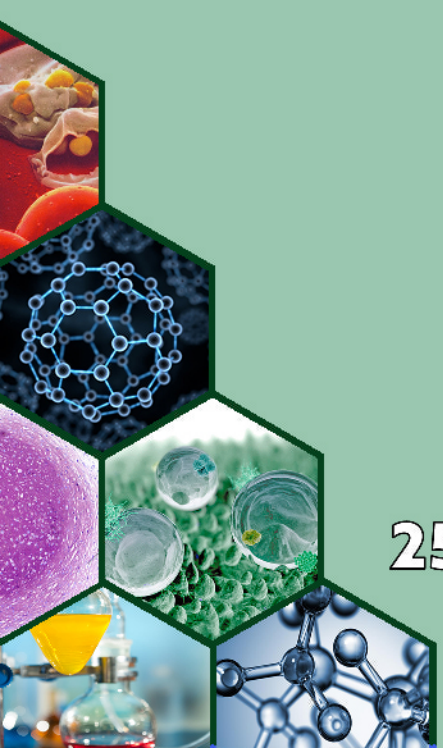
Serbian Chemical Society
Serbian Young Chemists' Club

11th Conference
of the Young Chemists of Serbia
Book of Abstracts



Kragujevac
25th OCTOBER 2025

11th Conference of Young Chemists of Serbia

Book of Abstracts

25th October 2025

University of Kragujevac – Faculty of Science

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	CB OP 01 – Andrija Gigić University of Kragujevac – Faculty of Science, Kragujevac, Serbia *"The effect of plant extracts, L. salicaria and S. pratensis on the interaction between copper(II) complexes and biomolecules"* **DCS OP 01 – Dunja Pupavac** Innovative Centre of the Faculty of Chemistry, Ltd., Belgrade, Serbia *"Synthesis and photochemical characterization of bridgehead nitrogen heterocyclic azobenzene photoswitches"* **EA OP 01 – Dragana Žmukić** University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia "*Extraction of polyhydoxyalkanoates from sludge using non-invasive surfactants*" **EA OP 02 – Marija Kuč** University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia "*Optimization and validation of the in-house procedure for the determination of bisphenol A in water: the importance of sample preparation*" **PCC OP 01 – Katarina Ćeranić** Innovative Centre of the Faculty of Chemistry, Ltd., Belgrade, Serbia *"How does coordination and the formation of the cation-π interaction affect the aromaticity of the benzene ring?"*

	PCC OP 02 – Zaharije Bošković University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia *"Alkaline electrolyzer with asymmetric electrolytes and nickel electrodes modified by spontaneous galvanic replacement"*
	PCC OP 03 – Andrej Dedić University of Belgrade – Faculty of Chemistry, Belgrade, Serbia *"Strong anion-π interactions between oxyanions and organic aromatic compounds – a DFT study"*
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	EA OP 03 – Lea Plavšin University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia "*Influence of current intensity on the efficiency of electrochemical removal of vinyl chloride*"
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	SCFM OP 01 – Tijana Vlašković University of Priština in Kosovska Mitrovica – Faculty of Sciences and Mathematics, Kosovska Mitrovica, Serbia *"Investigation of the obtaining method of $Ca_{0.9}Er_{0.1}MnO_3$ nanopowders applying the hydrazine nitrate procedure (HNP)"*
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All scientific contributions are divided into the following categories:

Chemistry and Society (CS)

Chemistry meets Biology (CB)

Developments in Chemical Synthesis (DCS)

Environmental Awareness (EA)

Physical and Computational Chemistry (PCC)

Phytochemistry and Food Chemistry (PFC)

Solution Chemistry and Chemical Equilibrium (SCCE)

Supramolecular Chemistry and Functional Materials (SCFM)

POSTER NUMBER is the last part of the contrubition code, e.g. XY PP 15.

VENUE:

- Lectures and oral presentations will take place at the **large amphitheater (A-II-1)** on the second floor, Faculty of Science, University of Kragujevac (address: Radoja Domanovića 12, Kragujevac).
- The Poster sessions will take place in the Faculty ceremonial hall **on the ground** floor.
- The lunch will take place in the Institute of Physics building.

Plenary Lecture

PL OP 01

Metal complexes as potential drugs for combating antimicrobial resistance

Tina P. Andrejević

University of Kragujevac – Faculty of Science, Kragujevac, Serbia

The increasing emergence of bacterial and fungal strains resistant to clinically used antimicrobial drugs poses a serious threat to global public health and a major challenge to the effective treatment of infectious diseases. This issue has prompted extensive research efforts focused on the synthesis of novel compounds with potential antimicrobial properties to combat the growing threat of drug-resistant infections [1]. The long-standing use of various metal-based compounds in treating numerous diseases has garnered attention for these compounds, highlighting their significant therapeutic potential. The vast diversity of metals, ligand types, and geometry of metal complexes make these compounds highly valuable for drug development, especially as potential new antimicrobial agents. In addition, coordination of organic ligands to metal ions leads to the formation of coordination compounds of various geometries. Moreover, metal complexes may have various mechanisms of action, including ligand exchange or release, redox activation, catalytic generation of reactive oxygen species (ROS), enzyme inhibition, and interactions with biomolecules such as DNA and proteins [2]. Therefore, it is crucial to design strategies for the development of new coordination compounds to limit the emergence and spread of antimicrobial resistance and improve their effectiveness against a broad spectrum of microorganisms.

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Acknowledgments

The study was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-136/2025-03/200122).

Invited Lectures

IL OP 01

Molecularly imprinted polymers as drug delivery systems

Miloš Pešić[1], Mladen Đurđević[1,2], Aleksa Vulićević[1], Uroš Marušić[1], Aleksandar Radovanović[1], Tatjana Verbić[1].

[1] *University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*

[2] *University of Belgrade – Institute of Chemistry, Technology, and Metallurgy, Belgrade, Serbia*

Molecularly imprinted polymers (MIPs) are functional materials with tailor-made binding sites selective towards the template, a molecule present during polymerization but not engaged in the process of polymer formation. Upon polymerization and template removal by extraction, the MIP has binding sites selective for template binding. These types of polymers can be used in various fields of application, such as solid-phase extraction, chromatography, catalysis, chiral separation, and polymeric receptors etc. One of the important areas of application is as drug delivery systems (DDS). MIPs can be prepared as a stimulus-responsive system, which is suitable for application in drug delivery. MIPs have shown potential for dermal, anticancer, ophthalmic, and other therapeutic areas. Release of the template should be monitored not only in the buffers, but also in the simulations of gastric and intestinal fluids in fasted and fed states to obtain more relevant data. In this work, MIPs for donepezil (Alzheimer's therapy) and furosemide (diuretic) were developed, and template release was evaluated in simulated intestinal fluids. The results highlight the potential of MIPs as DDS.

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1. Z. Liu, Y Huang, Y. Yang, Molecularly Imprinted Polymers as Advanced Drug Delivery Systems, Springer, **2021**.
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Acknowledgments

This research has been financially supported by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Contract No. 451–03–136/2025–03/200168 and 451–03–136/2025–03/200026).

IL OP 02

Synthesis of (–)-Goniofufurone Analogues: New Directions in Biological Activity Studies

Slađana Stanisavljević, Bojana Srećo Zelenović
University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia

Natural products and their derivatives represent an important starting point for the discovery of new drugs due to their structural diversity and pronounced biological activities.

Natural (+)-goniofufurone, isolated from the plant *Goniothalamus giganteus*, as well as its enantiomer (–)-goniofufurone, are well known for their cytotoxic activity.[1,2] However, other biological activities of these molecules, as well as the mechanism of their cytotoxic action, have not yet been investigated. In this study, new analogues of (–)-goniofufurone were synthesized, and the synthesis of divergent intermediates was optimized starting from L-xylose as a suitable chiral precursor. The cytotoxicity of the obtained compounds was evaluated using the MTT assay, while 3D-QSAR analysis provided insight into the influence of 3D conformation on activity against the K562 cell line. Based on the proposed target hypothesis, *in silico* studies were performed for selected analogues and PKCα, and the *in vitro* enzyme activity was investigated by ELISA assay. In addition, the effects of the compounds on cell cycle distribution, mitochondrial membrane potential, ROS generation, and induction of apoptosis/necrosis in K562 cells were analyzed.

The obtained results provide preliminary evidence of the pharmacological potential of the newly synthesized goniofufurone analogues, representing an initial step toward elucidating their mechanism of action and offering guidance for future investigations.

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Teaching Workshop

TW OP 01

Augmented reality and virtual reality in visualization of chemistry content

Jasna M. Adamov
University of Novi Sad – Faculty of Natural Sciences, Novi Sad, Serbia

Chemical particles are too small to be seen even under the most powerful microscope, and that makes chemistry concepts complex, abstract, and difficult to understand. Such concepts are: atomic and molecular structure, hybridization, the nature of chemical bonding, mechanisms of chemical reactions, etc. To explain them in textbooks and show them on paper or a computer screen, chemistry teachers use different two-dimensional visual representations. Students are required to create 3D mental pictures from them and to spatially manipulate them, so they need a well-developed set of visual skills. According to Wu and Shah (2004), most chemistry students are visual learners and need visual aids that make abstract chemical principles concrete and easier to grasp. That is why at the Chemistry Department of the University of Novi Sad, modern educational technology (augmented reality – AR, and virtual reality - VR) is used as a powerful tool for both teachers and students in overcoming difficulties with visualization of chemical models (Fig. 1). Using cell phones and QR codes students can place 3D models of atoms and molecules anywhere and see them from any angle. Holograms can be used to see the models of atoms, molecules, or orbitals, but also to represent the dynamics of chemical processes, such as bond formation, the change of configuration of organic molecules during substitution and addition, or to determine optical isomerism in molecules. When using VR goggles students are completely immersed into the 3D surroundings: they hold and move atomic and molecular models, or perform virtual chemical experiments. They also attend virtual tours, "see" technological processes in industrial plants, meet and talk to famous scientists and learn about their life and discoveries, or they visit thematic museums. Digital virtual escape rooms are used for gamification of learning, both in learning and reviewing chemical content, thus making studying chemistry more interesting and motivating.).

Figure 1. AR and VR in chemistry education.

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Oral Presentations

CB OP 01

The effect of plant extracts, *L. salicaria* and *S. pratensis* on the interaction between copper(II) complexes and biomolecules

Andrija D. Gigić[1], Ana S. Kesić[2], Jovana P. Bugarinović[1], Nikola Z. Srećković[1], Vladimir B. Mihailović[1], Jovana V. Bogojeski[1]

[1] *University of Kragujevac – Faculty of Science, Kragujevac, Serbia*

[2] *University of Kragujevac – Institute for Information Technologies Kragujevac, Kragujevac, Serbia*

Ferrocene derivatives have previously demonstrated a wide range of antifungal, antibacterial and anticancer activities [1]. Considering this, two copper(II) complexes were synthesized: one containing an amine ligand in a 1:1 ratio (Cu1), and the other incorporating an imine ligand in a 1:2 ratio (Cu2). These complexes were characterized using various spectroscopic methods. Their interactions with biomolecules were subsequently investigated. To potentially enhance their biological activity, the synergistic effects of the complexes in the presence of extracts from *Lythrum salicaria* and *Salvia pratensis* were examined. Extracts obtained from the aerial parts and roots of *L. salivaria* have previously been reported to display significant antimicrobial activity [2].

We investigated the binding affinity of these complexes toward calf thymus DNA (ct-DNA) and human serum albumin (HSA) in the presence of plant extracts, using fluorescence emission spectroscopy. The results indicated that the binding constants of the complexes increased upon addition of the extracts.

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Acknowledgments

The author, Andrija Gigić, gratefully acknowledges the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia through a scholarship grant.

CB OP 02

Cytotoxic and redox effects of curare on microglial cells

Ivona D. Ivanović, Đura J. Nakarada, Miloš D. Mojović
University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia

Curare is a plant-derived neurotoxin traditionally employed by South American tribes as a paralyzing agent [1]. Its action arises from competitive inhibition of acetylcholine (ACh) at nicotinic acetylcholine receptors (nAChRs), which prevents ion channel opening, membrane depolarization and subsequent muscle contraction [2]. In this study, we investigated the cytotoxicity and redox activity of curare on microglial cells, key mediators of immune defense in the central nervous system. Cells (Fig. 1) were thawed, cultured and exposed to a range of curare concentrations (0.1–100%). Cell viability was assessed using the MTT assay. A clear dose-dependent effect was observed: high concentrations (100% and 50%) caused near-complete cell death, whereas low concentrations (1% and 0.1%) maintained viability comparable to controls (98–100%). These results indicate that curare exerts pronounced toxicity only at elevated levels, with minimal effects at lower doses.

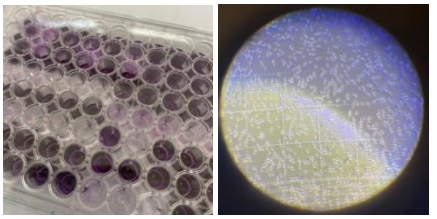

Figure 1. Cell viability assessed by MTT assay (left) and representative microscopic image (magnification 40×) of microglial cells (right).

Our findings highlight the concentration-dependent nature of curare's cytotoxic and redox properties, underlining the need to distinguish between its toxicological risks and potential pharmacological applications.

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Acknowledgments

This study funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-136/2025-03/200146 and 451-03-137/2025-03/200146).

DCS OP 01

Synthesis and photochemical characterization of bridgehead nitrogen heterocyclic azobenzene photoswitches

Dunja Pupavac[1], Andrea M. Nikolić[2], John-Paul Webster[3], Boban Anđelković[2], Timothy R. Newhouse[3] and Igor M. Opsenica[2]

[1]*Innovative Centre of the Faculty of Chemistry, Ltd., Belgrade, Serbia*
[2]*University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*
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Azobenzenes are among the most widely used molecular photoswitches, with application across different chemical fields. Their broad applicability stems from their photochromic properties, which depend on the substitution pattern on the azo-group.[1] Recent advances in molecular design show that replacing one or both phenyl rings with heteroaromatic systems is an effective strategy for accessing compounds with enhanced photoswitching properties and greater structural diversity.[2] This study introduces a new class of heteroaryl azobenzenes featuring privileged structures – pyrazolo[1,5-*a*]pyrimidine and 1,2,4-triazolo[1,5-*a*]pyrimidine, along with their synthesis and bidirectional photoisomerization. Experimentally obtained λ_{max} values of synthesized compounds were utilized for *in silico* prediction of the photochromic properties for the theoretical library of novel compounds. Three promising candidates from the library were synthetized and systematically characterized. Their photochemical behavior confirmed predicted red-shifted λ_{max} values.

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Acknowledgments

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EA OP 01

Extraction of polyhydoxyalkanoates from sludge using non-invasive surfactants

Dragana S. Žmukić[1], Anita S. Leovac Maćerak[1], Tamara D. Erceg[2], Sanja M. Rackov[2]
[1] *University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*
[2] *University of Novi Sad - Faculty of Technology, Novi Sad, Serbia*

Polyhydroxyalkanoates (PHAs) are polymers synthesized by microorganisms that accumulate glycogen and phosphate as intracellular reserves of carbon and energy in conditions of excess carbon [1]. PHAs are biodegradable polyesters whose properties can be compared with those of conventionally used plastics. Sludge, which is produced as a by-product in the wastewater treatment plant, is an organic substrate that contains microorganisms that accumulate PHAs. In this experiment, digested sludge was used as a source of PHA, and chloroform was used as a solvent. In the extraction, surfactants have the role of dissolving all non-PHA cell masses, in order to obtain a purer biopolymer. The effect of two surfactants Tween 80 and Glucopone 600 CS UP was monitored. Tween 80 (polyethylene sorbitol ester) is a non-ionic surfactant that has been shown to be effective in the extraction of biopolymers. Glucopone 600 CS UP (alkyl - polyglucoside) is a non-ionic, biodegradable surfactant. Both surfactants are less invasive, which makes the PHA extraction process more environmentally friendly. Polymer detection was performed by FT-IR analysis. The obtained FT-IR results were compared with the results of commercial PHA. In the sample with surfactant Glucopone 600 CS UP, FT-IR analysis showed vibrational stretching of the $-CH_2$ and $-CH_3$ groups at 3000-2800 cm^{-1}, which does not clearly indicate the presence of PHA. The peak corresponding to the ester carbonyl (C=O) group did not appear in this case. In the sample with surfactant Tween 80, with the peak corresponding to the ester carbonyl (C=O) stretching in the 1720 cm^{-1}, which confirms the presence of PHA. The vibrating mode of $-CH_2$ groups at 1455 cm^{1}. In our study, the surfactant Tween 80 proved to be more effective according to FT-IR analysis, while for the surfactant Glucopone 600 CS UP it is necessary to further optimize the extraction conditions.

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Acknowledgments

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-137/2025-03/ 200125 and 451-03-136/2025-03/ 200125).

EA OP 02

Optimization and validation of the in-house procedure for the determination of bisphenol A in water: the importance of sample preparation

Marija Z. Kuč, Tijana M. Marjanović Srebro, Tajana M. Simetić, Jelena J. Molnar Jazić, Jasmina R. Agbaba
University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia

Bisphenols, such as bisphenol A (BPA) and bisphenol S (BPS), are significant endocrine disruptors that are increasingly being detected in aquatic systems. The production, use, and disposal of materials containing BPA cause the release of this compound into the environment [1]. Due to their polarity, their direct determination by gas chromatography-mass spectrometry is limited, requiring chemical derivatization to increase the volatility and stability of the analyte. In this work, the effect of sample volume and solvent on the extraction efficiency of bisphenol A from the aqueous phase using the liquid-liquid method was investigated. Experiments were performed using hexane as the solvent and acetyl anhydride as the derivatization reagent. The results showed that a higher solvent volume with a higher water volume leads to high extraction efficiency, while a decrease in the volume results in lower efficiency due to the limited extraction capacity of the solvent. Method performance was evaluated by determining the limits of detection and quantification, linearity, method trueness, and precision. Trueness was expressed as recovery (86%), while method repeatability ranged from 1,08% to 3,26%, and instrumental repeatability from 0,55% to 2,30%. The optimized conditions resulted in an increase in signal intensity and improved chromatographic stability of BPA in the GC/MS analysis, allowing for lower detection and quantification limits compared to the non-derivatized forms.

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EA OP 03

Influence of current intensity on the efficiency of electrochemical removal of vinyl chloride

Lea P. Plavšin, Nataša S. Duduković, Tamara B. Apostolović, Jasmina R. Agbaba
University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia

Vinyl chloride is a toxic and persistent chlorinated compound that poses a significant ecotoxicological challenge due to its environmental accumulation and long-term toxicity. It frequently contaminates groundwater and surface waters as a result of industrial activities, leaching from waste disposal sites, and as a degradation product of other chlorinated solvents such as trichloroethylene and tetrachloroethylene. Once released into aquatic systems, VC exhibits high mobility and volatility, enabling its migration through soil into groundwater, where it can persist under anaerobic conditions for extended periods of time. Its presence in drinking water sources is particularly alarming due to its proven carcinogenicity and the associated risks to human health, while its toxicity also threatens aquatic organisms and overall ecosystem stability.

The removal of vinyl chloride from contaminated waters requires efficient and sustainable technologies, with electrochemical treatments gaining increasing attention because of their potential for rapid pollutant degradation. In this study, the influence of current intensity on the efficiency of electrochemical degradation of vinyl chloride in a synthetic water matrix was investigated. The experiments were conducted using titanium cathodes at currents greater than 40 mA. The results demonstrate that the electrochemical treatment achieved a high efficiency of more than 95% under the applied conditions. Treatment efficiency was consistently high, confirming that electrochemical treatment represents a promising, rapid, and energy-efficient method for removing vinyl chloride from water.

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PCC OP 01

How does coordination and the formation of the cation-π interaction affect the aromaticity of the benzene ring?

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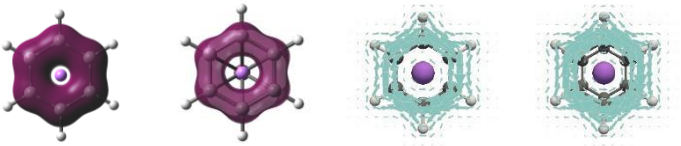
Benzene within the sandwich compounds was shown to form significantly stronger cation-π interactions than uncoordinated benzene [1]. In this work, the effect of coordination and the formation of cation-π iteractions on the aromaticity of the benzene ring was studied using two electron delocalization aromaticity indexes – Electron Density of Delocalized Bonds (EDDB) and Multi-Center Index (MCI), along with calculations of Magnetically Induced Current Densities (MICD). Studied cation-π systems included benzene, bis(benzene)chromium, bis(benzene)molybdenum, and bis(benzene)tungsten, as well as alkali (Li^+, Na^+, K^+) and alkaline earth cations (Be^{2+}, Mg^{2+}, Ca^{2+}). For the investigated systems, electronic delocalization indices (MCI and EDDB) are consistent with the trends observed in bond current strengths. In accordance with the differences in the strength of cation–π interactions between uncoordinated benzene and sandwich complexes, distinct effects on the aromaticity of the benzene units are observed. In complexes containing uncoordinated benzene, the interaction with cations leads to a reduction of aromatic character, whereas in sandwich complexes, cations enhance the aromatic nature of the benzene unit. These results highlight the dual role of cation–π interactions in modulating aromaticity, depending on the structural context of the benzene unit.



