Srpsko hemijsko društvo

Serbian Chemical Society

61. Savetovanje Srpskog hemijskog društva

KRATKI IZVODI RADOVA

61st Meeting of the Serbian Chemical Society

Book of Abstracts

Kragujevac 4. i 5. jun 2026. godine
Kragujevac, Serbia, June 4-5, 2026

CIP - Каталогизација у публикацији
Народна библиотека Србије, Београд

54(048)
577.1(048)
66(048)
66.017/.018(048)
502/504(048)

СРПСКО хемијско друштво. Саветовање (61 ; 2026 ; Крагујевац)
Kratki izvodi radova / 61. Savetovanje Srpskog hemijskog društva, Kragujevac 4. i 5. jun 2026. godine = Book of Abstracts / 61st Meeting of the Serbian Chemical Society, Kragujevac, Serbia, June 4-5, 2026 ; [glavni i odgovorni urednik, editor Biljana Glišić]. - Beograd : Srpsko hemijsko društvo = Serbian Chemical Society, 2026 (Kragujevac : Interprint). - 136 str. : ilustr. ; 25 cm

Apstrakti uporedo na srp. i engl. jeziku. - Tiraž 25. - Registar.

ISBN 978-86-7132-091-7

a) Хемија -- Апстракти b) Биохемија -- Апстракти v) Технологија -- Апстракти g) Наука о материјалима -- Апстракти d) Животна средина -- Апстракти

COBISS.SR-ID 194894089

61. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA
Kragujevac, 4. i 5. jun 2026.
KRATKI IZVODI RADOVA
61st MEETING OF THE SERBIAN CHEMICAL SOCIETY
Kragujevac, Serbia, 4-5 June 2026
BOOK OF ABSTRACTS

Izdaje/Published by
Srpsko hemijsko društvo/Serbian Chemical Society
Karnegijeva 4/III, 11000 Beograd, Srbija
tel./fax: +381 11 3370 467; www.shd.org.rs, E-mail: office@shd.org.rs
Za izdavača/For Publisher
Melina Kalagasidis Krušić, predsednik Srpskog hemijskog društva

Glavni i odgovorni urednik / Editor
Biljana Glišić, Prirodno-matematički fakultet, Univerzitet u Kragujevcu
Uređivački odbor / Editorial Board
Melina Kalagasidis Krušić, Biljana Glišić

Priprema za štampu i štampa/Prepress and printing
Interprint, Kragujevac
Tiraž/ Circulation
25 primeraka / 25 copies printing
ISBN 978-86-7132-091-7

Naučni odbor

Scientific Committee

Akademik Miloš Đuran, redovni profesor u penziji, Prirodno-matematički fakultet, Univerzitet u Kragujevcu, predsednik

Akademik Ivan Gutman, profesor emeritus, Univerzitet u Kragujevcu

dr Biljana Petrović, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Akademik Tanja Ćirković Veličković, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Igor Pašti, dopisni član SANU, redovni profesor, Fakultet za fizičku hemiju, Univerzitet u Beogradu

dr Melina Kalagasidis Krušić, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Aleksandra Dapčević, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Dragica Trivić, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Tatjana Anđelković, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Nišu

dr Zorka Stanić, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Igor Opsenica, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Maja Radetić, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Rada Petrović, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Milan Mladenović, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Jelena Mutić, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Nenad Janković, naučni savetnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

dr Marko Rodić, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Novom Sadu

dr Slavko Radenković, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Vladimir Petrović, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Jelena Đurđević Nikolić, docent, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Uroš Gašić, naučni savetnik, Institut za biološka istraživanja „Siniša Stanković”, Univerzitet u Beogradu

Organizacioni odbor

Organising Committee

dr Biljana Glišić, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu, predsednik

dr Jovana Bogojeski, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Milan Stanković, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Violeta Marković, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Dragana Stevanović, docent, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Tina Andrejević, naučni saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Nikola Srećković, naučni saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Žiko Milanović, naučni saradnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

dr Milena Petrović, naučni saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Nevena Stevanović, naučni saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Milica Međedović Stefanović, naučni saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Jelena Stepanović, asistent sa doktoratom, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Slađana Đorđević, asistent, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Jovica Branković, asistent, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Đorđe Petrović, asistent, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Jovana Dragojević, istraživač saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Katarina Postolović, istraživač saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Bojana Pantović, istraživač saradnik, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Emilija Milović, istraživač saradnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

Tamara Todorović, istraživač saradnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

Kristina Milisavljević, istraživač pripravnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

Recenzenti

Reviewers

dr Biljana Petrović, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Akademik Tanja Ćirković Veličković, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Igor Pašti, dopisni član SANU, redovni profesor, Fakultet za fizičku hemiju, Univerzitet u Beogradu

dr Melina Kalagasidis Krušić, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Aleksandra Dapčević, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Tatjana Anđelković, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Nišu

dr Zorka Stanić, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Igor Opsenica, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Rada Petrović, redovni profesor, Tehnološko-metalurški fakultet, Univerzitet u Beogradu

dr Milan Mladenović, redovni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Jelena Mutić, redovni profesor, Hemijski fakultet, Univerzitet u Beogradu

dr Nenad Janković, naučni savetnik, Institut za informacione tehnologije Kragujevac, Univerzitet u Kragujevcu

dr Marko Rodić, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Novom Sadu

dr Slavko Radenković, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

dr Vladimir Petrović, vanredni profesor, Prirodno-matematički fakultet, Univerzitet u Kragujevcu

Sponzori / *Sponsors*

Organizacioni odbor je zahvalan na donacijama:

Kefo d.o.o.

PRIMALAB d.o.o.

Projekat Vivendi

Savetovanje je podržalo / *Supported by*

Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije
Ministry of Science, Technological Development and Innovation of Republic of Serbia

Република Србија
МИНИСТАРСТВО НАУКЕ, ТЕХНОЛОШКОГ РАЗВОЈА И ИНОВАЦИЈА

Zahvalnost / Acknowledgement

Zahvaljujemo se Univerzitetu u Kragujevcu, Prirodno-matematičkom fakultetu na ustupanju prostorija fakulteta tokom 61. Savetovanja Srpskog hemijskog društva i tehničkoj podršci prilikom organizacije Savetovanja.

Ova knjiga sadrži kratke izvode
tri plenarna predavanja (PP),
tri predavanja po pozivu (PPP),
jedno predavanja dobitnika medalje SHD (MP),
dva predavanja u znak sećanja na nedavno
preminule zaslužne članove SHD (IM),
šesnaest usmenih izlaganja (O) i
pedeset osam posterskih saopštenja (P)
prihvaćenih za prezentovanje na
61. Savetovanju Srpskog hemijskog društva.

This book contains abstracts of
three plenary lectures (PP),
three invited lectures (PPP),
lecture of SCS medal awardee (MP),
two lectures in memory of recently deceased
distinguished members of the SCS (IM),
sixteen oral presentations (O), and
fifty eight poster presentations (P)
accepted for presentation at
the 61st Meeting of the Serbian Chemical Society.

SADRŽAJ / CONTENTS

Plenarna predavanja / Plenary lectures

Predavanja po pozivu / Invited lectures

Predavanje dobitnika medalje SHD za izvanredne rezultate u nauci / Lecture by the winner of the SCS medal for outstanding achievements in science

Predavanja u znak sećanja na nedavno preminule zaslužne članove SHD / Lectures in memory of recently deceased distinguished members of the SCS

Usmena saopštenja / Oral presentations

Saopštenja / Contributions

Biohemija / Biochemistry

Elektrohemija / Electrochemistry

Fizička hemija / Physical Chemistry

Hemija i tehnologija hrane / Chemistry and Technology of Food

Hemija i tehnologija materijala / Chemistry and Technology of Materials

Hemija životne sredine / Environmental Chemistry

Medicinska hemija / Medicinal Chemistry

Neorganska hemija / Inorganic Chemistry

Organska hemija / Organic Chemistry

Teorijska hemija / Theoretical Chemistry

Zelena hemija / Green Chemistry

P-ZH-1	Jelena Jovanović	Membranski potpomognuta ekstrakcija i stabilizacija parthenolida iz *Tanacetum parthenium* primenom PPG400	120

KRATKI IZVODI RADOVA

Short abstracts

Plenarna predavanja

Plenary Lectures

PP-1

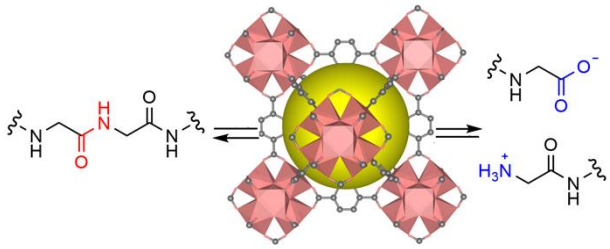
Veštački enzimi zasnovani na metal-okso klasterima: od diskretnih vrsta do metal-organskih mreža

Hong Giang Ly Thi, Siene Swinnen, Charlotte Simms, Francisco de Azambuja, Nada D. Savic, Kilian Declerck, Tatjana N. Parac-Vogt

KU Leuven, Odsek za hemiju,3001 Leuven, Belgija

tatjana.vogt@kuleuven.be

Efikasni katalizatori za kontrolisanu transformaciju velikih i kompleksnih biomolekula predstavljaju veliki izazov za dizajn. Posebno je teško postići selektivnu fragmentaciju proteina putem neenzimske katalize, iako je to od ključnog značaja za mnoge savremene primene u biotehnologiji i proteomici. Poslednjih godina razvili smo konceptualno novu strategiju za selektivno cepanje proteina kombinovanjem molekularnog prepoznavanja polioksometalata (POM-ova), velike grupe rastvorljivih metal-okso klastera, sa hidrolitičkom aktivnošću jakih Luisovih kiselih metalnih katjona (Zr, Hf) ugrađenih u POM strukturu. Koristeći ovaj pristup, demonstrirano je selektivno cepanje različitih proteina koji se razlikuju po veličini, strukturi i naelektrisanju. Nadovezujući se na ova istraživanja, pokazali smo da metal-organske mreže (MOF-ovi) zasnovane na $\{Zr_6O_8\}$ klasterima funkcionišu kao efikasni heterogeni katalizatori za hidrolizu peptidne veze. Ovi MOF-ovi pokazuju izuzetnu katalitičku aktivnost u širokom pH opsegu, uz značajno ubrzanje reakcije u poređenju sa nekatalizovanim reakcijama. Pored toga, UiO-66 Zr-MOF se pokazao sposobnim da katalizuje kako intra-, tako i intermolekularno formiranje peptidnih veza, pri čemu ne dolazi do epimerizacije. Potencijal metal-okso klastera kao nanoenzima za hidrolizu proteina dodatno je potvrđen i kod drugih diskretnih metal-okso klastera, koji su pokazali izuzetnu selektivnost pri cepanju različitih proteina. Zajedno, ovi rezultati ukazuju na to da materijali zasnovani na metal-okso klasterima predstavljaju veoma perspektivnu novu klasu dualno funkcionalnih nanoenzima, sposobnih da katalizuju i cepanje i formiranje peptidnih veza.



Shema 1. MOF-ovi za formiranje i cepanje peptidnih veza

1. K. Declerck, N. D. Savić, M. A. Moussawi, C. Seno, R. Pokratath, J. De Roo, T. N. Parac-Vogt, *J. Am. Chem. Soc*. **2024**, *146*, 11400.
2. S. Xie, S. S. Passadis, M. Gray, N. A. G. Bandeira, H. N. Miras, T. N. Parac-Vogt; *Angew. Chem. Int. Ed*. **2025**, e202515408.

PP-1

Artificial enzymes based on metal oxo-clusters: from discrete species to metal–organic frameworks

Hong Giang Ly Thi, Siene Swinnen, Charlotte Simms, Francisco de Azambuja, Nada D. Savic, Kilian Declerck, Tatjana N. Parac-Vogt

KU Leuven, Department of Chemistry,3001 Leuven, Belgium

tatjana.vogt@kuleuven.be

Effective catalysts for the controlled transformation of large, complex biomolecules remain rare and challenging to design. In particular, achieving selective protein fragmentation through non-enzymatic catalysis is difficult, yet critically important for many modern applications in biotechnology and proteomics. In recent years, we have developed a conceptually new strategy for selective protein cleavage by combining the enzyme-like molecular recognition ability of polyoxometalates (POMs), a large family of soluble metal-oxo clusters, with the hydrolytic activity of strong Lewis acid metal cations (Zr, Hf) embedded within the POM framework. Using this approach, selective cleavage has been demonstrated across a range of proteins differing in size, structure, and charge. Building on this, we have shown that metal–organic frameworks (MOFs) based on $\{Zr_6O_8\}$ clusters function as highly effective heterogeneous catalysts for peptide bond hydrolysis in various substrates. These MOFs exhibit excellent catalytic activity across a broad pH range, with significant rate accelerations compared to uncatalyzed reactions. Moreover, UiO-66 Zr-MOF has proven capable of catalyzing both intra- and intermolecular peptide bond formation, notably without inducing epimerization. The potential of metal-oxo clusters as nanozymes for protein hydrolysis has been further illustrated by other discrete metal-oxo clusters, which showed remarkable selectivity in the cleavage of different proteins. Together, these findings highlight that metal-oxo cluster-based materials hold strong promise as a new class of dual-function nanozymes, capable of catalyzing both peptide bond cleavage and formation.

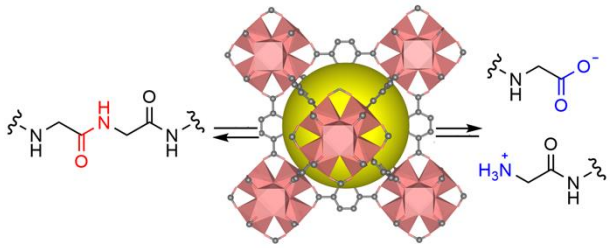


Figure 1. MOFs for peptide bond making and breaking

1. K. Declerck, N. D. Savić, M. A. Moussawi, C. Seno, R. Pokratath, J. De Roo, T. N. Parac-Vogt, *J. Am. Chem. Soc*. **2024**, *146*, 11400.
2. S. Xie, S. S. Passadis, M. Gray, N. A. G. Bandeira, H. N. Miras, T. N. Parac-Vogt; *Angew. Chem. Int. Ed*. **2025**, e202515408.

PP-2

Inovacije u istraživanjima mikro- i nanoplastike i njihovih efekata na zdravlje ljudi

Tanja Ćirković Veličković

[1] *Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
[2] *Srpska akademija nauka i umetnosti, Beograd, Srbija*
tcirkov@chem.bg.ac.rs

Mikro- i nanoplastika (MNP) predstavljaju značajan izazov za životnu sredinu i javno zdravlje zbog svoje široke rasprostranjenosti u vazduhu, vodi, hrani i ljudskim tkivima, uključujući krv, pluća i placentu. Nedavni napredak u analitičkoj hemiji, toksikologiji, biomonitoringu i računarskim pristupima značajno je unapredio razumevanje puteva izloženosti ljudi i potencijalnih bioloških efekata MNP-a. Međutim, i dalje postoje značajni naučni i metodološki izazovi, posebno u vezi sa karakterizacijom čestica relevantnih za životnu sredinu, dugotrajnom izloženošću niskim dozama i pouzdanom procenom rizika po zdravlje ljudi.

Ovo predavanje predstaviće inovacije u istraživanjima MNP-a razvijene u okviru nedavnih međunarodnih aktivnosti [1]. Posebna pažnja biće posvećena harmonizovanim analitičkim metodama [2], razvoju reprezentativnih referentnih materijala, naprednim in vitro i in vivo modelima, strategijama biomonitoringa, kao i novim bioinformatičkim pristupima i okvirima za procenu rizika. Biće razmatrano i kako fizičko-hemijske osobine MNP-a — uključujući veličinu, oblik, polimerni sastav, starenje i prisustvo pridruženih hemijskih kontaminenata — utiču na biološke odgovore.

Poseban akcenat biće stavljen na interdisciplinarnu saradnju i primenu inovativnih eksperimentalnih, analitičkih i računarskih pristupa neophodnih za podršku regulatornom odlučivanju i zaštitu zdravlja ljudi od rastućeg opterećenja izazvanog zagađenjem plastikom.

PP-2

Innovation in research on micro- and nanoplastics and their effects on human health

Tanja Ćirković Veličković
[1] University of Belgrade, Faculty of Chemistry, Belgrade, Serbia
[2] Serbian Academy of Sciences and Arts, Belgrade, Serbia
tcirkov@chem.bg.ac.rs

Micro- and nanoplastics (MNPs) have emerged as a major environmental and public health concern due to their widespread presence in air, water, food, and human tissues, including blood, lungs, and placenta. Recent advances in analytical chemistry, toxicology, biomonitoring, and computational approaches have significantly improved our understanding of human exposure pathways and the potential biological effects of MNPs. However, major scientific and methodological challenges remain, particularly regarding the characterization of environmentally relevant particles, long-term low-dose exposure, and reliable human health risk assessment.
This lecture will present innovations in MNP research developed within the recent international activities [1]. Particular attention will be devoted to harmonized analytical methods [2], development of representative reference materials, advanced *in vitro* and *in vivo* models, biomonitoring strategies, and emerging bioinformatics and risk assessment frameworks. The talk will also discuss how physicochemical properties of MNPs—including size, shape, polymer composition, ageing, and associated chemical contaminants—influence biological responses.
Emphasis will be placed on interdisciplinary collaboration and the application of innovative experimental, analytical, and computational approaches necessary to support regulatory decision-making and protect human health from the growing burden of plastic pollution.

References

1.Muncke, J., Pieters, R., Ćirković Veličković, T., Hernández Bonilla, A., Morrison, M., Reuther, R., & Vermeulen, R. (2025). CUSP Research Roadmap 2026-2032: Informing and advising on the state of the art, gaps, and future needs in micro- and nanoplastic and health research in Europe (1.0). Zenodo. https://doi.org/10.5281/zenodo.17467125.
2. Dmitrii D., et al., *Analytical Chemistry*, 2025, https://doi.org/10.1021/acs.analchem.4c05403

Acknowledgment: The author thanks the European Commission for supporting this work under the grant agreements, No. 965173 (IMPTOX), and Serbian Science Fund for supporting XPACT project under the grant agreement 7275.

PP-3

Balada o somborskom indeksu

Ivan Gutman
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija
gutman@kg.ac.rs

U predavanju će biti izloženi osnovni podaci o jednom novom topološkom indeksu, sa akcentnom na njegove primene u hemiji. Pre toga ćemo se podsetiti na to gde i kako se indeksi sreću u raznim oblastima ljudske aktivnosti, a zatim na njihovu upotrebu u hemiji. Indeks o kojem je reč nazvan je „*somborski"* po Somboru, rodnom gradu predavača. Somborski indeks je otkriven 2020. godine, na osnovu geometrijskih razmatranja (koja će biti ukratko opisana). Vrlo brzo je privukao pažnju neočekivano velikog broja istraživača. Autori iz pedesetak zemalja objavili su do sada više od 650 radova o somborskom indeksu. U završnom delu predavanja biće nabrojane primene somborskog indeksa, najviše u hemiji ali i daleko izvan hemije.

Ballad on Sombor index

Ivan Gutman
University of Kragujevac, Faculty of Science, Kragujevac, Serbia
gutman@kg.ac.rs

In the lecture, the basic facts on a new topological index will be presented, with emphasis on its chemical applications. Before that, we recall on where and how indices are encountered in various fields of human activity, followed by their uses in chemistry. The considered index is named "*Sombor index*", according to the lecturer's birthplace. It was invented in 2020, based on geometric arguments (which will be briefly outlined). Very soon, the Sombor index attracted the attention of surprisingly large number of scholars. Authors from some fifty countries published until now over 650 papers on it. In the concluding part of the lecture, the applications of Sombor index will be listed, most in chemistry, but also in areas far beyond chemistry.

1. I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem*. **86** (2021) 11-16.
2. H. Liu, I. Gutman, L. You, Y. Huang, Sombor index: Review of extremal results and bounds, *J. Math. Chem.* **66** (2022) 771-798.

Predavanja po pozivu

Invited Lectures

PPP-1

Novi elektrokatalizatori za proizvodnju vodonika alkalnom elektrolizom vode

Igor A. Pašti
Univerzitet u Beogradu, Fakultet za fizičku hemiju, Beograd, Srbija
Srpska akademija nauka i umetnosti, Beograd, Srbija
igor@ffh.bg.ac.rs

Razvoj savremenog društva nosi sa sobom stalno rastuću potrebu za energijom, koja, imajući u vidu ograničene rezerve fosilnih goriva, predstavlja jedan od glavnih problema održivog razvoja. Uprkos činjenici da se vodonik već duže vremena ističe kao gorivo budućnosti, njegova masivna proizvodnja je i dalje ograničena i dominantno bazirana na fosilnim gorivima. Stoga, kako bi se ova predviđanja ispunila, neophodno je unaprediti postojeće procese proizvodnje vodonika, prvenstveno takozvanog zelenog vodonika koji se dobija elektrolizom vode uz korišćenje obnovljivih izvora energije. U okviru ovog predavanja biće predstavljene strategije razvoja novih katalizatora za alkalnu elektrolizu vode, počevši od strategija u kompjutacionom dizajnu do površinskih modifikacija u cilju povećanja katalitičke aktivnosti. Konačno, biće diskutovana potreba da se pređe sa dizajna katalizatora na dizajn fazne granice (elektrode) i paralelnu optimizaciju elektrodnog materijala i elektrolita sa ciljem postizanja maksimalne katalitičke aktivnosti za proizovdnju vodonika.

New electrocatalysts for hydrogen production via alkaline water electrolysis

Igor A. Pašti
University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia
Serbian Academy of Sciences and Arts, Belgrade, Serbia
igor@ffh.bg.ac.rs

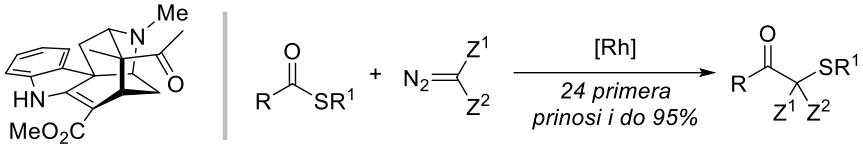
The development of modern society is accompanied by an ever-growing demand for energy, which, given the limited reserves of fossil fuels, represents one of the key challenges of sustainable development. Despite hydrogen's long-standing status as the fuel of the future, large-scale production remains limited and is still predominantly based on fossil resources. Therefore, to meet these expectations, it is necessary to improve existing hydrogen production processes, particularly the production of so-called green hydrogen obtained by water electrolysis using renewable energy sources. In this lecture, strategies for developing new catalysts for alkaline water electrolysis will be presented, ranging from computational design approaches to surface modifications aimed at enhancing catalytic activity. Finally, the need to move from catalyst design toward the design of the phase boundary (electrode) will be discussed, along with the parallel optimization of electrode materials and electrolytes to achieve maximum catalytic activity for hydrogen production.

PPP-2

Indolski alkaloidi - od totalne sinteze do razvoja novih reakcija

Filip J. Bihelović
Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija
filip@chem.bg.ac.rs

Strukturni diverzitet i konstituciona kompleksnost čine indolske alkaloide atraktivnim sintetskim metama. Dodatni motiv za hvatanje ukoštac sa sintezom ovih topološki složenih i često strukturno jedinstvenih molekula predstavlja njihov širok spektar bioloških aktivnosti, koje su neretko bez presedana. Najznačajnije reakcije za efikasne sinteze ovih molekula su one koje dovode do stvaranja više C—C ili C—heteroatom veza u jednom koraku – prevashodno domino-reakcije (tj. tandemne ili sekvencione reakcije). Izlaganje strukturno i funkcionalno složenih molekula standardnim uslovima za izvođenje željene transformacije katkada dovodi do neočekivanih ishoda i otkrića novih, opštih reakcija, koje nisu ciljano dizajnirane za rešavanje zadatog sintetskog poduhvata. Prezentovanjem totalne sinteze alstonlarsina A (Slika 1a) primenom domino-reakcije biće prikazan i razvoj nove reakcije za molekulsko (jednoatomsko) editovanje tioestara (Slika 1b).



Slika 1. a) Struktura alstonlarsina A; b) reakcija tiooestara sa karbenima.

Indole alkaloids - from total synthesis to the development of new reactions

Filip J. Bihelović
University of Belgrade, Faculty of Chemistry, Belgrade, Serbia
filip@chem.bg.ac.rs

The structural diversity and constitutional complexity of indole alkaloids make them attractive synthetic targets. An additional strong motivation for tackling the synthesis of these topologically complex and often structurally unique molecules lies in their broad spectrum of biological activities, which are frequently unprecedented. The most important reactions for the efficient synthesis of these molecules are those that enable the formation of multiple C—C or C—heteroatom bonds in a single step – primarily domino reactions (i.e., tandem or sequential reactions). Subjecting structurally and functionally complex molecules to standard conditions for carrying out a desired transformation occasionally leads to unexpected outcomes and the discovery of new, general reactions that were not intentionally designed to address the given synthetic challenge. Through the presentation of the total synthesis of alstonlarsine A (Figure 1a) using a domino reaction, the development of a new reaction for the molecular (single-atom) editing of thioesters will also be demonstrated (Figure 1b).

