temperature and air humidity, in shaping the seasonal water balance of *Urtica dioica*.

Keywords: stinging nettle, climatic factors, seasonal variation, water availability

Introduction

Urtica dioica is a perennial species widely spread across Europe, traditionally harvested as both food and medicine. One important feature of the physiology of the plant is water content. Water is required for metabolism, photosynthesis, nutrient transport as well as turgor maintenance. It has been reported that there is a decreasing water content with maturity, which results in a relative increase of the minerals and secondary metabolites concentration [5, 9]. This change has consequences for more than just the plant's nutritional value [7], but it also affects how it reacts to stress. Beyond this relative increase, minerals themselves are essential drivers of plant metabolism, as they function as cofactors in enzymatic reactions, structural components of cell walls, and regulators of osmotic balance [1].

Environmental conditions have a crucial influence on this balance. Elements such as soil water supply, rainfall, air temperature, and humidity interact closely to shape the plant's hydration status [11].

The aim of the study is to investigate how the seasonal interplay between mineral accumulation and water content shapes the developmental process of *Urtica dioica*.

A distinctive characteristic of *Urtica dioica* is its flexibility in adjusting the levels of bioactive compounds and minerals under stress or at different growth stages. Evidence suggests that when exposed to drought, nettle plants can accumulate more phenolic substances and antioxidants, which act as protective responses [4]. Such adaptive plasticity is not limited to secondary metabolites; mineral nutrients like magnesium, calcium, and potassium also fluctuate with

growth stage and environmental stress, directly influencing photosynthetic capacity and tissue resilience [3].

Experimental

2.1. Collection and preparation of samples

Nettle plants and soil samples were collected from Bazoș area, Timiș County, Romania, over a four-month period: October 2024, January, April and July 2025.

Soil samples were manually cleaned of impurities (leaves, roots, stones), then passed through a 2 mm laboratory sieve. After moisture determination, they were dried at room temperature (25°C) and prepared for further analyses.

Plant material was rinsed with distilled water to remove dust and contaminants. Roots, stems, and leaves were separated, cut, and homogenized individually to ensure uniform and representative samples.

Climatic data (temperature, precipitation, and atmospheric humidity) were obtained from local meteorological sources [12].

2.2. Analysis of samples

The moisture content [%] of the soil and nettle samples was assessed through thermogravimetric analysis, as presented by Bordean (2013), employing a Sartorius scale [2].

The total mineral content of nettle samples (roots, stems, leaves and flowers) was assessed using a portable X-ray fluorescence (XRF) spectrometer, which provided rapid and non-destructive elemental analysis [8]. The concentrations obtained were further processed and calculated to ensure accurate quantification of the mineral profile.

2.3. Statistical analysis

The experimental data were processed using Microsoft Excel 2010, which was employed for data organization, descriptive statistics, and graphical representation of the results.

Results and discussion

In Figure 1, we can observe the seasonal variability of *Urtica dioica* water status and mineral concentration, and their dependence on both soil and atmospheric parameters. Rainfall influenced mineral dynamics indirectly, since higher precipitation and soil moisture did not always correspond to lower mineral concentrations, highlighting the stronger role of atmospheric conditions in shaping nutrient balance. Temperature rises were associated with increased mineral concentration, suggesting that heat stress not only reduced tissue hydration but also enhanced nutrient accumulation as part of the plant's adaptive response. The data clearly indicate that soil water availability alone is insufficient to explain plant hydration levels; instead, the balance between precipitation, soil retention capacity, air temperature, and relative humidity exerts a combined influence [11]. The rise in mineral concentration (471 g/kg DM) indicates water stress, as dehydration concentrates solutes, a common adaptive response to drought and heat [11]. Such mineral enrichment may not only be a passive concentration effect but can also represent an adaptive advantage, since elements like potassium regulate stomatal function, calcium strengthens cell walls, and magnesium maintains photosynthetic efficiency under stress [6, 10].

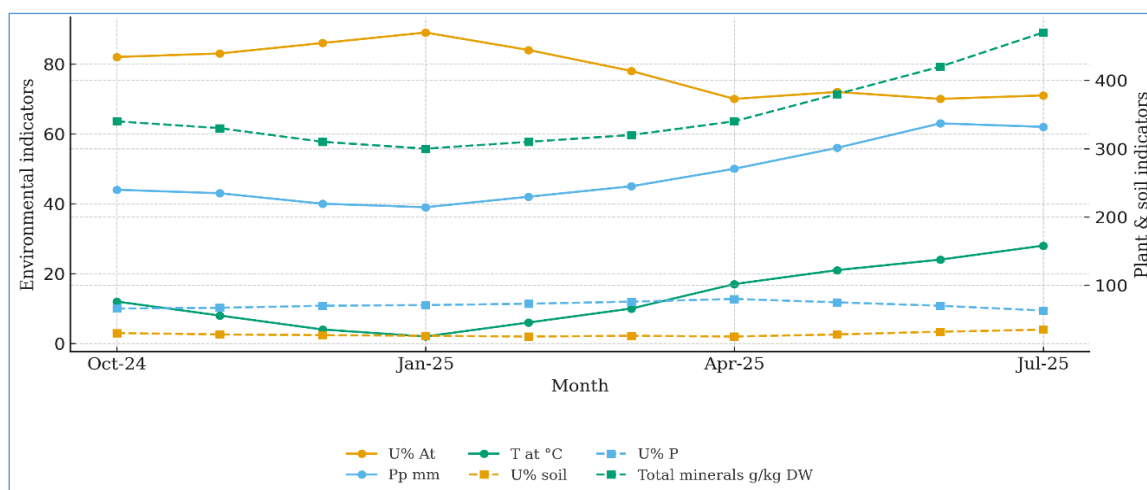


Figure 1. Seasonal Dynamics of Environmental and Plant Indicators (Oct-24 to Jul-25)

Legend: Oct-24=October 2024, Jan-25 =January 2025, Apr-25=April 2025

Jul-25=July 2025, U% soil= moisture content in the soil, U% P=Percentage of moisture content in *Urtica Dioica* plant, Total minerals g/kg DW=total mineral content in grams per kilogram of dry matter, U% At=Percentage of atmospheric humidity, Pp mm=Precipitation in millimeters (amount of rainfall), T at °C=Temperature in degrees Celsius.

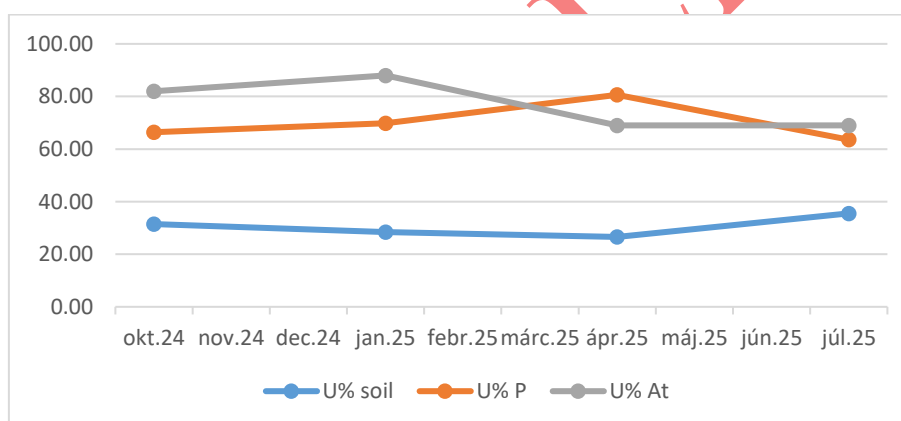


Figure 2. Comparison of Soil, Plant, and Air Moisture (Oct-24 to Jul-25)

In Figure 2, the seasonal changes of soil, plant, and air moisture in *Urtica dioica* are illustrated. Soil moisture dropped from autumn to spring, with the lowest point in April, then increased in July with higher rainfall. Plant water content followed another pattern, reaching its maximum in April under moderate temperature and balanced humidity. The plant was able to store more water even though the soil was relatively dry. By July, higher temperatures and lower air humidity reduced plant water content despite increased soil moisture. Atmospheric humidity peaked in winter but declined steadily with rising temperatures.

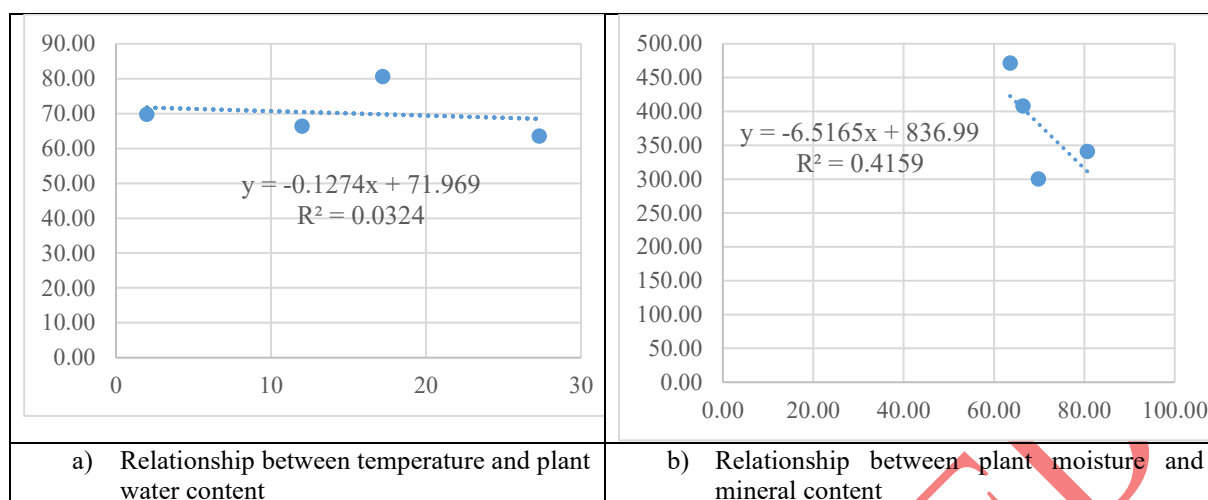


Figure 3. Association between investigated parameters

In Figure 3 a), the temperature trend and water content in the plant *Urtica dioica* are illustrated. The points show that as temperature rises, the plant contains less water in its tissues. The trendline reinforces a declining trend with slight slope but not greatly steep. The very low R^2 indicates that temperature cannot explain much of the variation in water content on its own. Other environmental factors, such as soil and atmospheric humidity, must play a larger role. The scatter plot reveals that as plant moisture increases, mineral content in *Urtica dioica* actually decreases (Figure 3 b). High tissue water in April (80.6%) corresponded to low mineral levels (340.9 g/kg SU), while reduced hydration in July (63.6%) coincided with the maximum (471.5 g/kg SU). This inverse pattern reflects both passive concentration through dehydration and active adjustment, as mineral accumulation aids osmotic balance and stress tolerance. Potassium, for instance, regulates stomatal aperture and water balance, calcium strengthens membranes and cell walls, while magnesium ensures chlorophyll stability and photosynthetic efficiency under fluctuating hydration [6,10].

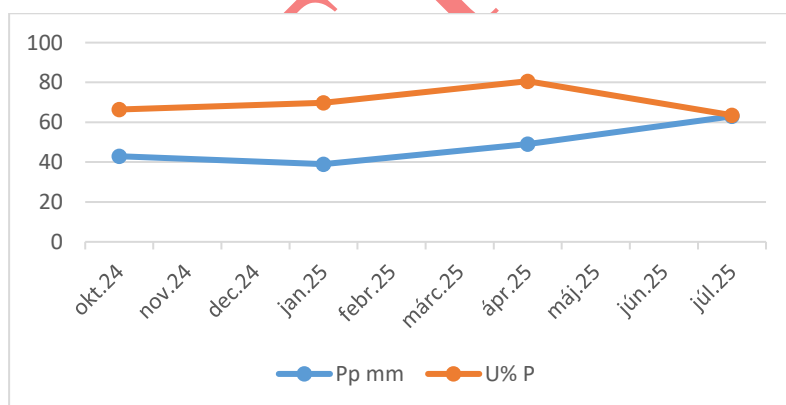


Figure 4. Effect of rainfall on plant moisture in *Urtica dioica*

Figure 4 shows that plant water content does not correlate with more rain. In April, *Urtica dioica* reached its maximum hydration (80.6%) with moderate rainfall, while in July, despite the highest rainfall (63 mm), plant moisture content dropped to 63.6%. This suggests that things like temperature and how much moisture is in the air have a greater impact on the water status of the plant than how much rain falls.

Conclusions

The analysis revealed that the growth of *Urtica dioica* is influenced by a variety of factors, such as soil conditions, climate, and plant physiology, rather than by rainfall alone. Spring was the most favorable period for hydration and growth, while summer imposed significant stress from high temperatures and low air humidity, even when soil moisture was plentiful. Minerals such as potassium, calcium, and magnesium play active roles in this adjustment by regulating stomatal behavior, reinforcing cell structure, and sustaining photosynthetic capacity, thereby enhancing the plant's tolerance to environmental stressors.

The inverse relationship between water content and mineral concentration reflects natural seasonal changes and the species' adaptive strategies under heat and drought stress. These results highlight the nettle's resilience and its ability to adapt its biochemical profile in response to environmental variations, providing valuable insights for ecological research and the sustainable use of this resource.

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STATISTICAL ANALYSIS METHODS IN EXPLAINING THE RELATIONSHIP BETWEEN THE BIOCONCENTRATION FACTOR AND MOLECULAR DESCRIPTORS - APPLICATIONS TO SMALL POLYCYCLIC AROMATIC HYDROCARBONS

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Abstract

The investigation of the chemical properties and potential environmental behavior of toxic compounds represents a subject of significant interest for researchers, as it allows them to develop strategies for protecting both human health and the integrity of the natural environment. In the present study, computational and statistical methods are employed to explore the relationship between the bioconcentration factor and surface area, polarizability, hydration energy, HOMO and LUMO energies, and the HOMO-LUMO gap, in a set of polycyclic aromatic hydrocarbon (PAH) molecules. This approach can be used as an alternative to existing QSAR methods to facilitate the assessment of bioaccumulation factors for a wider range of molecules, thereby extending the applicability of these existing procedures.

Introduction

The bioconcentration factor (BCF) can be defined as the ratio between the equilibrium concentration of a chemical in aquatic organisms and the corresponding concentration of the chemical dissolved in the surrounding aqueous environment: $BCF = C_f / C_w$. In the calculation formula, C_f (mg/kg) represents the steady-state concentration of the chemical within the organism (or the tissue) in question, while C_w (mg/L) represents the steady-state concentration of the chemical in the aquatic environment in which the organism is located [1,2]. The BCF is an estimate of a xenobiotic's tendency to concentrate and accumulate in an aquatic organism and is one of the most important criteria in both ecotoxicological assessment and hazard assessment [2,3]. The parameter most frequently employed as a preliminary screening tool to indicate bioaccumulation potential is the log P [4]. A variety of QSAR models utilize a range of theoretical molecular descriptors, encompassing molecular weight, connectivity indices, topological, geometric, or quantum-chemical descriptors, in addition to soil adsorption coefficients, fragment constants, and linear solvation energy relationships descriptors [5,6].

Polycyclic aromatic hydrocarbons (PAHs) are compounds constituted by two or more fused benzene rings, with varying structural configurations. The arrangement of the benzene rings determines the physical, chemical, and toxicological characteristics of the molecules. The behavior of PAHs in aquatic environments is contingent upon their chemical properties [7]. Numerous studies have been conducted over time to understand the distribution, fate, and environmental effects of this type of molecules, which have significant environmental and public health implications due to their presence in all environmental components, resistance to biodegradation, bioaccumulation potential, and carcinogenic activity. PAHs are considered among the first recognized environmental carcinogens that do not readily break down under natural conditions and have a persistence that increases with their molecular weight. Through environmental interactions, they may also contribute to pathogenic mechanisms such as DNA mutations, oxidative stress, protein dysfunction, or mitochondrial damage [8-10]. In order to better understand the impact of these compounds on human health and ecosystems, further

research into the mechanisms and models of PAH toxicity remains of paramount importance. The long-term goal is to develop more effective environmental protection strategies and implement appropriate measures to reduce the potential hazards posed by aromatic compounds [11].

In light of these considerations, the present study aims to evaluate the relationship between the toxicity (expressed as the bioconcentration factor) of a number of selected PAH molecules and several physical-chemical parameters, employing both computational and statistical techniques.

Experimental

The studied PAH molecules were drawn using HyperChem 8.0.10 software [12] and optimized using the ab initio, STO-3G basis set. Their physical-chemical parameters, generated at the same level include solvent-accessible surface area (S_A), polarizability (α), hydration energy (E_H), energy of HOMO and LUMO orbitals, and HOMO-LUMO gap (ΔE_{H-L}). The bioconcentration factor (BCF) was considered as a toxicity parameter and computed with ADMETlab 3.0 [13]. Statistical methods were used to analyze the data: Kolmogorov-Smirnov Test, Pearson correlation, and simple linear regression. All statistical calculations were performed using IBM SPSS Statistics 21 software.

Results and discussion

The PAH molecules in the working set are classified into four categories: linear catacondensates (LC), angular catacondensates (AC), angular pericondensates (AP), and cluster pericondensates (PC). Their surface area ranges from 341.37 to 553.95 ($M = 466.056$, $SD = 60.860$), the polarizability values range from 21.15 to 41.34 ($M = 34.098$, $SD = 6.117$), while the hydration energy values range from -3.89 to -1.63 ($M = -3.159$, $SD = 0.5366$). The highest recorded bioconcentration factor value ($M = 2.386$, $SD = 0.265$) is observed in the case of phenanthrene (3.091), while the lowest is observed for benzo(ghi)perylene (2.085). The physical-chemical and toxicity parameters are given in Table 1. Figure 1 shows the HOMO and LUMO distributions for several molecules in the working set belonging to the four classes.

Table 1. Molecular descriptors and the toxicity parameter of the selected PAHs

Name	Type	S_A	α	E_H	E_{HOMO}	E_{LUMO}	ΔE_{H-L}	BCF
Anthracene	LC	365.80	22.80	-2.69	-5.516	4.785	-10.301	3.069
Phenanthrene	AC	358.05	22.80	-2.59	-6.229	5.652	-11.880	3.091
Phenylene	CP	341.37	21.15	-1.63	-5.741	5.480	-11.221	2.601
Tetracene	LC	427.12	28.98	-3.09	-4.905	4.104	-9.010	2.254
Benz(a)anthracene	AC	421.50	28.98	-3.02	-6.222	5.541	-11.764	2.495
Chrysene	AC	415.03	28.98	-2.94	-5.864	5.209	-11.073	2.732
7H-Benzo(de)anthracene	AP	399.80	27.34	-2.19	-6.109	5.246	-11.355	2.973
Triphenylene	AC	421.75	28.98	-2.90	-6.209	5.609	-11.818	2.296
Pyrene	PC	375.25	25.50	-2.40	-5.506	4.787	-10.293	2.524
Pentacene	LC	491.89	35.16	-3.49	-5.472	4.871	-10.343	2.161
Benzo(a)naphthacene	AC	484.98	35.16	-3.42	-5.016	4.215	-9.232	2.270
Benzo(b)chrysene	AC	482.60	35.16	-3.37	-5.353	4.600	-9.953	2.359
Dibenz(a,h)anthracene	AC	480.00	35.16	-3.36	-5.621	4.958	-10.579	2.313
Pentaphene	AC	486.06	35.16	-3.45	-5.587	4.899	-10.486	2.203
Picene	AC	473.90	35.16	-3.30	-5.825	5.193	-11.018	2.455
Dibenz(a,c)anthracene	AC	475.08	35.16	-3.37	-5.658	4.940	-10.599	2.293
Perylene	AP	425.08	31.68	-2.75	-5.063	4.320	-9.382	2.198
Hexacene	LC	553.95	41.34	-3.89	-4.162	3.288	-7.449	2.095
Hexaphene	AC	533.12	41.34	-3.85	-5.095	4.289	-9.384	2.126

Benzo(a)pentacene	AC	551.90	41.34	-3.82	-4.580	3.727	-8.306	2.215
Dibenzo(a,j)naphthacene	AC	548.10	41.34	-3.76	-5.119	4.327	-9.446	2.362
Dibenzo(a,l)naphthacene	AC	543.31	41.34	-3.76	-5.122	4.327	-9.450	2.323
Dibenzo(a,h)pyrene	AP	488.67	37.87	-3.24	-4.787	3.996	-8.783	2.270
Dibenzo(a,e)pyrene	AP	485.57	37.87	-3.22	-5.277	4.550	-9.827	2.224
Benzo(pqr)picene	AP	490.96	37.87	-3.19	-5.158	4.410	-9.567	2.312
Naphtho(2,3-a)pyrene	AP	495.71	37.87	-3.25	-4.854	4.059	-8.912	2.376
Benzo(c)picene	AC	533.51	41.34	-3.66	-5.667	4.990	-10.657	2.407
Dibenzo(a,c)naphthacene	AC	541.06	41.34	-3.77	-5.091	4.281	-9.372	2.232
Anthanthrene	PC	447.50	34.39	-2.72	-4.774	3.940	-8.714	2.266
Benzo(ghi)perylene	AC	443.06	34.39	-2.68	-5.690	4.506	-10.197	2.085

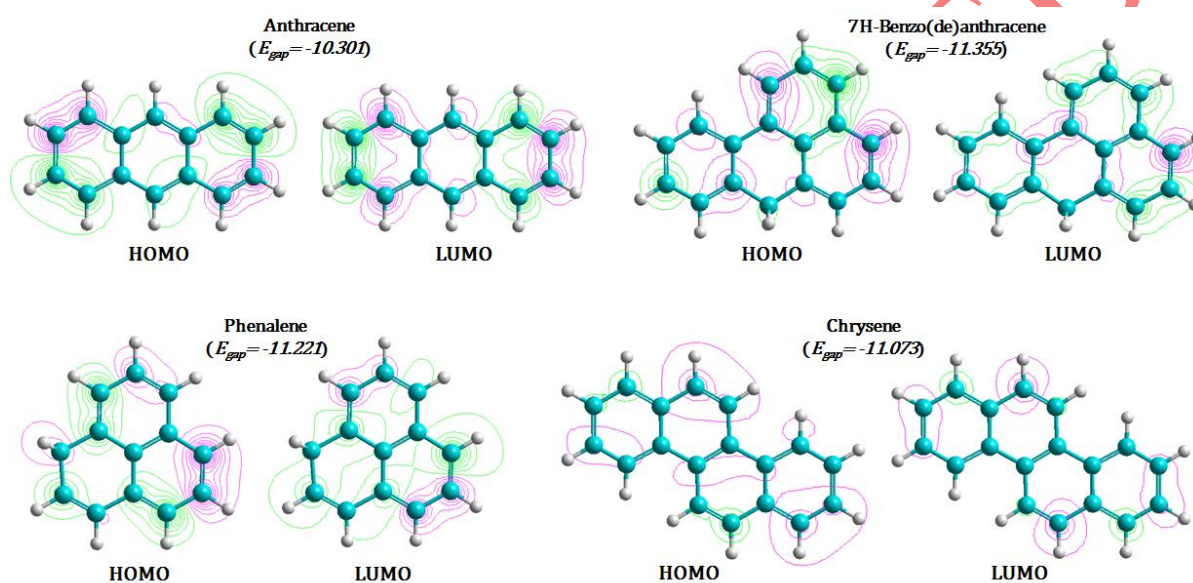


Figure 1. HOMO and LUMO distribution for several PAH molecules

The normality Kolmogorov-Smirnov Test returned $p > 0.05$ for all parameters, meaning that the data are normally distributed. As indicated by the Pearson analysis (Table 2) and following Schcher's interpretation [14], there is a moderate negative correlation observed between the bioconcentration factor and the surface area, the HOMO energy, and the HOMO-LUMO gap. Additionally, a strong negative correlation is observed between the bioconcentration factor and polarizability. Conversely, the bioconcentration factor shows a moderate positive correlation with hydration energy and LUMO energy. All correlations are statistically significant at the $p < 0.01$ level.

Table 2. Mean, standard deviation, and Pearson correlation coefficients for the studied variables ($N = 30$)

Variable	<i>M</i>	<i>SD</i>	<i>S_A</i>	α	<i>E_H</i>	<i>E_{HOMO}</i>	<i>E_{LUMO}</i>	ΔE_{H-L}
BCF	2.386	0.265	-0.648**	-0.709**	0.501**	-0.478**	0.494**	-0.488**
<i>S_A</i>	466.05	60.860	-	0.977**	-0.915**	0.550**	-0.575**	0.565**
α	34.098	6.117	-	-	-0.843**	0.551**	-0.585**	0.571**
<i>E_H</i>	-3.159	0.536	-	-	-	-0.436*	0.458**	-0.449**
<i>E_{HOMO}</i>	-5.375	0.510	-	-	-	-	-0.984**	0.996**
<i>E_{LUMO}</i>	4.636	0.585	-	-	-	-	-	-0.997**
ΔE_{gap}	-10.012	1.089	-	-	-	-	-	-

** $p < 0.01$, * $p < 0.05$

The relationship between the bioconcentration factor and the selected physical-chemical parameters was further investigated using simple linear regression, the results being presented in Table 3. The effect size was calculated using Cohen approach [15], after the formula:

$$f^2 = \frac{R^2}{1 - R^2} \quad (1)$$

Table 3. Results of simple regression analysis with the bioconcentration factor as dependent variable ($N = 30$)

Independent Variable	R^2	f^2	<i>B</i>	<i>SE_B</i>	β	<i>t</i>	<i>p</i>
Surface area solvent accessible	0.453	0.828	-0.003	0.001	-0.673	-4.818	< 0.001
Polarizability	0.502	1.008	-0.031	0.006	-0.708	-5.310	< 0.001
Hydration energy	0.327	0.485	0.283	0.077	0.571	3.684	0.001
HOMO energy	0.319	0.468	-0.294	0.081	-0.565	-3.621	0.001
LUMO energy	0.336	0.506	0.262	0.070	0.579	3.761	0.001
HOMO – LUMO gap	0.332	0.497	-0.140	0.038	-0.576	-3.729	0.001

The highest R^2 value was obtained for polarizability, followed by surface area; conversely, the lowest values corresponded to HOMO energy and hydration energy. Thus, polarizability accounts for approximately 50.2% of the variance of the bioconcentration factor, while surface area is responsible for 45.3% of the variation. In contrast, the HOMO energy accounts for only 31.9% of the variance, while the hydration energy accounts for 32.7%.

As indicated by the Cohen criteria [15], the effect size of hydration energy, HOMO energy, and HOMO-LUMO gap was moderate ($f^2 < 0.5$), large in the case of LUMO energy ($f^2 \approx 0.5$) and very large in the case of surface area ($f^2 \approx 0.8$). The highest value was obtained for polarizability ($f^2 = 1.008$), indicating that this parameter exerts the greatest influence on the bioconcentration factor. In contrast, the lowest effect size reported for HOMO energy indicates that this parameter exerts minimal influence on the bioconcentration factor.

Conclusion

The results of the correlation analysis indicate that an increase in the hydration energy and LUMO energies is associated with an increase in the value of the bioconcentration factor. Conversely, an increase in the polarizability, surface area, HOMO energy, and the HOMO-LUMO gap is predicted to result in a reversal of this effect. Regression analysis results indicate that polarizability may serve as an effective predictor when incorporated individually into a regression equation. Furthermore, the findings reveal that energy-related parameters contribute

to approximately 30% of the variation in the bioconcentration factor. As indicated by the effect size, it may be considered that the LUMO energy, surface area, and polarizability are the primary factors contributing to toxicity in the case of the studied molecules, meaning that these variables must be addressed in subsequent analyses. This study constitutes a preliminary investigation into the identification of the most suitable predictors for incorporation into multivariate analysis. Consequently, a novel predictive model can be developed to estimate the bioconcentration factor, thereby offering a potential alternative to existing models in literature.

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TOWARD Pt-FREE INDOOR DYE SENSITIZED SOLAR CELLS: PEDOT/GRAPHENE OXIDE SUSTAINABLE COUNTER ELECTRODES

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Abstract

Indoor photovoltaics are emerging as a key power source for IoT devices due to their ability to efficiently harvest LED and fluorescent light, with dye-sensitized solar cells (DSSCs) showing PCEs up to 34% under 1000 lux [1–4]. To enable sustainable large-scale deployment, Pt-free counter electrodes are needed, with PEDOT and PEDOT/graphene oxide hybrids [5] offering cost-effective, durable, and catalytically active alternatives.

In this work, we present a fast, environmentally friendly aqueous electrochemical deposition strategy to prepare Pt-free counter electrodes (CEs) composed of poly(3,4-ethylenedioxythiophene) (PEDOT) integrated with graphene oxide (GO). Characterization by XRD and Raman spectroscopy verified the successful incorporation of porous GO into the PEDOT framework, where strong π – π^* interactions promoted efficient charge transport.

The PEDOT/GO electrodes were evaluated for the first time in indoor DSSCs using two commercial LED sources and a quasi-solid I^-/I_3^- redox electrolyte. The optimized PEDOT/GO CE demonstrated superior electrocatalytic behavior ($\Delta E_p = 0.250$ mV; sheet resistance = 6.80 Ω/sq) and markedly improved device performance. Under 2700 K LED light, efficiency rose from 13.35% with PEDOT to 19.75% with PEDOT/GO, while illumination at 4000 K yielded a striking 60% gain, evidencing the synergistic catalytic contribution of GO. Importantly, the devices maintained stable operation for more than 720 hours.

Overall, PEDOT/GO hybrid electrodes provide a robust, sustainable alternative to Pt, combining high efficiency, durability, and eco-friendly fabrication, and represent a strong candidate for next-generation indoor DSSCs.

Acknowledgements

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USE OF HYDROQUINONE AS CORROSION INHIBITOR FOR CARBON STEEL IN ACETIC ACID / SODIUM ACETATE BUFFER SOLUTION

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Abstract

The present paper reports the results obtained in the research of the inhibitory effect of hydroquinone (HQ) on the corrosion of OLC 52 carbon steel in acetic acid 0.25 mol L⁻¹/sodium acetate 1 mol L⁻¹ buffer solution. The electrochemical stability of hydroquinone in the aggressive medium was analysed by cyclic voltammetry on platinum electrode within the potential window limited by hydrogen evolution reaction as cathodic limit and oxygen evolution reaction as anodic limit. Based on the potentiodynamic polarization curves (Figure 1), the surface coverage and inhibition efficiency have been determined (Table 1).

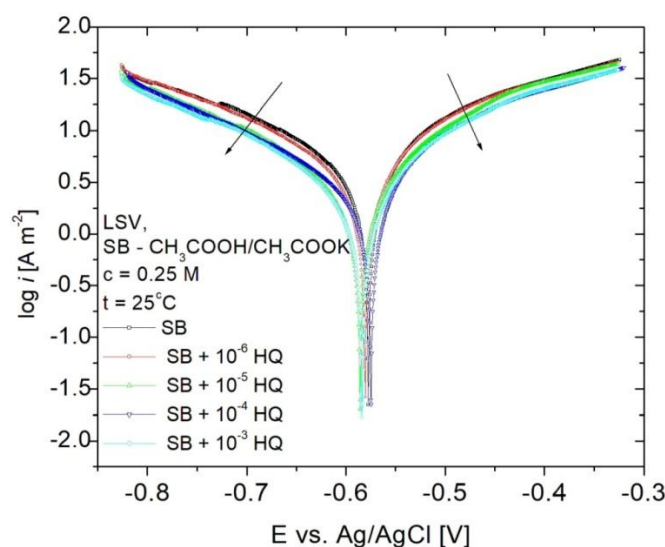


Fig. 1. Potentiodynamic polarization curves on Pt electrode in CH₃COOH 0.25 mol L⁻¹ / CH₃COOH 1 mol L⁻¹.

Table 1. Electrochemical parameters obtained by potentiodynamic polarization.

T [K]	Electrode	CHQ	E_{corr} [mV]	i_{corr} [$\mu\text{A}/\text{cm}^2$]	β_a	β_c	V_{corr}	IE [%]
							[mm/y]	
25	OLC52	0	-577.8	535.4	234	294	6.24	0.00
		1.00E-06	-581.8	330.3	152	216.7	3.84	38.30
		1.00E-05	-586.8	285.4	171	215	3.32	46.70
		1.00E-04	-575.0	239.6	138.8	209.3	2.79	55.24
		1.00E-03	-582.6	138.9	101.2	135.5	1.62	74.06

Molecular modeling have been employed to obtain the molecular descriptors of hydroquinone (Table 2), which provide information about its inhibitory capability.

Table 2.

E_{HOMO}	E_{LUMO}	ΔE [eV]	μ [Debye]	χ [eV]	η [eV]	σ [eV ⁻¹]	V [Å ³]	S [Å ²]	V/S [Å]
-7.02	-1.34	5.68	2.258	2.84	4.18	0.239	375	231	1.62

Based on the results presented, it can be appreciated that hydroquinone has an appreciable anticorrosive effect for OLC 52 even at low concentrations of 10^{-3} mol L⁻¹.

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EVALUATION OF SOME NUTRITIONAL PARAMETERS OF WILD ROSE HIP POWDER

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Abstract

Rosehip (*Rosa canina*) fruits are a valuable source of nutrients, widely appreciated for their nutritional value as well as their functional properties. This study aimed to evaluate the nutritional composition of powder obtained from rosehip fruits collected from wild flora. Standardized analytical methods were applied to determine several nutritional parameters, including moisture, mineral content (ash), protein, fat, crude fiber, and carbohydrates.

The results indicated that rosehip fruit powder contains considerable amounts of nutrients, with values varying depending on the origin of the fruits and the analyzed parameter: 10.45–11.06% moisture, 3.72–4.21% minerals, 4.78–5.56% protein, 2.11–2.66% fat, 8.54–9.11% crude fiber, and 68.31–70.05% carbohydrates.

These values demonstrate that the rosehip fruit powder obtained and analyzed in this experiment is a product rich in carbohydrates and fibers, with a moderate intake of proteins and minerals, low fat content and a low humidity level, which gives it stability and the possibility of long-term storage.

Taken together, these characteristics emphasize the nutritional potential of rosehip fruit powder and support its use as an ingredient in the development of functional foods with added nutritional value.

Keywords: Rosehip (*Rosa canina*), rosehip powder, nutritional composition, functional foods

Introduction

Wild rose hips, the fruits of *Rosa canina* L., are characterized by a balanced nutritional composition, being rich in carbohydrates (particularly dietary fiber) and minerals, and containing moderate amounts of proteins and lipids [1]. Proximate composition analyses highlight insoluble fibers, natural sugars, unsaturated fatty acids, and essential minerals such as calcium, magnesium, potassium, and iron [2]. In addition, rose hips are notable for their high levels of bioactive compounds—including polyphenols, flavonoids, carotenoids, and tannins—which contribute to strong antioxidant potential, as well as for their exceptional vitamin C content, a key determinant of their functional value [3,4].

Most previous research has focused on the bioactive profile of rose hips, with fewer studies addressing their nutritional composition. Nevertheless, available data show that, besides their bioactive richness, rose hips also provide significant amounts of essential nutrients [5–11], supporting their potential as a valuable source of functional ingredients in food formulations. According to the Frida fooddata.dk database, dried rosehip (*Rosa rugosa*) powder contains

94.2% dry matter, 5.8% water, 5.5% protein, 1.3% fat, 3.3% ash, 43.0% dietary fiber, 83.0% carbohydrates (by difference), and 40.0% available carbohydrates [5].

Comparative studies further illustrate variability in nutritional parameters depending on species, cultivar, and growing conditions. For instance, Shomirov et al. (2023) reported that dried wild rosehips contained 3.18% lipids, 5.89% protein, 4.1% ash, and 67.98% carbohydrates, with a high proportion of soluble fiber and simple sugars. Ivanova et al. (2023) found differences between wild and cultivated rosehips in Bulgaria, with wild fruits richer in protein and dietary fiber. Other studies confirmed that rosehip powders generally contain moderate protein (3–6%), low fat (<3%), appreciable fiber (8–39%), and a predominance of carbohydrates (38–70%) [7–11]. By-products of rosehip processing also retain nutritional value; for example, rosehip paste residues were reported to contain almost 7% protein, 3% fat, and over 37% crude fiber [12].

Overall, the nutritional composition of rosehip fruits and derived powders varies according to cultivar, climate, soil, ripening stage, and processing method [11]. Taken together, existing evidence highlights rosehip powder as a nutritionally valuable and functionally promising ingredient for the development of value-added foods [8–13].

Experimental

Fruit material

Fruits of rosehip (*Rosa canina* L.) were harvested in early October 2024, at full maturity (bright red color), from non-polluted areas suitable for culinary use. Approximately 1 kg of fruits was collected from three different locations, from which three composite samples were prepared. After removing damaged fruits and plant residues, the samples were washed and pre-dried for about 2–3 hours on filter paper. Subsequently, the fruits were dried in an oven at 55–60 °C for 8 hours. The dried fruits were ground using a household grinder, and the resulting powders were stored in polyethylene bags under refrigeration until analysis.

The rosehip fruit powders thus obtained were used as analytical material for determining moisture content, ash (minerals), protein, fat, crude fiber, and carbohydrates.

Analysis method

Standardized analytical methods used according to Velciov et al.'s recommendations, (2022) were applied to determine and nutritional parameters, including moisture, mineral content (ash), protein, fat, crude fiber, and carbohydrates [14,15]. For moisture content, dried apple peel powder was dried in an oven at 105°C to constant mass. The mineral substances (ash) were determined by the calcination method at 550°C. The protein content was determined by the Kjeldahl method, using a conversion factor for nitrogen of 6.25. The crude fat was determined using the Soxhlet method with hexane as solvent. Crude fibers were determined by using the method of acid base digestion. The carbohydrate content was obtained by difference. The crude fat was determined using the Soxhlet method with hexane as solvent. Crude fibers were determined by using the method of acid base digestion. The carbohydrate content was obtained by difference.

Table 1. Nutritional parameter values of rosehip (*Rosa canina*) powder obtained from fruits harvested in wild flora

Specification	Nutritional parameters, % from dry matter (DM)					
	Moisture	Ash	Protein	Fat	Brute fibre	Carbohydrates
Limits	10.45 – 11.06	3.72 – 4.21	4.78 – 5.36	2.11 - 2.66	8.54 - 9.11	68.31 - 70.05
Mean values	10.55±0.38	4.01± 0.20	4.99±0.26	2.34±0.23	8.91±0.26	69.16±0.71

Results and discussion

The results obtained from the analysis of the nutritional parameters of dried rosehip powder, harvested from plants grown in wild flora, are presented in Table 1.

The nutritional parameters of rosehip powders varied slightly depending on fruit origin, with values ranging between 10.45–11.06% moisture, 3.72–4.21% minerals, 4.78–5.56% protein, 2.11–2.66% fat, 8.54–9.11% crude fiber, and 68.31–70.05% carbohydrates. On average, the powders were characterized by high carbohydrate (69.16%) and dry matter content (89.45%), significant amounts of fiber (8.91%), protein (4.99%) and minerals (4.01%), and low fat levels (2.34%). These values, comparable to those reported by other authors, reflect the influence of cultivar, pedoclimatic conditions, and processing methods. The low moisture content supports microbial stability and longer shelf life, while bioactive compounds such as vitamin C, polyphenols, and carotenoids (not shown in the table) further enhance the functional and antioxidant value of rosehip powder as a potential ingredient for value-added foods.

The ash content of rosehip powders ranged between 3.72–4.21% (average 4.01%), indicating a considerable amount of minerals that can contribute to the intake of essential micro- and macroelements, thereby enhancing the biological value of food products. Protein levels were moderate (4.78–5.36%, average 4.99%), showing that although rosehips are not a primary protein source, they complement the nutritional profile of foods. Fat content was the lowest among the analyzed parameters (2.11–2.66%, average 2.34%), supporting the suitability of rosehip powder for formulations aimed at low-fat diets. Crude fiber was present in significant concentrations (8.54–9.11%), confirming the potential of rosehip powder as a valuable source of functional dietary fiber with beneficial effects on digestion, intestinal transit, and glycemic regulation. Carbohydrates represented the major component (68.31–70.05%, average 69.16%), providing energy while being balanced by the high fiber content. Overall, the nutritional profile supports the use of rosehip powder as a valuable ingredient for the development of foods with both nutritional and therapeutic value.

The analysis of proximate composition of rosehip (*Rosa canina*) powder obtained from fruits harvested in wild flora revealed a valuable profile, comparable to data reported in the scientific literature. Rosehip powder is characterized by a high content of carbohydrates and dry matter, a significant supply of crude fiber and minerals, as well as a moderate protein level. Its low fat content makes it suitable for food formulations with reduced lipid intake. The low moisture level enhances product stability and enables longer storage, while the richness in organic compounds and minerals supports its biological value. Therefore, rosehip powder represents a promising ingredient for the development of value-added foods, with potential applications both as a nutritional additive and as a functional component in various food products with prophylactic and therapeutic roles.

Conclusion

The results of the nutritional profile analysis of rosehip (*Rosa canina*) powders obtained from fruits grown in non-polluted wild flora indicated that they contain significant amounts of nutritional compounds, varying according to fruit origin and the analyzed parameter: 10.45–11.06% moisture, 3.72–4.21% minerals, 4.78–5.56% protein, 2.11–2.66% fat, 8.54–9.11% crude fiber, and 68.31–70.05% carbohydrates.

Rosehip powder is characterized by a high content of carbohydrates and dry matter, making it a nutritionally concentrated product. It is also an important source of crude fiber and minerals, with a moderate protein contribution. Its low-fat content makes rosehip powder suitable for diets with reduced lipid intake. Moreover, the low moisture level ensures storage stability and an extended shelf life. Altogether, these characteristics recommend rosehip powder as a valuable ingredient for the development of value-added foods.