(a) (b) (c) (d)

Figure 1. EDDB(r) isosurfaces and current density maps for systems: (a,c) Li^+-benzene and (b,d) Li^+-bis(benzene)chromium, calculated at the B3LYP-D3/def2-TZVP level of theory.

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PCC OP 02

Alkaline electrolyzer with asymmetric electrolytes and nickel electrodes modified by spontaneous galvanic replacement

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In the presented research, we developed an alkaline electrolyzer that allows independent optimization of anodic and cathodic operating conditions by employing two distinct electrolyte environments, along with galvanically modified nickel electrodes decorated with noble metals, platinum on the cathode and rhodium on the anode. The electrolyzer is constructed so that the anode and cathode compartments contain different electrolytes, separated by an ion-permeable but molecule-impermeable membrane. This configuration enables the precise adjustment of conditions for the individual half-reactions, hydrogen evolution (HER), and oxygen evolution (OER), thereby improving the overall energy efficiency of the process [1]. Nickel was used as the base electrode for its stability in alkaline solutions and relatively low price. At the same time, thin galvanically deposited layers of noble metals lowered overpotentials, enhanced catalytic activity, and minimized their usage compared to bulk electrodes. Compared to conventional alkaline electrolyzers, this system offers improvements in energy efficiency, catalyst durability, and operational flexibility. Key advantages include the absence of adhesives, binders, or high-temperature treatments, as galvanic deposition provides a rapid modification method (treatment time under 5 minutes) using only dilute noble-metal solutions. Additionally, the electrodes are immediately ready for use after preparation.

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PCC OP 03

Strong anion-π interactions between oxyanions and organic aromatic compounds – a DFT study

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Anion-π interactions have great biological significance, from protein structure stability and folding mechanisms to enzyme functions that rely on these interactions. Also, anion-π interactions have found applications in many fields, especially in catalysis and organic electronics. [1] In this work, we have studied anion-π interactions of oxyanions – chlorate, perchlorate, nitrite, nitrate, sulfite and sulfate, with electron-deficient aromatic rings – hexafluorobenzene, trifluorobenzene, trifluorotriazine, triazine and isocyanuric acid (Fig. 1). The anion-π systems were optimized in Gaussian 09 at the B3PW91-D3/def2-TZVP level of theory, with subsequent calculations of interaction energies. To study the nature of these interactions, an ETS-NOCV energy decomposition of interaction energies was performed using the ORCA 6.1.0 program.

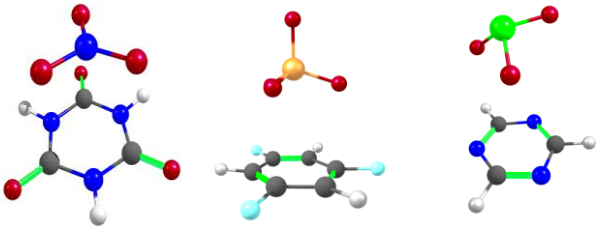

Figure 1. Anion-π interactions in isocyanuric acid/nitrate, trifluorobenzene/sulfate and triazine/perchlorate systems

The strongest anion-π interactions were observed for isocyanuric acid, particularly the one with sulfate (-52.11 kcal/mol). However, not all systems exhibited anion-π interactions as the strongest; addition of anion to the ring occurred in several systems, as well as the formation of hydrogen bonds. The energy decomposition analysis showed that the dominant contribution in anion-π interactions comes from electrostatic component, making them different in nature from cation-π interactions, which are dominated by polarization. [2]

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PCC OP 04

Tailoring carbon paste electrodes with $Ho_2Mo_4O_{15}$ nanoparticles for sensitive and selective Paracetamol sensing

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Paracetamol (PAR) or acetaminophen is an efficient pharmacological medication that reduces fever and relieves pain. For a successful impact, the therapeutic dose of paracetamol ranges from 10 to 20 μg/mL (or 66 to 132 μmol/L) [1]. Overuse of PAR can cause the accumulation of toxic metabolites, leading to hepatotoxicity, nephrotoxicity, skin rashes, inflammation of the pancreas, and liver and kidney problems [2]. A small amount of undecomposed PAR stays in human excretion after using a medication, which can be later found in water sources and become a drug pollutant. Following that, PAR has been detected in different water bodies, such as rivers, lakes, pond water, and drinking water.

Holmium-tetramolybdate nanoparticles have been employed for the first time to modify carbon paste electrodes, leading to the creation of an electrochemical sensor for the detection of PAR. These nanoparticles were synthesized using a simple, one-pot, organic solvent-free, hydrothermal method and were characterized both morphologically and electrochemically. The resulting material demonstrated remarkable electrocatalytic performance, attributed to its unique size and morphology. The developed sensor was subsequently utilized to establish a sensing platform for PAR detection. Under optimized square wave voltammetry (SWV) conditions, the sensor exhibited a wide linear range of 3-300 μM, a low limit of detection of 0.314 μM, and a sensitivity of 0.239 μA μM^{-1} cm^{-2}. These findings, along with satisfactory sensitivity, stability, and repeatability, underscore the potential of this sensor for routine paracetamol analysis. This study effectively illustrates the enhancement of carbon paste electrodes through the integration of holmium-tetramolybdate nanoparticles in the advancement of electrochemical sensors.

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PCC OP 05

The crystal structure of new platinum(II) complex with *N*-benzylphenothiazine

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Phenothiazine derivatives are widely used in medicine, with their effects depending on the side chains attached to the nucleus. Both phenothiazine, its *N*-alkyl derivatives, and metal–phenothiazine complexes show notable biological activity. However, while many transition metal–phenothiazine complexes have been synthesized and characterized, crystal structure reports are still limited [1].

Here we report the crystal structure determination of a new Pt(II) complex with *N*-benzylphenothiazine (L), formulated as [PtLCl$_2$MeCN]. The complex crystallizes in the monoclinic $P2_1/c$ space group, with unit cell parameters: a = 11.82798(12) Å, b = 11.22721(13) Å, c = 16.18722(17) Å, β = 108.8336(11)°, V = 2034.50(4) Å^3, and Z = 4. The structure was refined with HAR to R_1 = 2.65% based on 4131 independent reflections and 298 parameters. The asymmetric unit consist of one Pt(II) atom, one ligand molecule, two chloride anions, and one acetonitrile molecule (Fig. 1). The Pt(II) ion is four-coordinated in a square-planar arrangement by one sulfur atom from the phenothiazine ring, two chloride anions, and one nitrogen atom from the acetonitrile molecule. The *N*-benzylphenothiazine acts as an *S*-monodentate ligand.

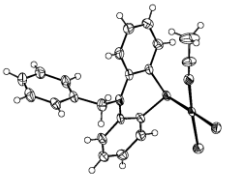

Figure 1. Molecular structure of [PtLCl$_2$MeCN] complex.

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PFC OP 01

Application of spherical coordinates for coding ternary solvent mixture in the optimisation of *Ganoderma resinaceum* extraction

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Mushrooms from the genus *Ganoderma* represent one of the most popular materials for studying the medicinal properties of fungi. Species *G. resinaceum*, while less popular than sister species *G.lucidum*, is still a goldmine of novel and potentially useful metabolites. Due to the complex array of compound classes in such material, complex solvent mixtures are needed to achieve the desired extract profile. A major obstacle in choosing a suitable solvent mixture is the optimisation of component ratios. Response surface methods, such as the Box-Behnken design (BBD), are widely employed to identify the optimal conditions for a desired outcome systematically [1]. Another important application involves determining the importance of each factor. Although specialised mixture-type designs may be employed, these designs preclude the incorporation of process parameters such as temperature, duration, and equipment power. Another problem is the exponential growth of experimental runs needed when adding more variables. In this work, the use of spherical coordinates [2] to code a ternary solvent mixture using two variables was described. This greatly reduced the number of experiments needed (about 35% less), saving time and resources. Within the framework of the BBD, process parameters such as extraction time and power were optimised in ultrasound-assisted extraction to identify the parameter combinations that maximise yield. The relative importance of each solvent in the mixture was also elucidated. To the best of our knowledge, this represents the first application of this methodology within the context of natural product chemistry involving medicinal mushrooms.

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SCFM OP 01

Investigation of the obtaining method of $Ca_{0.9}Er_{0.1}MnO_3$ nanopowders applying the hydrazine nitrate procedure (HNP)

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A $Ca_{0.9}Er_{0.1}MnO_3$ nanopowder of stoichiometric composition was obtained by combustion synthesis using the hydrazine nitrate procedure (HNP). Metal nitrate salts (Ca, Mn, Er) and hydrazine, which varied in different amounts, were mixed in an aqueous medium at room temperature. This procedure aims to determine the required hydrazine amount to control combustion in terms of releasing optimal fuel energy, as well as the amount that would complex the reactants present in the mixture. The voluminous powder obtained using the hydrazine nitrite procedure was then calcined for a 15-minute interval at three different temperatures (800, 900, and 1000 °C). Characterization of the obtained samples based on X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) gave results that unequivocally indicate that the amount of added hydrazine is crucial for the formation of single-phase $Ca_{0.9}Er_{0.1}MnO_3$ nanopowder. The possibility of incorporation of Er ions into position A of the perovskite structure was investigated by the X-ray method. The influence of Er on the unit cell volume of the perovskite compound, the occupation numbers, and the interatomic distance was analyzed using the Rietveld method. The importance of fuel dosing (hydrazine) in regulating the synthesis process and improving material properties was confirmed.

Acknowledgments

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Poster Presentations

Chemistry and Society (CS)

CS PP 01

Interest in chemistry and/or a good basis for studying: Students in Serbia on choosing a specialized grammar school track

Milica Raković, Filip Stašević, Jelena Đurđević Nikolić
University of Kragujevac - Faculty of Science, Kragujevac, Serbia

In the Republic of Serbia, only about one-quarter of students enroll in grammar schools after completing primary education. This situation poses complex challenges for society, as grammar schools are expected to serve as the primary pathway to higher education. Given that grammar school students often become key drivers of future societal development, it is essential to understand the reasons behind their decision to pursue this educational track. This issue gains additional importance in the context of STEM education. Although STEM disciplines are increasingly prominent in contemporary society, previous studies have highlighted a troubling decline in students' interest and engagement in these fields. Against this backdrop, the present study aimed to explore the factors that students themselves identify as influencing their decision to enroll in a specialized biology- and chemistry-focused grammar school track. The research was conducted on a sample of 55 grammar school students from two grammar schools in Kragujevac and Novi Sad. Responses to an open-ended question, in which students explained their reasons for choosing this specialized track, were analyzed using qualitative thematic analysis. The findings indicate that students' reasons can be grouped into three thematic categories: 1) interest in chemistry; 2) grammar school as preparation and a pathway to higher education; and 3) future professional orientation. These insights may inform the development of educational policies and career guidance practices in primary schools, providing students with more adequate support in making decisions about further education and offering a basis for future research on factors that shape educational choices.

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CS PP 02

Assessing the chemistry educational outcomes using PhET simulations: Analysis of primary school students' achievements in atomic structure

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Evaluating students' achievements is an important aspect of the educational process that, while seemingly straightforward, requires careful planning and implementation. Digital tools, particularly interactive simulations, have emerged as innovative methods for both teaching and assessing students' learning. PhET simulations, widely recognized for their accessibility and interactivity, offer built-in quiz features that provide immediate feedback and measurable data on student performance. This study investigated primary school students' chemistry educational outcomes on atomic structure using the Build an Atom simulation as an assessment tool. The sample included 57 seventh-grade students from a primary school in Kragujevac, Serbia. Students completed embedded quiz activities organized into three categories of five questions each, focused on identifying subatomic particles, determining atomic and mass numbers, predicting ion charges, and relating electron arrangement to an element's position in the periodic table. Correct responses were recorded and analyzed to evaluate students' conceptual understanding. Findings indicate that students demonstrated a satisfactory level of knowledge in atomic structure, though predicting ion charges emerged as the most common difficulty. These results suggest the need to improve students' understanding and refine instructional strategies, while highlighting that PhET simulations offer teachers a ready-to-use, interactive tool that facilitates assessment in an engaging and efficient way. Further research with a broader sample and additional outcomes is recommended to gain a more comprehensive view of students' chemistry achievements.

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CS PP 03

Perception vs. performance in chemical bonding concept among pre-service chemistry teachers: A case study at the Faculty of Science, University of Kragujevac

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University of Kragujevac - Faculty of Science, Kragujevac, Serbia

The development of effective strategies for teaching chemical bonding theory remains one of the central goals in chemistry education. For prospective chemistry teachers, a solid understanding of chemical bonding is essential not only for their own expertise but also for effectively conveying fundamental chemical principles to students. Mastery of this concept among students underpins comprehension of a range of topics relevant to real-world applications: physical and chemical properties of substances, chemical thermodynamics, and polymers. This study explored the alignment between self-perceived knowledge and actual understanding of chemical bonding among pre-service chemistry teachers at the Faculty of Science, University of Kragujevac. A total of 36 participants completed a short, five-item knowledge test, along with a five-item self-assessment scale measuring their confidence in understanding chemical bonding. The mean value of self-assessment scores was scaled to match the test range and compared with the actual test results, yielding a gap score. Based on this metric, participants were classified as overestimating, accurately estimating, or underestimating their knowledge. Scatter plot analysis with trendline inspection showed no meaningful linear relationship between self-perceived confidence and test performance ($R^2 \approx 0$), while distributional patterns indicated notable discrepancies, with several participants either overestimating or underestimating their competence. These findings highlight the importance of developing accurate self-assessment in teacher education, as the accuracy of self-assessment itself may influence the success of future teaching practice. Study limitations include the small sample size and the brevity of the test, which constrain the generalizability and depth of diagnostic conclusions.

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CS PP 04

Assessment of the effectiveness of using the Chemistry Cool application in 7th grade chemistry classes

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Modern chemistry education increasingly relies on innovative methods to enhance student engagement and facilitate deeper understanding of teaching contents. This study investigates the use of the mobile educational application Chemistry Cool (Fig. 1) in 7th-grade chemistry instruction, with a focus on student's perceptions of its effectiveness.
The research was conducted using an anonymous survey on a sample of 18 students. The questionnaire explored: students' ability to concentrate while using the application, their willingness to use the application in learning, perceived benefits in mastering the course material, and their achievements in learning outcomes using this method.
The results indicate that 84% of students reported improved concentration, 78% would choose to use the app voluntarily, 84% found it helpful for learning, and 75% felt confident in the knowledge gained. Interactivity, ease of use, and visual content were identified as key strengths of the application.

Figure 1. Chemistry Cool app icon.

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Chemistry meets Biology (CB)

CB PP 01

Biomimetic screening of the persistent pollutant PFOA to predict health outcomes

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Perfluorooctanoic acid (PFOA) is a perfluorinated carboxylic acid that belongs to the class of per- and polyfluoroalkyl substances (PFAS). The compound is globally present, very stable, frequently used, and as such has potential toxic effects on human health and the environment. The aim of this paper is to predict and understand the leading mechanisms of the biological behaviour of PFOA. The research combined various computational and mathematical models with experimental data to obtain the most important biomimetic profile, which is introduced under conditions that mimic the biological environment and as such indicates the behaviour of the tested molecules in the organism and the enviroment. The computational biomimetic profile is characterized through the prediction of compound biodistribution, clinical characteristics in relation to pharmacokinetics (OPERA-modeling), and its toxicological and ecotoxicological properties. Part of the experimental research included the application of a biomimetic chromatographic testing using an artificial membrane with immobilized phospholipids. This test successfully mimics the interaction of an experimental molecule with cell membrane phospholipids and consequently correlates with many physiologically based characteristics. The obtained results indicate high plasma concentrations of PFOA, as well as significant cardiotoxicity, nephrotoxicity and hepatotoxicity. Also, there is a risk of fetal malformation in pregnant women in accordance with high concentrations expected in the fetus' plasma, thyroid gland, kidneys, and arteries. The results show that the compound is preferentially absorbed from the upper parts of the small intestine, with a duration of 3-10 hours. Interaction with phospholipids correlates with lipophilic and toxicological characteristics of PFOA. The toxicity and ability of PFOA to bioaccumulate emphasize the need for control and caution when using this compound to reduce the harmful impact on human health. Furthermore, the successful application of biomimetic screening demonstrates their utility in the preliminary toxicological characterization of significant human health hazard molecules.

Acknowledgments

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CB PP 02

Ionic liquid-assisted investigation of Rh(III) complexes with biologically relevant ligands

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The limitations of platinum-based anticancer drugs, including high toxicity and resistance, have driven the search for alternative transition metal complexes with novel mechanisms of action [1]. Rh(III) complexes are particularly attractive due to their kinetic inertness, possible octahedral geometry, and potential for selective biomolecular interactions through ligand design [2]. In this study, Rh(III) complexes incorporating thiazole- and pyridine-based tridentate ligands N^2,N^6-bis(5-methylthiazol-2-yl)pyridine-2,6-dicarboxamide and N^2,N^6-di(benzo[d]thiazol-2-yl)pyridine-2,6-dicarboxamide were investigated. These rigid ligands provide stable coordination environments and opportunities for specific interactions with biomolecules. To address poor aqueous solubility, ionic liquids (ILs) were employed as cosolvents. Biocompatible ILs, particularly choline-based systems, enhanced solubility and stability, enabling comparative evaluation of ligand substitution kinetics and interactions with DNA and human serum albumin (HSA) in conventional and IL-containing media. DNA binding was examined using UV–Vis absorption and fluorescence spectroscopy, while HSA interactions were studied via fluorescence measurements. The results demonstrate that combining ligand design with IL-assisted solubilization can yield structurally robust Rh(III) complexes with potential for selective biomolecular targeting.

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CB PP 03

Development of bile acid-based compounds as dual NRF2 activators and FXR modulators

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Simultaneous targeting of the NRF2 and FXR pathways could hold the key to finding a cure to liver diseases, as these nuclear receptors regulate oxidative stress responses and bile acid metabolism, two processes tightly linked to hepatic inflammation and disease progression [1].
Key modifications included the introduction of enone moietie into the bile acid A ring, which is an essential feature for covalent interaction with Keap1 cysteine residues and subsequent NRF2 activation. Additionally, the introduction of a C7-ethylidene group, which is recognized as a pharmacophore for FXR antagonism, was accomplished via regioselective Wittig reaction. These structural modifications were guided by established structure–activity relations for 7-substituted bile acids, particularly by 7-ethylidene-lithocholic acid (7-ELCA) which is a potent FXR antagonist. The combination of targeted modifications within the steroidal framework is expected to afford compounds with a dual mechanism of action [1,2].

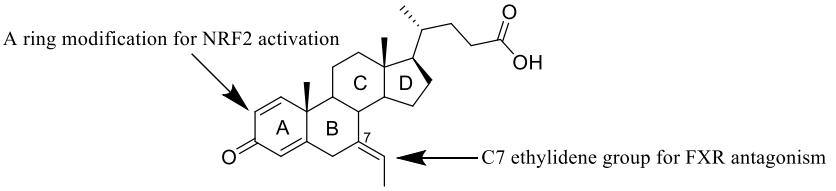

Figure 1. Example of a compound with NRF2 activating and FXR antagonistic pharmacophores

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CB PP 04

In vitro characterisation of gastrointestinal absorption of cinnamic acid

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Cinnamic acid, a naturally occurring phenolic compound, has been suggested as a potential agent in the treatment of obesity, hyperglycemia and prediabetes that stems from its insulin-mimetic and antidiabetic mechanisms of action. Cinnamic acid stimulates insulin secretion, mitigates glucose-induced damage due to hyperglycemia and prevents lipotoxic effects on pancreatic beta cells [1]. Permeability in the human gastrointestinal tract (GIT) influences the absorption of the tested molecule candidate. In this study, the permeability of cinnamic acid was assessed with the novel biomimetic barrier setup that mimics the passive absorption in the GIT in physiological conditions (temperature 37°C, phosphate buffer with pH value 7,4). The obtained apparent permeability coefficient $\log P_{app}$ (-6,3) is narrowly higher than the PAMPA $\log P_{app}$ (-6,5), the standard permeability assay for the passive absorption in the drug discovery process. However, the $\log P_{app}$ is lower than the $\log P_{app}$ in the Caco-2 assay (-4,7), which is used to simulate both passive and active absorption mechanisms [2]. *In silico* calculated physicochemical (logP, pKa, TPSA) and 3-dimensional solubility parameters indicate that cinnamic acid belongs to the group of moderately lipophilic and slightly water soluble compounds with the longest absorption time in the GIT and that the absorption occurs along the whole length of the GIT. The results point to the conclusion that the absorption of cinnamic acid likely occurs both through active and passive transport. Further studies are needed to optimize the delivery system for the use of cinnamic acid as a nutraceutical preparation.

