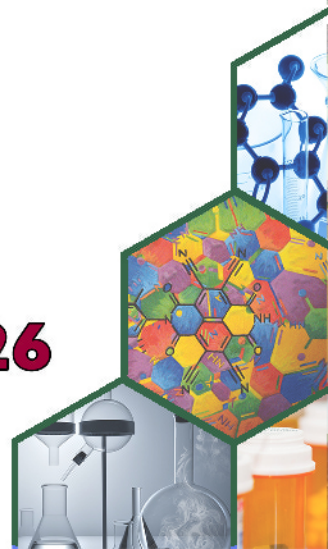
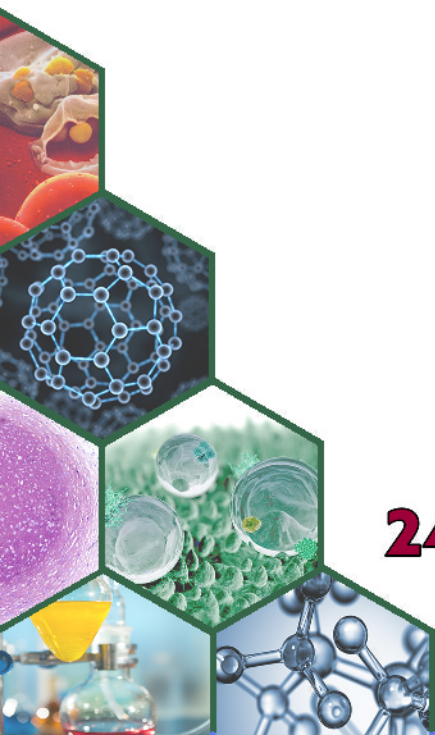


Serbian Chemical Society  
Serbian Young Chemists' Club



# **12<sup>th</sup> Conference of the Young Chemists of Serbia *Book of Abstracts***

**Novi Sad  
24<sup>th</sup> OCTOBER 2026**



**12<sup>th</sup> Conference of Young Chemists of Serbia**

# **Book of Abstracts**

**24<sup>th</sup> October 2026**

**University of Novi Sad – Faculty of Science**

**12<sup>th</sup> Conference of Young Chemists of Serbia**

Novi Sad, 24<sup>th</sup> October 2026

**Book of Abstracts**

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## Scientific Program

| Time schedule | Program                                                                                                                                                                                                                                          |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:00          | <i>Registration of the participants</i><br>Mounting posters for the Poster Session 1 ( <b>ODD POSTER NUMBERS</b> )                                                                                                                               |
|               | <i>Conference opening</i>                                                                                                                                                                                                                        |
| 10:00         | Serbian Chemical Society<br>Scientific Committee<br>Serbian Young Chemists' Club presentation                                                                                                                                                    |
| 10:15         | <i>Sponsor presentation</i><br><b>Olivera Popov, Teodora Ulić and Ana Marjanović</b> (Elixir Group)                                                                                                                                              |
| 10:25         | <i>Plenary Lecture</i><br><b>PP OP 01 – Izudin Redžepović</b><br>State University of Novi Pazar, Novi Pazar, Serbia<br><i>"New approaches to measure structural similarity of networks"</i>                                                      |
| 11:10         | <i>Sponsor presentation: MDPI Molecules</i><br><b>Tanja Nikolić and Milica Plazinić</b>                                                                                                                                                          |
| 11:20         | <i>Poster session 1 and Coffee break</i>                                                                                                                                                                                                         |
| 11:50         | <i>Coffee break</i>                                                                                                                                                                                                                              |
| 12:10         | <i>European Young Chemists' Network (EYCN) presentation</i><br>Jelena Tadić<br>Mounting posters for the Poster Session 2<br>( <b>EVEN POSTER NUMBERS</b> )                                                                                       |
| 12:20         | <i>Invited Lecture</i><br><b>PPP OP 01 – Jelena Tadić</b><br>University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia<br><i>"Natural products as sources of bioactive compounds: Insights from natural cleistanolate and its analogues"</i> |
| 12:50         | <i>Poster session 2</i>                                                                                                                                                                                                                          |
| 13:40         | <b>*GROUP PHOTO*</b>                                                                                                                                                                                                                             |
| 13:45         | <i>Lunch</i>                                                                                                                                                                                                                                     |
| 14:30         | <i>Popular Scientific Lecture</i><br><b>Luka Mihajlović, Analysis d.o.o.</b>                                                                                                                                                                     |
| 14:55         | <i>Invited Lecture</i><br><b>PPP OP 02 – Andrea Usenik</b><br>Faculty of Science, University of Zagreb, Zagreb, Croatia<br><i>"Old receptors, new tricks: intrinsic fluorescence of calixarenes and its applications"</i>                        |

|       |                                                                                                                                                                                                                                     |
|-------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 15:25 | <i>Presentation of guests from SS HKD</i><br><b>Josip Mikulić and Vedrana Stantić</b>                                                                                                                                               |
| 15:40 | <i>Oral presentations, Session 1 + flash presentation</i>                                                                                                                                                                           |
|       | <b>DCS OP 01</b> – Josip Mikulić<br><i>Faculty of Science, Zagreb, Croatia</i><br>"Regioselectivity of carbene-intermediate reactions modulated by hydrogen bonding"                                                                |
|       | <b>CB PP 23</b> – Andrej Nikolić<br><i>University of Rijeka, Rijeka, Croatia</i><br>"Porphyrin conjugation as a structural modulator of antimicrobial peptides"                                                                     |
|       | <b>PCC PP 15</b> – Luka Klemen<br><i>University of Zagreb, Faculty of Science, Zagreb, Croatia</i><br>"Intrinsic fluorescence of calix[6]arene as a probe for metal cation complexation"                                            |
|       | <b>CS OP 01</b> – Katarina Čeranić<br><i>Innovative Centre of the Faculty of Chemistry, Ltd., Belgrade, Serbia</i><br>"CSD4NCI workshop – a cheminformatics workshop on analyzing noncovalent interactions using the CSD Portfolio" |
|       | <b>CB OP 01</b> – Milena Petrović<br><i>University of Kragujevac, Faculty of Science, Kragujevac, Serbia</i><br>"Targeting HSP90 with pyrazoline-based derivatives: A docking-guided design, synthesis and biological evaluation"   |
|       | <b>EA OP 01</b> – Dragana Žmukić<br><i>University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia</i><br>"Optimization of polyhydroxyalkanoates production from biomass using response surface methodology"                      |
| 16:25 | <i>Coffee break</i>                                                                                                                                                                                                                 |
| 16:40 | <i>Oral presentations, Session 2</i>                                                                                                                                                                                                |
|       | <b>PCC OP 01</b> – Andrija Vukov<br><i>University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia</i><br>"Influence of alkyl chains on the physicochemical and thermophysical characteristics of nicotine-based ionic liquids"   |
|       | <b>PFC OP 01</b> – Anita Smailagić<br><i>Innovative Centre of the Faculty of Chemistry, Ltd., Belgrade, Serbia</i><br>"Different approaches for extraction of oil and polyphenols from grape seeds from Serbian wineries"           |

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**SCCE OP 01** – Milica Stefanović Pirković

*Institute of Chemistry, Technology and Metallurgy, National  
Institute of the Republic of Serbia, University of Belgrade,  
Belgrade, Serbia*

"Physicochemical changes in badlands under simulated climatic  
conditions - the interplay between mineralogical composition and  
texture"

**SCFM OP 01** – Milena Marković

*University of Priština, Faculty of Sciences and Mathematics,  
Kosovska Mitrovica, Serbia*

"MOF-derived nanoparticles for enhanced sensing of phenolic  
pollutants"

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|       |              |
|-------|--------------|
| 17:20 | <i>Break</i> |
|-------|--------------|

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|       |                         |
|-------|-------------------------|
| 17:30 | <i>Closing ceremony</i> |
|-------|-------------------------|

|  |                                   |
|--|-----------------------------------|
|  | <i>Awards and acknowledgments</i> |
|--|-----------------------------------|

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|       |                              |
|-------|------------------------------|
| 17:50 | <i>End of the Conference</i> |
|-------|------------------------------|

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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 contribution code, e.g. XY PP 15.

**VENUE:**

- Lectures and oral presentation will be taken place at the "Mihajlo Pupin" amphitheater on the ground floor at the Department of Mathematics and Informatics, Faculty of Science, University of Novi Sad (address: Trg Dositeja Obradovića 4, Novi Sad).
- The Poster sessions will take place in the hallway in front of the "Mihajlo Pupin" amphitheater.





## **Plenary Lecture**

**PP OP 01****New approaches to measure structural similarity of networks**Izudin Redžepović

State University of Novi Pazar, Novi Pazar, Serbia

Measuring similarity between complex systems represented as networks is a central challenge across disciplines such as network science, chemoinformatics, and social network analysis. Classical approaches, including exact graph matching, graph edit distance, and graph kernels offer powerful tools but often suffer from computational complexity or limited sensitivity to subtle structural variations.

In this talk, we present two new approaches to measure structural similarity of networks. First, we introduce a distribution-based framework for network similarity assessment [1]. In this approach, each network is represented by its degree and distance distributions, which capture key structural features in probabilistic form. These distributions are compared using Jensen-Shannon and Hellinger metrics, and we combine them into a unified similarity measure that reflects complementary aspects of network structures. Then, we introduce a novel class of similarity measure based on multiple topological indices [2]. This approach enables efficient polynomial-time computation while retaining sensitivity to fine structural information.

Importantly, both frameworks show strong potential in chemoinformatics, where capturing subtle molecular similarities is a critical step for drug design and molecular discovery, and we demonstrate their effectiveness on structured network families, random graph models, and real-world applications, highlighting promising directions for scalable and meaningful network comparison across diverse scientific domains.

**References**

- [1] M. Dehmer, I. Redžepović, N. Tratnik, P. Žigert Pleteršek, *Appl. Math. Comput.* **2026**, 531, 130179.
- [2] M. Dehmer, I. Redžepović, N. Tratnik, P. Žigert Pleteršek, *MATCH Commun. Math. Comput. Chem.* **2027**, 97 (1), 5.

**Acknowledgments**

I.R. gratefully acknowledges support received from the Serbian Ministry of Science, Technological Development, and Innovation (Agreement No. 451-03-34/2026-03/200252).

## **Invited Lectures**

**PPP OP 01****Natural products as sources of bioactive compounds: Insights from natural cleistanolate and its analogues**

Jelena Tadić

*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*

Natural products remain an important source of structurally diverse scaffolds for the discovery and development of biologically active compounds. Their structural and stereochemical complexity also present challenges that make them particularly valuable targets for synthetic and medicinal chemistry [1,2].

This lecture will present the story of natural product (–)-cleistanolate, from its isolation and synthesis to its stereochemical assignment. The use of the cleistanolate scaffold as a starting point for the synthesis of structurally modified analogues will also be discussed, together with their biological evaluation, including cytotoxic, cholinesterase-inhibitory and antimicrobial activities.

Through the example of (–)-cleistanolate, the lecture will illustrate how natural-product isolation, structure elucidation and organic synthesis can be integrated with analogue design and biological evaluation to explore new chemical space and identify biologically active compounds.

**References**

[1] D. J. Newman, G. M. Cragg, *J. Nat. Prod.* **2020**, 83, 770.

[2] D. J. Newman, *Nat. Sci. Rev.* **2022**, 9, nwac206.

**Acknowledgments**

The work was supported by a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-33/2026-03/ 200125 & 451-03-34/2026-03/200125), (in part) by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130), by the project of Croatian Science Foundation (HrZZ-9343) and by the Agency of Slovak Academy of Sciences VEGA (Grant No. VEGA 2/0094/23). The part of this lecture is based upon work from COST Action EURESTOP, CA21145, supported by COST (European Cooperation in Science and Technology).

**PPP OP 02****Old receptors, new tricks: intrinsic fluorescence of calixarenes and its applications**Andrea Usenik

Faculty of Science, University of Zagreb, Zagreb, Croatia

The monograph *Calixarenes and Beyond* [1] stated *Because the calixarenes are not fluorescent, they cannot be used as luminescent materials without introducing a luminescent center*. However, we have recently shown that tertiary-amide and ester calix[4]arene derivatives, as well as their monomeric analogue, do fluoresce, with the intensity and the position of the emission maximum shifting considerably upon binding of alkali and alkaline earth metal cations [2a]. This has since been explored for the more flexible calix[6]arene derivative, which can also form ternary complexes [2b]. Changes in fluorescence during metal-ion binding depend on the cation size and charge, whereby intensity in some cases increases, whereas in others it is quenched. These changes allow quantitative investigations at up to three orders of magnitude lower ligand concentrations than required by other methods. Large complex stability constants can be determined by direct fluorimetric titrations, avoiding time- and material-consuming competitive experiments. To investigate the origin of the emission and its complexation-induced changes, the structures and stoichiometries of the complexes were addressed experimentally (NMR, MS) and computationally (MD), and time-resolved fluorescence measurements were carried out. The different fluorimetric response of the monomeric, cyclotetra- and cyclohexameric compounds points to conformational rigidification and/or solvent inclusion in the calixarene basket as a driving force, together with reduced photoinduced electron transfer in the complexes. This paves a way to using calixarenes with no appended fluorophores as sensors for ionic species and their quantitative analysis.

**References**

- [1] P. Neri, J. L. Sessler, M.-X. Wang (Eds.), *Calixarenes and Beyond*, Springer International Publishing, Cham, 2016.
- [2] a) A. Usenik, I. Nikšić-Franjić, M. Belovari, M. Jurković, L. Klemen, N. Cindro, N. Došlić, I. Piantanida, V. Tomišić, *Anal. Chim. Acta* **2025**, 1377, 344648. b) A. Usenik, F. Sunjka, K. Kukina Gradečak, L. Klemen, K. Leko, N. Cindro, G. Horvat, I. Piantanida, V. Tomišić, *Analytica* **2026**, accepted for publication.

**Acknowledgments**

Croatian Science Foundation (IP-2024-05-3012, IP-2019-04-9560, IP-2022-10-9829, IP-2025-02-8238, IP-2024-05-5352), NextGenerationEU through the National Recovery and Resilience Plan 2021–2026. (NextGenChem and CryoLab), NPOO.C3.2.R2-I1.06.0043), and the European Regional Development Fund (infrastructural project CIuK, grant number KK.01.1.1.02.0016).



## **Oral Presentations**

## CS OP 01

## CSD4NCI workshop – a cheminformatics workshop on analyzing noncovalent interactions using the CSD Portfolio

Katarina Čeranić<sup>1,2</sup>, Slađana Đorđević<sup>3</sup>, Filip Stašević<sup>3</sup>, Dušan Malenov<sup>4</sup>

<sup>1</sup>Innovative Centre of the Faculty of Chemistry Ltd., Belgrade, Serbia

<sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

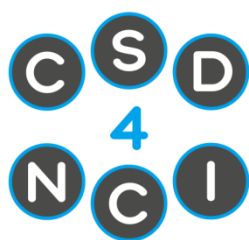
<sup>3</sup>University of Kragujevac, Faculty of Science, Kragujevac, Serbia

<sup>4</sup>University of Belgrade, Faculty of Chemistry, Belgrade, Serbia

The world's largest repository of experimental crystal structures is the Cambridge Structural Database (CSD), [1] with over 1.4 million structures, which makes it a rich dataset for analysis of noncovalent interactions. The Cambridge Crystallographic Data Centre (CCDC) has also developed the CSD Portfolio, a suite of programs that enable searching and analysis of crystal structures. In addition, CCDC aims to support the education activities that engage the wider public into structural sciences.

The CSD4NCI workshop (Fig. 1) is a student workshop developed at University of Belgrade and University of Kragujevac, and it is based on cheminformatics analysis of noncovalent interactions using the CSD Portfolio. Within this workshop students learn to use ConQuest for data mining and Mercury for visualization and data interpretation (Fig. 1). With the help of lecture slides, guided exercises, handouts and assessment materials, students gain hands-on experience in cheminformatics analysis of noncovalent interactions based on geometrical parameters.

The CSD4NCI workshop aims to increase awareness on the importance of noncovalent interactions, as well as to spread the use of CSD resources in both chemistry education and structural science.



CSD4NCI - logo

Programs:



Mercury



ConQuest

Find us on social media:



Website:



[in /company/csd4nci-workshop](https://www.linkedin.com/company/csd4nci-workshop)

Figure 1. CSD4NCI logo, programs, and social media.

### References

[1] C. Groom, I. Bruno, M. Lightfoot, S. Ward, *Acta Cryst.* **2016**, B72, 171.

### Acknowledgments

This work was enabled and funded by the Cambridge Crystallographic Data Centre (CCDC) within the framework of the CCDC Engagement Grants initiative.

## CB OP 01

# Targeting HSP90 with pyrazoline-based derivatives: A docking-guided design, synthesis and biological evaluation

Milena Petrović<sup>1</sup>, Jaka Dernovšek<sup>2</sup>, Tihomir Tomašič<sup>2</sup>, Violeta Marković<sup>1</sup>

<sup>1</sup>University of Kragujevac, Faculty of Science, Kragujevac, Serbia

<sup>2</sup>University of Ljubljana, Faculty of Pharmacy, Ljubljana, Slovenia

Heat shock protein 90 (Hsp90) is an ATP-dependent molecular chaperone involved in the proper folding, stabilization, and function of numerous client proteins.<sup>1</sup> Due to its essential role in the stabilization of several proteins involved in cancer development and progression, Hsp90 has emerged as an attractive therapeutic target. In the present study, 10 pyrazoline-based compounds were designed and synthesized as potential Hsp90 inhibitors using a rational design approach. Structural features present in previously reported Hsp90 inhibitors were considered in the design of the desired compounds. Molecular docking was subsequently employed to evaluate the proposed structures. The final compounds were synthesized from chalcones obtained *via* Claisen–Schmidt condensation of 3-acetylindole or 4-morpholinobenzaldehyde with an appropriate carbonyl compounds, followed by cyclization with (*non*-) substituted thiosemicarbazides.<sup>2</sup> The synthesized compounds will be subjected to biological evaluation, including assessment of their antiproliferative activity. The obtained results will provide preliminary insights into the potential Hsp90-inhibitory activity of the synthesized compounds and enable the selection of the most promising candidates for further investigation.

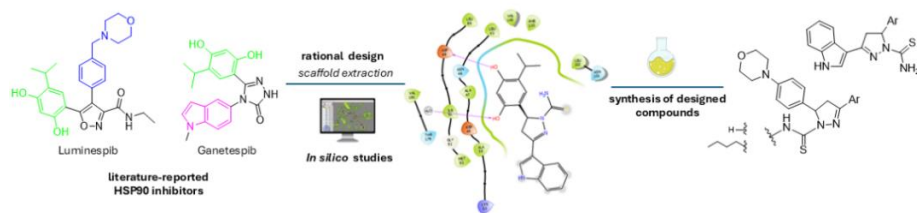


Figure 1. Design and synthesis of potential HSP-90 inhibitors.

## References

- [1] D. Picard, *Cell. Mol. Life Sci.* **2002**, 59, 1640.
- [2] M. Petrović, T. Andrejević, Ž. Milanović, K. Milisavljević, T. Stanojković, Ž. Žižak, V. Marković, *ChemMedChem.* **2025**, 00, e202500646.

## Acknowledgments

The authors are grateful to the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (grant nos. 451-03-34/2026-03/200122, and 451-03-33/2026-03/200122) for financial support.

## DCS OP 01

**Regioselectivity of carbene-intermediate reactions modulated by hydrogen bonding**Josip Mikulić<sup>1</sup>, Marko Purić<sup>2</sup>, Nikola Topolovčan<sup>2</sup><sup>1</sup>Faculty of Science, Zagreb, Croatia<sup>2</sup>Ruđer Bošković Institute, Zagreb, Croatia

Utilization of carbenes as highly reactive intermediates proves to be a valuable method for rapid construction of a diverse carbon scaffold. Thus, a number of innovative methodologies regarding their *in-situ* generation were consequently developed. Such a method is the visible-light-induced generation of carbenes from diazoesters – a high-yielding transformation under mild conditions [1]. This methodology was readily applied in generating substituted norcaradienes which can further undergo oxidation and ultimately provide synthetically valuable, highly functionalized compounds [2].

Though the mentioned carbenes are nowadays easy to generate, directing their reactivity remains a challenge. In this work, we explore means of directing their selectivity in a diversely functionalized system (Fig. 1). With carbazole as a model substrate, a series of organic bases and inorganic salts were utilized to investigate hydrogen bonding as a method of transient non-covalent protection. Furthermore, carbazole's reactivity relative to previously investigated carbene-trapping agents was explored to screen functionalities whose reactivity can further be selectively directed upon.

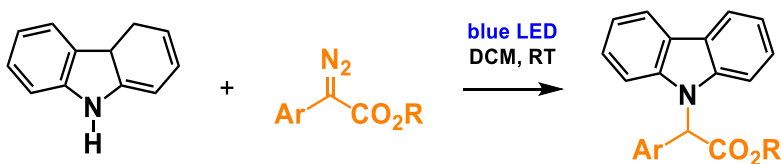


Figure 1. Reaction of a carbene precursor with the model substrate carbazole investigated for application of hydrogen bond acceptors as masking groups in organic synthesis.

**References**

- [1] Z. Yang, M. L. Stivanin, I. D. Jurberg, R. M. Koenigs, *Chem. Soc. Rev.* **2020**, 49 (19), 6833.  
[2] K. Petrić, A. Čikoš, I. Nikšić-Franjić, G. C. Lloyd-Jones, M. Gredičak, N. Topolovčan, *Org. Chem. Front.*, **2026**, 13 (9), 2794.

**Acknowledgments**

This work is supported through NextGenerationEU project (grant no. 01-893/1-2026)

## EA OP 01

**Optimization of polyhydroxyalkanoates production from biomass using response surface methodology**

Dragana Žmukić<sup>1</sup>, Ivana Mitrović<sup>2</sup>, Berta Barta Holló<sup>1</sup>, Branko Kordić<sup>1</sup>, Anita Leovac Maćerak<sup>1</sup>

<sup>1</sup>University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia

<sup>2</sup>University of Novi Sad, Faculty of Technology, Novi Sad, Serbia

Polyhydroxyalkanoates (PHAs) are biodegradable macromolecules produced by various types of intracellular microorganisms under conditions of carbon excess and lack of nutrients [1]. In order to produce a high yield of biopolymers from biomass, it is necessary to optimize the extraction conditions to overcome the existing limitations. Response surface methodology (RSM) is a set of statistical and mathematical techniques used to improve and optimize processes. In our study, we optimized the alkaline digestion process (hydrolysis of non-PHA cellular mass) by varying four parameters: mass of anaerobically digested sludge (biomass), volume of alkali, time and temperature. A Box-Behnken experimental design with four factors at three levels and three replications at the central point was used, resulting in a total of 27 experiments. For fitting the output mass, a coefficient of determination ( $R^2$ ) of 0.88 was achieved, which indicates that the model is adequate, because it explained 88% of the total variation in the observed response. After the optimization of the first step, the second step focused on the use of a non-ionic surfactant. In this stage, three parameters were varied: surfactant mass, time, and temperature. For the subsequent output mass fitting, an  $R^2$  of 0.95 was obtained, which explained 95% of the total variation in the observed response. FTIR analysis of the obtained biopolymers shows the vibrational stretching of long aliphatic chains  $-\text{CH}_2-$  and  $-\text{CH}_3$  groups at  $2918.96\text{--}2855.95\text{ cm}^{-1}$ , the stretching of the carbonyl group at  $1734.78\text{ cm}^{-1}$ , the vibrating mode of  $-\text{CH}_2-$  group at  $1458.41\text{ cm}^{-1}$ , and C–O bands at the  $1348.69\text{--}1296.39\text{ cm}^{-1}$  in the fingerprint region, which is consistent with commercial PHAs. The intensity of the carbonyl peak at the  $1734.78\text{ cm}^{-1}$  indicates the amorphous state of the biopolymer [2], which was also confirmed by XRD analysis.

**References**

- [1] G. Pesante, N. Frison, *Bioresour. Technol. Reports*. **2023**, 21, 101345.  
[2] M. Kansiz, A. Domínguez-Vidal, D. McNaughton, B. Lendl, *Anal. Bioanal. Chem.* **2007**, 388, 1207.

**Acknowledgments**

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants Nos. 451-03-33/2026-03/200125 & 451-03-34/2026-03/200125).

**PCC OP 01****Influence of alkyl chains on the physicochemical and thermophysical characteristics of nicotine-based ionic liquids**

Andrija Vukov<sup>1</sup>, Snežana Papović<sup>1</sup>, Domen Goste<sup>2</sup>, Bojan Šarac<sup>2</sup>, Magda Škvorová<sup>3</sup>,  
Milan Vraneš<sup>1</sup>

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Nicotine is a naturally occurring bicyclic alkaloid composed of a pyridine and a pyrrolidine ring. It is found most abundantly in the tobacco plant (*Nicotiana tabacum*). Global tobacco production is around 5.8 million tons, which equates to between 170 and 300,000 tons of pure nicotine. Despite the large global production capacity, nicotine has few uses, and its main market, tobacco products, is susceptible to significant fluctuations based on public opinion. This underutilized natural plant product is chemically interesting for further derivatization; the tertiary pyrrolidine nitrogen is both susceptible to quaternization and can act as a Brønsted base [1]. By alkylating nicotine with a homologous series of alkyl bromides, we obtained four nicotine-based surface-active ionic liquids (N-octyl-, N-decyl-, N-dodecyl-, N-tetradecyl-nicotinium bromide). Additionally, by neutralizing nicotine with fatty acids of analogous lengths, we obtained another set of nicotinium-alkylate ionic liquids (nicotinium octanoate, decanoate, dodecanoate, and tetradecanoate).

This work investigates how the physicochemical and thermophysical characteristics of nicotinium-based ionic liquids change with the positioning of an hydrophobic alkyl chain: whether it is present on the cation or anion. Densities, viscosities, and acoustic properties of the 8 synthesized ionic liquids are measured over a wide temperature range from 20 to 60 °C in 5 °C increments. Thermophysical characterization of the ionic liquids was performed by differential scanning calorimetry and thermogravimetric analysis. Results show significant differences in physicochemical behavior based on both alkyl chain length and whether the chain is on the cation or the anion. This indicates that the position of the alkyl chain, as well as its length, should be taken into consideration when predicting or designing the characteristics of ionic liquids.

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**PFC OP 01****Different approaches for extraction of oil and polyphenols from grape seeds from Serbian wineries**

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The production of high-quality wines is well-developed in Serbia, where both indigenous and international grape varieties are used. The winemaking process generates large quantities of by-products, including grape seeds, which are usually discarded. These by-products represent both an environmental challenge and an underexploited source of valuable natural compounds [1]. Grape seeds are particularly attractive because they contain two complementary classes of high-value constituents: a lipid fraction (oil) rich in unsaturated fatty acids and a non-lipid fraction rich in polyphenols such as flavan-3-ols and procyanidins [2]. However, their full potential remains underutilised. An integrated approach involving the production of oil followed by the extraction of polyphenols from the remaining residue could enable more complete utilisation of this raw material. The aim of this research is to explore different extraction techniques (supercritical fluid extraction and ultrasound-assisted extraction) for obtaining oil from grape seeds from Serbian wineries, followed by extraction of the remaining residue to obtain polyphenol-rich extracts. The total phenolic content (TPC) and radical scavenging activity (RSA) of the resulting phenolic extracts were determined. The oil yields obtained by different extraction techniques were comparable. The residues remaining after oil extraction from grape seeds were rich in polyphenols and showed high radical scavenging activity, with grape seeds from Serbian indigenous varieties Tamjanika and Grašac showing the highest TPC and RSA values.

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**SCCE OP 01****Physicochemical changes in badlands under simulated climatic conditions - the interplay between mineralogical composition and texture**

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Badlands are highly erodible landscapes in which weathering is strongly influenced by several interacting factors [1,2]. In this study, eight badland materials collected from Spain, Turkey, Romania, Israel, and Slovenia were investigated to assess how their initial mineralogical and textural characteristics influence their physicochemical response to simulated weathering. The samples represented different lithological types and were characterized in terms of grain size and mineralogical composition, with particular attention to presence of smectite, gypsum, analcime, and calcite. The weathering experiment consisted of two phases designed to simulate different climate conditions. In the first phase, the samples were subjected to repeated rainfall and snowmelt treatments followed by freezing–thawing cycles, while the second phase involved exposure to simulated rainfall and elevated temperature [2]. Surface changes, pH, electrical conductivity, and ion concentrations were monitored throughout each cycle of experiment. Despite differences in mineralogy and texture, sediments with gypsum exhibited similar physicochemical responses under the applied experimental conditions, suggesting that mineralogical composition, is crucial for their similar weathering behaviour [2]. The findings highlight that mineralogical, texture and physicochemical characteristics all influence the weathering behaviour of badland materials.