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UNRAVELLING THE COMPLEXITY OF HUMAN BRAIN
GLYCOSAMINOGLYCANS: A STUDY OF CHONDROITIN/ DERMATAN
SULFATES BY ION MOBILITY MASS SPECTROMETRY

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Abstract

Glycosaminoglycans (GAGs), particularly chondroitin sulfate (CS) and dermatan sulfate (DS), regulate brain processes through specific sulfation motifs. We report the first application of ion mobility spectrometry (IMS) mass spectrometry (MS) to neural GAG analysis. CS/DS octamers from mouse brain were profiled, revealing separation by sulfation content and glucuronic acid type. Eighteen distinct DS-rich domains were identified, including rare under- and oversulfated motifs. IMS MS/MS further resolved isomers and uncovered unusual trisulfated and pentasulfated structures. This approach advances brain glycosaminoglycomics and highlights novel, potentially bioactive CS/DS domains.

Introduction

Glycosaminoglycans are sulfated, linear O-glycan chains abundantly present in the extracellular matrix (ECM). Among these, CS and DS play key roles in the brain, where the specific pattern and positioning of sulfate groups along the CS/DS chains influence a wide range of biological processes [1]. The structural complexity and diversity of neural hybrid CS/DS in the brain have driven significant efforts to develop analytical techniques capable of identifying both regular and irregular sulfation patterns. In this context, we present here the first application of IMS MS to the study of brain glycosaminoglycans.

Experimental

Brains from 14-week-old C57BL/6 wild-type mice were incubated overnight in 4 M guanidinium chloride. Following the centrifugation, the supernatant was dissolved in Tris/HCl (pH 7.4) containing 150 mM NaCl. The solution was applied on a DEAE-anion exchange column. GAG chains were released by β -elimination. Depolymerization of CS/DS was carried out by digestion with 1 mU chondroitin AC lyase, which cleaved the linkage between GalNAc and D-GlcA. The size fractionation was performed on a Superdex Peptide HR10/30 column. The pooled octamer fraction was dissolved in methanol to a concentration of 10 pmol/ μ L and submitted to IMS MS. The IMS MS experiments were performed on a Synapt G2S (Waters, Manchester, UK) with nanoESI source, tuned in the negative ion mode, running MassLynx (version V4.1, SCN 855) and Driftscope (version V2.7).

Results and discussion

IMS MS profiling revealed that the species were not only separated according to the charge state, but, most importantly, to the sulfation content and the saturated (GlcA) or unsaturated (4,5- Δ -GlcA) type of glucuronic acid. The high separation efficiency of the IMS MS allowed

the discrimination of 18 distinct DS-rich CS/DS domains, of which nine undersulfated, five oversulfated and four regularly sulfated. Except for the most common motif, the tetrasulfated-[4,5- Δ -GlcAGalNAc(DoAGalNAc)₃], several unusual under- and oversulfated, as well as saturated structures were discovered. Among these, of major importance is the pentasulfated-[4,5- Δ -GlcAGalNAc(DoAGalNAc)₃], for which the IMS MS/MS disclosed the incidence of two isomers. Moreover, the generated fragment ions revealed an uncommon trisulfated and an uncommon pentasulfated motif.

Conclusion

By IMS MS and MS/MS, introduced here for the first time in brain glycosaminoglycomics, neural CS/DS domains of atypical sulfation patterns were discovered and structurally characterized in detail. This workflow discriminated isomers, defined sulfation signatures, and revealed novel motifs, pointing to potentially bioactive brain GAG species.

Acknowledgements

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AWARENESS OF MICROPLASTIC POLLUTION

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Abstract

Microplastics are defined as plastic particles ranging in size from 100 nanometers to 5 millimeters. Their appearance is highly diverse in terms of color, size, and shape. These particles can originate during the manufacturing process or from the fragmentation of larger plastic objects. In most cases, they end up in the environment after use, where they threaten entire ecosystems along with the organisms living within them. In recent years, this type of pollution has reached such proportions that the European Union, in 2019, initiated the ban of single-use plastics (such as straws). In 2023, this regulation was further expanded to include measures addressing packaging waste and microplastic pollution. Given the anthropogenic origin of the problem, informing students currently in education about the severity of the issue is of key importance. Taking this into account, the aim of this study was to conduct a survey to assess how well high school and university students in Vojvodina region, the north part of Serbia, are informed about microplastic pollution and to explore potential differences between the two groups. The research was conducted using a questionnaire completed by 50 respondents (25 high school students and 25 university students). The survey consisted of 19 questions designed to evaluate the respondents' demographic data, knowledge, and attitudes towards the topic. The results revealed some surprising findings, as the correlation between awareness and educational level proved to be less significant than initially expected. It was also confirmed that the majority of respondents had already heard of microplastics, although they did not necessarily possess more detailed knowledge. The importance of this research lies in the fact that, despite the popularity of the topic, the number of similar surveys remains limited. This represents a major issue, as human attitudes are a factor that exerts a substantial influence on today's global plastic pollution problems. Looking ahead, it will be essential to complement scientific investigations with social perspectives, as the combination of these two approaches can become truly effective in combating microplastic pollution.

Keywords: microplastics, pollution, consequences, students, environment

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USING ENERGY SAVING FUNCTIONS: PERSONAL OPINIONS

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Abstract

Conscious management of energy is a socio-technical problem. The spread of energy-saving features in technical devices contributes to cost savings and helps address climate change issues. However, such features are only useful when they are in use. Understanding personal approaches to energy savings is crucial for effective policy development, regardless of the structure of energy production systems. The pilot study results presented in the paper demonstrate an experiment designed to explore personal opinions. Based on a sample of Hungarian higher education students (n=197), this analysis aims to explore grouping options for further research.

Introduction

The rising energy consumption of humankind is a complex technical and social problem. The distribution of energy production and consumption among countries is diverse, depending on the availability of resources, population, and socio-economic development. Of course, small countries like Hungary cannot be compared to big ones like the United States or China, but similar problems can be expected at the household level. According to the data from the Hungarian Central Statistical Office for 2023 [1], the primary energy use was 4,080.8 million tonnes of oil equivalent (mtoe) in China, 2,253.4 mtoe in the United States, and 1,299.9 mtoe in the 27 countries of the European Union. Within that, Hungary's use is 24.3 mtoe, Slovakia's use was 16.4 mtoe, and Romania's use was 30.8 mtoe. The latter data are highlighted because the population of Hungary is approximately twice that of Slovakia's and half that of Romania's, which is not proportional to the energy use data. At the same time, electrical and other appliances, including smart devices, computers, air conditioners, cars, heating systems, and numerous other tools and services, contribute to overall well-being. Goal 7 of the SDGs [2] aims to ensure access to affordable, reliable, sustainable, and modern energy for all, emphasizing the big problem that 675 million people (80% of whom are in Sub-Saharan Africa) still live in the dark. That suggests structural differences and the need for local investigations: while electricity is fundamental and decisive in many countries, others are excluded from it. Furthermore, the complexity of the problem is underlined by the SDGs. Using fossil energy sources primarily affects climate change (Goal 13). The appreciation of renewable energy [3] [4] is unable to resolve the issues by itself, partly because consumption is still growing. Energy efficiency efforts [5] [6] cover the engineering efforts in the field, but these are worthless if the users' approach does not comply. A comprehensive overview of the trends and challenges is beyond the scope of this paper; the emphasis is on presenting the results of a survey, the purpose of which is to explore personal approaches to energy savings. Without the acceptance and proper use of energy-saving features of the devices, the expansion of economic goods further increases energy demand. It seems that bothering with individual use of energy-saving features is pale in comparison to national and international-level issues, such as climate change or economic impacts through the resource prices because of recent wars [7]; and accurate measurement on an aggregated level of such features is extremely limited. Despite the above,

pioneering exploration experiments can contribute to model-building for policy-making purposes and supporting energy efficiency in product development.

Experimental

A voluntary online survey was designed to collect information about personal opinions about energy-saving functions and their utilization. The pilot survey results in this paper are based on the responses of 197 higher education students of business and social programs in Hungary. The sample composition is presented in Table 1.

Table 1. Sample characteristics

Grouping factor	Option	No of respondents	%
Gender	female	128	65.0
	male	69	35.0
Age	24 years old or less	127	64.5
	more than 24 years old	70	35.5
Level of studies	bachelor	114	57.9
	master	83	42.1
Own income	no	32	16.2
	partly	73	37.1
	yes	92	46.7

The goal of the study is to provide preliminary information about personal approaches to using energy-saving features of home devices and to identify potential patterns in opinions.

To measure the opinions (see Table 2), statements were formulated, and respondents were asked to indicate their level of agreement using a 7-point scale (1: strongly disagree, 7: strongly agree). The statistical analysis included the descriptives by questions and checking the differences by gender, age, and level of study by the Kruskal-Wallis H test ($p=0.05$). Having one's own income is also included by hypothesizing that paying the bills from one's own income tends to use energy more sparingly. An additional question asked the respondents to mark which devices they use with energy-saving features.

Results and discussion

Smartphones, tablets, notebooks, and lightning are the focus of energy savings, while desktop computers as well as other household appliances are out of this scope (Figure 1). Although the use of devices deemed important is frequent or continuous, these are not typically the ones with high consumption. It is encouraging that only 1,5% of the respondents noted not using any energy-saving features of the devices.

The mean values and the distribution of the responses (Table 2) suggest that energy-saving is considered a social expectation among the students. The belief in the usefulness of energy-saving features to improve well-being, reduce costs, and strive against environmental problems is high. The respondents did not find the use of the features difficult and did not reject buying such devices, but this is not the main factor in their decision. However, it is essential to consider whether some responses reflect only social expectations and do not accurately describe the actual behavioral intentions.

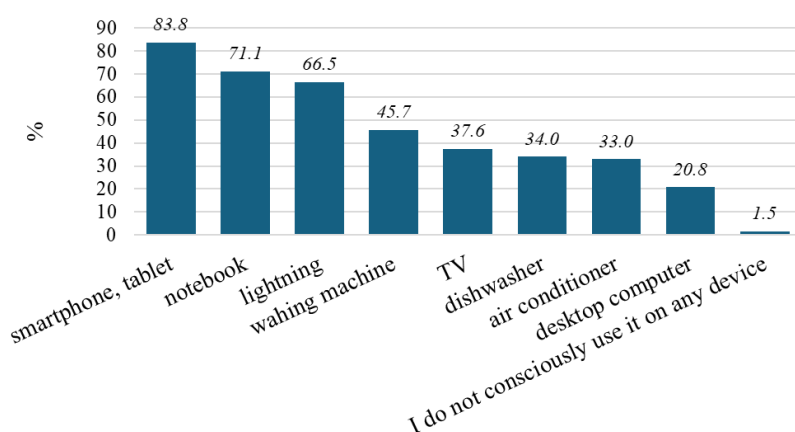


Figure 1. Using energy-saving features of the devices (% of the respondents)

Table 2. Descriptive statistics for the total sample (N=197)

	Mean	Std. Dev.	1 or 2 (%)	3, 4, or 5 (%)	6 or 7 (%)
Contribution: Energy-saving features of the devices...					
...help to reduce costs for me and my family.	5,43	1,333	2,5	47,7	49,8
...help to prevent global environmental problems.	4,85	1,463	7,1	59,4	33,5
...are worth a little discomfort.	5,13	1,397	4,5	49,2	46,2
...contribute to the well-being of society.	4,99	1,537	7,1	52,8	40,1
...help to increase the lifetime of the devices.	5,11	1,469	7,6	48,3	44,2
Personal aspects:					
Energy-saving features of the devices are easy to use.	5,68	1,219	1,5	38,5	59,9
Energy-saving options of the devices are not overcomplicated.	5,60	1,268	2,0	39,1	58,9
It will not take much time and effort to learn how to use energy-saving settings.	5,81	1,239	2,5	32,4	64,9
I have the knowledge, ability, and resources to use energy-saving options.	5,63	1,258	3,0	33,5	63,5
I intend to make efforts to save energy at home.	5,66	1,293	2,5	35,6	61,9
I measure or estimate my energy costs.	3,71	2,001	33,0	45,2	21,8
I prefer buying products with energy-saving features.	4,65	1,688	12,7	53,9	33,5
I usually buy energy-efficient household appliances.	4,63	1,696	12,7	52,3	35,0
I use energy-saving functions on many devices.	5,11	1,544	8,6	41,1	50,3
I encourage others to use energy-saving functions.	3,82	1,795	25,9	54,4	19,8
I always look for the energy-saving mode in the device settings.	4,31	1,761	19,3	50,8	29,9
I am satisfied with using the energy-saving features of the devices.	5,09	1,375	5,6	52,8	41,6

The sample shows a relatively uniform picture of the energy-saving features of devices. According to the contribution to well-being, the analysis found significant differences only by age. Elder respondents believe more that using these functions helps to reduce costs for the

family ($x_{\text{young}}=5,25$ $x_{\text{old}}=5,74$, Kruskal-Wallis $H=6,989$, $p=0,008$) and their contribution to preventing global environmental problems ($x_{\text{young}}=4,68$, $x_{\text{old}}=5,16$, Kruskal-Wallis $H=4,038$, $p=0,044$).

Among the personal aspects, females pay more attention to find the energy-saving mode in device settings ($x_{\text{female}}=4,55$ $x_{\text{male}}=3,86$, Kruskal-Wallis $H=7,692$, $p=0,006$), they are more satisfied with the features ($x_{\text{female}}=5,22$ $x_{\text{male}}=5,86$, Kruskal-Wallis $H=4,055$, $p=0,044$), and they more open to learn how to use them ($x_{\text{female}}=5,91$ $x_{\text{male}}=5,61$, Kruskal-Wallis $H=4,540$, $p=0,033$). Significant differences were found in the level of studies in the contribution of energy-saving features to well-being ($x_{\text{bachelor}}=5,20$, $x_{\text{master}}=4,71$, Kruskal-Wallis $H=4,163$, $p=0,041$) and increasing the lifetime of the device ($x_{\text{bachelor}}=5,29$, $x_{\text{master}}=4,86$, Kruskal-Wallis $H=4,013$, $p=0,045$), suggesting a more positive attitude of the bachelors compared to master students.

Table 3. Significant differences by the factor having his or her own income

Item	Mean value			Kruskal-Wallis H (df=2)	sig.
	No income	Partly	Having own income		
I measure or estimate my energy costs.	2.84	3.49	4.18	12.174	0.002
I prefer buying products with energy-saving features.	3.66	4.44	5.17	23.677	<.001
I usually buy energy-efficient household appliances.	3.44	4.6	5.08	25.224	<.001
I use energy-saving functions on many devices.	4.44	5.08	5.37	6.277	0.043
I always look for the energy-saving mode in the device settings.	3.44	4.32	4.61	10.594	0.005
I am satisfied with using the energy-saving features of the devices.	4.53	5.22	5.18	6.205	0.045

The results suggest, as hypothesized, that one's own income comes with greater responsibility; however, not all differences are significant (Table 3).

Conclusion

Saving energy is a social interest. New product development of corporations incorporates energy efficiency, partly due to policy and legal pressure. National and global results are measurable through energy production and consumption indicators; sustainability can be supported by increasing the share of renewable energy sources. Ultimately, technological development must be accepted and applied by households. Both measures and measurements are generating greater challenges at this level. Understanding the personal approaches and driving factors for energy-saving is essential to support future policy-making.

Considering that it is a pilot study, the generalization of the results is not possible. After validating the survey questions, a broader sample is required to test any hypothesis. Nevertheless, the survey results show that higher education students are aware of the energy-saving features of ICT tools and other household appliances; however, this awareness is not the primary driving force behind their product choices. It appears that small achievements are being made: devices with high power consumption are less in focus. At the same time, these devices

are in almost continuous use. A deep analysis is needed to build user profiles for estimating the energy use of individuals and households. Moreover, the hypothesis seems to be correct that managing one's own income has an impact on energy-conscious thinking; it is worth conducting further investigations in the field to map the influencing factors.

Acknowledgements

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MONITORING OF ORGANIC MATTER REMOVAL EFFICIENCY IN WASTEWATER AND SLUDGE TREATMENT PROCESSES BASED ON DIELECTRIC MEASUREMENTS

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Abstract

Organic compounds and the change of their concentration have effect on the polarizability of water molecules, ionic mobility and dielectric constant and loss. Measurements of dielectric parameters or electrical parameters related to the dielectric behavior (dielectric constant, dielectric loss, loss tangent, reflection coefficient, standing wave ratio, conductivity) can be gaining attention in water and wastewater quality monitoring because they can give non-destructive, rapid, and sensitive insights into changes in composition of multicomponent systems. These specifics allow early detection of process failures and real-time process control in continuously flow systems as well, such as wastewater purification technologies and bioreactors.

In our research wastewater and sludge samples of different types and origins (municipal, industry) as well as those originating from different stages of the purification/treatment process (raw wastewater, samples from clarifier, aeration step), were examined. A ZVL-3 (Rohde&Schwarz) VNA-connected open ended coaxial dielectric sensor (DAK 3.5, Speag) was used to measure the dielectric parameters in the 300-2400 MHz frequency range. The analytical parameters commonly used in wastewater and sludge treatment (pH, TS, TSS, COD, BOD, TN, TP) were also determined.

Our results verify that the change of concentration of organic pollutant (COD, BOD) show good correlation ($R^2 > 0.75$) with the dielectric parameters determined in the frequency range of 400-700 MHz. In this frequency range the effects of ionic conductivity is weaker, the dielectric parameters are influenced mainly by the polarization of water molecules, organic compounds, and interfacial polarization phenomena. The dielectric behaviour influenced by the polarization of water molecule and its interactions with other compounds, and the change in disruption of hydrogen bonding networks due to the change of dissolved organic matter fractions. These characteristics enable the organic content to be monitored during the process using a rapid, chemical-free dielectric method.

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PLASTICS HIT DIFFERENT: GRAM-NEGATIVE VS. GRAM-POSITIVE RESPONSES

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Abstract

The widespread use of agricultural plastics results in large amounts of microplastics (MPs) entering the environment, where their degradation and leaching processes may pose ecotoxicological risks not only to plants but also to microorganisms [1-2]. While phytotoxic effects of MPs have been relatively well-studied [3-5], their impacts on microbial species remain poorly understood. In this study, we investigated the toxicity of MPs derived from fresh and used polyethylene (PE) and biodegradable mulch films in aqueous medium (physiological saline). Two bacterial test species representing different cell wall structures were applied: the Gram-negative *Escherichia coli* and the Gram-positive *Bacillus licheniformis*. Microplastic suspensions were prepared at concentrations of 0.5% and 1% (w/v), and bacterial survival was assessed based on colony-forming unit (CFU) counts.

Our results revealed distinct sensitivity patterns: *E. coli* showed relatively high tolerance at lower MP concentrations, but its culturable cell numbers significantly decreased at 1% MP. In contrast, *B. licheniformis* exhibited pronounced sensitivity already at 0.5% MP, but no further significant decline was observed with increasing concentration. These responses suggest that both the physical interactions between MPs and cells (enhanced by agitation during incubation) and chemical leachates released from the plastics contributed to the observed toxic effects. Indeed, chemical characterization of MP leachates indicated increasing aromaticity and humification index with rising MP concentrations, confirming the role of dissolved compounds in bacterial stress responses.

Our findings highlight that agricultural MPs can negatively affect soil-relevant bacteria through multiple mechanisms, and that Gram-positive and Gram-negative taxa may respond differently to such stressors. These results contribute to a better understanding of how microplastics may alter microbial communities in terrestrial and aquatic environments.

Acknowledgements

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NOT FINALIZED

SYNTHESIS AND CHARACTERIZATION OF NITRIC OXIDE DONOR NANOSTRUCTURED DENDRITIC MESOPOROUS TETRASULFIDE-BRIDGED ORGANOSILICA WITH PROSPECTS FOR ENVIRONMENTAL APPLICATION

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Abstract

The objective of this study was to develop and optimize nanomaterials capable of enhancing the essential parameters of plant growth. To achieve this objective, nanoparticle-based nitric oxide (NO) donors and graphene oxide quantum dots (GQDs) were synthesized. Carbon quantum dots and graphene quantum dots (GQDs) exhibit minimal inhibition of the natural growth pathways of plants and have demonstrated potential to enhance growth while maintaining good biocompatibility. The NO donor was designed as nanostructured dendritic mesoporous tetrasulfide-bridged organosilica nanoparticles (DMON NPs), which have been modified with S-nitrosothiol (SNO) to facilitate a controlled and sustained release of NO. These characterizations are crucial to assess comprehensively the performance and potential applications of the nanoparticles in agricultural and plant biotechnology contexts.

Introduction

In response to various biotic (e.g., herbivores, pathogens, insects) and abiotic stress factors (e.g., drought, heavy metals, salinity), plants produce several redox molecules through enzymatic reactions to defend themselves. These highly reactive molecules, encompassing both free radicals and non-radical derivatives, include reactive oxygen species (ROS) and reactive nitrogen species (RNS). Although the excessive accumulation of these molecules can lead to oxidative burst, they are essential for homeostasis, self-defense, development, and hormonal signaling. Among the reactive oxygen and nitrogen species, nitric oxide (NO) is a predominant RNS. It is a diatomic, gaseous, uncharged free radical with a short lifespan, capable of migrating through both hydrophilic and hydrophobic regions of the cells (its existence spans three redox-active forms). NO rapidly reacts with other radicals and several other molecules. A notable example is its interaction with glutathione (GSH), to form a highly stable compound known as S-nitrosoglutathione (GSNO), which serves as a significant reservoir of NO within cells. However, the controlled delivery of NO to plants remains a challenge due to its instability and transient nature. For effective NO delivery in agricultural systems, dendritic mesoporous tetrasulfide-bridged organosilica nanoparticles (DMON) with S-nitrosothiol modification (DMON-SNO) were designed (Fig. 1).

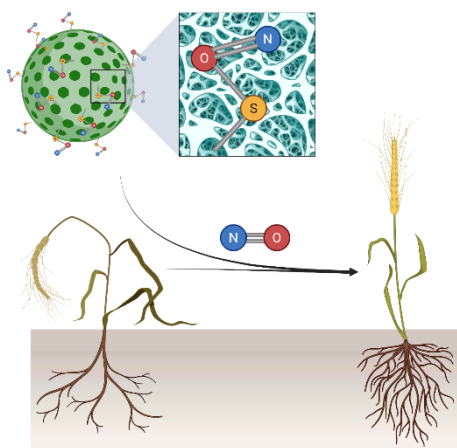


Fig 1.: Schematic figure of DMON-SNO and its effect to plant development as nitric oxide

Experimental

The DMON NPs were synthesized following a reported protocol. Firstly 380 mg of CTAB and 168 mg NaSal were added to the mixture of 25 ml deionized water and 68 mg of TEA. After this, 2 ml of TEOS and 1 ml of BTES were added and the mixture was vigorously stirred overnight at 80 °C. After an extraction of surfactant with 40 ml methanol and NaCl (25wt%) the product was centrifugated and collected.

For thiol modification 15 mg of the product was dispersed in 5 ml of ethanol. 150 μ l ammonium hydroxid (30 wt%) and 200 μ l MPTMS were added and stirred overnight at room temperature. The products were collected and washed with ethanol. For S-nitrosothiol modification 5 mg of these NPs were dispersed in 400 μ l of methanol and 200 μ l of 5 M HCl and stirred on ice. After cooling, a solution of 16 mg of NaNO₂ and 200 μ l of DTPA (500 μ M aqueous solution) was added to the mixture and stirred for 1 hour in dark and on ice. The DMON-SNO products were collected and washed twice with DTPA and methanol.

Results and discussion

The successful syntheses of DMON nanoparticles were validated using several physicochemical characterization methods including transmission electron microscopy (TEM), X-ray diffraction (XRD), dynamic light scattering (DLS) and ultraviolet-visible spectroscopy (UV-Vis) measurements (Fig. 2).

The chraracteristic of XRD pattern show one wide peak with spacings d of 21,36 Å. This large distance is characteristic of the mesostructure (pore structure).

Transmission electron microscopy was utilized to determine the size and morphological characteristics of the nanoparticles, with results detailed in Fig. 2B. The DMON nanoparticles were found to be spherical in shape, with an average size of approximately 200 nm.

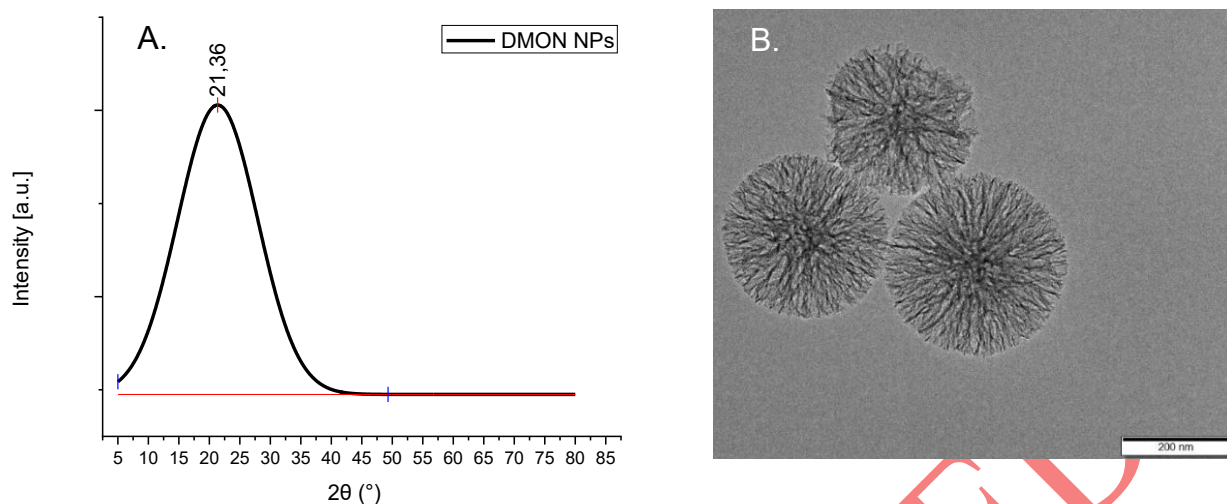


Fig 2.: A. X-ray diffraction pattern of DMON NPs;
B. Transmission electron microscopy image of DMON NPs

Ultraviolet-visible spectroscopy facilitated the measurement of localized surface plasmon resonance, revealing peaks at 320.75, 447.8, and 875.40 nm, which are consistent with values reported in the literature. Following thiol modification, new peaks emerged within the 478-528 nm range, confirming the successful functionalization, as illustrated in Fig. 3. The nitroso thiol modification was successful according to the color change of the product however the release speed needed to be examined further. Moreover the color was disappeared after a day. Dynamic light scattering analysis indicated that nanoparticles predominantly had a diameter of 220 nm and they exhibited a zeta potential of -11.4 mV.

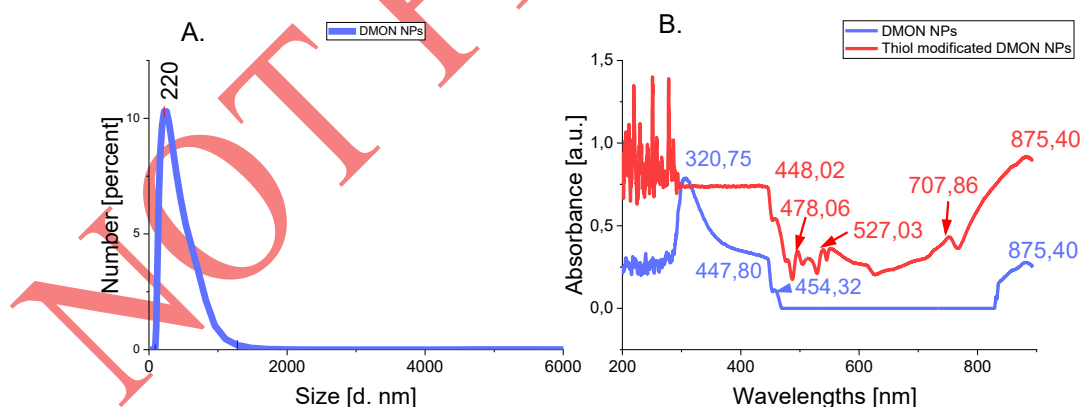


Fig 3.: A. Dynamic light scattering size distribution of DMON NPs by number; B. UV- visible light absorption spectra of DMON NPs and thiol modified DMON NPs

Conclusion

In conclusion, this study demonstrated the successful synthesis of dendritic mesoporous tetrasulfide-bridged organosilica. The products were homogeneous and spherical shaped, which were verified by dynamic light scattering and transmission electron microscopy measurements.

The product was suitable for both thiol and S- nitrosothiol modification. However, the release rate and ratio of NO content require further investigation. The UV-VIS characterisation results revealed distinct spectral peaks corresponding to both the modified forms and the initial DMON. This research anticipates the promising applications of DMON-SNO in promoting plant growth and development via the functional benefits of NO.

Acknowledgements

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PM10 AND PM2.5 EMISSION AND ANALYSIS FROM RESIDENTAL COMPLEX CONSTRUCION SITE IN SREMSKA KAMENICA, SERBIA

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Abstract

Construction sites are recognized as significant non-industrial sources of particulate matter (PM10 and PM2.5), contributing to the degradation of urban air quality and posing health risks for workers and nearby residents. The research quantified emissions from a residential complex construction site in Sremska Kamenica, Serbia, by applying the EMEP/EEA Air Pollutant Emission Inventory Guidebook (Tier 1 methodology). The active construction area was defined as 3,500 m², operating under a continuous 365-day work schedule. Annual emissions were estimated at 207 kg for PM10 and 59.5 kg for PM2.5, corresponding to daily emissions of 568 g and 163 g, respectively. Dispersion modeling using a box approach yielded hourly average concentrations of 112 µg/m³ for PM10 and 11.2 µg/m³ for PM2.5. Risk assessment, based on a 10-hour work shift and an inhalation rate of 1.25 m³/h, indicated daily doses of 1,400 µg of PM10 and 140 µg of PM2.5 per worker. When compared with WHO Air Quality Guidelines, PM2.5 remained within acceptable levels, while PM10 concentrations exceeded recommended thresholds by more than 2.5 times, yielding a Hazard Quotient of 2.49. These findings identify PM10 as the dominant polluting substance of concern, highlighting the necessity of implementing dust suppression measures such as watering, soil stabilization, vehicle speed control, and protective equipment.

Introduction

Suspended particulate matter (PM10 and PM2.5) is recognized as one of the most critical polluting substances in urban air, exerting a direct influence on public health and environmental quality [1]. Prolonged exposure to elevated concentrations of airborne particles has been linked to increased incidence of respiratory and cardiovascular diseases, as well as reduced overall life expectancy [2], [3]. According to the World Health Organization (WHO), there is no safe threshold for exposure to particulate matter, which underscores the importance of accurate monitoring and reliable emission assessment, particularly in urban areas undergoing rapid development.

Construction activities are among the most significant non-industrial sources of particulate matter emissions. Processes such as excavation, demolition, material handling, on-site transport, and equipment movement disturb soil and release dust into the atmosphere [4], [5]. Although temporary in nature, these emissions can lead to substantial short-term degradation of local air quality. Their impact is especially pronounced in densely populated areas where ventilation is limited and background pollution levels are already elevated.

Experimental

The observed construction site is situated in Sremska Kamenica (45°13'29"N, 19°51'23"E), a suburban settlement of Novi Sad, Serbia, positioned along the right bank of the Danube River (Figure 1.). The Parcel is 16,814 m² while estimated construction area is 10,000 m², as project is designed in 3 phases the observer area in the research covers a 3,500 m² complex, embedded

within a mixed-use urban environment. The immediate surroundings are characterized by low-rise residential housing, local commercial facilities, and public service infrastructure, with arterial roads of moderate traffic intensity contributing additional background air pollution. In the vicinity of the construction site is Institute of Cardiovascular Diseases, Sremska Kamenica, which is regional healthcare center. Vegetation is present in the form of fragmented green corridors and riverside belts; however, the effective Leaf Area Index is relatively low, providing limited mitigation capacity against airborne particulate matter. Due to the site's position within a partially enclosed urban canopy, natural ventilation is constrained, particularly under meteorological conditions of low wind speed and atmospheric stability. This creates conditions in which construction-generated dust can accumulate locally, significantly elevating ambient concentrations of PM₁₀ and PM_{2.5} and thus intensifying exposure risks for workers and nearby residents.



Figure 1. Residential complex construction site location in Sremska Kamenica, Serbia

The quantification of particulate matter (PM₁₀ and PM_{2.5}) emissions from the construction site was performed by applying the EMEP/EEA Air Pollutant Emission Inventory Guidebook (Tier 1 methodology). This methodology provides default emission factors for construction activities, expressed per unit area, and represents a transparent baseline for dust emission estimates in the absence of local measurements.

The active construction zone was defined as 3,500 m² (0.35 ha). Using Tier 1 factors, this produced 207 kg/year of PM₁₀ and 59.5 kg/year of PM_{2.5}. Unlike conventional approaches that distribute annual emissions over a standard working year of 250 days, in this scenario we used the real data from investors, where they have been working continuous operation over 365

days without interruption. Under these conditions, the calculated daily emissions were 568 g/day for PM₁₀ and 163 g/day for PM_{2.5}.

To estimate near-ground concentrations, a box-model dispersion approach was applied. The control volume was defined as the active surface (3,500 m²) with a mixing height of 10 m, yielding a dispersion volume of 35,000 m³. Daily emissions were divided by this volume to obtain average concentrations of 16.2 µg/m³ for PM₁₀ and 4.7 µg/m³ for PM_{2.5}. Assuming uniform distribution of emissions across the working day, the hourly concentrations were determined as 112 µg/m³ for PM₁₀ and 11.2 µg/m³ for PM_{2.5}.

The risk assessment was performed using the modeled concentrations. Worker exposure was evaluated under the assumption of 10-hour workdays, with an inhalation rate of 1.25 m³/h, yielding daily inhaled doses of approximately 1,400 µg/day for PM₁₀ and 140 µg/day for PM_{2.5}. A hazard quotient (HQ) approach was applied to assess non-carcinogenic risk, defined as the ratio of observed concentration to the reference value.

Results and discussion

Using the EMEP/EEA Tier 1 methodology, annual emissions for the 3,500 m² active construction zone were calculated as 207 kg/year (568 g/day) for PM₁₀ and 59.5 kg/year (163 g/day) for PM_{2.5}. By applying a box-model dispersion, distributed across the workday, hourly averages were 112 µg/m³ for PM₁₀ and 11.2 µg/m³ for PM_{2.5}. Modeled PM emission values are presented in Table 1. Assuming a 10-hour work shift with an inhalation rate of 1.25 m³/h, the estimated inhaled doses per worker were:

- 1,400 µg/day for PM₁₀
- 140 µg/day for PM_{2.5}

Table 2. PM emission modeled values

Pollutant	Modeled Concentration (µg/m ³)	WHO limits (µg/m ³)	Hazard Quotient
PM ₁₀	112	45	2.49
PM _{2.5}	11.2	15	0.75

The HQ for PM₁₀ was 2.49, indicating that concentrations substantially exceed WHO health-based thresholds, and therefore represent an unacceptable level of risk under continuous exposure. In contrast, the HQ for PM_{2.5} was 0.75, remaining below the guideline value and within acceptable limits, though chronic exposure could still contribute to cumulative health effects.

The results demonstrate that PM₁₀ concentrations exceed WHO air quality guidelines by approximately 2.5 times, representing an unacceptable risk level under continuous exposure. PM_{2.5} concentrations remain below the threshold but contribute to cumulative inhaled dose, particularly under year-round exposure conditions.

When compared to OSHA occupational exposure limits (5,000 µg/m³ for respirable dust), both pollutants are well below regulatory thresholds. However, OSHA standards are not designed to protect against long-term health impacts, while WHO guidelines are explicitly health-based. For this reason, PM₁₀ exposure remains the primary concern in terms of worker health and long-term morbidity. This indicates that PM₁₀ emissions require immediate attention, and that effective dust suppression measures — such as watering, soil stabilization, vehicle speed limits, and protective equipment — should be implemented to reduce risks.

Conclusion

The research applied the EMEP/EEA Tier 1 methodology to quantify emissions of suspended particulate matter from a construction site in Sremska Kamenica, with a focus on a 3,500 m² active area operating continuously for 365 days per year. The results indicate that annual emissions amount to approximately 207 kg of PM₁₀ and 59.5 kg of PM_{2.5}, corresponding to daily emissions of 568 g and 163 g, respectively.

Dispersion modeling using a simplified box approach yielded hourly concentrations of 112 µg/m³ for PM₁₀ and 11.2 µg/m³ for PM_{2.5}. When compared with the WHO Air Quality Guidelines, PM_{2.5} levels remain within acceptable limits, while PM₁₀ concentrations exceed recommended thresholds by more than 2.5 times, resulting in a Hazard Quotient of 2.49. This categorizes PM₁₀ exposure as a high-risk condition under continuous operation, while PM_{2.5} remains in the low-to-medium risk range.

The findings highlight PM₁₀ as the dominant polluting substance of concern for occupational exposure on construction sites. Although absolute concentrations are far below OSHA occupational exposure limits, these values do not account for long-term health impacts. Continuous exposure, especially during 10-hour work shifts, increases daily inhaled doses and raises the likelihood of adverse respiratory outcomes.

In conclusion, while Tier 1 modeling provides a conservative upper-bound estimate, it clearly demonstrates the necessity of implementing PM suppression measures (e.g., watering, soil stabilization, speed control, protective equipment) to mitigate worker exposure.

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EVALUATION OF ENERGY EFFICIENCY MEASURES IN PUBLIC INSTITUTIONS

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Abstract

This paper presents an empirical study on the energy efficiency of kindergartens in the city of Zrenjanin, Republic of Serbia, conducted in 2023. The research evaluated the implementation of basic energy efficiency measures across all 19 kindergartens, focusing on the differences between new and old buildings. A structured questionnaire was sent directly to the official email addresses of each kindergarten, and responses were linked to specific institutions. A survey was carried out covering key aspects such as wall and attic thermal insulation, type of windows and doors, lighting systems, heating and domestic hot water supply, as well as the quality of window and door sealing. Results revealed that energy efficiency is generally poor: only two kindergartens, Alisa u zemlji čuda and Bubamara, both constructed after 2010, met most criteria. Notably, 17 out of 19 kindergartens still use incandescent bulbs, and all rely on electric boilers for water heating, the least efficient option. External wall insulation exists in only five facilities, and roof insulation is present in just one.

Introduction

Energy efficiency represents the ratio between the benefit obtained (product or service) and the energy invested, and it can be improved not only by reducing energy consumption but also by optimizing this ratio. Unlike energy saving, which implies certain compromises, efficient energy use does not reduce comfort or working conditions; it enables the same amount of products or services to be delivered with lower energy consumption, resulting in financial savings. In buildings intended for human occupancy, ensuring the required level of comfort demands energy for heating, cooling, and ventilation. The total energy consumption depends on external factors (such as climate), as well as on the building's own energy characteristics and the duration of the required comfort conditions, the less energy needed to maintain the prescribed indoor comfort, the more energy-efficient the building is [1-3].

The characteristics of buildings in the Republic of Serbia in terms of energy efficiency largely depend on their period of construction. Buildings constructed before 1950 are characterized by massive, thick walls, with average heat losses between 200 and 250 kWh/m². After 1950, construction involved the use of new materials without any thermal requirements, and from 1970 onwards, mass construction of slender and thin structures with large glass surfaces began, which have extremely poor thermal performance, with average heat losses reaching up to 300 kWh/m². Buildings constructed between 1987 and September 2012 exhibit average thermal quality, with heat losses around 150 kWh/m². Studies and experiences with increasing the thermal insulation of exterior walls have shown that it is most effective to target buildings constructed before 1987, where energy savings of up to 70% can be achieved [2-5].

Experimental

The study employed a quantitative, survey-based methodology targeting all 19 kindergartens in Zrenjanin. The questionnaire was distributed via email in 2023 and included 11 structured questions covering the following aspects: year of construction, presence of external thermal

insulation, roof insulation, window type (wooden single/double glazing, PVC, aluminum), lighting type (incandescent, compact fluorescent, LED), heating system (gas, district heating, electric heaters, heat pumps), water heating method, perceived airtightness of windows and doors (rated on a 1–5 scale), and plans for future energy efficiency investments. The collected data were compared across kindergartens based on key characteristics, such as the year of construction, to identify patterns and differences in energy efficiency measures.

Results and discussion

The energy efficiency measure with the lowest impact on institutional budgets is the use of energy-efficient light bulbs (LED or compact fluorescent lamps). Survey results indicated that 17 out of 19 kindergartens continue to use incandescent bulbs, which do not contribute to building energy efficiency. The kindergartens that have adopted energy-efficient lighting are Alisa u zemlji čuda (compact fluorescent lamps) and Bubamara (LED bulbs). These two kindergartens are also the only facilities constructed after 2010, reflecting greater attention to energy efficiency in newer buildings compared to older ones, which were built when energy efficiency was less of a priority.

All kindergartens rely on electric boilers for water heating, which is the least economically and energetically efficient option. Regarding attic insulation, 18 kindergartens reported the absence of insulation, resulting in significant heat loss. Concerning windows, 9 kindergartens (47.3%) have energy-efficient window frames, while 10 (52.7%) do not. However, the presence of energy-efficient windows does not automatically guarantee energy savings; proper installation and quality are essential for achieving efficiency. Using a 1–5 scale to assess airtightness, energy-efficient windows received an average score of 3.77, and less efficient windows scored 2.4, highlighting the importance of window upgrades in Zrenjanin kindergartens.

Only 5 out of 19 kindergartens have external thermal insulation. Furthermore, only 4 kindergartens (Alisa u zemlji čuda, Bubamara, Kolibri, and Snežana) combine energy-efficient windows with external insulation, and only two buildings (Alisa u zemlji čuda and Bubamara) also use energy-efficient lighting. These two buildings were constructed after 2010. For space heating, 12 kindergartens use gas, while 6 rely on district heating (city network: natural gas and fuel oil).

Conclusion

The study showed that the energy efficiency of kindergartens in Zrenjanin largely depends on the age of the building. Newer facilities, constructed after 2010, demonstrate significantly better performance, particularly through the use of energy-efficient lighting combined with high-quality windows and external thermal insulation. Most older buildings still rely on outdated and inefficient heating and lighting systems, with insufficient insulation and window quality. The results indicate that upgrading window frames, installing insulation, and replacing inefficient lighting are key measures to improve the energy efficiency of kindergartens in Zrenjanin, which can substantially reduce energy losses and maintenance costs.