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CB PP 05

Modeling NA-HILIC retention of CNS drugs: insights into molecular interactions and ADMET relevance

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The retention of 25 central nervous system (CNS)-active compounds was examined using non-aqueous hydrophilic interaction liquid chromatography (NA-HILIC) to clarify molecular determinants of retention and evaluate its potential for biomimetic profiling. Experiments were conducted on a Zorbax C18 column with acetonitrile/methanol mobile phases containing ammonium formate and formic acid, while systematically varying acetonitrile content. Pharmacokinetic/ADME and molecular descriptors were computed using ADMETlab 3.0, and retention factors (logk) were modeled against the acetonitrile fraction (φ) using linear and quadratic functions. Abraham descriptors highlighted polarity and hydrogen bonding as major contributors to retention, supported by dipolarity and van der Waals volume. Linear models generally provided the best description of retention trends, though quadratic terms captured additional complexity in specific cases. Correlations between model coefficients and ADME parameters were notable, particularly for distribution (VDss), P-glycoprotein substrate status, and CYP inhibition profiles (CYP2C19, CYP2C9). Correlations were also observed with nuclear receptor and stress-response pathways (AhR, ER-LBD, PPARγ, ARE, ATAD5, MMP), indicating partial alignment between chromatographic retention and biological interactions. Solubility (LogS) and respiratory toxicity endpoints showed balanced but opposite correlations, further underscoring the pharmacokinetic and toxicological relevance of the retention models. The NA-HILIC modeling captured key physicochemical properties of CNS-active drugs and showed moderate predictive value for pharmacokinetic and toxicological behavior. While promising as a biomimetic tool, further improvements are required to achieve translational applicability in drug discovery.

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CB PP 06

Synthesis, characterization, biomolecular interactions and anticancer potential of [$RuCl_2(\eta^6$-*p*-cymene)(bph-κ*N*)] complex

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Ruthenium(II) half-sandwich complexes are promising anticancer candidates with advantages over platimnum drugs. We synthesized (Fig. 1), and characterized [$RuCl_2(\eta^6$-*p*-cymene)(bph-κ*N*)] via NMR, FTIR, spectrofluorimetric titration, and DFT studies. Fluorescence quenching indicated spontaneous, hydrophobic-driven binding to HSA and ctDNA, with static quenching. Ethidium bromide displacement and molecular docking studies confirmed strong intercalative DNA binding. EPR spectroscopy demonstrated efficient scavenging of hydroxyl and ascorbyl radicals. Cytotoxicity assays against A375, MDA-MB-231, MIA PaCa-2, and SW480 cells revealed selective activity, with pancreatic and colorectal cells most sensitive. QTAIM analysis confirmed favorable metal–ligand bonding and electronic stabilization. Overall, Ru(II)-complex integrates structural stability, biomolecular interactions, antioxidant capacity, and selective cytotoxicity, highlighting its potential as a lead anticancer compound [1].

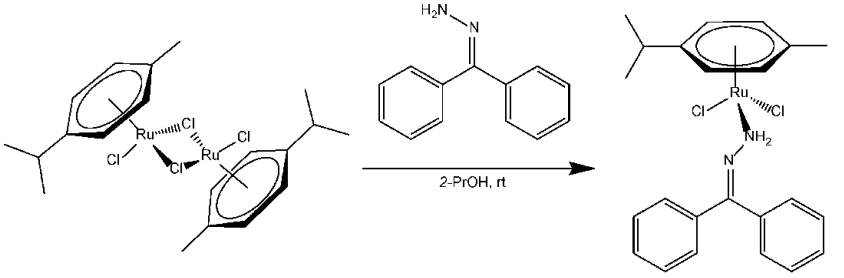

Figure 1. Synthesis of [$RuCl_2(\eta^6$-p-cymene)(bph-κN)].

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CB PP 07

Pd(II) complexes with anthracenyl Schiff bases as promising antimicrobial candidates

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Over the past two decades, numerous Schiff bases have been investigated and shown to possess antibacterial properties; however, their coordination to metals generally enhances this activity. Literature reports highlight that palladium-Schiff base complexes exhibit pronounced antimicrobial potential, positioning them as promising candidates for the development of antimicrobial metallodrugs [1].

Here, we present a series of four novel Schiff bases, one previously known in literature, and five newly synthesized Pd(II) complexes. All compounds were synthesized, fully characterized, and evaluated for their antimicrobial potential. Furthermore, the new ligands were obtained by condensing 9-anthracenecarboxaldehyde with various phenylenediamine derivatives. All ligands and complexes were characterized using NMR, IR spectroscopy, elemental analysis, and mass spectrometry, as well as molar conductivity measurements.

The antimicrobial activities of the synthesized compounds were tested *in vitro* against a representative set of microorganisms, including three Gram-positive bacteria and four Gram-negative bacteria. Streptomycin and chloramphenicol were employed as reference antibiotics to validate the assays and provide benchmarks for comparison. The **C2** complex showed remarkable potency across all tested bacterial species, with the following MIC values: *E. coli* (0.002 mg/mL), *S. enteritidis* (0.001 mg/mL), and *P. aeruginosa* 0.005 mg/mL), while also showing moderate antifungal activity against *C. albicans* (0.16 mg/mL).

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CB PP 08

Antimicrobial activity against *Staphylococcus* strains of "super essential oils", designed by means of Machine Learning algorithms

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The antibacterial activity of essential oils (EOs) has been intensively studied, generally revealing higher activity against Gram-positive (G+) than Gram-negative (G-) bacteria. Still, results are usually interpreted based on the EOs biological effects rather than their chemical composition, still implying that terpenes and their derivatives should be the bearers of EOs antibacterial features [1]. To outline the inner pharmacology, a dataset comprising 61 commercial EOs has been assessed against a palette of either (G+) or (G-) strains to define MIC values, subsequently submitting data to machine learning (ML) classification algorithms, including Support Vector Machines, Random Forest, Gradient Boosting, Decision Trees, and K-Nearest Neighbors, to generate Quantitative Composition-Activity Relationship models. Resulting Features Importance (FI) analysis identified key chemical components influencing EO activity: terpinen-4-ol, γ-terpinene, 1,8-cineole, α-pinene, terpinolene, β-pinene, and *p*-cymene.

Relying on the obtained Partial Dependence (PD) plots, 22 "super essential oils" mixtures were designed from the listed terpenes and determined of MIC against *Staphylococcus* (G+) strains, by means of a known resazurin-based protocol [2]. Most of the mixtures exerted remarkable clinical potential. The best antimicrobial activity (0.625%) was shown by a mixture with the following composition: terpinen-4-ol 51%, γ-terpinene 42% and terpinolene 7%. Cefalexin with an MIC value of 25 μmol/L was used as a positive control.

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CB PP 09

In silico exploration of caryophyllene binding modes to selected antibacterial protein targets in *Escherichia coli*

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Caryophyllene is a natural bicyclic sesquiterpene commonly found in the plant kingdom. This plant metabolite is of significant medicinal and pharmacological interest due to its diverse beneficial biological properties, including antibacterial activity [1,2]. In this work, the binding modes of caryophyllene to two *E. coli* proteins involved in fatty acid biosynthesis were assessed by molecular docking. The obtained results revealed significant binding affinities and favorable ligand - macromolecule interaction patterns. These findings suggest that caryophyllene possess the potential to interfere the fatty acid biosynthetic processes in *E. coli*, which could be employed for future design and development of antibacterial agents.

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CB PP 10

Anti-urease activity of *ortho*- and *para*-substituted cinnamoyl hydroxamic acids

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Urease is a nickel-dependent enzyme involved in the pathogenicity of *Helicobacter pylori* and *Proteus* spp., contributing to gastric ulcers and urinary stones. Hydroxamic acids inhibit urease by chelating its dinickel active site, making them promising therapeutic agents. Studies on cinnamoyl-hydroxamic acids show that substituent position and electronic properties significantly affect activity: *para*-position electron-withdrawing groups enhance inhibition by increasing β-carbon electrophilicity, aiding interaction with Cys residues and Ni^{2+} ions. *Meta*-substituents show weaker effects, while *ortho*-substituents remain unexplored [1].

Herein two pairs of *ortho*- and *para*-substituted cinnamoyl hydroxamic acids with electron-withdrawing groups (NO_2 and F) were synthesized and tested against Jack bean urease (Fig. 1). Derivatives **2o** and **1p** showed the strongest inhibition, surpassing the parent compound (**3**), while **2p** showed similar activity and **1o** was the least potent. These findings confirmed that both the electronic nature and positional orientation of the substituents significantly affect urease inhibition. The enhanced activity of derivative **2o** suggests that additional non-covalent interactions within the active site may contribute to potency.

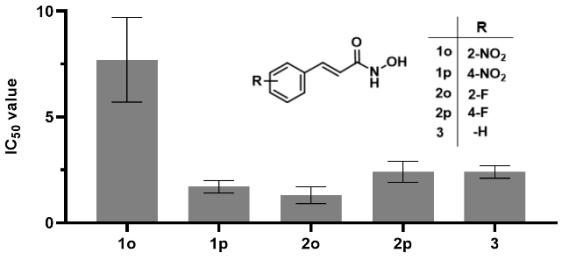

Figure 1. IC_{50} values of the tested cinnamoyl hydroxamic acids

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CB PP 11

Hands-on science: Formulating and assessing the efficacy of a propolis-infused hand sanitizing gel

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Hand hygiene plays a crucial role in preventing the transmission of infectious diseases, making hand disinfection an essential public health measure. Alcohol-based hand sanitizing gels are effective, accessible, and convenient tools for ensuring proper hand hygiene in everyday practice. The main goals of this study were to prepare a hand sanitizing gel with the addition of a natural antimicrobial substance, propolis, alongside ethanol as the primary disinfectant, and to evaluate its bactericidal properties. Propolis, a bee-derived resinous substance with antimicrobial and anti-inflammatory activity, was incorporated to enhance antimicrobial efficiency and reduce skin irritation. The gel was formulated with ethanol, glycerin (humectant), Carbomer 940 (thickening agent), triethanolamine (pH adjustment), water, ethanolic propolis extract, and tangerine essential oil for fragrance. The resulting gel was brownish-yellow, with a thick consistency and a pleasant smell of propolis and tangerine. Bactericidal activity was determined by contaminating glass coverslips with *S. aureus*, *S. enteritidis*, and *P. aeruginosa*, followed by treatment with gel for 1 and 3 minutes. After incubation of prepared coverslips in Mueller-Hinton broth for 48 h, bacterial growth was evaluated by OD_{650} measurements compared to an untreated control. Results showed significant bacterial reduction (3 minutes application), exceeding 80% for *S. enteritidis* and *P. aeruginosa*. A second experiment assessed bactericidal properties on Mueller-Hinton agar in Petri dishes, where four participants left fingerprints before using the gel and one minute after application. After 24 h of incubation at 37 °C, colony counts revealed that the gel reduced aerobic mesophilic bacteria by 94%. These findings confirm that the formulated gel is highly effective, while the presence of natural substances such as propolis may provide additional skin benefits beyond disinfection through their retention and bioactivity.

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CB PP 12

Characterization and antiradical activity of Vranac grape extracts using EPR and Orbitrap analysis

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Extracts from the grape variety Vranac were analyzed to evaluate their antiradical activity and chemical composition. Electron Paramagnetic Resonance (EPR) spectroscopy was used to assess the scavenging capacity of the extracts against DPPH, hydroxyl, and superoxide radicals. The chemical profiles were determined by Orbitrap mass spectrometry. Five different extract samples were prepared using supercritical CO_2 extraction with varying solvent compositions: (1) grape skin extract with 15% ethanol cosolvent, (2) grape skin and seed extract with 15% ethanol cosolvent, (3) grape skin extract without cosolvent, (4) liquid grape skin extract with 50% ethanol cosolvent, and (5) grape skin extract with 50% ethanol cosolvent. Additionally, a sixth sample was obtained via ultrasonic extraction in 50% ethanol.

EPR results showed the highest DPPH radical scavenging activity in sample 4 (53.77%), while samples 1 and 2 exhibited lower activities (32.41% and 15.79%, respectively). Hydroxyl radical scavenging ranged from 67.95% to 86.64%, with sample 4 again demonstrating the strongest activity. Superoxide radical scavenging was high across all samples (79.32% to 83.63%), with sample 4 showing the highest activity. Orbitrap analysis revealed that sample 4 was the richest in polyphenols, with major compounds including malvidin 3-O-glucoside, quercetin, kaempferol, and isorhamnetin. Other notable polyphenols such as catechin, epicatechin, procyanidins, and various anthocyanins were also identified, highlighting the complex phenolic composition of the extracts. These findings demonstrate that Vranac grape extracts possess significant antiradical activity and a diverse polyphenolic profile, which may contribute to their potential health benefits and applications in food and pharmaceutical industries.

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CB PP 13

Analysis of differential gene expression in Alzheimer's disease

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Alzheimer's disease (AD) is a neurodegenerative disorder that causes progressive loss of cognitive functions, and a growing number of studies point to the importance of the immune response in its pathogenesis [1]. In this research, data obtained by RNA sequencing of individual cell nuclei from the prefrontal cortex (10× Genomics v3; n=11 late stage AD, n=7 control) [2] were used in order to monitor the change in gene expression in specific cell types. Analysis of differential gene expression (DEG) indicated statistically significantly expressed genes in two cell types - microglia (MG) (32 DEG) and oligodendrocytes (ODC) (20 DEG). Then, GSEA (Gene Set Enrichment Analysis) was performed for statistically significant DEGs, which detects biological pathways affected by changes in gene expression. In microglia cells, two genes, HLA-B and CLEC5A, were statistically significantly differentially expressed and associated with the regulation of the immune response in Alzheimer's disease. Among the important genes are those involved in the production of heat shock proteins (HSP), which participate in antigen presentation. In oligodendrocyte cells, important immune response-related genes regulate the NF-κβ signaling pathway, linking pathogen signaling pathways and cellular responses to pathogen invasion. The obtained results can serve as a basis for further experimental research and help in understanding the pathogenesis and immune response in Alzheimer's disease.

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CB PP 14

In silico toxicity testing and docking study of 17-pyridin-2-yl estrane derivatives

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Due to their significant biological activity, steroid compounds are widely used in the treatment of various diseases. In our previous work [1], two novel steroidal compounds, 3-methoxy-17α-(pyridin-2-yl)estra-1,3,5(10)-trien-17β-ol (**1**) and 3-methoxy-17-(pyridin-2-yl)estra-1,3,5(10),16-tetraene (**2**) were synthesized (Fig. 1). Both compounds exhibited promising *in vitro* antiproliferative activity against MCF-7 (breast cancer) and HeLa (cervical cancer) cell lines, making them good candidated for futher biological testing. Due to this, *in silico* toxicity evaluations, target prediction and docking studies of these compounds were performed. Multiple online *in silico* tools predicted that these two compounds are less toxic than the reference compound abiraterone. Preliminary molecular docking analyses by AutoDock Vina suggested moderate binding of both of tested compounds to ligand-binding domains of human glucocorticoid and protegesterone receptors (~50% of estimated binding energy of positive controls for target receptors) and possible binding to aromatase, which support *in vitro* toxicity to MCF-7 (PR and aromatase) and HeLa cells (GR) and are consistent with target prediction studies.

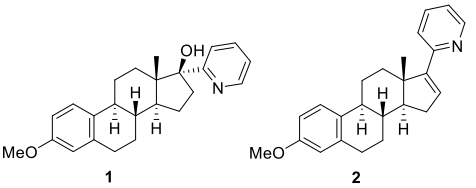

*Figure 1. Structure of compounds **1** and **2**.*

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CB PP 15

Synthesis of new aromatic steroid carbamates, their *in vitro* biological activity and *in silico* analysis

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Steroid hormones have a crucial role in the proliferation of hormone-dependent cancer cells, such as prostate and breast cancers. They manifest their physiological function by binding to steroid receptors, androgen (AR) and estrogen (ER). These receptors are highly expressed in most of hormone-dependent cancer cells, which makes them favorable targets for the development of new anticancer drugs [1]. Many synthetic drugs that are approved for cancer therapy are based on modified natural steroid molecules. Carbamate function, on the other hand, shows a wide range of biological effects. Because of the presence of three heteroatoms, it has the ability to form hydrogen bonds with amino acid residues in the active sites of enzymes and ligand-binding domains (LBD) of receptors [2]. For that reason, we synthesized new dehydroepiandrosterone derivatives with carbamate moiety containing aromatic substituent on *N*-atom and examined their binding affinity to androgen receptor and two isoforms of estrogen receptors, ERα and ERβ, using a fluorescent assay in yeast. Two of three newly synthesized compounds showed selective binding affinity to LBD-ERβ, while none of tested compounds showed binding affinity to LBD-AR and LBD-ERα. Docking analysis was performed for both active molecules, which helped us identify key interactions between these compounds and amino acid residues in the LBD-ERβ.

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CB PP 16

New Ru-arene complexes with 1,2,4-triazole Schiff base: synthesis, characterization, and cytotoxic evaluation

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Half sandwich Ru(II)-arene complexes show extraordinary anticancer activity due to their high selectivity for cancer cells and low toxicity to normal cells. The robust Ru(II)-arene unit, together with finely tuned chelate heterocycle ligands, can create structural models for interaction with common biological targets [1]. According to FDA database reports, 75% of heterocyclic drugs contain a nitrogen-based core, such as 1,2,4-triazoles, like Anastrazole and Letrozole, which are approved for clinical use against breast cancer [2].

Here we report the synthesis and biological evaluation of three novel Ru(II)-arene complexes **C1–C3**, prepared from $[RuCl_2(\eta^6\text{-p-cymene})]_2$, $[RuCl_2(\eta^6\text{-toluene})]_2$, $[RuCl_2(\eta^6\text{-benzene})]_2$, and the Schiff base ligand (anthracen-9-yl)-*N*-(3,5-di(pyridin-2-yl)-4*H*-1,2,4-triazol-4-yl)methanimine. The complexes were synthesized via reflux in methanol, and characterized by NMR, IR, and MS. Their cytotoxicity was assessed against human acute promyelocytic leukemia (HL-60) and normal lung fibroblast (MRC-5) cells. Compared to the IC_{50} of cisplatin, complex **C1** expressed the highest potency (0.18 μM) but also high toxicity to healthy cells. Complex **C2** showed good activity (8.46 μM), comparable to cisplatin, with reduced toxicity, while complex **C3** was less active than cisplatin (26.9 μM) but non-toxic to MRC-5 cells.

Overall, complex **C2** emerged as the most promising candidate, balancing anticancer efficacy with reduced toxicity compared to cisplatin, while complex **C3** was safest but least active.

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CB PP 17

Dengue drug discovery by repurposing approved drugs

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Dengue fever is caused by the dengue virus, an RNA virus belonging to the genus *Flavivirus*, and is transmitted to humans through the bite of infected mosquitoes. According to the World Health Organization, there is currently no specific treatment for the disease. Although 100–400 million people are infected annually, therapy is limited to drugs that alleviate symptoms such as muscle and joint pain, retro-orbital pain, fever, headache, nausea, and rash. This study aimed to identify potential therapeutic candidates for dengue fever using a theoretical approach based on drug repurposing. The method focused on existing FDA-approved drugs and combined electron-ion interaction potential (EIIP) analysis with molecular docking against a dengue virus coat protein (PDB ID: 3C5X). The research identified drugs that demonstrated stronger interactions with the target protein compared to the reference compounds NITD-2636, LCTA-949, and SA17. The obtained results related to LCTA-949 and SA17 indicate that the solution may be sought in antivirals, antineoplastics, drugs for maintaining bone density, and supplements (primarily vitamin B). The selected candidates related to NITD-2636 suggest that a potential drug or contribution to the therapy for dengue fever can be sought among a wide range of medications from antidepressants to antimalarials. Testing the synergistic effect of the obtained drugs or their combination in treatment is desirable, as it could contribute to the existing treatment for dengue fever.

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CB PP 18

Structural characterization and anticancer potential of a rhenium(V)-apigenin complex

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Apigenin is a plant-derived flavone commonly found in parsley, chamomile, celery, and other dietary sources, and has been linked to diverse biological activities relevant to human health [1]. High-valent oxo-rhenium(V) complexes have recently gained attention as chemically stable species with promising perspectives for therapeutic development [2].

In this work, we report the synthesis, structural characterization, and biological evaluation of a novel apigenin complex with $ReOBr_3(PPh_3)_2$. The compound was prepared via the reaction of apigenin with ReOBr3(PPh3)2 in acetone (1:1 molar ratio) under reflux conditions. Its composition and structure were confirmed using standard spectroscopic methods (NMR, IR), complemented by X-ray diffraction. The Re(V) center adopts a distorted octahedral geometry, with apigenin coordinating through two oxygen atoms in a nearly planar chelating mode. Cytotoxic properties were investigated using the resazurin reduction assay on a panel of cancer cell lines. The Re–apigenin complex demonstrated pronounced cytotoxicity toward the Jurkat cell line and moderate effects against other tested lines. The IC_{50} values for Jurkat were below 5 μM, indicating an enhancement of the cytotoxic effect compared to free apigenin. In summary, coordination of apigenin to a Re(V) center modulates its bioactivity and reinforces its anticancer potential, underscoring the relevance of oxorhenium(V) complexes as promising scaffolds for the development of novel therapeutic agents.