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**SCFM OP 01****MOF-derived nanoparticles for enhanced sensing of phenolic pollutants**

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The structural versatility and tunable surface chemistry of metal–organic framework (MOF)-derived materials enable the rational design of tailored sensing platforms featuring surface areas and abundant active sites, making them promising materials for the sensitive detection of phenolic pollutants [1]. Among these contaminants, bisphenol A (BPA) is of particular concern due to its widespread environmental occurrence, extensive industrial use, and potential endocrine-disrupting effects. In this study, metal oxide nanoparticles derived from the thermolysis of 1,3,5-benzenetricarboxylate-based metal–organic frameworks (MBTC; M = Cu, Bi, or Fe) were structurally characterized and subsequently incorporated into carbon paste electrodes (CPEs) for electrochemical investigation using electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV). Among the investigated materials, the Bi<sub>2</sub>O<sub>3</sub>-MOF-derived electrode exhibited the most pronounced electrocatalytic activity toward BPA oxidation, which was attributed to its high surface area, numerous accessible active sites, and favorable electron-transfer properties. Under optimized experimental conditions, the developed sensor demonstrated excellent analytical performance and high selectivity toward BPA in the presence of common interfering species. These results highlight the potential of Bi<sub>2</sub>O<sub>3</sub>-MOF-derived nanostructures as efficient sensing materials for BPA detection and their applicability in environmental monitoring.

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## **Poster Presentations**



## **Chemistry and Society (CS)**

## CS PP 01

**Developing entrepreneurial competencies in chemistry education: Insights from teachers' practices**

Stefan Gavrilović<sup>1</sup>, Emilija Dinčev<sup>2</sup>, Filip Stašević<sup>1</sup>, Jelena Đurđević Nikolić<sup>1</sup>

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Entrepreneurial competencies are increasingly recognized as important for personal development and future professional engagement. The aim of the study was to identify, through an analysis of chemistry teachers' responses, the activities implemented to develop students' entrepreneurial competencies, to examine existing practices, and to explore opportunities for further improvement. Data were collected through an electronic questionnaire from 132 secondary chemistry teachers who responded to an open-ended question. Reflexive thematic analysis was used to identify recurring patterns across the sample, while frequencies and percentages of coded occurrences were used descriptively to indicate how commonly particular activities were reported. The results revealed that only 47 respondents (36%) provided concrete examples of entrepreneurial activities, while 85 (64%) did not, suggesting limited implementation and/or recognition of entrepreneurial concepts in everyday teaching. The analysis resulted in five themes. Among responses providing concrete examples, the manufacture and sale of cosmetic and chemical products (e.g., soaps, balms, and candles) was the most prominent category (53%), followed by project-based learning tasks (21%), fairs and charity bazaars (11%), and environmental and recycling initiatives (8%). A fifth theme, critical reflections on barriers (6%), captured responses in which teachers did not identify specific activities but instead reflected on their lack of knowledge, experience, or opportunities for developing entrepreneurial competencies. The findings suggest that practical product development, particularly within organic and applied chemistry, represents the most commonly reported form of entrepreneurial activity, whereas explicit education in financial literacy, marketing, and formal student companies remains rare. The relatively small sample, combined with potential biases inherent in self-reported data, may limit the generalizability of the findings. Systematic and practice-oriented professional development could support teachers in more explicitly linking chemistry instruction with the development of creativity, initiative, problem-solving, and other key entrepreneurial competencies among students.

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## CS PP 02

**Educational apps and AI tools: Combining technologies in inorganic chemistry classes**

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Due to the abstract nature of the subject matter, teaching inorganic chemistry presents significant challenges. This study examines the synergy of two key technological pillars of modern education: educational applications designed to support learning and practice, on the one hand, and artificial intelligence (AI) tools, on the other. The application *Periodic Table Quiz* provides a structured and user-friendly learning environment, while AI supports the generation of individualized tasks, adaptive learning activities, and real-time feedback.

The study aims to demonstrate the potential of combining educational software and AI to support individualized learning and improve students' understanding and engagement in inorganic chemistry.



Figure 1. Software app icon Periodic Table Quiz

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**CS PP 03****Systemic analysis questions as a tool for assessing secondary school students' achievement in organic chemistry**

Valentina Periškić, Tamara Rončević, Saša Horvat, Dušica Rodić, Maja Bosanac  
*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*

The systemic approach to teaching and learning chemistry (SATL) views chemistry concepts and processes as interconnected elements of a broader system, aiming to foster the development of students' systems thinking [1,2].

One of the question types developed within the systemic approach is the systemic analysis questions, which require students to analyse a represented systemic (i.e., a closed diagram) and identify incorrectly established relationships between a selected set of concepts. Therefore, the aim of this study was to investigate the potential of systemic analysis questions as a tool for assessing secondary school students' achievement and understanding in organic chemistry, with a particular focus on hydrocarbons and oxygen-containing organic compounds.

The study was conducted at „Svetozar Marković“ grammar school in Novi Sad and involved 73 third-grade students. The students completed an assessment instrument with four systemic analysis questions that differed in the number of organic compounds included in the closed system and the number of relationships between them.

The maximum possible score on the instrument was 20 points, while the mean score was 11.77 points, corresponding to 58.85% of the maximum score. Analysis of individual questions showed that the highest achievement was observed on the first systemic analysis question (73.25%), which included a smaller number of organic compounds belonging to hydrocarbons and their halogen derivatives. The lowest achievement was observed on the third systemic analysis question (44.33%), which involved a larger number of organic compounds and relations between different classes of compounds. The findings suggest that systemic analysis questions have potential as assessment tool for evaluating students' achievement and their understanding of organic chemistry concepts and the relationships between them.

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## **Chemistry meets Biology (CB)**

## CB PP 01

## Structure–ADMET relationships in glycodeoxycholic acid-derived thiohydantoin candidates: an *in silico* study

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Thiohydantoin is a biologically relevant scaffold present in compounds with diverse pharmacological activities [1]. Glycodeoxycholic acid (GDCA, **1**) provides an attractive steroidal scaffold for structural modification. Here, a preliminary *in silico* ADMET assessment of **1** and proposed thiohydantoin (S-HDT) and their acetylated derivatives was performed using pkCSM and ADMETlab 2.0. Compared with **1** and its acetylated derivatives, S-HDT candidates showed lower aqueous solubility (2–4 vs. 39–56 mg/L), but higher Caco-2 permeability (log Papp 0.77–0.96 vs. 0.60–0.64), intestinal absorption (87–95% vs. 59–62%) and CYP-mediated interaction potential. Hydroxylated S-HDT (**5**) showed the highest Caco-2 permeability and intestinal absorption ( $0.96 \times 10^{-6}$  cm/s and 95%, respectively). Acetylated structures generally showed increased lipophilicity and reduced clearance. Compounds **1** and **5** displayed the lowest predicted toxicity across the series. Enzalutamide, an approved thiohydantoin-containing drug, showed markedly lower solubility (0.08 mg/L) but comparable intestinal absorption (93%). Overall, S-HDT incorporation substantially modifies the ADMET profile of GDCA, particularly enhancing permeability and intestinal absorption at the expense of aqueous solubility.

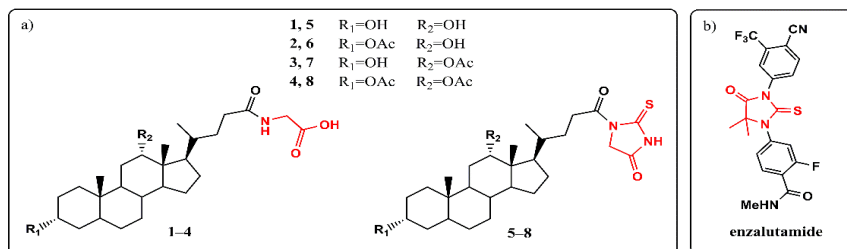


Figure 1. Chemical structures of (a) the analyzed compounds (**1–8**) and (b) the reference compound.

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## CB PP 02

**Elucidating subdomain IIA binding preferences of palladium(II) complexes with human serum albumin**

Marija Trifunović, Snežana Stojanović, Nenad Joksimović  
University of Kragujevac, Faculty of Science, Kragujevac, Serbia

The aim of this research was to investigate the interaction mechanisms and binding affinity of novel palladium(II) complexes with human serum albumin (HSA) in order to evaluate their transport properties, distribution, and potential *in vivo* efficacy. The interaction mechanisms of two novel palladium(II) complexes (**1** – **2**, Fig. 1) with HSA were investigated using steady-state fluorescence quenching measurements in both the absence and presence of specific site markers, namely eosin Y and ibuprofen [1]. Thermodynamic and binding evaluations revealed that complex **1** possesses the highest binding affinity toward HSA among the series. Furthermore, competitive binding assays with site-specific markers demonstrated that the investigated palladium(II) complexes preferentially bind to site I located within subdomain IIA of the protein structure, corresponding to the primary binding pocket shared with eosin Y.

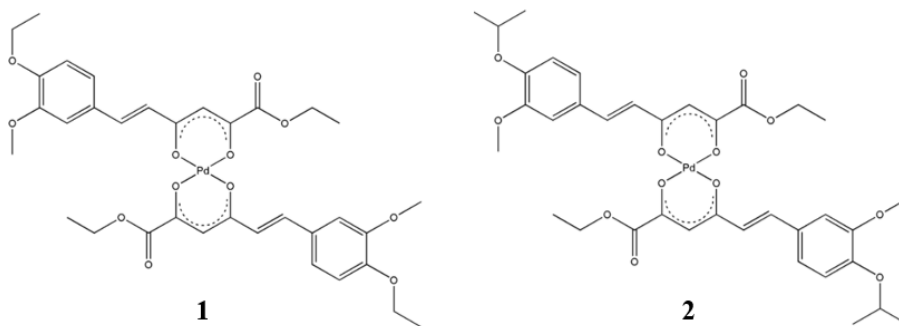


Figure 1. Structure of investigated complexes

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## CB PP 03

## Exploring the DNA recognition and minor groove binding of novel palladium(II) complexes

Snežana Stojanović, Marija Trifunović, Nenad Joksimović, Biljana Petrović  
University of Kragujevac, Faculty of Science, Kragujevac, Serbia

The interactions of four novel palladium(II) complexes (**1** – **4**) bearing *O,O*-bidentate  $\beta$ -diketo ester ligands (Fig. 1) with DNA were systematically investigated using UV-Vis absorption spectroscopy, competitive fluorescence quenching assays (utilizing ethidium bromide and Hoechst 33258), and viscometric titrations [1]. UV-Vis binding studies revealed that complex **3** possesses a significantly higher intrinsic binding constant, whereas complex **2** demonstrated a markedly superior Stern–Volmer quenching constant, prompting a detailed downstream evaluation. Viscosity measurements of CT-DNA upon the addition of increasing concentrations of complex **2** revealed only a negligible increase, effectively precluding a classical intercalation model. Supported by complementary competitive fluorescence data, these findings strongly suggest that the structural planarity of the investigated system facilitates a robust, non-intercalative minor groove binding mode with DNA. The aim of this research was to thoroughly elucidate the mechanism and binding affinity of novel synthetic palladium(II) complexes with DNA in order to evaluate their potential as new, biologically active agents for applications in pharmaceutical chemistry and metallodrug development.

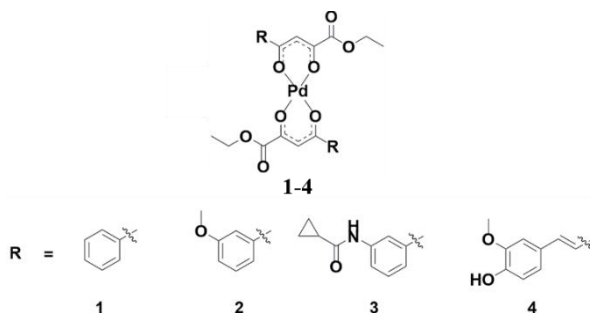


Figure 1. Structure of investigated complexes

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**CB PP 04****C-phycocyanin-derived peptide-conjugated, chemically crosslinked chitosan/carrageenan hydrogels for myoblast cultivation in reduced serum conditions**

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Fetal bovine serum (FBS) is commonly added to cell culture media, but for cultivated meat production to become truly sustainable, ethical and affordable, an alternative to it is necessary [1,2]. The purpose of this study was to demonstrate how myoblasts could be cultivated in reduced-serum media using animal-free scaffolds. Novel chitosan/carrageenan hydrogels were developed and conjugated with peptides obtained by digestion of C-phycocyanin from cyanobacteria *Arthrospira platensis*, their physico-chemical properties were assessed, and their ability to serve as scaffolds for myoblast cultivation in reduced-serum media was examined. These hydrogels were found to possess suitable physical characteristics to serve as scaffolds for cell culture, and it was demonstrated that their use made quail muscle clone 7 (QM7) cell cultivation possible in reduced-FBS media. These hydrogels, therefore, are a promising candidate for use as scaffolds in future cultivated meat production studies.

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**CB PP 05****Investigation of the interactions of Cu(II) complexes with DNA and human serum albumin using molecular docking**

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Copper(II) complexes attract considerable attention in bioinorganic and medicinal chemistry due to their ability to interact with biologically relevant macromolecules. In this study, molecular docking was applied to investigate the interactions of four Cu(II) complexes (C1–C4), which differ in ligand structure, with DNA and human serum albumin (HSA). Complexes C1 and C2 contain ligands derived from  $\beta$ -amino acids [1], whereas C3 and C4 contain tetradentate S,O-donor ligands derived from thiosalicylic acid [2]. The geometries of the complexes were optimized using the B3LYP functional and the def2-SVP basis set. Docking simulations were performed using Molegro Virtual Docker. DNA structures 1BNA and 1Z3F were used to evaluate minor-groove binding and intercalation, respectively, while the HSA structure 1AO6 was used to analyze binding sites I (IIA) and II (IIIA). All investigated complexes showed the ability to interact with both biomolecular targets. DNA binding was generally more favorable in the minor groove than through intercalation. Complex C3 showed the most favorable interaction with the DNA minor groove, whereas C4 showed the most favorable intercalative binding. For HSA, binding to site I was more favorable than binding to site II. The results indicate that ligand structure significantly influences the preferred binding mode and stability of Cu(II) complex interactions with DNA and HSA.

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**CB PP 06****Synthesis of oxazolidinone derivatives and determination of their inhibitory effects on acetylcholinesterase**

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The current approach to improving cognitive function in patients with Alzheimer's disease is primarily based on enhancing central cholinergic activity through the use of acetylcholinesterase inhibitors. Previous studies have shown that carbamate-containing compounds are highly effective acetylcholinesterase inhibitors. Molecular docking studies indicated that (S)-4-benzyl-2-oxazolidinone derivatives exhibit high binding affinity toward acetylcholinesterase. Based on the docking results, p-nitrophenyl and 1-adamantyl derivatives of (S)-4-benzyl-2-oxazolidinone were synthesized and evaluated for their inhibitory activity. Both compounds exhibited acetylcholinesterase inhibitory activity, with the p-nitrophenyl derivative showing an IC<sub>50</sub> value of 3.0 μM. The IC<sub>50</sub> value of the 1-adamantyl derivative could not be determined because of its poor solubility in water. These results suggest that (S)-4-benzyl-2-oxazolidinone derivatives represent promising scaffolds for the development of new therapeutic agents for Alzheimer's disease.

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**CB PP 07****Synthesis of novel androstane hydrazono-hydrazide derivatives and their binding affinity to androgen and estrogen receptors**

Đorđe Janković<sup>1</sup>, Sofija Bekić<sup>1</sup>, Maja Marinović<sup>2</sup>, Marina Savić<sup>1</sup>, Jovana Ajduković<sup>1</sup>

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Androgen (AR) and estrogen (ER) receptors belong to the superfamily of nuclear receptors that play a crucial role in regulating cell proliferation in both healthy and tumor cells. They exert their activity by binding their natural ligands, such as testosterone and estrone. Tumor cells often overexpress these receptors, making them convenient targets in medicinal chemistry [1]. Steroid compounds are natural ligands for steroid receptors, but they also show a wide range of biological activities, including anticancer activity. This makes the steroid core a privileged scaffold in medicinal chemistry. On the other hand, the hydrazono-hydrazide group represents a functional group with significant biological potential and serves as a pharmacophore for designing new anticancer molecules [2]. Guided by these facts, we synthesized new testosterone hydrazono-hydrazide derivatives and examined their binding affinity for ligand-binding domains (LBDs) of AR and ER. A compound bearing a (pyridin-3-yl) carbonylhydrazinylidene substituent showed notable binding affinity for AR. Docking studies provided insight into the key interactions between that compound and AR-LBD.

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**CB PP 08****Expression and Partial Immunochemical Characterization of a Recombinant BanLec-Based Chimera Containing Amb a 1 T-Cell Epitopes**

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Ragweed (*Ambrosia artemisiifolia*) pollen is one of the most important sources of respiratory allergy in Europe, and its major allergen, Amb a 1, is recognized by IgE antibodies in more than 90% of sensitized patients [1]. Classical allergen-specific immunotherapy (AIT) is effective but carries a risk of IgE-mediated adverse reactions. Hypoallergenic constructs based on T-cell peptide epitopes are being explored as a safer alternative, since they induce immune tolerance without IgE cross-linking [2]. To enhance the immunogenicity of isolated peptides, this study used banana lectin (BanLec) as an immunomodulatory carrier to generate, *in silico*, a fusion construct containing peptides representing the dominant T-cell epitopes of Amb a 1. The recombinant BanLec-based chimera containing Amb a 1 T-cell epitopes was cloned into the pET23b expression vector and transformed into *Escherichia coli* DH5 $\alpha$  cells for plasmid propagation and subsequently into BL21(DE3) cells for recombinant protein expression. After optimization of induction conditions, the fusion protein was expressed in strain BL21, accumulating mainly as insoluble inclusion bodies. A protocol was established for solubilization in 4 M urea and renaturation by stepwise dialysis; glycerol, particularly at 50%, markedly improved protein stability and yield. The renatured protein was purified on a Sephadex G-75 matrix, and its identity was confirmed by immunoblotting with anti-banana extract antibodies, revealing clear immunoreactive bands corresponding to the fusion construct. These results establish a functional experimental pipeline for the expression, solubilization, renaturation, and purification of the BanLec-based chimera containing Amb a 1 T-cell epitopes, providing a basis for its further functional characterization as a potential candidate for hypoallergenic immunotherapy of ragweed allergy.

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**CB PP 09****ACE-inhibitory potential of red and white wine lees from autochthonous Serbian grape cultivars**

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Wine lees are an underutilised winery by-product and a promising source of bioactive compounds, including proteins, peptides, phenolics and yeast-derived polysaccharides. Among their reported bioactivities, inhibition of angiotensin-converting enzyme (ACE) is of particular interest due to its relevance to blood pressure regulation and the identification of ACE-inhibitory peptides in wine lees [1]. This study investigated the ACE-inhibitory potential of red and white wine lees obtained from the autochthonous Serbian grape cultivars Probus and Grašac and its relationship with their previously characterised chemical composition. The two wine lees exhibited distinct chemical profiles, with white wine lees showing higher protein content and a more favourable essential amino acid profile, whereas red wine lees were substantially richer in phenolic compounds and exhibited stronger antioxidant activity. Despite these differences, both samples showed ACE-inhibitory activity within a comparable range, with IC<sub>50</sub> values indicative of promising inhibitory potency. ACE inhibition was evaluated using an HPLC-based assay according to Čakarević et al. [2]. The comparable activity of these chemically distinct matrices suggests that ACE inhibition may not be directly associated with the abundance of a single compound class. These findings support the potential of wine lees as sources of ACE-inhibitory bioactive compounds and provide a basis for further investigation of protein- and peptide-rich fractions.

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**CB PP 10*****In Silico* Structural Optimization of Boscalid Derivatives  
Targeting Acetylcholinesterase and Butyrylcholinesterase:  
Integrated Molecular Docking and ADMET Assessment**

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Excessive pesticide use leads to hazardous bioaccumulation and potential off-target neurotoxicity [1]. Given recent findings that boscalid, a widely used fungicide, exhibits inhibitory potential towards human acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) [2], *in silico* studies were conducted on its novel structural derivatives. This research aimed to assess the predicted binding of these compounds to the targets and to systematically compare computational approaches based on molecular docking and ADMET prediction platforms. By combining the docking results for both target enzymes, imidazole and benzoxazole-functionalized derivatives emerged as the most potent dual inhibitors. However, after integrating pharmacokinetic and ADMET parameters, specific derivatives stood out as the optimal pharmacological candidates due to their significantly improved safety profile including, but not limited to, the mitigation of cytochrome P450 binding and enhanced blood-brain barrier (BBB) permeability. Conversely, derivatives that demonstrated a non-toxic profile but lacked BBB permeability, specifically, the azole and benzoxazole classes excluding the *N*-imidazolyl pyridine modifications, are slated for synthesis and testing as safer agricultural agents. Overall, targeted structural optimization of boscalid successfully overcomes its toxicological limitations, yielding promising lead compounds for future neurodegenerative therapeutic development and sustainable agrochemistry.

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## CB PP 11

**Synthesis and biological evaluation of a novel heterocyclic  
16,17-secoandrost-5-ene derivative**

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Steroidal hormones and their analogues are an important class of compounds in medicinal chemistry due to their diverse pharmacological properties. In contrast to the rigid tetracyclic framework of conventional steroids, secosteroids possess greater conformational flexibility as a result of endocyclic carbon–carbon bond cleavage, which can affect their receptor binding and biological activity. Secosteroids have attracted considerable attention due to their diverse pharmacological properties, and several derivatives have shown activity against tumor cells as well as anti-inflammatory effects [1]. The incorporation of heterocyclic moieties into the steroidal framework may further affect their biological properties and selectivity [2].

We report the synthesis and biological evaluation of a novel heterocyclic 16,17-secoandrost-5-ene derivative. The target compound was obtained in a multistep synthesis involving selective D-ring cleavage, followed by further chemical transformations and formation of the heterocyclic ring in the final step. The target compound and the synthetic intermediate preceding heterocycle formation were *in silico* evaluated for their ADME/T profiles and showed generally favorable predicted oral bioavailability. Their binding affinities were then evaluated *in vitro* for the ligand-binding domains of estrogen receptors  $\alpha$  and  $\beta$  (ER $\alpha$  and ER $\beta$ ), androgen (AR), and glucocorticoid receptor (GR), together with inhibitory activity against AKR1C3 and AKR1C4. The compounds showed pronounced selectivity for GR, while inhibitory activity was observed against AKR1C4. These findings support further investigation of the synthesized compounds as selective GR ligands and AKR1C4 inhibitors.

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## CB PP 12

**Investigation of the potential of B-phycoerythrin from the microalga *Porphyridium purpureum* as albumin replacement in cell media for Japanese quail myoblasts cultivation**

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The critical challenge in the cultivated meat field is identifying and developing serum albumin alternatives as the key component in cell media. Phycoerythrins (PEs) from red algae are promising candidates for albumin replacement due to their high abundance and well-known excellent antioxidative and metal-binding activities of covalently attached tetrapyrrole chromophores [1]. Considering the importance of fatty acids (FA) binding by albumin for cell cultivation, the additional prerequisite for developing PEs as albumin replacement components is their validation for the ability to bind FA. This study aims to examine the ability of B-phycoerythrin (B-PE), the major PBP of red microalgae *Porphyridium purpureum*, to bind selected fatty acids and evaluate its potential as a serum albumin substitute in QM7 (Quail Muscle clone 7) cell culture. B-PE was isolated from lyophilized *Porphyridium purpureum* biomass by ammonium sulfate precipitation, dialysis, and hydroxyapatite chromatography. Binding to five fatty acids was studied by spectrofluorimetric titration. B-PE showed moderate to high affinity for all tested fatty acids, with the highest primary binding constant for stearic acid ( $4.1 \times 10^5 \text{ M}^{-1}$ ). Several binding constants observed for the majority of examined fatty acids suggest the presence of non-equivalent binding sites. The potential of B-PE to replace albumin was probed in albumin-depleted fetal bovine serum, using pure albumin and complete FBS as controls. Cell viability, metabolic activity, and growth were evaluated by neutral red and resazurin assays, cell counting, and light microscopy. At 0.2 g/L, B-PE increased the number of QM7 cells to approximately 260% of the albumin-depleted control, comparable to pure albumin at the same concentration. It also increased metabolic activity to levels similar to the complete FBS (1.5 %). Overall, B-PE binds both saturated and unsaturated fatty acids and supports QM7 cell viability and growth under albumin-depleted conditions. These results indicate that B-PE has potential as an alternative to serum albumin in cell culture media, although longer-term studies and multiple cell passages are needed to confirm its suitability.

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**CB PP 13****Synthesis of Biginelli compound loaded on chitosan and evaluation of its cytotoxic effect**

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In the present study, a suitable lead compound from previously synthesized tetrahydropyrimidines (THPMs) [1], is selected to incorporate into chitosan nano-based carrier.

THPM-loaded chitosan particles (THPM-CH) with different THPM contents (15 and 30 w.t.%) were successfully prepared by an adapted high-shear emulsification and glutaraldehyde crosslinking method. Chitosan was dissolved in 1 w.t.% acetic acid and combined with an ethanolic solution of the compound at controlled mass ratios, followed by high-speed homogenization and subsequent crosslinking. The obtained particles were isolated by centrifugation, lyophilized, washed, and dried to produce powdered THPM-CH materials. The incorporation of THPM into the chitosan matrix was investigated by Fourier-transform infrared spectroscopy (FTIR), while particle-size distributions were determined by SEM. FTIR spectra confirmed the characteristic structural features of both chitosan and compound, supporting the successful formation of the THPM–chitosan system. Both THPM-CH formulations exhibited predominantly submicron particle sizes, with most particles distributed within approximately 0.05–0.3 µm. Also, the cytotoxic activity of free THPM and corresponding chitosan-based nanocarriers was assessed against leukemia cell lines K562, and MOLT-4 using the MTT assay. Chitosan alone did not exhibit notable cytotoxicity, confirming its suitability as a carrier material. At equivalent concentrations of compound, the nanoforms demonstrated different cytotoxic profiles compared with the free THPM. After 72 h of treatment, the IC<sub>50</sub> values in K562 cells were 1.27 ± 0.10 µg/mL for free THPM, 1.73 ± 0.08 µg/mL for THPM15w.t.%, and 0.25 ± 0.06 µg/mL for THPM30w.t.%. In MOLT-4 cells, the corresponding IC<sub>50</sub> values were 1.38 ± 0.05, 1.16 ± 0.23, and 0.30 ± 0.04 µg/mL, respectively.

Overall, the study demonstrates the successful development of chitosan-based nanoforms of a selected THPM and highlights the influence of compound loading on their cytotoxic activity.

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## CB PP 14

**Lipophilicity assessment of selected phenolic acids using immobilized artificial membrane chromatography**

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Immobilized artificial membrane (IAM) chromatography is a biomimetic HPLC technique which utilizes stationary phases that mimic biomembranes for the profiling of compound–membrane interactions. The IAM stationary phase incorporates phospholipids that imitate structural features and fluidity of biomembranes. IAM chromatography can be used for lipophilicity assessment, an important physicochemical property related to membrane permeability, absorption, distribution, and tissue binding [1]. This approach provides a reproducible method for characterizing lipophilicity and could enable a more physiologically relevant alternative to standard *in vitro* methods. Gallic acid, 4-hydroxybenzoic acid, cinnamic acid, ferulic acid, caffeic acid, and *p*-coumaric acid are widely recognized for their health-promoting properties. The lipophilicity of the selected phenolic acids was assessed using a biomimetic chromatographic system consisting of an IAM stationary phase and UV detector. The mobile phase was composed of acetonitrile and 10 mM ammonium acetate (pH 6), the column temperature was maintained at 25 °C. IAM lipophilicity was expressed as the logarithm of the retention factor extrapolated to 100% aqueous mobile phase ( $\log k_\omega$ ), calculated according to the linear Snyder–Soczewinski model:  $\log k = \log k_\omega - S_\varphi$ , under reversed-phase conditions ( $\varphi = 0.2\text{--}0.4$ ). The obtained  $\log k_\omega$  values showed strong correlations with several predicted lipophilicity indices (iLOGP, XLOGP, WLOGP, MLOGP, SILICOS-IT, and  $\log D_{7.4}$ ) ( $r > 0.72$ ). The strongest correlation was observed between  $\log k_\omega$  and  $\log D_{7.4}$  ( $r = 0.77$ ), which represents the octanol/water distribution coefficient under physiological pH conditions. The results show a close relationship between IAM-measured and computationally predicted lipophilicity for the studied phenolic acids. In conclusion, biomimetic IAM chromatography could be utilized as an approach for lipophilicity characterization of bioactive phenolic compounds.

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## CB PP 15

**Synthesis and *in silico* biological investigation of  
3 $\beta$ -acetoxy-19-bromo-17-oxa-17a-homoandrost-5-en-16-one**

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Aromatase inhibitors play an important role in the treatment of hormone-dependent breast cancer by reducing estrogen biosynthesis. Since the C19 methyl group of the steroidal scaffold is involved in interactions within the aromatase active site, this position represents an interesting site for chemical modification aimed at developing novel steroid-based compounds with potential biological activity. In the present study, we synthesized 3 $\beta$ -acetoxy-19-bromo-17-oxa-17a-homoandrost-5-en-16-one, a 19-bromo derivative bearing a D-homo lactone moiety, starting from the corresponding 19-hydroxy derivative. The synthesized compound was further evaluated using *in silico* ADMET and toxicity prediction approaches. SwissADME [1] and ProTox 3.0 [2] predictions indicated favorable pharmacokinetic properties, including predicted gastrointestinal absorption and the ability to cross the blood-brain barrier. ProTox 3.0 predicted an LD<sub>50</sub> value of 5000 mg/kg and assigned the compound to toxicity class 5. At the same time, the analysis indicated a potential for immunotoxicity, which warrants further investigation. SwissTargetPrediction identified aromatase as the main predicted molecular target of the synthesized steroid derivative. Furthermore, PASS online analysis predicted antineoplastic activity with the highest probability among the evaluated biological activities. These findings suggest that 3 $\beta$ -acetoxy-19-bromo-17-oxa-17a-homoandrost-5-en-16-one represents a promising steroidal scaffold for further investigation, particularly in the context of aromatase-related and potential antineoplastic activity. The obtained *in silico* results provide a basis for subsequent experimental studies aimed at evaluating its biological activity and mechanism of action.