PPP-3

Fitohemijski profil i biološki potencijal lekovitih biljaka Srbije bogatih sekoiridoidima i ruzmarinskom kiselinom: od tradicionalne upotrebe do savremenih farmakoloških i nanotehnoloških primena

Vladimir B. Mihailović

Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Kragujevac, Srbija

vladimir.mihailovic@pmf.kg.ac.rs

Lekovite biljke predstavljaju značajan izvor bioaktivnih sekundarnih metabolita, naročito polifenola i terpena, sa izraženim antioksidativnim, antiinflamatornim, hepatoprotektivnim i antimikrobnim svojstvima, kao i potencijalnom primenom u farmaceutskoj, prehrambenoj i kozmetičkoj industriji. Ispitivanjem odabranih lekovitih biljaka Srbije utvrđeno je da vrste *Gentiana asclepiadea*, *Gentiana cruciata* i *Blackstonia perfoliata* sadrže visoke koncentracije sekoiridoidnih glikozida, jedinjenja iz grupe terpena, među kojima dominiraju genciopikrin, svertiamarin i sverozid. Sa druge strane, fitohemijski sastav proučavanih biljnih vrsta iz familije Lamiaceae (*Satureja hortensis*, *Salvia pratensis* i *Salvia verticillata*) odlikovao se raznovrsnim fenolnim profilom sa dominacijom ruzmarinske kiseline i njenih derivata. Biljke sa visokim sadržajem sekoiridoida, pre svega *G. asclepiadea* i *G. cruciata*, izdvojile su se izraženim hepatoprotektivnim efektom u modelu oštećenja jetre izazvanog ugljen-tetrahloridom. Ekstrakti bogati sekoiridoidima nisu pokazali citotoksičnost prema ispitivanim normalnim i tumorskim ćelijskim linijama, dok su metanolski ekstrakti vrsta *G. asclepiadea* i *B. perfoliata* ispoljili visok stepen inhibicije enzima COX-2. Ekstrakti vrsta *S. hortensis*, *S. pratensis* i *S. verticillata* pokazali su značajnu antioksidativnu aktivnost u različitim *in vitro* model-sistemima. U *in vivo* modelu oksidativnog stresa izazvanog cisplatinom, ekstrakt vrste *S. hortensis* značajno je ublažio oštećenja jetre, bubrega i testisa, normalizovao parametre oksidativnog stresa i ispoljio antiapoptotski efekat. Ekstrakti nadzemnih delova Lamiaceae biljaka pokazali su dobru biokompatibilnost sa eukariotskim ćelijama, dok su ekstrakti korena ispoljili citotoksičnu aktivnost prema pojedinim tumorskim ćelijskim linijama. Dodatno, ekstrakti vrste *S. pratensis* uspešno su korišćeni za zelenu sintezu nanočestica srebra sa izraženim biološkim i katalitičkim potencijalom, čime je potvrđena mogućnost povezivanja tradicionalne fitoterapije i savremenih nanotehnoloških pristupa. Dobijeni rezultati ukazuju da ispitivane biljke predstavljaju značajan izvor bioaktivnih jedinjenja sa potencijalom za razvoj novih fitopreparata, funkcionalne hrane i inovativnih nanoformulacija namenjenih prevenciji i tretmanu oboljenja povezanih sa oksidativnim stresom i inflamacijom.

PPP-3

Phytochemical profile and biological potential of Serbian medicinal plants rich in secoiridoids and rosmarinic acid: From traditional use to modern pharmacological and nanotechnological applications

Vladimir B. Mihailović

University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia

vladimir.mihailovic@pmf.kg.ac.rs

Medicinal plants represent an important source of bioactive secondary metabolites, particularly polyphenols and terpenes, characterized by pronounced antioxidant, anti-inflammatory, hepatoprotective, and antimicrobial properties, with potential applications in the pharmaceutical, food, and cosmetic industries. Investigation of selected medicinal plants from Serbia revealed that *Gentiana asclepiadea*, *Gentiana cruciata*, and *Blackstonia perfoliata* contain high concentrations of secoiridoid glycosides, terpenoid compounds predominantly represented by gentiopicrin, swertiamarin, and sweroside. In contrast, the phytochemical composition of the investigated plant species from the Lamiaceae family (*Satureja hortensis*, *Salvia pratensis*, and *Salvia verticillata*) was characterized by a rich phenolic profile dominated by rosmarinic acid and its derivatives. Plants with high secoiridoid content, particularly *G. asclepiadea* and *G. cruciata*, exhibited pronounced hepatoprotective effects in a carbon tetrachloride-induced liver injury model. Secoiridoid-rich extracts showed no cytotoxicity toward the tested normal and tumor cell lines, while the methanolic extracts of *G. asclepiadea* and *B. perfoliata* demonstrated strong COX-2 enzyme inhibition. Extracts of *S. hortensis*, *S. pratensis*, and *S. verticillata* showed significant antioxidant activity in various *in vitro* model systems. In an *in vivo* model of cisplatin-induced oxidative stress, the extract of *S. hortensis* significantly alleviated liver, kidney, and testicular damage, normalized oxidative stress parameters, and exhibited an antiapoptotic effect. Extracts of the aerial parts of Lamiaceae plants showed good biocompatibility with eukaryotic cells, whereas root extracts exhibited cytotoxic activity against certain cancer cell lines. Furthermore, extracts of *S. pratensis* were successfully used for the green synthesis of silver nanoparticles with pronounced biological and catalytic potential, confirming the possibility of integrating traditional phytotherapy with modern nanotechnological approaches. The obtained results indicate that the investigated medicinal plants represent a significant source of bioactive compounds with potential applications in the development of novel phytopharmaceuticals, functional foods, and innovative nanoformulations intended for the prevention and treatment of diseases associated with oxidative stress and inflammation.

Acknowledgment: This work was supported by the Serbian Ministry of Education, Science and Technological Development (Agreements No. 451-03-34/2026-03/200122)

Predavanje dobitnika medalje SHD za izvanredne rezultate u nauci

Lecture by the winner of the SCS medal for outstanding achievements in science

MP-1

Biougalj i zagađujuće supstance u zemljištu ka održivim rešenjima za zaštitu životne sredine

Snežana P. Maletić
Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija
snezana.maletic@dh.uns.ac.rs

Svake godine dragoceni resursi se gube kroz tokove otpada, dok organski materijali poput rezidualne biomase, ostataka hrane, stajnjaka i muljeva iz postrojenja za tretman otpadnih voda ostaju neiskorišćeni. Umesto odlaganja ili spaljivanja, gde nastaju značajne emisije gasova staklene bašte, ovi materijali mogu se transformisati u vredne produkte poput biouglja. Biougalj, dobijen pirolizom otpadnih tokova, predstavlja održivo rešenje za unapređenje kvaliteta zemljišta i upravljanje zagađujućim supstancama. Njegova visoka poroznost i velika specifična površina omogućavaju efikasnu sorpciju zagađujućih supstanci, poput teških metala i pesticida, čime se smanjuje njihova mobilnost i uticaj na životnu sredinu. Ipak, efekti biouglja zavise od karakteristika sirovine, uslova pirolize i tipa zemljišta, uz potencijalne rizike kao što su oslobađanje polutanata i nepredvidive interakcije u zemljištu. Ovo otežava opštu procenu njegovog uticaja na procese sorpcije, transformacije i transporta supstanci.

Biochar and soil contaminants towards sustainable solutions for environmental protection

Snežana P. Maletić
University of Novi Sad, Faculty of Sciences, Novi Sad, Republic of Serbia
snezana.maletic@dh.uns.ac.rs

Each year, valuable resources are lost through waste streams, while organic materials such as residual biomass, food waste, manure, and sewage sludge from wastewater treatment plants remain underutilized. Instead of disposal or incineration, which generate significant greenhouse gas emissions, these materials can be transformed into valuable products such as biochar. Biochar, produced by the pyrolysis of waste streams, represents a sustainable solution for improving soil quality and managing contaminants. Its high porosity and large specific surface area enable efficient sorption of pollutants, such as heavy metals and pesticides, thereby reducing their mobility and environmental impact. However, the effects of biochar depend on feedstock characteristics, pyrolysis conditions, and soil type, with potential risks such as pollutant release and unpredictable interactions in soil. This complicates the overall assessment of its impact on sorption, transformation, and transport processes.

Zahvalnica: Istraživanje sprovedeno uz podršku Fonda za nauku Republike Srbije, 6769, Natural based efficient solution for remediation and revitalization of contaminated locations using energy crops – ReNBES.

Predavanje u znak sećanja na nedavno preminule zaslužne članove SHD

Lecture in memory of recently deceased distinguished members of the SCS

IM-1

In memoriam Prof. dr Branislav Nikolić (1943 – 2025)

Vesna B. Mišković Stanković[1,2]
[1]*Srpska akademija nauka i umetnosti, Beograd, Srbija*
[2]*Univerzitet Union – Nikola Tesla, Fakultet za ekologiju i zaštitu životne sredine, Beograd, Srbija*
vesna.miskovicstankovic@sanu.ac.rs
vesna.miskovicstankovic@unionnikolatesla.edu.rs

Prof. Branislav Nikolić je bio redovni profesor na Tehnološko-metalurškom fakultetu Univerziteta u Beogradu, prodekan i šef Katedre za fizičku hemiju i elektrohemiju, a takođe i gostujući professor na Case Western Reserve Univerzitetu u Klivlendu, Ohajo, SAD. Držao je kurseve Fizička hemija, Elektrohemija i Elektrohemijsko inženjerstvo, i iz oblasti elektrohemije je objavio više od 120 naučnih radova, 130 radova saopštenih na simpozijumima i 3 knjige. Bio je potpredsednik, predsednik i počasni predsednik Srpskog hemijskog društva i glavni i odgovorni urednik časopisa *Journal of the Serbian Chemical Society.*

In memoriam Prof. dr Branislav Nikolić (1943 – 2025)

Vesna B. Mišković Stanković[1,2]
[1]*Serbian Academy of Sciences and Arts, Belgrade, Serbia*
[2]*University Union – Nikola Tesla, Faculty of Ecology and Environmental Protection, Belgrade, Serbia*
vesna.miskovicstankovic@sanu.ac.rs
vesna.miskovicstankovic@unionnikolatesla.edu.rs

Prof. Branislav Nikolić was Full professor at the Faculty of Technology and Metallurgy, University of Belgrade, Vice-Dean, and Chair of Department of Physical Chemistry and Electrochemistry, as well as Visiting Professor at Case Western Reserve University, Cleveland, Ohio, USA. He held courses Physical Chemistry, Electrochemistry and Electrochemical Engineering, and has published more than 120 scientific papers, 130 papers presented at symposiums and 3 books in the field of electrochemistry. He served as Vice-president, President and Honorary.

IM-2

In memoriam Prof. dr Ratko M. Jankov (1945 – 2026)

Natalija Đ. Polović
Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija
polovicn@chem.bg.ac.rs

Profesor Ratko M. Jankov ostavio je dubok i trajan trag u razvoju hemije, biohemije i visokog obrazovanja u Srbiji. Kao dugogodišnji profesor Hemijskog fakulteta Univerziteta u Beogradu, bio je jedan od utemeljivača prvog studijskog programa Biohemije u regionu i ključna ličnost u oblikovanju savremene škole biohemije. Posebno mesto u njegovom profesionalnom angažovanju imalo je Srpsko hemijsko društvo, čiji je bio veoma aktivan i posvećen član, zaslužni i počasni član, kao i dobitnik tri medalje za izuzetan doprinos razvoju Društva, nastavi i nauci. Decenijama je uređivao časopis Hemijski pregled i organizovao Aprilske dane, doprinoseći popularizaciji i unapređenju nastave hemije. Njegov naučni rad obuhvatao je hemiju prirodnih proizvoda i imunohemiju, uz pionirski doprinos istraživanjima alergena i primeni antitela u dijagnostici. Kao pedagog, mentor i vizionar, ostavio je neizbrisiv uticaj na generacije studenata, nastavnika i istraživača.

In memoriam Prof. dr Ratko M. Jankov (1945 – 2026)

Natalija Đ. Polović
University of Belgrade, Faculty of Chemistry, Belgrade, Serbia
polovicn@chem.bg.ac.rs

Professor Ratko M. Jankov left a profound and lasting mark on the development of chemistry, biochemistry, and higher education in Serbia. As a distinguished professor at the Faculty of Chemistry, University of Belgrade, he was one of the founders of the first Biochemistry study program in the region and a key figure in shaping the modern school of biochemistry. A special place in his professional engagement belonged to the Serbian Chemical Society, of which he was a highly active and dedicated member, distinguished and honorary member, and recipient of three medals for outstanding contributions to the development of the Society, education, and science. For decades, he served as editor of the journal Hemijski pregled and organized the April Days meetings, contributing significantly to the popularization and advancement of chemistry education. His scientific work encompassed natural products chemistry and immunochemistry, including pioneering contributions to allergen research and the application of antibodies in diagnostics. As a teacher, mentor, and visionary, he left an indelible impact on generations of students, educators, and researchers.

Usmena Saopštenja

Oral Presentations

O-AH-1

Primena elektrode od modifikovanog staklastog ugljenika za simultano određivanje triptofana, askorbinske i mokraćne kiseline

Katarina S. Postolović, Zorka D. Stanić
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Kragujevac, Srbija
katarina.postolovic@pmf.kg.ac.rs

Triptofan, askorbinska i mokraćna kiselina, biološki značajna jedinjenja, neophodna su za normalno funkcionisanje organizma[1]. Primenjen je nov, biokompatibilni senzor za simultano određivanje ovih jedinjenja, primenom adsorptivne diferencijalne pulsne voltametrije. Elektroda od staklastog ugljenika je modifikovana hidrogelovima polisaharida hitozana i pektina koji poboljšavaju adsorpciju analita na površini elektrode i omogućavaju jasno razdvajanje dobijenih pikova. Povećana provodljivost senzora postignuta je dodatkom redukovanog grafen-oksida. Optimizovani su sastav senzora i definisani radni uslovi (DPV parametri, pH vrednost, potencijal i vreme akumulacije). Dobijena je linearna zavisnost anodne struje od koncentracije navedenih analita. Postignut nizak limit detekcije i dobra selektivnost ukazuju na mogućnost dalje primene razvijenog senzora u farmaceutskoj industriji i kliničkim analizama.

Application of modified glassy carbon electrode for simultaneous determination of tryptophan, ascorbic and uric acid

Katarina S. Postolović, Zorka D. Stanić
University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia
katarina.postolovic@pmf.kg.ac.rs

Tryptophan, ascorbic and uric acid are biologically significant compounds essential for the normal function of the human organism[1]. A novel biocompatible sensor was used to simultaneously determine these compounds using adsorptive differential pulse voltammetry. The glassy carbon electrode was modified with hydrogels of polysaccharides chitosan and pectin, which enhanced analytes' adsorption onto the electrode surface and enabled clear separation of the obtained peaks. Improved sensor conductivity was achieved by the addition of reduced graphene oxide. The sensor composition was optimized, as well as the experimental conditions (DPV parameters, pH value, accumulation potential, and accumulation time). A linear dependence of anodic current on the concentration of the investigated analytes was obtained. The achieved low detection limit and good selectivity indicate the potential of the developed sensor for further application in the pharmaceutical industry and clinical analysis.

1. A. Arroquia, I. Acosta, M.P.G. Armanda, *Mater. Sci. Eng. C*. **2020**, *109*, 110602.

This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No: 451-03-34/2026-03/200122 and 451-03-33/2026-03/200122).

O-HTM-1

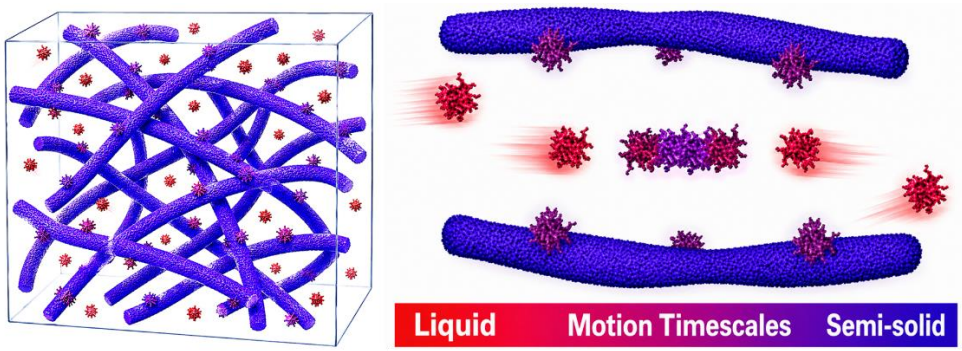
Dinamika iza funkcije u supramolekulskim biomaterijalima

Radoslav Z. Pavlović

Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Nacionalni institut Republike Srbije, Beograd, Srbija

radoslav.pavlovic@ihtm.bg.ac.rs

Supramolekulsko kretanje je nedavno prepoznato kao ključni faktor bioaktivnosti, ali ostaje nedovoljno istraženo. Koristeći peptidne amfifile (PA) pokazali smo da male promene u molekulskim strukturama dovode do značajnih razlika u pokretljivosti. Multifazna NMR merenja otkrivaju da je u visoko bioaktivnim sistemima povećana dinamika i populacije mobilnih vrsta, uspostavljajući direktnu vezu između dinamike i funkcije. Obrađene funkcije uključuju regeneraciju centralnog nervnog sistema i hrskavice. Pored hemijskog dizajna gradivnih jedinica, podešavanje dinamike je ključno za ostvarivanje prethodno nedostupnih funkcija i omogućava razvoj adaptivnih materijala visoke performanse koji se lako depolimerizuju i inherentno su reciklabilni i biorazgradivi.



Function from Dynamics in Supramolecular Biomaterials

Radoslav Z. Pavlović

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

radoslav.pavlovic@ihtm.bg.ac.rs

Supramolecular motion has recently been recognized as a key determinant of bioactivity, yet it remains underexplored. Using peptide amphiphiles (PAs), we show that small changes in molecular structure lead to significant differences in mobility. Multiphase NMR measurements reveal that highly bioactive systems exhibit enhanced molecular dynamics and larger populations of mobile species, establishing a direct link between dynamics and function. The functions addressed here include regeneration of the central nervous system and cartilage. Beyond chemical design, tuning dynamics is essential to access previously inaccessible functions and enables adaptive, high-performance materials that readily depolymerize and are inherently recyclable and biodegradable.

O-HZS-1

Sinergistički efekat sunčevog zračenja i hipohlorita na degradaciju 4-MBC u vodi

Marija Z. Kuč, Tajana M. Simetić, Tijana M. Marjanović Srebro, Jasmina R. Agbaba, Aleksandra M. Tubić, Jelena J. Molnar Jazić

Univerzitet u Novom Sadu, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Republika Srbija

marija.kuc@dh.uns.ac.rs

Organski UV filteri, poput 4-metilbenziliden kamfora (4-MBC), široko se koriste u proizvodima za zaštitu od sunčevog zračenja, ali njihovo prisustvo u vodenim sistemima izaziva zabrinutost zbog potencijalnih ekotoksikoloških efekata. U ovom radu ispitana je degradacija 4-MBC u vodi primenom kombinovanog procesa sunčevog zračenja i hipohlorita (SZ/OCl^-). Efikasnost uklanjanja 4-MBC povećavala se sa porastom koncentracije aktivnog hlora i vremena tretmana. Visok stepen degradacije (>95 %) postignut je nakon 1h tretmana pri koncentraciji hlora od 1,5 mg/L, što se pripisuje sinergističkom dejstvu visoko reaktivnih hidroksil i hlornih radikala generisanih tokom procesa. Nakon tretmana, toksičnost tretiranih uzoraka ispitivana je primenom bakterije *Pseudomonas putida.* Dobijeni rezultati pokazuju da je stepen inhibicije toksičnosti iznosio 31 %.

Synergistic effect of solar radiation and hypochlorite on the degradation of 4-MBC in water

Marija Z. Kuč, Tajana M. Simetić, Tijana M. Marjanović Srebro, Jasmina R. Agbaba, Aleksandra M. Tubić, Jelena J. Molnar Jazić

University of Novi Sad, Departmant of Chemistry, Biochemistry and Environmnetal Protection, Novi Sad, Republic of Serbia

marija.kuc@dh.uns.ac.rs

Organic UV filters, such as 4-methylbenzylidene camphor (4-MBC), are widely used in sunscreen products; however, their presence in aquatic systems raises concern due to potential ecotoxicological effects. This study investigated the degradation of 4-MBC in water using a combined solar radiation and hypochlorite process (SR/OCl^-). The removal efficiency of 4-MBC increased with higher active chlorine concentration and longer treatment time. A high degree of degradation (>95 %) was achieved after 1h of treatment at a chlorine concentration of 1.5 mg/L, attributed to the synergistic action of highly reactive hydroxyl and chlorine radicals generated during the process. After the treatment, the toxicity of the treated samples was tested using the bacterium *Pseudomonas putida*. The results showed a 31 % reduction in toxicity.

Acknowledgment: The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/200125 & 451-03-34/2026-03/200125.

O-MH-1

Od SMILES do konformacije vezivanja: automatizovani molekulski doking i validacija zasnovana na redokingu

Aleksa P. Alargić, Miloš M. Svirčev, Bojan D. Levovnik

Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Srbija

aleksa.alargic@gmail.com

Razvili smo automatizovan lokalni procesni tok za molekulsko dokovanje, namenjen prevođenju SMILES zapisa u geometrijski optimizovane trodimenzionalne strukture liganda, nakon čega slede priprema receptora, molekulsko dokovanje i validacija dokovanja. Radni tok integriše RDKit, Open Babel, Biopython i AutoDock Vina alate u računarski okvir pogodan za virtuelni skrining i istraživanja zasnovana na strukturi biomolekula. Procesni tok automatski priprema ligande i receptore, generiše GRID BOX parametre, vrši dokovanje i RMSD validaciju redokovanja. Validaciona ispitivanja pokazala su uspešnu reprodukciju kristalografskih orijentacija liganada, pri čemu su najbolje konformacije ostvarile RMSD vrednosti manje od 2 Å u odnosu na nativne konformacije.

From SMILES to binding conformation: automated molecular docking and redocking-based validation

Aleksa P. Alargić, Miloš M. Svirčev, Bojan D. Levovnik

University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia

aleksa.alargic@gmail.com

We developed an automated local molecular docking workflow for the conversion of SMILES representations into geometrically optimized three-dimensional ligand structures, followed by receptor preparation, molecular docking, and docking validation. The workflow integrates RDKit, Open Babel, Biopython, and AutoDock Vina into a computational framework suitable for virtual screening and structure-based biomolecular research. The workflow automatically performs ligand and receptor preparation, generates GRID BOX parameters, conducts molecular docking, and carries out RMSD redocking validation. Validation studies demonstrated successful reproduction of crystallographic ligand orientations, with the best conformations achieving RMSD values below 2 Å compared to the native conformations.

1. O. Trott, A. J. Olson, J. Comput. Chem. **2010**, *31*, 455.

Acknowledgment: This research is funded by the Ministry of Education and Ministry of Science, Technological Development and Innovation, Republic of Serbia, Grants: No. 451-03- 68/2022-14/200125 as well as a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

O-MH-2

In silico ispitivanje interakcija odabranih derivata piridina sa proteinima *Andes* hantavirusa

Vladimir P. Petrović, Milena D. Vukić, Jovica B. Branković
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Kragujevac, Srbija
jovica.brankovic@pmf.kg.ac.rs

Andes virus predstavlja soj zoonotskih hantavirusa koji prirodno inficiraju glodare. Virus se može preneti na ljude, pri čemu izaziva tešku i smrtonosnu respiratornu bolest poznatu kao hantavirusni kardiopulmonarni sindrom. Prema podacima SZO, trenutno ne postoji specifični antivirusni tretman ili vakcina za hantavirusnu infekciju. Primenom molekulskog dokinga, u ovom radu je izvedeno *in silico* ispitivanje interakcija odabranih derivata piridina sa nukleoproteinom[1] i glikoproteinom[2] *Andes* virusa kao potencijalnim antivirusnim metama.

In silico investigation of the interactions of selected pyridine derivatives with *Andes* hantavirus proteins

Vladimir P. Petrović, Milena D. Vukić, Jovica B. Branković
University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia
jovica.brankovic@pmf.kg.ac.rs

Andes virus represents a zoonotic hantavirus strain that naturally infects rodents. The virus can be transmitted to humans, causing a severe and often fatal respiratory disease known as hantavirus cardiopulmonary syndrome. According to the WHO, there is currently no licenced specific antiviral treatment or vaccine for hantavirus infection. Using molecular docking, this study performed an *in silico* investigation of the interactions of selected pyridine derivatives with the nucleoprotein[1] and glycoprotein[2] of the *Andes* hantavirus strain as potential antiviral targets.

References

1. Y. Guo, W. Wang, Y. Sun, C. Ma, X. Wang, X. Wang, P. Liu, S. Shen, B. Li, J. Lin, F. Deng, H. Wang, Z. Lou, *J. Virol.*, **2015**, 90, 1048.
2. A. Serris, R. Stass, E. A. Bignon, N. A. Muena, J.-C. Manuguerra, R. K. Jangra, S. Li, K. Chandran, N. D. Tischler, J. T. Huiskonen, F. A. Rey, P. Guardado-Calvo, *Cell*, **2020**, 183, 442.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/ 200122 and 451-03-33/2026-03/ 200122).

O-MH-3

Sinteza i *in vitro* ispitivanje vezivanja novih steroidnih derivata za androgene receptore

Đorđe D. Janković[1], Sofija S. Bekić[1], Maja A. Marinović[2], Milica Z. Stevanović[1], Ivana Z. Kuzminac[1], Marina P. Savić[1], Anđelka S. Ćelić[2], Edward T. Petri[2], Jovana J. Ajduković[1]

[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Srbija*

[2] *Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za biologiju i ekologiju, Trg Dositeja Obradovića 2, Novi Sad, Srbija*

djordje.jankovic@dh.uns.ac.rs

Androgeni receptori (AR) su prekomerno eksprimirani u hormon-zavisnim kancerima poput kancera prostate, gde imaju ključnu ulogu u regulaciji ćelijskog rasta i proliferacije vezivanjem prirodnih androgenih liganada. U ovom radu sintetizovana su dva nova hidrazono-hidrazidna derivata testosterona sa furanskim i tiofenskim ostatkom, sa ciljem razvoja jedinjenja sa selektivnim afinitetom prema androgenom receptoru. Oba jedinjenja pokazala su visok *in vitro* afinitet prema AR, dok je derivat sa tiofenskim prstenom ispoljio izraženu selektivnost u odnosu na estrogene (ER) i glukokortikoidne (GR) receptore. Molekulska doking analiza sprovedena je radi uvida u ključne interakcije između ispitivanih jedinjenja i aminokiselinskih ostataka ligand-vezujućeg domena androgenog receptora.

Synthesis and *in vitro* evaluation of binding of novel steroid derivatives to androgen receptors

Đorđe D. Janković[1], Sofija S. Bekić[1], Maja A. Marinović[2], Milica Z. Stevanović[1], Ivana Z. Kuzminac[1], Marina P. Savić[1], Anđelka S. Ćelić[2], Edward T. Petri[2], Jovana J. Ajduković[1]

[1]*University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad*

[2] *University of Novi Sad, Faculty of Sciences, Department of Biology and Ecology, Trg Dositeja Obradovića 2, Novi Sad*

djordje.jankovic@dh.uns.ac.rs

Androgen receptors (AR) are overexpressed in hormone-dependent cancers, such as prostate cancer, where they regulate cell growth and proliferation through androgen ligand binding. In this study, two novel hydrazono-hydrazide derivatives of testosterone bearing furan and thiophene moieties were synthesized to develop compounds selective toward the androgen receptor. Both compounds showed *in vitro* high affinity toward AR, while the thiophene derivative exhibited pronounced selectivity over estrogen (ER) and glucocorticoid (GR) receptors. Molecular docking analysis revealed key interactions of the investigated compounds within the androgen receptor ligand-binding domain.