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CB PP 19

DNA and HSA interactions of pyridine-based biogenic amine derivative

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DNA (Deoxyribonucleic Acid) and HSA (Human Serum Albumin) are highly interesting and essential biomolecules due to their fundamental roles in life, although their functions differ significantly. Albumin is one of the most medicinally interesting proteins which plays a crucial role in transporting essential medications to their targeted sites through the blood, while DNA is a potential target for many biological agents. Considering that the effectiveness of a potential drug depends both on its interaction with DNA and on its ability to bind to a protein carrier for transport in the bloodstream, we investigated the binding affinity of a synthesized imine, known for its excellent biological potential, to HSA and DNA molecules. The interactions of the tested compound with HSA were followed by the fluorescence quenching technique, while intercalation of ethidium bromide (EB) and minor groove binder Hoechst 33258 were used for DNA binding examinations, and the binding parameters [1] were calculated. The obtained values clearly indicated that the tested imine had a significant binding ability to the HSA molecule. Furthermore, a comparison of the binding constant values from EB and Hoechst 33258 quenching experiments suggests that the complexes interact with double-helical DNA through both binding modes: intercalation and minor groove binding.

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CB PP 20

INFOGEST 2.0 - Evaluation of peanut protein digestibility and IgE reactivity

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Peanut allergy is one of the most common and severe food allergies, often leading to systemic anaphylaxis [1]. The persistence of allergenic proteins during digestion contributes to their immunogenicity [2]. This study used the standardized INFOGEST 2.0 *in vitro* digestion model to assess the stability of peanut proteins under simulated oral, gastric and intestinal conditions. Protein breakdown was analyzed using SDS-PAGE, while IgE-binding capacity of digestion products was evaluated through immunoblotting with pool of sera from peanut sensitised individuals. SDS-PAGE analysis shows that bands that correspond to the mass of major peanut allergens (*Arachis hypogaea* L., Ara h 1–6) are present in different phases of gastrointestinal digestion. Bands corresponding to Ara h 1 (~60 kDa) and the acidic subunit of Ara h 3 (45–50 kDa) show reduced intensity compared to controls, with Ara h 3 being more extensively digested during the intestinal phase and Ara h 1 being similarly extracted and digested in both gastric and intestinal ohase. Ara h 2 (16-17 kDa) and Ara h 6 (15 kDa) also exhibit more pronounced digestion and extraction in the intestinal phase compared to the gastric phase. Immunoblot confirms immunoreactivity of these bands corresponding to main peanut allergens, as well as to some fragmens on lower masses that could correspond to digested Ara h proteins.

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CB PP 21

Green synthesis of pyrido-dipyrimidines: anticancer and DNA/HSA binding studies

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Our one-pot heterocyclization of thiobarbituric acid, vanillic aldehydes, and amines in water offers a green chemistry approach to synthesizing pyrido-dipyrimidine scaffolds, addressing the limitations of traditional methods that rely on hazardous solvents [1]. This synthetic strategy provides multiple advantages, including a sustainable aqueous medium, compatibility with diverse substrates, and very high yields. We synthesised series of 24 compunds and test them *in vitro* on cancer cell lines. Compounds **A** and **B** have showed most significant activity and values of IC_{50} bellow 18 μM on HeLa and K562 cell lines. Those two compunds are utilised for further investigation of DNA and HSA binding. Quenching constant (k_q) values above 10^{10} M^{-1} s^{-1} determined by competitive fluorescence spectroscopy study with ethidium bromide (EB) indicate intercalative binding by EB displacement. For HSA examination, we employed Eosin Y and ibuprofen as site-specific markers to investigate whether selected pyrido-dipyrimidines interact with site I in subdomain IIA and/or site II in subdomain IIIA of human serum albumin. Stern-Volmer (K_{sv}), binding (K_b) and quenching constants showed that both examined compounds exhibit a moderately high binding affinity for both, site I and site II. This researh will help better understanding of biological activity of green synthesised pyrido-dipyrimidines.

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CB PP 22

SAR analysis of novel hybrid analogues based on styryl-lactone scaffold with antiproliferative activity

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In our recent research, a series of novel hybrid molecules was designed and synthesized. These hybrid analogues were constructed by combining a furanofuranone bicyclic system, present in natural products such as (+)-protulactone A and (+)-asperilactone C, with a phenyl ring characteristic of styryllactones such as (+)-goniofufurone and 7-*epi*-(+)-goniofufurone. To correlate the structures of the synthesized hybrid analogues with their antiproliferative activities, we analyzed the influence of stereochemistry (Fig. 1), structural complexity and the presence of specific functional groups. This study aims to provide insights into structure–activity relationships that may guide the future design of bioactive lactone-based compounds.

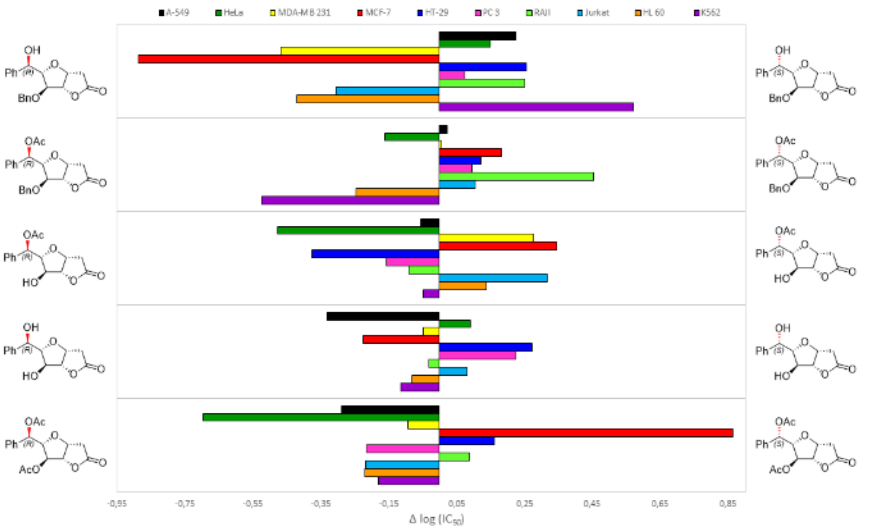

Figure 1. SAR analysis: influence of absolute stereochemistry at C-7.

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CB PP 23

Genipin- and potassium-crosslinked chitosan/carrageenan hydrogels as 3D scaffolds for cultivated meat production

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Cultivated meat (CM) is a promising future source of alternative protein. However, scaffolds often used in CM production are animal-derived; to develop completely animal product-free CM, alternative scaffolds are necessary. Algal polysaccharides such as carrageenan and chitosan form stable hydrogels which could possibly be used to grow CM due to their high-water content, porosity and cell-adhesive properties. Genipin, a biocompatible chemical cross-linker derived from *Genipa americana* and *Gardenia jasminoides,* can be used to produce chitosan hydrogels, and potassium ions can be used to physically cross-link carrageenan. Simultaneously cross-linking both polysaccharides in solution possibly results in them forming an inter-penetrating network (IPN), giving the resulting combined chitosan/carrageenan (CC) hydrogel greater strength and stability. The ability of quail muscle 7 (QM7) cells to adhere to, and grow on, these hydrogels was assessed using an Alamar blue assay, using gelatin hydrogels as a control. It was found that cell growth on CC gels over a period of 7 days was comparable to cell growth on gelatin hydrogels. CC gel structure was further studied using scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy.

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CB PP 24

DNA/BSA binding study of mononuclear gold(III) complexes containing miconazole and econazole as ligands

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Aromatic nitrogen-containing heterocycles (*N*-heterocycles) have attracted considerable attention as scaffolds for compounds with applications in various pharmacological areas, ranging from vitamins to antimicrobial and antitumor agents [1]. In this context, azoles are of particular importance due to their high potency and broad-spectrum activity, especially in the treatment of invasive fungal infections [2]. In the present study, the interactions of two gold(III) complexes with the general formula [$AuCl_3$(azole)], azole is miconazole (mcz, Au1) or econazole (ecz, Au2), were investigated with calf thymus DNA (ct-DNA) using fluorescence emission spectroscopy, in the presence of the intercalative agent ethidium bromide (EthBr) and the minor groove binder Hoechst 33258 (Hoe). Additionally, fluorescence competition experiments were conducted using specific site markers, eosin Y, ibuprofen, and digitoxin. These site markers were employed to gain better insight into the binding sites on BSA, where eosin Y serves as a marker for site I (subdomain IIA), ibuprofen for site II (subdomain IIIA), and digitoxin for site III (subdomain IB).

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CB PP 25

Recombinant production of the chimeric protein alpha-synuclein–mCerulean3–His6 in *Escherichia coli*, isolation and assessment of its thermal stability at different pH values

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Alpha-synuclein is a neuronal protein that regulates synaptic vesicle trafficking and neurotransmitter release. Synucleinopathies, such as Parkinson's disease, dementia with Lewy bodies, and multiple system atrophy, arise from accumulation of alpha-synuclein aggregates in neurons, neurites, or glial cells. mCerulean3 is a constitutively fluorescent protein derived from *Aequorea victoria*. The thermal stability of alpha-synuclein at different pH values is of great importance. Thermal stability reflects the conformational stability of a protein, which influences misfolding and aggregation. This study provides insight into the possibility that mCerulean3, when used to visualize the tissue and cellular localization of alpha-synuclein, may potentially affect alpha-synuclein's behavior and *vice versa*. Pathological conditions, such as the acidic environments of lysosomes or inflamed tissue, can destabilize alpha-synuclein, promoting aggregation. Drugs designed to stabilize alpha-synuclein must take into account the conditions in which alpha-synuclein is most susceptible to aggregation, in order to prevent pH-induced structural changes. This research focuses on defining *in vivo* methods for synthesizing a chimeric protein that can serve to study the molecular pathophysiology and etiology of synucleinopathies. The protein enables real-time visualization of alpha-synuclein's mechanisms of action, its pathological fibrils, and their localization in nervous tissue, representing one of the essential tools for future studies and therapeutic development for these diseases. The investigated thermal stability of the target protein demonstrates that the presence of alpha-synuclein confers increased stability to the mCerulean3 moiety in basic and neutral environments, whereas in acidic conditions the stability is not substantially altered.

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Developments in Chemical Synthesis (DCS)

DCS PP 01

Iminodiacetate-based gallium(III) complexes: synthesis, spectroscopic characterization and X-ray structural analysis

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The iminodiacetate anion (ida^{2-}), containing one amine nitrogen and two pairs of carboxylate oxygen donor atoms, is widely employed in coordination chemistry and forms stable complexes with various transition metal ions, including copper(II), nickel(II) and zinc(II) [1,2]. In this study, iminodiacetate was used as a ligand for the synthesis of two new gallium(III) complexes, $Na[Ga(ida)_2]\cdot 2H_2O$ (**1**) and $K[Ga(ida)_2]\cdot 3H_2O$ (**2**). Complexes **1** and **2** were synthesized in aqueous solution at 80 °C in 4 h by reacting $GaCl_3$ with iminodiacetic acid (H_2ida) in the presence of NaOH or KOH, respectively. Both complexes were characterized using IR and NMR (^1H and ^{13}C) spectroscopy, while their crystal structures were determined by single-crystal X-ray diffraction analysis. This analysis revealed that complexes **1** and **2** are related. In both, Ga(III) ion is coordinated by one nitrogen and two oxygen atoms from each of the two ida^{2-} ligands in octahedral coordination environment. Sodium or potassium cations are positioned in between the coordination anions in **1** and **2**, respectively. Due to the larger size of potassium, in the presence of the latter trihydrate is formed, while in the presence of smaller sodium cations dihydrate forms.

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DCS PP 02

Quantifying photon flux enhancement in a concave mirror photoreactor using ferrioxalate actinometry

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Accurate determination of photon flux is essential for evaluating and characterizing photochemical reactor setups. Knowledge of the effective photon flux not only ensures reproducible operation, but also facilitates rational scale-up and aids in the elucidation of the photochemical reaction mechanism. Ferrioxalate actinometry was employed as the benchmark method for quantifying optical power in visible-light photocatalysis.[1] Herein, we present a detailed assessment of photon flux enhancement in our recently published concave mirror photoreactor-data not included in the original report.[2] Comparative measurements reveal a significant increase in photon flux when the photoreactor is employed. Furthermore, a comprehensive measurement of photon flux is reported, including versatile vessel types, variable light source-sample distances, and irradiation in and without the photoreactor. These results highlight the influence of vessel geometry on illumination and provide a practical reference for reactor selection in photocatalytic applications. Finally, we observed that photon fluxes correlate directly with product yields in the thioxanthone catalyzed C–H functionalization of tetrahydrofuran with phenyl vinyl sulfone, confirming the impact of reactor design on synthetic efficiency.

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DCS PP 03

Synthesis, characterization and HSA binding studies of two novel palladium(II) complexes

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Two novel palladium(II) complexes, $[Pd(L)Cl_2]$ (**Pd1**) and $[Pd(L)_2]$ (**Pd2**) (Fig 1), where L is ethyl-2-hydroxy-4-[(*E*)-2-(3'-methoxy-4'-butoxyphenyl)vinyl]-4-oxo-2-butenoate, were successfully synthesized and characterized using ^{1}H NMR, IR spectroscopy and mass spectrometry. Their interactions with human serum albumin (HSA) were investigated through fluorescence quenching spectroscopy, both in the absence and presence of site-specific markers – eosin Y (site I, subdomain IIA) and ibuprofen (site II, subdomain IIIA)[1] – in order to elucidate their preferred binding sites. Both complexes exhibited significant binding affinity towards HSA, with **Pd2** showing notably higher binding constants. Competitive binding studies revealed that **Pd1** preferentially binds to subdomain IIA of HSA, while **Pd2** exhibits a stronger affinity for subdomain IIIA. These findings provide better insight into the structure–affinity relationship of palladium complexes with serum proteins and their potential implications in bioinorganic chemistry.

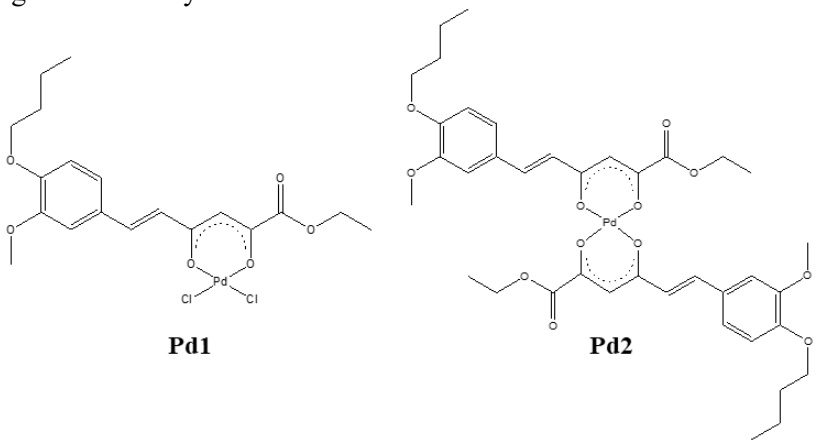

Figure 1. Structures of investigated complexes.

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DCS PP 04

New approaches to cyclohepta[*b*]indoles by intramolecular cyclization: gold(I)-catalysis vs Friedel–Crafts acylation

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Cyclohepta[*b*]indole is a privileged structure found in various natural products and potential pharmaceuticals, many of which exhibit diverse biological activities.[1] Despite its significance, only a limited number of general methods for its synthesis exist, providing strong motivation for the development of new synthetic methodologies.[2] Herein, we report a novel and efficient approach to cyclohepta[*b*]indoles that relies on the formation of a seven-membered ring via gold(I)-catalyzed cyclization of 3-alkylindoles possessing a triple bond in the alkyl-chain, under mild conditions. Alternatively, this tricyclic scaffold was also assembled through intramolecular Friedel–Crafts acylation of (indol-3-yl)valeric acids. Both of these methods proved efficient and we are therefore confident that the developed methodology will find application in total syntheses of complex indole alkaloids – an investigation currently underway in our research group.

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DCS PP 05

Synthesis and spectral characterization of 5-aminosalicylic acid esters

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5-Aminosalicylic acid (5-ASA) is a frontline agent for inflammatory bowel disease and also displays antioxidant and chemopreventive activities [1,2], motivating the preparation of new derivatives. We synthesized a small library of 5-ASA esters via Steglich esterification using structurally diverse alcohols (benzyl, 4-isopropylbenzyl, 1-(4-nitrophenyl)ethan-1-ol, 4-fluorobenzyl, and carvacrol). Five esters were obtained, including two compounds reported previously (benzyl and 4-isopropylbenzyl esters) that are fully spectroscopically characterized here for the first time, and three new esters. Comprehensive IR, MS, and NMR analyses —including 2D experiments (HSQC, HMBC, NOESY, and gradient-enhanced ^{1}H–^{1}H COSY) — confirmed the ester structures and enabled complete signal assignments.

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DCS PP 06

Synthesis and spectroscopy characterization of two Schiff bases and their Cu(II) and Co(II/III) complexes

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Schiff bases and their complexes have attracted considerable attention, due to their diverse biological activity, including antimicrobial, antifungal and anticancer effects [1,2]. In this study, two novel Schiff base ligands, N^1,N^2-bis(anthracene-9-methylene)-4-methylbenzene-1,2-diamine and N^1,N^2-bis(anthracene-9-methylene)-4,5-dimethylbenzene-1,2-diamine, were synthesized in high yields via condensation reactions. The ligands were characterised by IR, ^{1}H and ^{13}C NMR spectroscopy, and ESI-MS. Their Cu(II), Co(II) and Co(III) complexes were prepared in ethanol solution at 70ºC, in a molar ratio of 1:1 (metal:ligand). Characterization of the complexes was performed through the application of IR and UV spectroscopy. NMR analysis could not be performed due to the paramagnetic nature of the obtained complexes. The IR spectra confirmed coordination through shifts in the C=N stretching band, while the UV-Vis spectra exhibited electronic transitions characteristic of the oxidation states of the metals. These results indicate successful ligand coordination and distinct spectroscopy profiles. Further studies will focus on advanced characterisation, using EPR spectroscopy, single-crystal X-ray diffraction (SC-XRD), and evaluation of biological activity.

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Environmental Awareness (EA)

EA PP 01

Application of Fly Ash-Based Geopolymers for the Removal of Pesticides from Water

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Harmful effects of pesticides on human health have been observed even at very low concentrations. These chemicals are used in large quantities in agriculture to suppress the adverse impacts caused by various types of insects, bacteria, fungi, and algae [1]. Their extensive use has led to their penetration into natural ecosystems. On the other hand, modern societal development has resulted in an ever-increasing demand for electrical energy, which inevitably generates large amounts of waste originating from thermal power plants - fly ash [2]. The main aim of this study is to address the problem of environmental pollution by pesticides through the valorization of waste via the synthesis of a new type of inorganic polymeric material—geopolymers. In this work, geopolymers based on fly ash modified with chitosan and polyvinyl alcohol were synthesized. The obtained materials were characterized using scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRPD), and point of zero charge determination (pH_{PZC}). The adsorption capacity of the synthesized materials was examined for eight commercial pesticides: acephate, monocrotophos, dimethoate, carbofuran, carbaryl, linuron, malathion, and tebufenozide. The results showed that the adsorption efficiency depends on the type of pesticide and ranged from 19.1 % for acephate to 99.9 % for carbofuran, carbaryl, and malathion. These findings indicate that modified fly ash-based geopolymers have the potential to serve as an efficient and sustainable adsorbent for the removal of pesticides from contaminated water.

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EA PP 02

Photocatalytic degradation of Rhodamine B with laser synthesized indium- titanium(IV) oxide

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Water pollution caused by the textile industry is a major environmental concern due to the extensive use of synthetic dyes. Rhodamine B (Fig. 1), a xanthene dye widely applied in textiles, food additives, biological staining, and laser systems, exhibits severe toxic effects, including carcinogenicity, reproductive, developmental, and neurotoxicity [1]. Therefore, there is a need for effective methods for removing such organic dyes from industrial effluents. Titanium(IV) oxide is well known as an effective photocatalyst for dye degradation [2]. In this study, we report the synthesis and comparison of two nano-sized In/TiO_2 catalysts in the photodegradation of Rhodamine B dye under UV light irradiation. The catalyst was synthesized by laser ablation of a titanium plate in a diluted $InCl_3$ solution with a pulse energy of 35 mJ over a time interval of 20 minutes. The photodegradation process was monitored by UV-Vis spectroscopy for over 240 minutes. After 240 minutes of UV irradiation, the degradation efficiency reached 51.5% for the unannealed and 64.2% for the annealed titanium plate.