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NOT FINALIZED

ASSESSMENT OF ANTIBIOTIC RESISTANCE IN A GRAPEVINE-DERIVED *Bacillus* sp. ISOLATE

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Abstract

The irresponsible and excessive use of antibiotics has contributed to the rapid spread of antimicrobial resistance (AMR), which has emerged as a major global health concern. In this context, special attention must be devoted to the use of microorganisms in various sectors in order to minimize the risk of horizontal transfer and dissemination of AMR genes. In the present study, *Bacillus* sp. 17/S was isolated from the grapevine stem and investigated for its potential as a biocontrol agent. As an essential first step, the antimicrobial resistance profile of the isolate was evaluated. An *in vitro* antibiotic susceptibility assay was conducted using the disk diffusion method, and results were interpreted based on inhibition zone diameters: isolates were considered susceptible (≥ 21 mm), moderately susceptible (16–20 mm), or resistant (≤ 15 mm). In addition, the presence of antibiotic resistance genes was analyzed by the PCR (polymerase chain reaction)-based method. Several genes associated with different resistance mechanisms including *penP*, *blaOXA*, *vmiR*, *lmrB*, *ant-6*, *aac-3*, *tetL*, and *mphK* were selected as the molecular targets. The antibiotic susceptibility tests revealed the highest level of resistance towards β -lactam antibiotics, with the isolate being resistant to oxacillin, aztreonam, methicillin, cefepime, and cefixime, while showing moderate susceptibility to ceftaroline (20.00 ± 0.00 mm) and piperacillin (19.67 ± 0.58 mm). In contrast, the susceptibility was observed to penicillin G (37.33 ± 0.58 mm), ampicillin (22.33 ± 0.58 mm), imipenem (43.67 ± 0.58 mm), amoxicillin (29.00 ± 1.00 mm), and cephalexin (23.67 ± 0.58 mm). Within the lincosamide group, the isolate was susceptible to clindamycin (21.67 ± 0.58 mm) and moderately susceptible to lincomycin (15.00 ± 0.00 mm). Among tetracyclines, susceptibility was observed to minocycline (24.67 ± 0.58 mm), with moderate susceptibility to tetracycline (17.00 ± 0.00 mm) and doxycycline (18.67 ± 1.53 mm). Regarding aminoglycosides, the isolate was susceptible to gentamicin (24.67 ± 0.58 mm) and streptomycin (24.67 ± 0.58 mm), while tobramycin (19.00 ± 0.00 mm), kanamycin (19.00 ± 0.00 mm), and amikacin (18.67 ± 2.08 mm) exhibited only moderate activity, and the resistance was observed to neomycin. All tested macrolides (azithromycin, erythromycin, and clarithromycin) displayed strong growth inhibitory effects. Notably, none of the investigated resistance genes corresponding to these antibiotic groups was detected in the isolate's genomic DNA. It can be concluded that the *Bacillus* sp. 17/S isolate displays a heterogeneous antibiotic susceptibility profile. The absence of the tested resistance genes suggests that phenotypic resistance may not always be explained by the known genetic determinants. These findings highlight the importance of comprehensive safety evaluations of microbial strains prior to their potential application as biocontrol agents.

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ANALYSIS AND POSSIBLE USES OF CANNING PLANT WASTE

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Abstract

The research focuses on the valorization of plant-based waste and by-products generated in the canning industry. In light of growing environmental concerns, minimizing waste production and promoting the reuse of agricultural by-products for the development of value-added products has become increasingly important. The primary aim of this study was to utilize substandard green pea seeds, a by-product of green pea processing. Thereby contributing to the reduction of industrial food waste.

The research involved the development of a food product based on green pea flour, specifically a cracker. For this purpose the rejected green peas were dried and milled into flour, which was subsequently analyzed for its nutritional composition. The evaluation included the determination of fat, protein, fiber, and ash content to assess the flour's nutritional value and its potential applicability in food product development.

Introduction

Sustainable food production and waste reduction are gaining increasing importance in the food industry. The food industry generates a significant amount of plant-based by-products, which are often discarded as waste, despite their potentially valuable nutrient content. The canning industry, in particular, produces large quantities of such plant waste, including vegetable and fruit peels, stems, and also seeds. In 2004, companies in the European food industry generated nearly 222 million tons of processing losses. In the fruit and vegetable preservation sector, waste accounted for approximately 4.5% of the total production. (Baiano, 2014) These by-products are most commonly used as animal feed, compost, or disposed of as waste; however their reuse in food production offers promising opportunities.

During the canning process of green peas, substantial amounts of plant-based waste are generated, such as the green pea pods, seeds and other parts of the plant. These by-products are rich in fiber and protein, making them worth utilizing. In recent years, there has been a growing research interest focused on the alternative use of such plant-based residues,—such as grinding them into flour for application in bakery products.

The aim of the present study was to process green pea canning waste into flour and to use this flour to produce a simple, savory bakery product: crackers. The study focused on analyzing both the physical and sensory characteristics of the resulting flour and the properties of the crackers made from it.

Experimental

The green pea by-product used for the study originated from industrial canning processes. The waste material was collected immediately after processing and, due to its seasonal availability, it was stored frozen until use.

Prior to use, the green pea seeds were thawed and pureed, then dried in a drying oven at 60 °C for 20–22 hours. This relatively low-temperature, long-duration drying process was chosen to considering the high moisture content of the material and to prevent protein denaturation. After drying, the material was initially coarsely crushed, then further milled into a fine flour

consistency. The resulting flour was stored in airtight containers until further use. After milling, the nutritional composition of the green pea flour was analyzed.

Firstly, the **dry matter** content was determined according to the MSZ EN ISO 712 standard. A known amount of flour was dried at 130°C for one hour, after which the sample was weighed again to calculate moisture loss.

The **protein content** was assessed using the Kjeldahl method. The sample was digested in the presence of sulfuric acid at 400°C. After digestion, sodium hydroxide (NaOH) was added and the mixture was distilled. The resulting distillate was collected in boric acid, and then titrated with 0.100 M hydrochloric acid (HCl) solution using mixed indicator. The nitrogen content obtained from the titration was multiplied by a conversion factor of 6.25 to calculate the total protein content of the green pea flour.

The **fat content** of the green pea flour was determined gravimetrically using the Soxhlet extraction method, with a Soxtec extraction unit. The procedure began with a 1.5-hour hot extraction phase during which the sample was immersed in warm petroleum ether, followed by a 1.5-hour cold extraction phase, during which the sample was exposed only to the vapor of petroleum ether. After extraction, the recovered fat fraction was dried in a drying oven at 100 °C for approximately one hour, and the fat content was calculated based on the mass of the extracted material.

The **mineral content** of the sample was determined by measuring the ash content of the flour. The weighed samples were first incinerated over an open flame and then placed in a muffle furnace at 600 °C for 6 hours to complete the ashing process.

The **crude fiber** content was determined using an extraction-based method. The samples were first defatted by washing with ethanol, followed by boiling in diluted acid for 30 minutes, and then boiling in diluted alkali for another 30 minutes. After the chemical treatments, the residue was dried and weighed to determine the fiber content gravimetrically.

Following the analysis of the nutritional composition of the green pea flour, the next objective was to develop a food product. Green pea flour is gluten-free and nutritionally valuable due to its high fiber and protein content, as well as its low glycaemic index.

Based on these attributes, the aim was to create a product that is not only gluten-free but also free from common allergenic ingredients and animal-derived components, making it suitable for both vegetarians and vegans.

The choice fell on crackers, as they are simple to prepare yet widely popular snack products consumed by many people on a daily basis. Pea flour is rarely used alone; it is typically blended with other flours. For this purpose, rice flour and red lentil flour were applied separately, both of which are also gluten-free.

The selected basic recipe included green pea flour, rice flour or red lentil flour, water, olive oil, salt, and spices for a pleasant flavor. During the study, the addition of baking powder and yeast was also tested, but these formulations were discarded because the resulting product had a texture resembling shortcrust pastry rather than the desired crispiness expected in crackers.

As a texture improver, aquafaba—the cooking water of chickpeas—was used as an egg replacer. Depending on the amount, aquafaba can substitute egg yolk, egg white, or whole egg. The primary spices added were oregano, basil, and garlic, which imparted a pleasant flavor to the crispy crackers.

Baking conditions (temperature, duration, convection, etc.) were tested, and based on preliminary sensory evaluation, the optimal product was obtained by baking the crackers at 150 °C for 35 minutes.

The finished crackers were analyzed for protein, fiber, ash, and fat content, and their structural properties (e.g., hardness, crispness, brittleness) were evaluated using texture analysis.

In addition, a texture analysis was performed on three different cracker samples. During the texture analysis, I examined various parameters such as fracturability, hardness, and the required hardness work.

Results and discussion

The green pea flour obtained from canning industry by-products exhibited a fine texture with a characteristic greenish hue. The proximate analysis revealed a dry matter content consistent with expectations for dried legume-based flours. The obtained values for the various samples are summarized in Table 1. Protein content was notably high, reflecting the rich leguminous source, while the fiber content confirmed the potential of the flour as a valuable dietary fiber contributor. The flour has a protein content of 24.75% and a fiber content of 9.58%. Fat and ash contents were within typical ranges for pulse-derived flours, supporting its nutritional value. Fat content was found to be 2.39%. and the ash content 2.97%. For reference purposes, the compositional parameters of a flour produced using a similar method were utilized. (Sallam, El-Salam, & Abaza, 2021)

Table 1. Pea flour and crackers proximate composition

Proximate compositions				
Values are based on dry matter [%]	Green pea flour	Cracker with rice flour	Cracker with rice flour and aquafaba	Cracker with red lentil flour and aquafaba
Carbohydrates	56.62	56.44	55.97	53.16
Protein	26.42	24.76	24.83	27.50
Crude fiber	10.87	9.99	9.92	9.77
Fat	2.72	4.48	4.70	4.83
Ash	3.37	4.33	4.58	4.74
Energy content of 100g product	378.38 kcal	385.10 kcal	385.34 kcal	385.65 kcal

Formulation trials demonstrated that green pea flour could not be used as a sole flour in cracker production due to texture challenges. When combined with gluten-free rice or red lentil flours, the dough exhibited improved handling and baking properties. Attempts to incorporate leavening agents such as baking powder and yeast resulted in crackers with a softer, shortcrust-like texture rather than the desirable crispiness typical of crackers. leading to the exclusion of these additives. The use of aquafaba as an egg replacer proved effective in improving dough binding and texture without compromising the vegan and allergen-free objectives. Sensory evaluation favored crackers spiced with oregano, basil, and garlic, which enhanced the flavor profile and consumer acceptability.

Optimization of baking conditions identified 150 °C for 35 minutes as the ideal setting, producing crackers with optimal crispness and structural integrity. Texture analysis confirmed the products' desirable hardness, brittleness, and crunchiness, meeting expectations for a savory snack product. The nutritional composition of the final crackers retained significant levels of protein, fiber, and minerals, confirming that the valorization of green pea processing waste into a novel bakery product is both feasible and nutritionally advantageous. This approach not only contributes to reducing industrial plant waste but also offers a gluten-free, vegan-friendly snack option with promising market potential.

During the texture analysis, I recorded the characteristic texture profile curve of the product, which clearly illustrates the differences between the three samples (Figure 1.). The crackers show similar kind of response to the deforming force applied to them during measurements, in general. However, the results clearly indicate that the two different types of flour, as well as the addition of aquafaba, had a significant impact on the texture and structural properties of the crackers. Addition of rice flour and aquafaba led to weakest structure, showing lowest hardness among the samples.

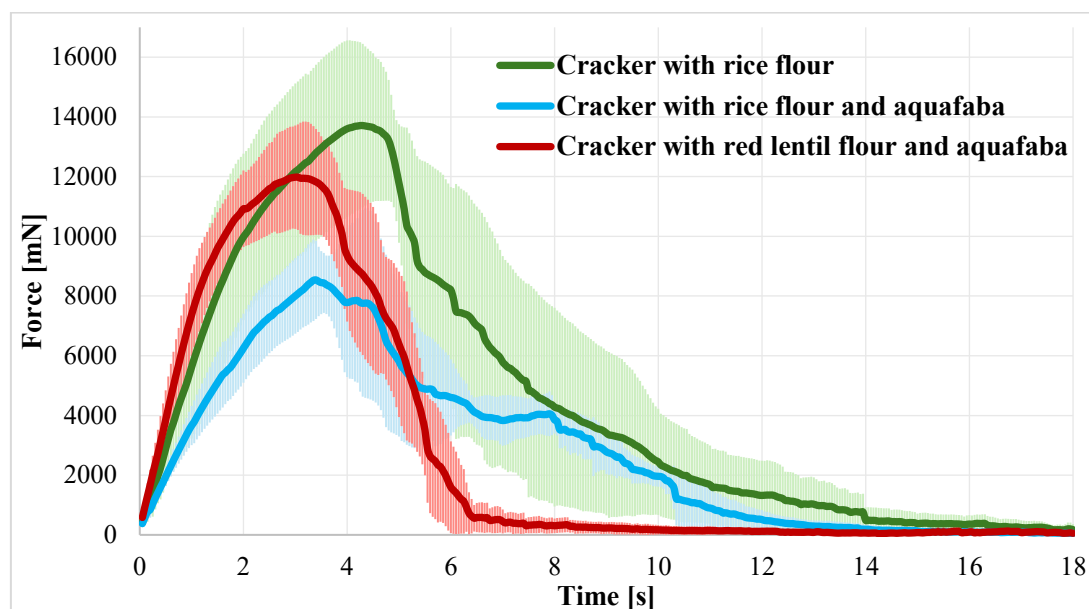


Figure 1. Texture curves of pea crackers

Conclusion

In my research, I investigated whether plant-based by-products generated during processing could be used to produce a raw material suitable for the development of various products. As a first step, I analyzed the nutritional composition of the material and compared the results with data found in the scientific literature. Based on my measurements, green pea proved to be an excellent source of protein and fiber, with a particularly favorable composition. Subsequently, crackers were produced from green pea flour using different formulations, and these were also examined. At this stage, the crackers serve as prototypes; further development is required, including sensory evaluations, in order to create a snack product that is both palatable and appealing to consumers. Future research could focus on a more detailed analysis of the protein and carbohydrate components, as well as digestibility experiments to determine the extent to which the flour or the final product can be utilized by the human body.

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EXPLORATION OF QuEChERS EXTRACTION FOR MULTICLASS EMERGING CONTAMINANTS

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In recent years, growing scientific and regulatory attention has been directed toward emerging contaminants (ECs) in soil and aquatic environments. Although frequently detected at trace concentrations, many of these substances exhibit high toxicity, environmental persistence, and the potential for bioaccumulation. They are continuously introduced into the environment through wastewater discharges, agricultural practices, and other anthropogenic activities, where they can be transferred into the food chain via plant uptake. Effluents from wastewater treatment facilities often contain carcinogenic, endocrine-disrupting, or otherwise hazardous compounds, further worsening contamination of surrounding soil and water resources. At the same time, climate change, rapid population growth, and increasing pollution pressure on limited natural resources highlight the urgent need for sustainable management of soil and freshwater. The widespread use of pharmaceuticals, personal care products, pesticides, and per- and polyfluoroalkyl substances (PFAS) adds to the complexity of long-term contamination scenarios. Consequently, environmental analytical chemistry has become increasingly focused on the development of sensitive, selective, and reliable methods for the simultaneous detection and quantification of multiple classes of ECs across diverse matrices. Yet, this remains particularly challenging due to the highly variable physicochemical properties of these compounds.

Within this framework, the present study explored the optimization of QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) extraction for the multiclass determination of 27 ECs with diverse polarities, molecular weights, and physicochemical characteristics. The QuEChERS protocol, coupled with UHPLC–MS/MS, enabled efficient extraction, clean-up, and high-throughput analysis of a wide range of ECs. The extraction performance was assessed in two different matrices: agar medium fortified with ECs and tomato plant tissues (stem and root) grown on fortified medium. Validation demonstrated satisfactory method performance in both matrices, with accuracy and precision within accepted limits, excellent linearity ($R^2 \geq 0.99$), recoveries ranging from 64 - 140%, and relative standard deviations below 20% in most cases. The limits of quantification ranged from 0.12 to 7.87 ng/g, confirming the method's sensitivity.

Overall, the study demonstrated that the optimized QuEChERS–UHPLC–MS/MS approach provides a robust and versatile platform for the simultaneous determination of multiclass ECs in complex matrices. Beyond controlled conditions, the method shows strong potential for application in real environmental scenarios, such as contaminated soils and edible plants cultivated on them. Its adaptability to additional classes of ECs further supports its use as a reliable analytical tool for advancing environmental monitoring, risk assessment, and strategies aimed at ensuring food and environmental safety.

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NOT FINALIZED

RESISTANCE STRUCTURE AND SOLUTE REMOVAL PATHWAYS IN UF–DF OF SWEET WHEY

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Abstract

Whey is a high-volume by-product of dairy processing, rich in valuable proteins, lactose, and minerals, yet its utilization remains limited in many regions due to challenges related to shelf life, transport, and processing infrastructure. Membrane-based separations such as ultrafiltration (UF) and diafiltration (DF) offer chemical-free, low-energy routes for valorizing whey streams, but their efficiency depends not only on the nominal molecular weight cut-off (MWCO) of the membranes, but also on fouling dynamics and concentration polarization phenomena. In this study, sweet whey was subjected to UF combined with up to four constant-volume DF steps using polyethersulfone (PES) membranes with MWCOs of 10, 30, and 50 kDa. Retention of chemical oxygen demand (COD) and lactose was determined, and the evolution of total hydraulic resistance (R_T) and its components – membrane resistance (R_M), reversible resistance (R_{REV}), and irreversible resistance (R_{IRR}) – was evaluated. Results showed that COD retention closely followed lactose concentration changes, with strong correlations ($r \approx 0.99$), confirming that small, permeable solutes dominated COD trends. UF exhibited clear MWCO-dependent retention (10 kDa > 30 kDa > 50 kDa), whereas during DF the sharpest decline occurred in the first diafiltration cycle (DF1), due to dilution-induced disruption of the concentration polarization layer and reduction of R_{REV} . Beyond DF2, resistance stabilized and the separation performance of the 30 and 50 kDa membranes converged, indicating that hydrodynamic control outweighed nominal MWCO differences. For the 10 kDa membrane, irreversible fouling became more prominent in later DF steps, increasing R_T . Overall, the first DF cycle resulted in the greatest removal of dissolved components with low molecular weight, while subsequent cycles contributed to a diminishing extent to the removal of these fractions, but further increased the purity of the protein fraction remaining in the retentate. These findings suggest that optimal industrial strategies should apply a limited number of DF steps and carefully consider fouling mechanisms to balance efficiency, product quality, and resource use.

Introduction

The dairy industry represents one of the largest and technologically most diverse sectors of the global food chain. During processing, it generates substantial by-product streams, particularly whey, with an annual production of approximately 180–190 million tons. Although whey contains considerable amounts of high biological value proteins, lactose, and minerals, it remains underutilized in many regions due to its short shelf life, geographically and seasonally fluctuating generation profile, and the lack of local valorization capacities. This underutilization results in both environmental burdens and economic losses [1]. With the growing emphasis on circular economy principles and sustainable food supply models, there is an increasing demand for technologies that selectively exploit whey as a feedstock for producing high value-added components, while simultaneously reducing energy and water consumption as well as the overall carbon footprint [2].

Membrane separation technologies – most notably ultrafiltration (*UF*) and its combination with diafiltration (*DF*) –, which generally avoid the use of chemicals and impose only mild thermal stress provide an industrially validated solution to this challenge. *UF* retains protein fractions, thereby enabling the production of whey protein concentrates (*WPC*) and isolates (*WPI*), whereas *DF* enhances the purity and stability of the retentate by removing small molecular weight permeating components such as lactose and minerals [3, 4, 5]. The “washing” effect of multiple *DF* cycles also modifies hydrodynamic conditions: dilution lowers ionic strength and viscosity, disrupts the concentration polarization (*CP*) layer formed during *UF*, and can thereby reduce reversible resistance while increasing flux [6]. This highlights that the efficiency of *UF/DF* separation is not determined solely by the nominal molecular weight cut-off (*MWCO*) of the membrane: permeate flux and separation selectivity are equally influenced by the dynamics of surface film formation and fouling, expressed as reversible resistance (R_{REV}) and irreversible resistance (R_{IRR}) [7].

Although the recovery of whey proteins via *UF/DF* and the conceptual and practical role of *DF* are widely addressed in the literature [3, 4, 8], only limited scientific studies are available that comprehensively evaluate both compositional parameter retention and the temporal evolution of total hydraulic resistance (R_T) and its components – namely membrane resistance (R_M), and the aforementioned reversible resistance (R_{REV}), and irreversible resistance (R_{IRR}) – over multiple *DF* cycles using membranes of different *MWCO* values. Joint analysis of membrane selectivity and resistance distribution is crucial for understanding how the outcome of separation is shaped by the interplay of membrane cut-off, fouling, and concentration polarization.

In this study, sweet whey was subjected to ultrafiltration combined with multiple diafiltration cycles using membranes with different molecular weight cut-offs. The process was monitored in terms of chemical oxygen demand (*COD*) and lactose retention, total hydraulic resistance (R_T), and the relative contributions of membrane resistance (R_M), reversible resistance (R_{REV}), and irreversible resistance (R_{IRR}). The aim was to quantitatively demonstrate that as *DF* progresses, the outcome of separation is increasingly determined by the rearrangement of the resistance distribution and the extent of low molecular weight washing-out, while the influence of the nominal *MWCO* gradually becomes secondary.

Experimental

For the laboratory-scale membrane separation experiments, an ultrafiltration cell (Millipore, Germany) with an active membrane surface area of 40 cm² was used. The membranes were based on polyethersulfone (*PES*) and had nominal molecular weight cut-off (*MWCO*) values of 10, 30, and 50 kDa. Before using, the membranes were preconditioned by soaking in distilled water for 1 hour. Experiments were carried out at room temperature (22 ± 1 °C), under a transmembrane pressure (*TMP*) of 2.5 bar and a stirring speed of 300 rpm. The initial feed consisted of 150 mL of sweet whey. During the ultrafiltration phase, the system was operated until a volume reduction ratio (*VRR*) of 3 was reached. This was followed by constant-volume diafiltration (*DF*), performed in up to four consecutive steps (*DF1–DF4*). At the beginning of each *DF* step, the retentate volume was restored to its original value (150 mL) by the addition of distilled water (approximately 100 mL). Sampling was performed at the end of each experiment from both the permeate and retentate fractions.

The organic matter content of the filtration fractions was determined as chemical oxygen demand (*COD*) using standard dichromate test cuvettes (Hanna Instruments, Hungary) followed by a spectrophotometric analysis. Lactose concentration was analyzed with a milk analyzer (Bentley Instruments, Inc., USA) operating with near-infrared (*NIR*) sensors. Based on

the compositional parameters of the permeate and retentate samples, retention values ($R\%$) were calculated.

The extent of membrane fouling and the underlying mechanisms were evaluated using the resistance-in-series model. According to this model, the total hydraulic resistance consists of three components: membrane resistance (R_M), reversible resistance (R_{REV}), which is associated with the concentration polarization layer and loosely bound deposits removable by hydraulic rinsing, and irreversible resistance (R_{IRR}), which persists even after rinsing.

Results and discussion

The results of the UF – DF series were evaluated based on chemical oxygen demand (COD) and lactose retention (Figure 1), as well as the evolution of total hydraulic resistance and its components (Figure 2). The changes observed in COD retention during UF – DF primarily reflected the behavior of the small molecular weight fraction (permeable to the membrane), particularly lactose, which is present in the highest concentration. This is because protein retention remained consistently high (85–88%) for all three tested $MWCO$ membranes. This interpretation is supported by the fact that, for each membrane, a strong positive Pearson correlation was observed between COD and lactose retention (10 kDa: $r \approx 0.997$; 30 kDa: $r \approx 0.992$; 50 kDa: $r \approx 0.996$). These findings confirm that the decrease in COD was primarily caused by the change in concentration of dissolved components washed out during diafiltration.

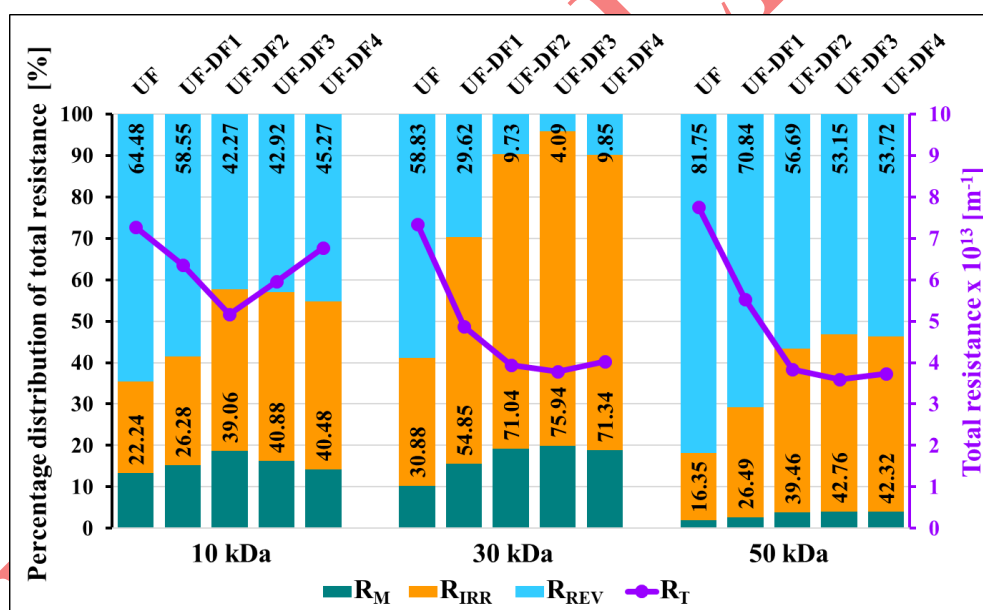


Figure 1. Distribution of resistances within the total resistance

During the UF phase, retention showed a clear $MWCO$ -dependent pattern: COD retention for the 10, 30, and 50 kDa membranes was 66.2%, 59.2%, and 56.2%, respectively, while lactose retention was 44.3%, 37.6%, and 35.8% (Figure 1). In other words, membranes with smaller nominal cut-offs resulted in higher retention of organic matter and lactose. The monotonic decrease in retention with increasing $MWCO$ is in agreement with previously documented trends in whey-based systems [3, 9].

Following UF , the absolute value of total resistance was high for all membranes tested, with the distribution of resistance components indicating dominance of the reversible fraction ($R_{REV} \approx 64.5/58.8/81.8\%$). This suggests that during UF a substantial concentration polarization (CP) layer formed on the membrane surface, restricting the free transport of small molecules and thus contributing to the high COD and lactose retention.

After the first diafiltration step (*DF1*), *COD* retention dropped to ~53.4/42.2/42.1% for the 10/30/50 kDa membranes, while lactose retention decreased to ~17.7/14.7/13.9%. This sharp change can be attributed to dilution induced by the water added during *DF1*, which reduced retentate concentration, ionic strength, and viscosity. Consequently, the concentration polarization layer that had developed during *UF* was likely loosened or partially collapsed [8]. As a result, total resistance – and especially its reversible fraction – decreased significantly, enabling enhanced migration of low molecular weight solutes to the permeate side [4, 5].

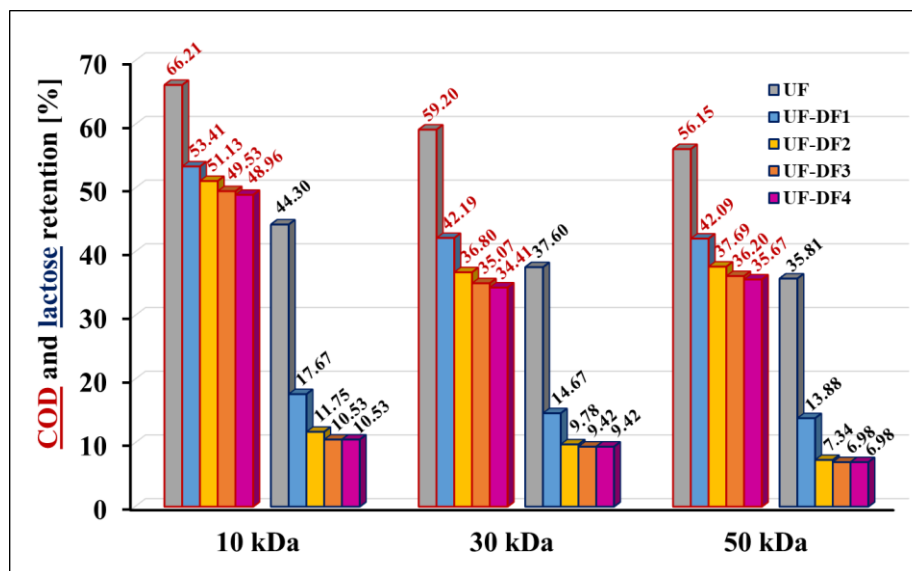


Figure 2. Evolution of *COD* and lactose retention across the different *MWCO* membranes

As diafiltration progressed (*DF2–DF4*), the further decreases in *COD* and lactose retention became more moderate. In parallel, the evolution of total resistance also stabilized: for the 30 and 50 kDa membranes, no significant changes were observed after *DF2*, and during this stage the retention trends and the values of R_T showed convergence. This indicates that as the process advanced, separation mechanisms were primarily governed by hydrodynamic factors and the transport of permeable components, while the influence of nominal *MWCO* differences diminished [4, 9].

In contrast, for the 10 kDa membrane it was evident that, alongside the relaxation and collapse of the *CP* layer, a more persistent (irreversible) protein/peptide deposit gradually developed, which in later *DF* stages led to renewed increases in R_T . This observation is consistent with literature reports indicating that for membranes with tighter pore structures, fouling can play a more pronounced role as diafiltration progresses [6].

Taken together, these results demonstrate that separation performance and the purity of the retained protein fractions during *DF* were shaped by two main effects: (i) the solvent-driven, diavolume-proportional depletion of low molecular weight fractions from the retentate, and (ii) the hydrodynamic disintegration of the concentration polarization layer responsible for reversible resistance. The combined action of these two processes explains the sharp decrease in *COD* and lactose retention observed during *DF1*, the more moderate changes in both resistance and retention during subsequent *DF* stages, and the emergence of separation patterns for the 30 and 50 kDa membranes that became independent of nominal *MWCO*.

Conclusions

The *UF–DF* experiments confirmed that *COD* and lactose retention are primarily determined by the removal of low molecular weight components and the hydrodynamic disintegration of

the CP layer. During the UF phase, a clear MWCO-dependent pattern was observed; however, as DF progressed, the separation behavior of the 30 and 50 kDa membranes became converged, indicating the dominance of hydrodynamic control. In contrast, for the 10 kDa membrane, the irreversible component of fouling became more prominent during the later DF stages. The DF1 step enabled the most substantial depletion of low molecular weight impurities (e.g., lactose, ions), while subsequent DF cycles produced diminishing incremental effects but nevertheless contributed to the purification of the retained protein fractions.

Our results suggest that for industrial applications it is advisable to apply a limited number of DF cycles, with careful selection of membrane type and cut-off value, while considering hydrodynamic factors and fouling mechanisms. These findings contribute to the optimization of whey-based membrane processes and may provide a basis for future studies on flux decline modeling and the development of cleaning strategies.

Acknowledgements

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PLANT GROWTH-PROMOTING POTENTIAL OF *Bacillus* sp. ISOLATED FROM VINEYARD SOIL

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Abstract

Conventional agrochemicals widely used in agronomic production raise serious environmental concerns, as their accumulation in soil, air, and water can lead to food chain contamination and adverse effects on animal and human health. These challenges have encouraged the search for alternative, eco-friendly approaches to sustainable agriculture. One promising strategy involves the application of microbial bioagents with plant growth-promoting (PGP) traits. This study aimed to evaluate the potential of *Bacillus* sp. 22/R isolated from vineyard soil as a candidate plant biostimulant by characterizing its PGP properties. Hydrolytic enzyme activities (cellulase, xylanase, pectinase, protease, gelatinase, and lipase) were assessed using semi-quantitative agar plate assays. The production of ACC deaminase was evaluated on DF minimal medium with ACC as the sole nitrogen source, while phosphate and zinc solubilization were determined on Pikovskaya and zinc-solubilizing agar, respectively. Indole-3-acetic acid (IAA) synthesis was determined spectrophotometrically after cultivation in nutrient broth supplemented with L-tryptophan. The isolate exhibited strong pectinolytic activity (EAI 4.28) and considerable xylanase activity (2.12), whereas cellulase, protease, gelatinase, and lipase activities were comparatively lower, with EAI values of 1.60, 1.29, 1.44, and 1.25, respectively. It demonstrated ACC deaminase activity with a growth diameter of 30.17 ± 0.29 mm, phosphate solubilization with an index of 1.06, and IAA synthesis at a concentration of $4.20 \mu\text{g/mL}$. Overall, these results highlight that the *Bacillus* isolate combines relevant enzymatic activities with ACC deaminase production and IAA biosynthesis, traits that are highly desirable in the context of plant growth promotion. Further studies, especially in greenhouse and field trials, are needed to validate its potential and applicability as a microbial biostimulant.

Acknowledgements

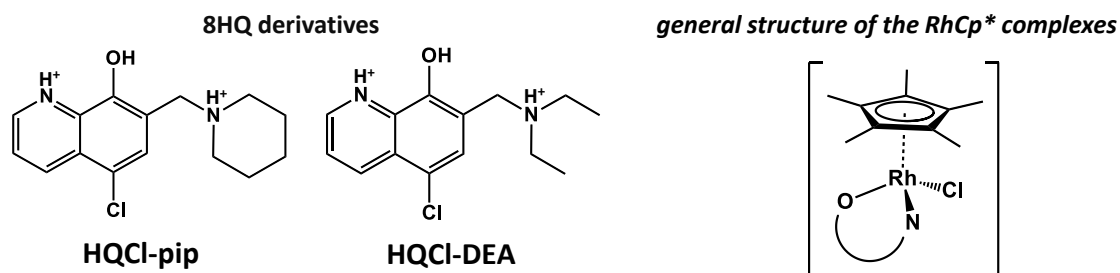
The research was supported by the programs 451-03-136/2025-03/200134 and 451-03-137/2025-03/200134 of the Ministry of Science, Technological Development and Innovations of the Republic of Serbia and by the Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina in the framework of the project "Development of industrial symbiosis in the AP Vojvodina through valorization of fruit processing by-products using green technologies" (project number 003075720 2024 09418 003 000 000 001 04 004).

A MULTIDRUG RESISTANCE SELECTIVE ANTICANCER 8-HYDROXYQUINOLINE DERIVATIVE AND ITS RhCp* COMPLEX

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In the field of developing more effective chemotherapeutic drugs with fewer severe side effects, 8-hydroxyquinoline (8HQ) derivatives are promising compounds. A group of these molecules was found to be selective against multidrug resistant (MDR) cancer cells, which occurs frequently when treating cancer [1]. Furthermore, several studies showed that these molecules form complexes with essential metal ions which is associated with the therapeutic effect [2]. In our research group several 8HQ Mannich base compounds have been developed and tested against MDR cancer cells, including HQCl-pip. Its complexation with half-sandwich Rh(III)(η^5 -petamethylcyclopentadienyl)(H₂O)₃]²⁺ (RhCp*) cation (see figure), has actually enhanced, rather than diminished the toxicity on MDR cells; moreover, the complex has better aqueous solubility in comparison to HQCl-pip alone [3].



HQCl-DEA is a close derivative of the former compound showing selective toxicity on MDR cancer cells. Therefore, we found it worth to investigate its behaviour in aqueous solution, complex formation with RhCp* cation and their interaction with human serum albumin. Proton dissociation processes and stability of HQCl-DEA and its RhCp* complex was followed by UV-Vis spectrophotometry and ¹H NMR spectroscopy. The same techniques were applied to determine the Cl⁻/H₂O exchange constant of the complex. Lipophilicity was determined by *n*-octanol/water partitioning experiments at various pH values and chloride ion concentrations. Albumin binding was investigated by equilibrium dialysis, ultrafiltration, UV-Vis and fluorescence spectroscopies. Based on our results, the complex shows promise as an anticancer agent against MDR.

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APPLICATION OF UV/SULFITE ADVANCED REDUCTION PROCESS FOR ELIMINATION OF THE PFOA, A „FOREVER CHEMICAL“

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Advanced oxidation processes (AOP) are effective for the elimination of most organic pollutants. However, its effectiveness is limited in the case of “forever chemicals”, such as per- and polyfluorinated compounds (PFs), responsible for several environmental and public health risks [1,2]. PF removal requires an advanced reduction process (ARP) [3-5], where a reducing agent, primarily the hydrated electron (e_{aq}^-), is formed. Photochemical water treatment practices typically use low-pressure mercury vapor lamps (LPM) emitting 254 nm UV light, and less often, 254/185 nm UV/VUV light. The wavelength determines the radical set and is decisive for the efficiency of radical generation and the transformation of target substances. UV light is generally absorbed by the additive (oxidizing or reducing agent), while VUV light is absorbed by the water, resulting in the formation of $\bullet OH$, $\bullet H$, and, with less efficiency, e_{aq}^- . Besides the formation of radicals from water, the direct VUV photolysis of the target substances cannot be excluded.

The UV-ARP substrate scope is weighted heavily toward contaminant classes that are resistant to degradation by AOPs, like PFs [23]. The underreported information about quality and the formation rates of reactive species has made it difficult to fully evaluate the impact of operating conditions and the role of water matrix components on efficiency. Investigating the impact of dissolved organic matter, inorganic ions, and dissolved O_2 content on efficiency is necessary. In this work, the effects of sulfite concentration, pH, dissolved oxygen, and biologically treated domestic wastewater as a matrix were investigated. Results showed that low-intensity VUV light can enhance the transformation efficiency. Besides direct VUV photolysis of PFOA, 185 nm light is responsible for the enhanced transformation of sulfite ions, and most probably, the photolysis of sulfate ions also contributes to the formation of e_{aq}^- . The effect of dissolved O_2 , pH, and radical scavengers proved the decisive role of e_{aq}^- in the transformation of PFOA. The HCO_3^- content of the matrix decreased the efficiency, while Cl^- had no effect.

Our results demonstrated that the UV/sulfite and UV/VUV/sulfite processes are capable of removing hardly oxidizable PFOA. The efficiency of the process is sensitive to the pH, and the presence of components that can compete with PFOA for e_{aq}^- . 185 nm low-intensity VUV light can significantly enhance the transformation rate of PFOA through various mechanisms; the contributions of direct VUV photolysis of PFOA and enhanced transformation of both sulfite and sulfate ions require further investigation.

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COMPLEXATION OF SALICYLIC ACID WITH SELECTED SURFACTANTS

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Abstract

Salicylic acid is a widely used compound in pharmaceutical and cosmetic formulations due to its keratolytic, anti-inflammatory, and antimicrobial properties. In topical applications, interactions with excipients such as surfactants may affect its availability and biological activity. Surfactants, as amphiphilic molecules, can form supramolecular complexes even below their critical micelle concentration (*cmc*). These interactions can enhance solubility but may also influence the fraction of salicylic acid that is free to act at the site of application. Understanding salicylic acid–surfactant interaction is therefore crucial for optimizing drug delivery and ensuring therapeutic efficacy.

The aim of this study was to experimentally investigate the propensity of salicylic acid to interact with selected surfactants at sub-*cmc* concentrations and to assess the effect of poloxamer modifiers on the binding process. UV–Vis spectroscopy was used to monitor changes in absorbance with increasing surfactant concentrations, and Job's method of continuous variation was employed to determine the stoichiometry of the complexes.

The results revealed that salicylic acid generally forms 1:1 complexes with the investigated surfactants. Nevertheless, significant deviations were observed in specific systems. The salicylic acid–Triton X-100 system demonstrated a 1:2 stoichiometry, suggesting that more than one surfactant molecule participates in stabilizing the system. Similarly, in the salicylic acid–Triton X-165 system with Poloxamer 188, a 1:2 binding ratio was identified, indicating that the poloxamer modifier influenced the equilibrium and enhanced the tendency of salicylic acid to interact with multiple surfactant molecules. In contrast, salicylic acid in the presence of Triton X-165 alone, or with Poloxamer 407, exhibited a predominant 1:1 binding ratio. Among the tested surfactants, Triton X-165 showed the highest affinity for salicylic acid, likely due to its longer polyoxyethylene chain, which provides more favorable hydrogen bonding and steric stabilization of the complex.

These findings highlight that both the chemical structure of the surfactant and the presence of polymeric modifiers affect the stoichiometry and stability of drug–surfactant systems. Understanding these interactions is crucial for improving the solubility, bioavailability, and delivery of salicylic acid in pharmaceutical formulations. The results contribute to a broader understanding of drug–surfactant interactions below the *cmc* and may support the rational design of surfactant-assisted drug delivery systems for poorly soluble compounds.

Keywords: salicylic acid; surfactants; drug–surfactant interactions; Job's plot; poloxamers

THE INCORPORATION OF PROPRANOLOL HYDROCHLORIDE INTO LIPOSOMES

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Abstract

Liposomes are nano-sized lipid-based vesicles used as drug delivery systems due to their hydrophilic and lipophilic characteristics. Moreover, when the active pharmaceutical agent (API) is incorporated inside the liposome, it protects them from degradation and provides improved targeting and drug release. The side effect is lower compared to other carriers. The properties of the liposomes are influenced by their lipid compositions, surface charge, size and method of preparation [1, 2].