Acknowledgment: The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/ 200125 & 451-03-34/2026-03/ 200125).

O-MH-4

TERNARYION: modeliranje PROTAC ternarnih kompleksa

Nevena Tomašević[1], Gordana Tasić[2], Predrag Jovanović[2], Milena Simić[2], Vladimir Savić[2], Sanja Lj. Matić[3], Milan Mladenović[1]

[1]*Centar za računarsku biohemiju Kragujevac, Prirodno-matematički fakultet, Univerzitet u Kragujevcu, Radoja Domanovića 12, 34000 Kragujevac, Srbija*

[2]*Univerzitet u Beogradu, Farmaceutski fakultet, Katedra za organsku hemiju, Vojvode Stepe 450, 11221 Beograd, Srbija*

[3] *Institut za informacione tehnologije, Univerzitet u Kragujevcu, Liceja Kneževine Srbije 1A, 24000 Kragujevac, Srbija*

milan.mladenovic@pmf.kg.ac.rs

TERNARYION je novi *in silico* protokol za modeliranje ternarnih kompleksa (TC) PROTAC molekula, koji podrazumeva korišćenje HADDOCK3 softvera za reprodukciju ko-kristalizovanih TC kompleksa, pametnu detekciju kontaktnih centara za protein–protein dokovanje binarnih kompleksa (BC) proteina od interesa (POI) i E3 ligaze, geometrijsku pred-orijentaciju PROTAC molekula unutar BC, odnosno reverzibilno ili ireverzibilno dokovanje PROTAC molekula unutar BC korišćenjem Vina softvera i njegovih derivata. Protokol je validiran na HDAC4 PROTAC molekulima, potencijalnoj palijativnoj terapiji za spinalnu mišićnu atrofiju.

TERNARYION: PROTACs ternary complexes modeling

Nevena Tomašević[1], Gordana Tasić[2], Predrag Jovanović[2], Milena Simić[2], Vladimir Savić[2], Sanja Lj. Matić[3], Milan Mladenović[1]

[1]*Kragujevac Center for Computational Biochemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia*

[2]*University of Belgrade, Faculty of Pharmacy, Department of Organic Chemistry, Vojvode Stepe 450, 11221 Belgrade, Serbia*

[3]*Institute for Informational Technologies, University of Kragujevac, Liceja Kneževine Srbije 1A, 4000 Kragujevac, Serbia*

milan.mladenovic@pmf.kg.ac.rs

TERNARYION is a novel *in silico* workflow for forming physiologically relevant ternary complexes (TCs) of PROTACs. It integrates structure-based alignment assessments of co-crystallized TCs, ambiguity-driven HADDOCK3 POI and E3 ligase protein–protein docking to construct binary complexes (BCs), geometry-guided pre-orientation of the PROTAC within BCs, and either reversible or irreversible docking of PROTACs into BCs using AutoDock Vina and its forks. The workflow was validated on HDAC4-targeting PROTACs as a palliative therapy for Spinal Muscular Atrophy.

Acknowledgments: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7490, Artificial Intelligence-Guided Design, Synthesis, and Pharmacological Evaluation of Innovative PROTACs as Degraders of HDAC4, an Epigenetic Target for Spinal Muscular Atrophy - SMAIPROTACs

O-MH-5

PhotoSCLART: Pregled projekta i rezultati ostvareni u prve dve godine projekta

Andrea M. Nikolić[1], Ljiljana Koračak[2], Pavle Stojković[1], Igor M. Opsenica[1]
[1]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
[2]*Inovacioni centar Hemijskog fakulteta u Beogradu d.o.o., Beograd, Srbija*
andrea@chem.bg.ac.rs

PhotoSCLART projekat za cilj ima je razvoj fotoreaktivnih agenasa protiv raka zasnovanih na derivatima prirodnih proizvoda. Novi derivati sklareola i artemizinina dizajnirani su i sintetisani na osnovu prethodno ostvarenih rezultata. Hibridi sklareola sa adamantanom sintetisani su primenom reakcija formiranja C–C veze katalizovane kompleksima paladijuma, a zatim reduktivnog aminovanja. Derivati artemizinina sa pirimidinom, dobijeni su primenom reakcija Suzuki-Miyaura, supstitucije i „*click*“ reakcije. Biološka aktivnost sintetisanih derivata ispitana je u modelima nesitnoćelijskog karcinoma pluća i glioblastoma rezistentnih na više lekova. Rezultati ovog projekta predstavljaće osnovu za teranostički pristup u dizajnu i sintezi bioaktivnih molekula, derivata prirodnih proizvoda.

PhotoSCLART: Project overview and the results accomplished in the first two years

Andrea M. Nikolić[1], Ljiljana Koračak[2], Pavle Stojković[1], Igor M. Opsenica[1]
[1]*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
[2]*Innovative Centre of the Faculty of Chemistry ltd., Belgrade, Serbia*
andrea@chem.bg.ac.rs

The goal of the PhotoSCLART project is to develop photoreactive anticancer agents based on derivatives of natural products. New derivatives of sclareol and artemisinin were designed and synthesized based on previously achieved results. Hybrids of sclareol with adamantane were synthesized utilizing C–C bond formation reactions catalyzed by palladium complexes, followed by reductive amination. Derivatives of artemisinin with pyrimidine were obtained using Suzuki-Miyaura reaction, substitution and click reactions. The bioactivity of the synthesized derivatives was determined in models of non-small cell lung cancer and glioblastoma, resistant to multiple drugs. The results of this project will represent the basis for a theranostic approach in the design and synthesis of bioactive molecules, derivatives of natural products.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, (grant No. 7005, Development of nature-inspired photoresponsive anticancer agents - sclareol and artemisinin derivatives in cancer multidrug-resistance models: a foundation for the theranostic approach – PhotoSCLART).

O-NH-1

Podešavanje katalitičkih svojstava renijum(V) kompleksa strukturnom modifikcijom liganada

Jana Timotijević[1], Ana Kandić[2], Tamara A. Petrović[1], Ljiljana E. Mihajlović, Stefan R. Nikolić, Antoine Dupé[3], Jelena M. Poljarević[1]

[1]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
[2] *Inovacioni centar Hemijskog fakulteta u Beogradu, Beograd, Srbija*
[3] *Iinstitut za hemiju, Univerzitet u Gracu, Grac, Austrija*
anak@chem.bg.ac.rs

Primena oksorenijum(V) kompleksa u homogenoj katalitičkoj epoksidaciji olefina intenzivno se proučava poslednjih desetak godina. U ovom radu ispitivan je uticaj strukturne modifikacije derivata 2-pikolininske kiseline kod 5 oksorenijum(V) kompleksa na katalitičku aktivnost u reakciji epoksidacije olefina sa terc-butil hidroperoksidom kao oksidansom. Svih pet kompleksa pokazalo je trenutnu aktivnost bez indukcionog perioda, a većina ciklooktena je konvertovana u prva tri sata. Među ispitivanim jedinjenjima, kompleks koji sadrži 6-hloropiridin-2-karboksilnu kiselinu pokazao je najveću katalitičku aktivnost, ostvarivši konverziju ciklooktena od 85%.

Modulating rhenium(V) catalysts through ligand structural modifications

Jana Timotijević[1], Ana Kandić[2], Tamara A. Petrović[1], Ljiljana E. Mihajlović, Stefan R. Nikolić, Antoine Dupé[3], Jelena M. Poljarević[1]

[1]*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
[2]*Innovation Center of the Faculty of Chemistry, Belgrade, Serbia*
[3]*Institute of Chemistry, University of Graz, Graz, Austria*
anak@chem.bg.ac.rs

Over the last ten years, the application of oxorhenium(V) complexes in homogeneous catalytic olefin epoxidation has been developed. We have evaluated the influence of structural modifications in the 2-picolinic acid derivatives' structure on the catalytic activity of five picolinate-based Re(V) complexes for the cyclooctene epoxidation using *tert*-butyl hydroperoxide as the oxidant. All five complexes showed immediate activity without an induction period, and most of the cyclooctene was converted within the first three hours. Among the investigated compounds, the complex containing 6-chloropyridine-2-carboxylic acid showed the highest catalytic activity, achieving a cyclooctene conversion of 85%.

Acknowledgments: This work was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (451-03-33/2026-03/200168, 451-03-33/2026-03/200288) and the European Union's Horizon Europe program under the Marie Skłodowska-Curie Actions grant agreement No. 101086373.

O-NH-2

Struktura i BSA/DNA interakcije $\{[Ba(H_2O)_4][Ba(2\text{-}OH\text{-}1,3\text{-}pdta)]\}_n \cdot 2H_2O$ kompleksa

Bojana V. Pantović[1], Darko P. Ašanin[2], Tina P. Andrejević[1], Nevena Lj. Stevanović[1], Nenad S. Drašković[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Radoja Domanovića 12, 34000 Kragujevac, Srbija*
[2]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*
[3]*Univerzitet u Prištini-Kosovska Mitrovica, Poljoprivredni fakultet, Kopaonička bb, 38228 Lešak, Srbija*
[4]*Srpska akademija nauka i umetnostii, Knez Mihailova 35, 11000 Beograd, Srbija*
bojana.pantovic@pmf.kg.ac.rs

Sintetisan je barijum(II) kompleks sa 2-hidroksi-1,3-propandiamin-*N,N,N',N'*-tetraacetatom (2-OH-1,3-pdta^{4-}), $\{[Ba(H_2O)_4][Ba(2\text{-}OH\text{-}1,3\text{-}pdta)]\}_n \cdot 2H_2O$. Kristalna struktura kompleksa određena je primenom rendgenske strukturne analize. Interakcije ovog kompleksa sa albuminom goveđeg seruma (BSA) i DNA izolovanim iz timusa teleta (ct-DNA) ispitivane su primenom fluorescentne emisione spektroskopije.

Structure and BSA/DNA interactions of $\{[Ba(H_2O)_4][Ba(2\text{-}OH\text{-}1,3\text{-}pdta)]\}_n \cdot 2H_2O$ complex

Bojana V. Pantović[1], Darko P. Ašanin[2], Tina P. Andrejević[1], Nevena Lj. Stevanović[1], Nenad S. Drašković[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Radoja Domanovića 12, 34000 Kragujevac, Serbia*
[2]*University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*
[3]*University of Priština-Kosovska Mitrovica, Faculty of Agriculture, Kopaonička bb, 38228 Lešak, Serbia*
[4]*Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia*
bojana.pantovic@pmf.kg.ac.rs

Barium(II) complex with 2-hydroxy-1,3-propanediamine-*N,N,N',N'*-tetraacetate (2-OH-1,3-pdta^{4-}), namely $\{[Ba(H_2O)_4][Ba(2\text{-}OH\text{-}1,3\text{-}pdta)]\}_n \cdot 2H_2O$, was synthesized and its crystal structure was determined by single-crystal X-ray diffraction analysis. The interactions of this complex with bovine serum albumin (BSA) and calf thymus DNA (ct-DNA) were examined using fluorescence emission spectroscopy.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122, and 451-03-33/2026-03/200378), and from the Serbian Academy of Sciences and Arts under the strategic projects program, with grant agreement No. 01-2026.

O-NH-3

Iridijum(III) kompleks: sinteza, karakterizacija i citotoksična aktivnost

Tamara A. Petrović, Sanja Grgurić-Šipka
Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija
tamarap@chem.bg.ac.rs

Karcinom predstavlja drugi vodeći uzrok smrtnosti u svetu, odmah nakon kardiovaskularnih bolesti, sa 2,74 miliona zabeleženih smrtnih slučajeva u 2022. godini. U poslednjih nekoliko godina, kompleksi iridijuma(III) izdvojili su se kao novi kandidati za razvoj antitumorskih lekova. U ovom radu sintetisan je novi Ir(III) kompleks opšte formule $[Ir(pyp)_2(L1)]PF_6$, gde je L1 derivat fenantrolina. Polazni kompleks $[Ir(pyp)_2Cl]_2$ reagovao je sa odgovarajućim ligandom u smeši metanola i dihlormetana, uz NH_4PF_6 kao kontrajona. Nakon 24 časa, proizvod je izdvojen u obliku narandžastog praha. Dobijeni kompleks je hemijski okarakterisan primenom ^1H i ^{13}C NMR, IC spektroskopije, EA i HRMS. Biološka ispitivanja pokazala su da novodobijeni Ir(III) kompleks ispoljava značajnu *in vitro* citotoksičnu aktivnost prema MDA-MB-231 (karcinom dojke) i HCT116 (kolorektalni karcinom) ćelijskim linijama, određenu MTT testom. Dodatno, konfokalnom mikroskopijom pokazano je da se ovaj Ir(III) kompleks predominantno akumulira u mitohondrijama MDA-MB-231 ćelija.

Novel iridium(III) complex: synthesis, chemical characterization, and cytotoxic potential

Tamara A. Petrović, Sanja Grgurić-Šipka
University of Belgrade, Faculty of Chemistry, Belgrade, Serbia
tamarap@chem.bg.ac.rs

Cancer remains the second leading cause of mortality worldwide, surpassed only by cardiovascular diseases, with 2.74 million recorded deaths in 2022. In recent years, iridium(III) complexes have emerged as attractive candidates for anticancer drug development. In this work, a novel Ir(III) complex of the general formula $[Ir(pyp)_2(L1)]PF_6$, where L1 is a phenanthroline derivative, was synthesized. The starting precursor $[Ir(pyp)_2Cl]_2$ was reacted with the corresponding ligand in a methanol/dichloromethane solvent mixture, using NH_4PF_6 as the counterion. After 24 hours of reaction, the product precipitated as an orange powder. The obtained complex was structurally and chemically characterized by ^1H and ^{13}C NMR, IR spectroscopy, EA, and HRMS. Biological evaluation revealed that the newly synthesized Ir(III) complex displayed notable *in vitro* cytotoxic activity against MDA-MB-231 (breast cancer) and HCT116 (colorectal cancer) cell lines, determined by MTT assays. Additionally, confocal microscopy studies revealed that this Ir(III) compound preferentially accumulates in mitochondria in MDA-MB-231 cells.

Acknowledgment: This work was funded by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia, under contract numbers 451-03-33/2026-03/200168.

O-OH-1

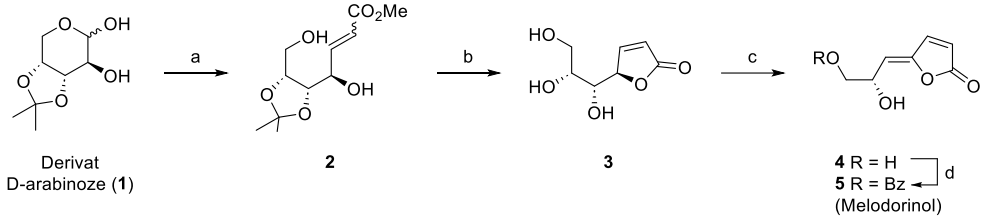
Totalna sinteza melodorinola i acetilmelodorinola iz D-arabinoze

Sanja M. Đokić, Jovana Francuz, Jelena Tadić, Mirjana Popsavin, Velimir Popsavin, Goran Benedeković

Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija

sanjadj@dh.uns.ac.rs

Melodorinol i acetilmelodorinol su prirodni laktoni[1] izolovani iz biljke *Melodorum fruticosum* Lour. (Annonaceae), a koji pokazuju značajnu citotoksičnost (2–6 μg/mL) prema odabranim humanim tumorskim ćelijskim linijama. U radu će biti opisana nova višefazna sinteza oba jedinjenja polazeći od D-arabinoze kao jeftinog hiralnog prekursora (Shema 1).



Shema 1. Sinteza melodorinola: (a) MCMP, $CHCl_3$, rt, 48 h; (b) aq 50% TFA; (c) Ph_3P, DEAD, THF, 0 °C to rt; (d) BzCl, Py/DCE, 0 °C to rt.

Total synthesis of melodorinol and acetylmelodorinol from D-arabinose

Sanja M. Đokić, Jovana Francuz, Jelena Tadić, Mirjana Popsavin, Velimir Popsavin, Goran Benedeković

University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental protection, Novi Sad, Serbia

sanjadj@dh.uns.ac.rs

Melodorinol and acetylmelodorinol are natural lactones[1] isolated from the *Melodorum fruticosum* Lour. (Annonaceae), which show significant cytotoxic activity (2–6 μg/mL) against selected human tumour cell lines. A new multistep synthetis of both compounds will be presented herein, starting from D-arabinose (Scheme 1).

1. J. H. Jung, C.-J. Chang, D. L. Smith, J. L. McLaughlin, S. Pummangura, C. Chaichantipyuth, C. Patarapanich *J. Nat. Prod*. **1991**, *54*, 500.

Acknowledgment: The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/ 200125 & 451-03-34/2026-03/ 200125) and Serbian Academy of Sciences and Arts (F-130).

O-TH-1

Regresija zasnovana na Gausovom procesu kao alat u teorijskoj spektroskopiji malih molekula

Stanka V. Jerosimić
Univerzitet u Beogradu, Fakultet za fizičku hemiju, Beograd, Srbija
stanka.jerosimic@ffh.bg.ac.rs

Regresija zasnovana na Gausovom procesu (Gaussian Process Regression, GPR) predstavlja metod mašinskog učenja pogodan za rad sa malim skupovima podataka tipičnim za teorijsku spektroskopiju i skupe *ab initio* proračune. U ovom radu prikazane su mogućnosti primene GPR pristupa na modelovanje površina potencijalne energije (PES), površi dipolnog momenta (DMS) i spin–orbitne sprege (SOC) kod malih molekula. Poseban naglasak stavljen je na izbor kernelskih funkcija, procenu neodređenosti predikcije i glatkih funkcija pogodnih za računanje rovibracionih nivoa i spektara. Diskutovane su i prednosti GPR pristupa u odnosu na druge metode mašinskog učenja u uslovima ograničenog broja kvantno-hemijskih podataka.

Applications of Gaussian Process Regression in Theoretical Spectroscopy of Small Molecules

Stanka V. Jerosimić
Univerzitet u Beogradu, Fakultet za fizičku hemiju, Beograd, Srbija
stanka.jerosimic@ffh.bg.ac.rs

Gaussian Process Regression (GPR) is a machine learning method particularly suitable for small datasets typical of theoretical spectroscopy and computationally demanding *ab initio* calculations. This contribution presents possible applications of GPR to the modeling of potential energy surfaces (PES), dipole moment surfaces (DMS), and spin–orbit coupling (SOC) in small molecules. Special emphasis is placed on kernel selection, uncertainty estimation, and the construction of smooth functions suitable for rovibrational calculations. Advantages of the GPR approach compared to other machine learning methods for limited quantum-chemical datasets are also discussed.

Acknowledgment: The author acknowledges the use of the LEO HPC infrastructure at the University of Innsbruck.

O-TH-2

Pojava σ-aromatičnosti kod dikatjona halogenovanih cikloalkana

Slađana Đorđević, Slavko Radenković
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija
sladjana.djordjevic@pmf.kg.ac.rs

Aromatičnost se najčešće definiše preko delokalizacije π-elektrona, dok je delokalizacija σ-elektrona manje istražen put stabilizacije u cikličnim sistemima. U ovom radu istraživali smo pojavu σ-aromatičnosti u halogenovanim cikloalkanima izazvanu oksidacijom. Primenom različitih kriterijuma aromatičnosti, poput gustine magnetno indukovanih struja (MICD), elektronske gustine delokalizovanih veza (EDDB) i aromatske stabilizacione energije (ASE), pokazali smo da su dikatjoni halogenovanih cikloalkana σ-aromatični sistemi.[1] Naša analiza otkriva da se određena odstupanja od Hikelovog pravila preciznije mogu objasniti pravilima orbitalne selekcije. Ovi rezultati pružaju jedinstveni okvir za razumevanje načina na koji oksidacija aktivira aromatični karakter u tradicionalno zasićenim molekulskim sistemima.

The emergence of σ-aromaticity in dicationic halogenated cycloalkanes

Slađana Đorđević, Slavko Radenković
University of Kragujevac, Faculty of Science, Kragujevac, Serbia
sladjana.djordjevic@pmf.kg.ac.rs

While aromaticity is classically defined through π-electron delocalization, the manifestation of σ-aromaticity offers a compelling yet less explored stabilization route in cyclic architectures. This study explores the emergence of σ-aromaticity in halogenated cycloalkanes triggered by two-electron oxidation. Through a comprehensive suite of electronic descriptors, including magnetically induced current densities (MICD), the electron density of delocalized bonds (EDDB), and aromatic stabilization energy (ASE), we demonstrate that dicationic halogenated cycloalkanes are σ-aromatic systems.[1] Our analysis reveals that certain deviations from Hückel's rule are more accurately rationalized through orbital selection rules rather than traditional counting models. These results provide a unified framework for understanding how oxidation activate aromatic character in traditionally saturated molecular systems.

1. S. Radenković, S. Đorđević, *Phys. Chem. Chem. Phys.* **2025**, *27*, 25422.

Acknowledgment: Supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia, contract 451-03-34/2026-03/200122.

O-TH-3

Od steking interakcija do vodoničnih veza – kristalografska i DFT priča o dimerima triazina

Katarina A. Ćeranić[1], Milenko M. Bunović[1,2], Dušan P. Malenov[2]
[1]*Inovacioni centar Hemijskog fakulteta u Beogradu, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
malenov@chem.bg.ac.rs

Sa ciljem pronalaženja steking interakcija između triazinskih jedinica, pretražene su kristalne strukture u Kembričkoj bazi strukturnih podataka koje sadrže međusobno paralelne triazinske prstenove. Međutim, uprkos značajnom broju tipičnih steking interakcija sa malim horizontalnim pomeranjima, na velikim pomeranjima se ne formiraju steking interakcije, već jako dominiraju dvostruke vodonične veze. Proračuni potencijalnih površi na ωB97X-D3BJ/def2-TZVP nivou teorije na model-sistemima pokazali su da steking interakcije između triazinskih jedinica mogu imati značajne energije (–4,5 kcal/mol za dimer triaminotriazina), ali da vodonične veze mogu biti značajno jače (preko –11,0 kcal/mol), čime se može objasniti njihovo često pojavljivanje u kristalnim strukturama.

From stacking interactions to hydrogen bonds – a crystallographic and DFT story on triazine dimers

Katarina A. Ćeranić[1], Milenko M. Bunović[1,2], Dušan P. Malenov[2]
[1]*Innovative Centre of the Faculty of Chemistry in Belgrade, Belgrade, Serbia*
[2] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
malenov@chem.bg.ac.rs

With the aim of finding stacking interactions between triazine units, crystal structures in the Cambridge Structural Database with mutually parallel triazine rings were analyzed. However, in spite of the large number of typical stacking interactions with small horizontal displacements, at large displacements stacking interactions are not preferred, but instead double hydrogen bonds are formed. Potential energy surface calculations on ωB97X-D3BJ/def2-TZVP level of theory using model systems showed that stacking interaction energies can be significant (–4.5 kcal/mol for triaminotriazine dimer), but hydrogen bonds can be significantly stronger (over –11.0 kcal/mol), which explains their frequent occurrence in crystal structures.

This research was inspired by our work on the project Empowering Chemistry Students to Discover Noncovalent Interactions via the Cambridge Structural Database – CSD4NCI Workshop, which was funded by the Cambridge Crystallographic Data Centre under the framework of CCDC Engagement Grants. Support by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (contracts number: 451-03-33/2026-03/200168 and 451-03-33/2026-03/200288) is appreciated.

O-ZH-1

Zelena ekstrakcija pektina iz jabučne kaše primenom dubokih eutektičkih rastvarača

Milica M. Vasović[1], Pavle M. Spasojević[2], Olga J. Pantić[3], Vesna V. Panić[2], Milica M. Spasojević-Savković[4], Maja D. Marković[2], Sanja I. Savić[1]

[1]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[3]*Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Rebuliku Srbiju, Beograd, Srbija*
[4]*Univerzitet u Beogradu, Inovacioni centar Hemijskog fakulteta, Beograd, Srbija*
sseslija@tmf.bg.ac.rs

U ovom radu ispitivana je ekstrakcija pektina iz otpadne jabučne kaše primenom dubokih eutektičkih rastvarača na bazi holin-hlorida u kombinaciji sa malonskom, jabučnom i mlečnom kiselinom, pripremljenih u molarnom odnosu 1:2. Ekstrakcija pektina sprovedena je primenom ultrazvučno potpomognute ekstrakcije, kao i ekstrakcije pod dejstvom povišene temperature, uz postizanje zadovoljavajućih prinosa. FTIR analiza potvrdila je pretežno pektinsku strukturu ekstrahovanih uzoraka, pri čemu prisustvo pojedinih pikova ukazuje na zaostale lignocelulozne komponente. Takođe, ispitivani uzorci pokazali su značajan antioksidativni potencijal, čime je ukazano na mogućnost valorizacije otpadne kaše jabuke primenom ekološki prihvatljivih postupaka ekstrakcije.

Green extraction of pectin from apple pomace using deep eutectic solvents

Milica M. Vasović[1], Pavle M. Spasojević[2], Olga J. Pantić[3], Vesna V. Panić[2], Milica M. Spasojević-Savković[4], Maja D. Marković[2], Sanja I. Savić[1]

[1]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[3]*University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia*
[4]*University of Belgrade, Innovation Centre of the Faculty of Chemistry, Belgrade, Serbia*
sseslija@tmf.bg.ac.rs

This study investigated the extraction of pectin from waste apple pomace using deep eutectic solvents based on choline chloride combined with malonic, malic, and lactic acids, prepared in a 1:2 molar ratio. Pectin extraction was performed using both ultrasound-assisted extraction and conventional solid–liquid extraction, reaching satisfactory yields. FTIR analysis confirmed the predominantly pectic structure of the extracted samples, although the presence of lignocellulosic residues was also detected. Furthermore, the obtained samples exhibited significant antioxidant potential, highlighting the possibility of valorizing apple pomace waste through environmentally friendly extraction approaches.