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**CB PP 16****Rational engineering of new glucose oxidase mutants through sequence-based modelling and molecular dynamics simulations**

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Engineering glucose oxidase (GOx) from *Aspergillus niger* is usually done by mutating residues surrounding the substrate-binding and catalytic regions [1]. Here, we investigated an alternative strategy targeting residues that interact directly with the FAD cofactor and may influence catalytic behaviour by modulating the protein-cofactor environment.

We represented mutant protein sequences as descriptor arrays obtained from the Informational Spectrum Method (ISM). Based on the descriptors, we built a partial least-squares regression (PLSR) model, relating sequence variation to catalytic turnover ( $k_{\text{cat}}$ ). The resulting model achieved an  $R^2$  of 0.99 and was subsequently used to evaluate the effects of individual amino-acid substitutions. We combined candidate mutations by considering their predicted effects on  $k_{\text{cat}}$ .

We examined the resulting triple mutant using three independent 200 ns molecular dynamics simulations in GROMACS. We calculated substrate binding energy from the trajectories using the MM-PBSA method. The simulations indicated that the proposed mutant remained structurally stable and preserved a catalytically favorable glucose orientation near the FAD cofactor. A persistent interaction between glucose and His516 supported this arrangement.

These results represent a sequence-based approach, combined with structure-based simulations, for prioritising multi-site enzyme variants. The proposed workflow provides a computational framework for identifying GOx mutants with potentially improved catalytic turnover and substrate-binding characteristics before experimental evaluation.

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**CB PP 17****Targeting envelope (E) dimer protein of Yellow Fever Virus**

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Yellow fever virus (YFV) is an enveloped, positive-sense single-stranded RNA virus whose genome encodes for a polyprotein that is post-translationally cleaved into seven non-structural and three structural proteins: capsid, pre-Membrane (prM) and Envelope (E). The E protein dimer plays a central role in viral entry. Upon exposure to the acidic environment of the endosome, the E protein undergoes a conformational transition from a dimeric to a trimeric state, leading to membrane fusion and release of the viral genome into the host cell [1].

Obtaining a stable E protein dimer for determining its structure has proven challenging, and several protein constructs were therefore designed. A specific sequence was seen in cryo-electron microscopy (cryo-EM) as interacting to the envelope dimer interface on the whole virion, and was thus added to the E protein to stabilize the dimer formation.

Two structural approaches were pursued to study those constructs. X-ray crystallography was investigated first, with purified protein subjected to extensive crystallization screening. Despite these efforts, suitable crystals for X-ray structure determination could not be obtained. Cryo-EM was then explored as an alternative approach. Since the size of the E-dimer (100kDa) is at the limit of resolution for the Cryo-EM approach, we have tested binding to known antibodies that could be added to increase the size of the protein. In parallel, cell viability was tested on two different cell lines with three control compounds as an initial evaluation of this assay for further investigation for the screening of novel virus inhibitors that we will receive from a collaborator.

Structural characterization of the YFV E protein dimer may contribute to a better understanding of the mechanisms underlying viral entry and guide the further investigation of compounds targeting this process. Although suitable crystals could not be obtained, cryo-EM is a promising alternative for determining the structure. Additionally, we have established a window of compound and vehicle (DMSO) concentrations that do not affect cell viability, providing a set-up for future assays.

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**CB PP 18****DNA-Binding Properties of Antimicrobial Potent Imine Derived from Tranexamic Acid**

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The rapid emergence and global spread of antimicrobial resistance (AMR) represent a major global health challenge, significantly reducing the efficacy of existing antimicrobial therapies and increasing morbidity, mortality, and healthcare costs [1]. Many organic compounds, as Schiff bases, have gained considerable attention as promising scaffolds for the development of biologically active molecules with diverse antimicrobial properties. Numerous antimicrobials, anticancer, and other biologically active agents exert their activity through interactions with DNA, emphasizing the need to elucidate their binding behavior. In this study, a Schiff base (compound C), derived from tranexamic acid (TXA) and a phenol-based aldehyde was investigated. This compound has previously demonstrated superior antimicrobial activity compared to commercially available antimycotics [3]. To better understand its mechanism of action, its DNA-binding properties were examined using competitive fluorescence assays with ethidium bromide (EB) and Hoechst 33258 (Hoe) as site-specific probes. The results indicate that compound C interacts with DNA via both intercalative and minor groove binding modes. Notably, a higher binding constant obtained in the presence of Hoechst 33258 compared to ethidium bromide suggests a preferential affinity for the minor groove of the DNA helix.

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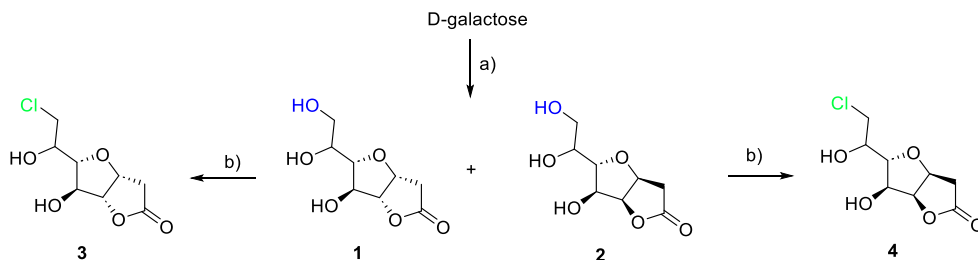
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## CB PP 19

**Synthesis and *in silico* ADME profiling of novel chlorinated furanofuranone analogues**

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Furanofuranone derivatives represent an interesting scaffold for the development of biologically active small molecules. Structural modification of this scaffold, including the introduction of chlorine, may influence its physicochemical and pharmacokinetic properties. In this work, the synthesis and characterization of novel chlorinated furanofuranone analogues will be presented (Scheme 1). The target compounds were obtained from furanofuranone derivatives previously synthesized according to a reported procedure starting from D-galactose [1]. The introduction of chlorine into the furanofuranone scaffold was explored with the aim of obtaining new structural analogues with potentially improved pharmacokinetic properties. In addition, the pharmacokinetic and drug-likeness properties of the synthesized compounds will be evaluated *in silico* using the SwissADME platform. The obtained results will provide insight into the physicochemical and pharmacokinetic profiles of the new chlorinated furanofuranone analogues and their potential for further biological evaluation.



Scheme 1. Reagents and conditions: a) Ref. [1]; b) CCl<sub>4</sub>, PPh<sub>3</sub>, Py, 0°C 30 min, rt, 3 h (for **1**), 10 h (for **2**), 65% **3** and 82% **4**.

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## CB PP 20

**Deoxycholic acid-based cyanoenones targeting the NRF2-KEAP1 pathway**

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Nuclear factor erythroid 2–related factor 2 (NRF2) represents a key regulatory factor in response to oxidative, inflammatory, and metabolic stress. Therefore it can be an attractive pharmacological target in inflammatory, neurodegenerative, metabolic, and cancer-related conditions. The primary controller of NRF2 is the Kelch-like ECH-associated protein 1 (KEAP1), whose reactive cysteines can be covalently modified by electrophilic molecules, thereby stabilizing NRF2 and promoting transcription of cytoprotective genes. [1]

Here we report the synthesis of deoxycholic acid-based compounds, containing A-ring electrophilic groups such as cyanoenones (Figure 1.) and dienones similar to omaveloxolone, a drug approved for Friedreich's ataxia. These electrophilic compounds were selected for their potential covalent interactions with KEAP1 cysteins. In this work we expanded on the chemical space of bile-acid based NRF2 modulators and provide synthetically accessible scaffolds for subsequent biological evaluation. Biological validation of the presented compounds is ongoing.

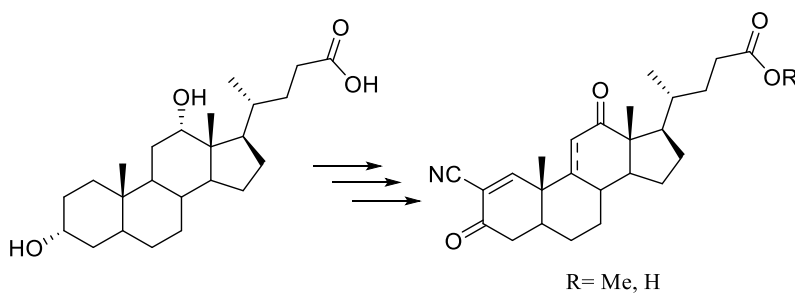


Figure 1. Deoxycholic acid modifications

**References**

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**Acknowledgments**

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## CB PP 21

**Plant-mediated synthesis and bioactivity of selenium nanoparticles using *Satureja hortensis* L.**

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The use of plant extracts in nanoparticle synthesis represents a sustainable approach to developing biologically active nanomaterials [1]. An aqueous extract of *Satureja hortensis* L. was used for the green synthesis of selenium nanoparticles (SeNPs). Their antioxidant,  $\alpha$ -amylase and  $\alpha$ -glucosidase inhibitory, and antimicrobial activities were compared with those of the plant extract and SeNPs synthesized using ascorbic acid.

For SeNPs synthesis, a 50 mM Na<sub>2</sub>SeO<sub>3</sub> solution was mixed with *S. hortensis* aqueous extract at a final concentration of 20% (v/v) or with 2 mM ascorbic acid. The pH was adjusted to 9, and the mixture was incubated under magnetic stirring at 60 °C for 2 h. Nanoparticle formation was monitored by UV–Vis spectroscopy. FTIR analysis indicated that compounds from the extract and ascorbic acid participated in SeNPs stabilization. Scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS) confirmed the formation of nanoparticles predominantly composed of selenium, with morphologies that varied depending on the reducing agent. In biological assays, the *S. hortensis* extract exhibited stronger antioxidant and  $\alpha$ -glucosidase inhibitory activities than the synthesized SeNPs. In contrast, SeNPs synthesized using the plant extract showed substantially stronger antimicrobial activity than the extract and ascorbic acid-mediated SeNPs, with MIC values of 0.625 mg/mL against several tested microorganisms.

These results demonstrate that *S. hortensis* is a promising natural resource for synthesizing biologically active SeNPs and suggest that their properties are strongly influenced by the reducing system.

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## CB PP 22

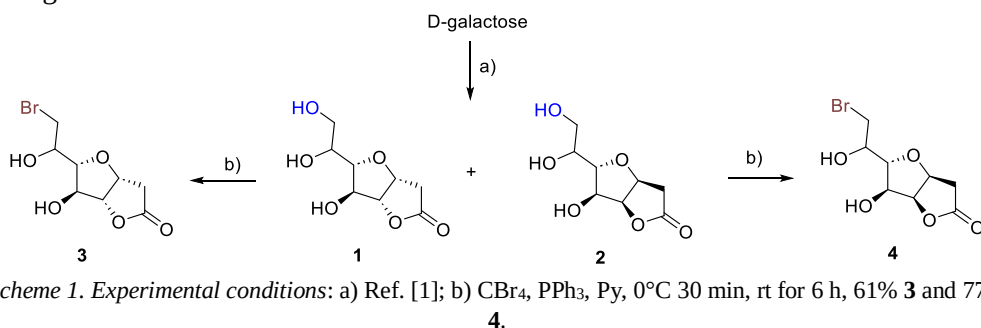
## Brominated furanofuranone analogues: synthesis, characterization and in silico pharmacokinetic profiling

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Furanofuranone-containing compounds have attracted attention as versatile scaffolds for the development of structurally diverse small molecules. In the present study, bromination was explored as a strategy for the structural modification of previously synthesized furanofuranone derivatives. The starting compounds were prepared according to a reported procedure using D-galactose as the initial carbohydrate source [1]. The corresponding brominated derivatives were synthesized and characterized, resulting in two novel furanofuranone analogues bearing a bromine substituent.

To further investigate the properties of the newly obtained compounds, their drug-likeness and ADME-related characteristics will be predicted using the SwissADME platform. The analysis will include relevant physicochemical and pharmacokinetic parameters and will enable comparison of the predicted profiles of the brominated derivatives with those of their parent compounds. The obtained data will contribute to a better understanding of the effect of bromine substitution on the molecular properties of this furanofuranone scaffold and provide a basis for selecting compounds for subsequent biological studies.



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## CB PP 23

**Porphyrin conjugation as a structural modulator of antimicrobial peptides**

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Antimicrobial peptides (AMPs) are promising candidates for the development of alternative antimicrobial agents in response to the growing challenge of antimicrobial resistance (AMR). Their antimicrobial properties are associated with peptide structure, membrane interaction and supramolecular organization [1]. Porphyrins, in turn, possess intrinsic antimicrobial potential through light-activated reactive oxygen species generation and light-independent membrane disruption [2]. Therefore, a conjugation between these two drug classes, porphyrin + AMP, to form peptide–drug conjugates (PDCs) is a promising strategy where the limitations of the individual components, porphyrin aggregation tendency and peptide serum stability can be successfully addressed [2].

In this study, we investigate how covalent attachment of porphyrin macrocycles affects the conformation and organization of selected AMP scaffolds. Four AMPs were synthesized by solid-phase peptide synthesis (SPPS) and subsequently conjugated on-resin with two porphyrin derivatives. Their structural properties were investigated using circular dichroism (CD) and nuclear magnetic resonance (NMR) spectroscopy, complemented by all-atom molecular dynamics simulations. Far-UV CD measurements revealed pronounced environment-dependent conformational changes, with anionic membrane-mimetic conditions producing spectral signatures consistent with increased  $\alpha$ -helical character. Porphyrin-associated CD signals further revealed sequence-dependent differences in the organization of the conjugates under membrane-mimetic conditions. NMR analysis provided additional evidence for close interactions between the peptide backbone and the attached porphyrin macrocycle. These findings demonstrate that porphyrin conjugation can reshape the structural landscape of antimicrobial peptides in a sequence- and environment-dependent manner.

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**Acknowledgments**

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## CB PP 24

**Design, synthesis, and ADME-Tox analysis of a new dephenylated analogue of (–)-goniofufurone with a 7-*O*-isobutyl group**

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The aim of this study was the design, synthesis, and *in silico* evaluation of the ADME-Tox properties of a novel dephenylated (–)-goniofufurone analogue bearing a 7-*O*-isobutyl substituent (compound **6**). Goniofufurone is a styryl-lactone natural product and a valuable scaffold for the development of structurally modified compounds with potentially improved pharmacological properties. The target analogue was synthesized starting from commercially available L-xylose through a five-step synthetic sequence with an overall yield of 3.38%. The synthetic pathway included construction of the furanofuranone lactone core using Meldrum's acid, benzyl protection, selective debenzylation, *O*-isobutylation, and final removal of the benzyl protecting group at the C-5 position.

*In silico* evaluation was performed using SwissADME and vNN-ADMET software [1]. The target compound **6** exhibited low lipophilicity and a favourable physicochemical profile according to Lipinski's Rule of Five. High gastrointestinal absorption was predicted, while significant blood–brain barrier penetration and P-glycoprotein substrate activity were not predicted. Compound **6** was also not predicted to inhibit the investigated CYP450 isoforms, indicating a low potential for CYP-mediated drug–drug interactions. Toxicological predictions did not indicate mitochondrial toxicity; however, potential drug-induced liver injury and hERG potassium channel inhibition were identified as relevant safety alerts. Overall, the obtained results indicate that compound **6** retains several favourable ADME characteristics of (–)-goniofufurone and represents a promising structural platform for further development of goniofufurone analogues, while the predicted hepatotoxicity and cardiotoxicity require experimental verification.

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**Acknowledgments**

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**CB PP 25****Allophycocyanin from cyanobacteria *Limnospira platensis*:  
Optimization of purification, stability testing and  
characterization of binding to concanavalin A**

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Simeon Minić<sup>1</sup>

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Phycobiliproteins (PBP) are a promising research subject due to their potential use in medicine, food and fundamental research [1]. Allophycocyanin (APC) is a blue fluorescent PBP from the cyanobacterium *Limnospira platensis* (blue spirulina). In this study, we showed that APC is more resistant to enzymatic digestion by bromelain (at pH 7.5) than C-Phycocyanin, the major PBP in spirulina. We purified APC by DEAE Sephadex A25 ion-exchange chromatography, followed by gel filtration on a Sephacryl S-200 column after bromelain digestion of spirulina water extract. APC was also purified from non-digested spirulina water extract by hydroxyapatite chromatography. We tested the impact of bromelain digestion on the thermal stability of APC by UV-far CD spectroscopy and spectrofluorimetry. The melting point of APC determined by spectrofluorimetry was 50.0 °C for APC purified with the enzymatic digestion step, and 50.1 °C for APC purified without digestion. The melting point of APC determined by CD spectroscopy was 67.6 °C and 67.2 °C for APC samples prepared with and without digestion, respectively. Microscale thermophoresis was used to determine the dissociation constant of the complex of APC and concanavalin A (ConA), a lectin from jack-bean (*Canavalia ensiformis*). The sample of APC purified with the digestion step didn't show any binding affinity to ConA, while APC purified without enzymatic digestion bound ConA with a dissociation constant of  $1.96 \times 10^{-5}$  mol dm<sup>-3</sup>. We also predicted the structure of the APC-ConA complex by protein-protein docking, which showed that the binding potentially occurs via two non-identical surfaces, which is in agreement with previous studies [2]. The results of this study suggest that bromelain digestion of spirulina water extract could induce minor hydrolysis of APC, leading to a change in binding to ConA, while not impacting its thermal stability.

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## CB PP 26

**Design, synthesis optimization, ADME-Tox analysis, and antiproliferative activity of (–)-goniofufurone analogue**

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The goal of this study was to optimize the synthesis of compound **6** (3,6-Anhydro-7-*O*-tridecyl-2-deoxy-*L*-ido-heptono-1,4-lactone), an analogue of (–)-goniofufurone (**1**). To reduce the number of synthetic steps and improve overall yield (13 from D-xylose and a total yield of 1.04%), the synthesis was optimized from L-xylose in 5 steps, affording the target compound with an overall yield of 8.60%. Subsequently, *in silico* ADME-Tox analysis was performed using the SwissADME platform, along with evaluation of the antiproliferative activity of compounds involved in the synthesis.

*In silico* studies included analysis of the lipophilicity of all synthesized compounds and of the passive permeability of compound **6**. The results showed that the average logP values for compounds **3** (3,6-Anhydro-2-deoxy-5,7-di-*O*-benzyl-*L*-ido-heptono-1,4-lactone), **4** (3,6-Anhydro-5-*O*-benzyl-2-deoxy-*L*-ido-heptono-1,4-lactone), and **6** were below 5, indicating a satisfactory balance between water solubility and membrane permeability. According to the BOILED-Egg model, compound **6** showed a high predicted probability of passive intestinal absorption and potential passive permeation across the blood–brain barrier. Furthermore, compound **6** was predicted not to be a substrate of P-glycoprotein. The obtained results indicate a relatively favourable ADME-Tox profile for compound **6**.

The antiproliferative activities of molecules **2** (3,6-Anhydro-2-deoxy-*L*-ido-heptono-1,4-lactone), **3**, **4** and **6** were examined by measuring their effects on the proliferation of seven malignant and one healthy cell line. The most significant results were achieved for analogue **2**, which revealed strong cytotoxic activity against six of the seven tested malignant cell lines. Analogue **6** showed the strongest cytotoxic activity against the HL 60 cell lines. Against the healthy MRC-5 cell line, compounds **3–6** were inactive, while compound **2** showed weak activity.

**Acknowledgments**

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## **Developments in Chemical Synthesis (DCS)**

**DCS PP 01****A refined approach in Zn<sup>2+</sup> detection: highly selective ESIPT-effect-based ratiometric sensors**

Galja Varga<sup>1</sup>, Borjana Karadžić<sup>1</sup>, Miloš Jović<sup>2</sup>, Olivera Marković<sup>3</sup>, Života Selaković<sup>1</sup>,  
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Zinc is a micronutrient, thus vital for humans and other living organisms, which makes its detection an important research topic. Considering the difficulties that arise with identifying the presence of ions with a d<sup>10</sup> electronic configuration, such as the absence of spectroscopic qualities that would provide selectivity in its detection process, there is an evident need for novelties that would allow circumvention of previously mentioned problems. Therefore, we present a ratiometric sensing system relying on the Excited-State Intramolecular Proton Transfer (ESIPT) effect, a fluorescence mechanism which photoexcited molecules that have the structural capacity to undergo tautomerization follow whilst relaxing their energy. Sensors **1** and **2** (Fig. 1) presented in this study have a structural moiety based on tetramic acid, a natural product found in a number of living organisms. Additionally, the synthetic approach is undemanding, since no more than two steps are needed for the acquisition of these sensors from commercially available starting materials, abiding by the principles of green chemistry, as a cost-effective, straightforward, and sustainable synthetic route.

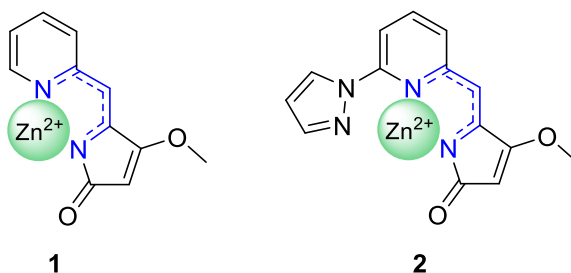


Figure 1. Ratiometric fluorescent sensors for zinc ions.

**Acknowledgments**

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## DCS PP 02

**Derivatization of pyrazole-3,5-dicarboxylic acid**

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<sup>2</sup>Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade

The objective of this study is the derivatization of pyrazole-3,5-dicarboxylic acid (PDC) to form hydrazone-type compounds of higher flexibility compared to the starting pyrazole-3,5-dicarboxylic acid. The experimental design involves the initial derivatization of PDC using aminoguanidine (AG) and hydrazine (HZ). The synthesis is carried out in DMF and MeOH, but the resulting compound is the same regardless of the reaction conditions. The traces of water in the reaction mixture hindered hydrazone formation and resulted in salt-type compounds AG-PDC·H<sub>2</sub>O and HZ-PDC. The salt AG-PDC·H<sub>2</sub>O crystallized in the form of a single crystal. Its molecular structure, determined by X-ray diffraction, is presented below (Fig. 1). The reaction of the salt-type derivatives with transition metals resulted in complexes of the composition [M(PDC)(H<sub>2</sub>O)<sub>4</sub>], M= Co<sup>II</sup>, Ni<sup>II</sup>, and Fe<sup>II</sup>. All the compounds were characterized by IR spectra.

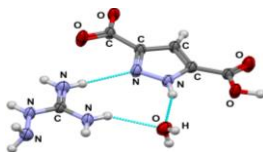


Figure1. Molecular structure of AG-PDC·H<sub>2</sub>O.

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**Acknowledgments**

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**DCS PP 03****Oxone-mediated oxidation of 5-monosubstituted tetrazoles -  
identification of complex reaction mixture constituents**

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*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*

Interest in the synthesis of high-energy-density materials (HEDMs) is ever-growing due to their wide range of applications. Among attractive HEDMs are hydroxytetrazoles, which combine the tetrazole moiety responsible for their high thermal stability and good detonation performance, and the hydroxyl group, which improves the oxygen balance. There are two synthesis approaches for obtaining hydroxytetrazoles: 1) via cyclization of azidoximes, which yields the 1,5-regioisomer exclusively, and 2) by direct oxidation of the corresponding 5-monosubstituted tetrazoles with oxone, which produces a mixture of 1,5- and 2,5-regioisomers [1]. In an attempt to obtain new hydroxytetrazoles using the second approach, we encountered a much more complicated reaction mixture than anticipated. This work deals with the characterization of several compounds from the reaction mixture using NMR techniques. According to the preliminary results, ring-opening reactions occurred leading to the formation of nitriles and amides.

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**Acknowledgments**

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**DCS PP 04****Synthesis and crystal structure of silver(I) complex with  
*N*-(pyrazin-2-yl)benzenesulfonamide**

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In this work, we present the synthesis and structural characterization of a silver(I) complex with *N*-(pyrazin-2-yl)benzenesulfonamide, [Ag(L-H)]<sub>n</sub>, where the ligand is coordinated in its deprotonated form. This complex was obtained by reacting silver(I) hexafluorophosphate with an equimolar amount of *N*-(pyrazin-2-yl)benzenesulfonamide in ethanol at room temperature. The reaction conditions were optimized to prevent the reduction of silver(I) ions. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by slow evaporation of a solution prepared by dissolving the white precipitate in an acetonitrile/water mixture (v/v = 1 : 1) at room temperature after 3 days. The purity and composition of the synthesized silver(I) complex were confirmed by elemental microanalysis, while the complex was further characterized by IR spectroscopy, UV-Vis spectrophotometry, molar conductivity measurements, and single-crystal X-ray diffraction analysis. In the [Ag(L-H)]<sub>n</sub> complex, each silver(I) center is coordinated by two nitrogen donor atoms, with Ag–N bond lengths of 2.168(3) and 2.174(3) Å and, additionally by one oxygen atom (Ag–O bond length of 2.1691(2) Å). Moreover, the distorted tetrahedral geometry around each silver(I) center is complemented by a very short Ag...Ag contact of 2.7742(4) Å. The combined spectroscopic and crystallographic results confirm the successful formation of the silver(I) complex and provide insight into its structural features.

**Acknowledgments**

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**DCS PP 05****Structural diversity of a cadmium(II) thiocyanate complex with 2-acetylthiazole semicarbazone**

Mima Jevtović<sup>1</sup>, Nevena Stevanović<sup>2</sup>, Marija Pavlović<sup>1</sup>, Božidar Čobeljić<sup>2</sup>, Matija Zlatar<sup>3</sup>

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Semicarbazone ligands are versatile coordination systems capable of stabilizing diverse metal environments and supramolecular architectures. In this work, a cadmium(II) thiocyanate complex with (*E*)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carboxamide (**HL**) was synthesized and structurally characterized. The complex was obtained from **HL**, a Cd(II) salt and ammonium thiocyanate in a methanol/water medium, yielding yellow single crystals after slow evaporation. The compound has the composition C<sub>16</sub>H<sub>16</sub>Cd<sub>2</sub>N<sub>12</sub>O<sub>2</sub>S<sub>6</sub>. Single-crystal X-ray diffraction revealed two distinct crystalline forms with the same chemical composition. One form crystallizes in the triclinic space group *P*1, while the second adopts the tetragonal space group *P*4<sub>2</sub>*c*. In both structures, cadmium(II) is six-coordinate and bound through donor atoms of the semicarbazone ligand and thiocyanate groups. The IR spectrum shows strong thiocyanate bands at 2130 and 2113 cm<sup>-1</sup>, supporting coordination of the SCN<sup>-</sup> groups. The results demonstrate pronounced solid-state structural diversity in this Cd(II)-semicarbazone-thiocyanate system and emphasize the influence of coordination geometry and crystal packing on the final crystalline structure.

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## DCS PP 06

**Synthesis and structural characterization of a mononuclear Ni(II) complex with a 2-acetylthiazole semicarbazone**

Marija Pavlović<sup>1</sup>, Mima Jevtović<sup>1</sup>, Nevena Stevanović<sup>2</sup>,  
Maja Šumar-Ristović<sup>2</sup>.

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A novel mononuclear Ni(II) complex with the semicarbazone ligand (*E*)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carboxamide (HL), obtained by the condensation reaction of semicarbazide hydrochloride and 2-acetylthiazole, in the presence of sodium cyanate, was synthesized. The complex was prepared by a solution-phase method, involving the dropwise addition of an aqueous solution of Ni(BF<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O and sodium cyanate to a methanolic solution of the ligand. The complex [Ni(HL)<sub>2</sub>](BF<sub>4</sub>)(OCN) (Fig.1) was characterized by single-crystal X-ray diffraction analysis. The analysis revealed that the complex crystallizes in the monoclinic crystal system, in the *P*2<sub>1</sub>/*c* space group. The central Ni(II) ion is coordinated by two neutral 2-acetylthiazole semicarbazone ligands, with each ligand acting as a tridentate NNO donor through the carbonyl oxygen, azomethine nitrogen, and thiazole nitrogen atoms. This coordination mode leads to the formation of four five-membered chelate rings, while the Ni(II) center adopts a distorted octahedral coordination geometry. The BF<sub>4</sub><sup>−</sup> and OCN<sup>−</sup> anions are located in the outer coordination sphere.

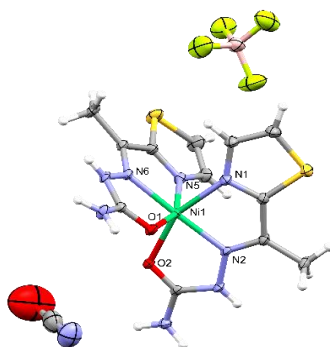


Figure 1. ORTEP representation of the [Ni(HL)<sub>2</sub>](BF<sub>4</sub>)(OCN) complex. Thermal ellipsoids are drawn at the 50 % probability level.

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Ministry of Science, Technological Development and Innovation of the Republic of Serbia, Contract numbers: 451-03-33/2026-03/200288 and 451-03-33/2026-03/200168.