The objective of this study was to successfully incorporate propranolol hydrochloride and to enhance the encapsulation efficiency (EE%). The charge of the phospholipid bilayer can be influenced by membrane additives such as stearylamine (SA) or dicetyl phosphate (DCP). The applied lipids were L- α -phosphatidylcholine (PC), dipalmitoylphosphatidylcholine (DPPC) and 1,2-distearoyl-sn-glycero-3-phosphocholine (DSPC). Furthermore, cholesterol (CH) and trehalose were utilised in the synthesis process. The molar ratios of the samples, as determined in a previous study [3], were found to be 8.5:4.5:6.5 for PC:CH:DCP, 12:5:5 for PC:CH:SA, 2.53:0.63:4.06:2.64 for DPPC:DSPC:CH:SA, and 2.53:0.63:1.53:3.96 for DPPC:DSPC:CH:DCP. Trehalose was present at a concentration of 5 w/w%, while propranolol hydrochloride was present at concentrations of 10, 20, or 50 w/w%, as indicated in the composition. The synthesis of liposomes was accomplished through the utilisation of the thin-film hydration method. The ethanol was evaporated from the alcoholic compositions at 100 mbar and 60°C (with the exception of trehalose and propranolol hydrochloride) in a rotary evaporator at 50 rpm. The lipid film was hydrated and ultrasonicated for a period of 30 minutes at a temperature of 60°C. The liposomes were then subjected to vacuum filtration, employing a 0.22 μ m membrane filter. Subsequently, the samples were subjected to immediate investigation with regard to their vesicle size, polydispersity and zeta potential in a liquid state. Following this, the samples were lyophilised for the purpose of further investigation. The drug release was examined over a period of one hour.

The size of the particles was found to be between 100 and 250 nm, and the polydispersity index (PDI) was approximately 0.3. The EE% and drug release were measured via HPLC. EE% was 2-36% and the drug release was 60-100%. The structures were examined via FT-IR, Raman and DSC. Further plans are to enhance the EE%.

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QUANTITATIVE INVESTMENT ANALYSIS AND PORTFOLIO MANAGEMENT: AN OPTIMIZATION PERSPECTIVE

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Abstract

Using mathematical models for maximizing returns and minimizing risk, this paper explores the process of dynamic portfolio optimization in the Republic of Serbia. The main focus is on the application of quantitative methods, including Markowitz's model and the fundamental principles of portfolio theory, adapted to real market data. Through a practical example of a portfolio consisting of domestic company stocks and government bonds, it is demonstrated how investors can make rational decisions under changing market conditions. The paper emphasizes the importance of a dynamic approach, where the portfolio is periodically adjusted based on shifts in the market and economic environment. Furthermore, the presented results highlight the significance of diversification and quantitative risk control for investors in small open markets. The use of real data from the Belgrade Stock Exchange and the inclusion of government bonds in the analysis provide a specific contribution to the study. The obtained findings can serve as a foundation for investment decision-making and the improvement of portfolio strategies in the contemporary business conditions.

Keywords: Markowitz model, portfolio optimization, investment analysis, risk, return.

Introduction

One of the key elements of financial management, both for individual investors and institutional funds, is the investment strategy. Portfolio optimization refers to the allocation of capital among different financial instruments in a way that maximizes expected return while simultaneously controlling risk.

The traditional approach to portfolio optimization, known as Markowitz's mean-variance model, is based on finding a balance between expected return and risk. While this model represents the foundation of modern portfolio theory, its static nature can be limiting in dynamic and volatile market conditions. On the Serbian capital market, such static optimization often proves insufficient, as it is characterized by relatively lower liquidity and higher volatility compared to developed markets. As noted in previous research, "frequent occurrences of extreme events, which are enhanced by the global economic crisis, significantly affect the return from investment activities". [3]

Dynamic optimization involves continuous adjustment of the portfolio structure – through changes in the weights of individual financial instruments – in accordance with fluctuations in stock prices, changes in interest rates, and movements in the exchange rate. In this way, investors can more effectively balance risk and return, while adapting to new information and macroeconomic developments.

The aim of this paper is to demonstrate, through a mathematical approach and a practical example of an investment portfolio in the Republic of Serbia, how dynamic optimization contributes to better risk control and more stable financial outcomes. Special emphasis is placed on the application of real data from the domestic market, which provides insight into the specific challenges and opportunities in the process of making investment decisions.

Markowitz Model

The portfolio optimization in this study is based on the Markowitz mean-variance model, which forms the foundation of modern portfolio theory [1]. The model was introduced to formally define the trade-off between risk and expected return, allowing investors to choose the optimal combination of different financial instruments [2]. The expected return of a portfolio is calculated using the formula:

$$E(R_p) = \sum_{i=1}^n \omega_i E(R_i), \quad (1)$$

where ω_i is the weight of the i -th asset in the portfolio and $E(R_i)$ is its expected return. The portfolio risk, defined as the standard deviation σ_p , is calculated using the covariances between assets:

$$\sigma_p = \sqrt{\sum_{i=1}^n \sum_{j=1}^n \omega_i \omega_j \cdot \text{Cov}(R_i, R_j)}. \quad (2)$$

The Markowitz model also allows the visualization of the Efficient Frontier, which represents the set of portfolios with the maximum expected return for a given level of risk. Portfolios below the efficient frontier are considered suboptimal because they do not provide the maximum return for a specific level of risk. As emphasized in earlier studies, "Markowitz considered that the relationship between realized return and risk can be expressed numerically and in that way the level of risk required for different levels of realized return can be determined".[4]

In this study, in addition to the static analysis, dynamic optimization is applied, which involves periodically adjusting the asset weights in the portfolio to maintain an optimal balance between risk and return under changing market conditions. The dynamic approach allows investors to respond to fluctuations in stock prices, interest rates, and exchange rates, thereby increasing the flexibility and efficiency of portfolio management [2].

Empirical Example – Serbia

Based on data from the Belgrade Stock Exchange and government bonds, the calculated returns are [5], [6]:

Table 1. Realized returns of selected securities

Asset	Initial Price	Final Price	Return
NIIS	900	745	-17.22%
DNOS	1252	1697	35.54%
GFOM	1500	1700	13.33%
Bonds	100	105	5.00%

Source: the authors' calculations

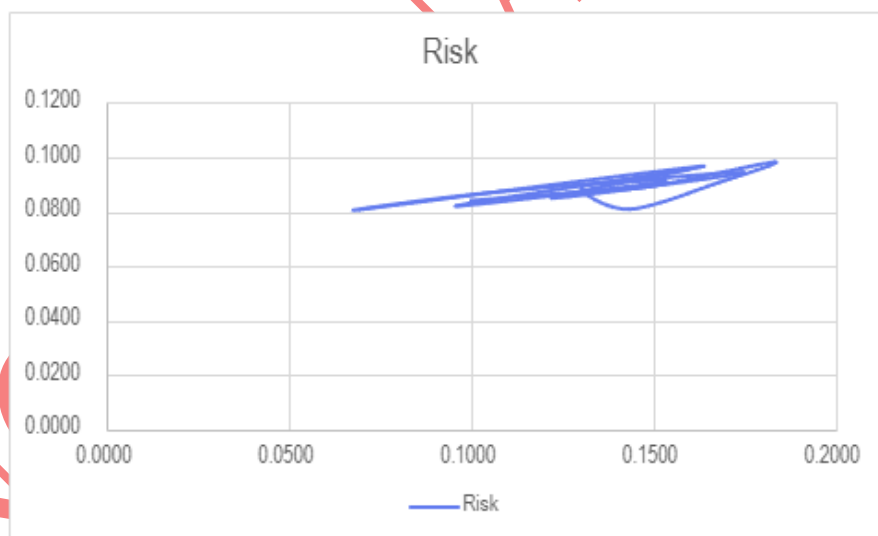
Using this data, 15 portfolios were created with different allocations of stocks and bonds. The expected return and risk (standard deviation) were calculated:

Table 2. Asset allocation, expected returns and risk metrics for selected investment portfolios

Portfolio	NIIS%	DNOS%	GFOM%	Bonds%	Expected Return	Risk
1	25%	50%	15%	10%	0.1596	0.0954
2	30%	40%	20%	10%	0.1222	0.0850
3	20%	50%	20%	10%	0.1749	0.0944
4	35%	40%	15%	10%	0.1069	0.0872
5	40%	30%	20%	10%	0.0694	0.0807
6	25%	50%	20%	5%	0.1638	0.0967
7	35%	35%	20%	10%	0.0958	0.0821
8	20%	45%	25%	5%	0.1527	0.0909
9	30%	40%	30%	0%	0.1305	0.0892
10	20%	40%	25%	5%	0.1435	0.0809
11	20%	45%	30%	5%	0.1680	0.0907
12	20%	50%	30%	0%	0.1833	0.0982
13	25%	45%	20%	10%	0.1485	0.0891
14	30%	40%	25%	5%	0.1263	0.0868
15	35%	35%	25%	5%	0.0999	0.0841

Source: the authors' calculations

The graphical representation of the Efficient Frontier shows how portfolio combinations move along the line that optimizes the risk-return trade-off. Portfolios near the upper part of the frontier represent the optimal combinations for a given risk level.

**Figure 1.** Efficient frontier – the risk–return trade-off for Optimized Portfolios

Source: the authors' calculations

The analysis reveals several key trends:

- **Risk and Return:** Portfolios with higher allocations to DNOS and GFOM stocks have higher expected returns but also higher risk. Portfolios with higher bond allocations show lower volatility but lower returns.
- **Optimal Portfolio:** Portfolio 12 (NIIS 20%, DNOS 50%, GFOM 30%, Bonds 0%) provides the highest expected return at an acceptable risk level (0.1833 return, 0.0982 risk).
- **Diversification:** Combining stocks and bonds reduces overall portfolio risk, confirming the importance of diversification and quantitative portfolio management.

- **Dynamic Optimization:** Adjusting asset weights over time allows the portfolio to move along the efficient frontier, enabling investors to maintain an optimal balance between risk and return in changing market conditions.
- **Advantages and Limitations of the Model:** The Markowitz model provides a clear mathematical basis and encourages rational decision-making, but requires additional adjustments in highly volatile and less liquid markets, confirming the need for a dynamic approach.

Conclusion

The implementation of quantitative analysis and dynamic portfolio optimization in the context of the Republic of Serbia demonstrates several key findings. First, the dynamic adjustment of asset weights enables more effective risk management, contributing to improved portfolio stability. Second, optimal portfolio configurations result in more consistent and predictable financial outcomes. Third, the utilization of real market data from the domestic financial environment enhances the relevance and practicality of investment decision-making. Moreover, the research underscores the value of diversifying across different types of financial instruments to achieve an efficient balance between risk and return. The results indicate that, even in smaller and more volatile markets, quantitative methodologies can support investors in making more informed, data-driven, and strategic decisions. Ultimately, the approach presented in this study provides a solid foundation for further research in dynamic portfolio optimization and opens opportunities for adapting advanced optimization models to the specific characteristics of emerging markets.

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INTERACTIONS OF As(III), Sb(III) AND Hg(II) SPECIES WITH HUMAN SERUM ALBUMIN

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Arsenic, antimony and mercury are among the most toxic elements of environmental and biomedical concern. They are associated with severe health effects, but their toxicity depends on the duration of exposure, dose and the molecular form that causes the poisoning. After entering the bloodstream, metal ions may interact with serum proteins. Human serum albumin (HSA), the most abundant protein in the serum, is particularly relevant due to its central role in the transport of organic hydrophobic compounds and metal ions. The molecular interactions and biochemical pathways of As^{III} and Sb^{III} in the human body remain poorly explored [1–3], and the binding properties of Hg^{II} and the metalloids to HSA are not thoroughly characterized, either.

In this study, we investigated the interactions of As^{III}, Sb^{III} and Hg^{II} with human serum albumin under physiologically relevant conditions. Two complementary spectroscopic methods were employed. First, we examined the potential binding of the metal ions to the free Cys34 thiol group of HSA using the 2,2-dithiodipyridine (DTDP) assay, monitored by UV-Vis absorption spectroscopy. In addition, tryptophan fluorescence quenching measurements were carried out to detect binding interactions near the Trp-214 group.

The experiments revealed that neither As^{III} nor Sb^{III} display significant affinity to HSA, since no consistent reactivity or fluorescence quenching was observed under the applied conditions. In contrast, the results of measurements carried out with Hg^{II} showed unambiguously the binding of this metal ion to HSA. Both the DTDP assay and the fluorescence quenching indicated strong binding to the protein, in line with the high affinity of thiol groups to Hg(II) and the known ability of Hg(II) to alter proteins' structure.

In summary, the present results provide a new insight into the molecular interactions and binding behavior of toxic metal ions with the blood transport protein (HSA). The lack of interaction observed for As^{III} and Sb^{III} indicates that other biomolecular targets may be more relevant in their transport in the human body. Exploring the binding characteristics of Hg^{II} to HSA is important for clarifying the mechanisms of the adverse effects of mercury and its transport in the bloodstream.

Acknowledgements

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TECHNICAL AND ANALYTICAL CHALLENGES
INVOLVED IN DRONE-BASED LASER-INDUCED BREAKDOWN
SPECTROSCOPY MEASUREMENTS FOR SECURITY APPLICATIONS

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Abstract

This presentation overviews the process of the development of drone-based LIBS instrumentation meant to be used primarily in security applications. We explain the difficulties faced and the potential solutions devised to tackle them. We also share our first results obtained during laboratory-based and field measurements with the system.

Introduction

Laser-induced breakdown spectroscopy (LIBS) is a versatile analytical laser spectroscopy method, which uses a focused laser beam to produce a microplasma on the surface (or inside) of a target and observes the light emitted by the plasma to reveal the chemical composition of the target (sample). The instrument can be made fairly compact and robust, considering that its main components are some optical elements (focusing and light collection optics), a pulsed and intense laser source, a spectrometer and some synchronization electronics. From an analytical point of view, LIBS offers uniquely advantageous features which can be exploited in multiple ways in industrial, security or scientific applications [1, 2]. Among these features, trace analytical sensitivity, very short measurement times, high information content in the collected dataset, field-based or stand-off measurement capabilities are perhaps the most important for security-related applications. Several successful related analytical demonstrations were already described in the scientific literature, including e.g. the stand-off detection of explosives [3], biological aerosols [4], nuclear materials [5], etc.

Along with the rapid development of ultracompact unmanned aerial vehicles (UAV, commonly referred to as “drones”) laser spectroscopy researchers started to explore the possibility to construct and use drone-based compact LIBS instruments [6], which would provide ultimate flexibility in security applications. Our pilot research projects financed by NKFIH (Hungary) aiming at demonstrating the potential of LIBS spectroscopy in chemical, biological, radiological, and nuclear (CBRN) security applications also belong to these efforts. The current paper describes the challenges involved in the realization of such a device and outlines our preliminary results related to specific applications.

Experimental

All LIBS experiments were performed using an in-house developed measurement system. This system is built around a GigaRotor6 type industrial-grade hexacopter drone and a LIBS setup whose main components are a compact, solid-state pulsed laser and a Nexos (Avantes, NL) fiber optic CCD spectrometer. For target distance measurements purposes, a Banner LT3 laser

distance sensor was incorporated. Communication, data storage and control functions were programmed in Python, and the program was run on a Raspberry Pi model 5 microcomputer.



Figure 1. System components, from left to right: hexacopter drone, compact fiber optic spectrometer, laser distance meter

Results and discussion

Our approach during the R&D project involved the following steps: 1) define/specify the analytical goal (application, expected performance) of the system, 2) identify the challenges and potential solutions involved, also considering operational safety and the capabilities of state-of-the-art industrial drones, 3) construct the system, 4) perform pilot measurements. In this abstract and in our presentation, we give a brief account of the results of all these steps.

Specifications. A drone-based pilot LIBS system should be considered as a remotely-controlled chemical sensor. Visually-driven human guidance is needed to spot a potential target and then initiate an analytical inspection to assess the chemical identity or composition of the target (sample). In later phases of the project, autonomous system operation may be imagined. Although stand-off LIBS measurements were already successfully demonstrated in the laboratory, but the challenges outlined below dictate that the drone-sample distance should be limited to a few meters. A LIBS analytical measurement only takes a fraction of a millisecond, the instrumentation is compact, lightweight (max. a few kg) and consumes small electrical power (ca. 50-100 W). Considering the operational distance, the necessity to record atomic spectra and the requirements for cost-efficiency and compactness, the system should incorporate a nanosecond laser source and a high resolution (around 0.1 nm), fiber-optic coupled CCD or CMOS spectrometer working in the UV-Vis range.

Challenges and solutions. Analytical, technical and operational safety issues are strongly interrelated. The following table attempts to give an overview of the most important aspects. Discussion of most challenges would exceed the limits of this abstract, therefore we only discuss a few here. For example, drone maneuvering accuracy and positional stability should be a high priority, given the very small analytical spot of LIBS. Vibrations and small movements should not be a problem though, given the very short measurement time. GPS-driven drone movement control is out of the question, as GPS accuracy is orders of magnitude poorer (e.g. 1 m) than what is required (ca. 1 mm). For less demanding applications, drone height (above ground distance) can be calculated by the barometric formula or by GPS, but it has a couple of meters accuracy only, and this is unacceptable for LIBS, where the target distance needs to be known/controlled with few mm accuracy. Only laser-guided distance measurements (e.g. laser pulse time-of-light measurements) are capable to provide both the height and directional (aiming) accuracy needed here.

In terms of safety, the issues are mostly drone-related, general ones. However, there is a couple of issues which are associated with the use of a pulsed, intense laser beam in the open

field. With respect to these, one countermeasure that must be implemented is that the laser is only turned on when a measurement is initiated and the drone is not directed to move (is supposed to be in a stable hover), this can be achieved by using an electromagnetic (or maybe electrooptical) safety interlock. In order to avoid (limit) any injuries or damages caused by joltlike, unintentional drone movements while measuring, the implementation of another safety switch can be suggested: this could be a tilt sensor, which can quickly shut the laser down (block the laser path) if the tilt of the drone exceeds a preset limit (please note that the laser beam is pointing vertically downwards under normal circumstances, thereby potential harm can only be done if the drone is excessively tilted). Last, but not least, the system should also be able to recognize if a human (or animal) is present directly under the drone. This feature can be implemented by using a shape recognition software working, in real time, on the camera data stream ("smart camera").

Table 1. An overview of some of the most important challenges concerning drone-based LIBS systems

Analytical (LIBS-centered) challenges	Technical (drone-centered) challenges	Safety issues
- increasing operational distance decreases sensitivity - dust particles, humidity, gases and turbulence in the optical path can have an influence on the performance - the higher the resolution of the spectrometer, the lower is the sensitivity - the broader is the spectral coverage, the lower is the resolution and sensitivity - aiming should have a high positional accuracy (mm-range) - laser wavelength should be not interfering with spectrometer - tilted target surfaces will decrease sensitivity	- sufficient load-carrying capacity - sufficient electrical power to subsystems - high maneuvering accuracy (positional control) is needed in the x-y plane - a continuous, high accuracy (mm) monitoring of drone-target distance is required - a continuous feed of imaging data is necessary to the operator - rotors generate dust and wind (turbulence) which dictates longer operational distances - on-board evaluation capability or high-speed streaming for measurement data (spectra + images) is needed - communication range	- danger of laser-inflicted eye or skin injuries to persons in the measurement path or caused by tilted, reflective targets - danger of laser-induced fire, explosions or release of CBRN materials - danger of rotor-inflicted damages to installations or injuries of persons in the measurement path - fall-inflicted damages to installations or injuries of persons in the measurement path, caused by drone failure/out-of-communication/out-of-power/EMI situations

Construction. The LIBS measurement module was built inside a plastic box (600×600×200 mm) attached to the bottom of the drone (in between the legs propping up the drone when standing on the ground). Fiber optic cables and a combination of reflective and transmissive optical elements were employed in the focusing and light collection optics. A compact, 532 nm laser was chosen as the excitation source, and the spectrometer was configured to measure in the 380-470 nm spectral range. The target distance is continuously monitored by a laser distance sensor which is aiming at the same spot as the excitation laser beam.

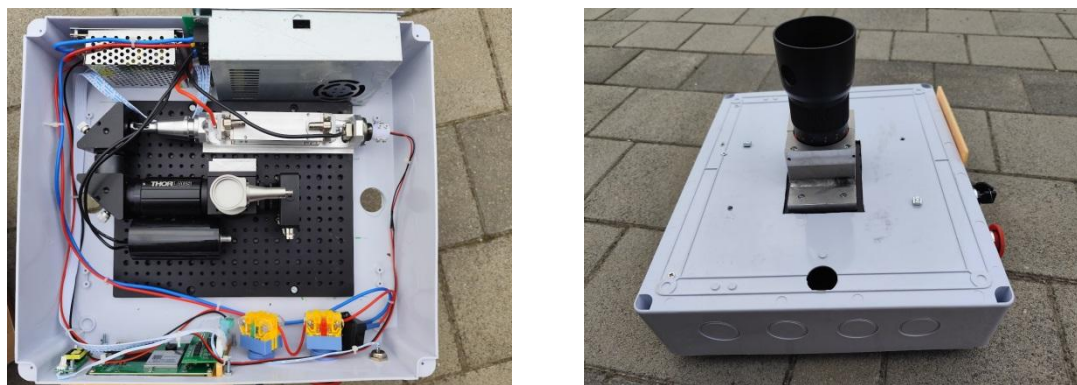


Figure 2. Photos of the internal system assembly (left) and the optics (right).

Measurements. The operational sequence of the system is the following. The operator steers the system over the target (suspicious object), at a height which is larger than the measurement distance. The target is locked by the operator and the drone enters a hovering mode, with no (intentional) lateral movements. The drone is then slowly lowered while the target distance is continuously monitored. At the moment when the target distance is equal to the measurement distance (set by the LIBS optics), the laser is fired, and the target's emission atomic spectrum is captured. This spectrum is time and position stamped and is wirelessly streamed down to the operator's computer along with the GPS coordinates and the camera image taken at the same moment when the laser is fired. In the presentation, we will also share some LIBS spectra collected with our system. Fertilizers and other metal salts were used as test samples.

Conclusion

We made significant steps towards the development of a functional drone-based LIBS measurement system. We assessed the technical and analytical challenges associated with the development and navigated them. Finally, we constructed a pilot system with which demonstrative field experiments were performed.

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PREPARATION AND STABILITY TESTING OF FLAVOURED WHIPPED CREAM WITH LYOPHILIZED INGREDIENTS

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Abstract

Flavored whipped cream, an innovative culinary creation, has garnered significant attention in recent years for its ability to elevate a wide array of dishes and beverages. Our poster delves into the diverse landscape of flavored whipped cream, shows its origins, production methods, and the multitude of delectable flavor profiles that have captivated the palates of gastronomes worldwide.

Our study begins by tracing the historical roots of whipped cream, from its inception as a simple cream topping to the modern culinary phenomenon it has become. Through a comprehensive review of literature, we explore the evolution of whipping techniques and the pivotal role of emulsifiers in achieving the desired texture and stability.

The production process of flavored whipped cream is then dissected, highlighting the incorporation of various natural and artificial flavoring agents. Techniques such as infusion, extraction, and emulsion are explored in detail, shedding light on the nuanced methods employed by culinary artisans to infuse creams with an array of enticing flavors, from classic vanilla and chocolate to salted caramel and vegan cheese.

Furthermore, our poster delves into the applications of flavored whipped cream in both sweet and savory culinary creations. Through case studies and sensory evaluations, we unveil the transformative impact of flavored whipped cream on diverse dishes, ranging from decadent desserts to innovative savory entrees.

In addition, the study examines the evolving consumer trends and market dynamics surrounding flavored whipped cream, shedding light on its growing popularity in the hospitality industry and its emergence as a staple in home kitchens.

Lyophilized fruits and cheese have emerged as indispensable components in the realm of flavoring, revolutionizing culinary creativity and product development. Their importance lies in their ability to impart concentrated, authentic flavors while offering practical benefits for both chefs and food manufacturers.

Lyophilized fruits, through the meticulous freeze-drying process, retain the essence of fresh fruits in a highly concentrated form. This allows for precise control over flavor profiles, enabling chefs to infuse dishes with vibrant, natural fruitiness regardless of seasonal availability. From adding intensity to desserts and beverages to enhancing the aromatic complexity of savory dishes, lyophilized fruits serve as versatile and reliable flavor enhancers. Similarly, lyophilized cheese undergoes a transformative preservation process that preserves its distinct taste while eliminating moisture. The resulting cheese products, whether in powdered or crumbled form, serve as potent flavor agents. These versatile cheese powders can be effortlessly integrated into a wide range of dishes, including sauces, dressings, snacks, and baked goods, elevating their taste with a rich, umami depth.

Beyond their flavor-intensifying capabilities, lyophilized fruits and cheese offer logistical advantages in the food industry. They boast extended shelf lives, reducing waste and allowing

for cost-effective inventory management. Their lightweight, compact nature simplifies storage, shipping, and handling.

In conclusion, lyophilized fruits and cheese play a pivotal role in modern culinary innovation and food manufacturing. Their concentrated flavors and practical benefits provide chefs and food professionals with a powerful toolset to craft exceptional and consistent taste experiences, while also addressing logistical concerns in the food supply chain. As essential components in flavoring, lyophilized fruits and cheese are poised to continue influencing the way we approach and savor food.

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COPPER(II) COMPLEXES OF THIOSEMICARBAZONES WITH EXCELLENT WATER SOLUBILITY: SOLUTION EQUILIBRIUM STUDIES AND NANOFORMULATION

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Thiosemicarbazones (TSCs) and their metal complexes are an important group of compounds due to their anticancer, antibacterial, and antiviral effects [1]. However their aqueous solubility is often limited, which may restrict their *in vivo* applicability. Therefore, one goal of their further development is to increase their hydrophilicity. However, their cytotoxic mechanism of action is based on passive transport across the cell membrane requiring proper lipophilicity, so the use of various carrier systems may be necessary to optimize the hydro-lipophilic character. One group of carrier systems consists of gold nanoclusters (Au NCs) stabilized with various proteins is very common [2].

In this work, the characterization of thiosemicarbazones containing four methylene trimethylammonium groups and their metal complexes is presented, in three cases with the group in a neighboring position and in one case in a distant position. We investigated the solution equilibrium and redox properties of the ligands and their metal complexes. Subsequently, we selected the two most active copper(II) complexes based on their biological activity and investigated their interaction with Au NCs stabilized with human serum albumin (HSA). The results showed that the stability of copper(II) complexes significantly affects the feasibility of drug delivery with Au NCs.

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USE OF UNMALTED CEREALS IN WORT PRODUCTION: TECHNOLOGICAL EVALUATION AND QUALITY ASSESSMENT

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In beer production, the quality of the four essential raw materials, barley malt, water, hops, and yeast, has a decisive and often crucial impact on the final quality of the beer. Malted barley is the primary raw material in traditional brewing. However, due to the complexity of the malting process, which is energy-intensive and requires large volumes of water, the use of unmalted raw materials – adjuncts – has become an increasingly viable alternative. Consequently, the use of unmalted cereals instead of malt has emerged as a promising approach to improve product quality, reduce production costs, and develop new types of beer. The most commonly used unmalted cereals in brewing include barley, wheat, oats, rice, and corn. Nevertheless, using substantial amounts of adjuncts poses technological challenges, and the sensory characteristics of beers with high adjunct levels remain unclear.

The aim of this study was to evaluate the quality of barley, oats, and dark wheat as unmalted raw materials for wort production, using the commercial enzyme Termamyl® BrewQ and a modified mashing regime (mash-in at 54 °C for 30 minutes; temperature raised to 64 °C with a 45-minute rest; and final mashing at 80 °C for 10 minutes). Worts were produced using two different proportions of native grains in grist: 25% and 50%. The results obtained in this study indicate that wort extract decreased as the proportion of native cereals in the mash increased, a trend observed in all tested samples. However, the wort produced with 25% dark wheat exhibited the highest extract content ($8.435 \pm 0.02\%$). The addition of the commercial enzyme resulted in an increase in wort extract, compared to the control sample (barley malt), since the selected enzyme—a thermostable α -amylase—enhanced starch degradation. Furthermore, enzyme application shortened the saccharification time of the worts, which has a significant impact on the overall quality of the mashing process. Wort color decreased with increasing proportions of native barley, oats, and dark wheat, with the highest color intensity observed in the wort produced from oats at a 25 % mash proportion. Based on the results, it can be concluded that unmalted dark wheat and barley can be used in wort production at proportions up to 25% of the grist with the application of a commercial enzyme. Since the lowest extract was obtained using oats, further research should focus on improving wort production to achieve more favorable extract content and optimal viscosity.

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ARSENIC(III) DETECTION USING A WHOLE-CELL BIOSENSOR

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Arsenic contamination poses a serious global environmental problem, with As(III) being a highly toxic form that threatens drinking water, soil, and human health [1]. While robust instrumental methods like ICP-MS provide sensitive and reliable detection, they are financially demanding, require specialized laboratory infrastructure, and involve complex sample preparation. This necessitates the development of alternative, portable, and cost-effective solutions for *in situ* arsenic monitoring [2]. Our research addresses this need by investigating the fundamental function of an ArsR protein using the I-Block technique within a bioreporter system.

The bioreporter system was constructed based on an ArsR metalloid sensor protein, relying on the principles of transcriptional regulation [3]. The key element of our system is the AfArsR metalloid regulator which acts as a repressor of transcription. In the absence of As(III), the protein binds to a specific promoter region of the DNA, effectively blocking the expression of the LacI protein. LacI inhibits the expression of a reporter protein, which is β -galactosidase in the I-Block system. Thus, upon binding of AfArsR to the DNA, β -galactosidase enables a simple, visual colour-detection related to the conversion of a specific substrate to a blue hydrolysis product. The presence of As(III) triggers a conformational change in the AfArsR protein, leading to its dissociation from the DNA. As a consequence of derepression, the LacI protein is expressed, which then inhibits the transcription of the reporter gene.

Our main objective was to investigate the functioning of the AfArsR protein via the operation of the bioreporter construct. The I-Block method allowed us to study the DNA-binding properties of AfArsR within the bacterial cells. Our experiments confirmed that the engineered cells respond sensitively to the presence of As(III). Furthermore, selectivity studies were conducted with metal ions possessing similar properties or a high affinity to active site of the protein, and the results were promising. This suggests that the AfArsR-controlled system holds promise for the efficient discrimination of As(III), which is a crucial attribute for environmental monitoring.

These findings highlight the potential of our bioreporter as a sensitive and sustainable biosensor for arsenic detection in environmental samples. This research also contributes to a better understanding of the metalloid-binding mechanisms of ArsR proteins and offers a valuable alternative to traditional analytical methods.

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OVERVIEW OF THE POTENTIAL ROLE OF LACTIC ACID BACTERIA IN THE REDUCTION OF MYCOTOXINS AND PESTICIDE RESIDUES IN FOOD AND FEED

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Abstract

Lactic acid fermentation and lactic acid bacteria (mainly *Lactobacillus* and *Streptococcus* species) are widely recognized for their nutritional and health benefits, including the promotion of a balanced gut microbiota, improved digestion, and immune support. Nevertheless, intensive agricultural practices, unauthorized pesticide applications, and inadequate post-harvest and storage conditions frequently result in the occurrence of pesticide residues and mold-derived mycotoxins in crops, feeds and food products. The presence of these contaminants in food and feed poses a major food safety and public health challenge. According to the scientific literature, lactic acid bacteria play a crucial role in the inhibition of pathogens, the neutralization of toxins, and the degradation of chemical contaminants (e.g., pesticide residues). Various mechanisms (e.g., cell wall binding, production of antifungal metabolites, and enzymatic degradation) have been reported to contribute to the direct and/or indirect reduction of mycotoxin and pesticide residue levels. Owing to their broad enzymatic repertoire and diverse beneficial biological activities, lactic acid bacteria constitute a promising natural strategy for the detoxification of food contaminants including mycotoxins and pesticide residues, particularly in the context of large-scale food production and growing environmental pollution.

1. Introduction

The beneficial effects of lactic acid fermentation and lactic acid bacteria are well recognized from both nutritional and health perspectives. During lactic acid fermentation, the presence of lactic acid bacteria (*Lactobacillus* and *Streptococcus* species) can promote the establishment and maintenance of a healthy gut microbiota, positively influence digestion, and strengthen the immune system [1–5]. Nowadays, the extensive use of pesticide formulations in intensive agricultural practices, the application of unauthorized chemicals, as well as inadequately chosen technological conditions during harvest and storage of crops, can substantially contribute to the occurrence of pesticide residues and mycotoxins produced by various molds in agricultural commodities and food products. The presence of mycotoxins and pesticide residues in food and feed poses significant food safety and public health risks. The pesticide active ingredients used in chemical plant protection, often persist throughout food processing, whereas mycotoxins (naturally occurring fungal secondary metabolites) generally exhibit remarkable stability and resistance to degradation [6–7]. Both contaminant groups are associated with severe adverse health outcomes, including carcinogenic, neurotoxic, immunotoxic, and endocrine-disrupting effects [7–9]. In response, stringent regulatory thresholds have been established by international

and national authorities. Currently, the conventional mitigation strategies (e.g., chemical decontamination and physical removal) are often costly, not permitted by law, or incompatible with the principles of sustainable food production [10–11]. Lactic acid bacteria have been shown to exert multiple detoxification functions, including the inhibition of pathogenic microorganisms, the neutralization of toxic metabolites, and the biotransformation of xenobiotic compounds [1, 5, 12–17]. Their diverse enzymatic repertoire and metabolic versatility, lactic acid bacteria can serve as a promising biotechnological tool for the detoxification of food contaminants in the context of industrial-scale production and increasing environmental pollution [1].

2. The role of lactic acid bacteria in the reduction of pesticide residues and mycotoxins

Lactic acid bacteria can contribute to the reduction of pesticide residues and mycotoxins in food and feed, providing a natural strategy that supports the food industry's sustainability objectives by reducing dependence on synthetic chemicals. Based on the results of the published studies, lactic acid bacteria are capable of mitigating residues of various pesticides including herbicides, fungicides, and insecticides (e.g., DDT, chlorpyrifos, malathion) as well as mycotoxins (e.g., aflatoxin B1, ochratoxin A, sterigmatocystin, and patulin) [1, 5, 12–19]. A remarkably wide range of mechanisms is reportedly involved in the reduction of pesticide residues and mycotoxins. The underlying mechanisms include: enzymatic degradation of contaminants, environmental modulation with synergistic effects, metabolic transformation, antioxidant activity and preventive effects, biofilm formation facilitating enhanced detoxification, adsorption through cell wall binding, and production of antifungal metabolites respectively the given food contaminants [1, 13–14, 20–23].

2.1. The potential for mycotoxin reduction by lactic acid bacteria

Mycotoxins are toxic secondary metabolites produced by fungi (e.g., *Aspergillus*, *Fusarium*, and *Penicillium* species) that contaminate agricultural products such as nuts, fruits, grains, and wine. They may develop in the field, post-harvest, or during processing and storage. Major representatives include aflatoxins, deoxynivalenol, zearalenone, ochratoxin, fumonisin, and patulin, all of which pose significant food safety and public health risks. Mycotoxins are associated with serious health risks, including carcinogenic, hepatotoxic, nephrotoxic, immunotoxic, and neurotoxic effects. Due to the high stability of mycotoxins against heat and conventional processing methods, the prevention and detoxification are particularly challenging [1, 7, 24].

The main direct and indirect mechanisms are involved in the reduction of mycotoxins:

- cell wall binding (non-covalent adsorption onto bacterial surface structures) [15]
- biological degradation (enzymatic breakdown into less toxic metabolites) [25]
- production of antifungal metabolites (inhibition of the growth of molds/other fungi) [23]
- biofilm formation (biofilms increase binding surfaces and environmental resistance to ensure effective detoxification) [26]

Lactic acid bacteria mitigate mycotoxin contamination through multiple mechanisms, including cell wall binding (e.g., aflatoxin B1), production of antifungal metabolites (e.g., 52–80% transcriptional inhibition of the *omt-A* gene responsible for the biosynthesis of aflatoxin B1), enzymatic degradation (e.g., >90% degradation of ochratoxin A by proteolytic activity), and modulation of fermentation conditions (e.g., pH, temperature). Both live and dead cells are effective, and biofilm formation further enhances detoxification by increasing binding surfaces and environmental stability [15, 23, 25–26]. Due to these beneficial properties of lactic acid

bacteria serves as a safe and sustainable strategy for natural food preservation and mycotoxin reduction in food and feed.

2.2. The potential for the reduction of pesticide residues by lactic acid bacteria

Pesticide formulations including insecticides, fungicides, and herbicides are widely used during the intensive agricultural practice to enhance crop yield and quality by controlling pests, diseases, and weeds [8]. The implications of pesticide use in food production, coupled with the recognition that residues may remain in consumable products, are of critical importance for food safety and are a growing concern among health-conscious consumers [27–28]. Additionally, the use of multiple agents on the same commodity can lead to the presence of multiple residues within a single product [29]. The residues of pesticide formulations are associated with a wide spectrum of health risks, encompassing both acute and chronic health effects and risks (e.g., cardiovascular and respiratory diseases, cancer, and endocrine disruptions) [27–29].

The main direct and indirect mechanisms are involved in the reduction of pesticide residues:

- enzymatic breakdown (specific enzymes catalyze the decomposition of pesticides) [21]
- environmental modulation synergistic effects (acidic environments destabilize the pesticide molecules) [14]
- metabolic transformation (convert compounds into less toxic/inactive forms) [12, 21]
- antioxidant effects and proactive action (mitigating oxidative damage associated with pesticide residues) [21]
- biofilm formation (more effective immobilization and degradation of pesticides) [21]

Lactic acid bacteria can degrade pesticides through multiple mechanisms, including enzymatic breakdown (e.g., dimethoate, parathion methyl, trichlorfon by phosphatase and antioxidation), metabolic transformation, and biofilm formation, which increase their detoxification capacity (e.g., biofilm-associated lactic acid bacteria can show enhanced degradation efficiency for organophosphorus pesticides compared to planktonic cells). Additionally, environmental modulation (e.g., enhanced degradation of λ -cyhalothrin, malathion, chlorpyrifos-methyl at low pH) and synergistic interactions further enhance the efficiency of lactic acid bacteria-mediated pesticide degradation in foods and beverages [1, 12, 14, 21, 30].

3. Advantages and limitations of lactic acid bacteria-based reduction approaches

Lactic acid bacteria offer several advantages as biological tool for pesticide and mycotoxin detoxification and reduction. Lactic acid bacteria are non-pathogenic and in many cases probiotic, making them highly suitable for application in foods and feeds [1–5]. Lactic acid bacteria-based strategies provide a sustainable alternative to chemical treatments while simultaneously conferring dual benefits, such as improving nutritional value, extending shelf-life, and enhancing the sensory properties of products [31–32]. Moreover, these microorganisms can be easily integrated into existing fermentation processes and silage production, supporting scalability in both food and feed systems [33]. However, despite the promising results, significant limitations remain. The efficiency of detoxification is highly strain-specific, meaning that not all lactic acid bacteria exhibit the same capability to degrade or bind contaminants (e.g., fumonisins) [34]. Furthermore, matrix effects, such as food composition and processing conditions, strongly influence detoxification performance. Stability is also a concern, as adsorption processes may be reversible, raising questions about the long-term effectiveness of toxin removal [35]. Finally, the mechanistic understanding of lactic acid bacteria detoxification remains incomplete, and further research into enzymatic pathways and genetic determinants is essential to optimize their use in food safety applications.

4. Conclusion

The presence of pesticide residues and mycotoxins in food and feed represents a major global food safety issue. Lactic acid bacteria provide a promising, natural, and sustainable tool for reducing pesticide residues and mycotoxins, while also contributing to gut health and overall well-being. Their detoxification ability through mechanisms related to adsorption, enzymatic degradation, and fermentation is increasingly supported by scientific evidence. Although challenges remain regarding strain specificity, stability, and scalability, lactic acid bacteria-based detoxification can complement or partially replace conventional chemical methods, contributing to safer food systems, improved public health, and more sustainable agricultural practices. Future research should focus on advancing biofilm-based applications, genomic and proteomic screening for high-performing strains, the use of mixed microbial cultures, and pilot-to-industrial scale validations to fully realize the potential of lactic acid bacteria in food and feed detoxification [26, 36].

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HRMS ANALYSIS OF SURFACTIN-TYPE COMPONENTS PRODUCED BY *BACILLUS* STRAINS ISOLATED FROM ENVIRONMENTAL SAMPLES

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Abstract

Surfactin-type components produced by *Bacillus* species are cyclic lipopeptides with broad potential across environmental sustainability, agriculture, and environmental protection. In addition to their ecological relevance, these compounds also exhibit practical bioactivities such as antibacterial, antifungal, antiviral, and antitumor properties. In this study, we successfully performed the taxonomic identification of 40 *Bacillus* strains isolated from fungal compost. The surfactin production by each strain, as well as the individual surfactin variants, was examined by High-Resolution Mass Spectrometry (HRMS). Of the 40 *Bacillus* strains, 18 were found to produce surfactins, representing members of the species *B. subtilis*, *B. halotolerans*, *B. licheniformis*, and *B. velezensis*. A total of 109 distinct surfactin variants were identified among the isolates. Following the spectrometric analysis, biological assessments were performed to determine the antimicrobial activity of the surfactin producing strains against phytopathogenic bacteria and fungi. *B. subtilis* strains were generally effective against phytopathogenic bacteria. For phytopathogenic fungi, *B. halotolerans* strains demonstrated the strongest activity. In general, our findings on the production of surfactin by *Bacillus* isolates provide a solid foundation for the identification of promising candidates for future biocontrol applications.

Introduction

The importance of studying surfactin production by *Bacillus* species is due to their role in environmental sustainability [1], health and medical uses [2], agriculture and environmental protection [3]. The use of biosurfactants at low concentrations exceeds the effectiveness of synthetic surfactants, they are more easily degraded and more stable under extreme conditions [4]. These properties make them suitable for industrial use. The study of their structure may contribute to the development of synthetic alternative surfactants with less environmental impact due to their easier degradation. In medicine, the antimicrobial effects of surfactins are exploited. The use of surfactins as antibiotics may offer an alternative to increasing antibiotic resistance [5]. Surfactins are also used in cancer research to efficiently deliver drugs to cancer cells [6]. Their use as biopesticides in agriculture can reduce the use of chemical pesticides, and their ability to solubilise and mobilise contaminants in soil and water can be used in bioremediation projects [7]. In the food industry, surfactins can act as natural emulsifiers in foods, improving texture, stability and shelf-life [8]. Research in this area focusses on the development of natural, safe food additives that can replace synthetic emulsifiers, often derived from chemicals or genetically modified organisms.