Saopštenja / Contributions

Biohemija

Biochemistry

P-BH-1

Skrining derivata žučnih kiselina kao novih liganda humanih enzima koji metabolizuju steroide

Yaraslau U. Dzichenka[1], Kristina I. Okhrimuk[2], Srđan Bjedov[3], Sergei A. Usanov[1], Suzana Jovanović-Šanta[3]

[1]*Institute of Bioorganic Chemistry of National Academy of Sciences, Minsk, Belarus*
[2]*Polessky State University, Pinsk, Belarus*
[3]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija*
suzana.jovanovic-santa@dh.uns.ac.rs

Enzimi koji metabolizuju steroide u organizmu čoveka učestvuju u metabolizmu oksisterola, steroidnih hormona i neurosteroida. Često su cilj delovanja leka, a poremećaji u njihovoj sintezi ili funkciji, kao i nekontrolisano delovanje leka na druge enzime povezani sa teškim poremećajima. U *in vitro* studiji koristili smo rekombinantne enzime CYP7B1, CYP17A1 i CYP21A2 da bi među derivatima žučnih kiselina identifikovali nove ligande za ove enzime. Među testiranim jedinjenjima, identifikovan je novi molekul koji se vezuje kao inhibitor za humani CYP7B1, sa K_d = 7,0±1,1 μM. Izvedena je *in silico* analiza da bi se otkrio način vezivanja i identifikovane ključne aminokiseline važne za vezivanje liganda. Dobijeni rezultati su veoma relevantni za identifikaciju potencijalnih neželjenih efekata vodećih jedinjenja sa obećavajućom biološkom aktivnošću.

Screening of bile acid-derived compounds for novel ligands of human steroid-metabolizing enzymes

Yaraslau U. Dzichenka[1], Kristina I. Okhrimuk[2], Srđan Bjedov[3], Sergei A. Usanov[1], Suzana Jovanović-Šanta[3]

[1]*Institute of Bioorganic Chemistry of National Academy of Sciences, Minsk, Belarus*
[2]*Polessky State University, Pinsk, Belarus*
[3]*University of Novi Sad Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental protection, Novi Sad, Serbia*
suzana.jovanovic-santa@dh.uns.ac.rs

Human steroid-metabolizing enzymes are involved in the metabolism of oxysterols, steroid hormones and neurosteroids. They are often targets for drugs action, so disruptions of their synthesis, function, but also uncontrolled action of the drug on other enzymes are associated with severe disorders. In the *in vitro* study, we used recombinant CYP7B1, CYP17A1, and CYP21A2 to find novel ligands of these enzymes among 20 bile acids derivatives. Among the tested compounds, a novel inhibitor-like molecule with a K_d = 7.0±1.1 μM for human CYP7B1 was identified. *In silico* analysis of the binding modes of the novel ligands was performed, and key amino acids involved in ligand binding were identified. The results obtained are highly relevant for identifying possible side effects of lead compounds with promising bioactivity.

Acknowledgements: Presented results are obtained in the frame of Belarus-Serbia bilateral project No X26SRBG-001/0001359152026134400030006200210300l.

P-BH-2

Evaluacija mehanizama antimelanogene aktivnosti ariliden-2-tiohidantoina

Petar B. Stanić[1], Nevena S. Jeremić[2], Biljana M. Šmit[1], Suzana Jovanović-Šanta[3]
[1]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Kragujevac, Srbija*
[2]*Univerzitet u Kragujevcu, Fakultet medicinskih nauka, Kragujevac, Srbija*
[3]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija*
suzana.jovanovic-santa@dh.uns.ac.rs

Melanogeneza je složen biohemijski proces regulisan višestrukim enzimskim i signalnim putevima. Ispitan je antimelanogeni potencijal serije ariliden-2-tiohidantoina kombinacijom *in vitro* i *in silico* pristupa u cilju razjašnjavanja mehanizama delovanja. Inhibitorni efekti na ključne enzime melanogeneze procenjeni su *in vitro* testovima merenja aktivnosti tirozinaze i proteina povezanog sa tirozinazom tipa 2 (eng. tyrosinase-related protein, TRP-2). Da bi se razjasnila molekularna osnova delovanja, sprovedene su studije dokovanja na tirozinazi i TRP-2, radi procene afiniteta vezivanja i važnih interakcija sa ostacima aminokiselina enzima. Molekularno dokovanje je prošireno i na proteine uključene u signalne puteve povezane sa melanogenezom. Generalno, rezultati ukazuju da su ariliden-2-tiohidantoini obećavajući kandidati za razvoj antimelanogenih agenasa sa potencijalnom primenom u dermatologiji.

Evaluating the mechanisms of antimelanogenic activity of arylidene-2-thiohydantoins

Petar B. Stanić[1], Nevena S. Jeremić[2], Biljana M. Šmit[1], Suzana Jovanović-Šanta[3]
[1]*University of Kragujevac, Institute for Information Technologies Kragujevac, Kragujevac, Sebia*
[2]*University of Kragujevac, Faculty of Medical Sciences, Kragujevac, Serbia*
[3]*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*
suzana.jovanovic-santa@dh.uns.ac.rs

Melanogenesis is a complex biochemical process regulated by multiple enzymatic and signaling pathways. Antimelanogenic potential of series of arylidene-2-thiohydantoins was investigated through combined *in vitro* and *in silico* approaches aimed to elucidate mechanisms of action. The inhibitory effects on key melanogenic enzymes were evaluated *in vitro* using tyrosinase and tyrosinase-related protein 2 (TRP-2) assays. To clarify the molecular basis of the activity, docking studies were performed on enzymes tyrosinase and TRP 2, as well as proteins belonging melanogenesis-associated signaling pathways, revealing binding affinities and interactions with important amino acid residues. Overall, the results indicate that arylidene-2-thiohydantoins are promising candidates for antimelanogenic agents with potential applications in dermatology.

P-BH-3

Fenolni profil metanolskih ekstrakata nadzemnog dela i korena biljke *Lysimachia vulgaris* L.

Nikola Srećković[1], Danijela Mišić[2], Uroš Gašić[2], Jelena S. Katanić Stanković[3], Vladimir Mihailović[1]

[1] *Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija*

[2] *Univerzitet u Beogradu, Institut za biološka istraživanja „Siniša Stanković" – Nacionalni institut Republike Srbije, Beograd, Srbija*

[3]*Univerzitet u Kragujevcu, Institut za informacione tehnologije, Departman za prirodno-matematičke nauke, Liceja Kneževine Srbije 1A, 34 000 Kragujevac, Srbija*

nikola.sreckovic@pmf.kg.ac.rs

Cilj ovog rada bio je ispitivanje fenolnog profila metanolskih ekstrakata nadzemnog dela i korena biljke *Lysimachia vulgaris* primenom UHPLC–MS/MS analize. Identifikovano je 94 sekundarna metabolita, uključujući fenolne kiseline, flavonoide i njihove glikozide. Nadzemni deo biljke pokazao je raznovrsniji fenolni sastav u odnosu na koren, sa dominantnim sadržajem galne kiseline, kvercetin-3-O-glukozida i ruzmarinske kiseline. Kao dominantna jedinjenja ekstrakta korena identifikovani su benzohinoni embelin i raponon. Dobijeni rezultati ukazuju da *L. vulgaris* predstavlja perspektivan prirodni izvor fenolnih jedinjenja sa potencijalnom farmakološkom primenom.

Phenolic profile of methanolic extracts of the aerial part and root of *Lysimachia vulgaris* L.

Nikola Srećković[1], Danijela Mišić[2], Uroš Gašić[2], Jelena S. Katanić Stanković[3], Vladimir Mihailović[1]

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

[2]*University of Belgrade, Institute for Biological Research "Siniša Stanković" – National Institute of the Republic of Serbia, Belgrade, Serbia*

[3]*University of Kragujevac, Institute for Information Technologies, Department of Science, Liceja Kneževine Srbije 1A, 34 000 Kragujevac, Serbia*

nikola.sreckovic@pmf.kg.ac.rs

The aim of this study was to investigate the phenolic profile of methanolic extracts of the aerial part and root of *Lysimachia vulgaris* using UHPLC–MS/MS analysis. A total of 94 secondary metabolites were identified, including phenolic acids, flavonoids, and their glycosides. The aerial part exhibited a more diverse phenolic composition compared to the root, with gallic acid, quercetin-3-O-glucoside, and rosmarinic acid being the predominant compounds. The benzoquinones embelin and rapanone were identified as the dominant constituents of the root extract. The results obtained indicate that *L. vulgaris* represents a promising natural source of phenolic compounds with potential pharmacological applications.

Acknowledgment: This work was supported by the Serbian Ministry of Science, Technological and Innovation (Agreement Nos. 451 03-33/2026-03/200122; 451-03-34/2026-03/200122 and 451-03 136/2025-03/200007).

Elektrohemija

Electrochemistry

P-EH-1

Koroziona stabilnost PEO oksidnih slojeva sa cerijumom

Anđela R. Simović[1], Dušan Berber[1], Kristina Mojsilović[2], Rastko Vasilić[2], Jelena B. Bajat[3]
[1]*Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Fizički fakultet, Studentski trg 12-16, Beograd, Srbija*
[3]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Karnegijeva 4, 11120 Beograd, Srbija*
jela@tmf.bg.ac.rs

Plazmena elektrolitička oksidacija (PEO) je inovativna, ekološki prihvatljiva metoda dobijanja oksidnih filmova na aluminijumu, magnezijumu, titanu. Dobijeni oksidni filmovi imaju odličnu adheziju, tvrdoću, otpornost na habanje i koroziju. U radu su ispitivane morfologija, hrapavost i koroziona stabilnost oksidnih slojeva dobijenih PEO postupkom (20 °C, 30 mA cm^{-2}) na aluminijumu u vodenom rastvoru Na_3PO_4 sa dodatkom CeO_2, $Ce(NO_3)_3$ ili $CeCl_3$. Oksidni slojevi sa cerijumom su značajni zbog inhibitorskih svojstava cerijuma. Koroziona stabilnost oksidnih filmova je praćena polarizacionim merenjima i spektroskopijom elektrohemijske impedancije u 3% NaCl tokom dužeg vremena. Diskutovana su uloga cerijuma i mehanizam zaštite koji pružaju različiti izvori Ce, kao i razlike u korozionoj stabilnosti ispitivanih zaštitnih sistema.

Corrosion stability of PEO oxide layers with cerium

Anđela R. Simović[1], Dušan Berber[1], Kristina Mojsilović[2], Rastko Vasilić[2], Jelena B. Bajat[3]
[1]*University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Physics, Studentski trg 12, Belgrade, Serbia*
[3]*University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia*
jela@tmf.bg.ac.rs

Plasma electrolytic oxidation (PEO) is an innovative, environmentally friendly method for oxide film formation on aluminium, magnesium, titanium. These oxide films have excellent adhesion, hardness, corrosion and wear resistance. The PEO coatings formed at 20 °C, 30 mA cm^{-2} on aluminium with the addition of CeO_2, $Ce(NO_3)_3$ or $CeCl_3$, were studied in this work. The corrosion stability of bare PEO films on aluminium, and the ones with Ce-based inhibitors was determined by polarization measurements and electrochemical impedance spectroscopy. The influence of Ce source was discussed, as well as differences observed in corrosion stability provided by different protective systems.

Acknowledgment: This research was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-34/2026-03/200135, 451-03-33/2026-03/200026, 451-03-33/2026-03/200162).

P-EH-2

Elektrohemijska stabilnost kompozitnih prevlaka za primenu u biomedicini

Ana Janković[1], Milena Stevanović[1], Marija Djošić[2], Vesna Mišković-Stanković[3,4]
[1]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2]*Institut za tehnologiju nuklearnih i drugih mineralnih sirovina (ITNMS), Beograd, Srbija*
[3]*Univerzitet Union – Nikola Tesla, Fakultet za ekologiju i zaštitu životne sredine, Beograd, Srbija*
[4]*Srpska akademija nauka i umetnosti, Beograd, Srbija*
ajankovic@tmf.bg.ac.rs

Kompozitne prevlake na bazi hidroksiapatita, poli(vinil alkohola) i hitozana, sa i bez gentamicina, dobijene su postupkom elektroforetskog taloženja iz vodenih suspenzija. Površinskim metodama potvrđeno je formiranje homogenih prevlaka sa odgovarajućom površinskom morfologijom. Elektrohemijska ispitivanja u simuliranoj telesnoj tečnosti pokazala su smanjenje gustine struje korozije i povećanje impedancije tokom 28 dana, što ukazuje na poboljšanu korozionu otpornost i površinsku stabilnost. Uvođenjem gentamicina očuvana su elektrohemijska svojstva, dodatno potvrđujući potencijal ovih prevlaka za primenu na titanskim implantatima.

Electrochemical stability of composite coatings for biomedical applications

Ana Janković[1], Milena Stevanović[1], Marija Djošić[2], Vesna Mišković-Stanković[3,4]
[1] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *Institute for Technology of Nuclear and Other Mineral Raw Materials (ITNMS), Belgrade, Serbia*
[3] *University Union – Nikola Tesla, Faculty of Ecology and Environmental Protection, Belgrade,Serbia*
[4] *Serbian Academy of Sciences and Arts, Belgrade, Serbia*
ajankovic@tmf.bg.ac.rs

Composite coatings based on hydroxyapatite, poly(vinyl alcohol), and chitosan, with and without gentamicin, were produced by electrophoretic deposition from aqueous suspensions. Surface characterization confirmed the formation of homogeneous coatings with favourable surface morphology. Electrochemical assessment in simulated body fluid demonstrated a decrease in corrosion current density and an increase in impedance over 28 days of immersion, indicating enhanced corrosion resistance and interfacial stability. The incorporation of gentamicin maintained the electrochemical properties, thereby further confirming the potential of these coatings for application on titanium implants.

Acknowledgment: This research is supported by SASA (Contract No. F-52), University Union - Nikola Tesla, Belgrade, Serbia (Contract No. 1318/1) and The Ministry of Science, Technological Development and Innovation, Republic of Serbia (Contracts No. 451-03-33/2026-03/200287, 451-03-33/2026-03/200023, 337-00-110/2023-05/13).

P-EH-3

Efekat morfologije bizmuta na aktivnost Pd@Bi katalizatora u elektrohemijskoj oksidaciji mravlje kiseline

Milica G. Košević, Nebojša D. Nikolić, Jelena D. Lović
Centar za elektrohemiju, Institut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija
milica.kosevic@ihtm.bg.ac.rs

Bimetalni Pd@Bi katalizatori su sintetizovani elektrohemijskom depozicijom Pd na prethodno pripremljene nanočestice Bi, a dobijeni katalizatori su testirani u reakciji elektrohemijske oksidacije mravlje kiseline (FAO). Nanostrukturni nataloženi bizmut u obliku zrna ili dendrita dobijen je primenom različitih katodnih potencijala, a zatim modifikovani sa Pd. Pd@Bi elektrokatalizator konstruisan od pojedinačnih Bi dendrita kao podsloja pokazao je 1,5 puta veću aktivnost i poboljšanu FAO kinetiku u poređenju sa Pd@Bi elektrokatalizatorom konstruisanim od Bi zrna. Zaključeno je da je kontrola morfologije obećavajuća i efikasna strategija za poboljšanje elektrokatalitičke aktivnosti i selektivnosti.

Effect of bismuth morphology on the activity of Pd@Bi catalysts in the electrochemical oxidation of formic acid

Milica G. Košević, Nebojša D. Nikolić, Jelena D. Lović
University of Belgrade, Institute of Chemistry, Technology and Metallurgy - National Institute of the Republic of Serbia, Belgrade, Serbia
milica.kosevic@ihtm.bg.ac.rs

Bimetallic Pd@Bi catalysts were synthesized by the electrochemical deposition of Pd onto previously prepared Bi nanoparticles, and the obtained catalysts were tested in the formic acid electrooxidation reaction (FAOR). Nanostructured bismuth deposits in the form of grains or dendrites were obtained by applying different cathodic potentials and subsequently modified with Pd. The Pd@Bi electrocatalyst consisting of individual Bi dendrites as the sublayer exhibited 1.5-fold higher activity than the Pd@Bi electrocatalyst consisting of Bi grains. It was concluded that morphology control is a promising and effective strategy for improving electrocatalytic activity and selectivity.

Acknowledgment: This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No. 451-03-33/2026-03/200026).

Fizička hemija

Physical Chemistry

P-FH-1

Oscilatorna Briggs–Rauscher reakcija u prisustvu dopirane cinkom fosfat-volframove bronze

Jovana S. Acković[1], Jelena P. Maksimović[2] , Pavle I. Tancić[3], Zoran P. Nedić[2], Jelena V. Senćanski[4], Ružica J. Micić[1], Maja C. Pagnacco[3]

[1]*Univerzitet u Prištini sa sedištem u Kosovskoj Mitrovici, Prirodno-matematički fakultet, Departman za hemiju, Lole Ribara 29, 38220 Kosovska Mitrovica, Srbija*

[2]*Univerzitet u Beogradu, Fakultet za fizičku hemiju, Studentski trg 12-16, Beograd, Srbija*

[3]*Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Njegoševa 12, 11000 Beograd*

[4]*Univerzitet u Beogradu, Institut za multidisciplinarna istrazivanja, Kneza Višeslava 1, 11030 Beograd, Srbija*

jovana.ackovic@pr.ac.rs

Briggs–Rauscher (BR) reakcija predstavlja osetljiv hemijski oscilatorni sistem, pogodan za ispitivanje antioksidativnog, antiradikalskog, ali i katalitičkog uticaja dodatih supstanci. U ovom radu analiziran je uticaj fosfat-volframove broze dopirane cinkom (Zn-PWB) na oscilatorno ponašanje BR reakcije. Dodate su različite mase Zn-PWB, a uticaj dopirane bronze na BR dinamiku procenjen je na osnovu dobijenih oscilograma. Rezultati pokazuju da dopirana bronza značajno menja dinamiku BR sistema, što ukazuje na potencijalna katalitička svojstva ove bronze.

The oscillatory Briggs–Rauscher reaction in the presence of zinc-doped phosphate-tungsten bronze

Jovana S. Acković[1], Jelena P. Maksimović[2], Pavle I. Tancić[3], Zoran P. Nedić[2], Jelena V. Senćanski[4], Ružica J. Micić[1], Maja C. Pagnacco[3]

[1]*University of Priština in Kosovska Mitrovica, Faculty of Sciences and Mathematics, Department of Chemistry, Lole Ribara 29, 38220 Kosovska Mitrovica, Serbia*

[2]*University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, Belgrade, Serbia*

[3]*University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia*

[4]*University of Belgrade, Institute for Multidisciplinary Research, Kneza Višeslava 1, 11030 Belgrade, Serbia*

jovana.ackovic@pr.ac.rs

The Briggs–Rauscher (BR) reaction is a sensitive chemical oscillatory system, suitable for examining the antioxidant, antiradical, as well as catalytic effects of added substances. In this study, the influence of phosphate-tungsten bronze doped with zinc (Zn-PWB) on the oscillatory behaviour of this reaction were investigated. Different masses of Zn-PWB were added, and the effect of the doped bronze on BR dynamics was evaluated based on the obtained oscillograms. The results show that the doped bronze significantly changes the dynamics of the BR system, indicates potential catalytic properties of this bronze.

Acknowledgements: This study was financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Grants No. 451-03-34/2026-03).

Hemija i tehnologija hrane

Chemistry and Technology of Food

P-HTH-1

Fitohemijski profil cvetova vrste *Chrysanthemum carinatum*

Sandra Vuković[1], Sofija Kilibarda[1], Marija Stojanović[1], Aleksandar Ž. Kostić[1]
[1]*Univerzitet u Beogradu, Poljoprivredni fakultet, Beograd, Srbija*
akostic@agrif.bg.ac.rs

Chrysanthemum carinatum Schousb. je ukrasna vrsta iz familije Asteraceae sa jestivim cvetovima. U ovom istraživanju, sveži cvetovi ekstrahovani su pomoću 80% acetona i 80% metanola radi procene njihovog fitohemijskog profila spektrofotometrijskim metodama, uključujući sadržaj fotosintetičkih pigmenata (hlorofil *a*, hlorofil *b* i ukupni karotenoidi), ukupnih fenola (TPC), ukupnih flavonoida (TFC) i derivata hidroksicimetnih kiselina (HCAs). Sadržaj pigmenata u acetonskim ekstraktima iznosio je 50,69 μg g^{-1} za hlorofil *a*, 23,87 μg g^{-1} za hlorofil *b* i 42,09 μg g^{-1} za ukupne karotenoide. Nisu utvrđene statistički značajne razlike između acetonskih i metanolnih ekstrakata u pogledu sadržaja TPC, TFC i HCAs. U acetonskim ekstraktima vrednosti su iznosile 6,06 mg g^{-1} GAE, 3,10 mg g^{-1} QE i 1,32 mg g^{-1} CGAE, redom, dok su u metanolnim ekstraktima izmerene vrednosti bile 6,69 mg g^{-1} GAE, 2,80 mg g^{-1} QE i 1,38 mg g^{-1} CGAE. U poređenju sa drugim vrstama iz familije Asteraceae, cvetovi vrste *C. carinatum* mogu se smatrati umereno bogatim izvorom bioaktivnih jedinjenja.

Phytochemical profile of edible flowers of *Chrysanthemum carinatum*

Sandra Vuković[1], Sofija Kilibarda[1], Marija Stojanović[1], Aleksandar Ž. Kostić[1]
University of Belgrade, Poljoprivredni fakultet, Beograd, Srbija
akostic@agrif.bg.ac.rs

Chrysanthemum carinatum Schousb. is an ornamental species from the Asteraceae family with edible flowers. In this study, flowers were extracted using 80% acetone and 80% methanol to evaluate their phytochemical profile by spectrophotometric methods, including photosynthetic pigments (chlorophyll *a*, chlorophyll *b*, and total carotenoids), total phenolic content (TPC), total flavonoid content (TFC), and hydroxycinnamic acid derivatives (HCAs). Pigments content in acetone extracts was 50.69 μg g^{-1}, 23.87 μg g^{-1}, and 42.09 μg g^{-1} for chlorophyll *a*, chlorophyll *b* and total carotenoids, respectively. No statistically significant differences were observed between acetone and methanolic extracts for TPC, TFC, or HCAs. In acetone extracts, values were 6.06 mg g^{-1} GAE, 3.10 mg g^{-1} QE, and 1.32 mg g^{-1} CGAE, respectively, while methanol extract contained 6.69 mg g^{-1} GAE, 2.80 mg g^{-1} QE, and 1.38 mg g^{-1} CGAE, respectively. Compared with other Asteraceae species, *C. carinatum* flowers can be considered a moderately rich source of bioactive compounds.

P-HTH-2

Opšti fitohemijski sastav pčelinjeg polena *Papaver* sp. različitog geografskog porekla

Duygu Nur Çobanoğlu[1], Ikranur Felek[1], Piroz Duzdaban[1], Danijel D. Milinčić[2], Mirjana B. Pešić[2], Aleksandar Ž. Kostić[2]

[1]*Univerzitet u Bingolu, Stručna škola za hranu, poljoprivredu i stočarstvo, Bingol, Turska*
[2]*Univerzitet u Beogradu, Poljoprivredni fakultet, Beograd, Srbija*
akostic@agrif.bg.ac.rs

Pčelinji polen predstavlja jedan od najpopularnijih pčelinjih proizvoda koji se često koristi kao funkcionalni dodatak hrani zbog izuzetnog sadržaja nutrijenata i bioaktivnih jedinjenja. Međutim, sadržaj svih komponenti u polenu snažno je uslovljen njegovim botaničkim ali i geografskim poreklom. Zbog toga, cilj ovog rada je bio da ispita opšti fitohemijski sastav 8 uzoraka polena istog botaničkog porekla (*Papaver* sp.) sakupljenog na području Turske. U tom smislu, određeni su sadržaji ukupnih karotenoida, fenolnih jedinjenja (Folin-Cicolteu, TPC), flavonoida (TFC) i derivata hidroksicimetne kiseline (HCA) standardnim spektrofotometrijskim metodama. Dok su se sadržaji ukupnih karotenoida (0,11-117,8 μg/g) značajno razlikovali, zavisno od geografskog porekla uzorka, vrednosti za TPC (11,1-14,1 mg/g GAE), TFC (5,3-6,6 mg/g RE) i HCA (5,6-8,7 mg/g CGAE) su pokazale manje ali značajne varijacije. Dobijeni rezultati ukazuju da osim botaničkog i geografsko poreklo može usloviti varijacije u fitohemijskom sastavu pčelinjeg polena.

Proximate phytochemical composition of *Papaver* sp. bee-collected pollen with different geographical origin

Duygu Nur Çobanoğlu[1], Ikranur Felek[1], Piroz Duzdaban[1], Danijel D. Milinčić[2], Mirjana B. Pešić[2], Aleksandar Ž. Kostić[2]

[1]*University of Bingöl , Vocational School of Food, Agriculture and Livestock, Bingöl, Türkiye*
[2]*University of Belgrade, Faculty of Agriculture, Belgrade, Serbia*
akostic@agrif.bg.ac.rs

Bee-collected pollen (BCP) is one of the most popular bee products that is often used as a functional food additive due to its exceptional content of nutrients and bioactive compounds. However, the content of all components in pollen is strongly conditioned by its botanical and geographical origin. Therefore, the aim of this work was to examine the general phytochemical composition of 8 BCP samples of the same botanical origin (*Papaver* sp.) collected in Türkiye. Accordingly, content of total carotenoids, phenolics (Folin-Cicolteu, TPC), flavonoids (TFC) and derivatives of hydroxycinnamic acid (HCA) were determined by standard spectrophotometric methods. While the content of total carotenoid (0.11-117.8 μg/g) differed significantly, depending on the geographical origin of the sample, the TPC (11.1-14.1 mg/g GAE), TFC (5.3-6.6 mg/g RE) and HCA (5.6-8.7 mg/g CGAE) content were with lower but significant variability. The obtained results indicate that beside the botanical, geographical origin of the BCP can influence on phytochemical composition.

P-HTH-3

Sadržaj odabranih bioaktivnih jedinjenja i antioksidativna aktivnost različitih sorti avokada

Marko Vukomanović[1], Ivana Grbić[1], Bogdana Simonović[1], Nebojša Đ. Pantelić[1]
[1] *Univerzitet u Beogradu, Poljoprivredni fakultet, Nemanjina 6, 11080 Beograd, Srbija*
markovukoman99@gmail.com

Avokado predstavlja značajan izvor bioaktivnih jedinjenja sa izraženim antioksidativnim svojstvima.[1] U ovom radu ispitane su tri sorte avokada (Arad, Pinkerton i Hass) sa ciljem određivanja sadržaja ukupnih polifenola, flavonoida i karotenoida, kao i antioksidativne aktivnosti primenom DPPH i FRAP metoda. Dobijeni rezultati ukazali su na razlike između ispitivanih sorti u sadržaju bioaktivnih komponenti i antioksidativnom kapacitetu. Sorta Hass pokazala je najveći sadržaj ukupnih polifenola i flavonoida, kao i najizraženiju antioksidativnu aktivnost primenom oba testa, dok je sadržaj karotenoida varirao između sorti. Rezultati potvrđuju značaj avokada kao funkcionalne namirnice i ukazuju na potencijal pojedinih sorti kao izvora prirodnih antioksidanasa.