## DCS PP 07

## Synthesis of manoyl oxide derivatives

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The labdane diterpene manoyl oxide, its stereoisomers and their semisynthetic derivatives exhibit various biological activities, including antibacterial, antifungal, anticancer and anti-inflammatory activities [1]. Synthesis of manoyl oxide from another labdane diterpene, sclareol, has been described in the literature [2]. In this study, we have found that sclareol derivatives with electron-rich aryl substituents at the terminal double bond readily undergo a cyclisation reaction, resulting in a mixture of manoyl oxide and 13-*epi*-manoyl oxide derivatives. On the basis of this reaction, we have developed a new methodology for the synthesis of manoyl oxide derivatives from sclareol (Fig. 1). In total, five manoyl oxide derivatives were synthesised and characterised with IR and NMR spectra. Spectral data confirmed that a cyclisation reaction occurred. Furthermore, attempts were made to gain control over the cyclisation reaction via the use of protecting groups. Simplification of the procedure into a one-pot reaction was also considered.

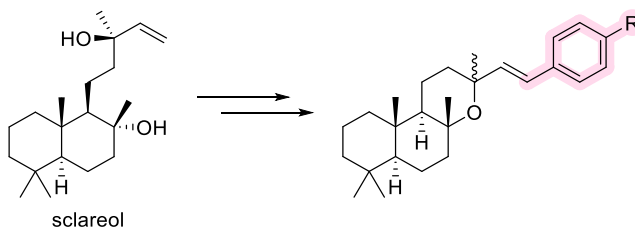


Figure 1. Synthesis of manoyl oxide derivatives from sclareol.

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**DCS PP 08*****N*-Alkyl and *N*-aryl acridone derivatives – a new class of photosensitizers for [2+2] cycloadditions**

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The activation of small organic molecules via an energy transfer mechanism (sensitization) represents a powerful tool for forming new chemical bonds. To generate reactive triplet states, various types of photosensitizers have been employed so far, such as (expensive) transition metal complexes and organic dyes. In this work, we demonstrate that various *N*-alkyl and *N*-aryl acridone derivatives can be utilized as efficient sensitizers for [2+2] cycloadditions, as well as for olefin *E/Z* isomerizations. Although structurally simple, the acridone scaffold possesses significant potential for derivatization and fine-tuning of photophysical properties. Of particular importance is the facile *N*-functionalization, which is not accessible in related xanthone and thioxanthone photosensitizers. Furthermore, the class of acridone photosensitizers has remained underexplored, with only one example recently published in the literature, independent of our research [1]. Finally, acridone photosensitizers enable the activation of substrates with exceptionally high triplet energies, indicating their potential for application in demanding photocatalytic transformations.

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**Acknowledgments**

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## DCS PP 09

**Synthesis and characterization of a Cu(II) complex with methyl 3-formyl-4-hydroxybenzoate and 4-methylphenanthroline**

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The mononuclear copper(II) complex (Fig. 1.) was obtained by reacting  $\text{Cu}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$  with methyl 3-formyl-4-hydroxybenzoate (HL) and 4-methylphenanthroline. Its crystal structure was determined by single-crystal X-ray diffraction analysis. The complex crystallizes in the triclinic space group  $P\bar{1}$  with two formula units per unit cell. The Cu(II) ion is five-coordinate and adopts an almost ideal square-pyramidal geometry ( $\tau_5 = 0.098$ ) with an  $\text{N}_2\text{O}_2\text{F}$  donor set. The basal plane is formed by the phenolate and aldehyde oxygen atoms of the bidentate methyl 3-formyl-4-hydroxybenzoate ligand and two nitrogen atoms of 4-methylphenanthroline, while a fluorine atom of the tetrafluoroborate anion occupies the apical position. Coordination of the O,O-donor ligand forms a nearly planar six-membered chelate ring. The crystal packing is additionally stabilized by  $\pi$ - $\pi$  interactions between aromatic rings of neighboring complex molecules, characterized by a centroid-to-centroid distance of 3.556 Å.

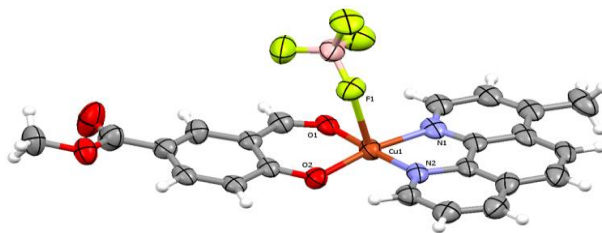


Figure 1. Molecular structure of Cu(II) complex.

**Acknowledgments**

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**DCS PP 10****Development of a method for the synthesis of ketones using an iron-based catalyst**

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Transition-metal-catalyzed cross-coupling reactions represent an important method for ketone synthesis. Since various biologically active molecules and pharmaceutical products contain a ketone functional group, methods for their synthesis are constantly being developed. The approaches for ketone synthesis primarily include cross-coupling reactions [1], which require catalysts. Iron offers numerous advantages over other metals when selecting a catalyst for cross-coupling reactions. Aiming to develop an iron-catalyzed method for ketone synthesis, this study investigated two synthetic approaches. The first approach involved the cross-coupling of benzoyl derivatives with various phenyl derivatives; however, it was demonstrated that the desired product was not formed under the tested reaction conditions. The second approach involved carbonylative coupling reactions, which resulted in the formation of the product in low yield under the tested conditions.

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## DCS PP 11

**Synthesis and characterization of octahedral Co(II) complex with condensation product of 2-acetylthiazole and semicarbazide hydrochloride**

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The ligand was synthesized in the reaction of 2-acetylthiazole and semicarbazide hydrochloride in molar ratio 1:1 in water. Two independent reactions involving the same starting compounds, the ligand, cobalt(II) tetrafluoroborate hexahydrate, and sodium cyanate, carried out in different solvent mixtures, afforded the same Co(II) complex. The first reaction was carried out in a MeOH/H<sub>2</sub>O mixture, whereas the second was performed in an MeCN/H<sub>2</sub>O mixture. Single-crystal X-ray diffraction revealed a mononuclear Co(II) complex crystallizing in the triclinic *P*1 space group. The Co(II) center is six-coordinate and adopts a distorted octahedral geometry, with an N<sub>4</sub>O<sub>2</sub> donor environment. The Co–N and Co–O bond lengths fall in the ranges 2.0744(15)–2.2065(15) Å and 2.0600(12)–2.0960(13) Å, respectively. The deviation from an ideal octahedral geometry is reflected in the coordination angles, with the trans angles ranging from 146.01(6)° to 162.01(6)°. The crystal structure also contains two lattice water molecules. The ligand was characterized by elemental analysis, NMR and IR spectroscopy, while the complex was characterized by elemental analysis and IR spectroscopy, and its crystal structure was determined by single-crystal X-ray diffraction.

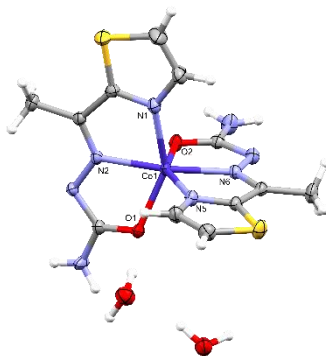


Figure 1. ORTEP representation of the Co(II) complex. Thermal ellipsoids are drawn at the 50% probability level.

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## DCS PP 12

**A pentacoordinate Zn(II) thiocyanate complex with 2-acetylthiazole semicarbazone: synthesis and crystal structure**

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Semicarbazones are versatile ligands containing multiple donor atoms and can exhibit different coordination modes upon binding to metal ions. In this work, (*E*)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carboxamide (HL) was synthesized by the condensation reaction of 2-acetylthiazole and semicarbazide hydrochloride in a 1:1 molar ratio in water. The Zn(II) complex was obtained by the reaction of HL with zinc(II) acetate and ammonium thiocyanate in a methanol/water medium. Slow evaporation of the reaction mixture afforded light-orange single crystals suitable for X-ray diffraction analysis. Single-crystal X-ray diffraction revealed a mononuclear complex of the composition [Zn(HL)(NCS)<sub>2</sub>], crystallizing in the monoclinic P2<sub>1</sub>/n space group. The Zn(II) ion is five-coordinate with an N<sub>4</sub>O donor environment formed by the tridentate N,N,O-coordinated semicarbazone ligand and two N-bound thiocyanate groups. The coordination environment around Zn(II) can be described as a distorted square-pyramidal geometry. The Zn–N bond lengths range from 1.9462(19) to 2.1135(18) Å, while the Zn–O bond length is 2.2292(16) Å. The results demonstrate the ability of 2-acetylthiazole semicarbazone to stabilize a pentacoordinate Zn(II) center in the presence of pseudohalide coligands.

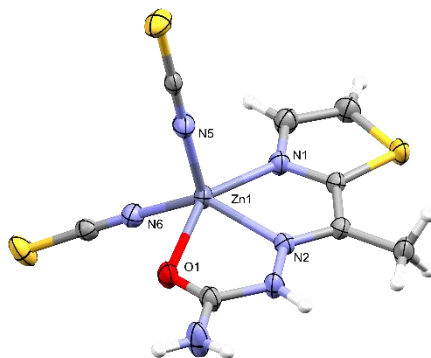


Figure 1. ORTEP representation of the complex. Thermal ellipsoids are drawn at the 50% probability level.

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Ministry of Science, Technological Development and Innovation of the Republic of Serbia, Contract numbers: 451-03-33/2026-03/200288, and 451-03-33/2026-03/200168.

## DCS PP 13

**A solvent-free form of the dinuclear zinc(II) complex  
[Zn<sub>2</sub>(L–2H)<sub>2</sub>]**

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In our previous work, we reported the synthesis and structural characterization of the Schiff base of 2,6-diacetylpyridine and adamantane-1-carbohydrazide (L) and its dinuclear zinc(II) complex [Zn<sub>2</sub>(L–2H)<sub>2</sub>]·EtOH [1]. Herein, we report the synthesis and structural characterization of [Zn<sub>2</sub>(L–2H)<sub>2</sub>], the solvent-free form of the previously described complex.

Yellow rod-shaped single crystals of [Zn<sub>2</sub>(L–2H)<sub>2</sub>] were obtained by evaporation of a 1:1 MeCN solution of L and Zn(OAc)<sub>2</sub>. The complex shows good solubility in DMF and a molar conductivity of 4 Scm<sup>2</sup>mol<sup>–1</sup>, indicating its non-electrolytic nature. In the novel complex, each Zn(II) center exhibits a 3+2 coordination mode, being coordinated by three donor atoms (pyridine N, azomethine N, and carbonyl O) from one hydrazide fragment and two donor atoms (azomethine N and carbonyl O) from the second hydrazide fragment. This coordination environment is identical to that observed in the previously reported [Zn<sub>2</sub>(L–2H)<sub>2</sub>]·EtOH complex [1]. Overlay of the molecular structures reveals a high degree of similarity in both the coordination environment and ligand conformation (RMSD = 0.62Å), indicating that the presence of solvent molecules in the crystal lattice has no significant effect on the complex geometry. The main differences concern intermolecular interactions and crystal packing.

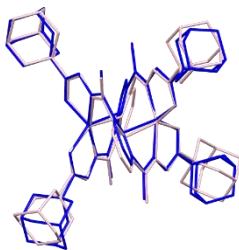


Figure 1. Overlay of the molecular structures of [Zn<sub>2</sub>(L–2H)<sub>2</sub>]·EtOH (blue) and [Zn<sub>2</sub>(L–2H)<sub>2</sub>] (pink).

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## **Environmental Awareness (EA)**

## EA PP 01

**Zeolite-based Geopolymer: Synthesis, Characterization and Ni<sup>2+</sup>, Cu<sup>2+</sup> and Cr<sup>3+</sup> Ion Removal**

Dušan V. Trajković<sup>1,2</sup>, Jelena K. Dikić<sup>1</sup>, Aleksandra S. Popović<sup>2</sup>, Katarina M. Sokić<sup>2</sup>,  
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Environmental pollution by heavy metal ions represents an increasingly pronounced ecological problem in recent years. Heavy metal ions are characterized by a pronounced ability for bioaccumulation and biomagnification, which leads to disruption of the natural balance and endangerment of human health. Natural zeolites are aluminosilicate materials that are often used as a natural material in adsorption process for water purification. However, there are two main problems associated with these materials: 1) agglomeration during application in real industrial systems, and 2) low adsorption efficiency for certain heavy metals (for example, Ni<sup>2+</sup> and Cr<sup>3+</sup>) [1]. Previous research has shown the potential of alkali-activated materials in the adsorption process [2]. The main objective of this work is to investigate the adsorption of the heavy metals by zeolite-based geopolymers. For this purpose, alkaline activation of natural zeolite - clinoptilolite, was performed in order to obtain zeolite-based geopolymer beads. The obtained materials were characterized by scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and X-ray powder diffraction (XRD). The possibility of adsorption of Cu<sup>2+</sup>, Ni<sup>2+</sup>, and Cr<sup>3+</sup> on these materials was investigated. The adsorption experiment was carried out using 1.00 g of adsorbent, 100 cm<sup>3</sup> of solution at concentrations of 100 and 200 mg/dm<sup>3</sup>, for 24 h at 25 °C, and the concentration of the metals was investigated by atomic absorption spectroscopy (AAS). The efficiency of the adsorption process ranged from 64.7-81.6% for Cu<sup>2+</sup>, 88.0-100.0% for Ni<sup>2+</sup>, and 50.6-97.0% for Cr<sup>3+</sup>, indicating the potential application of these materials in real industrial systems.

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**EA PP 02****Turning herbs into photocatalysts: Synthesis of *Thymus serpyllum* extract-based ZnO**

Dušica Jovanović, Daniela Šojić Merkulov, Vesna Despotović, Sabolč Bognar, Nina Finčur

*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*

Among other substances, pharmaceuticals, such as antibiotics and antipsychotics, contribute to water pollution – antibiotics can encourage bacterial resistance, while antipsychotics may disrupt the brain chemistry of non-target organisms [1]. Taking place in the presence of irradiation and a catalyst, heterogeneous photocatalysis is a process suitable for water purification. Over the last decade, there has been a shift towards the green synthesis of photocatalysts using plant extracts. The main advantage of this approach is the substitution of toxic reducing and stabilizing agents with biomolecules naturally occurring in plants. Due to having diverse functional groups (–OH, –NH<sub>2</sub>, –C=O), these biomolecules can obstruct the aggregation of formed photocatalyst particles acting as capping and stabilizing agents [2]. Therefore, the leading goal of this research was the synthesis of a novel ZnO-based photocatalyst (ZnO/TSE), by the precipitation method, using *Thymus serpyllum* aqueous extract as a biomolecule source, and zinc sulphate heptahydrate water solution as a corresponding metal precursor. Additionally, the study examined the photocatalytic activity of the ZnO/TSE (0.5 mg/cm<sup>3</sup>) in the removal of one fluoroquinolone antibiotic (ciprofloxacin, 0.05 mol/dm<sup>3</sup>) and one benzamide-class antipsychotic (sulpiride, 0.05 mol/dm<sup>3</sup>). The findings showed that ZnO/TSE achieved 62% ciprofloxacin and 36% sulpiride removal efficiency from the aqueous medium after 120 min of simulated solar irradiation.

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## EA PP 03

**Green synthesis of Fe/TiO<sub>2</sub> photocatalysts for wastewater treatment**

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<sup>2</sup>NOMATEN Centre of Excellence, National Center for Nuclear Research, Swierk/Otwock, Poland

<sup>3</sup>Scientific Research Center, Baku Engineering University, Baku, Azerbaijan

The development of sustainable photocatalytic materials has gained increasing attention due to the demand for environmentally friendly technologies for pollutant removal and water treatment. In this study, two novel Fe-based photocatalysts, FeVO<sub>4</sub>-bTiO<sub>2</sub> and Fe/TiO<sub>2</sub>/VOOH, were synthesized using bio-based TiO<sub>2</sub> (bTiO<sub>2</sub>) prepared through a green synthesis route employing citrus peel extract and titanium isopropoxide. The bioactive compounds present in the extract act as natural stabilizing and structure-directing agents, replacing conventional chemical additives and contributing to a more sustainable synthesis process [1].

The FeVO<sub>4</sub>-bTiO<sub>2</sub> photocatalyst was prepared by sequential deposition of vanadium and iron precursors onto the bTiO<sub>2</sub> support, followed by washing, drying, and calcination at 500 °C [2]. The Fe/bTiO<sub>2</sub>/VOOH photocatalyst was synthesized *via* precipitation under controlled conditions. Both synthesis routes enabled the successful incorporation of Fe- and V-based active phases while preserving the properties of the bio-derived TiO<sub>2</sub> support.

The synthesized materials were developed for photocatalytic applications, combining the advantages of bio-based TiO<sub>2</sub> with Fe- and V-containing active phases to obtain sustainable photocatalysts with enhanced potential for light-driven catalytic processes. The proposed synthesis strategy promotes the valorization of agricultural waste, reduces the use of hazardous chemicals, and supports the principles of green chemistry and the circular economy. These materials represent promising candidates for future photocatalytic environmental applications, particularly in wastewater treatment and pollutant degradation.

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**EA PP 04****Poly(*N,N*-Diethylacrylamide)/Graphene Oxide Composite for Methyl Violet 2B Removal: Synthesis, Morphological Characterization, and Adsorption Kinetics**

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A poly(*N,N*-diethyl acrylamide)/graphene oxide (pDEA/GO) composite adsorbent was successfully synthesized by the free-radical polymerization method. Scanning electron microscopy (SEM) revealed a porous, interconnected network morphology of the composite. The obtained pDEA/GO composite was applied to remove the cationic dye Methyl Violet 2B (MV2B) from aqueous solution. Following adsorption, the SEM micrograph showed a more compact structure with partially filled pores, indicating substantial changes in the surface upon dye uptake. The adsorption kinetics of MV2B were evaluated at different contact times using the pseudo-first-order, pseudo-second-order, Elovich, and intraparticle diffusion models. Among the investigated models, the pseudo-second-order model provided the best fit to the experimental data ( $R^2=0.960$ ), suggesting that the adsorption process is strongly influenced by the availability of active adsorption sites [1]. The equilibrium time was approximately 24 h. The observed adsorption behavior can be attributed, at least in part, to electrostatic interactions between the cationic MV2B molecules and negatively charged oxygen-containing functional groups on graphene oxide. Overall, the combined morphological and kinetic results demonstrate the potential of the pDEA/GO composite as an adsorbent for the removal of cationic dyes from aqueous media and provide further insight into the adsorption behavior of the composite material.

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**EA PP 05****Carcinogenic risk from polycyclic aromatic hydrocarbons in soils of different landfill types**

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Polycyclic aromatic hydrocarbons (PAHs) are common contaminants at landfills, where uncontrolled waste disposal and combustion can contribute to their accumulation in soil [1]. This study assessed PAH contamination and the associated carcinogenic risk in soils from different landfill types in Serbia. Fifteen of the 16 US EPA priority PAHs were detected in soils from the 14 investigated landfills, including ten illegal, three municipal solid waste, and one remediated illegal landfill.

Carcinogenic risk was estimated for adult exposure through soil ingestion, inhalation, and dermal contact using BaP-equivalent concentrations. Total risk ranged from  $3.29 \times 10^{-8}$  to  $2.87 \times 10^{-5}$ , with a median value of  $1.30 \times 10^{-6}$ . More than 55% of the samples fell within the generally accepted risk range of  $1 \times 10^{-6}$  to  $1 \times 10^{-4}$ , while the remaining samples showed negligible carcinogenic risk ( $< 1 \times 10^{-6}$ ). Dermal contact and soil ingestion contributed most to the overall risk, while inhalation was negligible.

Although the estimated carcinogenic risk was generally low to acceptable, the results should be interpreted with some caution. Differences in risk levels and localized hotspots were observed among the investigated landfills, highlighting the need for environmental monitoring and further investigation of individual sites, including other contaminant groups.

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**EA PP 06****Assessment of potentially toxic elements mobility in Zagreb urban soils using single-step extractions**

Marija Rosandić<sup>1</sup>, Aleksandar Popović<sup>2</sup>, Stanislav Frančišković Bilinski<sup>3</sup>, Nenad Sakan<sup>4</sup>, Igor Kodranov<sup>2</sup>, Sanja Sakan<sup>5</sup>

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Potentially toxic elements (PTEs) can harm human health, animals, and ecosystems. Their contamination is a major environmental issue due to their persistence and bioaccumulation [1]. Total elemental content does not reflect bioavailability, so this study used single-step extractions with three reagents of different strengths and properties: 1 M HCl, 2 M HNO<sub>3</sub>, and 1 M CH<sub>3</sub>COONH<sub>4</sub>. The contents of As, Ba, Cd, Co, Cr, Cu, Fe, K, Mn, Ni, Pb, Sb, and Zn were determined using ICP-OES. Extraction efficiency was evaluated by comparing element contents obtained with each reagent and their ratios to corresponding total element contents, determined in the work of Frančišković-Bilinski and co-authors [2], which preceded the present work.

Efficiency varied by element and location. Overall, 1 M HCl demonstrated the highest average efficiency, while 2 M HNO<sub>3</sub> showed the highest maximum values. 1 M CH<sub>3</sub>COONH<sub>4</sub> extracted small quantities but was more effective for K and Ba, indicating their higher mobility. Sb results were inconclusive due to low detection in many samples. The extraction efficiency of the two acids followed a clear pattern: some samples yielded similar extraction rates; HCl was favored in others, while HNO<sub>3</sub> was more efficient in the remaining samples. The observed differences are most likely due to variations in the geological composition of the investigated soil.

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**EA PP 07****Photocatalytic degradation of metformin in aqueous suspension using a biogenically synthesized catalyst**

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Widespread use of pharmaceuticals like metformin (MET) leads to their persistence in aquatic environments due to ineffective conventional wastewater treatment methods [1]. Advanced oxidation processes, particularly heterogeneous photocatalysis using semiconductor materials as photocatalysts, have emerged as efficient strategies for pollutant removal. Recent studies highlight the use of green photocatalysts synthesized using plant extracts, supporting green chemistry and circular economy principles, especially when derived from agricultural waste [2]. This study evaluated the efficiency of photocatalytic degradation of MET under simulated solar irradiation using bio-synthesized ZnO nanoparticles based on grape pomace extract, with ZnSO<sub>4</sub> used as a metal precursor. Factors affecting the efficiency of the photocatalytic degradation process were systematically investigated, including the effect of the initial pH of the suspension (~5, ~7, and ~10) at the optimal catalyst loading (1,0 mg/cm<sup>3</sup>). Under the optimal conditions (1,0 mg/cm<sup>3</sup>, pH ~10), the newly synthesized ZnO photocatalyst was compared with commercial ZnO. The highest degradation efficiency was achieved in an alkaline medium (pH ~10), with 12% of MET successfully removed after 180 min of irradiation. When comparing the newly synthesized ZnO with commercial ZnO under the optimized conditions, commercial ZnO exhibited higher photocatalytic efficiency, achieving 32% removal of the investigated pollutant after 180 min of irradiation. The results obtained confirm that green-synthesized ZnO from grape pomace extract has the potential to serve as an eco-friendly material for the removal of organic pollutants, such as pharmaceuticals, from water systems.

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**EA PP 08****Sustainable photocatalysis: plant-based ZnO nanomaterials in the 17 $\alpha$ -ethinylestradiol removal from water**

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The increasing occurrence of emerging pollutants in water poses serious environmental concerns. Different organics, such as active pharmaceutical ingredients, are important contaminants of aquatic ecosystems. 17 $\alpha$ -Ethinylestradiol (EE2) is a synthetic estrogen, widely used in oral contraceptives and recognized as one of the most potent endocrine-disrupting contaminants detected in waters [1]. Thus, EE2 was used as a target pollutant. Heterogeneous photocatalysis represents a promising approach for the sustainable removal of EE2. The employment of green nanomaterials as photocatalysts, synthesized using plant extracts instead of toxic chemicals, represents an innovative and sustainable approach in the removal of organics. The aim of this study was to examine the photocatalytic efficiency of the newly synthesized grape pomace-based ZnO (ZnO/GP) nanomaterials in the degradation of EE2 under various experimental conditions and in different water matrices, using simulated sunlight irradiation (SSI). Experiments were also conducted in the presence of scavengers to identify the predominant reactive species. The experiments, carried out under various initial suspension pH and catalyst loading, showed that the highest EE2 removal efficiency of 89% was achieved after 120 min of SSI at an initial suspension pH of 10.00 and a catalyst loading of 0.5 mg/cm<sup>3</sup>. The influence of the water matrix on the removal efficiency of EE2 was also assessed, using water collected from the Tisa River and under the above-defined optimal conditions. The results showed that the removal efficiency decreased (30%) compared to ultrapure water, probably due to the presence of naturally occurring ions in the surface water. Finally, the experiments with different scavengers (EDTA  $\times$  2Na, H<sub>2</sub>O<sub>2</sub>, and *p*-benzoquinone) indicated that the positively charged holes had the predominant role in the EE2 degradation, as the photocatalytic efficiency was significantly suppressed in the presence of EDTA  $\times$  2Na.

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**EA PP 09****Removal of paracetamol from aqueous environment using iron phosphate-based catalysts: the efficiency of heterogeneous photocatalysis and photo-Fenton systems**

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Water pollution represents one of the most eager problems of modern society. Pharmaceutical residues, such as paracetamol (PARA), are considered as dangerous micropollutants in water, as they cannot be completely removed by conventional wastewater treatment techniques. Advanced oxidation processes (AOPs), such as heterogeneous photocatalysis or photo-Fenton, represents sustainable and powerful alternatives for the efficient organic pollutant removal. The fabrication of new materials as photocatalysts is of great importance, since the most used commercial catalysts have drawbacks, which limit their employment in the AOPs. The aim of this study was to investigate the efficiency of the mentioned AOPs in PARA removal using (non)modified iron phosphate-based catalysts under simulated solar irradiation (SSI) and various experimental conditions. The nonmodified barboselite catalyst was labeled as MP289, while the modified, giniite catalysts as MP210, MP241, MP242, MP265, and MP271. Firstly, direct photolysis did not show any degradation of PARA, indicating the necessity of heterogeneous photocatalysis/photo-Fenton process. In the system with MP289 catalyst, neither the catalyst loading nor the initial suspension pH influenced the photocatalytic activity after 120 min of SSI. Thus, all the further experiments were carried out applying the lowest catalyst loading, i.e. 0.5 mg/cm<sup>3</sup>. Since the heterogeneous photocatalysis of PARA did not show satisfying efficiency, photo-Fenton process was examined, firstly using the nonmodified MP289 and H<sub>2</sub>O<sub>2</sub> (45 mmol/dm<sup>3</sup>), at different initial suspension pH values. The highest removal efficiency was achieved at initial suspension pH of 5.0, when 40% of PARA was removed after 120 min of SSI. Investigating the efficiency of the modified nanomaterials, the highest activity was observed with MP210 and MP241, when 60% of PARA was degraded after 120 min of SSI in both cases, under initial suspension pH of 5.0 and in the presence of H<sub>2</sub>O<sub>2</sub> (45 mmol/dm<sup>3</sup>).

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**EA PP 10****Aqueous systems with bio-derived ionic liquid as an alternative to organic solvents for the regeneration of dye-saturated silica gel**

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Adsorption is a well-established and widely investigated method for pollutant removal from aqueous streams, with activated carbon, silica gel, and zeolites among the most used adsorbents. However, the sustainability of this process is strongly influenced by adsorbent regeneration, which often relies on strong acids or bases and organic solvents [1]. Therefore, the development of alternative regeneration media with a lower environmental impact is of considerable interest. Ionic liquids (ILs) offer an alternative due to their negligible volatility, tunable physicochemical properties, and potential recyclability [2]. Nevertheless, their use for adsorbent regeneration remains limited.

In this work, a bio-derived choline dihydrogen citrate ([Ch][H<sub>2</sub>Cit]) was synthesized and investigated as an alternative regeneration medium for silica gel saturated with methylene blue (MB) and rhodamine B (RhB). Initially, this IL was synthesized through neutralization of choline hydroxide and citric acid at a 1:1 molar ratio. Then, the adsorption capacity of silica gel toward the dyes was investigated, reaching approximately 8 mg g<sup>-1</sup> for MB and 5 mg g<sup>-1</sup> for RhB after 1 h at 25 °C and a solid-to-liquid ratio of 5 mg mL<sup>-1</sup>. Subsequently, samples of dye-saturated silica gel were treated with a 20 wt% aqueous IL solution, ethanol, and water at 25 °C and the same solid-to-liquid ratio. For MB, recovered dye concentrations of 21.70, 18.58, and 1.28 mg L<sup>-1</sup> were obtained using the IL solution, ethanol, and water, respectively, while the corresponding values for RhB were 10.78, 10.86, and 3.51 mg L<sup>-1</sup>. The aqueous IL solution therefore exhibited regeneration performance comparable to ethanol and substantially higher than water. These results support the potential of investigated ILs as promising alternatives to conventional organic solvents, with their designer nature enabling broader application to other adsorbents and pollutants.

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## EA PP 11

**Kinetics of Malachite Green biosorption using a magnetically modified biosorbent in distilled and bottled water**

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The presence of synthetic dyes in aquatic systems represents a significant environmental concern due to their persistence and potential adverse effects on the environment [1]. Biosorption is a simple and environmentally friendly method for removing dyes from aqueous solutions, while water composition can affect the efficiency of the process due to possible competition between dissolved ions and dye molecules for the active sites of the biosorbent. Various natural and waste biomaterials can be used as biosorbents [2]. In this study, the biosorption efficiency of magnetically modified biomass of *Ambrosia artemisiifolia* for the removal of the cationic dye Malachite Green (MG) was investigated using aqueous dye solutions prepared in distilled and bottled water (ROSA). Experiments were conducted in both cases using an initial dye concentration of 50 ppm, 0.1 g of biosorbent, a contact time of 2 h, and an unadjusted pH of 8. Biosorption kinetics were evaluated using the pseudo-first-order, pseudo-second-order, and Elovich models, while the residual dye concentration was determined by UV-Vis spectrophotometry (NOVEL-102S, COLOLab Experts, Polje ob Sotli, Slovenia).