Experimental

For the strains taxonomic determinations, the *rpoB* gene sequences were amplified by PCR from purified template DNA of the bacteria. The surfactin production of each strain was examined by mass spectrometry. The individual surfactin variants were detected in each *Bacillus* strain by HRMS. The analysis of the surfactin variants was based on the characteristic fragmentation patterns of surfactin molecules. In the HRMS method surfactin molecules were analysed according to the mass of the sodium adduct from of the molecular ion (m/z 1016, m/z 1030, m/z 1044, m/z 1058, m/z 1072, m/z 1086, m/z 1100, m/z 1114).

Biological assays were carried out to determine the antimicrobial activity of surfactin producing strains. The inhibition zones were measured against phytopathogenic fungi and bacteria.

Results and discussion

We successfully performed the taxonomic identifications of 40 *Bacillus* strains from environmental samples. Following the taxonomic characterization, we carried out a detailed investigation of surfactin production by these strains. Of the 40 *Bacillus* strains, 18 were found to produce surfactins, representing members of the species *B. subtilis*, *B. halotolerans*, *B. licheniformis* and *B. velezensis*. A total of 109 distinct surfactin variants were identified among the isolates. The strains those produced the highest amount of surfactin were members of the *B. halotolerans* and *B. licheniformis* species.

Against the phytopathogenic bacteria, the *B. subtilis* strains were generally effective, although minor inhibition zones were observed. For the phytopathogenic fungi, most of the strains exhibited inhibition zones, with the largest inhibition were produced by members of the *Bacillus halotolerans* species.

Conclusion

The taxonomic identification of 40 *Bacillus* strains was performed using *rpoB* gene sequences. Through HRMS analysis, 18 surfactin producing strains were identified. A total of 109 distinct surfactin variants were identified among the isolates. Against phytopathogenic bacteria, *B. subtilis* strains were generally effective; for phytopathogenic fungi, *B. halotolerans* strains were the most effective.

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NOT FINALIZED

SEQUENTIAL EXTRACELLULAR ORGANIC MATTER-TREATMENT BOOSTS BIOREMEDIATION EFFICIENCY

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Abstract

Used lubricant oils (ULOs) often accumulate harmful compounds such as heavy metals and polycyclic hydrocarbons, causing persistent soil contamination that impairs habitat functions and future use [1–2]. Under these conditions, microorganisms, including hydrocarbon degraders, may enter a viable but non-culturable (VBNC) state with low or absent activity [3]. Thus, the outcome of bioremediation largely depends on sustaining microbial activity or reactivating VBNC cells via biostimulants. Resuscitation-promoting factors (Rpfs) have proven effective in the early stages of ULO bioremediation [2]. In this study, we aimed to extend the stimulatory effect of Rpf-containing extracellular organic matter (EOM) from *Micrococcus luteus* to improve ULO biodegradation. *Ex situ* soil microcosms were supplemented with EOM at the start (day 0) and after the first biodegradation phase (day 20). After 60 days of biostimulation (BS), extractable petroleum hydrocarbons (EPHs; 30,300 mg/kg) decreased by 56% with repeated EOM application (BS+2×EOM), compared to 46% with a single dose (BS+EOM). BS+2×EOM also enhanced colony-forming units (CFUs), respiration, and soil enzyme activities (dehydrogenase, catalase, sucrase, fluorescein diacetate hydrolase) relative to controls. Although BS+2×EOM and BS+EOM achieved the most effective hydrocarbon removal, the germination index of oilseed rape (*Brassica napus* L.) still decreased to 43% and 42%. These results indicate that improved microbial activity and pollutant reduction do not necessarily mitigate soil phytotoxicity.

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ASSESSMENT OF MIGRATION OF SUBSTANCES FROM BIODEGRADABLE PACKAGING MATERIALS INTO FOOD PRODUCTS USING ADVANCED ANALYTICAL TECHNIQUES: CHALLENGES AND POTENTIAL FOR SUSTAINABLE DEVELOPMENT

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Abstract

Contemporary requirements of sustainable development impose an increasing need to switch from conventional plastic packaging materials to sustainable, biodegradable and compostable alternatives with the aim of reducing the ecological footprint of the food industry, which is under pressure to reduce plastic waste. Biodegradable food packaging is gaining importance due to environmental and regulatory requirements, but the use of biodegradable materials raises new questions about food safety. Namely, intentionally added substances (IAS) - such as monomers, stabilizers or bioactive additives - and unintentionally present substances (NIAS) - such as degradation products or pollutants - can migrate from packaging to food [1,2]. These substances can change the organoleptic properties of food or pose a health risk, so the identification and quantification of IAS and NIAS is crucial for evaluating the safety of biodegradable packaging [3,4]. Modern analytical techniques, especially GC-MS/MS and LC-QToF, enable the detection of even the smallest traces of migrants and represent the basis for the development of regulatory guidelines and new materials [2]. Gas Chromatography–Tandem Mass Spectrometry (GC-MS/MS) is used for volatile and semi-volatile migrants of low molecular mass (<800 Da) originating from biodegradable packaging. The application of polar and non-polar columns in combination with "soft" ionization techniques ensures reliable identification and quantification of IAS and NIAS in food [2,5]. This technique is suitable for screening unknown substances because it can generate molecular ions and characteristic fragments necessary for structural identification. In contrast, Liquid Chromatography–Quadrupole Time-of-Flight Mass Spectrometry (LC-QToF) is the method of choice for nonvolatile migrants. LC-QToF enables identification even when no standards are available. By combining GC-MS/MS for volatiles and LC-QToF for non-volatile migrants, a comprehensive profile of IAS and NIAS from biodegradable packaging is achieved [6]. Previous research has shown that biodegradable polymers such as PLA and PHA can release a range of low molecular weight compounds, including additives, monomer residues and degradation products [7, 8]. Using GC-MS/MS and LC-QToF techniques, migrants such as phthalates, alcohols and esters, which may have a potential impact on food safety, were identified [9,10]. It was also found that the composition and structure of biodegradable packaging materials, as well as storage conditions, significantly affect the migration profile [11, 12]. Understanding the risks and benefits of using "green" packaging materials used for packaging food products is extremely important, in order to ensure not only food safety, but also environmental protection in accordance with the principles of sustainable development.

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COMPARATIVE KINETIC ANALYSIS OF ANAEROBIC BIOLOGICAL DEGRADATION OF SLUDGE

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The valorization of biologically derived raw materials is strongly influenced by their complex kinetic properties, which fundamentally affect both process efficiency and their applicability at industrial scale. Various mathematical, empirical, and semi-empirical models play a key role in accurately describing these processes, predicting yields, and optimizing operating conditions. In our research, we investigated the biogas fermentation of food industry-derived sewage sludges, with particular emphasis on their biokinetic characteristics and interpretation, as well as on the correlation between kinetic models and analytical and dielectric measurement methods applied for monitoring the fermentation process. Our aim was to determine which kinetic models provide the most accurate description of the biogas production processes of sludge samples subjected to different native and combined pretreatment methods, and whether process monitoring parameters correlate with the kinetic results. Cumulative biogas yields were evaluated using several commonly applied models, including the modified Gompertz model, integrated Monod model, first-order model, and logistic model. Among the kinetic models applied, several exhibited a high degree of fit to the experimental data ($R^2 > 0.98$) and accurately described the lag phase duration, the maximum product formation rate, and the asymptotic biogas potential. The best overall fit, as well as the lowest residual error and AIC values, was obtained with the modified Gompertz model for most sludge samples, confirming its broad applicability in the biogas valorization of the sludge types studied. Our results demonstrated the importance of selecting appropriate kinetic models for the evaluation and interpretation of experimental data, and highlighted the potential of combining biokinetic modeling with advanced process monitoring methods.

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BOOSTING ANAEROBIC LIGNOCELLULOSE UTILIZATION VIA SYNTROPHIC INTERACTIONS

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Lignocellulose-based biomass represents one of the most abundant renewable resources, holding great promise for sustainable energy generation and as a raw material for the chemical industry.

Our research aims to develop a stable, efficient microbial consortium capable of degrading lignocellulose under artificial conditions, relying on tight syntrophic interactions. To this end, we investigated the degradation efficiency of rumen-derived anaerobic fungi (AGF), methanogenic archaea (MA), and bacteria (BAC), cultivated on straw. Using SEM, HPLC, and metagenomic approaches, we observed intensive microbial proliferation and close cell-to-cell associations among AGF, MA, and BAC. Metagenomic sequencing provided insights into dynamic community shifts, while HPLC analyses revealed the composition of degradation products.

In line with previous findings on biomass pretreatment, we also applied biological pretreatment in our system. Both the anaerobic fungus–methanogen (AGF-MA) and the fungus–methanogen–bacterium (AGF-MA-BAC) consortia generated substantial methane yields when supplied with hydrogen. Notably, the AGF-MA-BAC community produced 27% more methane than AGF-MA alone, and under optimal microbial configurations, methane production increased by 50–60%. Subsequent biogas fermentation trials confirmed that the AGF-MA-BAC consortium consistently achieved the highest methane output. These results support our hypothesis that this minimal microbial community enhances structural breakdown of plant biomass and maximizes methane generation.

Since methane is the primary energy carrier in biogas and directly usable as a renewable fuel, the synergistic action of this microbial system offers a promising route for energy-efficient processing and utilization of lignocellulose-rich biomass and agricultural residues.

COLORIMETRIC QUANTIFICATION OF CYANOBACTERIAL BIOFILM UNDER DIFFERENT LIGHT ENVIRONMENT

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Abstract

Production of extracellular polymeric substance (EPS) in *Synechocystis* sp. PCC 6803 showed strong dependencies on both irradiance and growth regime. Biofilm forming cells secreted more EPS per biomass compared to planktonic cells regardless of light intensities, consistently with its structural role in biofilm matrix formation. Light-intensity dependence of EPS levels showed elevated production under both low ($10 \mu\text{mol photons m}^{-2} \text{ s}^{-1}$) and high light ($> 200 \mu\text{mol photons m}^{-2} \text{ s}^{-1}$) intensities, suggesting its induction by both carbon overflow and photoprotective mechanisms. In addition, EPS secretion showed a remarkable wavelength dependence, peaking under blue-green (460-510 nm) light and strongly declining under yellow-orange (560-590 nm) wavelengths. These findings highlight EPS secretion as a dynamic trait shaped by both light intensity and spectral composition, with the biofilm lifestyle further amplifying EPS yields.

Introduction

Some bacteria, cyanobacteria and algae have two major life forms during their growth and proliferation. In free-living, planktonic lifestyle, they exist as single, independent cells, whereas in biofilm form, they are embedded within a self-produced EPS matrix and adhere to each other and/or to a surface. Biofilms could be formed both on living and non-living surfaces.

Photosynthetic microorganisms (cyano-, purple- and green bacteria, diatoms and green algae) in terrestrial and aquatic environments can grow either as plankton or aggregates in phototrophic biofilms mats produced usually on surfaces when exposed to light [1]. The phototrophic biofilms have been used in various biotechnological applications, such as wastewater treatment in constructed wetlands, bioremediation, and aquaculture.

Cyanobacteria are ubiquitous photosynthetic microorganisms in aquatic environments, where they substantially contribute to primary production, nutrient cycling, and biofilm formation. Among them, *Synechocystis* sp. PCC 6803 (*Syn. sp.*) serves as a model organism for studying various aspects of physiology, including biofilm formation under diverse environmental conditions [2].

Light is one of the principal environmental parameters affecting cyanobacterial physiology. Both light quantity (intensity) and spectral quality (wavelength) shape photosynthetic efficiency and growth rates [3]. Despite these known effects on free-living planktonic cells, relatively less is understood about biofilm formation, structure, and function. Key question: How do different light intensities and spectral compositions influence the development and biomass of *Syn. sp.* biofilms? In this study we applied a colorimetric assay to quantify *Syn. sp.* biofilm levels across a matrix of light intensities and wavelengths.

Experimental

Strain and cultivation: *Syn. sp.* cells were grown in Erlenmeyer flasks with (planktonic) and without (biofilm) 2-3 mm diameter glass beads at 24°C in liquid BG-11 medium as semi-continuous batch cultures. The stock cultures were cultivated under warm-white, fluorescent

lamps ($25 \mu\text{mol photons m}^{-2} \text{s}^{-1}$). In the first session cultures exposed to 2, 10, 25, 50, 100, 250 and 400 $\mu\text{mol photons m}^{-2} \text{s}^{-1}$ diffuse warm white light, while in the second session, nine different monochromatic lights ($25 \mu\text{mol photons m}^{-2} \text{s}^{-1}$) were applied using a home-built cultivation apparatus (Fig.1), using a 16:8 h light-dark regime. Nine different growth wavelengths, from 430 to 690 nm, were applied, using power LEDs (Fig.1).



Figure 1. Home-built cultivation bench with nine different monochromatic growth lights from 430 to 690 nm.

EPS separation: Before harvesting, cells were grown to early stationary phase. 1 mL sample was collected from each flask and then were centrifuged (5000 g, 10 min, 4°C). The pellet was resuspended in Tris-HCl (pH: 7.5) buffer and gently shaken (room temperature, 60 min, 100 rpm) to release bound EPS from the cells. Then samples were centrifuged again (6000 g, 15 min, 4°C) to separate the soluble EPS fraction from the cells. The pellets (intact *Syn. sp.* cells) were resuspended in BG-11 medium and the OD₇₅₀ values were determined using a doublebeam spectrophotometer (Analytik Jena Specord 210 Plus) in order to determine the biomass for normalization. The supernatant of the samples containing soluble EPS was then used for the colorimetric assay.

EPS quantification - Colorimetric assay for total glucose: EPS are mostly composed of polysaccharides (exopolysaccharides), therefore a colorimetric method for carbohydrates was applied. The samples containing soluble EPS were precipitated with 100% cold ethanol (1:1) and incubated overnight at 4°C. After the ethanol treatment, the sample was dried out at 40-45°C temperature followed by rapid addition of 200 μL sterile distilled water, 200 μL 5% phenol, and 1 mL concentrated sulfuric acid [4]. After waiting 10 min for color development (Fig. 2) in the dark in a water bath at 22°C, optical absorbance was measured by a double beam spectrophotometer at 490 nm. For quantitative determination of the total soluble-glucose concentration, the colorimetric method was calibrated by a series of glucose solutions of known concentrations (0, 2, 5, 10, 20 $\mu\text{g/mL}$). To avoid possible interference from other substances different from glucose, corrections were made by running a parallel assay without phenol.

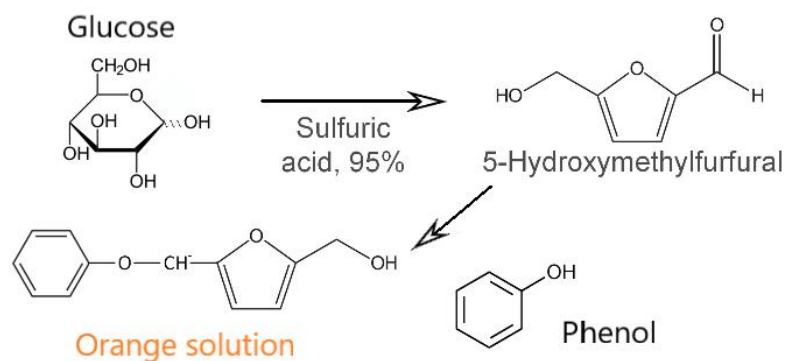


Figure 2. Schematic overview of the phenol-sulfuric acid method for the total glucose analysis.

Results and discussion

EPS production in *Syn. sp.* showed a strong dependency on both irradiance and growth type (Fig. 3). Biofilm forming cells secreted significantly more EPS per biomass compared to planktonic cells regardless of light intensities, consistent with the role of EPS in biofilm matrix formation and surface attachment [5]. In both cases, light-intensity dependence of EPS levels were relatively high under low light intensities ($10 \mu\text{mol photons m}^{-2} \text{s}^{-1}$), minimal under intermediate irradiances ($20\text{--}30 \mu\text{mol photons m}^{-2} \text{s}^{-1}$), and remarkably high under high light intensities (Fig. 2). This pattern suggests that EPS production is induced under both light limitations, possibly reflecting carbon overflow metabolism, as well as under high light stress, where EPS likely contributes to photoprotection and oxidative stress reduction [6]. These findings align with earlier reports that light intensity is a major regulator of cyanobacterial EPS yields [7] and further highlight the biofilm lifestyle as a driver of elevated EPS secretion in *Syn. sp.* cells.

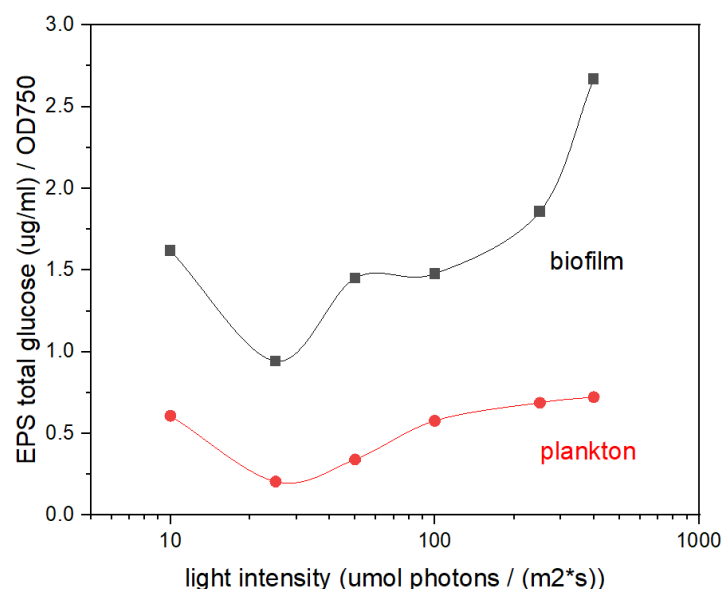


Figure 3. Light intensity dependent EPS production of *Syn. sp.* under biofilm and planktonic growth. Extracellular polysaccharide (EPS) levels were quantified using a colorimetric assay as glucose equivalents normalized to OD_{750} . Biofilm forming cells (black squares) consistently secreted more EPS per biomass compared to planktonic cells (red circles).

EPS production in *Syn.* sp. showed a strong wavelength dependence (Fig. 4). The highest EPS production were observed under blue-green light (460–510 nm), reaching more than six-fold higher levels compared to red light. In contrast, EPS secretion decreased markedly in the yellow-orange region (560–590 nm). Under longer wavelengths (630–690 nm), EPS production remained low but increased slightly again under near far-red illumination.

In several cyanobacterial species besides *Syn.* sp., blue light has been shown to have a pronounced impact on EPS production. In filamentous *Nostoc* sp. strains, exposure to blue light enhances EPS synthesis, a response often associated with stress signaling and the need for a protective extracellular matrix under fluctuating light conditions [8]. Studies on *Trichormus* sp. also demonstrate that high-intensity blue light increases EPS secretion, likely functioning as a photoprotective strategy under stress conditions [9]. Furthermore, in soil-crust-forming cyanobacteria such as *Microcoleus* sp., blue light contributes to EPS release that enhances soil aggregation and resistance to desiccation [10]. Collectively, these findings indicate that the stimulatory effect of blue light on EPS synthesis is widespread among cyanobacteria and is generally linked to protective and adaptive responses to environmental stresses.

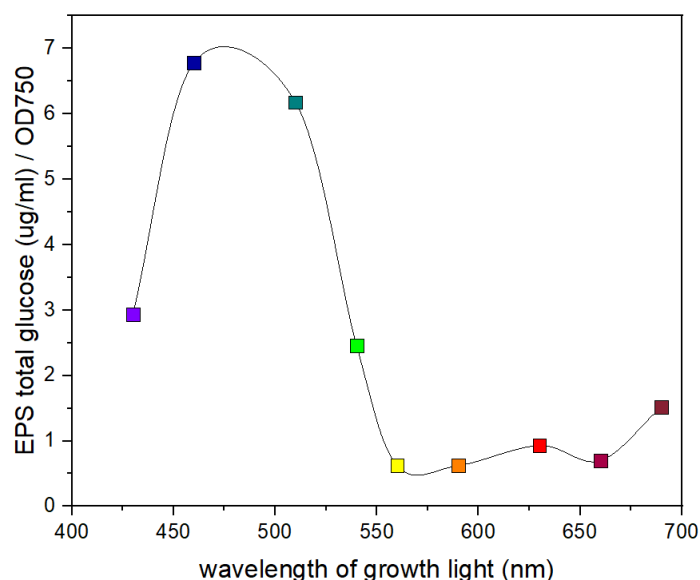


Figure 4. Wavelength dependence of EPS production in *Synechocystis* sp. PCC 6803. Cultures were grown under monochromatic light (430–690 nm) at $25 \mu\text{mol photons m}^{-2} \text{s}^{-1}$ light intensity, and extracellular polysaccharide levels (EPS) were quantified as glucose equivalents normalized to OD_{750} .

Conclusion

EPS secretion in *Syn.* sp. is strongly regulated by light intensity, spectral quality, and growth type. The enhanced production in biofilm forming cells highlights the ecological role of EPS in surface colonization, while the pattern of irradiance response and blue-green light stimulation suggest both metabolic overflow and stress protection as key drivers. Together, these results emphasize that EPS dynamics are central to cyanobacterial acclimation, linking environmental light conditions to biofilm development and ecological role.

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APPLICABILITY OF FLUORESCENCE-BASED IMMUNOBIOSENSOR ON HEAT SHOCK PROTEIN DETERMINATION IN GREEN ALGA *CHLORELLA VULGARIS*

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Members of 70 kDa heat shock protein (HSP70) family are highly conserved molecular chaperons and ubiquitously found in almost all living organisms, acting as crucial protectors of cellular integrity under various types of stress by stabilizing proteins and preventing their denaturation or aggregation [1]. HSP70s play a crucial role in protein homeostasis and stress response induced by environmental stressors (i.e. heat, desiccation, changes in salinity, UV radiation, etc.) or pollutants [2]. Algal organisms are usually investigated in ecotoxicity assays as indicator species of the aquatic ecosystem. HSP70s react quickly to these environmental stressors, thus they can be applied as biomarkers in ecotoxicity assays.

Various techniques have been presented for qualification or quantification of HSP70 proteins in different biological matrices. Methods to determine overall HSP70 levels, its intracellular localization, mRNA levels and functional binding include enzyme-linked immunosorbent assays [3–4], flow cytometry [5–6], immunohistochemistry [7–8], western blotting [9–10], quantitative reverse transcription polymerase chain reaction [11–12], fluorescence polarization [13–14] and immunocytochemistry [15].

In this study, the applicability of a double antibody sandwich enzyme-linked fluorescent immunoassay was investigated in HSP70 determination in *Chlorella vulgaris* green alga species. HSP70 calibration curves were obtained in standard assay dilution and in homogenized green alga samples prepared by sample assay diluent. Calibration curves were fitted by the Rodbard equation in the concentration range of 0–71.4 ng/mL. HSP70 standards were determined by both visual and fluorescent signals. Absorbance (optical density) and fluorescence were measured at 450 nm and 593 nm wavelengths (excitation: 535 nm), respectively.

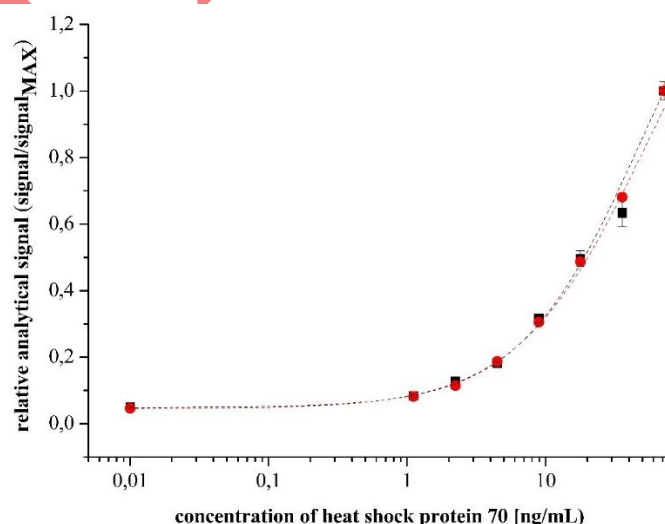


Figure 1. Calibration curves of the double antibody sandwich technique-based enzyme-linked fluorescent immunoassay obtained in assay standard diluent (black) and in homogenized green alga (*Chlorella vulgaris*) sample (red).

Determination by fluorescence provided a wider dynamic range for HSP70 detection. Application of the fluorescent signal provides a 4.5-times lower limit of detection value than that obtained with a visual absorbance signal. Parameters of calibration curves (IC_{50} and slope) did not significantly differ between calibration curves obtained in assay standard diluent and in green alga sample (Figure 1).

Acknowledgements

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THE HAPPY MARRIAGE OF METHANOGENIC ARCHAEA AND ANAEROBIC FUNGI

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Degradation of lignocellulose-rich material into biogas is an attractive strategy to face growing energy demands and moderate greenhouse gas emissions from the exploitation of fossil energy resources. Lignocellulose biomass is composed of interwoven cellulose and hemicellulose, coated by anaerobically almost undegradable lignin. This is the explanation why bacteria and archaea in the biogas reactor are not efficient in disintegration of the lignin, leaving a considerable portion of the more easily convertible sugars untouched. Anaerobic fungi (AF) from the phylum Neocallimastigomycota living in the rumen are of particular importance in the nutrition of herbivorous animals, as they are able to break down lignocellulose with high efficiency. The AF attach to the plant material and crack the fibres mechanically by growth and expansion of their rhizoids or bulbous holdfasts. To exploit this feature, we need to understand what the ideal conditions are for them and which microbes are their "favorite" partners. During our study, we isolated anaerobic fungi and their methanogenic partners from different herbivorous animals. In our experiments, we monitored the degradation efficiency using pure anaerobic fungal culture, AF enzymes and anaerobic fungal - methanogenic co-cultures. In this study, treatment with anaerobic fungi-methanogenic co-cultures (14-day) increased the total biomethane yield during the experimental period of 20 days. Pretreatment with anaerobic fungi significantly improved the degradability of substrates, the amount of methane produced increased by 100-300%, depending on the plant material. The results for AF biomethane yields correlated well with the organic acid concentrations measured by HPLC and with the enzyme activities. From these it can be concluded that the anaerobic fungi degraded the substrate efficiently during the 14-day long treatment. Based on these results AF isolates were effective in enhancing cellulose degradation and successfully increased biogas production.

INVESTIGATION OF RECOMBINANT B-GALACTOSIDASE FROM *RHIZOMUCOR PUSILLUS*

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Abstract

Zygomycetes fungi, especially members of Mucoromycota, represent a diverse group of filamentous fungi; many of which are saprotrophic and have industrial, biotechnological, and medical significance [7]. β -Galactosidase (lactase) hydrolyzes β -glycosidic bonds in β -galactosides and is widely used in the food industry to reduce the lactose sugar mass in dairy products and to process whey, a by-product of cheese production. [4], [5] Due to the prevalence of lactose intolerance, there is a growing demand for novel β -galactosidases with desirable biochemical properties and cost-effective production systems [2]. The Mucoromycota fungi can be exploited for enzyme production; however, their β -galactosidase activity and the molecular and functional features of the corresponding genes are less studied.

In this study, genome analysis of the thermophilic *Rhizomucor pusillus* SZMC 11025 revealed three putative β -galactosidase coding genes that show a high similarity to *Trichoderma atroviride* β -galactosidase [1], [3]. The predicted proteins differed in size, sequence length, and isoelectric point. A conserved domain characteristic of the glycoside hydrolase family 35, which may be responsible for activity, was identified in all predicted proteins. Coding cDNA sequences were isolated and cloned into *Komagataella phaffii* expression vectors, and the recombinant enzymes were produced and purified via affinity chromatography. Purification yield was superior to those of most fungal β -galactosidase expressed in heterologous systems to date [6]. The purified β -galactosidase exhibited optimal activity around 60 °C and pH 5.8-7.0.

To our knowledge, this is the first heterologous production of a β -galactosidase from a zygomycetous fungus. The targeted expression system allowed the isolation of the enzyme with sufficient purity for detailed biochemical characterization. Future work will focus on optimizing the heterologous production for higher enzyme yield as well as further characterization of the biochemical properties of the purified enzyme. The *R. pusillus* β -galactosidase can be a promising and cost-effective catalyst for food industry applications, including lactose removal from dairy products and the synthesis of galacto-oligosaccharide (GOS) and lactulose-derived GOS (OsLu) prebiotic sugars.

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NOT FINAL

CARBON QUANTUM DOTS: GREEN MICROWAVE-ASSISTED SYNTHESIS, PROPERTIES AND APPLICATION IN ROSE BENGAL DYE REMOVAL

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Abstract

Carbon Quantum Dots (CQDs) are an emerging class of carbon nanomaterials that have attracted growing research attention due to their unique physicochemical properties, including tunable photoluminescence, high stability, water solubility, and biocompatibility. [1] There environmentally friendly and low-cost synthesis routes, such as microwave-assisted methods, make them attractive candidates for practical applications in catalysis, sensing, and wastewater treatment. [2, 3] Among common water pollutants, organic dyes such as Rose Bengal, Methylene Blue, and Rhodamine B are particularly problematic due to their high stability and toxicity. [4, 5] In the present work, pristine CQDs were synthesized by the microwave-assisted method, which represents a simple, rapid and green synthesis approach that has proven to be suitable for the preparation of CQDs. [6] The obtained nanoparticles demonstrated dual functionality in the removal of Rose Bengal dye: 28% removal by adsorption in the dark and an additional 29% degradation under UV irradiation, giving a total efficiency of 57%. These results confirm the synergistic effect of adsorption and photocatalysis, as well as the potential of pristine CQDs for wastewater treatment.

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UNVEILING HOUSEHOLD FOOD WASTE: SURVEY RESULTS FROM THE HOUSEHOLDS FROM VOJVODINA REGION, SERBIA

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Introduction

The prevention and proper management of household food waste is a collective challenge. Food waste is a multifaceted and complex problem that raises social and ethical concerns, but also deeply affects the environment. In this sense, addressing the problem is a priority that requires actions that target our entire food system. Around 88 million tonnes of food waste is generated in the EU every year and the associated costs are estimated at €143 billion. While an estimated 20% of all food produced is lost or wasted, 33 million people cannot afford to eat quality food every other day (according to Eurostat, 2018). FAO reported, that 1.3 billion food wastes are generated worldwide in a year.

Experimental

The purpose of this study was to examine the attitudes and behavior of families in Vojvodina region in Serbia regarding food waste and to estimate the monthly amount and economic value of discarded food waste in households, using a self-filling method. The questionnaire consisted of 19 questions, which were filled in by a total of 193 people.

Results and discussion

The average age of the applicants were between 18 and 40 years old. According to the results 80,9% of the respondents are concerned about food waste trying to avoid it if possible. 64,8% of respondents are from the countryside, and 35.6% of those are involved in composting. The weekly amount of food waste in households was reported between 250 g-1kg.

The research revealed that the young and the middle-aged are concerned about food waste and avoid possible waste wherever possible, which does not reflect composting habits. Limiting food loss and waste can therefore help both the fight against hunger and environmental problems such as climate change. In order to reduce these values, it is definitely necessary to do something - not only here but throughout the world. For example: they must reduce the amount of food waste generated during production and distribution, they must reduce the amount of household waste, they must encourage food donation, they must monitor and evaluate the implementation of EU measures to prevent food waste. Many people are aware of the harmful factors of the activity, yet it is believed that they do little to avoid it.

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INVESTIGATION OF POLYMER SPECTRA WITH NANO- AND FEMTOSECOND LASER INDUCED BREAKDOWN SPECTROSCOPY

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Plastic products are a very common occurrence nowadays. Unfortunately this also means that plastic waste is generated on a giant scale, polluting the environment with plastic debris of all shapes, sizes and compositions. The majority of these pollutant particles end up being degraded nano- and microparticles, causing considerable environmental and even health concerns. Because of these problems it is an important task to identify them, both for recycling and for research purposes. The usual tools of identifying polymers is IR, Raman and fluorescence spectroscopy. A new direction in this field could be the use of laser induced breakdown spectroscopy (LIBS), because it provides a fast method, that requires minimal sample preparation and is easy to automate¹.

LIBS is an atomic spectroscopic method, which is based on aiming a focused, high energy laser beam onto the surface of the sample to generate a microplasma. By using a high-resolution spectrometer to record the spectrum the composition of the sample can be determined. The duration of the laser pulse used to generate the plasma is generally in the nanosecond range, but systems with shorter, femtosecond pulse lengths are also available. The pulse length can have a major influence on the plasma generation dynamics, thus the characteristics of the spectrum². In case of traditional ns-LIBS the plasma is hotter and the spectral features are more intense, but the produced craters are larger, as well as the UV and heat damaged zone around them. fs-LIBS plasmas are smaller and cooler, less intense, but provide smaller and very well defined craters that allows for a great spatial resolution, which may facilitate the measurement of small particles, e.g.: micron-sized plastics. Because of the aforementioned differences in plasma dynamics and spectra, it is probable that in ns-LIBS the well documented lines and bands characteristic to certain polymer types change when fs-LIBS is performed, also depending on the ambient gas.

In this study we compared the capabilities of nano- and femtosecond LIBS for polymer microparticle discrimination using both argon and air as ambient atmosphere. The sorting of the polymer spectra was done with machine learning methods (mainly LDA, CT, RF). We also investigated the effect of spectral masking, normalisation and other data treatments on the performance of the sorting.

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SCREENING OF WHEAT CULTIVARS FOR TRAITS RELATED TO WATER USE EFFICIENCY

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Abstract

The variability of climate and extreme weather events are likely to have a more profound effect on plant production, especially in rain-fed crops, like wheat. Climate change poses a significant threat to Serbia's grain production, impacting soil fertility, crop yields, and the sustainability of agriculture as a whole. Extreme weather events, changing precipitation patterns, and rising temperatures all interfere with grain production, resulting in financial losses and threats to food security. Maize and wheat, the main grain crops in Serbia, are especially susceptible to drought, soil degradation, and water scarcity.

The grain production in Serbia is crucial for the economy. In the Vojvodina region, wheat was cultivated on 327,892 hectares in 2024, yielding an average of 5.9 tons per hectare. Across Serbia, wheat was grown on 549,032 hectares, with an average yield of 5.3 tons per hectare. Nevertheless, there was a 15.9% decrease in wheat production in 2024, primarily due to a reduction in the sowing area compared to 2023, underscoring the sensitivity of wheat grain yields to climate fluctuations. Wheat production encounters threats from autumn droughts and elevated spring temperatures. The degradation of soil and a decline in organic matter further compromise the soil's ability to facilitate sustainable grain farming. In view of these challenges, it is vital to implement immediate adaptation strategies. Additionally, climate change amplifies the risks associated with mycotoxin contamination, plant diseases, and the heightened use of pesticides.

At present, considerable efforts are being directed towards the utilization of advanced techniques and methodologies to anticipate future climate scenarios and assess their implications for crop growth and yield. In this regard, the collaborative research project between Serbia and Italy, PHENO-DROP, aims to establish a shared hexaploid wheat germplasm panel that includes both modern varieties and local landraces. This panel will be the foundation for implementing complementary high-throughput phenomics, with monitoring conducted at both the individual plant and plot levels, as well as advanced genomics to identify climate-resilient phenotypes and their genetic determinants.

To tackle the biological complexities associated with plant climate resilience, the underlying principle of Pheno-DROP is that a combination of beneficial plant traits could unify various strategies for plants to adapt to environmental variability, thus providing synergistic advantages, as suggested by crop simulation modeling. Additionally, to uncover the plant capabilities for effective climate resilience that result in high yield performance and stability, the focus is on traits related to the plant's ability to enhance its water use efficiency (WUE), which facilitates achieving "more crop per (water) drop." This task is challenging and depends on a variety of plant traits, such as root architecture, osmotic adjustment capacity, stomatal

density and regulation, and vegetation indices. Therefore, the first step involves characterizing existing bread wheat cultivars and landraces in terms of their drought tolerance.

Preliminary results were obtained regarding the concentration of photosynthetic pigments in the flag leaves and stomatal densities for 30 bread wheat cultivars from the collection of the Institute of Field and Vegetable Crops in Novi Sad. There are significant differences in the concentration of chlorophyll *a* in the flag leaf and in ratio of stomata number on the abaxial and adaxial side of leaf blades between cultivars.

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INVESTIGATION OF SOME PHYSICAL AND PHYSICOCHEMICAL CHARACTERISTICS OF CORNELIAN CHERRY (*CORNUS MAS* L.) GENOTYPES

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Abstract

Due to the increasingly extreme climatic conditions in Hungary, the significance of wild-growing fruit species is rising year by year, particularly those that meet both the qualitative and quantitative demands of the processing industry and consumer markets. Cornelian cherry (*Cornus mas* L.) is gaining prominence owing to its resilience against harsh environmental factors, its suitability for organic cultivation due to the absence of major pests and pathogens, its outstanding nutritional composition, and, notably, its inclusion as a subsidized fruit crop in Hungary's agricultural support system from 2024 onward.

The aim of this study is to conduct a comparative analysis of the fruit quality characteristics of three cultivated Cornelian cherry varieties ('Lutea', 'Kazanlak' and 'Jolico') and nine wild-growing genotypes from different growing sites, with particular emphasis on physical (size parameters, weight, stone-to-flesh ratio) and physicochemical (°Brix, titratable acidity) properties.

The fruit weight of wild genotypes ranged from 1.11 g to 2.05 g; stone weight from 0.17 g to 0.55 g; and flesh-to-stone ratio from 50.8% to 86.1%. In contrast, the cultivated varieties exhibited fruit weights between 2.12 g and 6.00 g; stone weights between 0.42 g and 0.92 g; and flesh-to-stone ratios ranging from 80.2% to 87.7%. The soluble solids content of the cultivated varieties ranged from 15.5% to 22.8%, while titratable acidity varied between 0.89% and 2.55%. Significant differences were observed among the cultivated varieties depending on the growing region and cultivation technology.

For the successful domestic cultivation of Cornelian cherry, further variety evaluation studies and breeding - selection - research tailored to changing climatic conditions are essential. The fruit of Cornelian cherry is not only a unique raw material that enriches the product assortment, but also offers a competitive alternative for the food industry and holds considerable potential for food innovation.

Introduction

In recent years, there has been a growing interest in wild fruit species from both producers and consumers. Cornelian cherry (*Cornus mas* L.) is naturally widespread across a broad geographic range, from Central Europe to the southeastern regions of the continent (Ercisli et al., 2011; Bijelic et al., 2011; Karadeniz et al., 2009). Wild Cornelian cherry has demonstrated a relatively high adaptability to adverse environmental conditions and exhibits strong resistance to diseases. It is valued for its unique nutritional profile and physiological benefits (Klimenko, 2004; Bijelic et al., 2011).

Extreme environmental conditions and the resulting yield losses are increasingly observed in major cultivated fruit crops. At the same time, the importance of functional foods continues to grow - a domain in which wild fruit species represent promising candidates.

In Hungary, a significant wave of orchard establishment began in the 2010s, typically based on 2–3 foreign cultivars available through domestic nurseries: 'Lutea', the Austrian 'Jolico', and

the Bulgarian ‘Kazanlak’. In the context of our study, these are referred to as first-generation orchards.

A favorable development occurred in 2024 with the inclusion of Cornelian cherry as a subsidized crop under Hungary’s orchard establishment support scheme. This underscores the importance of sustainable cultivation practices for Cornelian cherry, including the development of suitable cultivars, varietal assortments, orchard systems, and technological frameworks. Future plantings should be guided by the knowledge and experience already accumulated in this field.

Experimental

The study was conducted on the fruits of 12 Cornelian cherry (*Cornus mas* L.) genotypes collected during the 2024 ripening season, including nine wild-growing genotypes and three cultivated varieties (‘Lutea’, ‘Kazanlak’, and ‘Jolico’). Fruits from wild genotypes were gathered from natural habitats and in part from plantations located in Győr-Moson-Sopron, Somogy, and Veszprém counties, while the cultivated varieties originated from orchards in Fejér, Somogy, and Veszprém counties.

Wild genotypes were selected based on their fruit characteristics, whereas the cultivated varieties represented the core of Hungary’s so-called “first-generation” orchards established in the mid-2010s and bearing fruit for approximately 5–10 years by 2024.

Sampling was performed manually, collecting at least 50 fruits and/or 100 grams per genotype and variety from all four cardinal directions of each tree. Fruits were harvested at full ripeness, prior to natural drop, once they had reached the characteristic color of the respective variety.

We determined the physical and physicochemical parameters of the fruits, including weight (g), size dimensions (mm), refractive index (°Brix, soluble solids content [SSC]), and titratable acidity (TA, %). Fruit size was measured using a caliper with 0.05 mm sensitivity, and weight was recorded with a digital scale accurate to 0.001 g. The flesh ratio (%) was calculated based on the mass of the fruit and its stone.

Refractive index was measured in °Brix (g/100g) using a digital refractometer on homogenized, filtered juice, following Codex Alimentarius standard 3-1-558/93. Titratable acidity was determined according to the Hungarian standard MSZ EN 12147:1998, expressed as total acidity (m/m%) in malic acid equivalents. The sugar-to-acid ratio was calculated as the quotient of soluble solids content and titratable acidity.