Content of selected bioactive compounds and antioxidant activity of different avocado cultivars

Marko Vukomanović[1], Ivana Grbić[1], Bogdana Simonović[1], Nebojša Đ. Pantelić[1]
[1]*University of Belgrade, Faculty of Agriculture, Nemanjina 6, 11080 Belgrade, Serbia*
markovukoman99@gmail.com

Avocado is an important source of bioactive compounds with pronounced antioxidant properties.[1] In this study, three avocado cultivars (Arad, Pinkerton, and Hass) were analyzed in order to determine the content of total polyphenols, flavonoids, and carotenoids, as well as antioxidant activity using DPPH and FRAP assays. The obtained results indicated differences among the investigated cultivars in the content of bioactive compounds and antioxidant capacity. The Hass cultivar showed the highest content of total polyphenols and flavonoids, as well as the strongest antioxidant activity using both assays, while carotenoid content varied among cultivars. The results confirm the importance of avocado as a functional food and highlight the potential of certain cultivars as sources of natural antioxidants.

1. A.P.S. Nascimento, M.E.M. Duarte, A.P.T. Rocha, A.N. Barros, *Foods*. **2025**, *14*, 2746.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia, grant number: 451-03-34/2026-03/200116.

Hemija i tehnologija materijala

Chemistry and Technology of Materials

P-HTM-1

Ekološki prihvatljivi hitozan–genipin sorbenti za tretman otpadnih voda nakon pranja veša

Marija Lj. Lučić Škorić[1], Nikola Z. Milašinović[2], Nedeljko B. Milosavljević[3], Melina T. Kalagasidis Krušić[4]

[1]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[2]*Kriminalističko-policijski univerzitet, Beograd, Srbija*
[3]*Univerzitet u Beogradu, Beograd, Srbija*
[4]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
mkrusic@tmf.bg.ac.rs

Hitozan–genipin hidrogelovi su sintetisani i ispitani kao sorbenti za uklanjanje model boje *C.I.* Acid Orange 7 (AO7) iz simuliranih otpadnih voda nakon pranja veša. Analiziran je uticaj vremena kontakta i temperature na proces sorpcije, kao i ispitivanje uklanjanja iz različitih sistema za pranje veša: česmenske vode, rastvora praškastog detergenta i tečnog detergenta za tamne tkanine. Proces sorpcije se karakteriše brzom kinetikom, pri čemu je ravnoteža postignuta u intervalu od 60 do 120 minuta, nakon intenzivnog početnog uklanjanja boje tokom prvih pola sata. Prisustvo detergenata blago smanjuje efikasnost sorpcije, ali je visok stepen uklanjanja zadržan u svim ispitanim sistemima. Hidrogelovi pokazuju dobru mogućnost ponovne upotrebe kroz više ciklusa. Dobijeni rezultati ukazuju na veliki potencijal primene ovih materijala za uklanjanje boja iz složenih vodenih sistema.

Eco-friendly chitosan–genipin sorbents for treating laundry wastewater

Marija Lj. Lučić Škorić[1], Nikola Z. Milašinović[2], Nedeljko B. Milosavljević[3], Melina T. Kalagasidis Krušić[4]

[1]*Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Criminal Investigation and Police Studies - Belgrade, Serbia*
[3]*University of Belgrade - Belgrade, Serbia*
[4]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
mkrusic@tmf.bg.ac.rs

Chitosan–genipin hydrogels were synthetized and employed for the removal of the dye *C.I.* Acid Orange 7 (AO7) from simulated laundry wastewater. The influence of contact time, temperature, and washing medium (tap water, washing powder solution, and liquid detergent for dark fabrics) on the sorption process was analyzed. Rapid adsorption was observed, with most dye removal occurring within the first 30 min and equilibrium was reached within 60–120 min. Increasing temperature enhanced both removal efficiency and adsorption rate. The presence of detergents slightly reduced adsorption efficiency, but high removal rates were maintained in all tested systems. The hydrogels demonstrated good reusability over multiple cycles. These results demonstrate the potential of chitosan–genipin hydrogels for dye removal from complex aqueous systems.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Contract No. 451-03-34/2026-03/ 200135 and 451-03-33/2026-03/200287).

P-HTM-2

Karboksimetilceluloza kao efikasan stabilizator emulzija tipa ulje u vodi

Marija Lj. Lučić Škorić[1], Melina T. Kalagasidis Krušić[2]
[1]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
mlucic@tmf.bg.ac.rs

U ovom radu je ispitana mogućnost formiranja emulzija tipa ulje u vodi korišćenjem prirodnih polimera, karboksimetilceluloze (CMC) i natrijum-alginata, kao emulgatora. Ispitan je uticaj različitih koncentracija polimera (0,5–2,0 mas.% CMC; 0,1–2,0 mas.% natrijum-alginat) i udela uljane faze (7,5–15 vol.%). Stabilnost dobijenih sistema praćena je vizuelnom i mikroskopskom analizom (veličina i raspodela kapi ulja u emulzijama), uz ispitivanje uticaja pH vrednosti, temperature (7 °C, 20 °C i 37 °C) i primenom testa ubrzanog starenja centrifugiranjem. Rezultati su pokazali da pomoću natrijum-alginata nije moguće dobiti stabilne emulzije, dok je kombinacija polimera dovela do kratkotrajne stabilnosti. Nasuprot tome, CMC je pokazala značajan emulgujući potencijal, pri čemu su stabilni sistemi dobijeni pri koncentracijama od 1,5 i 2,0 mas.%. Najbolju stabilnost pokazala je formulacija sa 2,0 mas.% CMC i 10 vol.% ulja. Dobijeni rezultati ukazuju da se CMC potencijalno može koristiti kao prirodni emulgator za emulzije tipa ulje u vodi.

Carboxymethyl cellulose as an effective stabilizer for oil-in-water emulsions

Marija Lj. Lučić Škorić[1], Melina T. Kalagasidis Krušić[2]
[1]*Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
mlucic@tmf.bg.ac.rs

This study evaluates the efficacy of natural polymers, carboxymethyl cellulose (CMC) and sodium alginate, as stabilizing agents in oil-in-water (O/W) emulsions. The concentrations of polymers (0.5–2.0 wt.% CMC; 0.1–2.0 wt.% sodium alginate) and the oil phase fraction (7.5–15 vol.%) were varied. The stability of the obtained systems was monitored using visual and microscopic analysis (droplet size and size distribution), along with the evaluation of pH effects, temperature (7 °C, 20 °C, and 37 °C), and accelerated stability testing by centrifugation. The results showed that sodium alginate did not form stable emulsions, while polymer combinations resulted only in short-term stability. In contrast, CMC demonstrated significant emulsifying potential, with stable systems obtained at concentrations of 1.5 and 2.0 wt.%. The best performance was achieved with a formulation containing 2.0 wt.% CMC and 10 vol.% oil phase. These findings indicate the potential of CMC as a natural emulsifier in O/W emulsions.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Contract No. 451-03-34/2026-03/200135 and 451-03-33/2026-03/200287).

P-HTM-3

Dopirani α-Bi_2O_3 za primenu u adsorpciji i fotokatalizi

Natalija D. Milojković[1], Bojana M. Simović[2], Andrija P. Kokanović[3], Lidija D. Radovanović[4], Slavica S. Lazarević[1], Aleksandra H. Dapčević[1]

[1]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Institut za multidisciplinarna istraživanja, Beograd, Srbija*
[3]*Inovacioni centar Hemijskog fakulteta, Beograd, Srbija*
[4]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
nmilojkovic@tmf.bg.ac.rs

Cilj ovog rada bio je sinteza i karakterizacija dopiranih oksida bizmuta sa poboljšanim svojstvima u odnosu na Bi_2O_3. Uzorci 1 mas.% M/Bi_2O_3 (M = Cu, Lu, Ru) sintetisani su hidrotermalnom metodom (12 h, 120 °C), dok je Bi_2O_3 dobijen pod istim uslovima, u odsustvu dopanata, radi poređenja. Sintetisani prahovi okarakterisani su XRD, FTIR, FESEM, EDS i UV-Vis metodama, dok su njihova adsorpciona i fotokatalitička svojstva ispitana kroz uklanjanje toksične boje RO16. Pokazano je da je monoklinični α-Bi_2O_3 dominantna faza u svim uzorcima. Svi uzorci pokazali su dobra adsorpciona i fotokatalitička svojstva. Najizraženiju adsorpciju boje (80,7 %) demonstrirao je 1 mas.% Cu/Bi_2O_3, dok je Bi_2O_3 pokazao najbolju fotokatalitičku aktivnost razgradivši 98,3 % boje nakon 240 min pod dejstvom simulirane sunčeve svetlosti.

Doped α-Bi_2O_3 for adsorption and photocatalytic application

Natalija D. Milojković[1], Bojana M. Simović[2], Andrija P. Kokanović[3], Lidija D. Radovanović[4], Slavica S. Lazarević[1], Aleksandra H. Dapčević[1]

[1]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia*
[3]*Innovative Centre of the Faculty of Chemistry, Belgrade, Serbia*
[4]*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
nmilojkovic@tmf.bg.ac.rs

The aim of this work was a synthesis and characterization of doped bismuth(III) oxides with improved properties compared to pristine Bi_2O_3. Samples 1 wt.% M/Bi_2O_3 (M = Cu, Lu, Ru) were synthesized by a hydrothermal method (12 h, 120 °C), while the pure Bi_2O_3 was prepared under the same conditions in the absence of dopants, for comparison. The obtained powders were characterized by XRD, FTIR, FESEM, EDS, and UV-Vis methods, while their adsorption and photocatalytic properties were examined toward removing toxic dye RO16. The monoclinic α-Bi_2O_3 was the dominant phase in all the samples. All the samples exhibited good adsorption and photocatalytic properties. The most pronounced dye adsorption (80.7 %) was observed for 1 wt.% Cu/Bi_2O_3, while Bi_2O_3 demonstrated the highest photocatalytic activity by degrading 98.3 % of the dye after 240 min under simulated solar light.

P-HTM-4

ZnO modifikovan ugljenikom iz poljoprivrednog otpada za prečišćavanje vode

Bojana M. Simović[1], Natalija D. Milojković[2], Jelena K. Dikić[3], Lidija D. Radovanović[3], Aleksandra H. Dapčević[2]

[1]*Univerzitet u Beogradu, Institut za multidisciplinarna istraživanja, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija,*
[3]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
nmilojkovic@tmf.bg.ac.rs

U radu je prikazana „zelena“ precipitaciona sinteza C/ZnO korišćenjem ekstrakta otpadne ljuske crnog luka (*Allium cepa*) kao redukcionog sredstva i izvora bio-ugljenika, nakon koje su uzorci kalcinisani na 350 i 500 °C. Rendgenskom difrakcijom potvrđeno je formiranje vurcitnog ZnO. Kristaliti u uzorku dobijenom na 350 °C su nešto manji nego u uzorku dobijenom na 500 °C: 28 prema 35 nm. FTIR i FESEM analize ukazale su na prisustvo ugljeničnih vrsta, pored nanočestica ZnO. Uzorci su pokazali visoku i međusobno sličnu fotokatalitičku aktivnost razgradivši tekstilnu boju Reactive Orange 16 za 120 minuta, kao i antibakterijsko dejstvo prema *Staphylococcus aureus* ATCC 25923 i *Escherichia coli* DSM 498, što ukazuje na njihov potencijal za primenu u prečišćavanju voda.

Carbon-modified ZnO from agricultural waste for water purification

Bojana M. Simović[1], Natalija D. Milojković[2], Jelena K. Dikić[3], Lidija D. Radovanović[3], Aleksandra H. Dapčević[2]

[1]*University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[3]*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
nmilojkovic@tmf.bg.ac.rs

This study presents a green precipitation synthesis of C/ZnO using waste onion peel (*Allium cepa*) extract as a reducing agent and a bio-carbon source, followed by calcination at 350 and 500 °C. X-ray diffraction analysis confirmed the formation of the wurtzite ZnO phase. The crystallite size of the sample obtained at 350 °C was slightly smaller than that of the sample calcined at 500 °C: 28 vs. 35 nm. FTIR and FESEM analyses indicated the presence of carbonaceous species alongside ZnO nanoparticles. The synthesized samples exhibited high and mutually similar photocatalytic activity by degrading Reactive Orange 16 textile dye for 120 min, as well as antibacterial activity against *Staphylococcus aureus* ATCC 25923 and *Escherichia coli* DSM 498, indicating their potential application in water purification.

P-HTM-5

Hidrotermalna modifikacija g-C_3N_4 dobijenog iz uree: uticaj dužine trajanja tretmana na fotokatalitičku redukciju Cr(VI)

Sofija Petković[1], Jana Petrović[1], Rada Petrović[2]
[1]*Inovacioni centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
spetkovic@tmf.bg.ac.rs

Grafitni ugljenik(IV)-nitrid (g-C_3N_4) je netoksičan poluprovodnik, stabilan u kiseloj sredini, sa velikim redukcionim potencijalom, što je od značaja za fotokatalitičku redukciju toksičnog šestovalentnog hroma (Cr(VI)) do manje štetnog Cr(III). Ipak, fotokatalitička efikasnost g-C_3N_4 je relativno niska, a jedan od razloga je i mala specifična površina, koja se može povećati raslojavanjem, odnosno eksfolijacijom. U tom cilju, g-C_3N_4 je u ovom radu sintetisan termičkom polimerizacijom iz uree, a zatim hidrotermalno tretiran na 180°C tokom 4, 8 i 12 h. Karakterizacija primenom FE-SEM, EDX, XRD, FTIR i DRS analiza, zajedno sa ispitivanjem fotokatalitičke redukcije Cr(VI), pokazala je da je optimalno vreme hidrotermalnog tretmana 4 h usled efikasne eksfolijacije i poboljšanih površinskih svojstava. Iako produženi hidrotermalni tretman povećava kristaliničnost i sužava energetsku zabranjenu zonu, dovodi do smanjenja fotokatalitičke aktivnosti usled prekomerne eksfolijacije (8 h) ili formiranja nove faze sa slabom sposobnošću adsorpcije Cr(VI) (12 h).

Hydrothermal modification of urea-derived g-C_3N_4: effect of treatment time on photocatalytic Cr(VI) reduction

Sofija Petković[1], Jana Petrović[1], Rada Petrović[2]
[1]*Innovation Center of Faculty of Technology and Metallurgy Ltd, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
spetkovic@tmf.bg.ac.rs

Graphite carbon(IV)-nitride (g-C_3N_4) is a non-toxic semiconductor, stable in an acidic environment, with a high reduction potential, which is important for the photocatalytic reduction of toxic hexavalent chromium (Cr(VI)) to less harmful Cr(III). Nevertheless, the photocatalytic efficiency of g-C3N4 is relatively low, and one of the reasons is the small specific surface, which can be increased by layering, i.e. exfoliation. In this work, g-C_3N_4 was synthesized by thermal polymerization from urea, and then hydrothermally treated for 4, 8 and 12 h. Characterization by FE-SEM, EDX, XRD, FTIR, and DRS analyses, together with photocatalytic reduction tests of Cr(VI), showed that the optimal hydrothermal treatment time was 4 h due to effective exfoliation and improved surface properties. Although prolonged hydrothermal treatment increased crystallinity and narrowed the band gap, it resulted in lower photocatalytic activity due to over-exfoliation (8 h) or formation of a new phase with poor Cr(VI) adsorption ability (12 h).

P-HTM-6

Fotokatalitička redukcija Cr(VI) pod dejstvom vidljivog zračenja upotrebom $ZnFe_2O_4/g\text{-}C_3N_4$

Jana Lj. Petrović[1], Sofija Petković[1], Đorđe Janaćković[2], Rada Petrović[2]
[1]*Inovacioni centar Tehnološko-metalurškog fakulteta, d.o.o. Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
petrovicj@tmf.bg.ac.rs

Fotokatalitička efikasnost poluprovodnika je u najvećem broju slučajeva ograničena velikom brzinom rekombinacije fotogenerisanih elektrona i šupljina. Kako bi se prevazišao ovaj nedostatak, $ZnFe_2O_4/g\text{-}C_3N_4$ (ZFO/CN) kompozitni fotokatalizatori su sintetisani jednostavnom hidrotermalnom metodom, gde je $g\text{-}C_3N_4$ dobijen termalnom polimerizacijom uree. ZFO/CN kompoziti su sintetisani pri različitim masenim odnosima (1/1, 0,5/1 i 0,1/1), kako bi se dobio optimalan heterospoj sa poboljšanom apsorpcijom vidljivog zračenja i boljom fotokatalitičkom aktivnošću. Za karakterizaciju dobijenih materijala korišćene su XRD, FTIR, BET, FESEM, EDS i DRS metode. Rezultati DRS analize su pokazali da su kompozitni fotokatalizatori imali užu zabranjenu zonu u odnosu na čist CN. Dobijeni uzorci su korišćeni za fotokatalitičku redukciju Cr(VI), a najveća efikasnost je postignuta pri odnosu ZFO : CN=0,1:1.

Visible-light photoreduction of Cr(VI) over $ZnFe_2O_4/g\text{-}C_3N_4$ heterojunction

Jana Lj. Petrović[1], Sofija Petković[1], Đorđe Janaćković[2], Rada Petrović[2]
[1]*Innovation Center of the Faculty of Technology and Metallurgy, Ltd, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
petrovicj@tmf.bg.ac.rs

The photocatalytic efficiency of semiconductors is mostly limited by the high recombination rate of photogenerated electrons and holes. To address this issue, $ZnFe_2O_4/g\text{-}C_3N_4$ (ZFO/CN) composite photocatalysts were synthesized using a simple hydrothermal method, while $g\text{-}C_3N_4$ was prepared by thermal polymerization of urea. Additionally, different ZFO/CN mass ratios were explored (1/1, 0.5/1 and 0.1/1) to construct a heterojunction system with improved visible-light absorption and enhanced photocatalytic performance. The materials were characterized by XRD, FTIR, BET, FESEM, EDS, and DRS analyses. DRS results showed a reduced band gap energy for all composites compared to the pristine samples. The samples were used for the photocatalytic reduction of Cr(VI), and the highest efficiency was achieved when the ZFO/CN ratio was 0.1:1.

Hemija životne sredine

Environmental Chemistry

P-HŽS-1

Detekcija arsena u uzorcima vode korišćenjem Au-dekorisanog MOF senzora

Aleksandar M. Đorđević[1], Kristina Radinović[2], Alexandre Viana[3], Salete S. Balula[3], Luís Cunha-Silva[3], Diogo M.F. Santos[4], Biljana Šljukić[2,4]

[1]*Institut za opštu i fizičku hemiju, Beograd, Srbija*

[2]*Univerzitet u Beogradu, Fakultet za fizičku hemiju, Beograd, Srbija*

[3]*LAQV-REQUIMTE, Odeljenje za hemiju i biohemiju, Fakultet prirodnih nauka, Univerzitet u Portu, Porto, Portugal*

[4]*Centar za fiziku i inženjerstvo naprednih materijala, Laboratorija za fiziku materijala i nove tehnologije, Odeljenje za hemijsko inženjerstvo, Viši tehnički institut, Univerzitet u Lisabonu, Lisabon, Portugal*

adjordjevic@iofh.bg.ac.rs

Kontaminacija voda arsenom predstavlja značajan ekološki i zdravstveni problem, pri čemu je As(III) posebno toksičan. U ovom radu razvijen je elektrohemijski senzor za određivanje arsena u uzorcima vode, baziran na Au@NH_2-MOF-808 materijalu. Optimizovani su parametri merenja, uključujući potencijal i vreme depozicije, kao i brzina polarizacije. Senzor pokazuje izražen elektrohemijski odgovor, dobru ponovljivost i selektivnost u prisustvu interferentnih jona, naročito Cu^{2+}. Primena na realnim uzorcima, vode iz Zrenjanina, potvrdila je njegovu pouzdanost i potencijal za brzu, osetljivu i ekonomičnu terensku analizu arsena.

Sensitive detection of arsenic in real water samples using an Au-decorated MOF sensor

Aleksandar M. Đorđević[1], Kristina Radinović[2], Alexandre Viana[3], Salete S. Balula[3], Luís Cunha-Silva[3], Diogo M.F. Santos[4], Biljana Šljukić[2,4]

[1]*Institute of General and Physical Chemistry, Belgrade, Serbia*

[2]*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*

[3]*LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Porto, Portugal*

[4]*Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal*

adjordjevic@iofh.bg.ac.rs

Arsenic contamination of water represents a major environmental and public health issue, particularly due to the high toxicity of As(III). In this work, an electrochemical sensor for arsenic determination in water samples was developed using Au@NH_2-MOF-808 material. Experimental parameters, including deposition potential, deposition time, and scan rate, were optimized to improve sensor performance. The optimized sensor exhibited a strong electrochemical response, good repeatability, and high selectivity in the presence of interfering ions, especially Cu^{2+}. Application to real water samples from Zrenjanin confirmed its reliability and potential for rapid, sensitive, and cost-effective on-site arsenic monitoring.

Acknowledgments: The authors acknowledge the financial support from the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (contract no. 451-03-34/2026-03/200146, 451-03-33/2026-03/200146), as well as Fundaçãao para a Ciência e a Tecnologia (FCT, Portugal) (funding under contract LA/P/0095/2020, LaPMET).

P-HŽS-2

Biosorpcija organskih boja iz vodenih rastvora

Natalija Ž. Nedić, Sandra S. Bulatović, Tamara T. Tadić, Bojana M. Marković, Aleksandra B. Nastasović

Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija

natalija.nedic@ihtm.bg.ac.rs

Biosorpcija predstavlja efikasan i ekološki prihvatljiv proces uklanjanja zagađujućih jedinjenja zahvaljujući niskoj ceni, jednostavnosti primene i upotrebi prirodnih materijala. Različiti biomaterijali mogu se koristiti za uklanjanje emergentnih zagađujućih jedinjenja, među kojima organske boje predstavljaju značajnu grupu polutanata. U ovom istraživanju kao biosorbent korišćena je biomasa ambrozije (*Ambrosia artemisiifolia* L.), invazivne biljne vrste sa negativnim uticajem na životnu sredinu i zdravlje ljudi. Cilj rada bio je ispitivanje biosorpcije anjonske i katjonske boje, Orange G (OG) i Crystal Violet (CV). Eksperimenti su izvođeni pri početnoj koncentraciji od 25 ppm, vremenu kontakta od 2 h i zapremini rastvora od 10 mL. Efikasnost biosorpcije određivana je UV-Vis spektrofotometrijom (NOVEL-102S, COLOLab Experts, Slovenia). Rezultati su pokazali efikasnost uklanjanja od 98% za CV i 2% za OG. FTIR analiza pre i nakon biosorpcije potvrdila je vezivanje boje (Nicolet SUMMIT, Thermo Fisher, USA).

Biosorption of organic dyes from aqueous solutions

Natalija Ž. Nedić, Sandra S. Bulatović, Tamara T. Tadić, Bojana M. Marković, Aleksandra B. Nastasović

University of Belgrade, Institute of chemistry, technology and metallurgy, Belgrade, Serbia

natalija.nedic@ihtm.bg.ac.rs

Biosorption is an efficient and environmentally friendly process for pollutant removal due to its low cost, simple application, and the use of natural materials. Various biomaterials can be used for the removal of emerging pollutants, among which organic dyes represent an important group of contaminants. In this study, *Ambrosia artemisiifolia* L. biomass was used as a biosorbent due to its negative impact on the environment and human health. The aim of this study was to investigate the biosorption of anionic and cationic dyes, Orange G (OG) and Crystal Violet (CV). Experiments were performed at an initial concentration of 25 ppm, a contact time of 2 h, and a solution volume of 10 mL. Biosorption efficiency was determined by UV-Vis spectrophotometry (NOVEL-102S, COLOLab Experts, Slovenia). Results showed a removal efficiency of 98% for CV and 2% for OG. FTIR analysis before and after biosorption confirmed dye binding (Nicolet SUMMIT, Thermo Fisher, USA).

Acknowledgment: This research has been financially supported by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Contract No. 451-03-33/2026-03/200026). The research presented in this study aligns with Goal 6 of the Agenda 2030 - UN SDGs.

P-HŽS-3

Enzimska i održiva degradacija sintetičkih boja primenom peroksidaze izolovane iz kupusa

Tanja M. Nedeljkov[1], Nataša Ž. Šekuljica[1], Zorica D. Knežević-Jugović[2], Dušan Ž. Mijin[2]
[1]*Inovacioni centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o., Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
nsekuljica@tmf.bg.ac.rs

Sintetičke boje pripadaju grupi izrazito postojanih, potencijalno kancerogenih i mutagenih zagađivača, koji se teško uklanjaju konvencionalnim metodama razgradnje i predstavljaju ozbiljnu pretnju po životnu sredinu. Održivu alternativu tradicionalnim pristupima predstavljaju enzimske tehnologije kao efikasna i ekološki prihvatljiva rešenja. U ovom radu ispitan je potencijal poljoprivrednog otpada kupusa kao izvora peroksidaze. Aktivnost enzima određena je ABTS (2,2'-azino-bis(3-etilbenzotiazolin-6-sulfonska kiselina)) spektrofotometrijskom metodom, dok je profil čistoće enzimskog ekstrakta analiziran SDS-PAGE elektroforezom u redukujućim uslovima. Molarna masa peroksidaze određena je SDS-PAGE analizom u neredukujućim uslovima. Maksimalna aktivnost enzima (6 IU) postignuta je pri blagim reakcionim uslovima (pH 6,0 i 35 °C), pri koncentraciji boje Acid Green 40 od 10 mg/L i koncentraciji vodonik-peroksida od 0,5 mM, pri čemu je uklonjeno približno 55% boje.