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EA PP 03

Influence of lithium-ion modification of zeolite 13X on CO_2 adsorption capacity

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In this study, the effect of lithium ion modification of zeolite 13X on CO_2 adsorption capacity was investigated, with the aim of developing more efficient adsorbents for application in greenhouse gas emission reduction processes. The ion exchange was conducted by mixing an 8.3 mol/L LiCl solution with a 13X zeolite suspension containing 220 g/L of the solid phase. Four different samples were synthesized, varying in temperature (45 and 55 °C), process duration (2 h), and the number of ion-exchange steps (single-step and two-step). The obtained materials were characterized using atomic absorption spectroscopy to determine the ion-exchange degree, X-ray diffraction (XRD) to verify the stability of the crystalline framework, laser diffraction for particle size distribution, the BET method for specific surface area and pore volume, as well as CO_2 adsorption capacity measurements. The results demonstrate that substitution of Na^+ with Li^+ induces slight lattice contractions without compromising the structural integrity, while simultaneously leading to a pronounced increase in CO_2 adsorption capacity. The highest value (5.71 mmol/g) was achieved for the sample obtained via two-step ion exchange at 55 °C, indicating that the degree of ion exchange, plays a critical role in optimizing the material for CO_2 capture. Overall, the findings confirm that Li-X is a promising adsorbent for applications aimed at reducing CO_2 emissions.

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EA PP 04

Obtaining a coloured stable nickel spinel-based compound by the process of ion-exchange and subsequent thermal treatment

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The enhanced rate of industrial development, over the past decades, has led to increased use of heavy metals, especially nickel, and their disposal in the environment. Nickel is a heavily used metal due to its anticorrosion properties. High concentrations of nickel ions in surface water are a consequence of industrial processes such as mining, electroplating, and battery manufacturing. Long-term exposure to high concentrations of nickel can be hazardous to both aquatic life and human health. Processes of ion exchange and subsequent calcination can be a promising way for the removal and permanent immobilization of Ni^{2+} ions. Thermal treatment of nickel-exchanged zeolites, at temperatures above 1000 ºC, leads to the formation of a newly formed Ni-spinel-based, stable compound that is coloured and thermostable. In this work, LTA zeolite is used as an ion-exchange precursor for a process of five successive cation exchanges with 0.1 M $NiSO_4$. A successful ion-exchange process has been confirmed by XRF analysis. After ion exchange, powder samples of Ni-exchanged were thermally treated at temperatures between 900 ºC and 1300 ºC. Formation of a new stable Ni-spinel based compound is analyzed by XRD and SEM. Distinct nuances of cyan coloured compound were studied by CIELab colorimetric analysis [1,2].

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EA PP 05

Adsorption kinetics of Cr (VI) ions using exhausted chestnut wood as a biosorbent

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Pollution that occurs due to the presence of high concentrations of heavy metal ions in aquatic ecosystems represents an increasing problem from the aspect of environmental protection. In recent years, biosorption has emerged as a new and efficient technique for removing metals from aquatic environments, using various natural and lignocellulosic materials, known as biosorbents (1). The aim of this study was to examine the potential of using exhausted chestnut wood (ECW), from a tannin production factory as a biosorbent for the removal of Cr (VI) ions, using various kinetic models. Biosorption was carried out in model water with an initial Cr (VI) ions concentration of 10 mg/l at pH 2, where the required contact time between the biosorbent and water was examined. Based on the obtained results, it can be concluded that the largest amount of ions is bound in the first 90 minutes. After 24 hours of contact, all ions in the solution were removed by ECW (100% efficiency), with the adsorption capacity 9,57 mg/g. The experimental data were processed using pseudo-first-order, pseudo-second-order, and Elovich models to describe how and at what rate adsorption occurs. The pseudo-second-order model appeared to be the best for fitting kinetic data (R^2 = 0,9999), which indicates that the limiting factor of the adsorption rate is the chemical binding to active sites. Also, the value of the adsorption capacity (9,66 mg/g), calculated using the pseudo-second-order model, agreed very well with the experimental data, which once again confirms that this model is suitable for describing the kinetics of Cr (VI) ions adsorption on ECW. Based on the obtained results, it can be concluded that the exhausted chestnut wood can be used as an adsorbent for Cr (VI) ions. Further tests will be focused on improving the adsoprtion characteristics of the biosorbent, using different modification procedures.

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EA PP 06

The bioaccumulation potential of the plant *Symphytum officinale* L.

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The bioaccumulation potential of comfrey (*Symphytum* sp.), collected from Mount Golija, Serbia, was investigated for ten elements: Al, Ba, Ca, Fe, K, Mg, Mn, Na, P, and Si. All parts of the plant were analyzed (Figure 1), for which the bioaccumulation coefficient (BAC) and translocation factor (TF) were determined. Potassium (K), phosphorus (P), and silicon (Si) were found to be strongly accumulated and efficiently translocated within the plant, as indicated by their high BAC and TF values. In contrast, aluminum (Al), iron (Fe), and sodium (Na) exhibited low BAC and TF values, suggesting limited uptake and poor internal mobility. Barium (Ba), calcium (Ca), magnesium (Mg), and manganese (Mn) demonstrated high TF values, indicating effective translocation, while their BAC values were moderate.

Figure 1. Comfrey (Symphytum sp.)

In the root, the bioaccumulation factor (BAF) was assessed. The highest BAF was recorded for K, followed by P. Low BAF values were observed for Al, Fe, and Mn. Overall, comfrey demonstrated a notable capacity for both bioaccumulation and translocation, particularly for Si and K, suggesting that it may act as a hyperaccumulator of these elements.

According to the available literature, no comparable study has been previously conducted on comfrey from Mount Golija to date.

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EA PP 07

Influence of pH on element leaching from plastic and glass bottles into water

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Monitoring of elemental composition in bottled waters is essential to assess both their nutritional contribution and potential health risks. In this study, six widely consumed Serbian bottled waters were analyzed to evaluate the influence of packaging material (PET vs. glass) and storage temperature (–20°C, 25°C, 40°C) on elemental stability [1,2]. A total of 18 elements were quantified by ICP–MS, and variations were compared across brands and conditions. The results revealed clear differences between PET and glass packaging. Antimony, originating from PET, was consistently higher in plastic bottles, with the maximum value of 15.6 µg/L detected in *Knjaz Miloš* at 40 °C. This level exceeded the drinking water guideline of 5 µg/L, while all glass samples remained below the limit. Cd and Pb showed sporadic occurrences, with maximum concentrations of 0.50 µg/L and 1.98 µg/L, respectively, both remaining within regulatory safety thresholds. Independent of packaging, each brand showed a unique geochemical fingerprint. *Knjaz Miloš* was distinguished by exceptionally high levels of strontium (up to 801 µg/L) and lithium (695 µg/L), in contrast to *Rosa*, which contained the lowest values of these elements. These markers proved stable across a range of temperatures, reflecting the geological origin of the source rather than packaging effects. pH values ranged between 5.9 and 6.9 for all PET samples and were nearly identical in the corresponding glass samples, indicating that pH had no significant influence on elemental migration. However, elevated temperatures enhanced Sb leaching from PET, confirming temperature as the dominant factor affecting packaging-related contamination.

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EA PP 08

Electronic Band Structure Modifications in $Fe/TiO_2/VO_4$ and $Fe/TiO_2/VOOH$ Systems: A Theoretical Study for Photocatalytic Applications

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This study theoretically investigates the electronic and photocatalytic properties of rutile-phase titanium dioxide (TiO_2) modified with Fe-doped iron vanadate ($Fe/TiO_2/VO_4$) and vanadium-substituted goethite ($Fe/TiO_2/VOOH$) using density functional theory (DFT) calculations [1]. Our analysis of the density of states (DOS), band structure, and work function reveals that both dopant systems significantly modify the electronic structure of pure rutile TiO_2. The incorporation of Fe and V alters the valence and conduction bands, resulting in a reduced band gap and a modified work function. This suggests enhanced visible light absorption and improved charge carrier separation, key factors for increasing photocatalytic efficiency. Specifically, the DOS analysis highlights the contribution of Fe 3d and V 3d orbitals, which create new electronic states within the band gap, facilitating charge transfer. These theoretical insights provide a strong foundation for the rational design of novel, highly efficient TiO_2-based photocatalysts for the degradation of organic pollutants [2].

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EA PP 09

Assessment of PAH contamination in soils from closed municipal landfills in Serbia

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In Serbia, a considerable number of landfills exist, the majority of which are not properly regulated [1]. These landfills represent a threat to human health and the environment, as they release various pollutants, with polycyclic aromatic hydrocarbons (PAHs) being among the most prevalent [1].

Samples were collected from three closed municipal landfills (*Kovin*, *Pančevo,* and the old part of *Vinča* landfill). Soil samples were extracted using Soxhlet extraction with an azeotropic mixture of dichloromethane and methanol. The obtained extracts were concentrated on a vacuum evaporator and dried to approximately 15 mg, then purified by column chromatography on silica gel deactivated with 5% water. Through this procedure, the purified extracts were prepared for analysis by Gas Chromatography–Mass Spectrometry (GC-MS). Although these landfills are no longer in use, the sum of the concentrations of all 16 PAHs at each location shows that more than 30% of the samples were classified as moderately polluted (> 0.600 mg/kg), while more than 38% were classified as highly polluted (> 1.000 mg/kg). The highest median concentration was observed for fluoranthene (1.19E-01 mg/kg), while the lowest was observed for acenaphthene (1.04E-03 mg/kg). These findings highlight the potential risks posed by the landfills and emphasize the need for continued monitoring and human exposure assessments. This knowledge also enables the identification of the most polluted locations and may help in reducing conscious exposure.

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EA PP 10

Sustainable biocomposites: valorization of agro-industrial by-products

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The search for sustainable alternatives to petroleum-based plastics has become a key goal in modern materials science. Biocomposites, which combine biodegradable polymers with natural fillers, are an important step toward reducing environmental impact and supporting circular economy practices. In this study, brewer's spent grain, one of the most abundant by-products of the beer industry, was investigated as a potential filler for polylactic acid (PLA). This material is attractive because it provides a low-cost, renewable source of reinforcement while also reducing agro-industrial waste. The research focused on the effect of filler particle size on the final properties of the composites. Several fractions, such as 150, 180, 335, 450, and 600 nm, were prepared and tested, and the results showed that finer particles, especially those around 150 nm, performed best. When particles were small and well dispersed in the polymer matrix, as confirmed by scanning electron microscopy (SEM) and dynamic mechanical analysis (DMA), the composites demonstrated improved stability, homogeneity, and functionality compared to those with larger particles. These findings highlight the importance of controlling filler morphology and dispersion to design effective bio-based materials. The study confirms that brewer's spent grain can be successfully incorporated into PLA to create biocomposites with promising properties, suitable for applications ranging from food packaging to technical products, where sustainability and performance must be balanced. Future research will focus on optimizing filler content and processing conditions to further enhance mechanical and functional characteristics, opening opportunities for wider industrial use of agricultural residues and supporting the global effort to replace conventional plastics with more environmentally friendly alternatives.

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EA PP 11

Pollution-related modifications enhance ragweed pollen allergenicity

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Air pollution can chemically modify aeroallergens and intensify symptoms, but how this shapes the allergen profile and bioactivity of ragweed pollen in different environments remains incompletely understood. We compared protein extracts from ragweed (Ambrosia artemisiifolia) collected at paired urban and rural sites for: (i) abundance of Amb a 1.2 (pectate lyase 1), (ii) oxidative/nitrative adduct (4-hydroxynonenal, 4-HNE; 3-nitrotyrosine), and (iii) IgE reactivity in ragweed-allergic patients. Mature pollen was sampled at appropriate phenological stages and processed under standardised conditions. Total protein was quantified and normalised before analysis. Amb a 1.2 was assessed by SDS-PAGE/Western blot, using rabbit anti-Amb a 1.2. Oxidative/nitrative stress markers were quantified by Western blot analysis with rabbit anti-4-HNE and rabbit anti-3-nitrotyrosine. Patient reactivity was assessed using sera from well-characterised ragweed allergy subjects (confirmed sensitisation by diagnostic immunoCAP). Urban extracts showed higher 4-HNE and 3-nitrotyrosine signals (normalised to total protein) compared to rural equivalents, with similar Amb a 1.2 immunoreactivity. Patient sera showed stronger IgE binding to urban extracts. Across all sites, IgE reactivity correlated with oxidative/nitrative adducts independently of total Amb a 1.2, while ELISA inhibition with Amb a 1 reduced - but did not abolish - IgE binding, implicating both Amb a 1-dependent epitopes and modified proteins. Pollution-related oxidative (4-HNE) and nitrative (3-nitrotyrosine) modifications coexist with increased allergenic activity of ragweed pollen.

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EA PP 12

Sunflower waste–derived activated carbon for efficient metol adsorption and its determination using a gold nanoparticle-modified carbon electrode

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Activated carbon (AC) is recognized as an efficient, versatile, and environmentally friendly material, widely used for the removal of diverse pollutants, even at low concentrations [1]. In this study, a porous carbon material was prepared from agro-industrial sunflower waste. The precursor material was first carbonized at 900 °C and subsequently chemically activated with potassium hydroxide at a mass ratio of 1:2 (carbonized material: KOH) to obtain the activated carbon. Adsorption experiments for metol removal were conducted using aqueous solutions (100 mg/L), to optimize adsorption parameters by evaluating the influence of pH (2–10) and contact time (1–180 min). After adsorption, metol in the supernatant was monitored by UV-Vis spectroscopy at 271 nm. The optimal conditions were identified at pH 8. In addition, the differential pulse voltammetry using a gold nanoparticle-modified carbon electrode was applied to monitor the removal efficiency of metol over different contact times in the potential range of –0.5 to 0.6 V at a scan rate of 25 mV/s. Metol removal efficiency reached 82.9% after 1 minute of contact, and complete adsorption was achieved after 120 minutes. The results highlight the potential of sunflower-derived activated carbon as a sustainable and efficient adsorbent for the removal of metol from aqueous solutions.

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EA PP 13

Efficient extraction of copper and lead from printed circuit boards using ionic liquid-based aqueous biphasic systems

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The growing demand for sustainable technologies in electronic waste recycling has stimulated the development of innovative separation methods for critical and toxic metals. Printed circuit boards (PCBs), a major component of e-waste, contain high levels of valuable and hazardous metals, whose efficient recovery is essential for both resource conservation and environmental protection [1]. In this work, real PCB samples were subjected to nitric acid leaching. Inductively coupled plasma analysis of the leachate revealed copper and lead concentrations of 2.8468 g/L and 0.7750 g/L, respectively, confirming their significant presence in PCB waste streams. To enable selective separation, the leachate was converted into an ammonium nitrate medium, after which the ionic liquid tetrabutylphosphonium salicylate ([TBP][Sal]) was introduced. Ionic liquids, widely recognized as green solvents for metal extraction [2], successfully induced the formation of an aqueous biphasic system (ABS), enabling the efficient partitioning of both metals into the ionic liquid-rich phase. Remarkably, extraction efficiencies of 99.8% were achieved for both copper and lead, clearly demonstrating the outstanding capability of [TBP][Sal]-based ABS to isolate these metals from complex acidic leachates. Such performance not only highlights the robustness of the method but also underlines its potential applicability to other multicomponent e-waste matrices. Overall, the presented study provides strong evidence that ionic liquid-based ABS can be utilized as a sustainable and highly effective strategy for treating real electronic waste leachates. The approach combines high selectivity, nearly quantitative extraction, and compatibility with circular hydrometallurgical concepts, thus offering a promising platform for future large-scale applications in e-waste recycling.

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EA PP 14

Application of nickel- and iron(III)-modified zeolite A for boron adsorption in wastewater treatment

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Boron contamination in aquatic environments is often associated with various industrial activities, including glass manufacturing, detergent production, and metallurgical processes. Although boron is an essential micronutrient for plants, excessive intake can pose risks to human health, such as skin irritation and inflammation [1]. Conventional boron removal methods, such as reverse osmosis and nanofiltration, are effective but associated with high operational costs. As a cost-efficient alternative, adsorption offers a simple and adaptable approach. This study investigates the application of zeolite A as an adsorbent for boron removal from water. Zeolites are aluminosilicate porous minerals widely used in wastewater treatment, and low-silica zeolite A is particularly promising due to its uniform pore structure and potential for chemical modification to enhance contaminant removal. To improve its adsorption performance, zeolite A was modified using nickel sulfate solution and iron(III) sulfate in an acetate buffer. Three adsorbents were examined: zeolite A, nickel-modified zeolite A, and iron(III)-modified zeolite A. The materials were characterized using X-ray powder diffraction (XRPD), scanning electron microscopy, and thermogravimetric analysis. XRPD analysis confirmed that the crystal structure of zeolite A remained intact after modification. Adsorption experiments were conducted using a synthetic boron solution at pH 9, where boron exists as both $B(OH)_3$ and $B(OH)_4^-$. The results showed that nickel- and iron(III)-modification substantially improved boron uptake, likely due to their ability to form complexes with $B(OH)_4^-$. Overall, the findings demonstrate that modified zeolite A represents a promising adsorbent for the removal of boron from wastewater.

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Physical and Computational Chemistry (PCC)

PCC PP 01

Platinum- and rhodium-enhanced electrocatalysis of hydrogen electrode reactions on cobalt in alkaline media

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Hydrogen electrode reactions are crucial processes regarding sustainable energy conversion technologies such as water electrolysis and fuel cells. In this study, we investigated the electrocatalytic activity of cobalt electrodes, whose surfaces were modified with noble metals – platinum (Pt) and rhodium (Rh) – towards the hydrogen evolution reaction (HER) and the hydrogen oxidation reaction (HOR) in alkaline media. The surface modification was achieved through a simple and rapid galvanic displacement process (30 seconds), enabling the efficient deposition of Pt and Rh onto polycrystalline cobalt electrodes, which resulted in a significant improvement in their electrocatalytic activity. Our results show that the Pt-modified electrode exhibited the highest activity for HER, surpassing even polycrystalline platinum, while the Rh-modified electrode also demonstrated substantial improvement compared to pure cobalt. However, for HOR, pure platinum retained superior electrocatalytic performance compared to the modified cobalt electrodes. These findings suggest that galvanic displacement of cobalt with Pt and Rh is an effective strategy to enhance HER kinetics and reduce noble metal utilization, offering a cost-efficient pathway for designing advanced electrocatalysts in hydrogen-based energy systems.

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PCC PP 02

Influence of halogen interactions on the energetic properties of halogen-substituated polycyclic nitroaromatic molecules

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Halogen interactions can have an effect on the electrostatic potential above the central regions of halogen-substituated high energetic materials (HEMs). By forming this interactions, it is possible to manipulate the potential values above the mentioned regions. [1] Recent research has shown that values of potentials above isolated polycyclic nitroaromatic molecules can depend on the type of halogen substituent and its position in relation to the nitro groups. [2]

In this paper, the halogen interaction energies between hydrogen chloride and 1,4-dihalo-5,8-dinitronaphthalene (1,4DXDN)/ 2,3-dihalo-5,8-dinitronaphthalene (2,3DXDN) were investigated. The interactions were calculated using the Gaussian program and the MP2/aug-cc-pVTZ level of theory. The wfn files were calculated in the PBE/6-311G** level of theory and they were used to calculate the electrostatic potential maps (MEPs) for those systems in WFA-SAS program. Obtained values of potentials were compared to the values above the isolated molecules of 1,4DXDN and 2,3DXDN. [2]

The results showed that in DXDN/HCl systems, when X = F or Cl, the interactions are stronger in systems in which dinitronaphthalene is a donor through its halogen substituent that participates in this halogen interaction (model system C) for 1,4 and 2,3 halogen supstituated molecules. The position is important for the case when X = Br. For the 2,3DBDN/HCl system more stable is model system C, while for the 1,4DBDN/HCl system it is more favorable for Br to be the acceptor in the halogen interaction (model system A). The acceptor role is preferred by both systems in which X = I. When comparing the results obtained by analyzing the MEPs of isolated DXDN molecules and 1,4DXDN/HCl or 2,3DXDN/HCl systems, it is noticeable that the most significant changes in values in all cases is in model systems C.

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PCC PP 03

Computational profiling of newly synthesized poly(ethylene terephthalate) derivatives: pharmacokinetic and quantum-chemical insights

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Plastic oligomers of poly(ethylene terephthalate) (PET) are increasingly recognized as non-intentionally added substances (NIAS) in food, yet their toxicological evaluation remains poorly defined [1]. We computationally characterized cyclic (cPET3) and linear (lPET3) PET trimers using molecular descriptors, ADMET predictions, Hansen solubility analysis, and ORCA-based quantum-chemical methods [2]. Pharmacokinetic modeling indicated low intestinal absorption (HIA < 0.1) but measurable BBB penetration, with marked differences between cPET3 and lPET3 in plasma protein binding (63% vs. 91%), distribution volume (0.37 vs. 0.99 L/kg), and lipophilicity (logD 2.9 vs. 3.5). Hansen solubility parameters suggested preferential absorption in the upper small intestine within 3–10 h and moderate dermal permeation. Quantum-chemical analysis revealed PET's large HOMO–LUMO gap (Δ = 7.1 eV; η = 3.55 eV; ω = 1.89 eV), consistent with chemical stability, whereas lPET3 exhibited a narrower gap ($\Delta \approx$ 5.1 eV; η = 2.54 eV; ω = 4.60 eV), higher electrophilicity, and stronger electron-accepting capacity ($\mu = -4.84$ eV), reflecting increased reactivity relative to cPET3. Compared with bisphenol A and phthalates, both PET oligomers demonstrated more favorable electronic and pharmacokinetic profiles. Overall, integrated modeling highlights lPET3 as more reactive than PET and cPET3, but still substantially safer than endocrine-active plastic-related toxicants.