Results and discussion

Significant differences were observed across all examined traits among Cornelian cherry genotypes and cultivars, as well as between growing sites and cultivation technologies. The physical parameters of the fruits from the studied varieties and genotypes are presented in Table 1. Previous studies have demonstrated that fruit weight and flesh-to-stone ratio are among the most variable traits in Cornelian cherry genotypes. In Serbia, fruit weight of genotypes ranges from 3.42 g to 8.00 g, with flesh-to-stone ratios between 79.32% and 88.55% (Bijelic et al., 2012; Ognjanov et al., 2009). In Slovakia, these values range from 0.5 g to 3.4 g (Brindza et al., 2009); in Poland, from 1.63 g to 2.21 g with flesh ratios between 84.68% and 89.87% (Szot et al., 2019); in Ukraine, from 4.5 g to 8.0 g and 89% to 92% (Moskalets et al., 2024; Klimentenko, 2004); and in Turkey, from 1.49 g to 9.11 g (Ercisli et al., 2011; Demir et al., 2003; Karadeniz, 2002; Karadeniz et al., 2009; Yilmaz et al., 2009), with flesh ratios between 79.08% and 89.99% (Ercisli et al., 2011; Karadeniz, 2019; Karadeniz et al., 2009; Yilmaz et al., 2009). In Iran, fruit weight has been reported between 1.23 g and 3.79 g (Moradi et al., 2019).

In our study, the fruit weight of the examined genotypes spanned a wide range from 1.11 g in the wild genotype ‘VAD-2’ to 6.00 g in the cultivated variety ‘Kazanlak’. The smallest stone

was recorded in 'VAD-6' at 0.172 g, while the largest was observed in 'Kazanlak' at 0.920 g. The percentage of fruit flesh relative to total fruit weight varied from 50.77% in the wild genotype 'VAD-3' to 87.68% in the 'Kazanlak' variety.

Table 1. Physical characteristics of the fruits of the examined Cornelian cherry genotypes

Genotypes	Location of cultivation / Habitat	Fruit weight (g)	Stone weight (g)	Flesh-to-stone ratio %
,Lutea'	Iszkaszentgyörgy	3,125	0,500	84,00%
,Lutea'	Kaposgyarmat	2,120	0,420	80,19%
,Kazanlak'	Iszkaszentgyörgy	3,373	0,600	82,21%
,Kazanlak'	Zselicszentpál	4,961	0,611	87,68%
,Kazanlak'	Kaposgyarmat	5,382	0,733	86,38%
,Kazanlak'	Bakonybél	6,000	0,920	84,67%
,Jolico'	Iszkaszentgyörgy	2,723	0,448	83,54%
,Jolico'	Zselicszentpál	2,966	0,533	82,02%
,VAD1'	Bakonybél	2,038	0,340	83,33%
,VAD2'	Bakonybél	1,112	0,198	82,23%
,VAD3'	Szentantalfa	1,122	0,553	50,77%
,VAD4'	Szentantalfa	1,258	0,270	78,57%
,VAD5'	Szentantalfa	1,238	0,320	74,14%
,VAD6'	Szentantalfa	1,116	0,172	84,55%
,VAD7'	Zselicszentpál	2,047	0,408	80,06%
,VAD8'	Pannonhalma	1,638	0,261	84,08%
,VAD9'	Pannonhalma	1,760	0,244	86,11%

The fruit weight of wild genotypes ranged from 1.11 g to 2.05 g; stone weight varied between 0.17 g and 0.55 g; and the flesh-to-stone ratio ranged from 50.8% to 86.1%. Among the cultivated varieties, 'Kazanlak' exhibited fruit weights between 3.37 g and 6.00 g, stone weights from 0.60 g to 0.92 g, and flesh-to-stone ratios between 82.2% and 87.7%. For 'Lutea', fruit weight ranged from 2.12 g to 3.13 g, stone weight from 0.42 g to 0.50 g, and flesh-to-stone ratio from 80.2% to 84.0%. In the case of 'Jolico', fruit weight ranged from 2.72 g to 2.97 g, stone weight from 0.45 g to 0.53 g, and flesh-to-stone ratio from 82.0% to 83.5%. Further investigations are required for the 'Jolico' cultivar, as drought conditions, water scarcity, and heat stress during the summer period inhibited fruit development and ripening.

Consistent with findings in the literature, our results confirm that measured fruit morphological traits are influenced by climatic conditions and cultivation technologies (Jaćimović et al., 2020). Under identical site conditions, the average fruit weight of wild Cornelian cherry genotypes cultivated with irrigation technology (2.038 g) was nearly twice that measured under non-irrigated conditions (1.112 g).

The soluble solids content (SSC) and titratable acidity (TA) values of the examined Cornelian cherry genotypes varied across a wide range, from 13.00% to 32.37% and from 0.89% to 3.15%, respectively. These extremes were observed primarily in wild genotypes and late-ripening cultivars (see Table 2). Among the cultivated varieties, 'Kazanlak' exhibited SSC values between 16.05% and 22.80%, and TA values ranging from 1.49% to 2.10%. For 'Lutea', SSC ranged from 16.20% to 20.10%, while TA values were between 1.55% and 2.55%. In the case of 'Jolico' SSC values ranged from 15.50% to 20.23%, and TA values from 0.89% to 1.54%. For 'Kazanlak', fruit samples collected from two different growing sites showed sugar-to-acid ratios between 9.71 and 10.89, indicating a more balanced flavor profile. In contrast, the 'Jolico' variety and wild-growing genotypes exhibited substantial variation in sugar-to-acid ratios, likely due to the previously mentioned drought conditions and heat stress, which adversely

affected fruit development and ripening. These findings highlight the need for further investigation.

Table 2. Physicochemical characteristics of the fruits of the examined Cornelian cherry genotypes, 2024

Genotypes	Production site	TA (%)		SSC (%)		Sugar-to-acid ratio
		$\bar{x}$	$\pm d$	$\bar{x}$	$\pm d$	
„Lutea“	Iszkaszentgyörgy	2,55	0,03	16,20	0,36	6,363
„Lutea“	Kaposgyarmat	1,55	0,02	20,10	0,10	12,944
„Kazanlak“	Iszkaszentgyörgy	2,10	0,03	22,80	0,18	10,875
„Kazanlak“	Zselicszentpál	1,56	0,01	17,00	0,12	10,893
„Kazanlak“	Kaposgyarmat	1,49	0,07	16,05	0,24	10,758
„Kazanlak“	Bakonybél	1,66	0,02	16,10	0,26	9,706
„Jolico“	Iszkaszentgyörgy	1,54	0,04	20,23	0,15	13,096
„Jolico“	Zselicszentpál	0,89	0,01	15,50	0,10	17,468
„VAD1“	Bakonybél	1,98	0,26	19,63	0,40	9,932
„VAD2“	Bakonybél	1,46	0,00	22,73	0,34	15,580
„VAD3“	Szentantalfa	1,31	0,04	32,37	0,35	24,719
„VAD4“	Szentantalfa	3,15	0,05	31,03	0,15	9,837
„VAD5“	Szentantalfa	1,29	0,02	31,93	0,40	24,835
„VAD6“	Szentantalfa	1,42	0,02	25,20	0,00	17,730
„VAD7“	Zselicszentpál	2,45	0,02	25,50	0,26	10,408
„VAD8“	Pannonhalma	2,56	0,04	13,00	0,40	5,071
„VAD9“	Pannonhalma	2,62	0,02	17,93	0,23	6,838

Previous studies have reported that SSC values of Cornelian cherry genotypes range between 14% and 28% (Kazimierski et al., 2019; Szot et al., 2019; Ercisli et al., 2006; Karadeniz et al., 2009; Ognjanov et al., 2009); titratable acidity (TA) values have been documented between 1.34% and 4.56% (Kazimierski et al., 2019; Szot et al., 2019; Karadeniz, 2002).

Conclusion

The physical and physicochemical parameters of Cornelian cherry cultivars and genotypes are significantly influenced by the production site and cultivation technology. It was established that, under identical ecological conditions, both irrigation practices (irrigated vs. non-irrigated) and differing production sites - when applying similar technological conditions - have a notable impact on fruit size and physicochemical characteristics.

There are promising wild genotypes with earlier ripening times (synchronous with ‘Kazanlak’) and shorter ripening periods, which may pose lower risk under prolonged or recurring extreme climatic conditions—such as high summer temperatures and mid-season drought—and thus represent valuable candidates for future breeding and selection programs.

This study also demonstrated that the fruit parameters of wild-growing genotypes can be significantly improved under cultivation.

For the successful domestic cultivation of Cornelian cherry, further variety evaluation and breeding–selection studies are essential, particularly those aligned with changing climatic conditions. The fruit of Cornelian cherry is not only a unique raw material that enriches product diversity, but also offers a competitive alternative for the food industry and holds considerable potential for innovation in food product development.

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NOT FINALIZED

CHARACTERISATION, COMPOSTING AND USE OF SPENT MUSHROOMS SUBSTRATE AS ORGANIC FERTILIZER

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Abstract

Spent mushroom substrate is byproduct of mostly champignon (*Agaricus bisporus*) and oysters (*Pleurotus ostreatus*) production. The substrate is used ones in the mushroom production due to deterioration of the properties and therefore, the increase of the production costs. Most of the spent substrate is disposed in landfills. Therefore, the aim of this study was to examine the composition of spent mushroom substrate from several producers in Vojvodina, Serbia, in order to assess their suitability and quality to be used as fertilizer. Also, the aim was to assess quality of the compost obtained from spent mushroom substrates by composting with different organic materials, as herb based activator (HA); tea compost (TC), and mixture of microorganisms (MM).

Collected samples of spent substrates have been analyzed on following parameters: pH value; electrical conductivity (EC); organic carbon content (C); total nitrogen (N); total P₂O₅ %; total K₂O %; mineral N; available P₂O₅, available K₂O, by standard methods, at the beginning and after 7, 14, 28, 56, 112, and 365 days of the composting. Whole proces was carried out without mixing or additional moistening.

The results show that all obtained composts of champignon can be used as NPK organic fertilizer of animal and plant origin, after 28 days of composting, according to Serbian regulation. The nitrification index (NI) showed that organic fertilizers are mature and stabilized, as NI values are below 0.5 (Meng et al., 2018). Other parameters as N, P, and K content and C/N ratio are suitable since the beginning of the experiment. On the other hand, the same applied technology for composting of the spent oysters substrate was not adequate (conditions and materials applied) and should be improved by better regulation of the C/N ration and moisture content.

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ENABLING THE REVERSE WATER GAS SHIFT REACTION AT HIGH PRESSURE AND LOW TEMPERATURE TOWARDS EFFICIENT CO₂ CONVERSION

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Abstract:

The reverse water gas shift (RWGS) reaction is a pivotal step for CO₂ valorization, yet it is often constrained by thermodynamic equilibrium and high energy demands. This study investigates a Process Intensification (PI) strategy by shifting the operational window to lower temperatures and elevated pressures using a conventional, commercially relevant catalyst: copper supported on γ -alumina (Cu/Al₂O₃) balls. We demonstrate that operating at high pressure significantly enhances the reaction rate and CO₂ conversion of the Cu/Al₂O₃ catalyst at temperatures below 400°C, a range where it traditionally exhibits low activity. The packed bed of catalyst balls, while simple, provides a robust system for evaluating this intensified process. The results indicate that high pressure compensates for the slower kinetics at low temperature, pushing the equilibrium and making the process more efficient. This approach demonstrates that significant process intensification for CO₂ conversion can be achieved not only with novel catalysts but also by strategically re-optimizing process parameters for existing, economically viable catalytic systems.

Introduction:

The conversion of CO₂ into carbon monoxide via the reverse water gas shift (RWGS) reaction ($\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{CO} + \text{H}_2\text{O}$, $\Delta H = +41.2 \text{ kJ/mol}$) is a fundamental route for producing syngas for fuel and chemical synthesis. Industrial application is currently limited by the need for high temperatures (>700°C) to achieve acceptable equilibrium conversion, leading to high energy costs and catalyst sintering. Copper-based catalysts are widely used in related reactions like methanol synthesis due to their cost-effectiveness and good activity, but they are typically considered less effective for low-temperature RWGS. This work challenges that notion by exploring a Process Intensification (PI) approach through parameter optimization. We hypothesize that operating a standard packed-bed reactor with a common Cu/Al₂O₃ catalyst at elevated pressures can dramatically improve its performance at lower temperatures. This strategy leverages Le Chatelier's principle, as the reaction proceeds without a change in the number of gas moles, making pressure a key yet underutilized variable for intensifying the RWGS process with standard catalyst materials.

Catalyst and High-Pressure, Low-Temperature Operation:

The focus of this work is on the operational intensification of a standard catalytic system, rather than the development of a new material. Catalyst System: The catalyst used was 10 wt% Cu supported on γ -Al₂O₃ balls (1-2 mm diameter), prepared by a standard incipient wetness impregnation method. This configuration represents a typical packed-bed reactor setup, chosen for its simplicity, low cost, and industrial relevance. Intensification Strategy: The key intensification strategy lies in operating this conventional system outside its typical window. High pressure has two major effects: Increased Reactant Concentration: The partial pressures of both CO₂ and H₂ are increased, leading to a higher frequency of reactant collisions with the

active Cu sites. This directly enhances the reaction rate, counteracting the slower kinetics inherent at lower temperatures.

Equilibrium Shift: Although the reaction volume change is zero, the presence of the water-gas shift equilibrium and the non-ideality of gases at higher pressures can influence the effective equilibrium constant, potentially favoring CO production under our specified conditions.

The combination of a robust Cu/Al₂O₃ catalyst in a simple packed bed with optimized high-pressure, low-temperature conditions represents a highly practical and easily scalable form of process intensification.

Future Outlook:

This finding opens a promising research direction for intensifying CO₂ conversion processes using cost-effective materials. Future work will focus on optimizing the Cu loading and particle size on the Al₂O₃ support specifically for this high-pressure, low-temperature regime. Furthermore, the integration of this intensified RWGS unit with a downstream pressurized process, such as methanol synthesis or Fischer-Tropsch, into a single, high-pressure operational train represents a logical and impactful next step for creating highly efficient and compact CO₂ conversion plants.

Conclusion:

This study successfully demonstrates that the reverse water gas shift reaction can be effectively intensified to operate efficiently at lower temperatures and higher pressures using a simple and economical Cu/Al₂O₃ ball catalyst in a packed bed. The improvement in CO₂ conversion and catalyst stability under these conditions challenges the conventional high-temperature paradigm for RWGS. It establishes that process intensification through strategic parameter optimization is a powerful and accessible tool, capable of unlocking new potential from existing catalytic systems. This approach significantly enhances the economic and practical feasibility of integrating the RWGS reaction into broader CO₂ utilization pathways, providing a viable step towards more sustainable chemical and fuel production.

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DEVELOPMENT AND EVALUATION OF PEAR JAM ENRICHED WITH POPPY SEEDS AS A FUNCTIONAL FOOD PRODUCT

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Abstract

This study aimed to develop an innovative functional food product — pear jam enriched with poppy seeds. Fruit jams are valuable sources of vitamins, minerals, simple sugars, soluble dietary fiber, phytonutrients, phytoestrogens, anti-inflammatory compounds, and antioxidants such as polyphenolic flavonoids, vitamin C, and anthocyanins. These bioactive compounds help neutralize free radicals, protecting the body against cancer, aging, and infections. Poppy seeds complement this profile, offering fats, proteins, manganese, calcium, linoleic acid, and vitamin E.

Two types of jams — plain pear jam and pear jam with poppy seeds — were evaluated through sensory and physicochemical analyses. Sensory results showed that the poppy seed variant excelled in taste, appearance, and consistency, receiving the highest possible score (5.0), while color and aroma scored 4.8 points. Physicochemical analysis assessed sugar content, vitamin C concentration, and refractive index. Pear jam with poppy seeds exhibited higher sugar content (61.2°Brix) and refractive index (1.4501) than plain pear jam. However, vitamin C levels were slightly higher in plain pear jam (64.2 mg/100 g) compared to the enriched version (58.7 mg/100 g).

Introduction

Functional foods – defined as products that provide health benefits beyond basic nutrition – have gained increasing attention in nutrition science due to their potential to prevent disease and promote well-being. These products often leverage naturally occurring bioactive compounds such as dietary fiber, polyphenols, vitamins, and unsaturated fatty acids to deliver added physiological value. Reviews highlight that dietary fiber and antioxidants are key targets in the development of functional formulations, since their synergistic presence can modulate oxidative stress, inflammation, and metabolic health [1,6]. Polyphenols, in particular, are plant secondary metabolites with antioxidant, anti-inflammatory, and anti-carcinogenic properties; their conjugation with dietary fiber further influences bioaccessibility and health impacts, making fruit-based matrices attractive delivery vehicles [3,5,7].

Fruit jams represent a promising carrier for such bioactive compounds, combining palatability, extended shelf life, and concentrated phytochemical content. Processing techniques and ingredient selection can markedly affect retention of phenolics, vitamin C, and overall antioxidant capacity, as shown in studies on polyphenol-enriched jams [2,11]. Moreover, the antioxidant profiles of diverse plant foods have been systematically catalogued, underscoring the value of selecting fruit sources with high intrinsic capacity to scavenge free radicals for functional formulations [4].

Pears are a rich source of polyphenolic compounds with emerging evidence of significant antioxidant, anti-inflammatory, and other bioactive effects; recent work has explored their polyphenol fraction and potential application in functional food development [12]. Their natural composition (providing soluble fiber, vitamin C, and phenolics) makes pear-based preserves a logical substrate for enhanced nutritional products. Complementing fruit-derived benefits, seed ingredients such as poppy seeds contribute additional functional attributes: they are dense in unsaturated fatty acids (notably linoleic acid), vitamin E, minerals (calcium and manganese), proteins, and other bioactive compounds, and have been recognized for their nutraceutical potential in food applications [8,9,10]. Their inclusion can increase lipid-soluble antioxidant capacity and supply essential fatty acids, while also influencing texture and sensory perception. Despite the individual recognition of pear-derived polyphenols and poppy seeds as health-promoting ingredients, their combined use in a single spreadable fruit product remains underexplored. Fruit jams enriched with complementary functional ingredients have previously shown that formulation changes can improve both nutritional profile and consumer acceptability, but the specific sensory and physicochemical trade-offs when incorporating poppy seeds into pear jam have not been systematically evaluated. This study therefore aimed to develop and characterize a novel functional product – pear jam enriched with poppy seeds – by assessing its sensory attributes alongside key physicochemical parameters (sugar content, refractive index, and vitamin C), thereby determining the extent to which poppy seed addition modifies both perceived quality and bioactive potential.

Experimental

2.1. Materials

Two types of jam were obtained – plain pear jam and pear jam with poppy seeds, following our original recipe. The raw and auxiliary materials needed in the production process were purchased from supermarkets or came from our own production.

The recipe for obtaining the 2 types of jam is presented below.

Raw / auxiliary materials	Plain pear jam	Pear jam with poppy seeds
Pear	500 g	500 g
Poppy seeds	-	15 g
Lemon juice	50 ml	50 ml
Sugar	150 g	150 g

2.2. Methods

The two types of jams were analyzed from a sensory and physicochemical point of view.

The sensory evaluation was carried out with the help of a number of 10 tasters, who filled in the sensory sheets following the organoleptic examination of the prepared products: pear jam with poppy seeds and plain pear jam. The tasters had to evaluate the following attributes of the jams: appearance, color, consistency, taste and smell.

The physicochemical analysis of the jams consisted of: determining the sugar content (using a DR201-95 digital refractometer), determining the vitamin C content (STAS 75588-87) and determining the refractive index (using an Abbe refractometer). The physicochemical analyses were done in triplicate.

Results and discussion

Following the results obtained on the basis of the questionnaires, for the assortment of pear jam with poppy seed, the most appreciated sensory characteristics were the appearance, consistency and taste, all these characteristics obtaining the maximum score of 5 points. Color and smell

achieved an average score of 4.8 points, with a small difference (0.2 points) compared to the other sensory characteristics.

For the plain pear jam assortment, the feature most appreciated by tasters was appearance, with an average score of 4.9 points. It was closely followed by consistency, smell (with an average score of 4.8 points) and color (4.7 points). The taste was the least appreciated, but nevertheless this feature also got a good average score of 4.6 points.

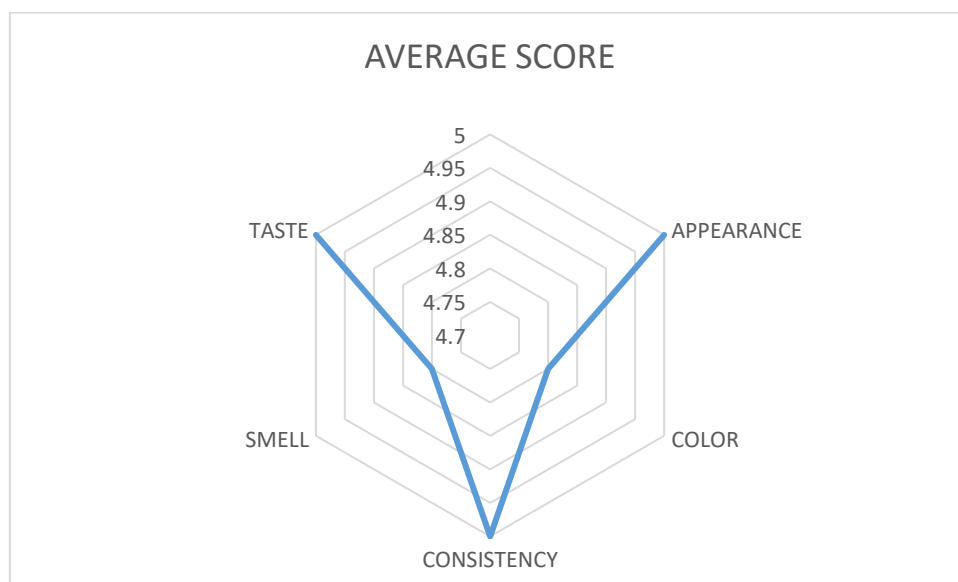


Figure 1. Sensory characterization of pear jam with poppy seeds

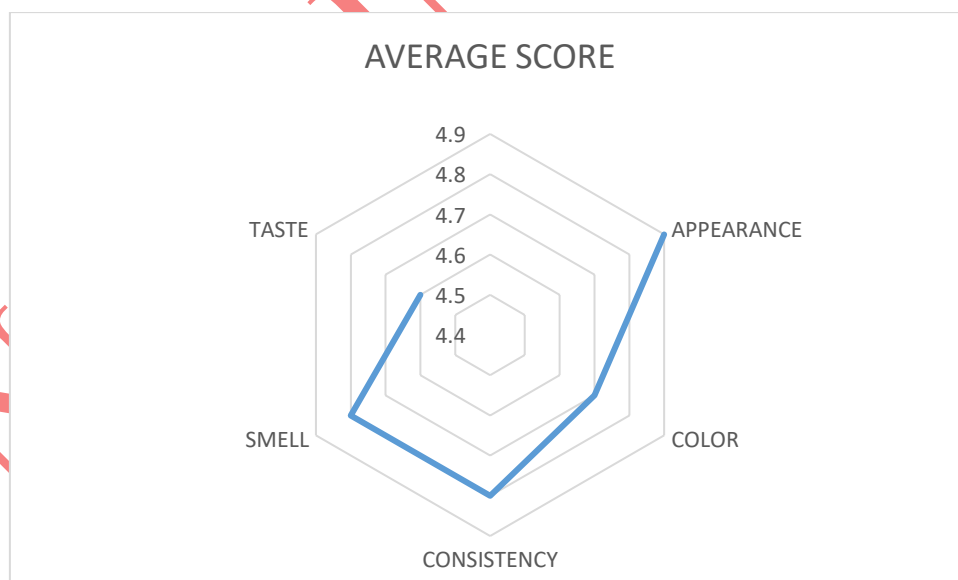


Figure 2. Sensory characterization of plain pear jam

The results of the physicochemical analysis for the 2 varieties of jam are presented in the table below.

Table 1. The results of the physicochemical analyzes for the 2 varieties of jam

Physicochemical analysis	Pear jam with poppy seeds	Plain pear jam
Sugar content (°Brix)	61.2	59.7
Vitamin C (mg / 100 g)	58.7	64.2
Refractive index	1.4501	1.4425

Conclusion

Following the sensory analysis of the studied products, the pear jam with poppy seeds was more appreciated by the tasters, obtaining a total average score of 4.92 points, while the pear jam obtained a total average score of 4.76 points.

The physicochemical analysis of the 2 varieties of jam showed a higher sugar content for the jam sample with poppy seeds (61.2°Brix), compared to 59.7°Brix for the sample without poppy seeds. The difference between the two jam samples is not very large, but can be felt in the taste and consistency. Also, the higher content of soluble solids (sugar + other dissolved substances) can make the product slightly sweeter and with a denser texture and can contribute to a longer shelf life by reducing water activity.

The refractive index increases with the soluble solids content, and the values confirm the difference observed in °Brix. Thus, poppy seed jam, having more dissolved solids, has a higher refractive index, which correlates with a denser texture and possibly a more pronounced gloss. The vitamin C content is slightly lower in the poppy seed version. Vitamin C is known to be sensitive to heat, oxygen, and processing. Thus, the decrease may be related to additional cooking time or exposure to higher temperatures. The difference between the two types of jam analyzed is modest, so the nutritional impact is not very high. Both variants remain moderate sources of vitamin C.

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**IN SILICO EVALUATION OF THE ECOTOXICOLOGICAL POTENTIAL
AGAINST *DAPHNIA MAGNA* OF SUCCINIMIDE DERIVATIVES FROM FOUR
HOMOLOGOUS SERIES**

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Abstract

Ecological monitoring analysis confirm that organisms in the environment are chronically exposed to complex multi-component pharmaceutical mixtures. Thus, the ecotoxicological evaluation of new pharmaceuticals and their negatively impact on ecosystems and aquatic life become integral step in the process of drug design and development. One of the most common model organisms for evaluation of freshwater toxicity of chemicals is *Daphnia magna*. Both experimental and computational methods are being developed for prediction of the ecotoxicological potential of new structures. In this paper ADMETlab 3.0 online program was employed for evaluating the concentration that kills 50% of *Daphnia magna* after 48h (LC₅₀DM) for 45 succinimide derivatives. The obtained results indicated that the observed compounds have less toxic effect in comparison to registered ethosuximide and similar toxic effect as phensuximide. The highest LC₅₀DM or the least toxic effect was recorded for most lipophilic compounds of the series F with statistically significant higher LC₅₀DM in comparison to series C, D and E respectively. In addition their toxic effect was positively associated with their polarity (TPSA, $p=0.001$), aquatic solubility (logS, $p<0.001$) and flexibility (Fsp3, $p<0.001$), respectively and negative associated with the Van der Waals volume (V, $p<0.001$) and lipophilicity (both logP and logD, $p<0.001$ for both), respectively.

Introduction

Ecotoxicological assessment has a crucial role in evaluating the environmental risks of pharmaceutical substances. Regulatory agencies worldwide require ecotoxicity testing as an integral component of the environmental risk assessment process, emphasizing proactive strategies to mitigate the impact of pharmaceutical contaminants. Green ecotoxicology introduces sustainable methodologies to evaluate the effects of compounds on ecosystems, reducing environmental harm while providing accurate information on chemical ecological hazards. This approach integrates advanced predictive tools and environmentally friendly techniques to facilitate the development of safer substances with minimized ecological effects [1]. *Daphnia magna* (water flea) is one of the most commonly used model organisms to assess freshwater toxicity of wide range of pharmaceuticals. The flexibility of *Daphnia magna* to cope with environmental stressors, its sensitive behavioural and physiological responses serve as reliable biomarkers for assessing the effects of diverse chemicals. Additionally, the use of *Daphnia* in toxicity testing aligns with the principles of the 3Rs (Replacement, Reduction, and Refinement) in animal research, making them an ideal model organism for developing and evaluating methods to assess emerging contaminants and environmental concerns [2, 3]. In

parallel with traditional ecotoxicity assessments, there is a growing shift toward the integration of *in vitro* testing and computational modelling approaches, reflecting a broader trend toward alternative, non-animal methods in environmental risk assessment.

Succinimide moiety has been recognized for various pharmacological effects [4, 5]. The design of new structures and development of potential pharmaceuticals with succinimide core undergo the testing for its ecotoxicological risk. The aim of this research was to assess *in silico* the toxicological effects of 45 compounds (Table 1) from four series (C, D, E and F) on *Daphnia magna* and to evaluate the influence of their physico-chemical features on these values.

Experimental

In this paper in ADMETlab 3.0 online program (<https://admetlab3.scbdd.com/>) was used for evaluating the ecotoxicological potential of 45 succinimide derivatives (Table 1). For each compound their two-dimensional structures were obtained by the ChemDraw Professional as Simplifies Molecular-Input Line-Entry System, SMILES. This form was used for evaluation of their properties. Various features of the analysed compounds were evaluated including the polarity expressed as total polar surface area (TPSA), solubility given as logS, lipophilicity calculated as partition coefficients (logP and logD), their size measured as volume (V) and their flexibility expressed as Fsp3 were determined. The ecotoxicological potential of each compound was evaluated as the concentration that kills 50% of *Daphnia magna* after 48h and presented as LC₅₀DM. The values were given in $-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$. All statistical analysis were conducted using OriginPro 8 and $p < 0.01$ was considered as statistically significant.

Results and discussion

The 48h-LC₅₀ for *Daphnia magna* based on the ADMETlab 3.0 online program were determined for all the observed compounds and are presented in Figure 1. Both series C and series D had statistically significant lower LC₅₀DM in comparison to series E and F respectively ($p < 0.01$), while series E also had statistically significant lower LC₅₀DM when compared to series F ($p < 0.01$). There were no statistically significant differences in the values of LC₅₀DM between series C and D. As model compounds phensuximide and ethosuximide, registered antiepileptic drugs were also tested. LC₅₀DM for phensuximide was 4.231 while for ethosuximide was 2.551. Based on the predicted values, all of the compounds analysed had higher LC₅₀DM (3.470-6.038) in comparison to ethosuximide, which means they have lower ecotoxicological potential in freshwater when compared to this medicine. All compounds of series F (LC₅₀DM interval 5.181-6.038) as well as some compounds of series C, D and E had also higher LC₅₀DM when compared to phensuximide as well. The lethal potential of the analysed compounds towards *Daphnia magna* according to the *in silico* screening results makes them less or equally hazardous in freshwater as medicines with succinimide moiety already present on the market.

The increment of LC₅₀DM was positively associated with the size of the analysed molecules calculated as Van der Waals volume (V) in statistically significant manner ($r^2 = 0.551$, $p = 3.193 \times 10^{-9}$). These results are in accordance with literature data about the influence of the size on the toxicological effects of the molecules, classifying small molecules as more hazardous [6]. In addition, the higher the lipophilicity (logP and logD, respectively) of the analysed compounds was, the higher were LC₅₀DM values. Namely, a statistically significant relationship was obtained between logP and LC₅₀DM ($r^2 = 0.857$, $p = 9.451 \times 10^{-12}$, Figure 2a) and logD and LC₅₀DM ($r^2 = 0.870$, $p = 8.913 \times 10^{-12}$), respectively for all 45 succinimides investigated in this study. It is generally accepted that the higher lipophilicity is associated to enhanced permeability and higher toxicity of the molecules [7]. However, experimental data often

contradict these claims. Our data are in concordance with the findings of Tafreshi et al. as more targeted alpha-particle therapy with higher lipophilicity exhibited less toxic effect in animal models [8].

Table 1. Structures of the compounds analysed

Series C			Series E		
Compound	-R ₁	-R ₂	Compound	-R ₁	-R ₂
C1	-H	-H	E1	-COOH	-H
C2	-CH ₃	-H	E2	-Cl	-H
C3	-OCH ₃	-H	E3	-Cl	-H
C4	-OH	-H	E4	-H	-Br
C5	-COOH	-H	E5	-H	-Cl
C6	-H	-COCH ₃	E6	-CH ₃	-H
C7	-COCH ₃	-H	E7	-OH	-H
C8	-NO ₂	-H	E8	-H	-H
C9	-Cl	-H	E9	-OCH ₃	-H
C10	-Br	-H	E10	-F	-H
C11	-I	-H	E11	-CN	-H
C12	-H	-Cl			
C13	-H	-Br			
Series D			Series F		
Compound	-R ₁	-R ₂	Compound	-R ₁	-R ₂
D1	-H	-H	F1	-CH ₃	-H
D2	-OH	-H	F2	-OCH ₃	-H
D3	-OCH ₃	-H	F3	-H	-H
D4	-COOH	-H	F4	-NO ₂	-H
D5	-CN	-H	F5	-F	-H
D6	-CH ₃	-H	F6	-Cl	-H
D7	-NO ₂	-H	F7	-Br	-H
D8	-Cl	-H	F8	-H	-Cl
D9	-Br	-H	F9	-H	-Br
D10	-H	-Cl	F10	-H	-I
D11	-H	-Br			

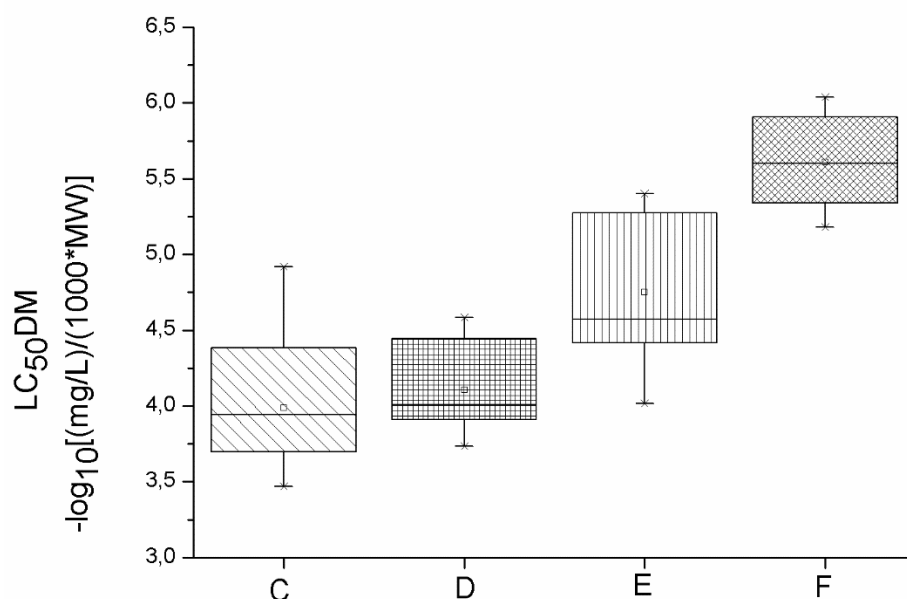


Figure 1. 48h-LC₅₀DM values of the analysed series of succinimide derivatives

The reduced toxicological potential of the more lipophilic compounds may be attributed to their restricted solubility, as higher lipophilicity is followed by poor aqueous solubility [9]. Accordingly, there was negative association between the solubility displayed as logS and the LC₅₀DM of the observed succinimides ($r^2=0.884$, $p=3.481 \times 10^{-12}$, Figure 2b). Moreover, the negative association was established between Fsp3 which presented the ratio of the number of sp³ hybridized carbons and the total carbon count and LC₅₀DM ($r^2=0.418$ $p=9.657 \times 10^{-7}$). This inverse relation between Fsp3 and LC₅₀DM which follows the negative association between logS and LC₅₀DM is expected as Fsp3 correlates with the aqueous solubility of the molecules.

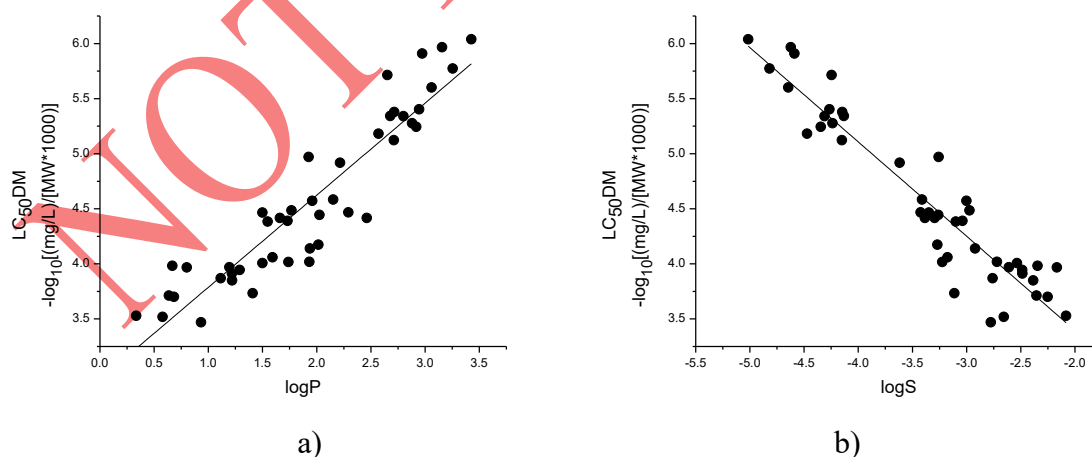


Figure 2. Statistically significant association of LC₅₀DM with a) logP and b) logS, respectively for the observed succinimide derivatives

Finally, the polarity (TPSA) was also negatively associated with the LC₅₀DM ($r^2=0.210$, $p=0.001$). Our results are supported by the previous finding that indicate that more polar

compounds exhibit higher toxicity especially in specific environmental samples such as freshwater [10].

Conclusion

Ecotoxicological assessment of newly synthesized compounds which are drug candidates becomes mandatory step in the drug development process. Forty-five succinimide derivatives based on the *in silico* evaluation had lower or similar toxicity potential against *Daphnia magna* in comparison to the drugs with succinimide core registered on the market. The most lipophilic structures of the series F had the least pronounced toxic potential in comparison to the compounds of the series C, D and E. The toxic potential towards *Daphnia magna* according to the *in silico* evaluation for the observed compounds is governed by their polarity, solubility and flexibility in a positive manner. On contrary, the Van der Waals volume and the lipophilicity of the compounds seem to decrease the toxic potential towards *Daphnia magna*.

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ECOTOXICITY OF DIHYDROPYRIDINES, CALCIUM CHANNELS BLOCKERS: *IN SILICO* SURVEY

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Abstract

There is growing evidence that the presence of pharmaceuticals in the environment results in exposure of biota, posing a potential threat to ecosystem health. Assessing the bioaccumulation of active pharmaceutical ingredients is critical, as it provides insight into the extent to which emerging contaminants may persist and concentrate within organisms. In this study, the ecotoxicological endpoints of selected twenty dihydropyridines were determined using the online ADMETlab 3.0 online programme. In addition, their polarity, solubility, and lipophilicity were determined based on their structure, followed by examination of the possible association of their physico-chemical properties and ecotoxicological endpoints. The obtained results suggested that their bioaccumulation factor is strongly positively associated with the lipophilicity of the observed dihydropyridines and negatively with their solubility and polarity, respectively. Moreover, the 48h 50% inhibition growth concentration of *Tetrahymena pyriformis*, the 48h-LC₅₀ of *Daphnia magna* and 96h-LC₅₀ of Fathead minnow for the analysed compounds were governed positively by the lipophilicity and negatively by their aquatic solubility, respectively, whilst the influence of the polarity of the molecules was not statistically significant. Further studies require experimental confirmation of the ecotoxicological potential of dihydropyridines as one of the most prescribed pharmaceuticals in the treatment of cardiovascular diseases.

Introduction

Most of pharmaceuticals excreted in urine are not effectively removed by wastewater treatment plants and consequently enter aquatic environments. Several active pharmaceutical ingredients (APIs) have been shown to exert toxic effects on aquatic organisms. The continuous prescription of APIs for various chronic disease contribute to the constant release of active pharmaceutical ingredients into waterways through wastewater treatment plants effluent. This sustained discharge raises serious environmental concerns, as APIs have been linked to a wide range of harmful impacts on both aquatic flora and fauna [1]. Thus, there is an urgent need for robust environmental risk assessment (ERA) of APIs. This has prompted the development of new approach methodologies (NAMs), which aim to generate hazard and risk information without the use of animals, in line with ethical frameworks of animal protection. Among these NAMs, computational or *in silico* methods, especially quantitative structure–activity relationship (QSAR) models, have become crucial, as they can predict toxicity across untested chemical-species combinations [2]. A QSAR model seeks to quantify how variations in chemical structure influence a molecule's biological activity or physico-chemical properties. These models are highly versatile, and can be applied to a broad spectrum of endpoints including pharmacological effects, toxicological outcomes, biokinetic behaviours, and physical or chemical characteristics. Finally, QSARs support chemical safety assessment by predicting

toxicity and biokinetics for both human health and environmental safety, enabling individual compound risk assessment and thus potentially reducing reliance on animal experiments [3]. Dihydropyridines as type of calcium channel blockers (CCBs) are among the most often prescribed drugs for the treatment of hypertension [4]. CCBs inhibit the influx of calcium by binding to L-type, long-acting voltage-gated calcium channels found in the heart, vascular smooth muscle, and pancreas. Dihydropyridines have minimal direct impact on the myocardium and act mainly as peripheral vasodilators at therapeutic doses. This makes them effective in treating conditions like hypertension, vasospasm following intracranial haemorrhage, and migraines [5], but also attributes to their harmful influence on various species in the environment. In this paper, the ecotoxicological potential of twenty dihydropyridines (Figure 1) has been examined *in silico*, with evaluation of the change in their physico-chemical properties on the obtained ecotoxicological endpoints.

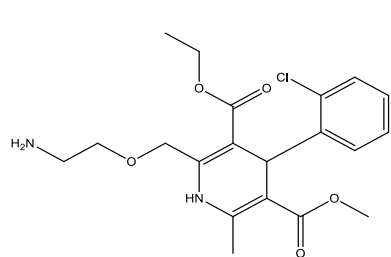
Experimental

In this paper in ADMETlab 3.0 online program (<https://admetlab3.scbdd.com/>) was used for evaluating the ecotoxicological potential of 20 dihydropyridines (Figure 1). Two-dimensional structures of the examined compounds were obtained by ChemDraw Professional as Simplified Molecular-Input Line-Entry System, SMILES and used for predicting their properties. Their polarity expressed as total polar surface area (TPSA), solubility given as logS as well as lipophilicity obtained in form of partition coefficients logP and logD were determined. The ecotoxicological potential of each compound was evaluated as bioconcentration factors (BCF), IGC₅₀, LC₅₀FM and LC₅₀DM, respectively. For all above predictors the unit is negative value of $\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$. BCF are used for considering secondary poisoning potential and assessing risks to human health via the food chain. IGC₅₀ presents the 50% inhibition growth concentration after 48h of *Tetrahymena pyriformis*. The concentration that kills 50% of Fathead minnow after 96h is given as LC₅₀FM, while the concentration that kills 50% of *Daphnia magna* after 48h is presented as LC₅₀DM.