Enzymatic and sustainable degradation of synthetic dyes using peroxidase isolated from cabbage

Tanja M. Nedeljkov[1], Nataša Ž. Šekuljica[1], Zorica D. Knežević-Jugović[2], Dušan Ž. Mijin[2]
[1]*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
nsekuljica@tmf.bg.ac.rs

Synthetic dyes belong to a group of highly persistent, potentially carcinogenic and mutagenic pollutants that are difficult to remove using conventional degradation methods and therefore represent a serious threat to the environment. Enzymatic technologies offer a sustainable alternative to traditional approaches as efficient and environmentally friendly solutions. In this study, the potential of agricultural cabbage waste as a source of peroxidase was investigated. Enzyme activity was determined using the ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)) spectrophotometric method, while the purity profile of the enzyme extract was analyzed by SDS-PAGE electrophoresis under reducing conditions. The molecular weight of peroxidase was determined by SDS-PAGE analysis under non-reducing conditions. Maximum enzyme activity (6 IU) was achieved under mild reaction conditions (pH 6.0 and 35 °C), at an Acid Green 40 dye concentration of 10 mg/L and hydrogen peroxide concentration of 0.5 mM, resulting in approximately 55% dye removal.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract number 451-03-34/2026-03/200135 and 451-03-33/2026-03/200287).

P-HŽS-4

Primena enzimski modifikovanog lignina iz piljevine u remedijaciji otpadnih voda

Nataša Ž. Šekuljica[1], Tanja M. Nedeljkov[1], Ivana V. Gazikalović[1], Zorica D. Knežević-Jugović[2], Dušan Ž. Mijin[2]

[1]*Inovacioni centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o., Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
nsekuljica@tmf.bg.ac.rs

Lignin se smatra otpadnim materijalom koji je, zahvaljujući svojoj obnovljivosti, biodegradabilnosti i netoksičnosti, prepoznat kao perspektivan adsorbens za remedijaciju otpadnih voda. U cilju unapređenja adsorptivnog kapaciteta, lignin se često podvrgava različitim metodama modifikacije. U ovom radu lignin izolovan iz piljevine bukve modifikovan je peroksidazom iz ljuske krompira radi dobijanja funkcionalnog materijala za prečišćavanje voda. Lignin je ekstrahovan u mikrotalasnom reaktoru korišćenjem eutektičke smeše mlečna kiselina–holin-hlorid (2:1) pri 150 °C tokom 20 min. Enzimski modifikovan lignin okarakterisan je ATR-FTIR analizom, raspodelom veličine čestica, ζ-potencijalom i sadržajem fenola, dok je dobijeni materijal pokazao poboljšanu efikasnost uklanjanja boje Acid Violet 109, pri čemu je nakon 10 min reakcije u smeši zaostalo približno 20% početne koncentracije boje.

Application of enzymatically modified lignin from sawdust in wastewater remediation

Nataša Ž. Šekuljica[1], Tanja M. Nedeljkov[1], Ivana V. Gazikalović[1], Zorica D. Knežević-Jugović[2], Dušan Ž. Mijin[2]

[1]*Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
nsekuljica@tmf.bg.ac.rs

Lignin is considered a waste material that, due to its renewability, biodegradability, and non-toxicity, has been recognized as a promising adsorbent for wastewater remediation. In order to improve its adsorption capacity, lignin is often subjected to various modification methods. In this study, lignin isolated from beech sawdust was modified using peroxidase extracted from potato peel to obtain a functional material for water purification. Lignin was extracted in a microwave reactor using a lactic acid–choline chloride deep eutectic solvent (2:1) at 150 °C for 20 min. The enzymatically modified lignin was characterized by ATR-FTIR analysis, particle size distribution, ζ-potential, and total phenolic content, while the obtained material exhibited enhanced dye removal efficiency toward Acid Violet 109, with approximately 20% of the initial dye concentration remaining in the reaction mixture after 10 min.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract number 451-03-34/2026-03/ 200135, 451-03-33/2026-03/ 200287 and bilateral project no. 337-00-216/2023-05/205).

P-HŽS-5

Optimizacija ekstrakcije i biokativnost voskovarine

Nikola Srećković[1], Vladimir Mihailović[1], Nevena Mihailović[1], Emilija Milović[2], Tatjana Panić[1]
[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija*
[2]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Srbija*
nikola.sreckovic@pmf.kg.ac.rs

Cilj ovog rada je ispitivanje sadržaja bioaktivnih jedinjenja, antioksidativne i antimikrobne aktivnosti otpada nastalog topljenjem iskorišćenog pčelinjeg saća, poznatog kao voskovarina. Etanolni ekstrakti pokazali su najviše sadržaje fenolnih i flavonoidnih jedinjenja, što je bilo praćeno i najjačom antioksidativnom aktivnošću. U celini, svi ispitivani uzorci ispoljili su umerenu, ali širokospektralnu antimikrobnu aktivnost, sa MIC vrednostima u rasponu od 1,25 do 10 mg/mL. Dobijeni rezultati ukazuju da voskovarina predstavlja perspektivan izvor bioaktivnih jedinjenja i potencijalno vrednu sirovinu za primenu u farmaceutskoj industriji. Njena valorizacija mogla bi imati značajnu ulogu u unapređenju održivog pčelarstva i razvoju prirodnih preparata sa antioksidativnim i antimikrobnim potencijalom.

Optimization of extraction and bioactivity of slumgum

Nikola Srećković[1], Vladimir Mihailović[1], Nevena Mihailović[1], Emilija Milović[2], Tatjana Panić[1]
[1]*University of Kragujevac, Faculty of Science, Kragujevac, Serbia*
[2]*University of Kragujevac, Institute for Information Technologies Kragujevac, Serbia*
nikola.sreckovic@pmf.kg.ac.rs

The aim of this study was to investigate the content of bioactive compounds, as well as the antioxidant and antimicrobial activities, of the waste material generated during the melting of used beeswax combs, known as slumgum. Ethanol extracts exhibited the highest contents of phenolic and flavonoid compounds, which were accompanied by the strongest antioxidant activity. Overall, all examined samples demonstrated moderate yet broad-spectrum antimicrobial activity, with minimum inhibitory concentration (MIC) values ranging from 1.25 to 10 mg/mL. The results obtained indicate that slumgum represents a promising source of bioactive compounds and a potentially valuable raw material for applications in the pharmaceutical industry. Its valorization could play a significant role in promoting sustainable beekeeping and in the development of natural products with antioxidant and antimicrobial potential.

Acknowledgment: This work was supported by the project BEEWASTEDERM (Agreement No. I01-1201/3), funded by the Center for Scientific Research of the Serbian Academy of Sciences and Arts and the University of Kragujevac, and by the Serbian Ministry of Education, Science and Technological Development (No. 451-03-33/2026-03/200122, 451-03-34/2026-03/200122 and 451-03-136/2025-03/200378).

P-HŽS-6

Praktična mikrotalasna sinteza *ms*-$BiVO_4$ sa unapređenim fotokatalitičkim performansama

Bojana R. Vasiljević[1], Nataša J. Tot[1], Dušan Mijin[2], Dragana J. Marinković[1]
[1]*Institut za nuklearne nauke Vinča, Univerzitet u Beogradu, Beograd, Republika Srbija*
[2]*Tehnološko-metalurški fakultet, Univerzitet u Beogradu, Beograd, Republika Srbija*
bojana.vasiljevic@vin.bg.ac.rs

Razvijena je praktična i ekološki prihvatljiva mikrotalasna (MW) metoda sinteze monokliničnog fotokatalizatora bizmut vanadata (*ms*-$BiVO_4$). Rad po prvi put jasno ističe povoljnu korelaciju između veličine kristala, efikasnosti MW zračenja i vremena formiranja u vodi kao jedinom rastvaraču. Nanokristali prosečne veličine oko 20 nm dobijeni su već nakon 10 minuta MW zračenja; visoka kristalnost potvrđena je TEM i XRD analizama. Energija zabranjene zone *ms*-$BiVO_4$ procenjena je na približno 2,55 eV. Fotokatalitička aktivnost ispitana je degradacijom Rodamina B (RhB), pri čemu je zabeležena izuzetno brza degradacija nakon 20 minuta osvetljavanja pri pH 2. Pored navedenog, studija detaljno analizira faktore koji utiču na performanse (dozu katalizatora, početnu koncentraciju boje, pH rastvora i vreme reakcije) i pruža smernice za optimizaciju uslova za maksimalnu efikasnost u prečišćavanju voda.

Practical microwave synthesis of *ms*-$BiVO_4$ with improved photocatalytic properties

Bojana R. Vasiljević[1], Nataša J. Tot[1], Dušan Mijin[2], Dragana J. Marinković[1]
[1]*Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*
[2]*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*
bojana.vasiljevic@vin.bg.ac.rs

A practical and environmentally friendly microwave (MW)-assisted method was developed for synthesizing monoclinic bismuth vanadate (*ms*-$BiVO_4$) photocatalyst. This work, for the first time, highlights a favorable relationship between crystal size, irradiation efficiency, and the time needed for its formation in water as the only solvent. Nanocrystals were obtained after 10 minutes of MW irradiation with a size of approximately 20 nm, and high crystallinity were determined using TEM and XRD, respectively. The band gap energy of *ms*-$BiVO_4$ is estimated to be about 2.55 eV. The photocatalytic efficiency was assessed through degradation studies using Rhodamine B (RhB) dye, demonstrating an impressive degradation rate after 20 min of illumination at a pH 2 environment. The present study further elucidates the photocatalytic performance of *ms*-$BiVO_4$, assessing factors influencing efficiency, including catalyst dosage, initial dye concentration, solution pH, and reaction time.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Project No. 451-03-33/2026-03/200017).

P-HŽS-7

Uticaj jonskog karaktera azo boja na fotokatalitičku aktivnost $BiVO_4$ pod vidljivom svetlošću

Nataša J. Tot[1], Bojana R. Vasiljević[1], Jovana R. Prekodravac Filipović[1], Vesna N. Despotović[2], Dragana J. Marinković[1]

[1]*Institut za nuklearne nauke Vinča, Univerzitet u Beogradu, Beograd, Republika Srbija*

[2]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine*

bojana.vasiljevic@vin.bg.ac.rs

U ovom radu ispitana je fotokatalitička aktivnost monokliničnog bizmut-vanadata (*ms*-$BiVO_4$) prema anjonskoj boji Acid Orange 7 (AO7) i katjonskoj boji Basic Yellow 28 (BY28) pod vidljivom svetlošću. Eksperimenti su izvedeni sa 15 ppm boje i koncentracijom fotokatalizatora od 0,8 g L^{-1}, nakon 15 min sonifikacije i 60 min mešanja u mraku, pri prirodnoj pH vrednosti. Nakon 120 min izlaganja vidljivoj svetlosti, za BY28 postignuto je 5 % uklanjanja, uz k = 0,002 min^{-1}, dok je za AO7 uklanjanje iznosilo 77 %, uz k = 0,009 min^{-1}. Kinetička analiza pokazala je dobro slaganje sa modelom pseudo-prvog reda (R^2 > 0,95), dok je veća efikasnost AO7 u odnosu na BY28 ukazala na selektivnost *ms*-$BiVO_4$ prema jonskom karakteru boja, što se može povezati sa površinskim naelektrisanjem fotokatalizatora.

Effect of the ionic character of azo dyes on the photocatalytic activity of $BiVO_4$ under visible light irradiation

Nataša J. Tot[1], Bojana R. Vasiljević[1], Jovana R. Prekodravac Filipović[1], Vesna N. Despotović[2], Dragana J. Marinković[1]

[1]*Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*

[2]*Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad*

bojana.vasiljevic@vin.bg.ac.rs

This work examines the photocatalytic activity of monoclinic bismuth vanadate (*ms*-$BiVO_4$) toward the anionic dye Acid Orange 7 (AO7) and the cationic dye Basic Yellow 28 (BY28) under visible light irradiation. The experiments were performed using 15 ppm dye and a photocatalyst concentration of 0.8 g L^{-1}, after 15 min sonication and 60 min stirring in the dark, at natural pH. After 120 min of visible-light irradiation, 5% removal was achieved for BY28, with k = 0.002 min^{-1}, whereas AO7 showed 77% removal, with k = 0.009 min^{-1}. Kinetic analysis showed good agreement with the pseudo-first-order model (R^2 > 0.95), while the higher AO7 efficiency compared with BY28 indicated *ms*-$BiVO_4$ selectivity toward dye ionic character, which may be related to the photocatalyst surface charge.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Project No. 451-03-33/2026-03/200017).

Medicinska hemija

Medicinal Chemistry

P-MH-1

Hibridi adamantana i sklareola sa aktivnošću prema višestruko rezistentnom nesitnoćelijskom karcinomu pluća

Pavle Stojković[1], Ema Lupšić[2], Nataša Terzić Jovanović[3], Andrea Nikolić[1], Ana Andrijević[4], Ana Stepanović[3], Ana Podolski Renić[3], Milica Pešić[3], Igor M. Opsenica[1]

[1]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Republika Srbija*

[2]*Institut za biološka istraživanja "Siniša Stanković" – Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Republika Srbija*

[3]*Univerzitet u Beogradu-Institut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Republika Srbija*

[4]*Inovacioni centar Hemijskog fakulteta u Beogradu, d.o.o., Beograd, Republika Srbija*

andrijevic@chem.bg.ac.rs

Sintetisana je serija hibrida sklareola i adamantana povezanih različitim diaminskim linkerima, čime su dobijena jedinjenja sa nanomolarnom aktivnošću prema nesitnoćelijskom karcinomu pluća. Ova jedinjenja dodatno poseduju sposobnost spontanog organizovanja u nanočestice, što ih čini perspektivnom platformom za razvoj savremene nanoterapije.

Adamantane-sclareol hybrids targeting multidrug-resistant non-small cell lung cancer cells

Pavle Stojković[1], Ema Lupšić[2], Nataša Terzić Jovanović[3], Andrea Nikolić[1], Ana Andrijević[4], Ana Stepanović[3], Ana Podolski Renić[3], Milica Pešić[3], Igor M. Opsenica[1]

[1]*University of Belgrade - Faculty of Chemistry, Belgrade, Republic of Serbia*

[2]*Institute for Biological Research "Siniša Stanković" - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Republic of Serbia*

[3]*University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Republic of Serbia*

[4]*Innovative Centre, Faculty of Chemistry, Ltd., Belgrade, Republic of Serbia*

andrijevic@chem.bg.ac.rs

A series of sclareol-adamantane hybrids bridged *via* distinct diamine linkers was synthesized, yielding lead compounds with nanomolar potency against non-small cell lung cancer cells. These compounds demonstrate spontaneous self-assembly into nanoparticles, establishing a viable platform for advanced nanotherapy.

This research was supported by the Science Fund of the Republic of Serbia, grant No. 7005, Development of nature-inspired photoresponsive anticancer agents - sclareol and artemisinin derivatives in cancer multidrug-resistance models: a foundation for the theranostic approach – PhotoSCLART.

P-MH-2

Sinteza i biološka aktivnost derivata žučnih kiselina kao aktivatora NRF2 signalnog puta

Sergej Cvijić[1], Milica Stevanović[1], Ivana Kuzminac[1], Đorđe Miljković[2], Albena Dinkova-Kostova[3], Srđan Bjedov[1]

[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija*
[2]*Univerzitet u Beogradu, Institut za biološka istraživanja „Siniša Stanković", Beograd, Srbija*
[3]*Univerzitet u Dandiju, Ujedinjeno Kraljevstvo*
srdjan.bjedov@dh.uns.ac.rs

NRF2 je transkripcioni faktor važan za ćelijsku odbranu od oksidativnog i elektrofilnog stresa, zbog čega predstavlja značajnu metu u razvoju hemoprotektivnih i citoprotektivnih agenasa. Naše istraživanje je usmereno na sintezu novih NRF2 aktivatora zasnovanih na strukturi žučnih kiselina, kao steroidnoj platformi pogodnoj za uvođenje elektrofilnih farmakofora. U ovom radu predstavljeni su linearni i ukršteni enonski derivati žučnih kiselina, njihova sinteza i biološka aktivnost. Biološka aktivnost ispitana je u humanoj ARPE-19 ćelijskoj liniji retinalnog pigmentnog epitela, praćenjem indukcije NQO1 aktivnosti kao funkcionalnog markera aktivacije NRF2 signalnog puta. Ispitivana jedinjenja su povećala NQO1 aktivnost, pri čemu je ukršteni enonski derivat pokazao izraženiji efekat od linearnog analoga. Dobijeni rezultati ukazuju na potencijal ovih derivata za dalji razvoj steroidnih NRF2 aktivatora.

Synthesis and biological activity of bile acid derivatives as activators of the NRF2 signaling pathway

Sergej Cvijić[1], Milica Stevanović[1], Ivana Kuzminac[1], Đorđe Miljković[2], Albena Dinkova-Kostova[3], Srđan Bjedov[1]

[1]*University of Novi Sad, Faculty of Science, Novi Sad, Serbia,*
[2]*University of Belgrade, Institute for Biological Research "Siniša Stanković", Belgrade, Serbia*
[3]*University of Dundee, United Kingdom*
srdjan.bjedov@dh.uns.ac.rs

NRF2 is a transcription factor important for cellular defense against oxidative and electrophilic stress, making it a significant target in the development of chemoprotective and cytoprotective agents. Our research is focused on the synthesis of new NRF2 activators based on the structure of bile acids, used as a steroidal platform suitable for the introduction of electrophilic pharmacophores. In this work, linear and cross-conjugated enone derivatives of BA are presented. Biological activity was evaluated in the human ARPE-19 retinal pigment epithelial cell line by monitoring the induction of NQO1 activity as a functional marker of NRF2 signaling pathway activation. The tested compounds increased NQO1 activity, with the cross-conjugated enone derivative showing a more pronounced effect than the linear analogue. The obtained results indicate the potential of these derivatives for the further development of steroidal NRF2 activators.

P-MH-3

Sinteza i *in silico* testiranje novih 17α-(piridin-3-il)-estra-1,3,5(10)-trien derivata

Milica Z. Stevanović[1], Sergej S. Cvijić[1], Srđan Bjedov[1], Đorđe D. Janković[1], Ivana Z. Kuzminac[1]
[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija*
srdjan.bjedov@dh.uns.ac.rs

Steroidna heterociklična jedinjenja predstavljaju važnu klasu biološki aktivnih supstanci. U ovom radu sintetisani su 17α-(piridin-3-il)estra-1,3,5(10)-trien derivati. Utvrđeni su povoljni *in silico* ADMET profili sa minimalnim odstupanjima, prvenstveno u vrednostima logP. Rezultati dobijeni korišćenjem PASS Online alata ukazuju na potencijalnu inhibitornu aktivnost svih sintetisanih jedinjenja prema lijazama, dok je primenom SwissTargetPrediction alata predviđeno da su glukokortikoidni receptori najverovatnije biološke mete. Dalje, rezultati CLC-Pred 2.0 analize ukazuju na potencijalnu antitumorsku aktivnost prema ćelijskim linijama melanoma (A2058) i karcinoma dojke (MDA-MB-231) kod svih sintetisanih jedinjenja. Prema predikcijama ProTox 3.0 platforme, sva jedinjenja svrstana su u klasu V toksičnosti (štetno ukoliko se proguta). Iako je imunotoksičnost identifikovana kao potencijalni neželjeni efekat, ovi rezultati ne isključuju dalja *in vitro* ispitivanja.

Synthesis and *in silico* studies of novel 17α-(pyridin-3-yl)-estra-1,3,5(10)-triene derivatives

Milica Z. Stevanović[1], Sergej S. Cvijić[1], Srđan Bjedov[1], Đorđe D. Janković[1], Ivana Z. Kuzminac[1]
[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija*
srdjan.bjedov@dh.uns.ac.rs

Steroidal heterocyclic compounds represent an important class of biologically active substances. In this study, we synthesized 17α-(pyridin-3-yl)estra-1,3,5(10)-triene derivatives. Favorable ADMET profiles were obtained *in silico* with only minor deviations, primarily related to logP values. According to the PASS Online predictions, all synthesized compounds demonstrated potential lyase inhibitory activity, while SwissTargetPrediction identified glucocorticoid receptors as the most probable biological targets. Furthermore, CLC-Pred 2.0 analysis indicated promising antitumor activity against melanoma (A2058) and breast cancer (MDA-MB-231) cell lines for all compounds. Based on ProTox 3.0 predictions, all compounds were classified as toxicity Class V (may be harmful if swallowed). Although immunotoxicity was identified as a potential adverse effect, these findings do not exclude them from further *in vitro* studies.

Acknowledgment: The authors acknowledge financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/200125&451-03-34/2026-03/200125).

P-MH-4

Predviđanje vremena zadržavanja BACE1 inhibitora primenom mašinskog učenja i molekulske dinamike sa pojačanim uzorkovanjem

Budimir S. Ilić
Katedra za hemiju, Medicinski fakultet, Univerzitet u Nišu, Niš, Srbija
budimir.ilic@medfak.ni.ac.rs

Ova studija predstavlja računarski pristup za predviđanje vremena zadržavanja BACE1 inhibitora, sa ciljem da se dizajn inhibitora Alchajmerove bolesti usmeri sa statičkog afiniteta vezivanja ka kinetički relevantnim parametrima[1]. Kombinovanjem molekulske dinamike sa pojačanim uzorkovanjem i modela mašinskog učenja, analiziraju se ključni dinamički deskriptori, uključujući postojanost i stabilnost vodoničnih veza, kao i konformaciona pokretljivost enzima. Ovaj kinetički zasnovan okvir može doprineti racionalnom dizajnu BACE1 inhibitora sa optimizovanim vremenom zadržavanja i boljem razumevanju molekulskih faktora koji određuju sporo odvajanje liganda od aktivnog mesta enzima.

Predicting BACE1 inhibitor residence time using machine learning and enhanced-sampling molecular dynamics

Budimir S. Ilić
Department of Chemistry, Faculty of Medicine, University of Niš, Niš, Serbia
budimir.ilic@medfak.ni.ac.rs

This study presents a computational framework for predicting the residence time of BACE1 inhibitors, shifting Alzheimer's drug discovery from static binding affinity toward kinetically relevant parameters[1]. By combining enhanced-sampling molecular dynamics with machine-learning models, this approach analyzes key dynamic descriptors, including hydrogen-bond persistence and stability, as well as enzyme conformational flexibility. This kinetic-driven framework may support the rational design of BACE1 inhibitors with optimized target engagement and provide mechanistic insight into the molecular determinants of slow ligand dissociation.

1. E. McDade, I. Voytyuk, P. Aisen, R. J. Bateman, M. C. Carrillo, B. De Strooper, C. Haass, E. M. Reiman, R. Sperling, P. N. Tariot, R. Yan, C. L. Masters, R. Vassar, S. F. Lichtenthaler. *Nat. Rev. Neurol.* **2021**, *17*, 703.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-137/2025-03/200113).

P-MH-5

Generativno mašinsko učenje i alhemijska perturbacija slobodne energije u otkrivanju nepeptidnih inhibitora agregacije tau proteina

Budimir S. Ilić
Katedra za hemiju, Medicinski fakultet, Univerzitet u Nišu, Niš, Srbija
budimir.ilic@medfak.ni.ac.rs

Ova studija predstavlja sažet računarski protokol za otkrivanje nepeptidnih inhibitora agregacije tau proteina, objedinjujući VAE/GNN modele obučene na pažljivo odabranom skupu tau/amiloidnih antiagregacionih jedinjenja, MD i FEP. Pristup je usmeren na agregaciono sklone PHF6*/PHF6 motive, odnosno VQIINK i VQIVYK sekvence, koje predstavljaju ključne strukturne pokretače fibrilizacije tau proteina[1]. Prioritizacija je izvedena dokovanjem u PHF6*/PHF6 regione i MD proverom poza; Gibsove energije vezivanja dobijene su FEP analizom. Odabrana jedinjenja blokiraju agregaciona mesta i narušavaju β-kontakte, čime se ovaj okvir pozicionira kao racionalna platforma za razvoj novih inhibitora agregacije tau proteina.

Generative machine learning and alchemical free-energy perturbation for the discovery of non-peptidic tau aggregation inhibitors

Budimir S. Ilić
Department of Chemistry, Faculty of Medicine, University of Niš, Niš, Serbia
budimir.ilic@medfak.ni.ac.rs

This study presents a concise computational pipeline for discovering non-peptidic tau aggregation inhibitors, integrating VAE/GNN models trained on a curated tau/amyloid anti-aggregation dataset, MD, and FEP. The approach targets the aggregation-prone PHF6*/PHF6 motifs, VQIINK and VQIVYK, which are key structural drivers of tau fibrillization and seeding[1]. Prioritization was performed by docking into PHF6*/PHF6 regions followed by MD-based pose filtering; Gibbs binding free energies were obtained by FEP analysis. Selected compounds block aggregation sites and disrupt β-contacts, positioning this framework as a rational platform for developing new tau aggregation inhibitors.

1. P. M. Seidler, D. R. Boyer, J. A. Rodriguez, M. R. Sawaya, D. Cascio, K. Murray, T. Gonen, D. S. Eisenberg, *Nat. Chem.* **2018**, *10*, 170.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-137/2025-03/200113).

P-MH-6

Sinteza novih derivata artesunata i njihova *in vitro* aktivnost prema ćelijama nesitnoćelijskog karcinoma pluća

Ljiljana Koračak[1], Vladimir Ajdačić[1], Milica Selaković[1], Milica Pajović[2], Miroslav Novaković[3], Ema Lupšić[2], Ana Podolski-Renić[2], Milica Pešić[2], Igor M. Opsenica[4]

[1]*Inovacioni centar Hemijskog fakulteta u Beogradu, d.o.o., Beograd, Srbija*

[2]*Institut za biološka istraživanja "Siniša Stanković" – Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija*

[3] *Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Srbija*

[4]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*

koracaklj@chem.bg.ac.rs

U okviru ovog istraživanja sintetisana je biblioteka hibridnih molekula, derivata artesunata i pirimidina i ispitana njihova antitumorska aktivnost na rezistentnim i osjetljivim ćelijama nesitnoćelijskog karcinoma pluća (NSCLC). Pokazano je da uvođenjem 1,2,3-triazolskog strukturnog fragmenta dolazi do povećane citotoksičnosti prema rezistentnim NCI-H460/R ćelijama, što ukazuje na kolateralnu senzitivnost.

Synthesis of novel artesunate derivatives and their *in vitro* activity against non-small cell lung cancer cells

Ljiljana Koračak[1], Vladimir Ajdačić[1], Milica Selaković[1], Milica Pajović[2], Miroslav Novaković[3], Ema Lupšić[2], Ana Podolski-Renić[2], Milica Pešić[2], Igor M. Opsenica[4]

[1]*Innovative centre of the Faculty of Chemistry in Belgrade, Ltd., Belgrade, Serbia*

[2]*Institute for Biological Research "Siniša Stanković" – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

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

[4]*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

koracaklj@chem.bg.ac.rs

In this study, a library of hybrid artesunate–pyrimidine derivatives were synthesized and their antitumor activity was evaluated against resistant and sensitive non-small cell lung cancer (NSCLC) cells. The introduction of a 1,2,3-triazole structural fragment resulted in enhanced cytotoxicity toward resistant NCI-H460/R cells, indicating the collateral sensitivity.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, grant No. 7005, Development of nature-inspired photoresponsive anticancer agents - sclareol and artemisinin derivatives in cancer multidrug-resistance models: a foundation for the theranostic approach – PhotoSCLART.