The dye removal efficiency was 93.4% in distilled water and 88.5% in bottled ROSA water. The higher efficiency in distilled water may be attributed to the absence of dissolved ions, resulting in reduced competition for the active sites of the biosorbent ( $\text{Ca}^{+2}$ ,  $\text{Mg}^{+2}$ , and  $\text{Na}^{+}$ ). For both aqueous systems, the pseudo-second-order model showed the best fit to the experimental data ( $R^2 = 0.999$ ), indicating that chemisorption limits the biosorption process. The obtained results indicate the potential of magnetically modified biomass of *A. artemisiifolia* as an efficient biosorbent for MG removal from distilled and bottled water.

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**EA PP 12****Efficiency of the photocatalytic degradation of metformin using ZnO-based green catalyst and grape pomace extract**

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The widespread use of pharmaceuticals has led to their persistence in aquatic environments, with metformin (MET), a widely prescribed antidiabetic drug, raising particular concern due to its accumulation and associated ecological risks [1]. Among advanced oxidation processes, heterogeneous photocatalysis offers an effective and eco-friendly approach for degrading pollutants. Heterogeneous photocatalysis relies on semiconductor catalysts, with recent research increasingly promoting green alternatives synthesized from plant extracts, which reduce hazardous chemical usage and support circular economy principles by utilizing agricultural waste [2]. The aim of this study was to evaluate the efficiency of green-synthesized ZnO nanoparticles, derived from grape pomace extract with  $\text{Zn}(\text{CH}_3\text{COO})_2$  used as the metal precursor, in the photocatalytic degradation of MET under simulated solar irradiation. At an optimized catalyst loading ( $1,0 \text{ mg/cm}^3$ ), the influence of the initial pH value of the suspension (5, 7, and 10) was examined. The best results were achieved in a neutral medium ( $\text{pH} \sim 7$ ), where 18% of MET was removed after 180 min of irradiation. Furthermore, the activity of the newly synthesized ZnO nanoparticles was compared with that of commercial ZnO ( $1,0 \text{ mg/cm}^3$ ) at neutral pH ( $\text{pH} \sim 7$ ). Both catalysts demonstrated very similar efficiency, removing 18% of MET after 180 min of irradiation. Finally, evaluating the direct influence of pure grape pomace extract at various mass fractions (3%, 5%, 7% and 10%) showed that the system containing 10% of pure grape pomace extract was the most effective, removing 25% of the targeted pollutant. The experimental results demonstrated the potential of newly synthesized green ZnO and pure grape pomace extract for the removal of MET from aqueous media.

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**EA PP 13****From Agricultural Waste to Functional Adsorbent: Sunflower Husk for Rhodamine B Removal**

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The valorization of agricultural residues into functional materials represents a sustainable approach to resource recovery and wastewater treatment. Sunflower husk, an agro-industrial residue generated during edible oil production, is a promising biosorbent due to its lignocellulosic structure and the presence of various surface functional groups, which can contribute to the removal of different pollutants from aqueous solutions [1]. Rhodamine B is a widely used synthetic dye of environmental concern due to its persistence, limited biodegradability, and potential toxicity to aquatic organisms and humans [2]. In this study, the sunflower husk treated with 0.1% HCl is used for the removal of Rhodamine B from aqueous solutions. Adsorption experiments were conducted using Rhodamine B solutions with an initial concentration of 5 mg/L to evaluate the effect of adsorbent dosage (1–40 g/L) and contact time (1–120 min) on the removal efficiency. After adsorption, the residual Rhodamine B concentration was determined by UV–Vis spectroscopy at 554 nm. The optimal adsorbent dosage was 5 g/L, and equilibrium was reached after 30 min, resulting in a removal efficiency of 79.5%. FTIR analysis was employed to identify the functional groups present on the adsorbent surface and to provide evidence of interactions between Rhodamine B and the adsorbent. The obtained results demonstrate that sunflower husk exhibits high removal efficiency for Rhodamine B, confirming its potential for application in wastewater treatment processes.

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**EA PP 14****CO<sub>2</sub> adsorption and regeneration performance using an amino-modified polymer**

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The continuous increase in anthropogenic CO<sub>2</sub> emissions has become a major concern due to their contribution to global warming and climate change, highlighting the need for efficient carbon capture technologies [1]. Among the available CO<sub>2</sub> capture technologies, adsorption using amino-modified polymers has emerged as a promising approach due to their high affinity toward CO<sub>2</sub> and tunable surface properties [2]. In this study, an amino-modified polymer was investigated as a CO<sub>2</sub> sorbent. Adsorption and desorption experiments were conducted using pulse gas chromatography in a dynamic flow system, complemented by temperature-programmed desorption (TPD) analysis. At the optimum adsorption temperature of 20 °C, the amino-modified polymer exhibited a CO<sub>2</sub> uptake of 3.61 mmol CO<sub>2</sub>/g ( $4.00 \times 10^{-2}$  mmol CO<sub>2</sub>/m<sup>2</sup>). TPD analysis revealed an activation energy of 28.72 kJ/mol for CO<sub>2</sub> desorption. Furthermore, the amino-modified polymer maintained a stable CO<sub>2</sub> uptake over ten consecutive adsorption/desorption cycles, demonstrating its potential as an efficient and reusable sorbent for CO<sub>2</sub> capture.

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**EA PP 15****Photocatalytic degradation of methyl orange using Pt-modified TiO<sub>2</sub> photocatalysts**

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The contamination of water bodies by synthetic dyes represents a significant environmental concern due to their high chemical stability, persistence, and potential toxicity to aquatic ecosystems. Methyl orange, a widely used anionic azo dye, is particularly problematic because of its resistance to conventional degradation processes and its potential adverse effects on aquatic organisms and water quality [1]. Therefore, the development of efficient methods for the removal and degradation of methyl orange from contaminated water is of considerable environmental importance. Photocatalysis has emerged as a promising advanced oxidation process for water treatment, enabling the degradation of persistent organic pollutants into less harmful products through the generation of highly reactive species. Among semiconductor photocatalysts, TiO<sub>2</sub> is particularly attractive due to its high photocatalytic activity, chemical stability, low toxicity, and relatively low cost. A key limitation of TiO<sub>2</sub> is its wide band gap, which restricts its photocatalytic activity mainly to the UV region and limits the efficient utilization of solar light. Therefore, TiO<sub>2</sub> was modified with Pt to enhance its photocatalytic performance and improve the utilization of photogenerated charge carriers [2]. In this study, TiO<sub>2</sub> photocatalysts modified with 0.5, 1, and 2 at% Pt were synthesized to evaluate the effect of platinum modification on the photocatalytic degradation of methyl orange in comparison with unmodified TiO<sub>2</sub>. The photocatalytic degradation efficiencies were 62.3%, 91.1%, and 95.2% for 0.5, 1, and 2% Pt-modified TiO<sub>2</sub>, respectively, compared with 42.3% for pristine TiO<sub>2</sub>. The results demonstrate enhanced photocatalytic performance of Pt-modified TiO<sub>2</sub>, with the degradation efficiency increasing with increasing Pt content.

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**EA PP 16****Green synthesis of silver nanoparticles using aqueous extract of black goji berries (*Lycium ruthenicum* Murr.)**

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This study focused on the green synthesis and physicochemical characterization of silver nanoparticles (AgNPs) using an aqueous extract of black goji berries (*Lycium ruthenicum* Murr.) as a plant-derived source of reducing and stabilizing agents. Plant-mediated synthesis represents a promising alternative to conventional nanoparticle synthesis methods, owing to its simplicity, low environmental impact, and potential to produce biologically active nanomaterials [1]. The formation of AgNPs was monitored by UV–Vis spectroscopy in the range of 300–700 nm. The appearance of a characteristic surface plasmon resonance (SPR) band in the approximately 400–450 nm region provided the first indication of Ag<sup>+</sup> reduction and the formation of silver nanoparticles. Optimization of the synthesis conditions demonstrated that a pH of 10, 10 mM AgNO<sub>3</sub>, and a 10% (v/v) concentration of the aqueous berry extract provided the most favorable conditions for nanoparticle formation. The involvement of metabolites naturally present in black goji berries in both the reduction of silver ions and stabilization of the formed nanoparticles was further supported by Fourier-transform infrared (FTIR) spectroscopy. Scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS) confirmed the formation of predominantly spherical nanoparticles and provided information on their morphology and elemental composition. Overall, the results demonstrate the potential of black goji berry aqueous extract as a natural source of reducing and stabilizing agents for the green synthesis of AgNPs. The synthesized nanoparticles will be subjected to further investigations aimed at evaluating their biological properties and potential applications.

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## EA PP 17

**Mechanical Activation of Deposited Ash for Enhanced Reactivity in Cementitious Composites**

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Disposal of ash originating from coal combustion in thermal power plants presents an environmental challenge and highlights the need for sustainable approaches for its reuse as a secondary raw material in the construction industry. Previous studies have demonstrated the potential of beneficiation and mechanical activation of ponded ash to improve its properties and reactivity [1, 2]. Building upon these findings, the aim of this study was to investigate the potential application of deposited (ponded) ash (PA) as a partial cement replacement and to analyse the effects of mechanical activation of PA on the properties of the resulting materials. Deposited ash from the “Nikola Tesla B” thermal power plant was used in the study. Mechanical activation of PA was performed by grinding in a planetary ball mill, with a PA-to-grinding-medium ratio of 1:5 identified as the optimal ratio, and the resulting material was designated as PA5. Mechanical activation reduced the mean particle diameter of PA from 250.2  $\mu\text{m}$  to 8.65  $\mu\text{m}$ . Mechanically activated PA was used to prepare mortars in which 10, 20, and 30 wt.% of cement was replaced with PA. It was found that replacing 30 wt.% of cement with PA5 resulted in mortars with compressive strength close to that of the reference mortar prepared using neat cement. The results obtained indicated a positive effect of mechanical activation on the reactivity of PA and its potential use as a partial cement replacement.

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**EA PP 18****Removal of bezafibrate from water using hydrochar as an adsorbent**

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Pharmaceutically active compounds in aquatic environments are an increasing concern due to their potential adverse effects on ecosystems and human health. Hydrochar (HC), produced through hydrothermal carbonization of biomass, is a promising adsorbent for pharmaceutical removal from water [1]. Bezafibrate adsorption was investigated using hydrochars produced from waste woody biomass at 300 °C without process-water recirculation (HC-1) and with process-water recirculated twice (HC-R2). Kinetic experiments were conducted at pH 5 and 25 °C using 0.020 mg/L bezafibrate and 2 g/L adsorbent. For HC-R2, most of the adsorption occurred within the first 10 min, and the kinetic data were adequately described by the pseudo-first-order and pseudo-second-order models ( $R^2 = 0.994$  and  $0.988$ ), with the pseudo-first-order model providing a slightly better fit and  $q_e = 0.0091$  mg/g. For HC-1, the kinetic models were not considered further because of poor fit ( $R^2 < 0.70$ ). Equilibrium experiments were conducted at 25–55 °C by varying the adsorbent concentration from 0.5 to 5 g/L at a constant initial bezafibrate concentration of 0.020 mg/L. The equilibrium data were evaluated using the Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich models, with no acceptable fit obtained at 25 and 35 °C. At 0.5 g/L, HC-1 and HC-R2 achieved comparable removal efficiencies of 94.27% and 94.17%, with adsorption capacities of approximately 0.038 mg/g. For HC-1, Freundlich gave the best fit at 45 °C ( $R^2 = 0.95$ ), with a comparable Dubinin–Radushkevich fit ( $R^2 = 0.94$ ), suggesting nonlinear adsorption on a heterogeneous surface. At 55 °C, Freundlich showed a weaker fit ( $R^2 = 0.80$ ). For HC-R2, no model consistently provided the best fit across temperatures. Overall, both hydrochars showed high and comparable bezafibrate removal, while only HC-R2 kinetic data were adequately described by the applied models. Twice-recirculated process water altered adsorption behavior without reducing removal efficiency and may improve resource efficiency in hydrochar production, although further process level evaluation is needed.

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## EA PP 19

**Betaine-based NADESs as designer solvents: tailoring plant bioactivity profiles for cosmetic applications**

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Natural deep eutectic solvents (NADESs) are tunable extraction media whose composition can be rationally designed to preferentially recover specific classes of bioactive compounds [1]. Rather than seeking a universal solvent, this study investigated whether bioactivity could be tailored by matching plant matrices with specific NADES. Three equimolar betaine-based NADESs paired with sorbitol, proline, and urea (constituents selected for their recognized skin benefits), were used to extract six different plant materials. Ultrasound-assisted extraction (30 min, room temperature, 1:10 w/v) of six plant materials using three equimolar betaine-based NADESs, methanol, and glycerol yielded 30 extracts, with methanol and glycerol serving as analytical and cosmetic benchmarks, respectively. Radical-scavenging, tyrosinase-inhibitory, and elastase-inhibitory activities were measured spectrophotometrically, for both NADES extracts, as well as their respective pure solvents (blanks). NADES blanks showed negligible or low activity, indicating that the effects arose predominantly from extracted phytochemicals. Each plant–NADES pair produced a distinct activity fingerprint. Betaine/proline yielded the highest DPPH capacity for five plant matrices, while betaine/urea–*Paeonia officinalis* L. gave the highest value overall (1650 ± 40 µmol TE/g), exceeding the corresponding methanol and glycerol extracts by 2.4- and 8.3-fold, respectively. Betaine/proline–*Syringa vulgaris* L. showed the strongest tyrosinase inhibition (55 ± 7%, 1:100 dilution), while both reference extracts were inactive. Betaine/sorbitol–*P. officinalis* showed the greatest elastase inhibition (60 ± 2%, 1:50 dilution), surpassing both benchmarks. These findings highlight plant–NADES pairing as a key determinant of bioactivity and a promising strategy for designing multifunctional cosmetic extracts.

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**EA PP 20****Exploring Co-Au synergy in CNT- based electrodes for As(III) detection**

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Arsenic (As) is an extremely hazardous metalloid; its presence in water resources, soil, and food poses a significant risk to human health and environmental quality. Long-term exposure to arsenic, particularly its more toxic form, As(III), is associated with various adverse health effects, including carcinogenesis and damage to the liver and nervous system. Although historically known as a toxic substance, arsenic contamination remains a critical environmental issue, both globally and in the northern region of our country [1,2]. This study presents a comparative investigation of Co/CNT, Au/CNT, and CoAu/CNT (CNT - carbon nanotube) nanocomposite electrodes for the electrochemical detection of As(III) in an acidic medium using anodic stripping voltammetry (ASV). ASV parameters (deposition potential and time) were systematically optimized to achieve higher sensitivity. The applicability of the developed electrochemical sensing approach was further validated through the analysis of real water samples. Catalysts were tested under established experimental conditions, providing insight into their performance in complex aqueous matrices. The results demonstrate the potential of nanocomposite electrodes based on CNTs and metal and/or bimetallic systems for the sensitive and practical detection of As(III), and highlight the importance of electrode composition for the development of electrochemical sensors intended for trace arsenic analysis.

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## EA PP 21

**Gold-Modified MnO<sub>2</sub> electrodes for sensitive electrochemical detection of As (III)**

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Arsenic contamination of water represents a significant environmental and public health concern due to the high toxicity of arsenic species and their potential adverse effects following long-term exposure [1]. The World Health Organization has established a guideline value of 10 ppb for total arsenic in drinking water [2]. In this study, three MnO<sub>2</sub>-based electrodes with different crystalline phases,  $\alpha$ -K<sub>0.15</sub>MnO<sub>2</sub>,  $\alpha$ -K<sub>0.18</sub>MnO<sub>2</sub>, and  $\beta$ -MnO<sub>2</sub>, were comparatively investigated for the electrochemical detection of As(III). The materials were synthesized by a hydrothermal procedure and subsequently modified with gold. Anodic stripping voltammetry was employed in 0.5 M H<sub>2</sub>SO<sub>4</sub> to evaluate the analytical response of the Au-modified MnO<sub>2</sub> electrodes to arsenic presence. All investigated electrodes exhibited a well-defined anodic stripping peak at approximately 0.25 V vs. SCE, attributed to the oxidation of deposited arsenic. The analytical performance was found to depend on the MnO<sub>2</sub> phase, with the Au/ $\beta$ -MnO<sub>2</sub> electrode exhibiting the lowest limit of detection of 1.34 ppb. The practical applicability of the developed electrodes was further assessed using real water samples collected from the Drina River and tap water. Direct analysis without prior sample treatment resulted in clearly distinguishable anodic responses, demonstrating the applicability of the Au-modified MnO<sub>2</sub> electrodes for As(III) detection in complex aqueous matrices.

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## EA PP 22

**Viscose substrates as delivery systems for anthocyanin extracts**

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Anthocyanins are natural pigments with pronounced pH-dependent structural and colorimetric changes, making them promising candidates for sustainable pH indicators. This study examines anthocyanin extracts and viscose fibers as carriers and stabilizing matrices. Cyanidin-3,5-diglucoside was extracted from red cabbage and characterized by UV–Vis spectroscopy [1]. Interactions with viscose were analyzed using FTIR, surface tension, conductometry, and hyperspectral imaging. FTIR confirmed predominantly physical interactions, while surface tension revealed concentration-dependent behavior. Conductometric analysis demonstrated sensitivity to environmental composition, particularly in fertilizer-enriched soil. Hyperspectral imaging recorded spectral shifts under acidic and alkaline conditions, highlighting pH responsiveness. These findings confirm the suitability of anthocyanins as natural indicators and underscore the potential of viscose substrates as bio-based carriers for innovative, environmentally friendly systems [2].

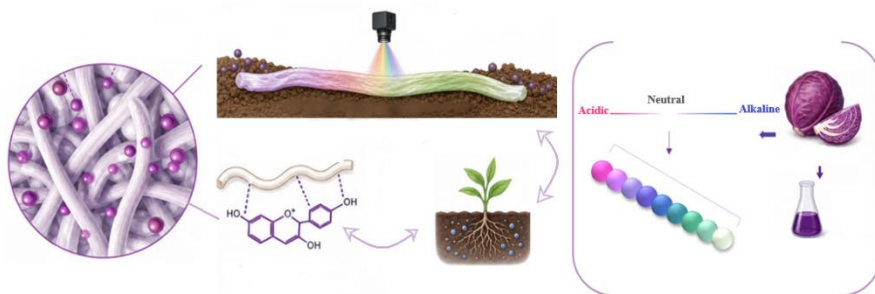


Figure 1. Interactions between anthocyanins and viscose fibers.

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## **Physical and Computational Chemistry (PCC)**

**PCC PP 1****Structural and toxicological similarity of selected organic pollutants**

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This study investigates the structural and toxicological similarity of 67 selected organic pollutants using extended-connectivity fingerprints (ECFP) and similarity indices. SMILES representations were used to generate ECFP fingerprints, a widely applied circular fingerprint approach for encoding local atomic environments [1]. Tanimoto and Dice indices were then calculated to quantify pairwise structural similarity [2]. Toxicological similarity was evaluated using experimental logLC<sub>50</sub> values, followed by comparison with structural similarity to examine the relationship between molecular structure and toxicity. The results showed a very strong correlation between the Tanimoto and Dice indices ( $r \approx 0.99$ ), indicating a high level of agreement between these structural similarity measures. In contrast, a very weak negative correlation was observed between structural and toxicological similarity, suggesting that structurally similar molecules do not necessarily exhibit similar toxicological properties. ANOVA confirmed statistically significant differences between the analyzed similarity measures. These findings emphasize the usefulness of chemoinformatics approaches for the analysis of organic pollutants while also highlighting limitations of the similarity property principle when structural similarity is used to infer toxicological behavior.

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## PCC PP 2

**An insight into the complex world of s-triazine – a crystallographic and quantum-chemical study**

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1,3,5-triazine, or more commonly known as s-triazine, can be viewed as an important building block in supramolecular chemistry due to its deceptively simple, yet rich structure<sup>1</sup>. This structure is known to establish multiple types of noncovalent interactions<sup>2</sup>, such as stacking and ion- $\pi$  interactions, as well as hydrogen bonds. In this work, we have decided to examine stacking interactions between molecules containing a triazine unit by querying the Cambridge Structural Database. This was later followed by performing DFT calculations in order to assess the strength of the given interactions. Our search yielded a significant number of stacking interactions, which were both face-to-face and parallel-displaced, with the antiparallel orientation being very dominant. A significant number of aminotriazine systems with double N-H $\cdots$ N hydrogen bonds were also found, as well as C-H $\cdots$ N hydrogen bonds of unsubstituted triazine. Meanwhile, DFT calculations showed that the strength of the stacking interactions and hydrogen bonds not only changes with reorientation of the triazine units but also depends on the type of substituent group present in the structure. The most pronounced example is melamine (triaminotriazine), which forms significantly stronger hydrogen bonds (–11.0 kcal/mol) and somewhat stronger stacking interactions (–4.5 kcal/mol) than unsubstituted triazine, where these interactions are of comparable strength (about –4.0 kcal/mol).

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## PCC PP 3

**Detection of chloramphenicol using a glassy carbon electrode modified with Ni/Co-ZIF-67 and silver nanoparticles**

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In this study, an electrochemical sensor for the detection of chloramphenicol was developed, based on a glassy carbon electrode (GCE) modified with silver nanoparticles and zeolitic imidazolate frameworks (ZIFs). ZIFs exhibit high adsorption capacities due to their highly porous structure, as well as significant catalytic properties, which, in combination with silver nanoparticles that enhance electrical conductivity, enable high sensor sensitivity [1,2]. Several GCE modifications were prepared, including ZIF-67, Ni/Co-ZIF-67, Ag-ZIF-67, and Ag-Ni/Co-ZIF-67, and characterized by cyclic voltammetry. Among them, Ag-Ni/Co-ZIF-67 demonstrated the highest electrochemical response. Chloramphenicol detection was performed using the GCE | Ag-Ni/Co-ZIF-67 electrode by differential pulse voltammetry within a concentration range of 40  $\mu\text{M}$  to 200  $\mu\text{M}$ . A linear relationship between the electrode response and chloramphenicol concentration was obtained, with a high correlation coefficient ( $R^2 = 0.998$ ) and a detection limit of 40  $\mu\text{M}$ . Analysis of a real sample (eye drops) showed a deviation of only 1.34% compared to HPLC/UV analysis, indicating that the GCE | Ag-Ni/Co-ZIF-67 sensor has strong potential for rapid and reliable chloramphenicol detection.

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**PCC PP 4*****In silico* evaluation of the antioxidant and potential antibacterial activity of lawsone**

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Lawsone (2-hydroxy-1,4-naphthoquinone) is a natural pigment found in *Lawsonia inermis*. Its conjugated quinone system allows it to react with reactive oxygen species and to interact with different biological targets. This study aimed to determine the pathways by which lawsone reacts with the hydroxyl radical and to assess its potential interaction with a bacterial target protein. The Gaussian 09 software package and Density functional theory at the M06-2X/6-311++G(d,p) level of theory were used to investigate the thermodynamic properties of hydrogen atom transfer (HAT), separated electron and proton transfer (SET-PT and SPLET), and radical adduct formation (RAF) mechanisms. The effect of solvent polarity was studied using the CPCM solvation model for water and benzene. Potential antibacterial activity was explored by molecular docking of lawsone against the DNA gyrase from *Escherichia coli* (PDB ID: 3NUH), using AutoDock4 [1]. Its pharmacokinetic and toxicological properties were additionally predicted using the ADMETlab 3.0 platform [2]. The results showed that the dominant mechanism of hydroxyl radical deactivation by lawsone depends primarily on the polarity of the solvent. Direct hydrogen atom transfer was found to be thermodynamically favorable, whereas multistep mechanisms were limited by the unfavorable thermodynamics of individual reaction steps. Among the examined pathways, radical adduct formation showed the most negative reaction enthalpy, with the C3 position identified as the preferred site for hydroxyl radical addition. Molecular docking predicted a binding pose supported by hydrogen bonds and interactions involving the aromatic system. The predicted ADMET profile indicated acceptable basic drug-like properties, along with potential limitations related to absorption, metabolic interactions, and toxicity. Overall, the results support further experimental evaluation of lawsone's antioxidant potential and its ability to interact with the studied bacterial protein.

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## PCC PP 5

## Are C<sup>α</sup>H/O hydrogen bonds of glycine transition metal complexes and water relevant?

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After comprehensive analysis of NH/O and two types of O/HO hydrogen bonds, O1/HO via  $\alpha$ -hydroxyl O1 oxygen, and O2/HO via  $\alpha$ -carbonyl O2 oxygen, of coordinated glycine and water, [1] we investigated the often-neglected C<sup>α</sup>H/O hydrogen bond [2]. Interaction energy calculations at B3LYP-D4/def2-TZVP level reveal that linear C<sup>α</sup>H/O hydrogen bonds are quite strong for both neutral glycine complexes (-1.99 to -3.70 kcal/mol) and singly positively charged complexes (-6.16 to -8.12 kcal/mol). Although they are much stronger than conventional CH/O interactions, their relevance was examined because of the stronger NH/O and O/HO hydrogen bonds that are possible in the vicinity. After the search of Cambridge Structural Database (CSD), we examined a few crystal structures in more detail by calculating the total interaction energy and performing Quantum Theory of Atoms In Molecules (QTAIM) analysis (Fig. 1). The results confirmed the presence of the bond critical point (orange dots) corresponding to C<sup>α</sup>H/O interaction, even with multiple interactions present. We conclude that C<sup>α</sup>H/O hydrogen bonds are very important for crystal packing and orientation of the water molecule.

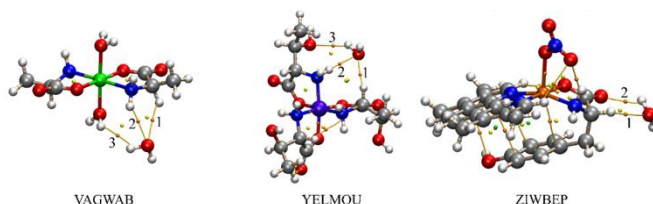


Figure 1. QTAIM analysis of geometries from the CSD search with CH/O hydrogen bonds.

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## PCC PP 6

**Electrochemical activity of a glassy carbon electrode modified with ZnO particles synthesized using a hydroethanolic extract of *Pinus nigra* needles for doxorubicin detection**

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Plant extracts rich in bioactive compounds have attracted considerable attention due to their antioxidant properties and potential application in sustainable material synthesis. In this study, needles of the coniferous species *Pinus nigra*, a reported source of phenolic compounds, flavonoids, and terpenes, were extracted using 50% (v/v) ethanol [1]. The antioxidant activity of the extract was evaluated by electron paramagnetic resonance (EPR) spectroscopy using DPPH, OH<sup>•</sup>, and O<sub>2</sub><sup>•-</sup> radicals, revealing pronounced radical-scavenging activity. ZnO particles were synthesized by microwave processing of Zn(OH)<sub>2</sub> in the presence of the hydroethanolic extract and subsequently used to modify a glassy carbon electrode for electrochemical detection of doxorubicin (DOX). To investigate the effect of extract amount, ZnO particles were synthesized using different volume ratios of aqueous ZnCl<sub>2</sub> solution to plant extract (10:1, 20:1, and 40:1). The obtained materials were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), field-emission scanning electron microscopy (FESEM), and photoluminescence (PL) spectroscopy. Cyclic voltammetry measurements demonstrated an enhanced electrochemical response of ZnO-modified electrodes toward DOX compared with bare glassy carbon electrodes. The electrochemical activity was influenced by the volume ratio of ZnCl<sub>2</sub> solution to plant extract, and particle morphology.

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**PCC PP 7****Anion– $\pi$  interactions of oxyanions with strongly electron-deficient aromatic rings – a DFT study**Andrej B. Dedić<sup>1</sup>, Dušan P. Malenov<sup>2</sup><sup>1</sup> Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade<sup>2</sup>University of Belgrade, Faculty of Chemistry, Belgrade, Serbia

Noncovalent interactions involving oxyanions and electron-deficient aromatic systems play a fundamental role in supramolecular chemistry and anion recognition [1]. In this work, quantum chemical calculations at the B3PW91-D3/def2-TZVP level of theory were performed to systematically investigate the binding behavior, geometry, and energetic features of six oxyanions ( $\text{ClO}_3^-$ ,  $\text{ClO}_4^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ,  $\text{SO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ ) interacting with three strongly electron-deficient aromatic rings: 1,3,5-tricyanobenzene (TCNB), 1,3,5-trinitrobenzene (TNB), and hexacyanobenzene (HCNB). To study the nature of these interactions, an ETS-NOCV energy decomposition of interaction energies was performed using the ORCA 6.1.0 program. Geometry optimizations revealed that the interaction strength follows the order  $\text{TCNB} < \text{TNB} < \text{HCNB}$ , driven by the increasing positive surface electrostatic potential above the aromatic ring. HCNB exhibits exceptionally strong interactions, achieving an interaction energy of -132.86 kcal/mol with  $\text{SO}_3^{2-}$  (Fig. 1). Regarding the anions, the interaction strength generally increases as  $\text{ClO}_4^- \approx \text{NO}_3^- < \text{ClO}_3^- < \text{NO}_2^- < \text{SO}_3^{2-}$ . Energy decomposition analysis demonstrates that electrostatics is the main driving force of these interactions (Fig. 1). Additionally, the low-lying  $\pi^*$  orbitals of the cyano and nitro groups enable strong orbital mixing with electron-rich anions. These insights highlight the tunable nature of strongly electron-deficient aromatic acceptors for targeted anion binding.