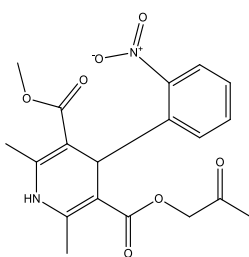
Results and discussion

Bioaccumulation serves as a key parameter in environmental risk assessment, particularly for evaluating long-term ecological impacts. This focus is essential not only for understanding population-level effects but also for assessing risks to individual organisms across trophic levels [6]. The BCF for the compounds analysed varied between 0.763 and 2.134 with mean value of 1.426 ± 0.299 (Figure 2). Although, there are no data for BCF among humans, there is a list of BCF values expressed in wet weight or dry weight bases in L/kg for different aquatic species. The variation of bioaccumulation for different pharmaceuticals suggested BCF values such as 3981 L/kg in fish for cefotaxime, 49,000 L/kg for ibuprofen in trout, with up to 209,500 fluoxetine in shrimps [7].

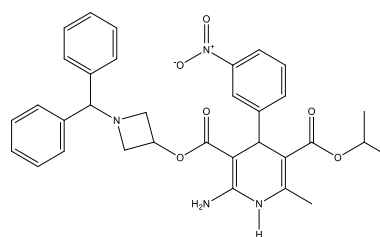
Tetrahymena pyriformis a protozoan model organism used for environmental toxicology analyses. *Daphnia magna* (DM), a small freshwater crustacean and *Pimephales promelas* (fathead minnows, FM), a small fish model, are routinely used for regulatory programs aimed at assessing potential risks of chemicals including pharmaceuticals. The 48h 50% inhibition growth concentration of *Tetrahymena pyriformis*, IGC₅₀ was in the interval of 3.571 and 4.714, while LC₅₀DM varied between 4.315 and 5.863 for the analysed dihydropyridines (Figure 2). The experimental data for verapamil, a non-dihydropyridines, calcium channel blocker indicated that 48h-LC₅₀ was 7.04 mg/L [8]. Finally, the LC₅₀FM levels for the selected dihydropyridines were between 4.896 and 6.332 (mean value of 5.673 ± 0.423 , Figure 2). Experimental data for verapamil suggested that although FM survival was not impacted by verapamil exposure, the growth was significantly decreased at 600 µg/L [9].



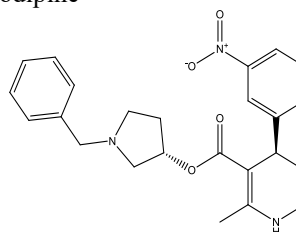
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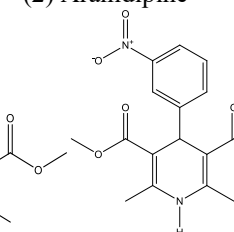
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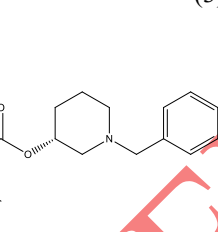
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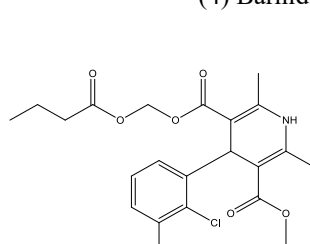
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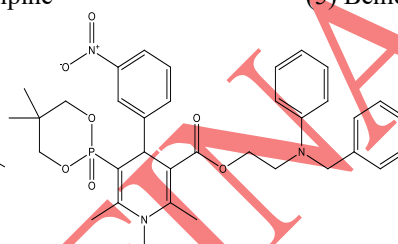
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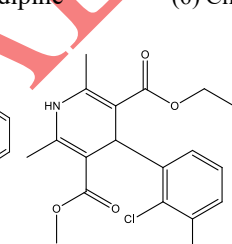
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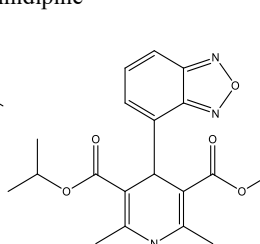
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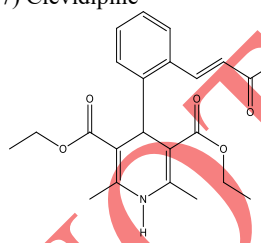
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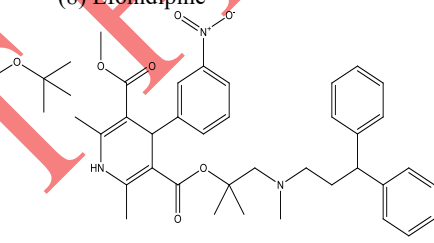
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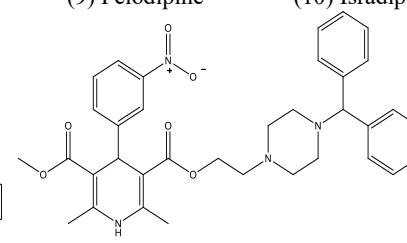
(10) Isradipine



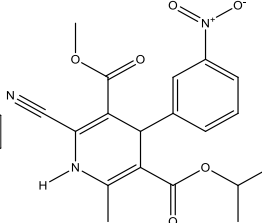
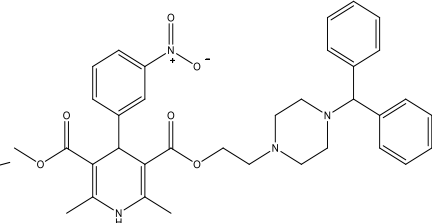
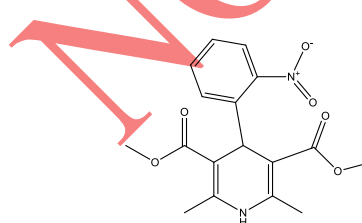
(11) Lacidipine



(12) Lercanidipine



(13) Manidipine



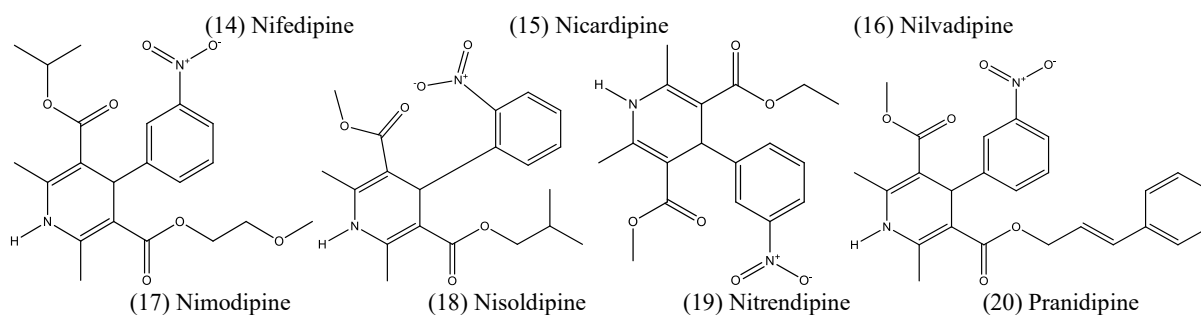
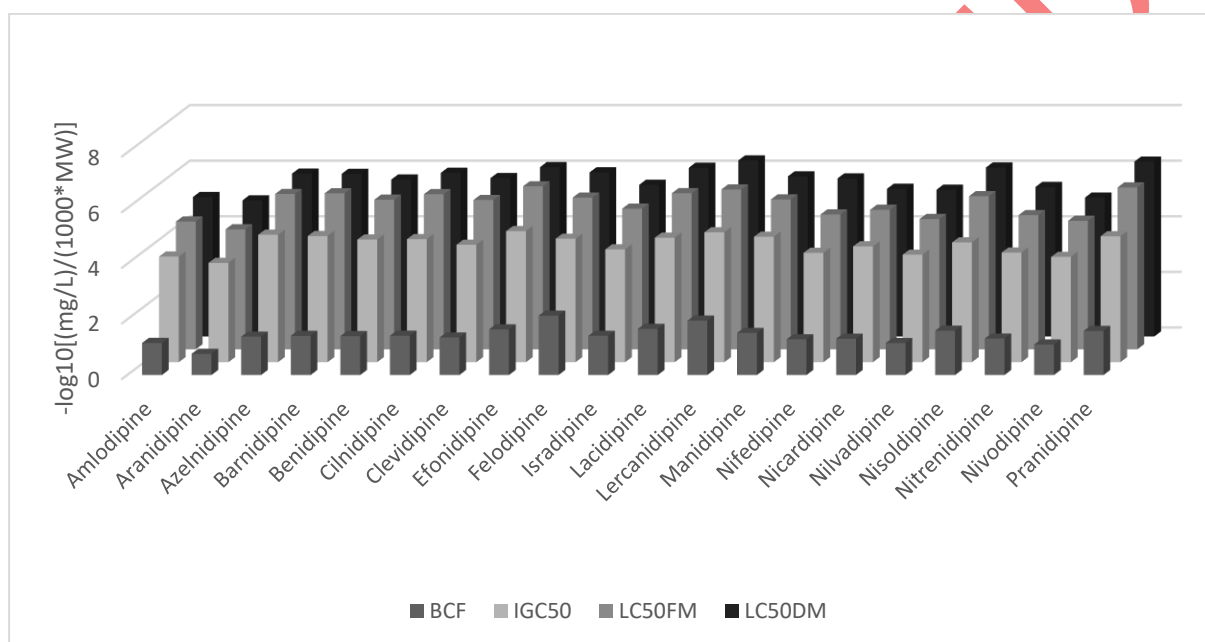
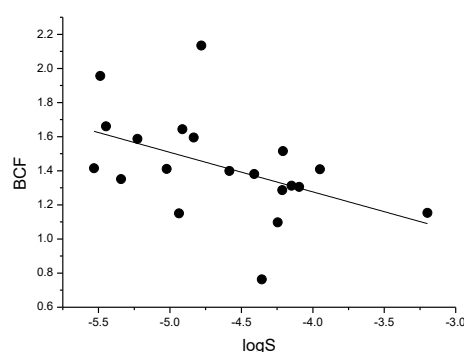
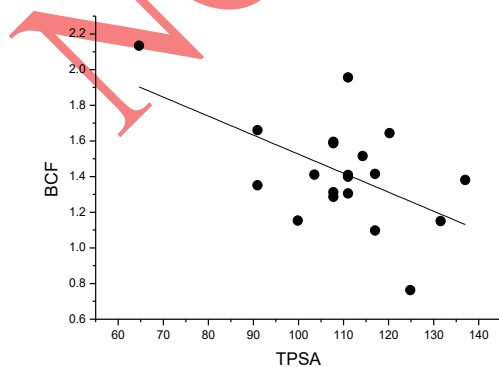


Figure 1. Structures of the analysed dihydropyridines

Figure 2. *In silico* evaluated ecotoxicological endpoints for the selected dihydropyridines

The BCF values seem to be governed negatively by the polarity, TPSA ($r^2=0.268$, $p=0.011$, Figure 3a), and the solubility, $\log S$ ($r^2=0.182$, $p=0.034$, Figure 3b), respectively. The association of BCF with lipophilicity of the compounds ($r^2=0.494$, $p=3.30 \times 10^{-4}$ with $\log P$, $r^2=0.472$, $p=4.95 \times 10^{-4}$, with $\log D$) was directly proportional (Figures 3c-d).



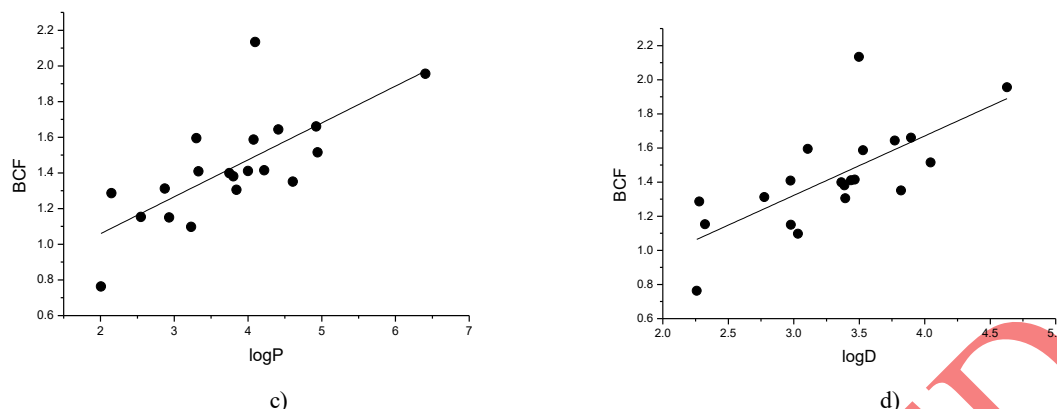


Figure 3. The association of BCF with a) TPSA, b) logS, c) logP and d) logD of the analysed dihydropyridines

The IGC_{50} , LC_{50FM} and LC_{50DM} were associated only with solubility and lipophilicity of the analysed compounds, while the influence of the polarity on these values was not statistically significant. Namely, IGC_{50} was negatively correlated with solubility, $\log S$ ($r^2=0.163$, $p=0.044$) and positive with lipophilicity ($r^2=0.562$, $p=8.484 \times 10^{-5}$ with $\log P$; $r^2=0.580$, $p=5.782 \times 10^{-5}$ with $\log D$, respectively). Solubility, $\log S$ was inversely associated with both LC_{50FM} and LC_{50DM} ($r^2=0.275$, $p=0.010$, $r^2=0.349$, $p=0.004$), respectively. The positive proportionality between LC_{50FM} and $\log P$ ($r^2=0.519$, $p=2.054 \times 10^{-4}$) and $\log D$ ($r^2=0.535$, $p=1.483 \times 10^{-4}$), respectively as well as LC_{50DM} positive relationship with $\log P$ ($r^2=0.437$, $p=9.075 \times 10^{-4}$) and $\log D$ ($r^2=0.435$, $p=9.48 \times 10^{-4}$), respectively was in accordance with the literature data. Namely, lipophilicity was recognized as a suitable predictor of bioconcentration of various pharmaceuticals in fish [10]. However, other studies indicated lack of association between lipophilicity of pharmaceuticals, within a specific category or across all classes, and their acute toxicity to individual species or groups of organisms. Despite these findings, the best relation between measured and estimated lipophilicity of pharmaceuticals and acute toxicity was reported towards *Daphnia magna* [11]. The inverse influence of solubility on the toxic potential of the observed molecules on contrary to their solubility is in line with the negative connection between a molecule's aquatic solubility and lipophilicity: higher lipophilicity generally indicates lower aquatic solubility, and vice versa [12].

Conclusion

The ecotoxicological endpoints can be determined *in silico* due to advanced new methodology techniques that apply machine learning. Lipophilicity is the crucial factor that governed the ecotoxicological endpoints of twenty selected dihydropyridines, while the aquatic solubility and polarity have exerted less emphasized influence. There is rapid concern regarding the influence of pharmaceuticals including dihydropyridines on aquatic environment.

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NOT FINALIZED

A NEW Zn(II) COMPOUND WITH A MACROCYCLIC LIGAND *tpmc*. SYNTHESIS AND CHARACTERIZATION

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Abstract

Zinc is an important transition metal in the biological intracellular environment of living organisms which plays critical roles in important physiological process [1]. Zinc complexes have kindled interest, as they are less toxic than complexes of non-essential metals and have been used as drugs for the treatment of Alzheimer's disease, showing bactericidal, antimicrobial and cytotoxic activity [2]. Zinc complexes can adopt diverse geometries with different ligands and coordination numbers. This paper reports the synthesis and characterization of new complex Zn(II) with N,N',N'',N'''-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane (*tpmc*).

The new complex was prepared in mixture acetonitrile/water in reaction $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ and *tpmc* (mole ratio 2:1) with reflux and stirring for 2 h in a water bath (80 °C). Obtained complex is stable on the air

The complex was characterized by elemental analysis (C, H, N), FTIR spectroscopy, and molar conductivity determination. The analytical data show the formation of binuclear $[\text{Zn}_2(\text{OH})\text{tpmc}](\text{ClO}_4)_3 \cdot 3\text{H}_2\text{O}$ complex. The elemental analyses data correspond well to the proposed formula. The molar conductance measurements of the complex in acetonitrile correspond to 1:3 electrolyte [3].

FTIR spectrum of the complex is very much consistent with the proposed formula and with data obtained by other methods.

Comparing the FTIR spectrum of the new complex with the spectra of related *tpmc* hydroxo complexes and different central ions, it was concluded that the macrocyclic ligand is coordinated to metal ions through eight N atoms. Also, based on the comparison, it was concluded that OH^- connects two Zn(II) forming a bridge between them [4].

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SECOND-LIFE ASSESSMENT OF AUTOMOTIVE BATTERIES AT THE UNIVERSITY OF SZEGED

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Abstract

The growing number of electric vehicles has led to an increasing amount of end-of-life batteries that no longer satisfy user requirements, while efficient recycling practices are still in their early development stages. At the University of Szeged, we established a standardized analytical protocol based on the UL 1974 framework, enabling objective evaluation of various large-capacity battery types. In addition, we built the necessary laboratory infrastructure to safely disassemble cells and conduct post-mortem analyses. To date, more than ten batteries have been systematically tested using the developed methodology, and several dozen cells have been dismantled and examined in detail. This approach not only provides a reliable pathway for assessing second-life potential but also lays the foundation for future recycling strategies.

Introduction

The management of used lithium-ion batteries poses significant environmental and industrial challenges. Although some cells remain partially functional, their performance no longer meets the required characteristic and safety requirements for transportation. Nevertheless, their secondary use potential and the recovery of valuable raw materials are highly relevant. Based on international standards (e.g., ANSI/CAN/UL 1974), we set out to develop a laboratory-feasible, standardized protocol for the systematic characterization of second-life batteries.

Experimental

The following procedures were applied:

- physical inspection,
- insulation resistance
- open-circuit voltage measurements,
- charge–discharge cycling,
- state-of-health (SOH) estimation,
- self-discharge tests and internal resistance determination,
- micro CT-scan
- disassembly of the bad cells,
- postmortem analysis of the cell materials.

Before disassembly, the cells were first examined using micro-CT imaging to identify apparent structural issues. Following this non-destructive screening, defective cells, primarily LiFePO₄ cathode-based, were dismantled under safe conditions, either in a glovebox or under a fume hood with humidity monitoring. The cell casing was opened by scoring and cutting, followed by electrolyte removal through puncturing and draining. After unrolling the jelly roll,

electrodes and separators were inspected for typical failures such as separator perforation, black spots, discontinuities, and graphite detachment from the copper foil.

Results and discussion

We successfully developed and applied a systematic battery analysis method at the university. Open-circuit voltage and insulation values were adequate in several cells, while others fell below acceptable limits. Charge–discharge tests revealed stable performance within the operational voltage range in many analyzed cells, without significant temperature rise. Autolab measurements indicated SOH values of ~98% for new cells, and as low as 60% for used ones. Degraded cells exhibited a threefold increase in internal resistance and self-discharge rates of ~0.5–0.7% per month.

Prior to disassembly, micro-CT imaging was carried out to identify hidden structural anomalies. This technique revealed, in one case, the presence of iron filings inside a cell, likely introduced during the manufacturing process. Subsequent post-mortem analysis of faulty cells confirmed typical structural damages, including separator punctures, ceramic coating detachment, and graphite loss. These combined results demonstrate the complementary value of non-destructive imaging and destructive inspection in identifying both operational degradation and assembly-related defects.

Conclusion

The proposed methodology allows for an objective assessment of used battery cells and facilitates the distinction between units suitable for reuse and those requiring disposal and recycling. Our results may support the standardization of battery recycling processes in Hungary and provide a foundation for future second-life applications.

Acknowledgements

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EFFECT OF UNMALTED TRITICALE AND MASHING REGIME ON WORT AMINO ACID PROFILES

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Abstract

Nitrogen compounds, which play a key role in determining the quality and stability of the final product, are considered highly important in brewing technology. Representing 3–5% of the total wort extract, these compounds include amino acids, peptides, proteins, nucleic acids, and their degradation products. The complex profile of nitrogen compounds in beer is influenced by multiple factors, with the malting process being the most critical. Additionally, the choice of cereal variety and growing conditions also affect their composition. The quantity of nitrogen compounds and the availability of oxygen are key factors for yeast growth and development. However, yeast does not assimilate all nitrogen present; it primarily utilizes ammonium ions and free amino nitrogen, comprising amino acids and smaller peptides. Amino acids are essential for barley malting, wort production, and fermentation, as they influence the activity of cereal proteolytic enzymes during malting, support yeast metabolism during fermentation, and contribute to the final sensory profile of beer. Malt contains 19 of the 20 essential amino acids, and yeast assimilates them in a specific sequence throughout fermentation. Based on their assimilation patterns, amino acids are categorized into four groups—A, B, C, and D—ranging from those most readily assimilated to those assimilated most slowly.

The effects of mashing with unmalted triticale variety 'Odisej' at proportions of 10%, 30%, and 50% of the grist were examined, with the addition of 5 µL of the commercial enzyme Shearzyme® 500L, which was used to reduce the viscosity characteristic of triticale worts, with analysis of the amino acid profile of the resulting worts. Two mashing regimes were applied: a standard congress mash and a modified mash with temperature rests designed to enhance enzymatic activity and compared with barley malt wort. A markedly higher proportion of group "B" amino acids—valine, methionine, leucine, isoleucine, and histidine—was observed compared to groups "A," "C," and "D," consistent with previous studies (Glatthar et al., 2004). The modified mashing regime, adjusted to enhance proteolytic degradation, led to higher amino acid content across all tested triticale proportions compared to the standard congress method. Worts containing unmalted triticale consistently showed lower amino acid levels than those produced from barley malt, with the lowest amino acid content observed at the highest triticale proportion (50% ratio). Increasing the proportion of unmalted triticale in the grist resulted in a noticeable decrease in amino acid content, confirming that substantial use of unmalted raw materials at the expense of barley malt reduces amino acid availability in beer.

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EFFECTS OF CADMIUM ON THE MINERAL CONTENT OF SWISS CHARD AND STRATEGIES FOR REDUCING ITS HARMFUL IMPACT

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Abstract

Cadmium (Cd) contamination in agricultural soils is a critical threat to crop productivity, food security, and human health. Cadmium contamination continues to be a major constraint in the safe and sustainable cultivation of Swiss chard (*Beta vulgaris* subsp. *cicla*) and other leafy vegetables. Swiss chard, a mineral-rich leafy vegetable, is highly susceptible to Cd accumulation, leading to nutrient imbalances, oxidative stress, impaired root growth, and diminished crop quality. Cadmium ion competes with transporters of essential macro- and micronutrients, including K^+ , Ca^{2+} , Mg^{2+} , and Fe^{2+} , and promotes reactive oxygen species (ROS) formation, disrupting cellular homeostasis. To mitigate Cd toxicity, soil amendments such as biochar, compost, and zeolites can be used to immobilize Cd and improve soil health. Beneficial microorganisms, including plant growth-promoting rhizobacteria (PGPR) and arbuscular mycorrhizal fungi (AMF), enhance nutrient uptake, stress tolerance, and Cd sequestration. Foliar applications of zinc, iron, and selenium, as well as chelating agents, provide additional defense, while breeding programs targeting low-Cd-accumulating cultivars offer long-term solutions.

In this experiment was evaluated the effect of *Bacillus mycoides* on nutrient uptake in Swiss chard under Cd stress. Although Cd remained below detection level in plant tissues, Cd exposure significantly altered nutrient distribution. *B. mycoides* inoculation alleviated these imbalances, supporting root health and nutrient absorption. The promising results observed with microbial treatments, such as those involving *Bacillus mycoides*, highlight the role of plant growth-promoting rhizobacteria in enhancing nutrient uptake and mitigating heavy metal stress.

These results suggest that integrated management approaches, which combine soil remediation, microbial inoculation, nutrient supplementation, and cultivar selection are the best sustainable strategies to mitigate Cd toxicity while maintaining crop nutritional quality. Future research should focus on optimization of microbial applications under field conditions, and evaluation of environmental and economic sustainability to advance safe crop production in Cd-contaminated soils.

Keywords: cadmium contamination, Swiss chard, nutrient uptake, *Bacillus mycoides*, heavy metal stress, food safety

Acknowledgements

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DIFFUSE REFLECTANCE SPECTROSCOPY OF (Y,Me)NbO₄:Er,Yb PHOSPHORS (Me = In, Al)

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Abstract

Yttrium niobate (YNbO₄) is a self-activated phosphor exhibiting intense blue-band emission, with additional red and green emissions when doped with selected rare-earth ions. In this study, diffuse reflectance spectroscopy (DRS) was employed to investigate the electronic transition bands, optical band gap, and the influence of trivalent dopant ions (Me³⁺ = In³⁺, Al³⁺) on these properties. Nanocrystalline (Y,Me)NbO₄:Er³⁺,Yb³⁺ powders were synthesized via a solid-state reaction in a planetary ball mill (100 rpm, 8 h), followed by pre-annealing at 800 °C for 4 h and final annealing at 1200 °C for 4 h. Er³⁺ and Yb³⁺ ions were introduced to facilitate up-conversion (UC) luminescence, functioning as activator and sensitizer ions, respectively. Dopant Me³⁺ ions were incorporated to partially substitute Y³⁺ in the host lattice, thereby inducing local structural distortions and modifying the optical environment [1]. Microstructural characterization was carried out using X-ray diffraction (XRD) and scanning electron microscopy (SEM). DRS revealed characteristic Er³⁺ absorption bands, corresponding to the ⁴I_{15/2} → ²H_{11/2}, ⁴S_{3/2}, ⁴F_{9/2}, and ⁴I_{9/2} transitions, consistent with those observed in the up-conversion emission luminescence spectra. The optical band gap, estimated from the DRS data using the Kubelka-Munk function, was approximately 3.7 eV [2].

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AMBIENT MONITORING: A POTENTIAL APPROACH TO ENHANCING EMPLOYEE PERFORMANCE AND PRODUCTIVITY

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Abstract

Human productivity refers to the optimal use of human talent, knowledge, and skills to achieve maximum organisational performance. Personal, organisational, social, and environmental factors, such as noise, lighting, temperature, and air quality, determine the level of benefits for the company [1]. To increase human productivity, it is primarily necessary to ensure a healthy working environment. In addition to the negative impact on human health, the reduction of concentration, fatigue, and absence from work due to monotony and an inappropriate ambient environment also negatively affect human performance during working hours [2]. It has been estimated that an inappropriate work environment results in significant material losses for companies. One practical approach to addressing this issue is to conduct periodic employee surveys [3].

The research study involved 85 respondents, consisting of 35 men (41.2%) and 50 women (58.8%). The questionnaire evaluated several dimensions, including habits, which analysed respondents' daily routines and preferences for catering facilities and venues. It assessed perceptions of everyday noise within the immediate environment and evaluated subjective assessments of ambient factors, including noise, lighting, and air quality, in workplace settings. Additionally, the study investigated the impact of noise on employee productivity and performance levels and examined the adverse effects of noise on employee health.

The analysis of employee surveys examines the relationships between ambient factors (such as noise, lighting, and air quality), daily habits, productivity, and health, with a particular focus on the adverse effects of noise. Key findings include a positive correlation between ambient factors and adverse outcomes. Research shows significant correlations between everyday noise ($r = 0.430$) and ambient factors ($r = 0.394$) and productivity, as well as between everyday noise ($r = 0.625$) and ambient factors ($r = 0.353$) and health. Higher noise levels and poor conditions are linked to decreased productivity and health deterioration, with the strongest correlation between health and productivity ($r = 0.811$), suggesting that noise affects well-being first, which then impacts efficiency.

Notably, daily habits exhibit weak correlations with ambient factors (e.g., $r = -0.234$ for daily noise), indicating that personal choices, rather than environmental conditions, have a greater influence on them.

Implications for practice include the need to reduce noise and improve ambient conditions in the workplace to enhance productivity and overall health. Strategies such as using acoustic panels, optimising lighting (300–500 lux), and improving ventilation can mitigate the adverse effects by 30–60%. These insights are especially relevant for catering establishments, where ambience significantly affects customer satisfaction.

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UTILIZATION OF SILICON-MODIFIED CORN WASTE BIOCHAR FOR CADMIUM AND LEAD REMOVAL FROM AQUEOUS SOLUTIONS

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Abstract

In this study, we investigated the potential of biochar derived from corn harvest residues, modified with silicon, to enhance the removal efficiency of cadmium and lead ions from aqueous solutions. Our characterization of pristine and silicon-modified biochars using Fourier-Transform Infrared Spectroscopy (FTIR) confirmed the successful incorporation of silicon on the modified biochar's surface, a crucial factor for the enhanced adsorption of metals, especially Cd. The metal residue was quantified by Inductively Coupled Plasma - Optical Emission Spectrometry (ICP-OES). Our adsorption experiments demonstrated that the silicon-modified biochar exhibited significantly improved adsorption capacity, achieving removal efficiencies exceeding 99% in various pH conditions. This high removal efficiency was achieved with a minimal amount of Si, and in combination with the use of a low-cost and widespread biochar precursor, this approach demonstrates its potential as a cost-effective strategy for the removal of metal contaminants from water.

Introduction

Lead and cadmium are recognized as two of the most toxic and persistent heavy metals in the environment, notorious for their ability to bioaccumulate in living organisms. Their widespread presence primarily results from various anthropogenic activities, including mining, smelting, and waste disposal. Owing to their high persistence, these metals remain in the environment for extended periods, posing a significant and long-term risk to ecosystem integrity and public health [1]. To mitigate this risk, several removal approaches have been proposed. Among these, adsorption is considered one of the most suitable and promising methods for the remediation of heavy metals [2]. Over time, researchers have experimented with various materials as sorbents for adsorption, and each material brings its unique characteristics to the adsorption process. Recently, biochar-based materials have gained attention as innovative and cost-effective options for adsorbing various heavy metals [3].

Biochar is a black, carbon-rich, and porous material, obtained by carbonization of biomass at temperatures higher than 250 °C in an inert atmosphere of nitrogen [4]. These carbonaceous materials possess several advantageous properties, including low density, extensive porosity, and a large surface area, making them highly effective, even in their unmodified state [5]. However, strategic modifications are often employed to enhance their surface chemistry and textural properties, improving targeting efficiency for specific contaminants and enhancing overall removal performance.

Modified biochar can be prepared through various physical, chemical, and microbial methods to improve its performance. Among these, silicon modification has emerged as a particularly effective strategy [6].

This study focuses on biochar produced from corn harvest residues (corn cobs and corn stalks) as adsorbent materials, comparing their pristine forms with silicon-modified variants. The research examines their effectiveness in the removal of cadmium and lead from contaminated water, with the dual objective of evaluating their applicability in water treatment and their potential use as amendments for assisted phytostabilization. This approach aims to identify the samples that exhibit the most promising characteristics for removing lead and cadmium from the media, providing a foundation for future *in situ* investigations.

Experimental

Materials and Methods

The precursor biomass (corn stalks and corn cobs) was collected from an agricultural site near Belgrade, Serbia, following the harvest. The precursor material was modified using an aqueous solution of sodium metasilicate nonahydrate ($\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$), commonly known as water glass. Carbonization was conducted in a horizontal tube furnace, Adamel-Lhomargy CT7, under a nitrogen atmosphere. Cadmium and lead stock solutions (50 ppm) were prepared by dissolving $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ and $\text{Pb}(\text{NO}_3)_2$ in deionized water. The initial pH was modified by adding 0.1 M HCl or 0.1 M NaOH to achieve target pH values of 3 and 5, respectively. Concentrations of the analytes after the adsorption process were quantified using a Thermo Fisher iCAP DUO 7000 inductively coupled plasma optical emission spectrometer (ICP-OES). The surface chemistry of pristine and silicon-modified biochar was characterized by Fourier-transform infrared spectroscopy (FTIR) using a Thermo Fisher Scientific Nicolet iS5 spectrometer.

Synthesis of pristine and Si-modified biochar

Biomass was air-dried at room temperature, mechanically ground to a fine powder, and homogenized in a 1:1 mass ratio of corn cobs to corn stalks. The biomass was treated in a horizontal tube furnace under a nitrogen atmosphere for carbonization. The heating rate was maintained at 5 °C per minute until the target temperature of 800 °C was achieved. The temperature was held constant for 2 h to ensure complete carbonization. After the carbonization process, the biochar was subjected to cooling to room temperature inside the furnace, and then ground into a fine powder. The resultant unmodified biochar was labeled NoSi, corresponding to zero additional silicate content.

The synthesis of silicon-modified biochars was carried out using a soaking method. Specifically, biomass samples were impregnated with sodium silicate solution (1.5 g/mL) before carbonization, at three different biomass-to-silicate ratios (4:1, 2:1 and 1:1). The silicon-modified samples were subjected to the same carbonization conditions as the unmodified ones. The resultant modified biochars were labeled LowSi, MedSi, and HighSi, corresponding to the low, medium, and high additional silicate content.

Adsorption experiments

The obtained materials were immersed in a 50 ppm mixed solution of cadmium and lead salts, which was adjusted to two different pH values and agitated using an orbital shaker at 180 rpm for 24 h. Upon completion of the adsorption experiment, the solutions were filtered and analyzed using ICP-OES. The adsorption efficiency was evaluated based on the residual metal concentration, where the lowest concentration indicated the highest adsorption capacity.

Results and discussion

FTIR analysis

FTIR spectra of the analyzed samples are presented in Figure 1. The characteristic vibrational peak at region 3300 cm^{-1} is assigned to OH stretching vibrations of free or intercalated water. The peak at 1620 cm^{-1} may be assigned to $\text{C}=\text{C}$ bonds. Two vibrational peaks at 470 cm^{-1} and 1110 cm^{-1} are assigned to Si-O-Si or Si-O stretching vibrations [7]. These two peaks confirm the successful binding of silicon to the surface of the materials carbon structure. An increase in the intensity and peak area at 1110 cm^{-1} is also visible, which is increasing in samples with a higher Si content, which is an additional confirmation of the successful modification of the biochar.

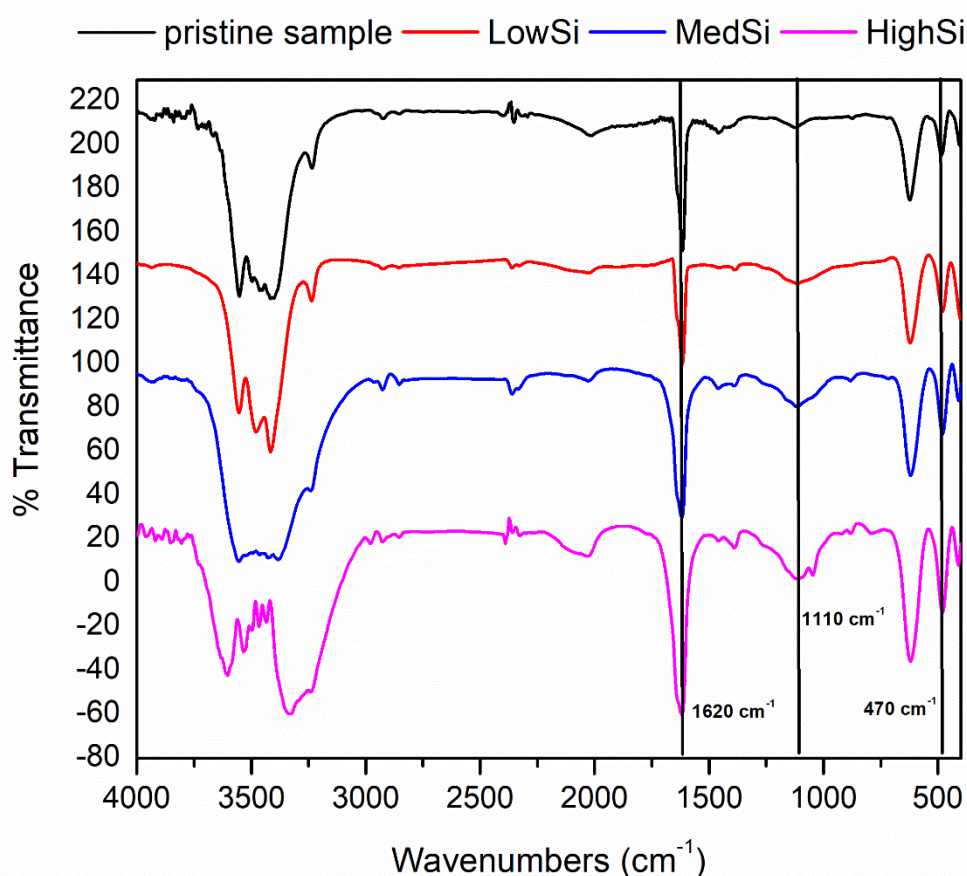


Figure 1. FTIR spectrum of synthesized samples with different ratios of silicon

Adsorption study

The adsorption of Cd and Pb was investigated at pH 5 and pH 3, a range selected to prevent metal precipitation, which typically occurs at higher pH values. The adsorption trends for the different biochar samples at each pH are presented in Figure 2. At pH 5, complete removal of Pb is observed for the pristine and LowSi samples. For samples with higher Si content, the percentage removal slightly decreases up to 90% for the HighSi sample, but it is still a very high percentage of Pb removal. In Cd adsorption, the pristine sample shows a low removal efficiency of 64%, while the Si modified samples show drastically better adsorptive characteristics, from 99% for the LowSi sample to 91% for the HighSi sample. Even in the case of Cd adsorption, a slight decrease in adsorption efficiency is observed in modified samples,

around 9%. The trends of decrease in the efficiency of Pb and Cd removal in samples with a higher Si content, as well as the reduced removal percentage of Cd in the pristine sample, can probably be explained by the saturation of the material surface and active sites in the HighSi sample, which reduces the availability of active sites for binding other metals. Further research will give a more detailed and complete answer to this very interesting phenomenon.

Adsorption at pH 3 showed a similar trend with a slight decrease in removal efficiency of both Pb and Cd for the HighSi sample compared to at pH 5. Pristine sample at pH 3 shows a low removal efficiency for Cd, only 37%, which can be explained by the fact that in acidic conditions, there is competition between metal ions and H^+ ions, leading to reduced adsorption of the target analyte [7]. Consequently, achieving an optimal degree of modification is crucial for utilizing the full potential of Si-functionalization as a targeted strategy for biochar enhancement.

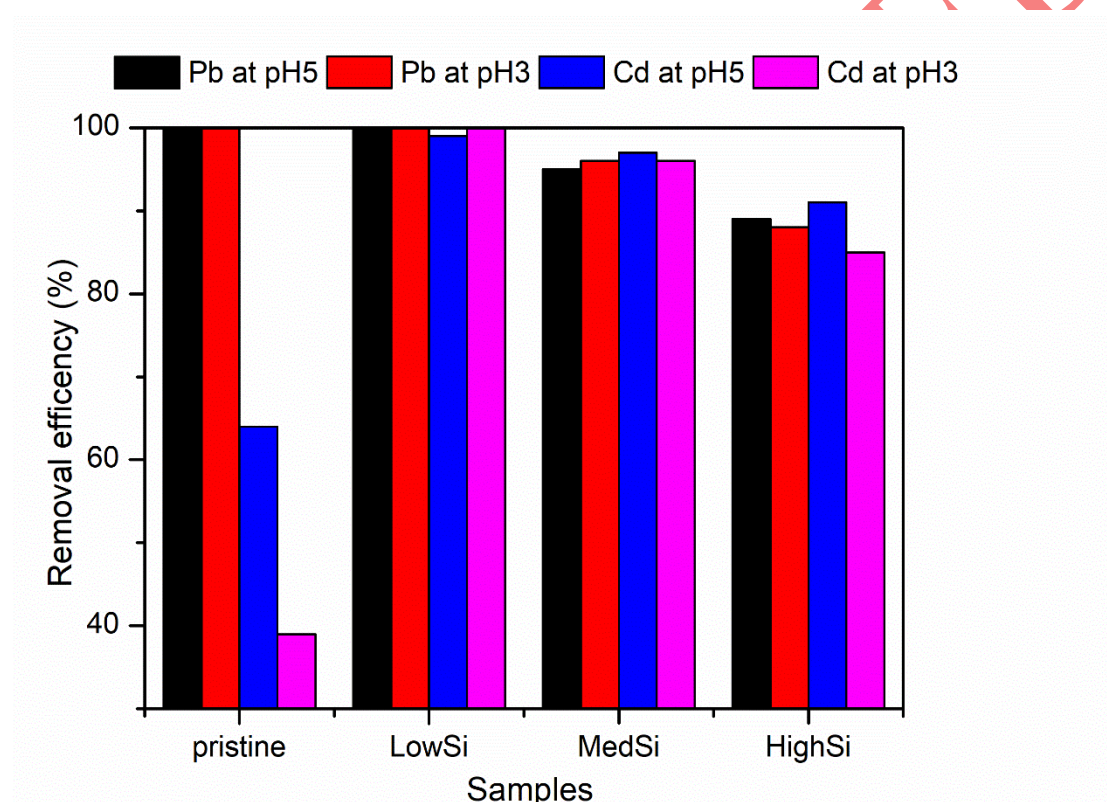


Figure 2. Removal efficiency for Pb and Cd at pH 3 and pH 5

Conclusion

FTIR analysis confirmed the successful modification of pristine biochar with different silicon content. All silicon-modified biochars exhibited excellent heavy metal removal capabilities, especially the sample with low Si content, which demonstrated exceptional efficiency (>99%) for both Pb and Cd across distinct pH conditions. The study highlights the importance of optimal silicon dosage, as the lowest silicate modification (4:1 ratio) achieved better results while minimizing material costs. Combined with abundant agricultural waste biomass, this approach presents a highly cost-effective strategy for the remediation of heavy metal-contaminated media. In future research, the mechanism of silicon binding to the biochar surface during modification and the mechanism of metal adsorption onto biochar will be thoroughly examined.