P-MH-7

In Silico dizajn i enzimska evaluacija HDAC4 PROTAC degradera

Nevena Tomašević[1], Gordana Tasić[2], Predrag Jovanović[2], Milena Simić[2], Vladimir Savić[2], Sanja Lj. Matić[3], Milan Mladenović[1]

[1]Centar za računarsku biohemiju Kragujevac, Prirodno-matematički fakultet, Univerzitet u Kragujevcu, Radoja Domanovića 12, 34000 Kragujevac, Srbija

[2]Univerzitet u Beogradu, Farmaceutski fakultet, Katedra za organsku hemiju, Vojvode Stepe 450, 11221 Beograd, Srbija

[3] Institut za informacione tehnologije, Univerzitet u Kragujevcu, Liceja Kneževine Srbije 1A, 24000 Kragujevac, Srbija

milan.mladenovic@pmf.kg.ac.rs

Histon deacetilaza 4 (HDAC4) je uključena u razgradnju mišićnih proteina i progresiju spinalne mišićne atrofije, što je čini privlačnom terapijskom metom. U ovom radu, dizajnirani su selektivni HDAC4 PROTAC molekuli korišćenjem skraćenog 6FYZ warhead fragmenta, vođeni preliminarnim Py_CoMFA i Py_ComBinE 3-D QSAR modelima. PROTAC molekuli generisani su pomoću RDKit biblioteke kuplovanjem sa dostupnim linkerima i VHL-1 ili CRBN ligandima. Nakon sinteze, jedinjenja sa oznakama PJ12 i PJ590 su podvrgnuta enzimskom fluorogenom ispitivanju i pokazala su značajnu inhibiciju HDAC4, sa IC_{50} vrednošću od 500 nM za oba jedinjenja. Dalja istraživanja biće usmerena na procenu njihovog degradacionog potencijala na nivou HDAC4 unutar ćelije.

In Silico-guided design and enzymatic evaluation of HDAC4 PROTAC degraders

Nevena Tomašević[1], Gordana Tasić[2], Predrag Jovanović[2], Milena Simić[2], Vladimir Savić[2], Sanja Lj. Matić[3], Milan Mladenović[1]

[1]Kragujevac Center for Computational Biochemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia

[2]University of Belgrade, Faculty of Pharmacy, Department of Organic Chemistry, Vojvode Stepe 450, 11221 Belgrade, Serbia

[3]Institute for Informational Technologies, University of Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia

milan.mladenovic@pmf.kg.ac.rs

Histone deacetylase 4 (HDAC4) is involved in muscle protein degradation and the progression of spinal muscular atrophy, making it an appealing therapeutic target. In this study, selective HDAC4-targeting PROTAC degraders were designed using a truncated 6FYZ warhead, guided by preliminary Py_CoMFA and Py_ComBinE 3-D QSAR models. PROTACs were generated using the RDKit library by merging them with in-house linkers and either VHL-1 or CRBN ligands. After synthesis, compounds PJ12 and PJ590 underwent enzymatic fluorogenic evaluation and showed significant HDAC4 inhibition, each with an IC_{50} value of 500 nM. Further studies will assess their potential for HDAC4 cellular degradation.

Acknowledgments: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7490, Artificial Intelligence-Guided Design, Synthesis, and Pharmacological Evaluation of Innovative PROTACs as Degraders of HDAC4, an Epigenetic Target for Spinal Muscular Atrophy – SMAIPROTACs.

P-MH-8

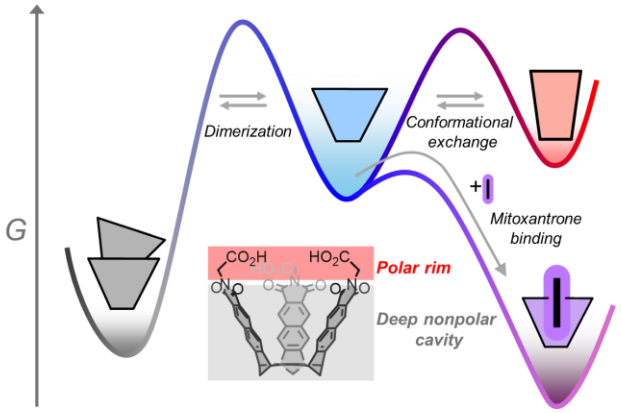
Molekulske korpe u dizajnu naprednih terapija

Radoslav Z. Pavlović

Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Nacionalni institut Republike Srbije, Beograd, Srbija

radoslav.pavlovic@ihtm.bg.ac.rs

Dizajnirali smo i sintetisali duboku molekulsku "korpu" rastvornu u vodi koja vezuje mitoksantron (MTO), lek koji se koristi u terapiji multiple skleroze i određenih karcinoma. Ustanovili smo da korpa reverzibilno dimerizuje, dok monomeri fluktuiraju između relaksiranih i komprimovanih konformacija. Relaksirana konformacija vezuje MTO u mikromolarnom opsegu blizu fizioloških uslova. Ova dinamika omogućava svetlosno ili pH-responzivno uklanjanje leka. Na osnovu *in vivo* studija toksičnosti, kavitand pokazuje dobru biokompatibilnost, otvarajući mogućnosti za supramolekulski dizajn naprednih terapija.



Molecular baskets in the design of advanced therapies

Radoslav Z. Pavlović

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

radoslav.pavlovic@ihtm.bg.ac.rs

We designed and synthesized a water-soluble molecular basket that can bind and release mitoxantrone (MTO), a drug used to treat multiple sclerosis and certain cancers. We found that basket dimerizes reversibly, while monomers fluctuate between relaxed and squeezed conformations. Relaxed conformer binds MTO in the micromolar regime near physiological conditions. These dynamics enable light or pH-responsive removal of the drug. The cavitand seems biofriendly based on *in vivo* work, offering opportunities for supramolecular design of advanced therapies.

P-MH-9

Antiradikalska aktivnost odabranih derivata 1,4-dihidropiridina

Vladimir P. Petrović, Milena D. Vukić, Jovica B. Branković
Univerzitet u Kragujevcu, Prirodno-matematički fakultet , Institut za hemiju, Kragujevac, Srbija
vladimir.petrovic@pmf.kg.ac.rs

1,4-Dihidropiridini predstavljaju važan skelet u medicinskoj hemiji, čiji su derivati poznati po raznovrsnom biološkom potencijalu.[1] Pored dobro poznatih kardiovaskularnih efekata, ova jedinjenja ispoljavaju antioksidativna, antitumorska, antimikrobna i druga benefitna svojstva.[2] U ovom radu je ispitana sposobnost inaktivacije radikalskih vrsta odabranih derivata 1,4-dihidropiridina primenom DPPH metode. Dobijeni rezultati ukazuju na povoljan antiradikalski potencijal pojedinih derivata, naročito onih sa prisutnim elektron-donorskim grupama na fenil fragmentu.

Antiradical activity of the selected 1,4-dihydropiridine derivatives

Vladimir P. Petrović, Milena D. Vukić, Jovica B. Branković
University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia
vladimir.petrovic@pmf.kg.ac.rs

1,4-Dihydropyridines represent a valuable scaffold in medicinal chemistry, whose derivatives are recognized for their diverse biological potential.[1] Beyond their well-established cardiovascular effects, these compounds also exhibit antioxidant, antitumor, antimicrobial, and other beneficial properties.[2] In this study, the radical scavenging ability of selected 1,4-dihydropyridine derivatives was assessed employing the DPPH assay. The results obtained indicate a promising antiradical potential of certain derivatives, particularly those bearing electron-donating substituents on the phenyl moiety.

References

1. A. de Fátima Silva Lago, D. F. C. de Benedicto, L. da Silva, S. S. Thomasi, *Curr. Org. Chem.,* **2023**, 27, 1567–1610.
2. A. Parthiban, P. Makam, *RSC Adv.*, **2022**, 12, 29253.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/ 200122 and 451-03-33/2026-03/ 200122).

P-MH-10

Novi hibridi artesunata suzbijaju rezistenciju posredovanu P-glikoproteinom u ćelijskoj liniji nesitnoćelijskog karcinoma pluća

Milica Selaković[1], Ljiljana Koračak[1], Vladimir Ajdačić[1], Milica Pajović[2], Miroslav Novaković[3], Ema Lupšić[2], Ana Podolski-Renić[2], Mario Zlatović[4], Milica Pešić[2], Igor M. Opsenica[4]

[1]*Inovacioni centar Hemijskog fakulteta u Beogradu, d.o.o., Beograd, Republika Srbija*

[2]*Institut za biološka istraživanja "Siniša Stanković" – Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Republika Srbija*

[3]*Univerzitet u Beogradu-Intitut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Republika Srbija*

[4]*Univerzitet u Beogradu-Hemijski fakultet, Beograd, Republika Srbija*

milica_videnovic@chem.bg.ac.rs

Nova serija hibridnih jedinjenja artesunata i pirimidina pokazala je kolateralnu senzitivnost prema rezistentnoj ćelijskoj liniji NCI-H460/R *in vitro* u MTT eseju. Ispitan je mehanizam delovanja najaktivnijih derivata u kontekstu inhibicije P-glikoproteina u *in vitro* uslovima i molekulskim dokovanjem primenom Glide algoritma iz Schrödinger Suite 2021–1 programa (extra precision mode XP).

Novel artesunate hybrids combat P-gp-mediated multidrug resistance in non-small cell lung carcinoma

Milica Selaković[1], Ljiljana Koračak[1], Vladimir Ajdačić[1], Milica Pajović[2], Miroslav Novakovic[3], Ema Lupšić[2], Ana Podolski-Renić[2], Mario Zlatović[4], Milica Pešić[2], Igor M. Opsenica[4]

[1]*Innovative centre of the Faculty of Chemistry in Belgrade, Ltd.,Belgrade, Republic of Serbia,*

[2]*Institute for Biological Research "Siniša Stanković" - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Republic of Serbia*

[3]*University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Republic of Serbia*

[4]*University of Belgrade - Faculty of Chemistry, Belgrade, Republic of Serbia*

milica_videnovic@chem.bg.ac.rs

A new series of pyrimidine-artesunate hybrids showed enhanced cytotoxicity toward the resistant NCI-H460/R cell line *in vitro* in the MTT assay, indicating collateral sensitivity. Mechanistic studies were performed for the most potent derivatives to investigate their inhibition of P-glycoprotein both *in vitro* and via docking simulations using Glide from Schrödinger Suite 2021–1, extra precision mode (XP).

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, grant No. 7005, Development of nature-inspired photoresponsive anticancer agents - sclareol and artemisinin derivatives in cancer multidrug-resistance models: a foundation for the theranostic approach – PhotoSCLART.

P-MH-11

Sinteza i *in silico* ispitivanja novog defenilovanog diacetatnog analoga (–)-goniofufurona

Teodora Vujanić, Slađana Stanisavljević, Bojana Srećo Zelenović
Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija
bojana.sreco@dh.uns.ac.rs

(–)-Goniofufuron (**1**), enantiomer prirodnog proizvoda (+)-goniofufurona, pokazao je značajnu citotoksičnu aktivnost.[1] U ovom radu ostvarena je efikasna sinteza novog diacetilovanog analoga (–)-goniofufurona polazeći od L-ksiloze, pri čemu je ciljno jedinjenje dobijeno u dva sintetska koraka. U okviru *in silico* ispitivanja potencijalni biološki targeti predviđeni su primenom programa SwissTargetPrediction, pri čemu je protein kinaza C alfa (PKCα) identifikovana kao jedan od najverovatnijih ciljnih molekula. Molekulskim dokovanjem utvrđen je afinitet vezivanja novog analoga za PKCα i mogućnost ostvarivanja povoljnih interakcija unutar aktivnog mesta enzima. Dobijeni rezultati ukazuju na to da je novosintetizovani analog perspektivan kandidat za dalja biološka ispitivanja.

Synthesis and *in silico* evaluation of a novel dephenylated diacetate analogue of (–)-goniofufurone

Teodora Vujanić, Slađana Stanisavljević, Bojana Srećo Zelenović
University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
bojana.sreco@dh.uns.ac.rs

(–)-Goniofufurone (**1**), the enantiomer of the natural product (+)-goniofufurone, has demonstrated significant cytotoxic activity.[1] In this work, an efficient synthesis of a novel diacetylated analogue of (–)-goniofufurone starting from L-xylose was achieved, with the target compound obtained in two synthetic steps. Within the *in silico* study, potential biological targets were predicted using the SwissTargetPrediction program, whereby protein kinase C alpha (PKCα) was identified as one of the most probable target molecules. Molecular docking revealed the binding affinity of the newly synthesized analogue toward PKCα and its ability to establish favorable interactions within the enzyme active site. Based on the obtained results, the newly synthesized analogue represents a promising candidate for further biological evaluation.

1. V. Popsavin, G. Benedeković, B. Srećo, J. Francuz, M. Popsavin, V. Kojić, G. Bogdanović, V. Divjaković, *Tetrahedron*, **2009**, *65*, 10596.

Acknowledgment This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia through Grant Nos. 451-03-33/2026-03/200125 and 451-03-34/2026-03/200125, as well as by the Serbian Academy of Sciences and Arts through Grant No. F-130.

P-MH-12

Sinteza, *in silico* i *in vitro* biološka ispitivanja novog defenilovanog analoga (–)-goniofufurona

Anastasija Dimčić, Slađana Stanisavljević, Tatjana Majkić, Ivana Beara, Bojana Srećo Zelenović
Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija
bojana.sreco@dh.uns.ac.rs

U ovom radu ostvarena je sinteza novog defenilovanog analoga (–)-goniofufurona sa metoksi grupom u položaju C-5 i 7-*O*-dodecil nizom. Ciljno jedinjenje dobijeno je u četiri sintetska koraka, iz L-ksiloze, u ukupnom prinosu od 17 %. Nakon sinteze sprovedena su *in silico* ispitivanja, uključujući procenu ADME-Tox parametara i molekulsko dokovanje sa lipazom, glukozidazom i acetilholinesterazom, a potom i *in vitro* analiza biološke aktivnosti. Dobijeni rezultati pokazuju da je novosintetizovani analog pogodan kandidat za dalju strukturnu optimizaciju u cilju unapređenja biološke aktivnosti.

Synthesis, *in silico* and *in vitro* biological evaluation of a novel dephenylated analogue of (–)-goniofufurone

Anastasija Dimčić, Slađana Stanisavljević, Tatjana Majkić, Ivana Beara, Bojana Srećo Zelenović
University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
bojana.sreco@dh.uns.ac.rs

In this work, the synthesis of a novel dephenylated (–)-goniofufurone analogue bearing a methoxy group at the C-5 position and a 7-*O*-dodecyl chain was achieved. The target compound was obtained in four synthetic steps, from L-xylose, in an overall yield of 17 %. Following the synthesis, *in silico* studies were performed, including ADME-Tox evaluation and molecular docking with lipase, glucosidase, and acetylcholinesterase, followed by *in vitro* biological evaluation. The obtained results indicate that the novel analogue represents a suitable candidate for further structural optimization aimed at improving biological activity.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia through Grant Nos. 451-03-33/2026-03/200125 and 451-03-34/2026-03/200125.

P-MH-13

Dizajn, sinteza i inicijalna biološka karakterizacija selektivnih HDAC degradera

Gordana D. Tasić[1], Predrag M. Jovanović[1], Milena R. Simić[1], Nevena M. Tomašević[2], Sanja Lj. Matić[3], Milan P. Mladenović[2], Vladimir M. Savić[1]

[1]*Univerzitet u Beogradu, Farmaceutski fakultet, Katedra za organsku hemiju, Vojvode Stepe 450, 11221 Beograd, Srbija*

[2]*Centar za računarsku biohemiju Kragujevac, Prirodno-matematički fakultet, Univerzitet u Kragujevcu, Radoja Domanovića 12, 34000 Kragujevac, Srbija*

[3]*Institut za informacione tehnologije, Univerzitet u Kragujevcu, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*

gordanat@pharmacy.bg.ac.rs

Histonske deacetilaze (HDAC) su enzimi koji regulišu ekspresiju gena modulirajući interakcije u hromatinu, čime utiču na brojne ćelijske procese.[1] Sa idejom razvoja selektivnih degradera HDAC enzima, proučavane su mogućnosti strukturne transformacije poznatih, literaturnih inhibitora u PROTAC molekule.[2] Primenom računarskih metoda i analize SAR-a dizajnirana je inicijalna serija molekula koja je zatim i preliminarno biološki okarakterisana.

Design, synthesis and initial biological characterisation of selective HDAC degraders

Gordana D. Tasić[1], Predrag M. Jovanović[1], Milena R. Simić[1], Nevena M. Tomašević[2], Sanja Lj. Matić[3], Milan P. Mladenović[2], Vladimir M. Savić[1]

[1]*University of Belgrade, Faculty of Pharmacy, Department of Organic Chemistry Vojvode Stepe 450, 11221 Belgrade, Serbia*

[2]*Kragujevac Center for Computational Biochemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia*

[3]*Institute for Information Technologies Kragujevac, University of Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*

gordanat@pharmacy.bg.ac.rs

Histone deacetylases (HDACs) are enzymes that regulate gene expression by modulating chromatin interactions, thereby influencing numerous cellular processes.[1] With the aim of developing potential HDAC enzyme degraders, the possibilities for structural transformation of known literature inhibitors into PROTAC molecules were explored.[2] Using computational methods and SAR analysis, an initial series of molecules was designed and then subjected to preliminary biological characterization.

References

1. S.Y. Park, J. S. Kim, *Experimental & Molecular Medicine*, **2020**, *52*, 204.
2. C. A. Luckhurst, O. Aziz, *et all*, *Bioorganic & Medicinal Chemistry Letters*, **2019**, *29*, 83.

Acknowledgements: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7490, Artificial Intelligence-Guided Design, Synthesis, and Pharmacological Evaluation of Innovative PROTACs as Degraders of HDAC4, an Epigenetic Target for Spinal Muscular Atrophy – SMAIPROTACs ; Ministry of Science, Technological Development, and Innovation of the Republic of Serbia through two grant agreements with the University of Belgrade – Faculty of Pharmacy (Nos. 451-03-33/2026-03/200161 and 451-03-34/2026-03/200161).

Neorganska hemija

Inorganic Chemistry

P-NH-1

Sinteza i strukturna karakterizacija novog kompleksa bakra(II) sa *N*-benziltiabendazolom

Tina P. Andrejević[1], Violeta R. Marković[1], Marta Počkaj[2], Darko P. Ašanin[3], Nevena Lj. Stevanović[1], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Radoja Domanovića 12, 34000 Kragujevac, Srbija*
[2]*Univerzitet u Ljubljani, Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, SI-1000 Ljubljana, Slovenija*
[3]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*
tina.andrejevic@pmf.kg.ac.rs

N-Benziltiabendazol (*N*-BzTBZ) korišćen je kao ligand za sintezu novog kompleksa bakra(II), $[Cu(NO_3)_2(N\text{-BzTBZ})(H_2O)]\cdot H_2O$. Sintetisani kompleks je okarakterisan primenom spektroskopskih metoda i rendgenske strukturne analize. Stabilnost kompleksa bakra(II) ispitivana je primenom UV-Vis spektrofotometrije, ciklične voltametrije, kao i merenjem molarne provodljivosti neposredno nakon rastvaranja u odgovarajućem rastvaraču i nakon 48 h.

Synthesis and structural characterization of new copper(II) complex with *N*-benzylthiabendazole

Tina P. Andrejević[1], Violeta R. Marković[1], Marta Počkaj[2], Darko P. Ašanin[3], Nevena Lj. Stevanović[1], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Department of Chemistry, Radoja Domanovića 12, 34000 Kragujevac, Serbia*
[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia*
[3]*University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*
tina.andrejevic@pmf.kg.ac.rs

N-Benzylthiabendazole (*N*-BzTBZ) was used as a ligand for the synthesis of a new copper(II) complex, $[Cu(NO_3)_2(N\text{-BzTBZ})(H_2O)]\cdot H_2O$. The synthesized complex was characterized using spectroscopic methods and X-ray structural analysis. The stability of the copper(II) complex was investigated by UV-Vis spectrophotometry, cyclic voltammetry, and molar conductivity measurements performed immediately after dissolution in an appropriate solvent and again after 48 h.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122 and 451-03-33/2026-03/200378), as well as the Slovenian Research and Innovation Agency (ARIS) under grants P1-0175 and IO-0022.

P-NH-2

Srebro(I) kompleks sa *N*-benziltiabendazolom: sinteza i kristalna struktura

Tina P. Andrejević[1], Violeta R. Marković[1], Marta Počkaj[2], Darko P. Ašanin[3], Nevena Lj. Stevanović[1], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Radoja Domanovića 12, 34000 Kragujevac, Srbija*
[2]*Univerzitet u Ljubljani, Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, SI-1000 Ljubljana, Slovenija*
[3]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*
tina.andrejevic@pmf.kg.ac.rs

Tiabendazol (TBZH) je dobro poznat antifungalni agens i antihelmintik, dok supstitucija N–H grupe benzil grupom povećava njegovu lipofilnost i može uticati na njegovu biološku aktivnost. Sintetisan je novi srebro(I) kompleks, $[Ag(N\text{-BzTBZ})_2]SbF_6$, u reakciji *N*-benziltiabendazola (*N*-BzTBZ) sa $AgSbF_6$ u ekvimolarnom odnosu u etanolu na sobnoj temperaturi, a njegova kristalna struktura određena je rendgenskom strukturnom analizom.

Silver(I) complex with *N*-benzylthiabendazole: synthesis and crystal structure

Tina P. Andrejević[1], Violeta R. Marković[1], Marta Počkaj[2], Darko P. Ašanin[3], Nevena Lj. Stevanović[1], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Department of Chemistry, Radoja Domanovića 12, 34000 Kragujevac, Serbia*
[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia*
[3] *University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*
tina.andrejevic@pmf.kg.ac.rs

Thiabendazole (TBZH) is a well-known antifungal and antihelmintic agent, while substitution of the N–H group with a benzyl group increases its lipophilicity and may influence its biological activity. A new silver(I) complex, $[Ag(N\text{-BzTBZ})_2]SbF_6$, was synthesized by reacting *N*-benzylthiabendazole (*N*-BzTBZ) with $AgSbF_6$ in an equimolar ratio in ethanol at room temperature, and its crystal structure was determined by single-crystal X-ray diffraction analysis.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122 and 451-03-33/2026-03/200378), as well as the Slovenian Research and Innovation Agency (ARIS) under grants P1-0175 and IO-0022.

P-NH-3

Sinteza, karakterizacija i ispitivanje interakcije mononuklearnog platina(II) kompleksa sa helatnim merkaptopirimidinom i derivatom malonske kiseline

Anđela A. Franich[1], Jakob Kljun[2], Marija Živković[3], Snežana Rajković[1]
[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, R. Domanovića 12, 34000 Kragujevac*
[2]*Univerzitet u Ljubljani, Fakultet za hemiju i hemijsku tehnologiju, Institut za hemiju i biohemiju, Večna pot 113, SI-1000 Ljubljana, Slovenija*
[3]*Univerzitet u Kragujevcu, Fakultet medicinskih nauka, S. Markovića 69, 34000 Kragujevac*
andjela.franich@pmf.kg.ac.rs

Platina(II) kompleksi igraju važnu ulogu u hemioterapiji, ali zbog neželjenih efekata i pojave rezistencije njihova klinička upotreba je ograničena. U cilju pronalaska kompleksa sa boljim antitumorskim efektom, sintetisan je [Pt(Me_2-mal)(B2)] kompleksa gde je Me_2-mal dimetilmalonat, a B2 je 2-(metiltio)-4-(pirazin-2-il)pirimidin. Ligand B2 je sintetisan i okarakterisan ^{1}H i ^{13}C NMR spektroskopijom, dok je karakterizacija kompleksa izvršena pomoću X-ray analize, elementalne mikroanalize, IR, UV-Vis i ^{1}H i ^{13}C NMR spektroskopije. Rezultati ispitivanja su pokazali da se kompleks vezuje za vezivno mesto I u HSA biomolekulu.

Synthesis, characterization and investigation of the interaction of a mononuclear platinum(II) complex with chelating mercaptopyrimidine and a malonic acid derivative

Anđela A. Franich[1], Jakob Kljun[2], Marija Živković[3], Snežana Rajković[1]
[1]*University of Kragujevac, Faculty of Science, Institute of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia*
[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Department of Chemistry and Biochemistry, Večna pot 113, SI-1000 Ljubljana, Slovenia*
[3]*University of Kragujevac, Faculty of Medical Sciences, S. Markovića 69, 34000 Kragujevac, Serbia*
andjela.franich@pmf.kg.ac.rs

Platinum(II) complexes play an important role in chemotherapy, but their clinical use is limited due to side effects and the development of resistance. To obtain complexes with improved antitumor activity, the [Pt(Me_2-mal)(B2)] complex was synthesized, where Me_2-mal is dimethylmalonate and B2 is 2-(methylthio)-4-(pyrazin-2-yl)pyrimidine. The B2 ligand was synthesized and characterized by ^{1}H and ^{13}C NMR spectroscopy, while the complex was characterized using X-ray analysis, elemental microanalysis, IR, UV–Vis, ^{1}H and ^{13}C NMR spectroscopy. The results of the study showed that the complex binds to binding site I in the HSA biomolecule.

Acknowledgements: This work was funded in part by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (No. 451-03-34/2026-03/200122, 451-03-34/2026-03/200111) and in part by the Slovenian Research Agency (ARIS) through Infrastructure program No. I0-0022 and research program No. P1-0175.