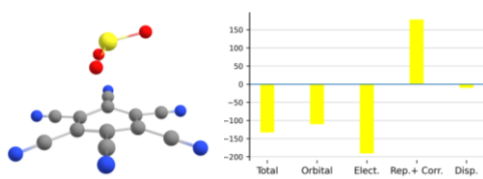


Figure 1. Structure (left) and interaction energy decomposition (right) of the HCNB–sulfate complex.

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**PCC PP 8****Ghrelin-Ca<sub>v</sub>1.2 interactions explored by informational spectrum analysis and molecular docking**

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Ghrelin is a peptide hormone and the endogenous ligand of the growth hormone secretagogue receptor 1a (GHS-R1a). This study explored a possible interaction between ghrelin and the human L-type voltage-gated calcium channel Ca<sub>v</sub>1.2 by combining the informational spectrum method (ISM) with molecular docking.

The amino acid sequences of ghrelin, GHS-R1a, and Ca<sub>v</sub>1.2 were converted into numerical signals using electron-ion interaction potential values and analyzed by Fourier transformation [1]. Spectral comparison highlighted the normalized frequency  $F = 0.264$ . Analysis of channel sequence segments at this frequency suggested a putative recognition region. The  $\alpha 1C$  subunit from the human Ca<sub>v</sub>1.2 cryo-EM structure (PDB ID: 8WE8, chain A) [2] was used as the target for molecular docking. The resulting model placed ghrelin near the ISM-predicted region on the channel surface. This qualitative spatial correspondence supports further investigation of the proposed recognition region, while direct binding and functional effects on channel activity remain to be established. The findings provide a basis for targeted experimental testing of a possible ghrelin-Ca<sub>v</sub>1.2 interaction.

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**PCC PP 9****Unravelling rhodamine B degradation kinetics on TiO<sub>2</sub>/CF:  
model comparison and mechanistic insights**

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Rhodamine B (RhB), as a representative synthetic dye, poses a significant challenge for environmental protection due to its persistence and potential toxicity. Electrochemical oxidation is a promising approach for the degradation of persistent organic pollutants such as RhB through the generation of strong oxidizing species, primarily hydroxyl radicals [1,2]. In this study, the degradation kinetics of RhB using a TiO<sub>2</sub>/CF electrochemical system were investigated under controlled operating conditions (RhB concentration of 10 ppm and applied current of 8 mA). To assess the kinetic behavior of the degradation process, the experimental data were fitted to pseudo-first-order and pseudo-second-order kinetic models using nonlinear regression. The models were compared both in the absence and in the presence of radical scavengers, methanol and tert-butanol (TBA), to evaluate changes in the apparent degradation kinetics associated with the contribution of reactive radical species. The pseudo-first-order model provided an excellent fit for the control experiment, with an R<sup>2</sup> value of 0.9958 (vs. 0.9740 for the pseudo-second-order model), indicating a very good agreement between the experimental data and the model. In the presence of radical scavengers, lower R<sup>2</sup> values were obtained for both models, although the pseudo-second-order model showed marginally higher R<sup>2</sup> values for methanol (0.7336 vs. 0.7295) and TBA (0.9273 vs. 0.9130). However, the differences between the models remained small ( $\Delta R^2 < 0.015$ ), indicating that the concentration of reactive radicals remains approximately constant under steady-state conditions, making the overall rate proportional only to the RhB concentration. Overall, the TiO<sub>2</sub>/CF system exhibited pseudo-first-order kinetic behavior under control conditions, while the lower R<sup>2</sup> values in the presence of radical scavengers suggest greater kinetic complexity. These findings highlight the value of combining kinetic modelling with radical scavenger experiments for a more reliable understanding of electrochemical degradation mechanisms.

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**PCC PP 10****Electrochemical detection of fluoxetine in aqueous solution using ZnO/SnO<sub>2</sub>-modified screen-printed carbon electrodes**

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Fluoxetine (FLX) is an antidepressant belonging to the class of selective serotonin reuptake inhibitors (SSRIs) and is one of the widely used second-generation antidepressants. Due to its widespread use, stability, and resistance to degradation, FLX is considered an emerging pharmaceutical contaminant that can persist in the environment and potentially affect aquatic organisms. Therefore, the development of sensitive, selective, and rapid sensors for its detection is essential.

In this study, a ZnO/SnO<sub>2</sub> composite material with a ZnO:SnO<sub>2</sub> mass ratio of 9:1 was used to modify screen-printed carbon electrodes (C-SPEs) for the electrochemical detection of FLX. The ZnO/SnO<sub>2</sub> composite was synthesized by mechanical milling of commercial ZnO and SnO<sub>2</sub>, and subsequently calcined at 400 and 700 °C. Structural and morphological properties of the composites were characterized using X-ray powder diffraction (XRD) and field-emission scanning electron microscopy (FESEM).

For the modification of C-SPEs, an ink containing ZnO/SnO<sub>2</sub> composite, carbon black, Nafion, ethanol, and distilled water was prepared. Electrochemical measurements were performed using differential pulse voltammetry (DPV) in 25 mL of phosphate buffer (0.1 M, pH 7.0) with successive additions of 50 µL of a methanolic FLX solution. All modified electrodes exhibited two distinct oxidation peaks. The limit of detection (LOD), limit of quantification (LOQ), dynamic range, and sensitivity were evaluated.

**Acknowledgments**

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## PCC PP 11

**Quantum chemical assessment of the N,N-dihaloamino groups as potential explosives**

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Molecular Electrostatic Potentials (MEPs) are among the most commonly studied indicators of sensitivity of molecules towards detonation. More information about the stability of the molecule can be obtained by calculating the bond dissociation energies (BDE) of the "trigger bond" [1]. In nitroaromatic molecules, the most common "trigger bonds" are C-NO<sub>2</sub>, so the presence and number of -NO<sub>2</sub> substituents in the molecule can have a significant impact on the sensitivity of molecules towards detonation [2]. In this work, DFT calculations were used to study the influence of different numbers of -NO<sub>2</sub> and -NX<sub>2</sub> substituents on the high-energy properties of the group of nitroaromatic compounds. The MEPs, BDE and Wiberg bond indexes (WBI) were calculated for optimized geometries. The results of calculations performed at the PBE/6-311G\*\* level with the addition of GD3JB dispersion show a trend of increasing BDE values with a decreasing number of -NO<sub>2</sub> or -NX<sub>2</sub> substituents in the molecule. For the molecules without -NO<sub>2</sub> substituents but only -NX<sub>2</sub>, the BDE values decrease as the halogens in the -NX<sub>2</sub> substituents change in the following order: I, Br, Cl, F. The calculated WBI values are in good agreement with these results. In the molecule with three -NI<sub>2</sub> groups, the WBI for the C-NI<sub>2</sub> bond is 1.27, while for the C-NF<sub>2</sub> bond in the molecule with three -NF<sub>2</sub> groups, it decreases to 1.20. The results obtained by analyzing MEPs show an increase in the potential values in the central regions of the studied molecules in the same order as the BDE values decrease, so it can be noticed that the observed trends are mutually consistent.

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**PCC PP 12****Development of a carbon paste-based sensor modified with a CeO<sub>2</sub>/MWCNT nanocomposite for sensitive detection of diuron in water and food samples**

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Diuron is a systemic herbicide from the phenylamide family and the subclass of phenylurea herbicides. It is widely used for different types of crops, such as corn, fruit, cotton, sugar cane *etc.*, as well as a sterilization agent for non-crop areas such as roads and railway lines. Diuron migrates into aquatic environments by soil leaching and its threat to water and soil ecosystems is not only posed by diuron itself, but also by its secondary degradation products, which may include a highly toxic 3,4-dichloroaniline that persists in soil and aquatic environments for an extended period of time, as it is relatively chemically stable under soil and aquatic conditions. Because of its harmful potential to different ecosystems, an affordable, quick, and sensitive detection method of diuron is integral [1]. Nanocomposites consisting of rare earth metal oxides and multiwalled carbon nanotubes (MWCNT) have been proven to have an outstanding effect on electrocatalytic performance through modification of a working electrode in voltammetric measurements, which in turn leads to increases in sensitivity of developed methods using the aforementioned modifications [2]. A sensitive, novel carbon paste-based sensor was developed using a CeO<sub>2</sub>/MWCNT modified carbon paste electrode (CeO<sub>2</sub>/MWCNT/CPE). The material was characterized both morphologically and electrochemically and it demonstrated potent electrocatalytic activity, attributed to its unique morphological structure and synergistic effect of the two used modifiers. The optimized detection method of choice for diuron using the CeO<sub>2</sub>/MWCNT/CPE is developed through the use of square-wave voltammetry. The sensor showed two linear ranges for the detection of diuron, from 2-20 µM and 20-165 µM. Diuron was successfully detected and quantified in spiked real samples of tap water and polenta.

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**PCC PP 13****Electrochemical Determination of Vanillin Using an Eu<sub>x</sub>Mo<sub>y</sub>O<sub>z</sub>/MWCNT-Modified Glassy Carbon Electrode**

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Vanillin is a widely occurring phenolic compound extensively used in the food, pharmaceutical, and cosmetic industries, therefore the development of rapid and sensitive methods for its determination is highly relevant. The presence of an electroactive phenolic group in the vanillin structure makes it a suitable analyte for the development of electrochemical sensors [1]. Nanostructured molybdenum oxides have demonstrated significant potential as electrocatalytic materials in electrochemical sensors due to their active surface area and ability to facilitate electron transfer [2]. The goal of this study was to investigate a newly synthesized Eu<sub>x</sub>Mo<sub>y</sub>O<sub>z</sub> material for the potential electrochemical detection of vanillin. The Eu<sub>x</sub>Mo<sub>y</sub>O<sub>z</sub>/MWCNT nanocomposite was used to modify a glassy carbon electrode (GCE), which was subsequently employed in this study. The modified GCE exhibited an enhanced electrochemical response and high sensitivity toward vanillin. A linear relationship between the current and vanillin concentration was obtained over the range of 0.5–25 μM, described by the equation  $I(\mu A) = 4.7819c - 2.9631$ , with excellent linearity ( $R^2 = 0.9987$ ). The limit of detection (LOD), calculated as  $3.3\sigma/s$ , was 1.40 μM, while the limit of quantification (LOQ), calculated as  $10\sigma/s$ , was 4.25 μM. These results show that the Eu<sub>x</sub>Mo<sub>y</sub>O<sub>z</sub>/MWCNT-modified GCE could be used as a simple and reliable platform for the electrochemical detection of vanillin.

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**PCC PP 14****Effect of small changes in basis-set parameters on the description of hydrogen bonding in the water dimer**Danijela Kretić*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

Hydrogen bonds play an important role in determining stability and properties of many natural and synthetic materials. As a result, hydrogen-bonded systems have been extensively studied using both experimental and theoretical approaches. An important goal of theoretical chemistry is to improve the accuracy of computational methods for describing and predicting the properties of chemical systems, including their ability to form hydrogen bonds and the strength and characteristics of these interactions. Reliable hydrogen-bond descriptions are therefore important [1]. In this study, small changes were introduced to the exponents of diffuse and polarization functions in the aug-cc-pVDZ basis set, making the basis set either more diffuse and flexible or more compact. This approach allowed us to investigate how small changes in individual basis-set parameters affect the description of hydrogen bonding in the water dimer. The calculated interaction energies showed only small differences among the modified basis sets. The largest deviations in BSSE-corrected energy were observed for basis sets with modified polarization-function exponents. In contrast, more pronounced changes were observed in the electrostatic potential at the critical point between the donor H and acceptor O atoms. Deviations of approximately 4 kcal/mol were obtained when diffuse and polarization-function exponents were modified for the donor water molecule. Polarization functions allow the electron density to deviate from a simple spherical atomic shape and provide additional flexibility for describing electron-density redistribution, which is particularly relevant to the directional nature of hydrogen bonding. Energy decomposition analysis further showed deviations of approximately 10–22% in the electrostatic energy contribution for model systems in which the polarization-function exponents of the acceptor water molecule were modified. The small changes in the steric contribution indicate that the electron-density changes have a limited energetic effect. However, the results show that small modifications of basis-set parameters can produce substantially larger changes in local electrostatic properties at the H $\cdots$ O interaction region than in the overall interaction energy. These findings highlight the sensitivity of local hydrogen-bond descriptors to basis-set parameters, even when the calculated interaction energy remains relatively stable.

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## PCC PP 15

## Intrinsic fluorescence of calix[6]arene as a probe for metal cation complexation

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Changes in the intrinsic fluorescence of a tertiary-amide calix[6]arene derivative **L** (Fig. 1) were investigated as a sensitive probe for monitoring and quantitatively characterizing the complexation of alkali and alkaline earth metal cations. As demonstrated previously for the corresponding calix[4]arene analogue [1], despite the absence of an appended fluorophore, **L** exhibits moderate intrinsic emission that is strongly influenced by cation binding, providing a direct spectroscopic response to complex formation. Spectrofluorimetric titrations enabled the determination of stability constants for both 1:1 and 2:1 cation:**L** complexes. The obtained values showed very good agreement with those determined independently by absorption spectrophotometry and microcalorimetry, demonstrating the reliability of fluorescence-based characterization. The stoichiometries and structures of the complexes were further investigated by <sup>1</sup>H NMR spectroscopy and mass spectrometry, while molecular dynamics simulations provided additional insight into the cation binding processes and the structural features of the resulting complexes. Owing to its high sensitivity and low receptor requirements, fluorimetry provides clear advantages over conventional spectrophotometric and calorimetric methods, particularly for poorly soluble systems and highly stable complexes. These findings highlight the potential of intrinsic calixarene fluorescence for sensitive detection and differentiation of metal cations and for future molecular sensing applications.

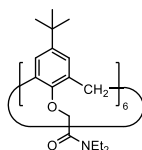


Figure 1. Structure of the investigated calix[6]arene **L**.

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## PCC PP 16

## The formation of cation- $\pi$ interactions and pnictogen bonds between $\text{XH}_4^+$ cations ( $\text{X} = \text{N}, \text{P}, \text{As}$ ) and benzene sandwich compounds

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Cation- $\pi$  interactions are significantly stronger when the cation interacts with a coordinated benzene ring in a sandwich compound than with an (uncoordinated) benzene [1]. Small alkaline earth metal cations form remarkably strong cation- $\pi$  interactions, while larger alkali metal cations form interactions of moderate strength [1]. It was shown that the strengthening of cation- $\pi$  interactions of sandwich compounds occurs due to involvement of transition metal d orbitals [2].

In this work, we analyzed the interactions between pnictogen onium cations ( $\text{NH}_4^+$ ,  $\text{PH}_4^+$ ,  $\text{AsH}_4^+$ ) and aromatic rings of three benzene sandwich compounds ( $\text{Cr}(\text{benzene})_2$ ,  $\text{Mo}(\text{benzene})_2$  and  $\text{W}(\text{benzene})_2$ ). All complexes were optimized at the B3LYP-D3/def2TZVP level of theory, which was also used for interaction energy calculations. The strength of interactions (somewhat unexpectedly) follows the order:  $\text{NH}_4^+ > \text{PH}_4^+ \approx \text{AsH}_4^+$ , even though the  $\text{AsH}_4^+$  cation is larger than the  $\text{PH}_4^+$  cation. With the help of different analyses, we determined that the  $\text{NH}_4^+$  cation and the  $\pi$ -systems form only the cation- $\pi$  interaction, while with the  $\text{PH}_4^+$  and  $\text{AsH}_4^+$  cations both the cation- $\pi$  interaction and the charge assisted pnictogen bond form simultaneously (Fig. 1).

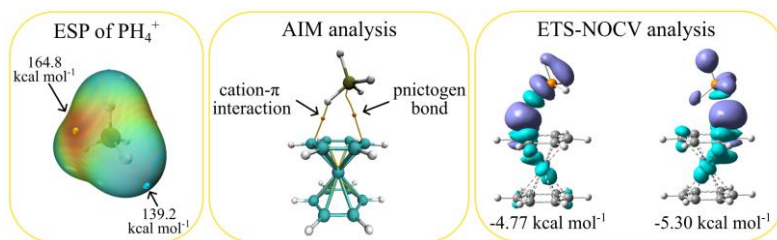


Figure 1. The analysis of the interaction between the  $\text{PH}_4^+$  cation and bis(benzene)chromium.

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## PCC PP 17

**Effect of Pd-Fe ratio on the electrochemical and capacitive performance of carbon aerogel electrodes in acidic media**

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Carbon aerogels (CA) are highly porous 3D carbon-based materials characterized by their ultra-low density, high specific surface area, and excellent electrical conductivity. These unique properties make them particularly attractive as electrode materials for supercapacitors, where a large accessible surface area facilitates efficient charge storage, while high electrical conductivity enables rapid charge and discharge. Also, their tunable porous structure and the possibility of doping with transition metals can further enhance their electrochemical performance, making CA promising materials for high-performance energy storage applications [1]. In this study, CAs were doped with Pd and Fe nanoparticles in different ratios Pd<sub>x</sub>-Fe<sub>100-x</sub>/CA (x = 0, 30, 50, 70, 100) to investigate the influence of the metal composition on the capacitive behavior in 1 M H<sub>2</sub>SO<sub>4</sub>. Electrochemical measurements were performed using the cyclic voltammetry at scan rates from 5 to 400 mV s<sup>-1</sup>. Pd/CA showed the highest specific capacitance value of 120.8 F g<sup>-1</sup> at 20 mV s<sup>-1</sup>, while Fe/CA gave the lowest value of 10.2 F g<sup>-1</sup>. The same trend is observed at other scan rates. Increasing the Pd content enhances the specific capacitance and capacitive performance. The dominant presence of Pd primarily contributes to the charge storage process, while the increase in Fe content disrupts the pore structure due to instability and passivation/dissolution of Fe and thus leads to the degradation of the working electrode. The findings show how careful tuning of the CA structure and metal composition influence the optimization of the capacitive properties, in order to design efficient electrodes for supercapacitors.

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**PCC PP 18****Simultaneous determination of dopamine, serotonin, and tryptophan using a modified glassy carbon electrode**

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Dopamine and serotonin represent important neurotransmitters in the central nervous system [1]. L-tryptophan is an essential amino acid, necessary for normal functioning of human organism [1]. Dopamine, serotonin, and tryptophan are coexisting compounds in biological fluids, and their levels can be used in the diagnosis of various diseases [1,2]. In this study, a novel sensor was developed for their simultaneous determination using square wave voltammetry. The sensor was prepared by modifying a glassy carbon electrode with  $\beta$ -cyclodextrin, graphene oxide, and CuO nanoparticles. The results indicated that the presence of  $\beta$ -cyclodextrin enabled the dispersion of the added modifiers on the electrode surface. Furthermore, thanks to the inner cavities of  $\beta$ -cyclodextrin and its ability to form stable host-guest inclusion complexes with biological compounds, the separation of the analytical peaks of the target molecules was achieved in this work. The presence of all modifiers improved sensor conductivity and adsorption of analytes onto the electrode surface, resulting in significantly higher voltammetric peak currents. Variation of the pH values demonstrated that highly acidic and basic media were not suitable for determination of the analytes. It was found that an equal number of protons and electrons was exchanged in the redox reactions of all analytes. Utilizing the determined optimal experimental conditions, the sensor exhibited a broad linear response of the anodic current as a function of the concentration of each analyte, achieving low detection limits. Finally, the developed sensor was effectively applied for the detection of target compounds in a synthetic serum solution. Considering the obtained low detection limits, electrode stability, good selectivity, and reproducibility of results, it can be concluded that the developed sensor possesses significant potential for the simultaneous determination of dopamine, serotonin, and tryptophan over broad concentration ranges in various samples.

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**PCC PP 19****Hydrogen bonds of imidazole transition metal complexes with water molecule**

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The molecule coordination leads to stronger hydrogen bonds. This has been shown for various types of interactions, such as NH/O [1], where free ethylenediamine (en) bonds to the water molecule with an interaction energy of -2.3 kcal/mol, while neutral en complexes have hydrogen bonds from -4.0 to -6.7 kcal/mol. The same trend applies to CH/O hydrogen bonds of 2,2'-bipyridine (bipy) [2], whose hydrogen bond strength rises from -2.1 kcal/mol for noncoordinated bipy to the range from -3.0 to -5.6 kcal/mol for neutral bipy complexes.

In this work, we studied the influence of coordination on the hydrogen bonds between imidazole and water using quantum chemical calculations of interaction energy at the B3LYP-D4/def2-TZVP level. We investigated NH/O and CH/O hydrogen bonds in non-coordinated imidazole and its neutral complexes: octahedral cobalt(II) and nickel(II), square pyramidal copper(II), square planar copper(II), and linear silver(I). For NH/O hydrogen bonds, a non-coordinated imidazole-water bond has an interaction energy of -6.5 kcal/mol, while imidazole complexes have significantly stronger interactions, from -8.3 to -9.5 kcal/mol. The same trend applies to weaker CH/O interactions, which have an interaction energy of -2.4 kcal/mol for non-coordinated, and in the range from -3.6 to -4.6 kcal/mol for imidazole complexes. The hydrogen bonds become stronger as the coordination number decreases; the NH/O interaction energies are from -8.3 to -8.4 kcal/mol for coordination number six, -8.6 kcal/mol for coordination number five, -9.0 kcal/mol for coordination number four, and -9.5 kcal/mol for coordination number two, while the corresponding CH/O energies are from -3.6 to -3.7, -3.8, -4.1, and -4.6 kcal/mol.

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## PCC PP 20

**Electrochemical oxidation of Rhodamine B: kinetic analysis and impact of reactive oxygen species**

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Electrochemical oxidation is a promising approach for the removal of organic pollutants from water, relying on the generation and action of reactive oxygen species (ROS). Understanding the contribution of individual reactive species is essential for elucidating the degradation process [1,2]. In this study, the degradation of Rhodamine B (10 mg L<sup>-1</sup>), used as a model organic pollutant, was investigated in an electrochemical system consisting of a Ti anode and carbon felt (CF) cathode at a constant current of 8 mA. Rhodamine B degradation was monitored by UV–VIS spectrophotometry, and the degradation kinetics were described using a pseudo-first-order model, yielding an apparent rate constant of 0.0318 min<sup>-1</sup>. To evaluate the contribution of reactive species, methanol (MeOH, 100 mM), which can scavenge both hydroxyl radicals (•OH) and sulfate radicals (SO<sub>4</sub>•<sup>-</sup>), and tert-butanol (TBA, 250 mM), used as a selective •OH scavenger, were employed. The addition of MeOH and TBA markedly suppressed Rhodamine B degradation, decreasing the apparent rate constant to 0.0009 and 0.0017 min<sup>-1</sup>, corresponding to inhibition of 97.2% and 94.7%, respectively. The pronounced inhibition observed in the presence of both scavengers indicates a dominant contribution of hydroxyl radicals (•OH) to Rhodamine B degradation, while the small difference between the effects of MeOH and TBA suggests a limited contribution of sulfate radicals (SO<sub>4</sub>•<sup>-</sup>). These findings demonstrate the predominant role of •OH in Rhodamine B degradation and provide insight into the contribution of reactive species in the investigated electrochemical system.

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## **Phytochemistry and Food Chemistry (PFC)**

**PFC PP 1****Comparative analysis of bioactive compound content and antioxidant potential in selected berry fruits**

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Berries are widely recognized as rich dietary sources of phenolic compounds, flavonoids and other bioactive metabolites that contribute to their antioxidant capacity and various health-promoting effects, including a reduced risk of cardiovascular disease and other chronic disorders [1,2]. Among cultivated berries, raspberry (*Rubus idaeus* L.), blackberry (*Rubus fruticosus* L.) and blueberry (*Vaccinium spp.*) are particularly valued for their nutritional and functional properties. This study aimed to evaluate and compare the total phenolic content (TPC) and total flavonoid content (TFC), as well as the antioxidant potential, of raspberry, blackberry and blueberry fruit extracts. TPC and TFC were determined spectrophotometrically using the Folin–Ciocalteu and aluminum chloride methods, respectively, while antioxidant potential was evaluated using the DPPH free radical scavenging assay and the FRAP (Ferric Reducing Antioxidant Power) assay. Among the tested fruits, blackberry exhibited the highest TPC ( $5059.83 \pm 317.29$  µg gallic acid equivalents (GAE)/g fresh weight (FW)) and TFC ( $201.90 \pm 5.48$  µg catechin equivalents (CE)/g FW), followed by blueberry ( $2628.21 \pm 429.10$  µg GAE/g FW;  $170.75 \pm 15.02$  µg CE/g FW) and raspberry ( $2439.39 \pm 432.84$  µg GAE/g FW;  $109.23 \pm 4.74$  µg CE/g FW). Consistently, blackberry showed the strongest DPPH inhibition (77.67%) and the highest FRAP value ( $8837.74 \pm 682.18$  µg Trolox equivalents (TE)/g FW), compared to raspberry (58.96% and  $4045.27 \pm 292.75$  µg TE/g FW, respectively) and blueberry (41.67% and  $3206.14 \pm 378.88$  µg TE/g FW, respectively). These results highlight berry fruits as valuable dietary sources of bioactive compounds with antioxidant potential, with blackberry exhibiting the most pronounced antioxidant properties among the analyzed samples.

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**PFC PP 2*****Porphyridium purpureum*-based hydrogels as delivery systems for vitamin D<sub>3</sub> and coenzyme Q10: digestibility and antioxidant potential**

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The red microalga *Porphyridium purpureum* represents a promising source of bioactive compounds, such as phycobiliproteins and sulfated polysaccharides. In our previous study<sup>1</sup>, we characterised its ability to form hydrogels under acidic conditions. In this study, *P. purpureum*-based hydrogels were investigated as delivery systems for vitamin D<sub>3</sub> and coenzyme Q10. Encapsulates were prepared by electrostatic extrusion of an aqueous *P. purpureum* extract containing 0.5% sodium alginate and either vitamin D<sub>3</sub> or coenzyme Q10 at a final concentration of 100 µM. The droplets were collected in 50 mM glycine buffer containing 2% CaCl<sub>2</sub>, yielding intensely coloured purple hydrogel particles up to 2 mm in diameter. The particles were subsequently lyophilised and subjected to simulated *in vitro* gastrointestinal digestion. Following digestion, the samples were analysed by SDS-PAGE electrophoresis. Also, the resulting digests were evaluated for antioxidant capacity using the reducing power (FRP) assay. Both vitamin D<sub>3</sub> and coenzyme Q10 loaded hydrogels, as well as unloaded hydrogels, remained stable under simulated gastric conditions, whereas digestion occurred predominantly during the intestinal phase. In the absence of digestive enzymes, pepsin and pancreatin, no appreciable digestion was observed, indicating an enzyme-dependent degradation process. Vitamin D<sub>3</sub> loaded hydrogels exhibited the highest antioxidant activity, followed by coenzyme Q10 loaded and unloaded hydrogels. These findings highlight the potential of *P. purpureum*-based hydrogels as delivery systems for bioactive compounds and their potential to enhance antioxidant activity following gastrointestinal digestion. This approach may support the development of functional food formulations.

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## PFC PP 3

**Development and validation of an ion chromatography method for the determination of oxalic acid content in honey**

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The application of oxalic acid for controlling *Varroa destructor* has been increasing in recent years due to its effectiveness, safety, and low cost. However, improper treatment can leave residues of oxalic acid in honey, which influences its chemical composition and quality [1]. Therefore, to address the need for a reliable analytical approach for monitoring oxalic acid content in honey, this study proposed a method based on ion-exchange chromatography with conductometric detection (IC-CD), as oxalic acid predominantly exists in anionic form at basic pH conditions [2]. Optimisation of elution parameters revealed that gradient elution with potassium hydroxide as the mobile phase (0–10 min, 40 mmol/L; 10–18 min, 40–50 mmol/L; 18–22 min, 50 mmol/L; 22–40 min, 50–40 mmol/L) provided the optimal peak shape and separation of oxalic acid. The method demonstrated satisfactory selectivity, with resolutions between adjacent peaks of 1.8 and 5.8, as well as a high linearity coefficient within the concentration range of 1 mg/L to 10 mg/L ( $r = 0.9998$ ). Based on the calibration curve, the limit of detection (LOD) and the limit of quantification (LOQ) were calculated to be 2.9 mg/kg and 8.8 mg/kg, respectively. The working range of the method covers concentrations from 8.8 mg/kg to 108 mg/kg. Repeatability and intermediate precision of the method were in agreement with the Horwitz model ( $\text{HorRat}_r = 0.39$  and  $\text{HorRat}_R = 0.41$ ). Analysis of spiked samples across three concentration levels revealed satisfactory accuracy, with recovery values above 92%. Lastly, the method was successfully applied to real samples of *acacia* honey, where the oxalic acid content was relatively low, often remaining below the method's detection limit.