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PCC PP 04

Strong CH/O hydrogen bonds of phenanthroline transition metal complexes and water

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CH/O hydrogen bonds are considered weak, but we have recently shown that these interactions between a coordinated 2,2'-bipyridine and water can even be stronger than hydrogen bonds between waters. [1] Continuing this work, we investigated CH/O hydrogen bonds of coordinated phenanthroline and a water molecule using Cambridge Structural Database (CSD) search and quantum mechanical (QM) calculations. CSD results showed that water molecules tend to form bifurcated CH/O interactions. For QM calculations, the following interaction types were investigated: C2, C3, C4, and bifurcated C1-C2, C2-C3, C3-C4, and C4-C4 (Fig. 1). The strongest interaction energy at DLPNO-CCSDT/CBS level of -4.935 kcal/mol was obtained for a square planar palladium(II) complex with C3-C4 interaction type, which is almost as strong as the water-water hydrogen bond (-5.0 kcal/mol). [2]

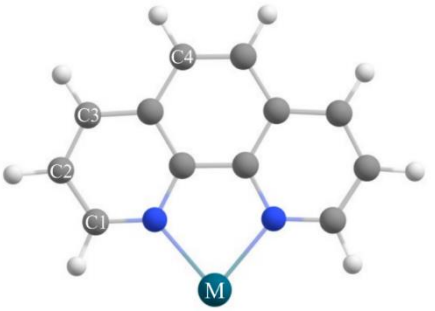

Figure 1. Schematic view of a coordinated phenanthroline with types of CH/O hydrogen bonds.

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PCC PP 05

Electrochemical investigation of Rh(III) Schiff base complex and its interaction with human serum albumin

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The electrochemical properties of a Schiff base ligand and its rhodium(III) complex were investigated in aqueous (PBS, pH 7.4) and non-aqueous solvents (acetonitrile, dimethylformamide). Distinct differences in electrochemical behavior were observed depending on the solvent, with aprotic media providing more defined and stable signals. For the study of protein binding, phosphate buffer saline with 10 mM NaCl was selected as the medium to examine the interaction of the Rh(III) complex with human serum albumin (HSA). Cyclic voltammetry was employed to monitor these interactions, and the obtained binding constants (10^4–10^5 M^{-1}) indicated an optimal binding affinity.[1] These findings suggest favorable pharmacokinetic properties of the Rh(III) complex, highlighting its potential as a novel therapeutic agent or drug carrier.

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PCC PP 06

Hydrogen bonds in hydroquinone dimer. Crystallographic and DFT study

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Hydrogen bonds are an important noncovalent interaction type in various systems. In this work, hydrogen bonds between two hydroquinone (benzene-1,4-diol) molecules were analyzed using crystallographic and computational studies. Hydroquinone possesses two hydroxyl groups, which are an essential structural feature, enabling it to form strong bonds with other polar substances as well as with other hydroquinone molecules. The performed Cambridge Structural Database search resulted in 79 classical hydrogen bonds between two hydroquinone molecules, that are characterized by a hydrogen bond distance of ≤ 3 Å and a hydrogen bond angle of ≥ 120°.[1,2] DFT calculations were performed using the B2PLYP-D3BJ method and the def2-TZVP basis set for all 79 hydrogen bonds. It was found that the interaction energy for hydrogen bonds varies from -4.0 kcal/mol to -8.8 kcal/mol, and that for most hydrogen bonds, the interaction energy is higher than -6.0 kcal/mol. To better explain the nature of hydrogen bonds, SAPT analyses were performed. The results from SAPT analysis show that the main attractive force for hydrogen bonds in two hydroquinone molecules is electrostatic, which is in general the most dominant component for hydrogen bonds. It is noteworthy to mention that the exchange term has the highest contribution, but it is partially canceled by the dispersion term.

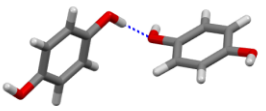

Figure 1. Hydrogen bond between two hydroquinone molecules in the crystal structure BUSPAG.

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PCC PP 07

Influence of the type of substituent adjacent to the C–NO_2 group on the impact sensitivity of trinitroaromatic molecules

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Nitroaromatic compounds are widely used high-energy materials (HEMs). Many studies have focused on studying the geometrical parameters—particularly the strength of C–NO_2 bonds—due to its significance in initiating the detonation of nitroaromatic molecules. Most important indicators of the strength of the C-NO_2 bonds are BDE values and Wiberg bond index values. [1] This study focuses on the systematic analysis of geometrical parameters of the C–NO_2 fragment, its tilting in the presence of various substituents, and the potential impact on the detonation properties of trinitroaromatic compounds. [2]

All geometries of the trinitroaromatic molecules were extracted from the Cambridge Structural Database (CSD) and structurally analyzed. Few selected geometries were used for further quantum chemical calculations (QC). Structural analysis results suggest that nitroaromatic molecules with larger deviations of the NO_2 groups from the aromatic plane are usually more sensitive to impact (TNB: 10.2◦, 100 cm and TETRYL: 43.5 ◦, 32 cm). QC results have shown that different substituents can affect the strength of weakest C-NO_2 bond through repulsing interactions between NO_2 group and neighboring substituents, formation of attractive non-covalent interactions and through electronic effect of specific neighboring substituents which cause the depletion of electron density in C-NO_2 bond fragment. Voluminous substituents such as iodine or alkyl groups can induce the tilting of the NO_2 group and the weakening of the C-NO_2 bond. On the other hand, the NH_2 substituents in TATB molecules can "lock" the neighboring NO_2 group in the same plane with the aromatic ring and enhance electron delocalization which prevents the dissociation of the observed NO_2 group.

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PCC PP 08

Clar goblet isomers: electronic structure, stability, and aromaticity

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Clar's goblet presents the first synthesized example of a concealed non-Kekulé polycyclic benzenoid hydrocarbon.[1,2] This is a class of molecules for which it is not possible to draw classical Kekulé structures without unpaired electrons. According to Ovchinnikov's rule, such systems are predicted to have a singlet ground state. This study examines the stability, electronic structure and aromaticity of Clare's goblet along with its seven structural isomers. All compounds were examined in both their lowest singlet and triplet states. The singlet states were analyzed using both restricted and unrestricted broken-symmetry approaches. All calculations were performed at the B3LYP/def2-SVP level of theory. It was shown that all studied molecules exhibit a singlet ground state, consistent with Ovchinnikov's rule. The singlet states exhibit pronounced open shell diradical character and lie energetically very close to their triplet states. The observed stability and electronic structure can be rationalized through aromaticity analysis, which revealed that the singlet and triplet states exhibit remarkably similar aromatic character.

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PCC PP 09

Amyloid-like ovalbumin fibrils as novel electrode modifiers for electrochemical detection of pharmaceutical compounds

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In recent years, amyloid-like aggregates derived from food proteins have been actively studied because to their unique nanostructure, mechanical robustness, and surface functionality. Their large surface area, diverse surface chemistry and ability to form π–π and electrostatic interactions make them promising candidates for electrode modification. In this work, amyloid-like ovalbumin fibrils, whose formation was influenced by lead(II) and cadmium(II) ions[1], were employed to modify different types of electrodes for the determination of active pharmaceutical compounds. The types of modification used include drop casting amyloid solutions on surfaces of glassy carbon(GCE), carbon paste (CPE), gold and platinum electrodes, as well as modifying the CPE by incorporating the fibrils directly into the CPE mixture. To the best of our knowledge, there are currently no reports describing amyloid-like ovalbumin fibrils as modifiers for electroanalytical sensors. The electron transfer properties of the modified electrodes were evaluated using the standard redox couple $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$. The determination of antibiotics was performed by pulse voltammetry, including differential pulse voltammetry (DPV) and square wave voltammetry (SWV). The active pharmaceutical compounds investigated in this study were sulfamethoxazole, chloramphenicol, ciprofloxacin, and diazepam. Results show that drop-cast modification enhanced the cyclic voltammetric signal of 100 µM diazepam by 150.5%. Incorporating amyloid fibrils into the CPE increased the DPV signal of 100 µM sulfamethoxazole by 698.7%. Furthermore, after additional drop-casting on the CPE surface, SWV signal of 100 µM chloramphenicol increased by 631.6%.

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PCC PP 10

Effect of benzo-annelations on the HOMO-LUMO gap in polycyclic conjugated compounds

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This study investigates how different types of benzo-annelation influence the electronic properties of polycyclic conjugated compounds. The analysis is conducted using tools from chemical graph theory, yielding results equivalent to those obtained at the level of simple Hückel molecular orbital (HMO) theory.[1] The focus is on determining how angular, linear, and combined annelation modes influence the value of the HOMO-LUMO gap, which serves as an indicator of the stability and reactivity of π-conjugated systems, as well as a valuable parameter in the design of electronic and optoelectronic materials.[2] The analysis includes nine molecules, among them anthracene, biphenylene, phenanthrene, and fluorene in both cationic and anionic forms. The obtained results show that the dominant factor influencing the effect of annelation on the HOMO-LUMO gap is the size of the central ring in the studied molecules. Specifically, when the central ring contains $4n+2$ carbon atoms (e.g., anthracene), angular (linear) annelation tends to increase the HOMO-LUMO gap, while linear annelation decreases it. On the other hand, for molecules with $4n$ central rings (e.g., biphenylene), the opposite trend was observed. Overall, this study highlights the effectiveness of chemical graph theory in providing fast end insightful relations between molecular structure and electronic properties. However, as the results are based on the HMO model, further validation using more advanced quantum chemical methods remains a task for future work.

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PCC PP 11

Green production of hydrogen peroxide via selective two-electron oxygen reduction at Cu_{30}-Fe_{70}/GA

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Hydrogen peroxide (H_2O_2) is an essential chemical that, due to its strong oxidizing properties and environmental friendliness, has numerous applications in industry, laboratories, and households. However, the largest quantities of H_2O_2 are currently obtained by the anthraquinone autoxidation process, a multi-step process that uses complex infrastructure, energy-intensive procedures, costly Pd-based catalysts, and generates organic waste. Additional costs are required for transportation and storage of large quantities of concentrated H_2O_2 produced, along with high safety risks. In this work, the catalytic performance of Cu- and Fe-doped graphite aerogel, Cu_{30}-Fe_{70}/GA, towards selective 2-e^- ORR for green H_2O_2 production was investigated in an alkaline medium. Graphite aerogel is characterised by 3D porous structure, ultra-low density, high active surface area and excellent conductivity.[1] The ORR activity of this material was investigated by linear sweep voltammetry (LSV) using a rotating disk electrode (RDE) in O_2-saturated 1 M KOH. The onset potential (at -0.1 mA cm^{-2}) and the half-wave potential were determined to be 0.73 and 0.64 V vs. RHE, respectively. The Tafel slope of 122 mV dec^{-1} was obtained and the number of exchanged electrons of 2 was determined. The initial stability was tested by the chronoamperometry method. Based on the electrochemical performance, this material could potentially be used as a 2-e^- ORR catalyst for the in-situ electroproduction of green H_2O_2 in the electro-Fenton process, which is one of the most important technological procedures for wastewater treatment, thereby significantly reducing environmental pollution, facilitating work and reducing costs.

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PCC PP 12

Design of a rechargeable hybrid cell utilizing seawater electrolyte

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The growing global demand for energy necessitates the development of sustainable and cost-effective storage systems. Among the promising candidates, seawater-activated batteries are particularly attractive due to their high operating voltage and ability to deliver power at elevated current densities [1,2]. However, the instability of cathode materials remains a critical limitation. In this study, a novel hybrid electrochemical cell was developed with a rechargeable composite cathode composed of functionalized carbon felt (FCF) and electrochemically synthesized polypyrrole (PPy), further coated with silver chloride (AgCl) using a modified successive ion layer adsorption and reaction process (SILAR). The FCF/PPy–AgCl electrode demonstrated stable electrical and electrochemical properties. When paired with an AZ63 magnesium alloy anode, which functioned as a sacrificial electrode during discharge and as a hydrogen-evolving electrode during charge, the cell achieved specific energy values ranging from 120 to 32 mWh g^{-1} and specific power outputs between 52 and 450 mW g^{-1}. These findings emphasize the potential of the AZ63 | 3.5% NaCl | FCF/PPy–AgCl system for practical applications such as emergency power sources in lifeboats and short-term monitoring of shallow seawater environments.

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PCC PP 13

Exploring the Euler–Sombor index of benzenoid and phenylene molecular graphs

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The Euler–Sombor index of a graph, denoted by *EU(G)*, is a recently introduced topological index based on vertex degrees and inspired by geometric considerations of a graph. It is defined as:

$$EUG=uv\in E(G)du2+dv2+dudv$$

where d_u is a degree of a vertex u.

In this paper, we investigate the Euler–Sombor index in the context of molecular graphs corresponding to benzenoid and phenylene systems (Fig. 1), which are important families of polycyclic aromatic hydrocarbons. These compounds are widely studied in theoretical chemistry due to their stability and electronic properties. We derive general formulae for computing *EU(G)* for benzenoid and phenylene molecular graphs, based on their structural parameters and connectivity patterns [1]. The results not only simplify the computation of the index for large classes of such molecules but also highlight structural factors influencing the index values. These findings may contribute to further studies on the correlation between molecular structure and physicochemical properties of organic compounds.

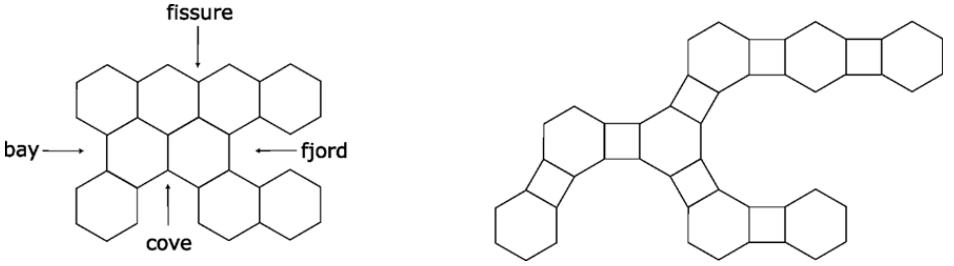

Figure 1. Benzenoid (left) and phenylene (right) molecular graphs.

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PCC PP 14

Double aromaticity in halogenated monocyclic conjugated hydrocarbons

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The cationic hexaiodobenzene, $C_6I_6^{2+}$, is a prototypical example of double aromatic molecules, exhibiting both π and σ cyclic electron delocalization. This study analyzes the double aromaticity in perhalogenated derivatives of benzene, the cyclopentadienyl anion and the tropylium cation. Aromaticity was examined using magnetically induced current density (MICD) calculations performed at the B3LYP/def2-TZVP level of theory. The selected molecules provide insight into how the size of the central carbon ring, and the nature of halogen substituents influence aromaticity. It was demonstrated that only the doubly oxidized Br- and I-derivatives of benzene and the tropylium cation exhibit double aromaticity. This behavior can be explained by the structural features of the central ring, which determine the distance between halogen atoms and facilitate the overlap of their in-plane lone pair orbitals. Additionally, substitution of Br or I atoms with BH_2 units also leads to doubly aromatic derivatives.

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PCC PP 15

Electronic structure and magnetic properties of a novel carbon allotrope: C_{48}

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A recent study has demonstrated the synthesis of a novel molecular carbon allotrope, cyclo[48]carbon, which is stable in solution at room temperature. [1] Cyclo[48]carbon was synthesized as a catenane, with a C_{48} ring threaded through three macrocyclic structures. In this work, we investigated the electronic structure and magnetic properties of the isolated C_{48} macrocycle at the B3LYP/def2-SVP level of theory. Our analysis demonstrated that the carbon ring exhibits two orthogonal, cyclically delocalized π electronic subsystems (π_{in} and π_{out}), each containing 24 electrons. A comprehensive analysis of aromaticity, conducted using both electronic and magnetic aromaticity indices, showed that the C_{48} ring is double antiaromatic (both π_{in} and π_{out}), consistent with Hückel's rule. Our results support previous claims[1] that the three surrounding macrocycles play a crucial role in stabilizing the highly reactive and antiaromatic C_{48} ring by providing steric protection.

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PCC PP 16

Influence of pnictogen interactions on the sensitivity of nitroaromatic high-energy molecules

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Non-covalent interactions have significant impact on detonation properties of high-energy molecules (HEM). [1] Generally, the non-covalent interactions can affect detonation performance of nitroaromatic HEMs in two ways: by adjusting the values of electrostatic potential over the central regions of molecular surface and by tilting the nitro groups. While the influence of hydrogen bonds on the detonation characteristics of HEMs is well established, the role of other types of non-covalent interactions is yet to be revealed and systematically analysed. [2]

In this work, we combined analysis of crystalographic data with the Density Functional Theory (DFT) calculations to reveal how pnictogen interactions affect the sensitivity of high-energy nitroaromatic molecules. The Cambridge Structural Database (CSD) was searched to identify all crystal structures containing trinitroaromatic fragments in which nitro-group was involved in intermolecular pnictogen interactions. DFT calculations at M062X/aug-cc-pVDZ level were used to calculate the interaction energies and electrostatic potential maps in selected crystal structures.

The results of the analysis of crystalographic data indicate that pnictogen interactions may affect the sensitivity of nitroaromatic explosives by tilting the nitro group in respect to the aromatic plane. The results of the DFT calculations showed that non-neglible pnictogen interactions (ΔE = -2.86 kcal/mol) are present in the crystal structure of 1,3,5-trinitrobenzene. The results also showed that in many crystal structures pnictogen interactions are accompanied by other non-covalent contacts.

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PCC PP 17

Sigma holes and halogen bonding of dihalogenated arenes – influence of regioisomerism and transition metal coordination

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Sigma hole is a region of positive electrostatic potential on an electronegative atom, which enables the formation of noncovalent interactions known as halogen bonds.[1] To study the mutual influence of halogen substituents, as well as the influence of transition metal coordination on sigma holes of halogenated benzenes, we have performed a series of DFT calculations in the Gaussian 09 (D.01) suite of programs, using the M06-2X-D3/def2-QZVP level of theory, which was previously shown to be the best methodological approach for studying halogen bonds.[2] The ability of regioisomers of dihalogenated benzenes to form halogen bonds was then assessed by studying their interactions with ammonia. The maps of electrostatic potentials showed that dihalogenated arenes exhibit larger sigma holes than monohalogenated arenes (Fig. 1). However, upon transition metal coordination, the size of sigma holes decreases for both types of these molecules (Fig. 1). Energies of halogen bonds of these molecules with ammonia show good correlation with the size of the observed sigma holes. This study shows that fine-tuning of halogen bonding and related properties can be achieved by changing mutual positions of halogen substituents in both organic and organometallic compounds.

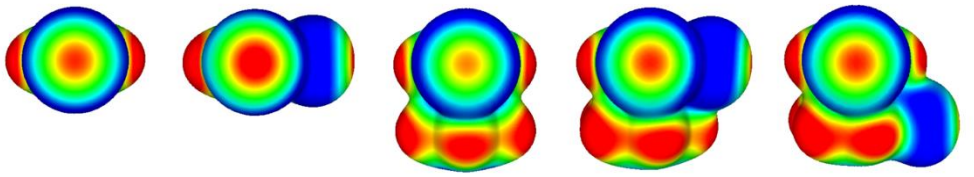

Figure 1. Electrostatic Potential (ESP) maps of bromobenzene, 1,2-dibromobenzene, (benzene)(bromobenzene)chromium, (benzene)(1,2-dibromobenzene)chromium, and (1-bromobenzene)(2'-bromobenzene)chromium. The ESPs were mapped on the molecular surface defined by electron density of 0.001 a.u. The colors denote different values of ESP in kcal/mol: blue < -9.4, -9.4 < green < 0.0, 0.0 < yellow < +9.4, red > +9.4.

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Phytochemistry and Food Chemistry (PFC)

PFC PP 01

Comparative study of maceration, ultrasound, and microwave-assisted extraction of dandelion roots

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Taraxacum officinale (dandelion) is a widely distributed medicinal plant traditionally valued for its diuretic, hepatoprotective, and antioxidant properties due to its diverse secondary metabolites. In this study, dandelion root extracts were prepared using maceration (6 days), ultrasound and microwave-assisted extraction with 70% ethanol at different solvent-to-solid ratios (1:10, 1:15, 1:20). Antioxidant activity was evaluated by FRAP, DPPH assays, while total phenolic and flavonoid contents were quantified using standard spectrophotometric methods (Folin Ciocalteu for phenolics, $AlCl_3$ for flavonoids).