Acknowledgements

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DETERMINATION OF PHENOLIC COMPOUNDS IN INDUSTRIAL WASTE

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Abstract

The aim of this work was to validate the concentration of phenolic compounds in waste using an aminoantipyrine spectrophotometric method. The validation of the method was carried out with leachate from industrial waste. Leachates from various industrial wastes were treated by an extraction process in which soluble components were removed from the solids. Millipore water was used as a solvent. The concentration of phenolic compounds was determined in leachates from the following materials: filter dust from the abrasives industry and filter dust from the aluminium industry. The validation included the determination of the measuring range, the detection limit, the limit of quantification, the linearity, the precision of the measurements, the accuracy and the influence of interferences. The results confirmed the precision and accuracy of the method. The method is suitable for determining the phenolic compounds content in industrial waste from the metal industry.

Introduction

Phenol is classified as an organic aromatic compound, which is not harmful to health in minimal concentrations of up to 0.1 mg/kg, but can become very harmful with prolonged exposure to the body. The European Community (EC) has classified them as priority compounds [1]. Phenol is used in the production of synthetic fibers, in the production of phenolic resin, in chemicals that kill bacteria (slimicides), is used as a disinfectant, is also an antiseptic and is found in medicinal preparations (e.g. throat lozenges, mouthwash, etc.). It is biodegradable, reacts with OH⁻ radicals and ozone. Its estimated half-life in the atmosphere is approximately 14 days.[2] Phenol is produced in large volume, mostly as an intermediate in the production of other chemicals. Phenol index is an indicator of phenolic contamination expressed as total content of phenolic compounds in water [3]. Various materials are used in the production of grinding wheels. These include corundum-based particles, organic binders (e.g. phenol-formaldehyde resins to hold abrasive grains together) and various other additives. The gas and dust products generated in the production of grinding wheels are led through a cleaning device with filters, where the filter dust is collected. This dust contains high levels of phenol. It is disposed off in hazardous waste landfills. Due to the discharge of effluent from wastewater treatment plants, the concentrations of phenol in surface water increases [4].

Foundry sand is a byproduct produced during the aluminum casting process. It is primarily composed of quartz sand and contains approximately 1 % binder, typically a mixture of polymerized phenolic resin and isocyanurate. Classified as non-hazardous, this material can be repurposed for various applications, such as the production of floor tiles.

The aim of this work was to partially validate the concentration of phenolic compounds in leachate from industrial waste. The following validation requirements, such as correlation coefficient (*R*), the accuracy, precision, the limit of detection (*LOD*) and the limit of quantification (*LOQ*) were evaluated.

Experimental

The implementation of the method includes preliminary leaching according to the SIST EN 12457- 4:2004 standard [5], sample distillation, liquid-liquid extraction and measurement on a spectrophotometer. The preparation of the test sample was carried out in accordance with the SIST EN 15002:2006 standard [6].

The validation of the analytical method includes the working and measuring range, determination and confirmation of the detection limit and the quantification limit, linearity, precision (repeatability and reproducibility), accuracy (calculation of average recoveries) and interference study. The measurement uncertainty of the leaching was estimated from the repeatability uncertainty (*RSD*) of all samples. Figure 1 shows the real sample.



Figure 1. Grinding wheel filter dust real sample

Phenol reference material (Phenol [CAS:108-95-2] 1000 mg/L in Water), was prepared by dissolving in freshly boiled and cooled millipore water, transferred to a 1000 mL volumetric flask. The solution was stable for 1 week.

UV-Visible Spectrophotometer Cary 50 Bio, Agilent, USA, Multi 3410 WTW pH meter and COND 3110 WTW conductometer were used.

Samples were crushed and sifted, then leaching was done with HNO_3 in laboratory. After filtration (0.45 μm filter) and distillation the solid-liquid extraction with chlorophorm followed. 500 mL of destilate was extracted with 25 mL of chloroform. Blank and control samples are extracted the same way. Always control sample was treated the same way. The absorbance was measured at 456 nm. The dillution factor must be calculated. After extraction dry weight was calculated (SS).

The laboratory should be able to determine, whether imprecision or bias is the reason for its inaccuracy. Interlaboratory tests are one of the most important external quality assurance tools to assure comparability with all the other laboratories. Another option is based on the recovery calculation according to equation 1. Recovery for standard solutions was calculated at multiple concentration levels of a given linear concentration range. We set the criterion that the method is accurate when the average recovery value is within the interaval from 90.0 % to 110.0 %.

$$\text{recovery} = x_m / x_t \cdot 100 \quad (1)$$

x_m : is the result reported by the measurement.

x_t : is the theoretical value.

Results and discussion

The dry weight was determined by dividing the mass of dried sample (at 105 °C) and the mass of sample which was not dried. The results showed, that the SS value was 99.8 % and 99.6% in dust from Al production and from grinding wheels production, respectively.

LOD was determined to be 0.2 $\mu\text{g/L}$, based on the standard deviation of the blank signals (s_b) and the slope of the calibration curve (m) after dilution of the standard solutions ($3s_b/m$). LOQ was determined at 0.7 $\mu\text{g/L}$.

Accuracy

To check the accuracy, we prepared standard solutions with concentrations of 50.0 $\mu\text{g/L}$ (V1), 100 $\mu\text{g/L}$ (V2), 250 $\mu\text{g/L}$ (V3), 500 $\mu\text{g/L}$ (V4) and 800 $\mu\text{g/L}$ (V5) in the same way. Measured concentrations and recoveries, calculated according to equation (1), are seen from Table 1.

Table 1. Measured values and recoveries

Sample	x_m ($\mu\text{g/L}$)	x_t ($\mu\text{g/L}$)	Recovery (%)
V1	46	50	92
V2	109	100	109
V3	237	250	95
V4	522	500	104
V5	850	800	106

It is seen from Table 1 that all results were determined within the confidence interval 92 % – 109 %. Recovery meets the criterion and the method is accurate.

Linearity

The concentration of phenolic compounds was measured in a chloroform extract. Figure 2 represents the calibration curve.

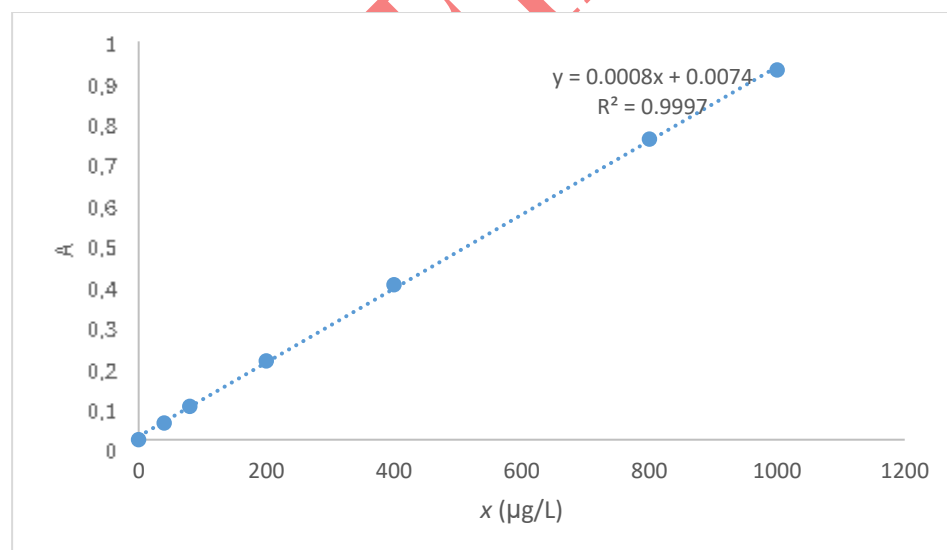


Figure 2. Calibration curve

The phenol concentration in the extract was first measured using a spectrophotometer, and then we calculated the initial leachate sample the 20times dilution was considered. The calibration

curve with equation $A = 0.0008 \cdot x + 0.0074$ and high correlation coefficient $R^2=0.9997$ was determined. Quality coefficient was determined at 2.01.

Precision

The repeatability of the leaching was performed on four types of real leachate samples. From each sample, 6 leachate samples were prepared and analyzed under reproducible conditions (the same analyst, same analytical procedure, the same equipment, the same chemicals, etc.). From the obtained data, we calculated the standard deviation (s) and relative standard deviation (RSD). The RSD was obtained from 6 measurements of each sample. It was demonstrated that the RSD meets the standard requirements. The results of precision study are presented in Table 2.

Table 2. Data for precision determination

Sample number	$\bar{x}$ ($\mu\text{g/L}$) wheels	$\bar{x}$ ($\mu\text{g/L}$) Al dust
1	860	4.3
2	895	4.1
3	880	4.4
4	820	3.9
5	850	4.1
6	880	3.8
Average	864.2	4.1
s	26.9	0.2
RSD (%)	3.1	5.5

The results of reproducibility (under different conditions) showed low RSD value 3.1 % which is in accordance with requirements.

Interferences study

Interferences due to biological degradation, sulphur compound content or oil content as well as amine presence could influence the measurements. In such cases a preservative must be added. However, in our samples it was impossible. Therefore, the interference of amine addition was checked. Known volumes of trihydroxytriethylamine were added to 500 ml of a standard control solution of phenol with a concentration of $c = 0.40$ mg/L in chloroform. The procedure was carried out without distillation to avoid the removal of the interfering compound.

Table 3. Influence of trihydroxytriethylamine (amine) to the sample (N =sample number)

N	V_{amine} (mL)	$\bar{x}$ measured (mg/L)
1	0	0.41
2	0.5	0.41
3	1.0	0.40
4	4.0	0.42
5	8.0	0.42

Trihydroxytriethylamine was at least partially extracted into chloroform, which was also noticeable during the measurement, but the presence of this interference, as can be seen from

the Table 3, did not have a significant effect on the determination of the concentration of phenolic compounds. The recovery was in range from 95 % to 105 % within the 95 % confidence interval.

Conclusion

The partly validation of the concentration of phenolic compounds was carried out on waste samples generated in the aluminum industry. The following validation requirements, such as correlation coefficient (R), quality coefficient (QC), the accuracy, the limit of detection (LOD) and the limit of quantification as well as interferences were evaluated. Linearity was checked with the quality coefficient QC , which was 2.01%, and the correlation coefficient R^2 was 0.999. The relative standard deviation (RSD) of repeatability was below 15 %. The accuracy of the analysis method was confirmed by the calculation of recovery. The concentration of phenolic compounds in waste sample generated in the aluminum industry was low, while it was quite higher in a waste sample from the grinding wheel industry.

Acknowledgements

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EFFECT OF *ASCOPHYLLUM NODOSUM* EXTRACT ON THE GROWTH PARAMETERS AND YIELD OF WILD ROCKET (*DIPLLOTAXIS TENUIFOLIA*)

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Abstract

The aim of the research was to assess the significance of variations in yield, morphological (stem length, leaf length, mean number of leaves, root length) and physiological (nitrogen balance index, chlorophyll, flavonoids, anthocyanins) traits of wild rocket under application of different doses of *Ascophyllum nodosum* extract (ANE) mixed with distilled water (0, 2, 4 and 6 ml/l). The experiment was conducted in greenhouse, in pots, from the fourth week of April to the second week of July 2025. Each pot was filled with 1.4 kg/pot of homogenized Vertisol, soil with a very clayey texture and acidic reaction. Physiological parameters were determined using a Dualex leaf clip sensor. The obtained results indicated a very noticeable influence of all applied doses of ANE on all tested plant parameters in relation to soil not treated with ANE. The most pronounced effect on plant morphological traits and yield had ANE dose at 4 ml/l, while on physiological parameters - ANE doses at 2 and 4 ml/l. Concluding, improved plant nutrition with 4 ml/l of ANE promoted the root growth, reflecting on the growth, development and yield of wild rocket plants. Further research in this area of study on larger soil areas could suggest new possibilities for *A. nodosum* application in the cultivation of rocket plants and other vegetable crops from an ecological point of view.

Introduction

Perennial wild rocket (*Diplotaxis tenuifolia* (L.) D.C.) is a plant from the cabbage family (Brassicaceae) with a specific smell and taste. Its taste is very similar to that of cultivated arugula, but is more intense. The young plants are also edible. Traditionally grown as a spontaneous plant along roadsides and in abandoned places, it was mostly domesticated in Europe and western Asia. Nowadays, it is a cultivated crop species of increasing importance with worldwide distribution.

Wild rocket can grow in any moderately fertile soil, slightly acidic to neutral, partially sunny and moist, but well-drained, with high drought resistance. This is due to the presence of a well-developed taproot, suggesting limiting irrigation. Nutritional requirements of wild rocket are modest, and can be supplied through fertigation [1].

Wild rocket is recognized for various medicinal and therapeutic properties and thus health beneficial effects in bactericidal and anti-inflammatory use. The leaves of wild rocket have notable nutritional properties related to their contents of flavonoids, fibre, calcium, iron, potassium, phosphorus, richness in vitamins such as A, B, C, and K, essential proteins, as well as a number of other microelements essential for the human health [1, 2].

The plant can be grown in open fields but more often in greenhouses, particularly in organic production [3]. Rocket grown in organic conditions without pesticides and inorganic fertilizers is an increasingly common choice for health-conscious consumers [2].

Methods in organic production imply the application of natural processes (crop rotation, intercropping, cover crops, minimal tillage) and substances (organic fertilizers, symbiotic associations, biostimulators), and limit or completely eliminate the use of synthesized agents, promoting ecosystem preservation by integrating biodiversity and biological cycles [4].

Among the innovative and promising solutions for improving the sustainability and profitability of organic agriculture, biostimulants are being considered, especially those based on seaweed extracts. The use of natural seaweeds as fertilizer enables the gradual substitution of conventional inorganic fertilizers. These fertilizers are biodegradable, non toxic and non polluting in nature, and also non hazardous to humans, animals and birds.

A wide range of beneficial effects of seaweed extracts, necessary for plant growth and development, are based on the presence of multiple growth regulators (cytokinin, auxins, gibberellins, betaines), macronutrients (Ca, K, P), and micronutrients (Fe, Cu, Zn, B, Mn, Co and Mo) [5].

Due to their ability to be used in organic agriculture, extracts of the brown seaweed *Ascophyllum nodosum* (L.) are well-known and commercially present as a suitable alternative to reduce the use of chemical inputs and has the potential to increase the quantitative and qualitative yield of various cultivars [6]. Aly et al. [7] observed the highest chlorophyll content, grain yield and essential oil content in parsley when using foliar application of *A. nodosum* extract. Nasiri et al. [8] reported the increased content of carvacrol in essential oil of savory under the application of *A. nodosum* extract. The extracts are also well-established plant biostimulants that improve stress tolerance and crop vigour, expressing ability to stimulate soil microbes [9].

The use of *A. nodosum* extract in agriculture, mostly in organic, significantly improved the germination rate, thus increasing the growth of lateral roots, enhancing water and nutrient use efficiencies, increasing the content of flavonoid, chlorophyll and nutrient, alleviating the effects of abiotic and biotic stresses in different crop plants [10].

This research aimed to evaluate the effect of different doses of *A. nodosum* extract (ANE) on the yield, morphological and physiological traits of wild rocket, grown on Vertisol, performed in semi-controlled greenhouse conditions.

Experimental

This study was performed under semi-controlled greenhouse conditions at the Institute of Soil Science, using plastic pots, from the fourth week of April to the second week of July 2025. Each pot was filled with 1.4 kg/pot of homogenized Vertisol soil [11], sourced from a field located in Mala Ivanča, Sopot Municipality (grid reference: 44°35' N, 20°36' E), about 35 km from Belgrade in Serbia. Our previous study [12] revealed high clay fraction, acidic reaction, high available K, very low available P, medium total N and SOM supply in Vertisol.

In every plastic pot, fifteen rocket seeds were sown on April 28. After the plants have grown 2.5-3 cm above the ground ten plants per pot were left. Plants were grown using standard growing methods (regular watering, manual weed control, and without chemical protection). The following four designed treatments were carried out in three replications: ANE (0.2%, 2 ml/l distilled water); ANE (0.4%, 4 ml/l distilled water); ANE (0.6%, 6 ml/l distilled water); Control (ANE 0 ml/l distilled water). According to the manufacturer's packaging, the extract of *A. nodosum* is a nitrogenous liquid organic fertilizer of plant origin (algae).

After sowing, soils were sprayed with appropriate doses of ANE, and when the plants grew to 2.5-3 cm above the soil and after triage, soil and foliar spraying were performed every 7 days. Regular watering was done as needed, so that the grown plants always had enough moisture. Seven days before the complete removing the plants, morphological traits (stem length, SL; leaf length, LL; mean number of leaves, MNL), and physiological parameters (nitrogen balance index, NBI; chlorophyll, Chl; flavonoids, Flv; anthocyanins, Ant) of the plants aerial biomass were measured. Physiological parameters were measured using portable Dualex optical leafclip sensor (FORCE-A, Orsay, France). After seven days, on July 14, the rocket plants were completely removed from the pots, taking care to separate the root from the soil in the safest

way possible. The root was then thoroughly cleaned of soil using distilled water and its length (root length, RL) was measured for each treatment. The yield of the rocket aerial biomass from each treatment was first measured for fresh weight, then air-dried and measured for dry weight, both parameters expressed in g/pot.

Analysis of variance (ANOVA, SPSS 22.0), followed by Duncan's multiple range tests (DMRT) at $p < 0.05$, were used to statistically analyse the data relevant to the treatment effects on all plant parameters.

Results and discussion

The values of the yield, morphological and physiological traits of wild rocket showed distinct responses under influence of treatment with different doses of *A. nodosum* extract (ANE). Statistical analysis of the differences between the treatments for individual comparison of plant morphological traits is presented in Table 1. The obtained results indicated a statistically significant effect ($p < 0.05$) of all applied doses of ANE on plant morphological traits in relation to soil not treated with ANE. The most pronounced significant effect ($p < 0.05$) on all plant morphological traits compared to other tested treatments was determined in the treatment where ANE at dose of 4 ml/l was applied, followed by treatments sprayed with ANE at doses of 6 and 2 ml/l. Accordingly, improved plant nutrition with 4 ml/l of ANE promoted the root growth, reflecting on the growth and development of an aerial biomass of wild rocket plants (Figure 1).

Table 1. Effect of treatments on morphological traits of wild rocket

Treatments	Morphological traits ¹			
	SL (cm)	LL (cm)	MNL	RL (cm)
T1 - ANE (0 ml/l)	9.17 c (± 1.26)	3.53 c (± 0.93)	3.33 c (± 0.58)	6.83 d (± 2.08)
T2 - ANE (2 ml/l)	13.45 b (± 3.25)	4.18 bc (± 0.66)	5.77 b (± 0.58)	8.63 c (± 0.85)
T3 - ANE (4 ml/l)	16.33 a (± 1.44)	6.50 a (± 1.32)	6.53 a (± 0.58)	10.83 a (± 1.61)
T4 - ANE (6 ml/l)	13.53 b (± 1.63)	4.33 b (± 1.53)	5.89 b (± 1.00)	9.67 b (± 1.61)

¹Means $\pm$ STDEV (n = 3); Duncan's test at $p \leq 0.05$ - values followed by the same letter in a column are not significantly different.

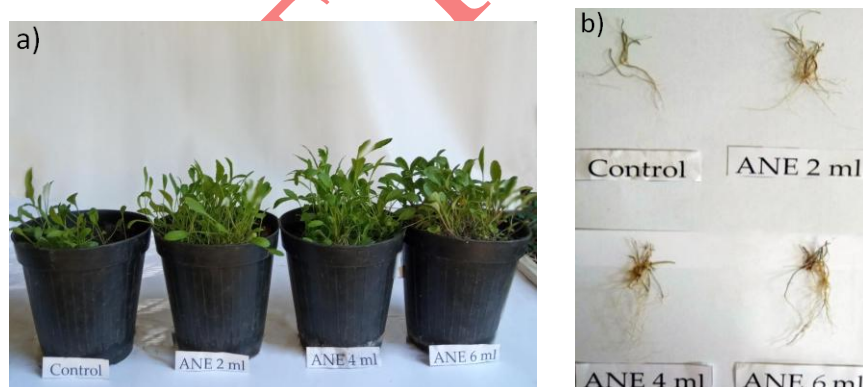


Figure 1. Growth and development of wild rocket plants: a) aerial biomass; b) root

Contrary to obtained results, Morelatto and Silva [13] determined that none of the tested doses of ANE (0, 1, 2 and 4 ml/l) promoted improvements in the growth and root length of cultivated rocket. Nevertheless, other authors [8] reported significance in the response of the savory to the *A. nodosum* soil and foliar application, regarding plant height and number of lateral branches. In some studies pot foliar application and pot root application of 0.05% and 0.10% of *A. nodosum* extract ameliorated the growth performance of *Vigna aconitifolia* [14].

Statistical analysis of the differences between the treatments for individual comparison of plant physiological parameters is presented in Table 2. The obtained results indicated a statistically significant effect ($p < 0.05$) of all applied doses of ANE on all plant physiological parameters in relation to soil not treated with ANE. The most pronounced significant effect ($p < 0.05$) on all plant physiological parameters compared to T1 (0 ml/l ANE) and T4 treatments (6 ml/l ANE) was determined in the treatments where ANE doses at 2 and 4 ml/l were applied. Overall results revealed that the treatments with ANE at doses of 2 and 4 ml/l, rather than ANE at dose of 6 ml/l, had the greatest influence on physiological parameters.

A. nodosum extract is significant as having bioactive ingredients that potentially regulate the molecular, physiological, and biochemical processes of crop plants [15]. Previous research on grapes revealed that repeated foliar sprays with *A. nodosum* extracts improved vine physiological performances, leaf assimilation, and water use efficiency, preserving photosystems integrity and resilience when water deficit is moderate [6].

Table 2. Effect of treatments on physiological parameters in wild rocket

Treatments	Physiological parameters ¹			
	NBI	Chl (μcm^2)	Flav (μcm^2)	Ant (μcm^2)
T1 - ANE (0 ml/l)	19.97 c (± 5.95)	17.00 c (± 1.75)	0.59 c (± 0.12)	0.15 c (± 0.01)
T2 - ANE (2 ml/l)	32.90 a (± 1.65)	23.02 a (± 5.40)	0.76 a (± 0.01)	0.19 a (± 0.01)
T3 - ANE (4 ml/l)	33.77 a (± 8.47)	23.33 a (± 2.62)	0.77 a (± 0.08)	0.20 a (± 0.02)
T4 - ANE (6 ml/l)	26.93 b (± 3.78)	20.30 b (± 1.74)	0.66 b (± 0.12)	0.17 b (± 0.01)

¹Means $\pm$ STDEV (n = 3); Duncan's test at $p \leq 0.05$ - values followed by the same letter in a column are not significantly different.

Differences in the values of fresh and air-dried biomass yield between the treatments indicated a statistically significant effect ($p < 0.05$) of all applied doses of ANE on plant yield in relation to soil not treated with ANE. The treatments where ANE doses at 4 ml/l, followed by treatments sprayed with ANE at doses of 6 and 2 ml/l, were applied showed the most pronounced significant effect ($p < 0.05$) on plant yield. Overall data on biomass yield were in accordance with morphological traits and physiological parameters, meaning that the highest yield was registered in pot treatment with the dose of ANE at 4 ml/l (Table 3).

Table 3. Effect of treatments on yield of wild rocket

Treatments	Yield (g/pot) ¹	
	Fresh biomass	Air-dried biomass
T1 - <i>A. nodosum</i> (0 ml/l)	3.62 c (± 0.10)	0.48 c (± 0.05)
T2 - <i>A. nodosum</i> (2 ml/l)	7.95 b (± 0.16)	0.97 b (± 0.03)
T3 - <i>A. nodosum</i> (4 ml/l)	9.15 a (± 0.04)	1.17 a (± 0.02)
T4 - <i>A. nodosum</i> (6 ml/l)	9.13 a (± 0.03)	1.02 b (± 0.03)

¹Means $\pm$ STDEV (n = 3); Duncan's test at $p \leq 0.05$ - values followed by the same letter in a column are not significantly different.

The use of *A. nodosum*-based biostimulant in improving plant growth and yield was reported previously [8, 15, 16, 17]. In evaluating the effect of *A. nodosum* extract on the growth and yield of savory it was reported that the soil or foliar application of seaweed has significant effects on increasing the dry weight of plant [8]. Analyzing the effect of soil and foliar application of ANE in improving the growth of fennel plants grown under salinity stress, significant increase in the fennel yield and yield components was determined [15]. Studying the role of ANE in improving the productivity of *Zea mays* under phosphorus-limited conditions

and in nutrient-deficient soils, Shukla and Prithiviraj [16] reported an increase in the agricultural productivity of this plant. Also, Shukla et al. [17] emphasize multiple and beneficial effects of *A. nodosum* extracts on plants growth and their defense responses.

Conclusion

The results of the paper indicate that the most pronounced effect on morphological and physiological parameters had the treatment where ANE at dose of 4 ml/l was applied, followed by treatments sprayed with ANE at doses of 2 and 6 ml/l. All applied doses of ANE (2, 4, and 6 ml/l) showed a significant effect on all tested rocket parameters in relation to soil not treated with ANE. Overall data on biomass yield were in accordance with morphological and physiological parameters, meaning that the highest yield was registered in treatments with the dose of ANE at 4 ml/l, which could be proposed in the wild rocket cultivation in greenhouse pots conditions. Nevertheless, further research in this area of study on larger soil areas is desirable.

Acknowledgements

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PESTICIDE RESIDUES IN AGRICULTURAL SOILS: EMPHASIZING THE NEED FOR NATIONAL-LEVEL MONITORING

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Abstract

This study emphasizes the importance of establishing a comprehensive national monitoring program for pesticide residues in agricultural soils, especially in regions with intensive crop production. Due to widespread use, herbicides pose significant environmental and health risks, with soil being particularly vulnerable to contamination. Monitoring was conducted in agricultural soil in Vojvodina (Serbia) in 2023 and 2024. Samples were collected from surface layer and analyzed using LC-MS/MS and GC-MS/MS techniques for 41 herbicidal active substances. The 2023 analysis revealed that all samples contained multiple herbicide residues, with up to 19 active substances detected in a single sample. In 2024, high detection frequencies were noted for clopyralid, 2,4-D-methyl ester, terbuthylazine, fenoxaprop-ethyl, and aclonifen, although most were found at low concentrations. These findings confirm the persistence and accumulation of herbicide residues in agricultural soils, underscoring the urgent need for more effective regulation, improved agricultural practices, and sustainable weed management strategies to protect soil health and the environment.

Introduction

In order to protect crops from a wide range of pests and ensure optimal yields, contemporary plant protection relies almost completely on the use of chemical agents, mostly herbicides. Nowadays, the risks associated with pesticide use have outweighed their benefits [1]. Pesticides are regarded as particularly important for the environment due to their potential toxicity and the physicochemical characteristics of certain active ingredients, which enable them to interact with the environment, resulting in high mobility and/or persistence [2]. Thus, as a consequence of their intensive use, the growing trend of environmental protection and food safety, monitoring of the presence of pesticide residues is crucial.

The soil is particularly vulnerable. Although a non-renewable resource with a possible high degradation rate, soil represents the foundation for agricultural production. The land is most threatened by anthropogenic factors through activities related to agricultural production.

Pollution caused by pesticide use in agriculture requires particular attention, especially in regions with intensive crop production. In these areas, the economy heavily depends on agriculture, and high pesticide use per hectare is common to ensure adequate yields [2].

Much research demonstrated that pollution of surface soil leads to pesticide contamination of both groundwater and surface freshwater [3]. Therefore, controlling pesticide levels in surface soil is crucial for protecting public health [4].

However, extensive surveys of pesticide residues in agricultural soils are surprisingly scarce [5-8], nor is the monitoring of pesticide residues in soil regulated appropriately. Healthy soils form the basis for 95% of the food, support over 25% of the world's biodiversity, and represent the largest terrestrial carbon reservoir. However, soil is a limited resource, and more than 60% of

soils in the EU are not in good condition. Significant change of the existing conditions in this area, aiming to ensure that all EU soil ecosystems are in a healthy state, could be done by the Soil Surveillance and Resilience Law, as well as a new EU Soil Strategy for 2030 [9].

This study aims to highlight the importance of establishing and maintaining a comprehensive national-level monitoring program for pesticides in agricultural soil, which is essential for assessing environmental impact, ensuring food safety, and promoting sustainable farming practices.

Experimental

Sampling area.

Sampling area covered region under intensive agricultural production, located in the northern part of Serbia (Vojvodina) (Figure 1). In two monitoring programs of pesticide residues in agricultural soil, analysis was done at 128 localities in 2023 and 260 localities in 2024.

Soil was sampled at the surface layer (0-30 cm) by collecting 20 sub-samples at various points diagonally in the plots within the production area, using a soil sampling probe or shovel. Covered with chernozem as the most widespread type of soil, this region is recognized for its intensive agricultural production of maize, soybean, sugar beet, and sunflower.

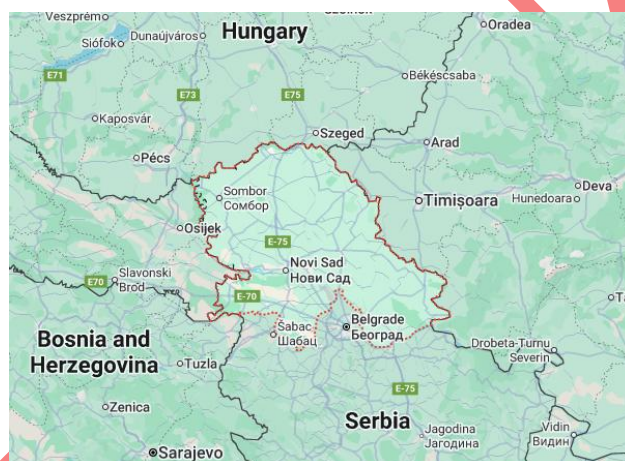


Figure 1. Sampling area

Extraction and analysis.

Certified analytical standards of herbicides with a purity greater than 98% were sourced from Dr. Ehrenstorfer. The solvents used for the extraction and chromatography were supplied by Fisher Scientific (Leicestershire, UK). Individual stock standard solutions of herbicides were prepared by accurately dissolving the analytical standards in a suitable solvent. These solutions were then protected from light and stored at -20 °C in dark glass bottles. Working standard solutions of different concentrations were subsequently prepared by appropriate dilution.

For the extraction of herbicide residues from soil, a modified QuEChERS-based method was applied. The extraction was preceded by sample preparation, which included air-drying, grinding, and sieving of soil samples. Afterward, a 10 g sample was weighed and transferred to a 50 mL polypropylene cuvette with 3 mL of deionized water and 10 mL of acetonitrile acidified with 2% formic acid.

The mixture was shaken for 1 min, vortexed for 1 min, and after which, a salt buffer mixture was added (4 g of magnesium salt, 1 g of sodium chloride, 1 g of Na citrate, and 0.5 g of disodium citrate sesquihydrate). The prepared samples were shaken for 1 min, vortexed for 1 min, left for 10 min in an ultrasonic bath, and centrifuged for 5 min at 4000 rpm. In the next step, the aliquot was evaporated to dryness, dissolved in acetonitrile or acetone, filtered through

a 0.45 µm membrane filter, transferred to a vial, and analyzed. Depending on the herbicide nature, residues were analyzed by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) and chromatography–tandem mass spectrometry (GC-MS/MS). Analysis covered 41 herbicide active substances.

Results and discussion

In the 2023 analysis (Figure 2), herbicide residues were found in all soil samples, with the minimum number of detected residues being 6, while the maximum number of active substances per location increased to 19. The most frequently detected herbicides were prosulfocarb, napropamide, and bentazon. Additionally, 2,4-D methyl ester, flumioxazine, metazachlor, oxyfluorfen, and propyzamide were present in a significant number of soil samples (50-90%). The highest concentration found was 18.90 µg/kg for terbuthylazine [10]. The monitoring program was carried out in 2024 to assess the current situation (Figure 2). Herbicide residue analyses revealed a high frequency of clopyralid, 2,4-D-methyl ester, terbuthylazine, fenoxaprop-ethyl, and aclonifen. While the concentrations of clopyralid, fenoxaprop-ethyl, and aclonifen were all below 0.5 µg/kg, clomazone, ethofumesate, metsulfuron-methyl and s-metolachlor stood out with a concentration of 11.856, 24.335, 26.137 and 29.878 µg/kg, respectively. Among the 41 herbicides analyzed, three were either not detected or were below the limit of detection (LOD), while twenty-three had occurrence frequencies below 10% [11].

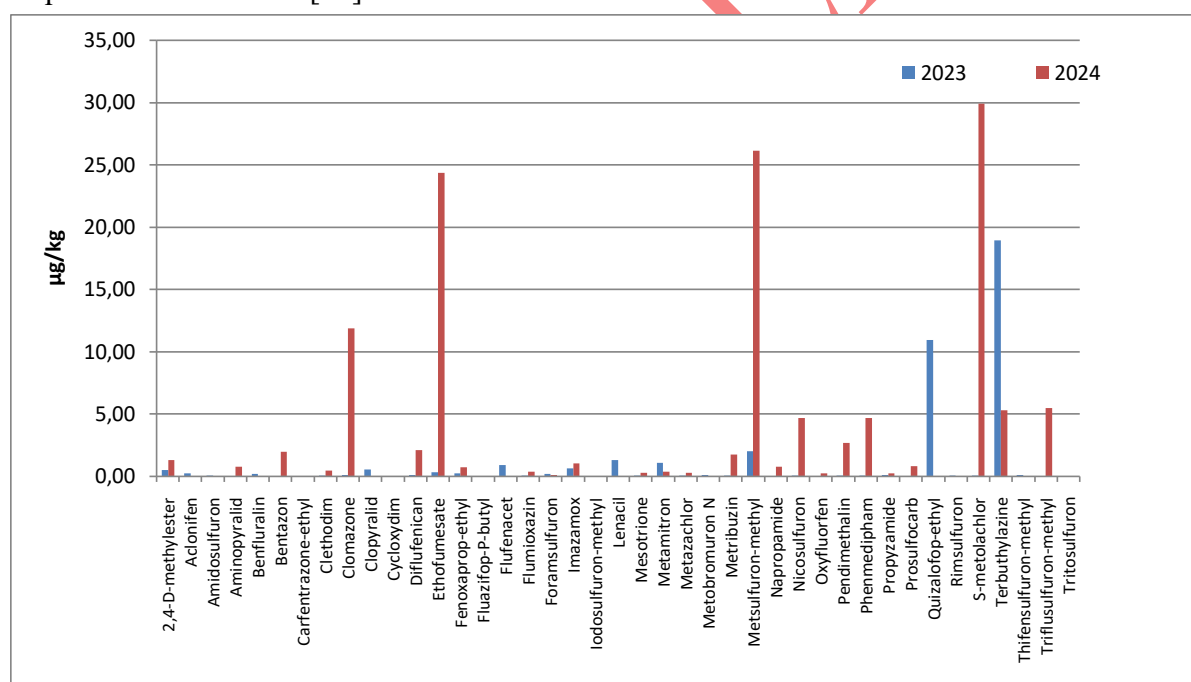


Figure 2. Herbicide residues in soil samples.

The monitoring results from 2023 and 2024 indicate a persistent and complex presence of herbicide residues in agricultural soils. In 2023, all soil samples contained herbicide residues, with up to 19 active substances detected in a single sample, reflecting a high level of chemical diversity and accumulation. Particularly concerning was the exceptionally high concentration of terbuthylazine.

In 2024, although the concentrations of the most frequently detected herbicides were generally low, the consistently high detection rates suggest widespread use and environmental

persistence. S-metolachlor emerged as a compound of particular concern due to its notably high concentration at one location, despite its moderate average value.

Conclusion

The data from both years underscore ongoing and intensive herbicide application, leading to cumulative contamination and potential ecological risks. These findings highlight the need for more stringent monitoring, responsible herbicide management, and consideration of alternative weed control strategies to mitigate long-term impacts on soil health and the broader environment.

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INNOVATIVE BIOFERTILIZATION STRATEGIES FOR MITIGATING EMERGING CONTAMINANTS IN SUSTAINABLE AGRICULTURE

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Climate change, biodiversity loss, and increasing environmental pollution constitute a “triple planetary crisis,” demanding innovative and sustainable approaches across all sectors, particularly food production and agriculture. The increasing demand from consumers for safe, chemical-free agricultural products, including those free from pesticide residues and other pollutants, further drives the need for alternative farming practices. While the extensive application of fertilizers and agrochemicals has historically enabled high yields, it poses significant risks to human health, including farmers, and the environment. Transitioning from conventional intensive agriculture to sustainable organic practices requires the implementation of green solutions and the active transfer of knowledge from research and development to end users.

In this context, the present study investigated the effects of *Bacillus licheniformis* and *Bacillus safensis* on tomato (*Solanum lycopersicum*) growth cultivated on the medium (agar) contaminated with selected pharmaceutical active compounds (PhACs) and pesticides, as well as their potential to mitigate the uptake of contaminants of emerging concern (CECs). Tomato plants were initially grown on CEC-contaminated media for 14 days, followed by bacterial treatment, with cultivation continuing for an additional 10 days. Subsequently, an optimized QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) extraction protocol was applied to isolate selected CECs from the medium, roots, and stems, with extracts analyzed using ultra-high-performance liquid chromatography coupled to tandem mass spectrometry (UHPLC-MS/MS). The results demonstrated that the presence of selected CECs did not significantly affect stem biomass. However, treatment with *B. safensis* significantly increased root biomass, highlighting its potential for plant growth promotion. Differential accumulation patterns were observed for the tested CECs: phosphamidone, imazalil, furosemide, and losartan predominantly remained in the medium; methidation, linuron, sotalol, and salbutamol accumulated in roots; whereas carbofuran, dimethoate, carbamazepine, and propranolol were enriched in stems. Notably, foliar treatment reduced the uptake of certain compounds, including omethoate and ethoprophos, indicating an effective mitigation strategy.

These findings underscore the potential of *Bacillus*-based biofertilization/biofortification technologies to enhance plant growth while reducing CEC accumulation in edible tissues. The study provides a framework for developing sustainable agricultural practices that integrate microbial interventions to mitigate environmental contamination and protect food quality.

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ADDITION OF ENCAPSULATED *LACTOBACILLUS HILGARDII* IN PEA PROTEIN FOR OBTAINING KOMBUCHA BEVERAGE WITH PROBIOTIC PROPERTIES

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Abstract

Kombucha is a traditional beverage, which is usually prepared by fermenting sweetened black tea using a symbiotic consortium of acetic acid bacteria (AAB) and yeast. Kombucha exhibits several functional properties such as antioxidant, antimicrobial, anticancer, etc. However, its probiotic potential is limited due to low and variable concentrations of lactic acid bacteria (LAB) and their number most often does not reach the specified criteria. LAB should be able to survive sometimes harsh conditions during fermentation, storage and passing through the gastrointestinal tract, to exhibit health benefits. Several methods of microencapsulation of probiotic microorganisms are widely used to improve their viability. The aim of this work was to enhance the probiotic properties of kombucha beverage by incorporating encapsulated *Lactobacillus hilgardii* into the fermentation system. The probiotic culture was encapsulated in pea protein by lyophilization method and added at the beginning of kombucha fermentation. Encapsulation in pea protein protected the cells under acidic and oxidative conditions, enabling their survival throughout the process. Obtained results indicated a slightly higher titratable acidity in samples enriched with encapsulated *L. hilgardii* compared to the control. The number of viable LAB remained stable during fermentation, with 7.28 log CFU/mL on the final day, exceeding the recommended minimum level for probiotic products defined as 6-7 log CFU/mL. The growth of native yeasts and acetic acid bacteria was not negatively affected. These findings suggest that pea protein-based encapsulation is a promising strategy for the development of kombucha with improved probiotic properties.

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VALUE-ADDED UTILIZATION OF OAT PROCESSING RESIDUES VIA *RHIZOMUCOR MIEHEI*-BASED ENZYMATIC TREATMENT

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Abstract

The utilization of oat grain has shown an increasing trend in recent years, due to its favorable nutritional properties. However, large amounts of hull are generated during the processing, which are not suitable for human consumption. Nevertheless, oat hull contains a wide variety of bioactive compounds, for example vitamins, dietary fibers and phenolic compounds [1-3]. Phenolics can exert antioxidant, antimicrobial and anti-inflammatory properties, however majority of these compounds occur in carbohydrate-ester and carbohydrate-glycoside forms, which decreases their bioavailability [4-5]. Traditional solvent-based extraction methods can be harmful to the environment, therefore the development and testing of eco-friendly approaches have become a key research focus in recent years [6]. Extracellular hydrolases (cellulases, esterases) produced by *Mucoromycota* fungi [7], for instance, can be well-utilized for such phenolics extraction. In this study an enzyme-assisted extraction approach using the enzyme cocktail with cellulolytic and esterolytic properties from the *Mucoromycota Rhizomucor miehei* was applied to liberate phenolic compounds from the hull of a black-hulled oat cultivar. The enzyme cocktail was produced in a wheat-bran based solid state fermentation system and partially purified by gel filtration prior to treatments. Relevant enzyme activities of the *R. miehei* cocktail were also determined. During enzyme-assisted extraction a mass of 1 g grounded oat hull was treated with 10 mL of enzyme cocktail, and the mixtures were incubated for 7 hours at 50 °C, under constant stirring at 130 rpm. Samples were taken at predefined intervals (0, 1, 3, 5 and 7 hours), then total phenolic content (TPC), total flavonoid content (TFC) and antioxidant activity measurements (e.g., radical scavenging and metal ion reducing capacities) were carried out. Results indicated that the enzyme treatment had a positive effect on both free phenolic and flavonoid yields, moreover the antioxidant activity generally increased in parallel with the TPC and TFC. The highest values were detected in samples collected during the later stages of the treatment, indicating that a longer incubation time is necessary to achieve higher bioactivity. In conclusion, treatment with enzymatic cocktail of *R. miehei* had a positive effect on the liberation of bioactive phenolic compound from pigmented oat hull.

Acknowledgements

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