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**PFC PP 4****Extraction and determination of nitrates in vegetables by ion chromatography**

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Nitrates are naturally occurring components of plant-based foods and represent an important source of nitrogen required for plant growth and development. However, excessive nitrate accumulation in edible plant tissues may raise concerns about food quality and safety, making reliable nitrate determination in vegetables particularly important. This study investigated nitrate content in selected vegetables, including lettuce, spinach, and celery root. Nitrates were extracted from the plant matrices, appropriately diluted, and analyzed by ion chromatography (IC). This technique enabled selective determination of nitrate ions in the presence of other anionic species naturally occurring in the extracts, without interference with the nitrate signal. Lettuce had the highest nitrate concentration (5868 mg/kg), followed by spinach (2359 mg/kg), while celery root showed a considerably lower content (743 mg/kg). These results demonstrate pronounced differences in nitrate accumulation among the investigated vegetables and are consistent with the greater tendency of leafy vegetables to accumulate nitrates compared with root vegetables. In addition to nitrate determination, we performed non-purgeable organic carbon (NPOC) analysis to provide complementary information on the organic matter extracted from the plant matrices. Celery root extract had the highest organic carbon concentration (31.86 mg/L), whereas lettuce and spinach extracts contained 19.64 and 17.34 mg/L, respectively. The results highlight ion chromatography as a selective and reliable analytical approach for nitrate determination in complex vegetable matrices, while TOC analysis provides additional insight into extract composition. This combined approach supports more comprehensive characterization of vegetable extracts and demonstrates its potential for assessing food quality and safety.

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**PFC PP 5****Chemical characterisation of *Satureja montana* L. (Lamiaceae) extracts obtained employing microwave-assisted extraction and choline chloride-based natural deep eutectic solvents**

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Phytochemicals, especially phenolic compounds, play a pivotal role in improving health and well-being [1]. Although widely recognized as a culinary herb, winter savory (*Satureja montana* L., Lamiaceae) possess medicinal potential due to its rich content of phenolics. Selecting appropriate extraction methods and solvents is crucial for maximizing the recovery and stability of these compounds. Negative impact of conventional extraction methods and solvents on environment and human health has prompted their replacement with greener alternatives. The coupling of microwave-assisted extraction (MAE) with natural deep eutectic solvents (NADES) represents an eco-friendly, efficient, versatile and cost-effective approach [2]. In this study, two choline chloride-based NADES were evaluated for their phenolic compound extraction efficiency from winter savory and compared with the conventional solvents, 70% ethanol and water. MAE was performed at a microwave power of 180 W for three cycles of 5 s each, employing choline chloride:lactic acid NADES, choline chloride:malic acid NADES, 70% ethanol, and water as extraction solvents. The high-performance liquid chromatography with diode-array detection (HPLC-DAD) analysis of the savory extracts resulted in the identification and quantification of rosmarinic acid, trans-cinnamic acid, rutin, quercetin, and naringenin. The choline chloride:lactic acid system yielded extracts with higher levels of rutin, quercetin, and trans-cinnamic acid compared with those obtained using other applied solvents. Water was observed to be the least efficient solvent in this study. The enhanced extraction efficiency of the choline chloride:lactic acid NADES compared with the choline chloride:malic acid system may be related to its lower viscosity, which facilitates mass transfer and diffusion of phenolic compounds. This green approach enhances extraction efficiency, offers a sustainable alternative to conventional solvents, and supports the potential application of phenolic-rich savory extracts.

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**PFC PP 6****Valorization of invasive *Ailanthus altissima* (Mill.) Swingle biomass using natural deep eutectic solvents**

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*Ailanthus altissima* (Mill.) Swingle, also known as Tree of heaven, is a member of the Simaroubaceae family. While native to China, it is one of the most invasive plant species in northern Serbia, in the Vojvodina region, with anthropogenic environments being most susceptible to its invasion. Due to its heightened fecundity, it threatens the survival of autochthonous species, causes changes in food chains and destroys biodiversity in doing so, while its roots crack building foundations, warp pavements, and block underground drainage systems [1]. Developing sustainable strategies for the utilization of *A. altissima* biomass can transform an ecological challenge into a valuable source of bioactive compounds. The aim of this study was to explore the leaves of *A. altissima* as a potential source of antioxidant agents using natural deep eutectic solvents (NADES) as environmentally friendly extraction media [2]. The extraction efficiency of various NADES formulations combined with microwave-assisted extraction (MAE) was evaluated based on total phenolic content (TPC), total flavonoid content (TFC), and antioxidant activity of the obtained extracts. Water and 70% ethanol (v/v) were used as reference solvents. Four NADES systems based on choline chloride, glycerol, lactic acid, glucose and urea were synthesized by heating and stirring. MAE was performed at 180 W in three 8-second cycles. The TPC and TFC were determined spectrophotometrically, while the antioxidant activity of extracts was evaluated via the DPPH radical scavenging test and the CUPRAC assay. Among the tested formulations, the urea:lactic acid (1:4) NADES yielded the highest TPC and TFC, whereas the choline chloride:glycerol (1:2) NADES exhibited the strongest antioxidant potential in both DPPH and CUPRAC assays, outperforming conventional solvents. These findings demonstrate that NADES represent highly efficient, green alternatives for transforming invasive biomass into high-value antioxidant bioactive compounds.

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**PFC PP 7****Phycocyanins as a substitute for serum in adipocyte differentiation media in cellular agriculture**

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Cultivated meat offers a compelling alternative to conventional livestock farming, lowering the demand for resources such as land and water while cutting down on environmental pollution. In this process, myoblasts are differentiated to adipocytes using a differentiation medium that typically relies on animal-derived chicken serum. This ingredient, however, poses major limitations for scaling up production, since it is costly, variable in composition, and raises ethical concerns. Phycocyanins (PCs) derived from algae and cyanobacteria may offer a way to enhance cellular differentiation, potentially allowing for a reduction in the serum content of cell culture media. This, in turn, could lower the overall cost of cultivated meat production while making it more ethically sound.

This study explores how R-phycocyanin (R-PC) from red microalgae *Prophyra haitanensis* and C-phycocyanin (C-PC) from cyanobacteria *Arthrospira platensis* can help Qual myoblast cell line (QM7) to differentiate in medium with reduced serum level. We tested viability of cells in differentiation media with Neutral Red Uptake assay, stained lipids in cells with Oil Red dye, and measured cell differentiation markers with real-time PCR.

NRU assay showed us not only that PCs have no toxic effect on cells, but slightly boost their metabolism in modified differentiation medium, while PCR results shows that PCs increased differentiation markers for adipocyte differentiation compared to control. Also, Oil Red staining detected increased amount of lipids in cells cultured in medium for adipogenic differentiation, compared to medium without PCs.

This study shows that phycocyanins from algae and cyanobacteria can boost adipogenic differentiation in medium with reduced serum. This can help in lowering the need for chicken serum in meat cultivation, which can potentially decrease the price of industrial production.

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**PFC PP 8****Influence of different distillation methods on the chemical composition of plum distillate**

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Distillation is a crucial step in fruit spirit production, since it separates and concentrates the volatile aromatic fraction of the fermented mash, thereby shaping the spirit's chemical profile. The distillation system used has a direct impact on the final chemical composition of the resulting alcoholic beverage, altering the relative proportions of higher alcohols, esters, furfural, methanol, aldehydes, hydrogen cyanide, volatile acids, primary aroma compounds and other congeners that contribute to its aroma and overall quality [1,2].

This study aimed to investigate the influence of two distillation methods, fractional column distillation and double pot still distillation, on the chemical composition of plum spirit. Volatile compounds were analyzed using gas chromatography with flame ionization detection (GC-FID). The double pot still distillate showed markedly higher titratable acidity (165.6 mg/L vs. 39.6 mg/L), as well as higher contents of ethyl acetate (1537.3 vs. 1165.3 mg/L of absolute alcohol (a.a.)) and aldehydes (140.9 vs. 122.8 mg/L a.a.). Methanol, furfural, benzaldehyde and higher alcohol contents were comparable between the two methods. These results indicate that the distillation method influences the chemical composition of plum spirit, with double pot still resulting in higher titratable acidity and increased concentrations of ethyl acetate and aldehydes, while contents of several other examined congeners remained comparable between the two methods.

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**PFC PP 9****Relationship between extraction yield and antioxidant potential of Lamiaceae herbal teas**

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Lamiaceae includes many aromatic and medicinal plants commonly used as herbal teas. Although extraction yield is often used to describe extraction efficiency, a higher yield does not necessarily indicate higher antioxidant activity. This study examined the relationship between extraction yield and antioxidant activity in aqueous extracts of ten Lamiaceae species prepared by traditional infusion and microwave-assisted extraction. Antioxidant activity was evaluated using DPPH and ABTS radical-scavenging assays based on IC<sub>50</sub> values, together with FRAP and CUPRAC assays. For infusion extracts, extraction yield showed weak negative correlations with DPPH and ABTS IC<sub>50</sub> values ( $r = -0.213$  and  $-0.227$ ), while moderate positive correlations were observed with FRAP and CUPRAC ( $r = 0.401$  and  $0.453$ ). For microwave-assisted extracts, the strongest positive correlation was observed between extraction yield and FRAP ( $r = 0.409$ ), while weak negative correlations were observed with DPPH and ABTS IC<sub>50</sub> values. None of the correlations were statistically significant ( $p > 0.05$ ). Savory showed strong DPPH radical-scavenging activity despite its relatively low extraction yield, whereas high-yielding species such as mentha and lemon balm did not consistently show higher antioxidant activity. These findings indicate that extraction yield alone may not reliably reflect the antioxidant potential of aqueous Lamiaceae extracts. Therefore, both extraction efficiency and antioxidant activity should be considered when evaluating Lamiaceae herbal teas.

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**PFC PP 10****Elemental profiles of Saffron Flower Petals and the Petal Preserve**

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Saffron (*Crocus sativus* L.) is traditionally valued primarily for its dried stigmas, which are widely used as a spice and in food products [1]. In recent years, increasing attention has been directed towards the saffron petals, which are generally considered an agricultural by-product of saffron spice production. Saffron petals are good source of proteins, carbohydrates and essential elements and contain a range of bioactive compounds (carotenoids, phenolic compounds, flavonoids, and anthocyanins), highlighting their potential for valorization in food and nutraceutical applications [1,2]. In this study, the contents of 28 macro- and microelements in saffron flower petals and the petal preserve were analyzed by means of ICP-OES analytical technique. The aim was to compare the initial plant material and the final product. Petals and the petal preserve were obtained from the saffron producer "Prvi Srpski Šafran". The results showed that As, Be, Cd, Cr, Li, Pb, Sb, Se, Ti, Tl and V were below the limits of detection in both saffron petals and the preserve. K had the highest concentration with 4303 mg/kg in saffron petals, and 431.3 mg/kg in the preserve. It was followed by P (387 vs. 56.6 mg/kg), S (277 vs. 40.2 mg/kg), Mg (211 vs. 34.5 mg/kg), and Ca (178 vs. 102 mg/kg) in petals and the preserve, respectively (all  $p < 0.05$ ). Fe was the most abundant microelement, with concentrations of 92.2 mg/kg in the petals and 7.20 mg/kg in the preserve, followed by Zn (6.17 vs. 1.50 mg/kg), Mn (3.80 vs. 0.30 mg/kg), B (2.22 vs. 0.30 mg/kg) and Cu (1.79 vs. 0.40 mg/kg) (all  $p < 0.05$ ). Concentrations of Al and Ba were 83.0 and 0.65 mg/kg (petals) and 13.6 and 0.10 mg/kg (the preserve), respectively ( $p < 0.05$ ). In contrast to other elements, concentration of Na, increased in the preserve, while Ni, Sr, Mo, and Co were detected only in the petals. Overall, the high concentrations of K, P, S, Mg, Ca, and Fe in saffron petals indicate their potential for food fortification and support their valorisation as an underutilized agricultural by-product.

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**PFC PP 11****Chemical characterization and food-grade extraction of *Coprinus comatus* powder as a potential functional food ingredient**

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Edible mushrooms are increasingly recognized as valuable food resources due to their combination of nutritional components and diverse bioactive compounds [1]. *Coprinus comatus* is of particular interest as a source of polysaccharides, phenolic compounds and other constituents with potential functional properties [2]. This study aimed to characterize the chemical composition of commercial *C. comatus* powder and to evaluate food-grade extraction approaches for the recovery of bioactive compounds. Proximate composition, dietary fiber and cellulose contents were determined by standard analytical procedures, while the mineral profile was analysed by atomic absorption spectroscopy. Aqueous and ethanol-based extractions were performed, followed by spectrophotometric determination of total phenolic and flavonoid contents and total soluble carbohydrates. The chemical characterization showed that *C. comatus* powder is a protein- and carbohydrate-rich material (24.86 and 60.73%, respectively), with a substantial fiber fraction (31.05%), predominantly represented by insoluble fiber (27.12%). The cellulose content was 6.40%, accounting for approximately 23.6% of the insoluble fiber fraction. The mineral profile further revealed considerable amounts of potassium, magnesium and calcium, while iron was present at  $1062.16 \pm 4.92$  mg/kg. Aqueous extraction resulted in a higher extraction yield than 70% ethanol (69.30 vs. 42.34%) and provided higher levels of total phenolic compounds and soluble carbohydrates. These results demonstrate that *C. comatus* combines a nutritionally valuable composition with the potential for food-grade recovery of bioactive compounds, providing a basis for further optimization of the extraction conditions and evaluation of the resulting extracts for functional food applications.

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**PFC PP 12****Evaluation of different lactic acid bacterial strains  
for bean fermentation**

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Fermentation of beans is a promising approach for improving their biological and functional properties, and reduction of antinutritional compounds [1]. Lactic acid bacteria (LAB) widely used in fermentation process and valued for their ability to improve the taste and texture of fermented products [2]. The aim of this study was to evaluate the potential of different lactic acid bacteria for fermentation of two Serbian bean varieties ('Dvadesetica' and 'Šareni'). Selected 15 bacterial cultures belonging to the genera *Lactococcus* (B212, S44, S66), *Leuconostoc* (L44, L64, S1010, L614, B771, S154, S141, S91), *Lactobacillus* (S109, B62, I143) and *Pediococcus* (B204) were used for the fermentation of samples under controlled conditions. The fermentation process was evaluated by monitoring changes in the pH value, total bacterial count and protein profile assessed by electrophoresis, after 24h of fermentation. The tested strains showed growth during the fermentation of both bean varieties. The highest bacterial counts were recorded for strain S44 in both 'Dvadesetica' (9.54 log CFU/g) and 'Šareni' (9.59 log CFU/g). pH values differed depending on the bean variety and the applied strain of lactic acid bacteria. The lowest pH was recorded in 'Dvadesetica' (4.34) fermented with strain S91 and in 'Šareni' (4.25) fermented with strain I143, compared to the relevant control samples (5.43 and 5.77, respectively). The same proteins were present in all protein isolates from the same bean variety after fermentation, although there were variations in the total amount of protein extracted, as well as between two bean varieties.

The obtained results highlight the potential of selected LAB for the fermentation of studied bean varieties.

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**PFC PP 13****Fatty acid composition of grapevine leaves (*Vitis vinifera* L.)  
from ‘Grašac’ and ‘Probus’ cultivars**

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Grapevine leaves represent an abundant but still underutilized source of biomass generated during routine vineyard management. In addition to dietary fibre, proteins, minerals, and phenolic compounds, grapevine leaves contain lipids rich in polyunsaturated fatty acids, which may contribute to their nutritional and functional value (Tomić et al., 2026). However, the fatty acid composition of grapevine leaves can vary depending on cultivar and growing conditions, while information on the fatty acid profiles of ‘Grašac’ and ‘Probus’ leaves remains limited. Therefore, this study aimed to characterise and compare the fatty acid composition of these two autochthonous cultivars from Vojvodina. Lipids were extracted using chloroform–methanol (2:1), converted to fatty acid methyl esters (FAME), and analyzed by gas chromatography with flame ionization detection (GC-FID). The analysis revealed a slightly higher fat content in ‘Probus’ leaves compared with ‘Grašac’, while both cultivars showed similar fatty acid profiles, characterized by a predominance of polyunsaturated fatty acids, particularly  $\alpha$ -linolenic acid (C18:3 n-3), followed by palmitic acid (C16:0). Despite differences in total fat content, the proportion of polyunsaturated fatty acids was comparable between the cultivars, with omega-3 fatty acids representing the major fraction of total fatty acids. The n-3/n-6 ratio was also relatively high in both cultivars, indicating a consistent predominance of omega-3 over omega-6 fatty acids. Overall, the study provides additional phytochemical insight into grapevine leaves, revealing cultivar-related differences in lipid content with a broadly conserved fatty acid pattern, and highlights their potential for valorization as a plant-derived lipid source in food applications.

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## PFC PP 14

**High-affinity binding of concanavalin A to C-phycocyanin**

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The growing demand for natural food colorants has increased interest in microalgae as a source of natural pigments. *Arthrospira platensis* (Spirulina) is a rich source of C-phycocyanin (C-PC), a blue phycobiliprotein (PBP) with considerable potential for applications in the food industry. However, the limited stability of C-PC remains a major challenge for its wider application. In order to replace synthetic pigments with PBPs, it is necessary to keep them stable during industrial processing. One possible approach to modify the properties of C-PC is the formation of specific interactions with other proteins. This study aims to characterize the interaction of C-PC with concanavalin A (ConA), a lectin from *Canavalia ensiformis* (jack bean), and to investigate the factors contributing to their binding. Fluorescence spectroscopy was used to characterize the interactions between C-PC and different oligomeric states of ConA at pH 5.5 (dimer) and pH 7.2 (tetramer). ConA-induced enhancement of fluorescence of C-PC chromophore revealed a stronger affinity for the tetramer form of ConA ( $K_a$  of  $7.35 \times 10^6 \text{ M}^{-1}$ ) than for the dimer form ( $K_a$  of  $3.10 \times 10^6 \text{ M}^{-1}$ ). We demonstrated that the presence of sugars (glucose and mannose) inhibited the binding at pH 7.2. Whereas at pH 5.5 only mannose decreased the binding affinity, indicating that the presence of specific carbohydrates can alter the conformation of ConA and reduce their affinity for C-PC. VIS-CD spectroscopy revealed that ConA binding influences the chiral environment of the C-PC chromophore. Thermal stability study demonstrated higher stability of C-PC chromophore in the presence of ConA at pH 7.2. Overall, these findings suggest that lectin interactions may contribute to improving C-PC stability and support its potential use in the food industry [1,2].

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**PFC PP 15****Organochlorine pollutants: persistence, bioaccumulation and food safety concerns**

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Organochlorine pesticides and polychlorinated biphenyls (PCBs) are persistent organic pollutants of particular concern due to their high chemical stability, lipophilicity and ability to bioaccumulate and biomagnify through food chains. Despite restrictions and bans on the use of many of these compounds, their residues can still be found in the environment [1]. Therefore, these pollutants are routinely monitored as important food safety parameters, with maximum permitted levels defined by relevant legislation.

This study analyzed samples of food of animal origin and animal feed for the presence of 20 organochlorine pesticides and 6 PCB residues. Extraction of the target compounds was performed using a QuEChERS procedure. Samples were extracted with acetonitrile, followed by a clean-up step to remove interfering matrix components. The obtained extracts were subsequently evaporated and reconstituted in hexane prior to instrumental analysis. Qualitative and quantitative determination of organochlorine pesticides and PCB congeners was performed by gas chromatography coupled with mass spectrometry (GC-MS).

The results showed that most of the analyzed samples contained no detectable residues of the investigated compounds. Occasional findings of PCB congeners were observed in a limited number of samples, with PCB 138 and 153 being the congeners most commonly detected. These findings were predominantly associated with fish and fish-derived matrices, which may be related to the lipophilic nature and bioaccumulative properties of these compounds. More importantly, all determined concentrations were within the maximum residue levels permitted by applicable legislation. The obtained results indicate a generally satisfactory level of safety of the analyzed food and feed samples, while also emphasizing the importance of continuous monitoring of persistent organochlorine contaminants, particularly in matrices with a higher potential for their accumulation.

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**PFC PP 16****Chemical and Physical Characterization of Grain Quality in Five Wheat Genotypes**

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Wheat (*Triticum aestivum* L.) is one of the most important cereal crops worldwide and plays a major role in human nutrition due to its nutritional value and wide range of applications in food production. Grain quality is determined by a combination of chemical, physical, and technological properties, which can vary among genotypes and growing conditions. Among these characteristics, protein content is one of the most important chemical parameters because it contributes not only to the nutritional value of wheat but also significantly influences dough properties, processing quality, and suitability for different end uses [1]. Moisture content is also an important quality parameter, as it affects grain storage stability and susceptibility to deterioration. Physical traits such as thousand-seed weight and test weight provide important information about grain size, density, yield potential, and overall grain quality. The aim of this study was to evaluate the protein content, moisture content, thousand-seed weight, and test weight of five wheat genotypes.

The field experiment was conducted at the Experimental Field of the “Tamiš” Research and Development Institute, during the 2026 growing season. Genotype W4 had the highest protein content (12.58%) and the lowest moisture content (10.20%), whereas W3 showed the lowest protein content (12.11%) and thousand-seed weight (34.720 g). The highest moisture content (11.30%) and test weight (77.0 kg hL<sup>-1</sup>) were recorded in W2, while W5 had the lowest test weight (64.3 kg hL<sup>-1</sup>). Genotype W1 showed the highest thousand-seed weight (38.520 g).

The study highlights the importance of chemical characterization in assessing wheat grain quality. Protein and moisture content are important indicators of nutritional value, stability, and technological quality, demonstrating the relevance of analytical chemistry in wheat quality evaluation.

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**PFC PP 17****Antioxidant and skin-related enzyme inhibitory potential of blueberry waste extracts obtained using natural deep eutectic solvents**

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Fruit processing by-products represent sustainable sources of bioactive compounds with potential for value-added applications. Blueberry waste is particularly interesting due to its abundance of anthocyanins and other phenolic compounds associated with antioxidant and skin-related activities [1]. Oxidative stress contributes to skin ageing, excessive melanogenesis, and the degradation of extracellular matrix components. Therefore, the extracts were evaluated for antioxidant activity and their ability to inhibit tyrosinase and elastase, key enzymes involved in melanin synthesis and elastin degradation, respectively. This study proposes a green approach for blueberry waste valorisation using 18 natural deep eutectic solvents (NADES), with water and methanol as reference solvents. Binary NADES (1:1) and ternary systems with ascorbic acid (1:1:0.05) containing 25% water (w/w) were used for ultrasound-assisted extraction (45 min, 1:10 g/mL). Total phenolic content (TPC), DPPH radical scavenging activity, and tyrosinase and elastase inhibition were evaluated. The glycerol-proline-ascorbic acid (GPA) extract exhibited the highest TPC ( $360.24 \pm 0.98$  mg GAE/g) and DPPH activity ( $2909.38 \pm 53.58$   $\mu$ mol TE/g), while also achieving  $89.7 \pm 2.5\%$  tyrosinase inhibition. The glycerol-citric acid (GC) extract showed the strongest inhibition of both skin-related enzymes, reaching  $96.7 \pm 0.2\%$  for tyrosinase and  $84.6 \pm 4.3\%$  for elastase. High inhibitory activity was also observed for betaine-citric acid (BC) extract, with  $80.2 \pm 3.4\%$  tyrosinase and  $79.1 \pm 2.6\%$  elastase inhibition, whereas the reference extracts were considerably less effective. The pronounced antioxidant activity and inhibition of enzymes involved in skin pigmentation and elasticity highlight the potential of NADES-based blueberry waste extracts as sustainable multifunctional ingredients for further development of cosmetic formulations.

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**PFC PP 18****Valorization of grape pomace using green NADES extraction for natural antimicrobial formulations**

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Grape pomace represents a rich source of bioactive compounds which can be valorized for natural antimicrobial formulations. For the recovery of these biocompounds in an eco-friendly way, Natural Deep Eutectic Solvents (NADES) can be used as sustainable alternatives to conventional organic solvents [1]. This study evaluated the antimicrobial activity of grape pomace extracts obtained using binary and ternary NADES systems composed of glycerol or betaine combined with organic acids (lactic, malic, and citric acid), polyols (xylitol, sorbitol), amino acids (glycine, proline), and vitamin C. The antimicrobial activity of both grape pomace extracts and pure polar NADES formulations was evaluated *via* agar well diffusion test against *Escherichia coli*, *Bacillus cereus*, *Salmonella* Typhimurium, and *Listeria monocytogenes*. Results showed that antimicrobial activity was driven by the synergistic contribution of extracted bioactive compounds and the chemical composition of the eutectic solvents. Extracts prepared with organic acid-based NADES displayed pronounced antibacterial activity across all tested pathogens, exhibiting enhanced inhibition compared with pure NADES solvents. In contrast, polyol- and amino acid-based NADES exhibited negligible activity. This confirms that bioactive phytochemicals recovered from grape pomace directly contribute to antibacterial efficacy [2]. These findings highlight the potential of combining green NADES extraction with agro-industrial by-product valorization for the development of natural antimicrobial formulations.

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**PFC PP 19****Antibacterial activity of lettuce (*Lactuca sativa* L.) extracted with polar and non-polar NADES**

Milica Jankov<sup>1</sup>, Mila Lazović<sup>1</sup>, Nevena Kićović<sup>2</sup>, Petar Ristivojević<sup>2</sup>, Jelena Trifković<sup>2</sup>

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Plant extracts represent a significant source of phytochemicals that can exhibit a wide spectrum of biological activities. Lettuce (*Lactuca sativa* L.) extracts possess powerful antioxidant, antimicrobial, and anti-inflammatory activities, making them valuable candidates for various applications [1]. The aim of this study was to evaluate and compare the antibacterial activity of polar and non-polar NADES lettuce extracts against selected food-bacterial pathogens. Extraction of the plant material was performed using polar and non-polar NADES, after which the antibacterial activity was tested against *Bacillus cereus*, *Listeria monocytogenes*, *Escherichia coli*, and *Salmonella typhimurium* strains, using the agar-well diffusion assay. The results showed that polar NADES extracts exhibited antibacterial activity against all tested pathogens. This activity was strongly influenced by the chemical composition of the NADES formulations, indicating that these solvents act as active functional components rather than passive extraction media. These findings confirm the high efficiency of polar NADES systems for extracting antibacterial compounds from lettuce for potential use as natural preservatives. On the other hand, due to the presence of thymol in all non-polar NADES extracts, its volatile nature at 37°C led to accumulation in the headspace, delaying bacterial growth across the petri dishes [2]. Despite this diffuse vapor effect, distinct bactericidal and bacteriostatic zones were clearly visible for all tested bacteria except for *Listeria monocytogenes*, where no zones were observed. In summary, these results show that both polar and non-polar NADES extracts exhibit antibacterial activity.

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## **Solution Chemistry and Chemical Equilibrium (SCCE)**

**SCCE PP 1****Aqueous solubility, and hydration properties of methylliberine from density, viscosity, and acoustic measurements, supported by DFT and MD simulations**

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Methylliberine, a naturally occurring purine alkaloid and metabolic derivative of methylxanthines, has recently attracted attention as a potential ergogenic and cognitive-enhancing ingredient for dietary supplements [1,2]. Despite its growing use and investigation in human studies, fundamental knowledge of its physicochemical properties remains limited. Understanding these properties is essential for evaluating its behavior during processing, formulation, dissolution, and biological exposure. Therefore, this study provides a comprehensive physicochemical characterization of methylliberine through experimental measurements of solubility, density, speed of sound, viscosity, and thermal stability, combined with molecular dynamics simulations. The integrated experimental and computational approach provides molecular-level insight into solute–solvent interactions, hydration behavior, solution organization, and thermal stability, contributing to a better understanding of methylliberine and its potential application as a functional ingredient in food and dietary supplement formulations.

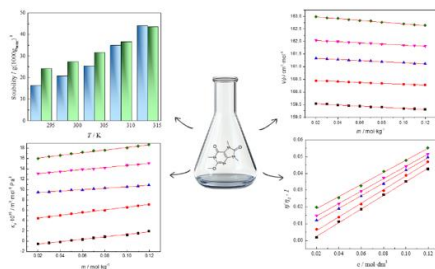


Figure 1. Methylliberine solubility, apparent molar volumes, compressibility and specific viscosity in aqueous solution

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## SCCE PP 2

**Catalytic performance of a copper(II) complex in the oxidation of *o*-aminophenol**

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Copper is an essential element for living organisms and plays a crucial role in numerous biological processes. It is present in the active sites of various metalloproteins and enzymes, such as superoxide dismutase, cytochrome *c* oxidase, and tyrosinase, where its biological activity is largely associated with its ability to undergo redox processes. [1]. One of the major multicopper oxidases belonging to the type-2 copper proteins is phenoxazinone synthase, which catalyzes the oxidative coupling of *o*-aminophenols, resulting in the formation of the phenoxazinone chromophore during the final stage of actinomycin D biosynthesis [2]. The kinetics of the oxidase biomimetic catalytic activity of the copper(II) complex, [CuCl<sub>2</sub>(py-2tz)]<sub>2</sub>, where py-2tz is dimethyl 2-(thiazol-2-yl)pyridine-4,5-dicarboxylate, was investigated using *o*-aminophenol as a substrate in a reaction.

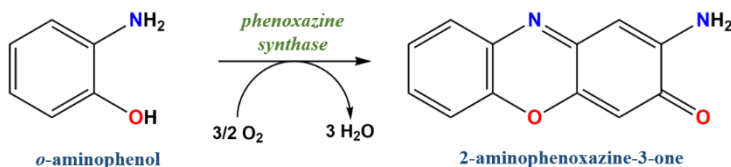


Figure 1. Scheme of the reaction catalyzed by the copper-containing enzyme phenoxazinone synthase.