Maceration led to a gradual increase in antioxidant capacity up to 72-96 h, followed by a decline, whereas ultrasound extraction reached the highest FRAP values after 20 min. Microwave-assisted extraction showed the strongest activity, achieving the highest FRAP absorbance (1.030) after 2 min at a 1:15 ratio. DPPH inhibition confirmed this trend, while the microwave extracts demonstrated markedly superior radical scavenging. HPLC analysis was applied for phytochemical profiling of phenolic compounds, while ICP-OES provided quantitative data on the mineral composition of the extracts.

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PFC PP 02

Rare sacculatane-type diterpenes from *Porella cordaeana*: complete NMR-based structural elucidation

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A series of chromatographic separations of the diethyl ether extract of *Porella cordaeana* (Huebener) Moore afforded two sacculatane-type diterpene dialdehydes. These compounds were identified as perrottetianal A and perrottetianal B, originally reported by Asakawa and co-workers (Fig. 1) [1]. The structure of perrottetianal A was later confirmed by total synthesis, while the initially proposed structure of perrottetianal B was revised in 1996 [2]. Despite these advances, complete NMR spectroscopic data for these metabolites (particularly the full ^{1}H NMR assignment of perrottetianal A) have remained unavailable. In this work, we provide the first comprehensive NMR assignment of both diterpenes. The structural elucidation was achieved through an extensive set of 1D and 2D NMR experiments, supported by spin simulations and molecular modeling.

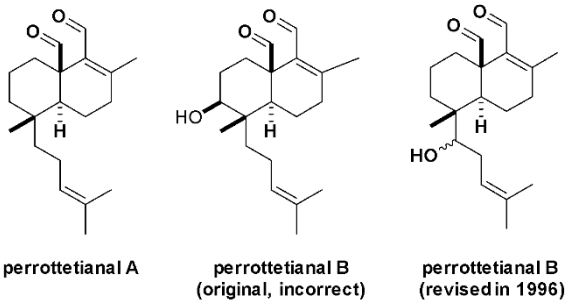

Figure 1. Structures of perrottetianal A and B.

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PFC PP 03

Comprehensive NMR characterization of isopinguisone from the liverwort *Porella cordaeana*

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The essential oil of the liverwort *Porella cordaeana* (Huebener) Moore is a known source of pharmacologically active pinguisane-type sesquiterpenes [1]. Chromatographic separation of the essential oil of *P. cordaeana* collected on Suva Mt. (Serbia) yielded a pinguisane ketone, whose structure was determined to correspond to isopinguisone [2]. To date, this compound has only been reported in a PhD thesis and has not yet been described in a scientific journal [2]. Its structure was unequivocally confirmed by 1D and 2D NMR experiments (NOESY and gradient ^{1}H–^{1}H COSY, HSQC, HMBC) and as well as by NMR spin simulation and computational modelling.

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PFC PP 04

Structural characterisation of iridoid glycosides in the aerial parts of *Nepeta nuda* L.

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Within the family Lamiaceae, the genus *Nepeta* contains approximately 280 species, with the greatest diversity found in southwestern Asia and the western Himalayan region [1]. Belonging to the cyclopenta[c]pyran monoterpenoid family, iridoids form a large and continually increasing group of compounds present in many folk medicinal plants, where they serve as bitter tonics, fever reducers, sedatives, blood pressure regulators, and agents for healing wounds and skin-related disorders, due to the wide spectrum of bioactivity of both aglyconic and glycosidic forms [2]. In this study, iridoid glycoside was isolated from air-dried aerial parts of *Nepeta nuda* L. The plant material underwent maceration in methanol over a period of three days, which was then evaporated. The obtained extract was suspended in water and extracted with chloroform. The remaining aqueous fraction was then further extracted with *n*-butanol, and this butanol extract was evaporated to yield the extract used for iridoid isolation. The purification procedures included chromatography using a Sephadex LH-20 column, implementation of dry flash chromatography, and semi-preparative high-performance liquid chromatography (HPLC). Isolated compound, identified as one of the predominant iridoid glycosides beside 1,5,9-*epi*-deoxyloganic acid, was comprehensively analyzed by detailed NMR spectroscopic analysis, employing both 1D (^{1}H and ^{13}C) and 2D (COSY, HSQC, HMBC, and NOESY) experiments. This compound, to the best of our knowledge, has not been fully investigated so far either in the plant species *N. nuda* L.or in the genus *Nepeta*.

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PFC PP 05

Cosmetic Safety Evaluation of Cultivated Serbian Plant Petals via *Danio rerio* Toxicity Test

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Flower petals are a sustainable and eco-friendly source of bioactive compounds, as their harvesting does not compromise plant survival or ecosystem balance. Rich in phenolics, flavonoids, and other valuable metabolites [1], petals remain largely underexplored compared to leaves, roots, or aerial parts, making them a promising source of bioactive ingredients for innovative cosmetic applications. To ensure their safe use, four methanolic petal extracts (PEs) with strong cosmetic potential—prairie rose (*Rosa setigera* Michx.), common peony (*Paeonia officinalis* L.), common lilac (*Syringa vulgaris* L.), and ivy geranium (*Pelargonium peltatum* (L.) L'Hér. ex Aiton)—were evaluated for toxicity using zebrafish (*Danio rerio*) embryos across six concentrations (15.62–500 μg/mL), assessing survival and hatchability. Notably, rose caused only 20% lethality at the highest concentration but significantly inhibited hatching at ≥31.25 μg/mL, whereas geranium exhibited the highest lethality, with 100% mortality at ≥125 μg/mL. Hatchability assays revealed species-specific embryotoxicity: rose completely inhibited hatching at ≥62.5 μg/mL, peony at 125 and 62.5 μg/mL, lilac showed minimal impact up to 125 μg/mL, and geranium affected hatching only at 31.25 μg/mL. Overall, in vivo results confirmed safe concentrations of ≤31.25 μg/mL for peony, lilac, and ivy geranium, and ≤15.62 μg/mL for rose. These findings establish safe concentration ranges for the tested PEs, providing guidance for their sustainable and safe incorporation into cosmetic formulations.

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PFC PP 06

Isolation and structural elucidation of abietane-type diterpene from *Euphorbia spinossa*

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The genus *Euphorbia*, which has long been used in traditional medicine for the treatment of diverse disorders, has attracted substantial scientific attention, as reflected in the extensive body of published research. *Euphorbia spinossa L*. (Euphorbiaceae) is a small perennial xerophilous shrub, distributed mainly in Mediterranean climates with a wider range on the western Adriatic (from southeastern France through the Apennine Peninsula, Sardinia, and Corsica) than on the eastern Adriatic coast (Croatia to Albania) [1]. In the present study, the root of *E. spinossa,* collected from Maglič (Serbia), was examined. The hexane-ethyl acetate extract was using conventional chromatographic methods, resulting in the isolation of bioactive metabolites, among which was the abietane-type diterpene jolkinolide B. Structural elucidation of the isolated metabolite was carried out using NMR spectroscopy and further confirmed by LC–MS analysis. Numerous studies have highlighted the diverse pharmacological properties of jolkinolide B, including its anticancer, anti-inflammatory, anti-osteoporotic and anti-tuberculosis effects, among others [2].

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PFC PP 07

The comparison of the antioxidant activity of three different teas using the Briggs-Rauscher oscillatory reaction

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The Briggs-Rauscher (BR) oscillatory reaction involves the iodination and oxidation of an organic substrate (typically malonic acid) by acidic iodate in the presence of hydrogen peroxide, catalyzed by Mn^{2+} ions. When starch is used as an indicator, the solution cycles through color changes (colorless-amber-blue) before stabilizing; however, in this study starch was omitted, and oscillations were monitored potentiometrically [1]. The BR reaction is abundant with free radical species such as reactive oxygen species (HO•, HOO•) and iodine radicals. These radicals are generated during the BR reaction course. This enables the BR reaction should be applied as an antioxidant test, in both pure compounds and plant extracts [2]. Antioxidants are compounds capable of neutralizing free radicals, and are generally classified as either synthetic or natural, with natural antioxidants being commonly found in fruits, vegetables, and various vitamins (e.g., B-complex, C, E, K). Their activity is largely influenced by their structural characteristics, particularly the degree of ring substitution [2]. When antioxidant compounds are added to the BR reaction mixture, the oscillations are temporarily suppressed. The duration of this suppression-known as inhibition time, is directly proportional to the amount and potency of the antioxidant [2]. In this study, the BR reaction was successfully applied to compare the antioxidant activity of green tea, mint tea, and chamomile tea, which are prepared in the same way. The results showed that green tea had the highest antioxidant capacity, followed by mint, while chamomile exhibited the lowest, with the shortest inhibition time. These findings demonstrate that the BR reaction is a simple, sensitive, and effective method for assessing and comparing the antioxidant potential of plant-based extracts.

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PFC PP 08

Developing a method for direct detection of erinacine A in mycelium of *Hericium erinaceus* (Bull.) Persoon

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Hericum erinaceus represents one of the most promising functional foods, with potential benefits in the treatment of neurodegenerative diseases, such as Alzheimer's disease. In addition to neuroprotective activity, *H. erinaceus* exhibits several other pharmacological effects, such as anti-hypercholesterolemic, anti-tumor, and antioxidant activities, which have been well documented [1]. Neuroprotective potential of the mycelium is best demonstrated on the two main compounds, erinacine A, and C, stimulators of nerve growth factor (NGF) synthesis [2]. Numerous *Hericium*-based supplements are currently marketed for the treatment of dementia; however, their therapeutic efficacy largely depends on the concentration of bioactive constituents, such as erinacines, underscoring the importance of rigorous standardization. In the present study, two complementary analytical methods were integrated as a quality control approach for the detection of erinacine A in *H. erinaceus* mycelium extracts. Specifically, nuclear magnetic resonance (NMR) spectroscopy was employed alongside semi-preparative high-performance liquid chromatography (HPLC). The presence of erinacine A was initially confirmed through comprehensive 2D NMR spectroscopy and detailed analysis of the resultant mixture. Subsequently, HPLC analysis was performed using both the conventional 210 nm wavelength and an additional wavelength specific to erinacine A. The applied methodology represents a reliable and promising approach for the determination of erinacines, offering enhanced speed, improved efficiency, and increased reliability.

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PFC PP 09

Phytochemical profile and biological activities of *Myrtus communis* essential oil: An HPTLC-based approach combined with GC-MS analysis

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Myrtus communis L. (Myrtaceae) is a Mediterranean aromatic plant with numerous beneficial properties [1]. This study aimed to evaluate the chemical composition of its leaf essential oil using gas chromatography–mass spectrometry (GC-MS) and to investigate its antioxidant and antibacterial activities through high-performance thin-layer chromatography combined with direct bioautography (HPTLC/DB). GC-MS analysis identified 26 compounds, accounting for 98.68% of the total oil content. The major constituents were α-pinene (41.61%) and 1,8-cineole (38.79%). HPTLC fingerprinting was performed on silica gel as the stationary phase using toluene:ethyl acetate (85:15, *v/v*) as the mobile phase, followed by derivatization with *p*-anisaldehyde–sulfuric acid (ASA) reagent. The ASA derivatization enabled the visualization of oil constituents as distinct brown, violet, and pink zones. Derivatization with 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical revealed a yellow zone at hR_F 50, corresponding to the compound with the strongest antioxidant potential. In addition, bioautographic assays against *Staphylococcus aureus* and *Klebsiella pneumoniae* showed several active zones for both tested strains, with the most pronounced antibacterial activity observed at hR_F 50. Based on the characteristic coloration after ASA derivatization, as well as literature data, this zone can be attributed to 1,8-cineole. To quantify the antibacterial activity, bioautogram images were processed using ImageJ software, and results were expressed as streptomycin equivalents per µL of oil. The calibration curve for streptomycin was obtained by plotting peak area against applied concentrations (µg/band). The results demonstrated strong antibacterial activity of essential oil, with *S. aureus* showing higher sensitivity than *K. pneumoniae*. This combined approach provided valuable insights into the antibacterial and antioxidant potential of *M. communis* essential oil and highlighted the compounds with the most promising bioactivity.

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PFC PP 10

Lacto-fermentation enhances antioxidant and digestive enzyme inhibitory activity of *Cotinus coggygria* leaf extracts

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Cotinus coggygria Scop., commonly referred to as the smoke tree or smoke bush (Anacardiaceae), is a medicinal plant with a wide range of therapeutic benefits, such as hepatoprotective, anti-inflammatory, antioxidant, antibacterial, antiviral, anticancer, and antigenotoxic effects [1]. Through modulating enzyme inhibition, boosting antioxidant and antibacterial activity, and improving phytochemical bioavailability, lacto-fermentation further expands the therapeutic potential of plant extracts [2]. This study aims to investigate the impact of lacto-fermentation on the antioxidant activity and digestive enzyme inhibitory activity of *Cotinus coggygria* leaf extracts. Fermentation-induced changes in the antioxidant profile were clearly observed using the high-performance thin-layer chromatography (HPTLC)-DPPH bioautographic approach. The bioactivity of both fermented and non-fermented ethyl acetate extracts was further assessed through spectrofotometric assays targeting the inhibition of key digestive enzymes, specifically pancreatic lipase and α-amylase. Using a moderately polar mobile phase, the HPTLC-DPPH assay showed stronger antioxidant activity in the fermented ethyl acetate extract, with intense yellow zones indicating an increased presence of active phenolic compounds due to fermentation. Fermented ethyl acetate extract of *C. coggygria* exhibited potent lipase inhibitory activity, comparable to orlistat, suggesting that lacto-fermentation enhances the formation or bioavailability of active constituents. While α-amylase inhibition by *C. coggygria* has been scarcely reported, our results indicate a significantly higher inhibitory potential in regional samples. Our results demonstrate the plant's therapeutic potential in managing obesity-related metabolic disorders and warrant further bioactivity-guided molecular investigations, while also revealing that fermentation enhances the bioactivity of smoke tree leaves.

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PFC PP 11

Turning Waste into Value: NADES-Based Extraction of Bioactives from Red Onion, Ginger, and Apple Peels

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The valorization of agri-food by-products represents a promising strategy to promote sustainability and circular economy in the food sector [1]. In this study, three types of food waste (red onion peel, ginger peel, and apple peel) were extracted using natural deep eutectic solvents (NADES) composed of combination of L-proline, malic acid, betaine, xylitol, and glycerol, alongside two conventional solvents for comparison. The obtained extracts were evaluated for their biological activities. Antimicrobial activity was tested against four foodborne pathogens (*E. coli*, *B. cereus*, *L. monocytogenes* and *S. Typhimurium*), antioxidant capacity was assessed using three spectrophotometric assays, and tyrosinase inhibitory activity was evaluated as an indicator of anti-browning potential in fruits and vegetables. The results demonstrated that NADES-based extracts showed better activities compared to conventional solvents. Since the NADES components themselves can act as functional ingredients, this approach not only ensures safe and efficient extraction but also gives the opportunity for the creation of green-labelled functional food enriched with natural antioxidants, antimicrobials, and anti-browning agents, thereby supporting waste reduction and sustainable product development.

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PFC PP 12

Beyond the fruit: polyphenols and biological activity in branches and leaves of selected Prunus and Pyrus species

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It is widely aknowledged that fruits from generas *Prunus* and *Pyrus* possess theraputical proterties, while other parts of the plants are often disregrded [1]. Over the past few decades, however, there has been increasing interest in the biological activity of these overlooked parts [2]. The main goal of this study was to investigate polyphenolic composition and antioxidant capacity of the branches and leaves of nine *Prunus* species (wild *P. avium*, cultivated *P. avium*, *P. mahaleb*, *P. fruticosa*, *P. cerasus*, *P. domestica*, *P. persica*, *P. cerasifera*, *P. cerasifera pissardii*) and one *Pyrus* species (*P. communis*). Branches and leaves were extracted in 70% ethanol using ultrasound. The polyphenolic content was analyzed spectrophotometrically to determine the total phenolic content, total flavonoid content, total hydroxycinnamic acid content, and total anthocyanins content. Antioxidant was evaluated using FRAP and DPPH assays. The highest total phenolic content was observed in *P. communis*, both branches (591.55 mg gallic acid equivalents/g dry weight) and leaves (685.62 mg GAE/g dry weight). FRAP and DPPH assays revealed *P. communis* as the most potent antioxidant source. Within the *Prunus* species, *P. cerasifera pissardii* demonstrated high antioxidant capacity, along with elevated levels total anthocyanins, phenolic acids, and total phenols. These findings highlight that by-products of these fruit species, particularly *Pyrus communis* and *Prunus cerasifera pissardii*, are potent antioxidants, but the potential of other species, should not be neglected, also.

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Solution Chemistry and Chemical Equilibrium (SCCE)

SCCE PP 01

Determination of pK_a values and water solubility of amino-modified β-CDs

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Commonly used molecules for enhancing solubility, solution stability, and photoprotection of active pharmaceutical ingredients (APIs) are cyclodextrins (CDs), glucose oligomers (6-8 glucose molecules). Different modifications of β-CD were synthesized to address the limitations in solubility and acid-base properties of unmodified β-CD. Three derivatives were synthesized: piperazine (PIP), 1,2-ethylenediamine (EDA), and 1,3-propylenediamine (PDA) modified β-CD [1-2]. Literally, modified β-CDs were not significantly physicochemically characterized. As one of the most essential molecular descriptors of molecules, pK_a values were determined with potentiometric titrations at constant ionic strength (0.15 mol/L NaCl) using a pSOL Model 3 titrator (pION) equipped with a Ross combined glass electrode and pS software package, and standard HCl and NaOH solutions. Determined pK_a values varied among derivatives, 5.39±0.02 and 9.17±0.03 for EDA-β-CD, 7.41±0.04 and 10.02±0.05 for PDA-β-CD, and 3.28±0.06 and 9.07±0.01 for PIP-β-CD. The water solubility of the derivatives was determined using the shake-flask method, with a mixing time of 6 hours and a sedimentation time of 18 hours. UV-Vis spectroscopy was used to measure the modified β-CD contents in supernatants at a wavelength of 488 nm. Solubility of unmodified β-CD was 13.88±0.07 g/L, of EDA-β-CD 87.95±2.22 g/L, of PDA-β-CD 40.73±3.54 g/L, and of PIP-β-CD 38.96±2.29 g/L. EDA-β-CD has up to 6.5 times higher water solubility than unmodified β-CD. The obtained results indicate that modifications have the potential to enhance the properties of unmodified β-CDs in all mentioned areas, especially when acidic APIs are the molecules of interest.

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Supramolecular Chemistry and Functional Materials (SCFM)

SCFM PP 01

Fabrication and surface functionalization of TiO_2/TiN thin films toward visible-light photocatalysis

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Thin film photocatalysts offer advantages over nanoparticle systems, including high mechanical stability, reusability, and straightforward integration onto solid supports. In this study, TiO_2/TiN thin films were fabricated using reactive DC sputtering, a technique that provides precise control over stoichiometry, thickness, and homogeneity. Post-deposition annealing in air at 600°C yielded polycrystalline anatase TiO_2 while preserving TiN domains, with TEM and SEM analyses revealing distinct changes in surface morphology as a function of the TiO_2/TiN ratio. Surface characterization showed variations in wettability and surface free energy, indicating that subtle modifications of the TiO_2 top layer strongly influence photocatalytic behavior. Optical measurements confirmed band gap tuning toward the visible range, while photocatalytic tests using methylene blue degradation demonstrated stable activity and reproducibility across multiple cycles. Additional surface functionalization with ultrathin gold films further adjusted surface chemistry and contributed to improved light harvesting. These results show that photocatalytic efficiency is closely linked to the surface characteristics of the films, such as morphology, wettability, and optical response, while reactive sputtering provides a reliable and scalable method to obtain such thin film heterostructures [1].

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SCFM PP 02

Effect of ethanol on the thermoresponsive behavior of P(NiPAM) hydrogels

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Thermoresponsive hydrogels have been a key focus of research and are among the most widely used materials in polymer-based biomedicine. Despite decades of investigation, certain aspects of the behavior of N-isopropylacrylamide (NiPAM) remained insufficiently understood. This monomer was selected due to the pronounced temperature responsiveness of its hydrogels, particularly within the transition range around 32°C, which is close to physiological temperatures [1]. This study investigates how ethanol, both as an additive and as a pure solvent, affects the properties of P(NiPAM) hydrogels, using water-based synthesis as the reference. One of the objectives of this work was to gain insight into how ethanol affects the quality and properties of the resulting hydrogels. After synthesis, the gel phase was examined, followed by FTIR analysis to assess the crosslinking degree. The hydrogels underwent swelling measurements during heating and cooling to determine the volume phase transition temperature (VPTT) and assess material reproducibility. SEM analysis confirmed structure–property relationships.

The results show that water-synthesized hydrogels had the highest gel content, the most robust surface, and the best temperature response. The introduction of ethanol as a cosolvent significantly reduced the gel fraction, pointing to a pronounced cononsolvency [2] effect that hindered network formation. When synthesized in pure ethanol, although the structure was defined, the yield was extremely low, preventing triplicate characterization. These findings underscore the crucial role of solvent choice in designing thermoresponsive hydrogels and provide valuable guidance for optimizing synthesis conditions for biomedical applications.