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**SCCE PP 3****Physicochemical changes in badlands under simulated climatic conditions - the interplay between mineralogical composition and texture**

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Badlands are highly erodible landscapes in which weathering is strongly influenced by several interacting factors [1,2]. In this study, eight badland materials collected from Spain, Turkey, Romania, Israel, and Slovenia were investigated to assess how their initial mineralogical and textural characteristics influence their physicochemical response to simulated weathering. The samples represented different lithological types and were characterized in terms of grain size and mineralogical composition, with particular attention to presence of smectite, gypsum, analcime, and calcite. The weathering experiment consisted of two phases designed to simulate different climate conditions. In the first phase, the samples were subjected to repeated rainfall and snowmelt treatments followed by freezing–thawing cycles, while the second phase involved exposure to simulated rainfall and elevated temperature [2]. Surface changes, pH, electrical conductivity, and ion concentrations were monitored throughout each cycle of experiment. Despite differences in mineralogy and texture, sediments with gypsum exhibited similar physicochemical responses under the applied experimental conditions, suggesting that mineralogical composition, is crucial for their similar weathering behaviour [2]. The findings highlight that mineralogical, texture and physicochemical characteristics all influence the weathering behaviour of badland materials.

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## **Supramolecular Chemistry and Functional Materials (SCFM)**

**SCFM PP 1****Beyond the band gap: exploring the role of oxidation states and defects in the electronic properties of vanadium oxides**

Jelena Georgijević<sup>1</sup>, Lazar Rakočević<sup>1</sup>, Tatjana Vulić<sup>1</sup>, Nikola Ilić<sup>1</sup>, Tijana Đorđević<sup>1</sup>,  
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Vanadium oxides exhibit diverse electronic properties owing to the multiple accessible oxidation states of vanadium and their ability to form oxygen-deficient, non-stoichiometric phases. Consequently, their electronic structure cannot be adequately interpreted from a single band-gap value alone. Here, two contrasting vanadium oxide systems, amorphous VO<sub>x</sub> thin films and crystalline V<sub>2</sub>O<sub>5</sub> powders, were comparatively investigated using X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and X-ray photoelectron spectroscopy (XPS). Amorphous VO<sub>x</sub> films were deposited by reactive magnetron sputtering at three oxygen partial pressures, whereas crystalline V<sub>2</sub>O<sub>5</sub> powders were obtained by hydrothermal synthesis and direct thermal calcination. Optical analysis was adapted to each material form: film absorption coefficients were determined by combining transmittance with specular and diffuse reflectance, while powder diffuse-reflectance spectra were analyzed using the Kubelka-Munk transformation. The film deposited at the lowest oxygen partial pressure displayed metallic optical behavior without a clearly defined band gap, consistent with the XPS detection of V<sup>0</sup> and V<sup>3+</sup> species. Increasing oxygen availability promoted higher vanadium oxidation states and the emergence of semiconducting optical transitions. The most oxidized film exhibited an apparent indirect optical gap of approximately 2.23 eV, consistent with an increasing contribution from V<sup>5+</sup>-containing oxide species. Both crystalline V<sub>2</sub>O<sub>5</sub> powders showed comparable indirect band gaps of 2.14–2.18 eV, despite differences in their V<sup>4+</sup> and oxygen-defect contents. The results demonstrate that changes in oxygen stoichiometry, reflected in the distribution of vanadium oxidation states, govern the major evolution from metallic to semiconducting behavior. In contrast, differences in defect content were not accompanied by substantial changes in the fundamental absorption edge of crystalline V<sub>2</sub>O<sub>5</sub>. Combining structural, optical, and surface-sensitive characterization is therefore essential for interpreting the electronic complexity of vanadium oxides.

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**SCFM PP 2****Comparative analysis of MBAA-crosslinked PNiPAM hydrogels at different irradiation doses**

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One of the prominent topics in contemporary research over the past several decades has been temperature-sensitive hydrogels, a class of materials that exhibit reversible changes in their structure and properties in response to variations in the surrounding temperature. Poly(N-isopropylacrylamide) (PNiPAM) has found widespread use as a monomer in hydrogel synthesis due to its pronounced temperature sensitivity over a range near physiological temperatures [1]. The conditions of radiation synthesis play a crucial role in determining the structure, physicochemical properties, and potential applications of the synthesized hydrogels. Parameters such as the absorbed dose and presence of a crosslinking agent influence the degree of crosslinking, gel fraction, porosity, biocompatibility, and other functional characteristics of the resulting materials [2]. This study investigates the effects of the total absorbed gamma-radiation dose and N, N'-methylenebisacrylamide (MBAA), used as a crosslinking agent, on the design and physicochemical properties of the synthesized PNiPAM hydrogel. The hydrogels were characterized by gel fraction and dynamic swelling behavior at different temperatures to determine equilibrium swelling time (Qe). Swelling measurements over a broad temperature range were conducted to evaluate thermoresponsiveness and determine the volume phase transition temperature (VPTT). Biocompatibility was also evaluated to assess their potential applications. The results show that irradiation dose slightly increased the gel fraction of PNiPAM hydrogels, while decreasing Qe without affecting VPTT (~30 °C). The samples exhibited similar swelling kinetics, reaching equilibrium within 4–5 days below the VPTT, whereas equilibrium was attained within a few hours above the VPTT. All hydrogels showed favorable biocompatibility, confirming that synthesis conditions affect their properties and potential applications.

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**SCFM PP 3****Batch removal of Cr(VI) using chitosan/cellulose fiber composite beads: effect of adsorbent dose, pH and citric acid functionalization**

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Hexavalent chromium, Cr(VI), is a highly toxic and carcinogenic pollutant frequently found in wastewaters from electroplating, tanning and metal-finishing industries, posing risks to human health and aquatic ecosystems. Adsorption onto low-cost, biodegradable biopolymer-based materials is a promising and sustainable removal approach. Chitosan, rich in amino and hydroxyl groups, is an attractive biosorbent whose combination with cellulose fibers can further improve mechanical stability and sorption performance. Building on previously characterized chitosan hydrogel beads and their cellulose fiber composite [1], this study evaluates CHB-CF-GLA (chitosan/cellulose fiber composite crosslinked with 0.05% glutaraldehyde) and its citric acid-functionalized counterpart (CHB-CF-GLA-CA) as Cr(VI) adsorbents, via batch sorption tests: effect of adsorbent dose, pH, initial concentration and contact time. Increasing the adsorbent dose (75 mg/L Cr(VI), pH ≈ 3) reduced the equilibrium capacity,  $q_e$  (from ≈ 90 to ≈ 15 mg/g), for both composites, while removal efficiency,  $E$ , stayed consistently high for CHB-CF-GLA and kept increasing for CHB-CF-GLA-CA, reaching ≈ 89%. pH also strongly affected adsorption: both composites performed best near the solution's natural pH (≈ 2.8–2.9), where CHB-CF-GLA achieved the higher capacity but collapsed above pH ≈ 3.5, whereas CHB-CF-GLA-CA declined more gradually and still removed Cr(VI) even at pH 5.6 — indicating improved pH-stability upon citric acid functionalization. Equilibrium data (Cr(VI) 10–250 mg/L) showed the expected concentration-dependent increase in  $q_e$  for both composites, reaching ≈ 85 mg/g. Kinetics, investigated for the more pH-stable CHB-CF-GLA-CA, showed fast initial uptake ( $E \approx 47\%$  at 60 min) followed by a slower approach to equilibrium, reaching ≈ 61% after 24 h. These results confirm chitosan/cellulose fiber composites, particularly the citric acid-functionalized form, as effective, low-cost and pH-stable Cr(VI) adsorbents, promising for future use in continuous fixed-bed treatment systems.

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**SCFM PP 4****Assessing the adsorption performance of chitosan-based hydrogels for heavy metals removal: from batch experiments to continuous fixed-bed column**

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Heavy metals are among the most hazardous water pollutants due to their toxicity and non-biodegradability. Consequently, considerable efforts have been devoted to developing efficient materials for heavy metal removal. Chitosan is a promising adsorbent for heavy metal cations due to its abundant amino and hydroxyl groups, while cellulose can improve the mechanical stability of chitosan-based materials. In this study, glutaraldehyde-crosslinked chitosan hydrogel beads functionalized with citric acid (CHB-GLA-CA) and chitosan-cellulose fiber composite beads (CHB-CF-GLA) were investigated for heavy metal removal, with their successful modification confirmed by physicochemical characterization reported previously [1,2]. The adsorption of Cu(II), Pb(II), Zn(II), and Cd(II) ions onto CHB-GLA-CA and CHB-CF-GLA hydrogels was investigated through pH, kinetic, and equilibrium studies. For both adsorbents, the highest removal efficiency was achieved at pH<sub>i</sub> = 5.5, following the order Cu(II) > Pb(II) > Zn(II) > Cd(II). Kinetic data obtained at initial concentrations of 25 and 100 mg dm<sup>-3</sup> were best described by the pseudo-second-order model, while equilibrium data showed better agreement with the Langmuir than the Freundlich isotherm model. Following batch experiments, both hydrogels were evaluated in continuous fixed-bed columns using Cu(II) as a representative metal ion. Although CHB-GLA-CA exhibited higher adsorption capacity, its application in continuous operation was limited by bed clogging and excessive bed expansion, preventing breakthrough curve establishment. In contrast, CHB-CF-GLA demonstrated stable column performance and well-defined breakthrough behavior, indicating that cellulose incorporation significantly enhanced the mechanical stability and suitability of the hydrogel for continuous adsorption processes.

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## SCFM PP 5

**Immobilization of surfactant-modified phillipsite in chitosan hydrogel beads: does it improve Congo red removal?**

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Congo red (CR) is a stable anionic diazo dye widely used in the textile and paper industries, associated with allergic reactions and carcinogenic effects, and difficult to remove from wastewater by conventional treatments [1]. Surfactant-modified zeolites show high affinity toward anionic dyes, but their powdered form limits practical use. In this work cetylpyridinium-modified phillipsite (P2), previously synthesized and characterized [2], was immobilized in chitosan hydrogel beads to facilitate easier recovery and reuse. Four bead formulations were compared: plain chitosan hydrogel (Ch), glutaraldehyde-crosslinked chitosan hydrogel (Ch-GLA), chitosan hydrogel-P2 composite (Ch-P2, with ratio Ch:P2 = 4:1), and its glutaraldehyde-crosslinked counterpart (Ch-P2-GLA), to assess whether P2 incorporation and/or crosslinking improve CR removal relative to free P2 powder. Batch adsorption used 10 mL of 25 mg L<sup>-1</sup> CR, with doses of 5 and 25 mg at 60 min, and kinetics up to 240 min at a fixed dose of 5 mg. Free P2 removed nearly all CR at the highest dose (~100%), while all bead formulations removed only 31-50%, regardless of composition. Plain Ch performed comparably to, or better than, the P2-loaded composites (Ch-P2, Ch-P2-GLA), showing that embedding P2 does not improve dye uptake, likely due to restricted surface accessibility. Crosslinking consistently lowered CR uptake throughout the kinetic run in both P2-free (Ch vs. Ch-GLA) and P2-loaded (Ch-P2 vs. Ch-P2-GLA) beads, consistent with consumption of free amino groups that act as CR adsorption sites. Thus, despite the practical advantage of beads over powders in terms of handling, they do not enhance - and in fact reduce - the CR removal performance of modified phillipsite, highlighting the need for further formulation optimization.

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**SCFM PP 6****Radiation-induced synthesis and characterization of temperature-responsive P(NIPAM/HEA) copolymeric hydrogels**

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Temperature-sensitive hydrogels are polymeric materials that change physicochemical properties with temperature, making them promising for biomedical and drug delivery applications. Hydrogels based on N-isopropylacrylamide (NIPAM) are widely studied due to a sharp phase transition near 32 °C, leading to pronounced temperature-dependent changes in swelling that can be exploited in biomedical applications [1]. However, the copolymerization of 2-hydroxyethyl acrylate (HEA) with NIPAM hydrogels by radiation-induced synthesis remains scarcely investigated.

In this study, we synthesized P(NIPAM/HEA) hydrogels with a 50/50 molar ratio of NIPAM and HEA by radiation-induced crosslinking and polymerization at absorbed doses of 5, 10, 15, and 25 kGy. We evaluated their gel fraction, equilibrium swelling, and volume phase transition temperature (VPTT) over a wide temperature range at pH 7.4. Dynamic swelling behavior was further investigated at temperatures below, near, and above the VPTT (5, 25, and 35 °C), and biocompatibility was assessed.

Whereas NIPAM has been reported in the literature to have a VPTT of approximately 32 °C, the synthesized P(NIPAM/HEA) hydrogels exhibited a VPTT of approximately 25 °C regardless of the applied radiation doses. The obtained results indicate that the copolymerization of NIPAM with HEA influences the thermosensitive behavior.

The results provide insight into how irradiation dose influences the swelling behavior, temperature responsiveness, and biocompatibility of P(NIPAM/HEMA) hydrogels, supporting their further modification and development for potential biomedical applications.

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## SCFM PP 7

**Titanium-based implant materials surface response to laser treatment under different atmospheres**

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The interaction between biomaterials and surrounding tissues is strongly influenced by the implant's surface characteristics, making surface modification an important approach to improved biointegration [1]. In this study, commercially pure titanium (CP-Ti), coarse-grained (CG) Ti-45Nb alloy and nano-grained (NG) Ti-45Nb alloy were subjected to surface treatment with ultrashort laser pulses under different processing atmospheres. The results showed that laser-induced alterations at the macro- and micro-scales occur primarily in the material's surface and subsurface regions. The absorption of laser energy by the material's surface layer led to the development of surface craters, accompanied by the appearance of hydrodynamic phenomena manifested through the formation of valleys, droplets, and wave-like features. However, differences in crater morphology and dimensions were observed between CP-Ti, CG, and NG Ti-45Nb samples and between air and argon irradiation conditions. These surface modifications were most pronounced in the argon-irradiated NG Ti-45Nb alloy sample. Moreover, the presence of titanium oxide on all irradiated surfaces was observed, with more pronounced oxide formation during irradiation in air. Furthermore, surface analysis confirmed variations in the degree of surface damage along the crater depth, with more pronounced surface and subsurface alterations detected after irradiation in an argon atmosphere, particularly in the NG Ti-45Nb sample. The results demonstrate that the selection of implant material and processing atmosphere significantly affect laser-induced surface modifications, which may influence the surface properties, biocompatibility, and osseointegration potential of titanium-based implant materials.

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## SCFM PP 8

**Gamma irradiation-induced chemical and structural modification of polystyrene-based nanomaterials**

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Gamma irradiation is an effective approach for synthesizing and modifying nanomaterials derived from polymeric precursors. Commercial polystyrene (PS) is one of the most widely used polymers [1]. In this study, we investigated the physical and chemical properties of a material synthesized by gamma irradiation of polystyrene dissolved in chloroform. The resulting colloidal system was irradiated at doses ranging from 300 to 600 kGy. Atomic force microscopy (AFM) was used to examine the samples' morphological and topographical characteristics, while X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy were used to analyze structural and chemical changes. AFM analysis revealed pronounced dose-dependent morphological changes. At 300 kGy, a network-like structure associated with crosslinking of the polymer chains was observed, whereas at 600 kGy, nanoparticles with a characteristic ring-like morphology were formed. XPS analysis showed that gamma irradiation affected carbon bonding and revealed chlorine in all irradiated samples. High-resolution Cl 2p spectra indicated the presence of chlorine in both ionic form and as covalently bound C–Cl species. FTIR analysis revealed irradiation-induced changes in the characteristic absorption bands of polystyrene, including spectral features associated with C–Cl and C=O groups. Raman spectroscopy further demonstrated dose-dependent structural changes, particularly in the phenyl-ring vibrations. The increasing I(1582)/I(1602) intensity ratio with irradiation dose indicated a gradual reduction in local structural symmetry. The combined AFM, XPS, FTIR, and Raman analyses indicate that the properties of the resulting material can be tailored by varying the irradiation dose.

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**SCFM PP 9****Targeted elimination of sertraline as a pharmaceutical pollutant by functional poly(methacrylic acid) based hydrogels**

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Pharmaceutical contaminants are increasingly detected in aquatic systems, raising concerns due to their persistence and potential environmental impact and motivating the development of efficient and sustainable removal strategies [1]. In this study, a crosslinked poly(methacrylic acid-co-poly(ethylene glycol) methyl ether methacrylate), P(MAA-co-PEGMEMA), hydrogel was synthesized and evaluated as a sorbent for sertraline, a widely prescribed antidepressant frequently identified in the environment. The hydrogel was prepared via free-radical polymerization of neutralized methacrylic acid and PEGMEMA, with monomer selection guided by Hansen Solubility Parameters (HSP) to optimize compatibility and interactions with the target compound. A crosslinking agent generated a stable three-dimensional polymer network. Ionizable carboxylate groups from MAA enable electrostatic attraction with the protonated amine group of sertraline, while PEGMEMA segments provide chain flexibility and promote interactions with its hydrophobic and aromatic groups. Swelling studies confirmed substantial water uptake and accessibility of functional groups within the network. Sorption experiments demonstrated high removal efficiency, achieving 96.8% elimination of sertraline from an aqueous solution with an initial concentration of 50 ppm under the tested conditions. These results highlight the importance of rational functional group design and solubility parameter-based monomer selection in enhancing adsorption performance. Overall, crosslinked P(MAA-co-PEGMEMA) hydrogels represent promising functional polymeric materials for water remediation, with tunable chemistry and high sorption efficiency within the broader framework of supramolecular chemistry and advanced environmental materials.

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## SCFM PP 10

**CQDs derived from natural precursor as novel pro-oxidant agents in polyurethane composite**

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The increase of bacterial infections is one of the important problem worldwide. In addition to direct transmission, bacterial infections can be transmitted through contaminated inanimate surfaces. Therefore, new strategy to prevent the spread of infections is using antibacterial coatings [1]. In this study we demonstrated the preparation of polyurethane coatings with prooxidant activity through the encapsulation of carbon quantum dots (CQDs). Commercial polyurethane film was used as matrix during swelling-encapsulation-drying process [2]. Prepared extract of the commercial aerial parts of St. John's wort (*Hypericum perforatum*) was used as precursor in synthesis of prooxidant CQDs. The synthesis was performed in laboratory beaker at 200 °C in the presence of H<sub>3</sub>PO<sub>4</sub> and H<sub>2</sub>SO<sub>4</sub>. Size distribution of CQDs and their distribution within the polyurethane matrix were investigated using atomic force microscopy (AFM). The chemical composition of the obtained materials was characterized by Fourier-transform infrared spectroscopy (FTIR). The pro-oxidant activity of the composite was evaluated by photoluminescence spectroscopy using Singlet Oxygen Sensor Green (SOSG) as a specialized fluorescent probe.

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## SCFM PP 11

**Structural and optical characterization of  $\text{MgGd}_2\text{Zr}_2\text{O}_8$  nanoparticles doped with  $\text{Eu}^{3+}$  and  $\text{Yb}^{3+}/\text{Tm}^{3+}$** 

Andrijana Pantelić<sup>1</sup>, Vesna Lojpur<sup>1</sup>, Ljiljana Veselinović<sup>2</sup>, Lidija Mančić<sup>2</sup>, Tijana Stamenković<sup>2</sup>

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This study introduces an innovative host material,  $\text{MgGd}_2\text{Zr}_2\text{O}_8$ , examined for its up- and down-conversion characteristics. Nanoparticles doped with 15 at%  $\text{Eu}^{3+}$  ions for down-conversion, and with 0.5 at%  $\text{Tm}^{3+}$  and 4 at%  $\text{Yb}^{3+}$  for up-conversion, were synthesised via the sol-gel method using urea as a chelating agent. The resulting powders were subjected to structural, morphological and optical characterization. X-Ray Powder Diffraction (XRPD) analysis confirmed the crystalline nature of both samples, indexed to  $Fm\bar{3}m$  space group, with crystallite of a few nm. Transmission Electron Microscope (TEM) revealed agglomerated clusters approximately 200 nm in size, formed by accumulation of smaller particles. High-Resolution TEM (HR-TEM) further showed that these clusters consist of crystallites with an average size of 7 nm, while Energy Dispersive Spectroscopy (EDS) confirmed a homogeneous elemental distribution. The optical properties, examined by UV-Vis spectroscopy, revealed  $f-f$  transitions characteristic for lanthanide ions in both up- and down-conversion samples. Room temperature Photoluminescence (PL) measurements under 313 nm excitation showed emission lines corresponding to the  $^5\text{D}_0 \rightarrow ^7\text{F}_J$  transitions of the  $\text{Eu}^{3+}$  ions ( $J = 0, 1, 2, 3, 4$ ), while excitation at 978 nm produced emission bands characteristic for  $\text{Tm}^{3+}$  ions.

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## SCFM PP 12

## From microwaves to $\gamma$ -rays: *ms*-BiVO<sub>4</sub> for methylene blue removal

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Combining rapid microwave synthesis with post-synthetic  $\gamma$ -irradiation offers a way to modify the functional properties of monoclinic BiVO<sub>4</sub> (*ms*-BiVO<sub>4</sub>) nanoparticles while preserving their crystalline framework. The *ms*-BiVO<sub>4</sub> was synthesized by microwave treatment at 170 °C for 10 min, with an approximate yield of 98%, and was subsequently exposed to an absorbed dose of  $20 \pm 1$  kGy using a <sup>60</sup>Co  $\gamma$ -ray source (Figure 1). X-ray diffraction analysis confirmed that the monoclinic scheelite structure was retained after irradiation, while the crystallite size decreased only slightly, from approximately 24 to 22 nm. Methylene blue (MB) removal was investigated using 40 mg of photocatalyst suspended in 50 mL of a 5 mg L<sup>-1</sup> MB solution under a 300 W Osram Vitalux lamp. After dark equilibration, the removal achieved during the subsequent 120 min of illumination, calculated relative to the initial MB concentration, was 27.66% for pristine *ms*-BiVO<sub>4</sub> and 40.50% for *ms*-BiVO<sub>4</sub> irradiated at 20 kGy. However,  $\gamma$ -irradiation markedly reduced dark adsorption from 67.97% to 6.00%, resulting in total MB removal of 95.63% and 46.50% for pristine and irradiated *ms*-BiVO<sub>4</sub>, respectively. Thus, the 20 kGy treatment increased the contribution of the light-driven stage but reduced overall MB removal by altering the balance between dark adsorption and light-driven removal, while preserving the monoclinic structure [1].

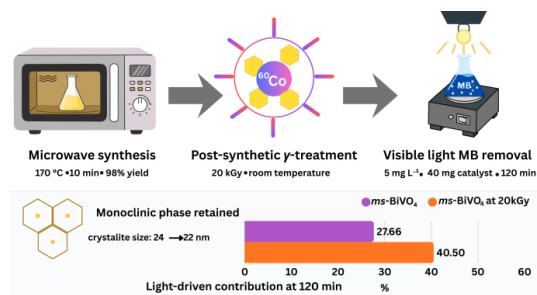


Figure 1. Microwave synthesis,  $\gamma$ -irradiation, and MB removal over *ms*-BiVO<sub>4</sub>

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## SCFM PP 13

**Influence of fluoride-containing additives on the structural, morphological, and stability properties of FAPbI<sub>3</sub> perovskite thin films**

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Metal halide perovskites are promising materials for next-generation photovoltaics due to their excellent optoelectronic properties and high device efficiencies. However, their practical application is limited by environmental instability and the toxicity of lead-containing compositions[1] . Here, we investigate the effect of fluoride-containing additives on the structural, morphological, optical, and stability properties of formamidinium lead iodide (FAPbI<sub>3</sub>) perovskite thin films. Fluoride is of particular interest due to its high electronegativity and strong interaction with metal cations, which may modify the local chemical environment, crystallization, and defect formation[2] . PbF<sub>2</sub> and NH<sub>4</sub>F were incorporated into the FAPbI<sub>3</sub> precursor at different concentrations, including combined PbF<sub>2</sub>/NH<sub>4</sub>F compositions. The resulting films were characterized using UV–Vis spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM). Fluoride-containing additives produced distinct changes in crystal structure, morphology, surface roughness, and atmospheric stability, depending on their type and concentration. Selected samples also showed indications of an intermediate phase during crystallization, which was further investigated through annealing-time experiments. Overall, the results demonstrate that fluoride-containing additives can significantly influence the crystallization, morphology, and stability of FAPbI<sub>3</sub> thin films. The differences between PbF<sub>2</sub>, NH<sub>4</sub>F, and their combined compositions highlight the role of fluoride chemistry in possibly controlling perovskite formation and may suggest a promising approach for tuning defect-related properties, such as morphology and environmental stability.

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## SCFM PP 14

**Sustainably obtained carbon-modified ZnO: an efficient photocatalyst for psychiatric drug removal**

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Pharmaceuticals have emerged as significant wastewater pollutants due to their adverse effects on aquatic organisms and human health even at trace concentrations [1]. Psychiatric drugs are among the most frequently prescribed pharmaceuticals, and their occurrence in aquatic environments has become an emerging environmental concern. Heterogeneous photocatalysis is a promising approach for pharmaceutical removal, but its efficiency depends mainly on the properties of the applied catalyst. Therefore, this study, aligned with circular economy, aimed to synthesize highly efficient carbon-modified ZnO photocatalysts via sustainable routes and evaluate their efficiency on psychiatric drug removal from water. Samples C/ZnO-350 and C/ZnO-500 were synthesized using onion peel waste (*Allium Cepa*) extract and zinc acetate by the precipitation method, followed by calcination at 350 and 500 °C, respectively. Sample C/talc/ZnO-350 was obtained from expired supplement (Zn Max Medica) through grinding, rinsing, and calcination at 350 °C. Samples were characterized by XRD, FTIR, and FESEM, while their photocatalytic activity was tested on the photodegradation of diazepam under simulated solar light. XRD results showed that hexagonal wurtzite ZnO (PDF#99-0111, space group  $P6_3mc$ ) was present in all the samples. In addition to wurtzite, C/talc/ZnO-350 contained monoclinic talc  $Mg_3Si_4O_{10}$  (PDF#13-0558, space group  $C2/c$ ). FTIR analysis revealed COO<sup>-</sup> and C=C stretching bands in C/ZnO-350 and C/ZnO-500, originating from residual onion peel extract derived species, while C/talc/ZnO-350 exhibited Mg–OH and Si–O vibrations of preserved talc, alongside C=O stretching band of residual pharmaceutical excipients. FESEM analysis revealed that the average particle size amounted to 43, 57, and 205 nm for C/ZnO-350, C/ZnO-500, and C/talc/ZnO-350, respectively. C/ZnO-500 was the most efficient photocatalyst: it removed 92 % of the drug after 240 min. Samples C/ZnO-350 and C/talc/ZnO-350 also exhibited pronounced photocatalytic efficiency, since 89 and 83 % of diazepam was degraded after 240 min, respectively. The enhanced photocatalytic efficiency of C/ZnO-500 may be associated with its relatively cleaner surface and lower organic content resulting from higher calcination temperature.

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## SCFM PP 15

## One-step synthesized silica nanoparticles functionalized with mushroom extract exhibited extraordinary antimicrobial activity

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The increasing prevalence of antimicrobial resistance (AMR) necessitates the development of novel strategies that combine high efficacy with reduced therapeutic doses. Natural products, such as medicinal mushroom extracts, exhibit promising biological activity; however, their practical application is often limited by high effective concentrations and solubility. In this study, nonporous silica nanoparticles (SiO<sub>2</sub> NPs) were synthesized in the presence of a hot-water extract of *Fomes fomentarius*, enabling the incorporation of bioactive components within the nanoparticle matrix and yielding a silica-based nano-system with enhanced antimicrobial performance. The SiO<sub>2</sub> NPs were synthesized via a modified sol–gel (Stöber) method, with the extract added prior to TEOS addition, enabling its incorporation within the silica matrix. The nanoparticles were characterized using UV–Vis, FTIR, DLS, and TEM. Antimicrobial activity was evaluated using the minimum inhibitory concentration (MIC) assay against a panel of Gram-positive and Gram-negative bacterial strains. The obtained results demonstrate a remarkable enhancement in antimicrobial efficiency, with MIC values reduced by up to 1500 times compared to the pure mushroom extract.



Figure 1. Schematic illustration of SiO<sub>2</sub> NP<sub>s</sub> nanoparticle synthesis and characterization

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**SCFM PP 16****Removal of emerging contaminants from water using ultrafiltration and nanofiltration in a hybrid membrane system**

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The presence of pharmaceutical residues and contaminants of emerging concern (CECs) in water bodies poses a growing environmental challenge. The objective of this study was to evaluate the removal efficiency of eight persistent micropollutants (Sotalol, Carbamazepine, Clarithromycin, Erythromycin, HCTZ, Ofloxacin, Acetamiprid, and Atenolol) from water using membrane technologies on a pilot-scale system. Three operational system configurations were evaluated: ultrafiltration (UF), nanofiltration (NF), and a combined hybrid process (UF+NF). Concentration changes were monitored, and rejection factors were calculated based on mass balance evaluations. Ultrafiltration alone demonstrated limited efficiency (17–50%), with removal relying predominantly on adsorption onto the membrane surface and within the pores rather than physical size exclusion. Nanofiltration proved to be significantly more efficient, achieving over 93% rejection for macrolide antibiotics due to size exclusion mechanisms and electrostatic repulsion (Donnan effect). The combined hybrid system (UF+NF) exhibited a synergistic effect and achieved the highest overall performance, with total rejection rates for most compounds ranging between 70% and 97.44% (the highest efficiencies recorded were 97.44% for clarithromycin and 90.75% for ofloxacin). Multistage hybrid filtration (UF+NF) represents a highly effective and robust technological solution for removing complex organic micropollutants and pharmaceutical residues from water.

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