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SCFM PP 03

Microscale surface topography evolution of a new-generation titanium alloy subjected to laser treatment

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Enhancing the surface characteristics of metallic biocompatible materials is essential for the production of long-lasting medical implants [1]. This study investigates the effects of laser surface treatment on the surface chemistry, morphology, and roughness of a new-generation titanium alloy, both before and after severe plastic deformation by high-pressure torsion (HPT). Field-emission scanning electron microscopy (FE-SEM), energy-dispersive spectroscopy (EDS), and profilometric analysis were employed to assess the morphological and chemical changes induced by laser treatment. The picosecond laser pulses' interaction with the surface of as-received and HPT-deformed alloy led to notable morphological alterations, including ripple-like structures, re-solidified droplets, and crater-like features. These alterations were dependent on the applied laser energy. Namely, usage of low laser energy caused localized melting and re-solidification, while high energy application resulted in more pronounced surface damage due to ablation and rapid material vaporization. Moreover, increased oxygen content at the alloy surface was revealed by EDS analysis at lower laser pulse energy, higher in the case of the as-received alloy. Furthermore, profilometric measurements showed a clear correlation between laser pulse energy and surface roughness for both pre- and post-HPT alloy states, with surface roughness increasing with energy increase in both cases, and the highest values being observed in the HPT-deformed alloy. Overall, the results demonstrate that laser surface treatment, especially when combined with HPT processing, can significantly alter the surface characteristics of titanium alloys, potentially improve their functional performance and contribute to the development of advanced titanium-based implant systems.

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SCFM PP 04

A novel La_2O_3/rGO aptasensor for rapid and sensitive electrochemical spore biosensing

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Bacillus cereus is an opportunistic pathogen that poses a major risk to food safety and public health by producing thermostable toxins responsible for food poisoning and gastrointestinal disorders. The high resistance of its spores to adverse environmental conditions highlights the need for rapid and reliable detection methods [1]. Lanthanum (La) and other rare earth elements have gained increasing attention in electrochemistry due to their catalytic activity, oxygen mobility, and electrical conductivity, making them promising for biosensor development [2]. In this study, a La_2O_3/reduced graphene oxide (rGO) composite (1:5 ratio) was synthesized via the Pechini method and used to modify screen-printed carbon electrodes (SPCEs). Structural and morphological analyses (XRD, FTIR, SEM, TEM) confirmed the formation of La_2O_3 nanostructures and successful composite integration. An aptasensor for spore detection was fabricated through direct aptamer immobilization, and key parameters (pH, temperature, aptamer concentration, interaction time) were optimized. The sensor was validated on real samples, confirming its potential for practical biosensing applications.

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SCFM PP 05

Alginate-coated jute non-woven sorbent for removal of cationic dyes from aqueous solutions

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The rising levels of textile waste are negatively influencing the environment. At the same time, effluents originating from textile dyehouses pose a threat not only to aquatic life, but also to terrestrial biota, including humans, due to the presence of various organic and inorganic compounds that are visible in the water and difficult to degrade. To tackle these challenges, an effort has been made to develop a non-woven sorbent made from recycled jute carpet fringes, which can be utilized for the removal of cationic dyes from effluents produced by textile dyehouses. The non-woven sorbent was modified with biopolymer alginate, providing carboxyl groups as potential binding sites for the basic dye C.I. Basic Red 46 from water. FESEM and FTIR analyses confirmed the presence of alginate coating on the fiber surface. A series of experiments was conducted in batch mode to evaluate the influence of contact time, concentration, pH, and temperature on dye uptake. The alginate-coated sorbent demonstrated a maximum sorption capacity of 51 mg/g, in contrast to the 43 mg/g capacity of the non-coated sorbent, suggesting that the alginate coating improves the sorption performance of the non-woven sorbent. The largest sorption capacity was achieved at pH 8. The variation in temperature did not significantly affect the sorption process. The findings of this research indicate that the alginate-coated non-woven sorbent, which is produced from recycled jute, has the potential for repeated sorption of cationic dyes from effluents. Nevertheless, a 50% reduction in sorption capacity was noted following five cycles of sorption.

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SCFM PP 06

Carrageenan-anthocyanins/chitosan films supported by artificial neural network model for food freshness monitoring

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Various polysaccharides and color-sensing compounds, along with different methods, have been utilized for the preparation of active and smart packaging formulations [1,2]. In this research, novel multifunctional packaging for monitoring and maintaining food freshness, significant from the aspect of quality control and food safety, has been developed. Bilayer films, based on carrageenan and chitosan hydrogels incorporating anthocyanins extract from red cabbage, were prepared using the layer-by-layer technique. Anthocyanins, as pH-sensitive indicators, were loaded in the inner layer based on κ-carrageenan hydrogel, while the chitosan hydrogel was utilized as a protective outer layer. The developed films demonstrated excellent homogeneity, fast and reversible pH and NH_3 responsiveness, while the chitosan layer ensured the stability of the encapsulated anthocyanins. The films exhibited excellent antioxidant activity (87%) against DPPH free radicals, thus indicating the potential of developed films to be used as active packaging as well. The applicability of the films in the process of fish freshness monitoring was evaluated through monitoring the storage of trout fillets for 12 days at 4 °C. The color of the films changed from brown to green as storage proceed, thus confirming the suitability of the films to predict food freshness. Additionally, in order to provide a more precise, appropriate, and non-destructive method to determine fish freshness, different machine learning algorithms were established using the correlation between film color and ammonia content, as a fish spoilage indicator. The application of an artificial neural network algorithm achieved the most precise prediction (R^2=0.984). Based on all the obtained results, it can be concluded that the prepared chitosan-carrageenan films with encapsulated red cabbage anthocyanins have good potential for food preservation and, in combination with machine learning models, these films could successfully be applied for monitoring fish quality.

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SCFM PP 07

Magnetic properties of the hybrid polymer containing incorporated magnetite nanoparticles

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An innovative approach in polymer synthesis involves the incorporation of nanoparticles into their structure. These hybrid systems offer a wide range of applications, enable simple and efficient separation from mixtures (particularly useful in complex matrices) using an external magnetic field, further increasing their applicability and efficiency, replacing time-consuming centrifugation and filtration steps[1]. Magnetite (Fe_3O_4) is one of the most commonly used magnetic materials due to its low toxicity, biocompatibility, and ease of preparation[2]. Surface modification of a magnetite particle can improve thermodynamic stability and dispersion, reduce agglomeration between particles, change the physical and chemical properties of its surface, and change its compatibility with other components in the system. Various types of silanes, such as tetraethyl orthosilicate, TEOS, are the most commonly used inorganic compounds for surface modification and protection, as they provide many functional groups that can easily be converted into other desirable groups. In this work, the magnetic properties of the polymer were examined using a SQUID magnetometer. The saturation magnetization value, *Ms*, for the analyzed polymer is 4.8 emu/g, while the isothermal magnetization curve has low coercive field values (*Hc* = 0.17 kOe) and remanent magnetization, *Mr,* 0.63 emu/g, which are a characteristic of superparamagnetism. The *Mr/Ms* value of 0.13 indicates that polymer possesses a multidomain structure and has nearly uniform magnetization.

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SCFM PP 08

Enhancing environmental stability of perovskite absorbers through polyionic liquid engineering

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Metal halide perovskites are promising photovoltaic materials due to their excellent optoelectronic properties and low-cost fabrication, but their rapid degradation under moisture, UV light, and heat hinders commercialization. To address this, we incorporated polyionic liquids (PILs) into formamidinium lead iodide ($FAPbI_3$) thin films to improve stability. [1] Two PILs, Poly(lithium bis(trifluoromethanesulfonyl)imide) (for short w/PIL 1) and 1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (for short w/PIL 2) were added to the precursor solution, and the resulting films were tested under controlled environmental stress. Their evolution was tracked using UV–Vis spectroscopy, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and scanning electron microscopy (SEM). Pristine $FAPbI_3$ films degraded within 45 minutes of moisture exposure, while δ-phase formation was delayed to 75 minutes with [PMTFSI]Li and 115 minutes with [PMTFSI][Imid]. Under UV stress, [PMTFSI]Li showed stronger morphological stability, whereas [PMTFSI][Imid] exhibited minor PbI_2 formation. Thermal tests further confirmed the delayed emergence of PbI_2 in PIL-modified films. Overall, PILs suppressed degradation, preserved film morphology, and improved environmental stability, underscoring their potential for more durable perovskite solar cells.

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SCFM PP 09

Investigation of $MgGd_2Zr_2O_8$ doped with Eu^{3+} ions as an innovative luminescent material

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A new luminescent down-conversion material, composed of $MgGd_2Zr_2O_8$ doped with different concentrations of Eu^{3+} ions (2, 5, 10, 15, 20 and 25 at. %), was synthesized *via* sol-gel method, using urea as a chelating agent. The X-ray Powder Diffraction (XRPD) pattern indicated that the sample crystallizes as a pure cubic phase of $MgGd_2Zr_2O_8$ with space group Fd-3m (227). Transmission Electron Microscopy (TEM) discovered agglomerated clusters containing nanoparticles measuring approximately 5 nm in size, while energy dispersive spectroscopy (EDS) confirmed a uniform elemental distribution of all constituting elements. Luminescence was observed after excitation at 313 nm and revealed emission lines that originate from the $^5D_0 \rightarrow {}^7F_J$ transitions of the Eu^{3+} ions, with J=0, 1, 2, 3, 4. Intensity of the luminescence emission increased with increasing the concentration of europium ions, up to 15 at. %, after which the concentration quenching led to its decrease. Examination of luminescence properties demonstrated the predominance of red emission transitions, and a potential for the material to be used in light emitting devices.

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SCFM PP 10

Design and synthesis of P(MAA-co-PEGMA) hydrogels as functional sorbents for fluoxetine as a pollutant

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Pharmaceuticals are increasingly recognized as persistent pollutants in aquatic environments, necessitating the development of efficient and sustainable removal strategies [1]. In this study, we synthesized a crosslinked poly(methacrylic acid-co-poly(ethylene glycol) methacrylate) [P(MAA-co-PEGMA)] hydrogel and evaluated its potential as a sorbent for fluoxetine, a widely prescribed antidepressant of environmental concern. The hydrogel was prepared via free radical polymerization using the neutralized form of methacrylic acid together with PEGMA, guided by Hansen Solubility Parameters (HSP) to ensure compatibility and optimize interaction with the target pharmaceutical. A crosslinking agent was employed to generate a stable three-dimensional polymer network. The combination of ionizable carboxylate groups from MAA and the flexible PEGMA chains provided complementary binding sites, enabling electrostatic attraction with the protonated amine of fluoxetine and enhanced compatibility of its aromatic and hydrophobic groups with the PEG segment. Swelling studies confirmed favorable water uptake, while sorption experiments demonstrated nearly complete removal of fluoxetine (~93%) from solution under the tested conditions, starting from an initial concentration of 100 ppm. The high affinity of the hydrogel toward fluoxetine highlights the importance of functional group design and solubility parameter-driven monomer selection in achieving efficient uptake. These findings indicate that crosslinked P(MAA-co-PEGMA) hydrogels represent a promising class of functional polymeric materials for water remediation. Their tunable chemistry, and high sorption efficiency underscore their potential within supramolecular chemistry and functional materials frameworks for addressing pharmaceutical pollution.

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SCFM PP 11

Antibacterial activity of silver-immobilized polymer composite

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Polymeric materials represent a versatile platform for designing functional composites with tailored properties. Among them, glycidyl methacrylate (GMA)-based polymer composites have attracted considerable attention due to their chemical reactivity, structural stability, and adaptability for various functionalizations, including the incorporation of silver ions.[1] Silver is recognized as one of the most effective antimicrobial agents, with broad activity against microorganisms. When immobilized within a polymer composite, silver ions may remain biologically active and exhibit antimicrobial activity.

In this study, the antibacterial potential of the GMA/Ag polymer composite was evaluated against gram-positive bacteria (*Micrococcus luteus* and *Bacillus subtillis*) using the agar well diffusion method.[2] Agar plates were prepared under sterile conditions and inoculated with test bacteria. Then wells were filled with the composite sample (30 mg in 100 μL of sterile distilled water). Following 24 h of incubation at 37 °C, inhibition zones were measured with a ruler to assess antibacterial efficiency. The results revealed clear inhibition zones of approximately 4 mm against the tested bacteria, confirming the pronounced antibacterial activity of the polymer with immobilized silver. This shows that the GMA/Ag polymer composite could be used as an antibacterial agent in diverse fields.

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SCFM PP 12

Structure–property relationships in P(OEGDA/OPGMA) copolymeric hydrogels: A study on composition, crosslinking, and thermal sensitivity

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This study investigates the synthesis and characterization of copolymeric hydrogels composed of oligo(ethylene glycol) diacrylate (OEGDA) and oligo(propylene glycol) methacrylate (OPGMA), prepared in three different monomer ratios and synthesized with or without an external crosslinker via gamma radiation polymerization and crosslinking. The hydrogels were produced in a water/ethanol (50/50, v/v) solvent system, using a fixed monomer-to-solvent molar ratio of 10:90. Although OEGDA has been occasionally reported in the literature as a crosslinker [1], in this work it was used primarily as a co-monomer and, in selected formulations, ethylene glycol dimethacrylate (EGDMA) to investigate its potential to contribute to network formation. The thermal responsiveness of the resulting hydrogels was assessed by conducting swelling measurements over a wide range of temperatures, as a function of monomer composition and crosslinking strategy. FTIR spectroscopy revealed distinct structural differences between hydrogels crosslinked solely by irradiation and those additionally crosslinked with EGDMA. Gel content analysis confirmed more efficient network formation in the presence of EGDMA. Consistently, SEM analysis of P($OPGMA_{50}$/$OEGDA_{50}$) hydrogels highlighted clear morphological differences between irradiation-crosslinked networks and those formed with the chemical crosslinker.

These results provide insight into how monomer composition and the use of a crosslinker influence hydrogel structure and behavior, and demonstrate both the potential and limitations of using OEGDA in the design of temperature-responsive hydrogel networks. The findings may support the development of smart materials for environmental applications.

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SCFM PP 13

Femtosecond laser-induced micro- and nanostructuring of silicon surfaces for biomedical applications

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The experimental investigation of Ti/Zr/Ti thin films deposited on silicon substrates pre-patterned by dynamic femtosecond laser processing is presented. High-aspect-ratio micrometer-scale conical spikes (~2 μm height, 40° opening angle, density ~13×10^6 cm^{-2}) were generated on crystalline silicon under 0.65 bar SF6 ambient using femtosecond laser pulses, producing black silicon surfaces tailored for biomedical applications. Subsequent ion sputtering deposition formed a 400 nm-thick composite Ti/Zr/Ti thin film over the laser-structured surface. Detailed characterization by FESEM-EDS, XPS, TEM, and EDX revealed the surface morphology, elemental composition, and interdiffusion phenomena within the Ti and Zr layers after deposition. This study demonstrates the integration of femtosecond laser surface texturing and multilayer thin-film deposition for engineered silicon surfaces with potential biomedical functionality.

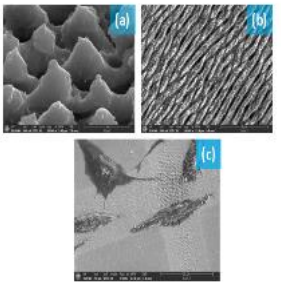

Figure 1. *FE-SEM micrographs of laser-modified silicon surfaces with thin film deposition showing: (a) conical spike structures, (b) laser-induced periodic surface structures (LIPSS), and (c) fibroblast cells adhered on LIPSS.*

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SCFM PP 14

Amino-modified β-cyclodextrin as a solubilizer for folic acid

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Folic acid (FA), also known as vitamin B9, is a water-soluble micronutrient, involved in folate-mediated one-carbon transfer reactions, crucial for *de novo* nucleotide synthesis as well as for cellular methylation reactions, that maintain genome integrity and regulate gene expression. Adequate FA intake is critical during pregnancy, where supplementation in the preconceptional and early gestational period is well established to reduce neural tube defects, highlighting its key role in embryonic development and maternal health [1]. However, FA's low aqueous solubility and light sensitivity limit formulation robustness. Previous attempts to overcome these limitations involved the use of native cyclodextrins (CDs), well established supramolecular hosts for improving drug solubility and stability, as well as glucose- and maltose- substituted monoderivatives of β-CD [2]. In this work, two derivatives, propylenediamine-modified β-CD (PDA-β-CD) and piperazine-modified β-CD (PIP-β-CD), were evaluated as hosts for improving FA solubility and stability. We have shown that in 6 mM solutions of these derivatives, solubility of FA increased 2.28-fold with PDA-β-CD, and 2.29-fold with PIP-β-CD, compared to that of the unmodified β-CD, as determined by HPLC analysis. Under UV irradiation (254 nm), complexation with PIP-β-CD conferred superior protection relative to both buffer and unmodified β-CD. Correspondingly, the FA half-life ($t_{1/2}$) increased from 33.1 min in buffer and 33.9 min in β-CD to 50.7 min in PIP-β-CD. Chemical stability was profiled at pH 7.4, 6.5, and 5.5, and in biorelevant FaSSIF and FeSSIF media. After three days, substantial FA degradation was observed only in FaSSIF, and protection followed the order PIP-β-CD > β-CD > buffer, consistent with tighter binding affording greater suppression of degradative pathways under intestinally relevant conditions. These results position both derivatives as promising formulation tools for simultaneous FA solubilization and photoprotection.

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Many thanks to Shimadzu for providing the HPLC LC2050C 3D PDA for use.

SCFM PP 15

Enhanced photostability of naproxen through complexation with amino-modified beta-cyclodextrin

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Cyclodextrins, cyclic oligomers containing 6-8 glucose units, are frequently used as complexing agents for a broad group of active pharmaceutical ingredients (APIs) in the pharmaceutical industry. Their use as enhancers of APIs solubility, as well as formulation stabilizers, photoprotectors and antioxidants, makes them an integral part of drug formulation development [1]. β-Cyclodextrins (β-CDs, 7 glucose units) are widely used for their purposes, but they have limited water solubility and form low-stability complexes with APIs. To enhance the solubility and complexation potential of β-CD, 1,2-ethylenediamine (EDA) was used to synthesize amino-modified β-CD [2]. In this study, modified β-cyclodextrin was applied to improve the photostability of naproxen, a non-steroidal anti-inflammatory drug. The obtained results suggest that upon irradiation with a 254 nm UV lamp, complexes of naproxen with EDA-β-CD are more stable than with unmodified β-CD. Photodegradation was followed using reversed phase (C18) HPLC with PDA detection. Determined photodegradation constants (according to zero-order kinetics) were 2.13×10^{-6} mol/L×min for unmodified β-CD and 1.98×10^{-6} mol/L×min for EDA-β-CD. Degradation half times at 1.0×10^{-3} mol/L β-CD concentrations were 42.46 ± 2.68 min for unmodified β-CD and 45.01 ± 2.93 min for EDA-β-CD.

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Many thanks to Shimadzu (Japan) for providing the HPLC LC2050C 3D PDA for use.

SCFM PP 16

Polyaniline/TiO_2 heterostructure: the efficient photocatalyst for diazepam degradation under simulated solar light

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As pharmaceuticals have become significant wastewater pollutants [1], the objective of this work was to design efficient PANI/TiO_2 photocatalysts for degradation of psychiatric drug diazepam since both, titanium dioxide (TiO_2) and polyaniline (PANI) are highly appropriate for photocatalytic application. Hence, PANI/TiO_2 heterostructures with different amounts of PANI (0, 1, 3, 5 wt.%) were obtained by mixing TiO_2 synthesized by using hydrothermal method and PANI prepared via chemical oxidative polymerization. The obtained samples were characterized by XRD, FT-IR, FESEM, EDS, DLS, and UV/Vis methods, while their photocatalytic efficiency was examined by UV/Vis and TOC methods. The tetragonal anatase with preserved structure was obtained in all the samples, with crystallites sized of about 25 nm. EDS analysis revealed that the PANI/TiO_2 heterostructures were successfully formed. According to FESEM, TiO_2 created spherical particles with an average size of 23 nm, while PANI consisted of fibers with an average length of 300 nm. Interestingly, with an increase in PANI content, particle size distribution was wider. According to the absorption spectra, the absorption edge of PANI/TiO_2 was shifted to the visible light region compared to pristine TiO_2. All the samples showed photocatalytic activity towards diazepam, while 1%PANI/TiO_2 was the most efficient by degrading 95.9% of this drug after 210 min under simulated solar light. Moreover, this heterostructure showed high mineralization efficiency as well, which was confirmed by TOC measurements. The performed kinetic analysis revealed that the photocatalytic degradation of diazepam in this work can be well described by pseudo-first kinetic order. The highest value of reaction rate constant (0.017(1) min^{-1}) was obtained for the 1%PANI/TiO_2. Finally, based on scavenger tests and electrochemical calculations, the diazepam photocatalytic degradation in the presence of 1%PANI/TiO_2 heterostructure under simulated solar light follow direct Z-scheme type of mechanism.

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