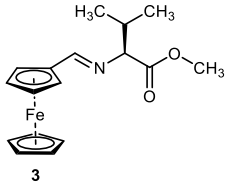
P-NH-4

Sinteza i karakterizacija bakar(I) kompleksa sa derivatom ferocena

Andrija D. Gigić[1], Dragana Stevanović[1], Jovana Bugarinović[1], Ana Kesić[2], Jovana Bogojeski[1], Jakob Kljun[3]

[1]*Univerzitet u Kragujevcu - Prirodno-matematički fakultet, Kragujevac, Srbija*
[2]*Univerzitet u Kragujevcu - Institut za informacione tehnologije Kragujevac, Kragujevac, Srbija*
[3]*Univerzitet u Ljubljani – Fakultet za hemiju i hemijsku tehnologiju, Ljubljana, Slovenija*
andrija.gigic@pmf.kg.ac.rs

Kompleksi bakra(I) imaju značajno mesto u savremenoj koordinacionoj i bioneorganskoj hemiji zbog svojih redoks svojstava, strukturne raznovrsnosti i potencijalne primene u katalizi, materijalima i medicinskoj hemiji. Kompleks bakra(I) sintetisan je reakcijom tetrakis(acetonitril)bakar(I)-heksafluorofosfata, $[Cu(MeCN)_4]PF_6$, sa metil 2-((ferocenilmetilen)amino)-3-metilbutanoatom (Slika 1) u hloroformu na sobnoj temperaturi, pri molskom odnosu 1 : 2. Formiranje kompleksa praćeno je NMR spektroskopijom, dok je njegova struktura potvrđena rendgenskom strukturnom analizom monokristala.



3

Slika 1. Metil 2-((ferocenilmetilen)amino)-3-metilbutanoat

Synthesis and characterization of a copper(I) complex with a ferrocene derivative

Andrija D. Gigić[1], Dragana Stevanović[1], Jovana Bugarinović[1], Ana Kesić[2], Jovana Bogojeski[1], Jakob Kljun[3]

[1]*University of Kragujevac,- Faculty of Science, Kragujevac, Serbia*
[2]*University of Kragujevac - Institute for Information Technologies Kragujevac, Kragujevac, Serbia*
[3]*University of Ljubljana - Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia*
andrija.gigic@pmf.kg.ac.rs

Copper(I) complexes occupy an important place in modern coordination and bioinorganic chemistry due to their redox properties, structural diversity, and potential applications in catalysis, materials science, and medicinal chemistry. A copper(I) complex was synthesized by reacting tetrakis(acetonitrile)copper(I) hexafluorophosphate, $[Cu(MeCN)_4]PF_6$, with methyl 2-((ferrocenylmethylene)amino)-3-methylbutanoate (Figure 1) in chloroform at room temperature, using a molar ratio of 1 : 2. The formation of the complex was monitored by NMR spectroscopy, and its structure was confirmed by single-crystal X-ray diffraction analysis.

P-NH-5

Ispitivanje uticaja hibridnih nanočestica srebra na humane fibroblaste

Bojana B. Laban[1], Sandra Petrović[2], Andreja Leskovac[2], Ana Vujačić Nikezić[2], Vladimir Rajić[2], Uroš Ralević[3]

[1]*Univerzitet u Prištini, Prirodno-matematički fakultet, Kosovska Mitrovica, Srbija*
[2]*Univerzitet u Beogradu, Institut za nuklearne nauke „Vinča" – Institut od nacionalnog značaja, Beograd, Srbija*
[3] *Univerzitet u Beogradu, Institut za fiziku, Beograd, Srbija*
bojana.laban@pr.ac.rs

Nanočestice plemenitih metala, njihova sinteza i površinska modifikacija, se poslednjih decenija intenzivno istražuju zbog specifičnih svojstava i potencijalne primene u različitim oblastima. U ovom radu ispitan je uticaj hibridnih nanočestica srebra (Ag@LM/ICG NPs) na normalne humane MRC5 fibroblaste. Ag@LM/ICG NPs, sintetisane primenom zelene metode, pokazale su se kao netoksične prema humanim limfocitima.[1] Njihova interakcija sa MRC5 ćelijama ispitana je primenom Ramanske spektroskopije (RS), Skenirajuće elektronske mikroskopije (SEM) i analizom vijabilnosti ćelija. RS i SEM studija ukazuju na interakciju NPs sa ćelijskom membranom, dok analiza ćelijske vijabilnosti pokazuje blago smanjenje vijabilnosti, bez značajnog citotoksičnog efekta.

Study of hybrid silver nanoparticles in human fibroblasts

Bojana B. Laban[1], Sandra Petrović[2], Andreja Leskovac[2], Ana Vujačić Nikezić[2], Vladimir Rajić[2], Uroš Ralević[3]

[1]*University of Priština in Kosovska Mitrovica, Faculty of Sciences and Mathematics, Kosovska Mitrovica, Serbia*
[2]*University of Belgrade, Vinča Institute of Nuclear Sciences-National Institute of the Republic of Serbia, Belgrade, Serbia*
[3]*University of Belgrade, Institute of Physics Belgrade, Belgrade, Serbia*
bojana.laban@pr.ac.rs

Noble metal nanoparticles have been extensively studied in recent decades due to their unique properties and potential applications. This study investigated effects of hybrid silver nanoparticles (Ag@LM/ICG NPs) in normal human MRC5 fibroblasts. The green-synthesized NPs were previously shown to be non-toxic to human lymphocytes [1]. Their interaction with MRC5 cells was examined using Raman spectroscopy (RS), Scanning Electron Microscopy (SEM), and cell viability assays. RS and SEM analyses indicate interactions between the NPs and the cell membrane, while cell viability analysis shows a slight reduction in viability without significant cytotoxicity.

Reference

1. B. Laban, U. Ralević, A. Leskovac, S. Petrović, M. Stoiljković, M. Rosić, A. Vujačić Nikezić, *Spectrochim. Acta, Part A*. **2025**, 3*40*, 126360.

Zahvalnica: Rad je finansiran od strane Ministarstva nauke, tehnološkog razvoja i inovacija Republike Srbije, broj: 451-03-34/2026-03 i 451-03-33/2026-03/200017.

P-NH-6

Spektroskopska i kristalografska karakterizacija kompleksa $[Mg(H_2O)_6][Ni(2\text{-}OH\text{-}1,3\text{-}pdta)]\cdot 4H_2O$

Bojana V. Pantović[1], Darko P. Ašanin[2], Tina P. Andrejević[1], Nevena Lj. Stevanović[1], Nenad S. Drašković[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Radoja Domanovića 12, 34000 Kragujevac, Srbija*
[2]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*
[3]*Univerzitet u Prištini-Kosovska Mitrovica, Poljoprivredni fakultet, Kopaonička bb, 38228 Lešak, Srbija*
[4] *Srpska akademija nauka i umetnostii, Knez Mihailova 35, 11000 Beograd, Srbija*
bojana.pantovic@pmf.kg.ac.rs

Diaminopolikarboksilatni 2-OH-1,3-pdta^{4-}-anjon (2-hidroksi-1,3-propandiamin-*N,N,N',N'*-tetraacetat) je korišćen kao ligand za sintezu novog nikal(II)-kompleksa, $[Mg(H_2O)_6][Ni(2\text{-}OH\text{-}1,3\text{-}pdta)]\cdot 4H_2O$. Karakterizacija ovog kompleksa je izvršena pomoću IR spektroskopije, UV-Vis spektrofotometrije i rendgenske strukturne analize.

Spectroscopic and crystallographic characterization of $[Mg(H_2O)_6][Ni(2\text{-}OH\text{-}1,3\text{-}pdta)]\cdot 4H_2O$ complex

Bojana V. Pantović[1], Darko P. Ašanin[2], Tina P. Andrejević[1], Nevena Lj. Stevanović[1], Nenad S. Drašković[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Radoja Domanovića 12, 34000 Kragujevac, Serbia*
[2]*University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*
[3]*University of Priština-Kosovska Mitrovica, Faculty of Agriculture, Kopaonička bb, 38228 Lešak, Serbia*
[4] *Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia*
bojana.pantovic@pmf.kg.ac.rs

Diaminopolycarboxylate 2-OH-1,3-pdta^{4-} anion (2-hydroxy-1,3-propanediamine-*N,N,N',N'*-tetraacetate) was used as a ligand for the synthesis of nickel(II) complex, $[Mg(H_2O)_6][Ni(2\text{-}OH\text{-}1,3\text{-}pdta)]\cdot 4H_2O$. Characterization of this complex was performed using IR spectroscopy, UV-Vis spectrophotometry, and single-crystal X-ray diffraction analysis.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122, and 451-03-33/2026-03/200378), and from the Serbian Academy of Sciences and Arts under the strategic projects program, with grant agreement No. 01-2026.

P-NH-7

Sinteza i kristalna struktura kompleksa bakra(II) sa 3-(((piridin-2-ilmetil)imino)metil)-4*H*-hromen-4-onom

Nevena Lj. Stevanović[1], Jakob Kljun[2], Tina P. Andrejević[1], Darko P. Ašanin[2], Milena Vukić[1], Bojana V. Pantović[1], Nenad Vuković[1], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Radoja Domanovića 12, 34000 Kragujevac, Srbija*

[2]*Univerzitet u Ljubljani, Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, 1000 Ljubljana, Slovenija*

[3]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*

nevena.stevanovic@pmf.kg.ac.rs

Novi kompleks bakra(II), $[CuCl_2(L)]\cdot 2H_2O$, dobijen je u reakciji $CuCl_2\cdot 2H_2O$ i 3-(((piridin-2-ilmetil)imino)metil)-4*H*-hromen-4-ona (L) u 1 : 2 molskom odnosu u etanolu na sobnoj temperaturi. Ovaj kompleks je okarakterisan primenom spektroskopskih i elektrohemijskih metoda, dok je njegova kristalna struktura određena pomoću rendgenske strukturne analize. U $[CuCl_2(L)]\cdot 2H_2O$ kompleksu, ligand L je tridentatno koordinovan za Cu(II) jon, pri čemu kompleks ima distorgovano kvadratno-piramidalnu geometriju.

Synthesis and crystal structure of a copper(II) complex with 3-(((pyridin-2-ylmethyl)imino)methyl)-4*H*-chromen-4-one

Nevena Lj. Stevanović[1], Jakob Kljun[2], Tina P. Andrejević[1], Darko P. Ašanin[2], Milena Vukić[1], Bojana V. Pantović[1], Nenad Vuković[1], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia*

[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000, Ljubljana, Slovenia*

[3]*University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*

nevena.stevanovic@pmf.kg.ac.rs

A new copper(II) complex, $[CuCl_2(L)]\cdot 2H_2O$, was obtained by reacting $CuCl_2\cdot 2H_2O$ with 3-(((pyridin-2-ylmethyl)imino)methyl)-4*H*-chromen-4-one in a 1 : 2 molar ratio in ethanol at room temperature. The complex was characterized using spectroscopic and electrochemical methods, while its crystal structure was determined by single-crystal X-ray diffraction analysis. In the $[CuCl_2(L)]\cdot 2H_2O$ complex, the ligand L is tridentately coordinated to the copper(II) ion, whereas the coordination environment around the metal center is best described as a distorted square-pyramidal geometry.

Acknowledgments: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122 and 451-03-33/2026-03/200378) and by the Slovenian Research Agency (grants P1-0175 and IO-0022).

P-NH-8

Sinteza i stukturna karakterizacija kompleksa srebra(I) sa azakonazolom

Nevena Lj. Stevanović[1], Jakob Kljun[2], Tina P. Andrejević[1], Darko P. Ašanin[3], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Radoja Domanovića 12, 34000 Kragujevac, Srbija*

[2]*Univerzitet u Ljubljani, Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, 1000 Ljubljana, Slovenija*

[3]*Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Srbija*

nevena.stevanovic@pmf.kg.ac.rs

U ovom radu je prikazana sinteza i strukturna karakterizacija kompleksa srebra(I) sa azakonazolom (azc). Kompleks $[Ag(NO_3)(azc)]_n$ je dobijen u reakciji srebro(I)-nitrata i azakonazola u molskom odnosu 1 : 1 u etanolu na sobnoj temperaturi. Čistoća i sastav sintetisanog kompleksa srebra(I) su potvrđeni primenom elementalne analize, dok je kompleks srebra(I) okarakterisan primenom ^{1}H NMR i IR spektroskopije, merenjem molarne provodljivosti i rendgenske strukturne analize.

Synthesis and structural characterization of the silver(I) complex with azaconazole

Nevena Lj. Stevanović[1], Jakob Kljun[2], Tina P. Andrejević[1], Darko P. Ašanin[3], Bojana V. Pantović[1], Biljana Đ. Glišić[1]

[1]*University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia*

[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000, Ljubljana, Slovenia*

[3]*University of Kragujevac, Institute for Information Technologies Kragujevac, Liceja Kneževine Srbije 1A, 34000 Kragujevac, Serbia*

nevena.stevanovic@pmf.kg.ac.rs

This work presents the synthesis and structural characterization of a silver(I) complex with azaconazole (azc). The $[Ag(NO_3)(azc)]_n$ complex was obtained by the reaction of silver(I) nitrate with azaconazole in a 1 : 1 molar ratio in ethanol at room temperature. The purity and composition of the synthesized silver(I) complex were confirmed by elemental analysis, while the complex was further characterized by ^{1}H NMR and IR spectroscopy, molar conductivity measurements, and single-crystal X-ray diffraction analysis.

Acknowledgments: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/200122, 451-03-33/2026-03/200122 and 451-03-33/2026-03/200378) and by the Slovenian Research Agency (grants P1-0175 and IO-0022).

P-NH-9

Ispitivanje načina vezivanja dva nova kompleksa paladijuma(II) za DNK

Marija D. Trifunović[1], Nenad M. Joksimović[1], Milica G. Međedović-Stefanović[1], Ana M. Rilak Simović[2], Dušan S. Ćoćić[1], Biljana V. Petrović[1], Snežana R. Stojanović[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, Kragujevac, Srbija*

[2]*Univerzitet u Kragujevcu, Institut za informacione tehnologije, Odeljenje za prirodne nauke, Kragujevac, Srbija*

snezana.stojanovic@pmf.kg.ac.rs

Interakcije dva nova paladijum(II) kompleksa, $[Pd(L)_2]$, u kojima je L = etil-2-hidroksi-6-(4-etoksi-3-metoksifenil)-4-oksoheksa-2,5-dienoat (**Pd1**) ili etil-2-hidroksi-6-(4-izopropoksi-3-metoksifenil)-4-oksoheksa-2,5-dienoat (**Pd2**), sa DNK ispitivane su UV–Vis spektrofotometrijom i fluorescentnom tehnikom korišćenjem etidijum-bromida (EB) u cilju rasvetljavanja načina vezivanja. Na osnovu UV–Vis eksperimenata, kompleks **Pd1** pokazao je veću konstantu vezivanja za DNK, dok je Stern–Volmerova konstanta gašenja bila nešto viša za kompleks **Pd2**. Na dobijene rezultate značajno su uticali supstituenti u bočnom nizu liganada, koji mogu otežati ili olakšati interkalativni način vezivanja. Dobijeni rezultati su ukazali na umerenu sposobnost paladijum(II) kompleksa da istisnu EB i ostvare interakciju sa DNK.

DNA binding studies of two novel palladium(II) complexes

Marija D. Trifunović[1], Nenad M. Joksimović[1], Milica G. Međedović-Stefanović[1], Ana M. Rilak Simović[2], Dušan S. Ćoćić[1], Biljana V. Petrović[1], Snežana R. Stojanović[1]

[1]*University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia*

[2]*University of Kragujevac, Institute for Information Technologies, Department of Natural Science, Kragujevac, Serbia*

snezana.stojanovic@pmf.kg.ac.rs

The interactions of two novel palladium(II) complexes, $[Pd(L)_2]$, where L is ethyl-2-hydroxy-6-(4-ethoxy-3-methoxyphenyl)-4-oxohexa-2,5-dienoate (**Pd1**) or ethyl-2-hydroxy-6-(4-isopropoxy-3-methoxyphenyl)-4-oxohexa-2,5-dienoate (**Pd2**), with DNA were investigated by UV–Vis spectroscopy and competitive fluorescence measurements using ethidium bromide (EB) in order to elucidate their binding mode. Based on the UV–Vis experiments, complex **Pd1** exhibited a higher DNA binding constant, whereas the Stern–Volmer quenching constant was slightly higher for complex **Pd2**. The obtained results were strongly influenced by the substituents in the side chain of ligand, which may either hinder or facilitate the intercalative binding mode. The results indicated a moderate ability of palladium(II) complexes to displace EB and interact with DNA.

Acknowledgment: This work was supported by the Serbian Ministry of Science, Technological Development and Innovation (Agreement No. 451-03-33/2026-03/200122 and 451-03-34/2026-03/ 200122).

P-NH-10

Sinteza i karakterizacija novih pirolil-terpiridin rutenijum(II) kompleksa

Milica G. Međedović Stefanović[1], Ana M. Rilak Simović[2], Biljana V. Petrović[1], Snežana R. Stojanović[1], Dušan S. Ćoćić[1]

[1]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija*

[2]*Univerzitet u Kragujevcu, Institut za informacione tehnologije, Kragujevac, Srbija*

snezana.stojanovic@pmf.kg.ac.rs

U velikoj grupi koordinacionih jedinjenja prelaznih metala sintetisanih sa ciljem da uspešno zamene komplekse platine i pruže bolju selektivnost i manju toksičnost, kompleksi rutenijuma zauzeli su važno mesto. U ovom radu predstavljena je sinteza i karakterizacija dva nova mononuklearna Ru(II)-polipiridil-kompleksa opšte formule *mer*-[Ru(L_3)(*N*-*N*)Cl]Cl, gde je L_3 2,2':6',2''-terpiridin sa dodatnom funkcionalnom grupom (2-pirolil) u položaju 4', dok je *N*-*N* 2,2'-bipiridin ili fenantrolin. Karakterizacija Ru(II)-kompleksa izvršena je elementalnom analizom, UV-Vis, IR, 1D (^{1}H, ^{13}C) i 2D (^{1}H-^{1}H COSY i ^{1}H-^{13}C HSQC) NMR spektroskopijom, kao i masenom spektrometrijom sa elektrosprej jonizacijom (ESI-MS). Metode korišćene za karakterizaciju potvrdile su uspešnu sintezu i visoku čistoću dobijenih kompleksa.

Synthesis and characterization of new pyrrolyl-terpyridine ruthenium(II) complexes

Milica G. Međedović Stefanović[1], Ana M. Rilak Simović[2], Biljana V. Petrović[1], Snežana R. Stojanović[1], Dušan S. Ćoćić[1]

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

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

snezana.stojanovic@pmf.kg.ac.rs

In a huge number of transition metal complexes synthesized to replace platinum-based ones and provide better selectivity and smaller toxicity, ruthenium complexes occupied an important place. In this study, we presented the synthesis and characterization of new mononuclear Ru(II) polypyridyl complexes of the general formula *mer*-[Ru(L_3)(*N*-*N*)Cl]Cl, where L_3 is 2,2':6',2''-terpyridine with the additional functional group in the 4'-position (2-pyrrolyl) and *N*-*N* is 2,2'-bipyridine or phenanthroline. Characterization of the Ru(II) complexes was performed using elemental analysis, UV-Vis, IR, 1D (^{1}H, ^{13}C) and 2D (^{1}H-^{1}H COSY and ^{1}H-^{13}C HSQC) NMR spectroscopy, as well as electrospray ionization mass spectrometry (ESI-MS). Collectively, these analyses confirmed the successful synthesis and high purity of the desired complexes.

Zahvalnica: Ovaj rad podržan je od strane Ministarstva nauke, tehnološkog razvoja i inovacija, 451-03-33/2026-03/200122; 451-03-34/2026-03/200122.

Organska hemija

Organic Chemistry

P-OH-1

Sinteza i strukturna karakterizacija odabranih C4-aril-funkcionalizovanih Hantzsch-ovih estara

Jovica B. Branković, Đorđe M. Pavlićević, Milena D. Vukić, Vladimir P. Petrović
Univerzitet u Kragujevcu, Prirodno-matematički fakultet , Institut za hemiju, Kragujevac, Srbija
jovica.brankovic@pmf.kg.ac.rs

U ovom radu prikazana je sinteza odabranih C4-aril-funkcionalizovanih Hantzsch-ovih estara modifikacijom klasične multikomponentne Hantzsch-ove reakcije,[1,2] uz primenu različito supstituisanih aromatičnih aldehida. Struktura i čistoća dobijenih proizvoda potvrđeni su primenom NMR i IR spektroskopskih metoda. Dobijeni rezultati ukazuju na potencijal primenjene metodologije kao i na mogućnost njene dalje optimizacije u cilju obogaćivanja hemijske biblioteke ovih jedinjenja i njihovih daljih sintetičkih transformacija.

Synthesis and structural characterization of selected C4-aryl-functionalized Hantzsch esters

Jovica B. Branković, Đorđe M. Pavlićević, Milena D. Vukić, Vladimir P. Petrović
University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia
jovica.brankovic@pmf.kg.ac.rs

In this work, the selected C4-aryl-functionalized Hantzsch esters were synthesized *via* a modified multicomponent Hantzsch reaction,[1,2] utilizing diverse aromatic aldehydes. The structure and purity of the obtained products were confirmed by NMR and IR spectroscopy. The obtained results demonstrate the potential of the applied methodology and offer opportunities for further optimization, expansion of the chemical library of target compounds and their synthetic transformations.

References

1. Arthur Rudolph Hantzsch (1857–1935) and the synthesis of nitrogen heterocycles, *Synform,* **2021**, 12, A201–A210.
2. A. M. F. Phillips, A. J. L. Pombeiro, *Catalysts*, **2023**, 13, 419.

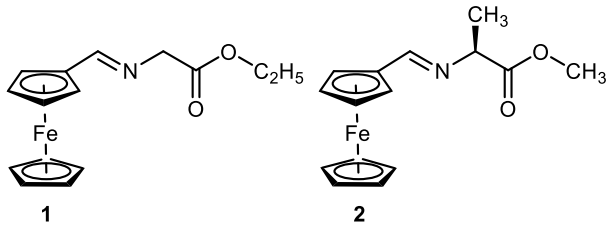
Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/200122 and 451-03-33/2026-03/200122).

P-OH-2

Lipofilnost ferocenskih imina dobijenih iz estara aminokiselina

Andrija D. Gigić, Dragana Stevanović, Jovana Bugarinović, Marko Pešić
Univerzitet u Kragujevcu - Prirodno-matematički fakultet, Kragujevac, Srbija
andrija.gigic@pmf.kg.ac.rs

Derivati ferocena imaju značajno mesto u savremenoj bioorganometalnoj i medicinskoj hemiji zbog svoje stabilnosti, redoks-svojstava i potencijala za dobijanje biološki i farmakološki značajnih jedinjenja.[1] Ferocenski imini **1** i **2** (Slika 1) su sintetisani polazeći od estara amino kiselina i okarakterisani standardnim spektroskopskim metodama. Lipofilnost, kao važan parametar koji može uticati na rastvorljivost, permeabilnost i ukupno farmakokinetičko ponašanje jedinjenja, ispitana je eksperimentalnim određivanjem logP vrednosti i *in silico* analizom primenom SwissADME platforme.



Slika 1. Strukturne formule ispitivanih ferocenskih imina

Lipophilicity of ferrocene imines derived from amino acid esters

Andrija D. Gigić, Dragana Stevanović, Jovana Bugarinović, Marko Pešić
University of Kragujevac - Faculty of Science, Kragujevac, Serbia
andrija.gigic@pmf.kg.ac.rs

Ferrocene derivatives play an important role in modern bioorganometallic and medicinal chemistry due to their stability, redox properties, and potential for the development of biologically and pharmacologically important compounds.[1] Ferrocene imines **1** and **2** (Figure 1) were synthesized starting from amino acid esters and characterized by standard spectroscopic methods. Lipophilicity, as an important parameter that can affect solubility, permeability, and the overall pharmacokinetic behavior of compounds, was investigated experimentally by determining logP values and by *in silico* analysis using the SwissADME platform.

1. Patra, M., Gasser, G, *Nat. Rev. Chem.* **2017**, *1*, 66.

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

P-OH-3

Wittig-ova olefinacija androstanskih C19 aldehida: put ka novim steroidnim jedinjenjima sa antitumorskim dejstvom

Ivana Z. Kuzminac[1], Sofija S. Bekić[1], Dimitar S. Jakimov[2], Anđelka S. Ćelić[3], Đorđe D. Janković[1], Marina P. Savić[1], Marija N. Sakač[1]

[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Srbija*

[2]*Institut za onkologiju Vojvodine, Put dr Goldmana 4, Sremska Kamenica, Srbija*

[3]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za biologiju i ekologiju, Trg Dositeja Obradovića 2, Novi Sad, Srbija*

djordje.jankovic@dh.uns.ac.rs

C19-derivatizovani steroidi su jedinjenja sa značajnim biološkim aktivnostima kod kojih je metil grupa na C10 modifikovana različitim funkcionalnim grupama. U ovom radu izvedene su Wittig-ove olefinacije na androstanskom C19 aldehidu sa 17a-homo laktonskom funkcijom. Iako 19-hlormetilidenski derivat nije dobijen, a 19-cijanometilidenski nije pokazao dovoljnu stabilnost za biološka ispitivanja, dva novosintetisana 19-metilidenska derivata su pokazala značajnu citotoksičnu aktivnost prema MDA-MB-231, HT-29 i A549 ćelijama. Pored povoljnih *in silico* ADMET svojstava, ovi derivati nisu pokazali vezivanje za androgeni i estrogene receptore (α i β), što ukazuje na manji rizik od neželjenih efekata.

Wittig olefination of androstane C19 aldehydes: access to novel steroid-based antitumor agents

Ivana Z. Kuzminac[1], Sofija S. Bekić[1], Dimitar S. Jakimov[2], Anđelka S. Ćelić[3], Đorđe Janković[1], Marina P. Savić[1], Marija N. Sakač[1]

[1]*University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad*

[2]*Oncology Institute of Vojvodina, Put dr Goldmana 4, Sremska Kamenica, Serbia*

[3]*University of Novi Sad, Faculty of Sciences, Department of Biology and Ecology, Trg Dositeja Obradovića 2, Novi Sad*

djordje.jankovic@dh.uns.ac.rs

C19-derivatized steroids are compounds in which the C10 methyl group is modified by various functional groups, showing diverse biological activities. In this study, Wittig olefinations were performed on an androstane C19 aldehyde with a 17a-homo lactone moiety. While the 19-chloromethylidene derivative was not obtained and the 19-cyanomethylidene derivative lacked stability, two 19-methylidene derivatives demonstrated significant cytotoxic activity against MDA-MB-231, HT-29, and A549 cell lines. These compounds showed favorable *in silico* ADMET properties and no binding to androgen and estrogen receptors (α and β), indicating a lower risk of adverse effects.

Acknowledgment: The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/ 200125 & 451-03-34/2026-03/ 200125).

P-OH-4

Sinteza odabranih bis-pirazola primenom Knoevenagel–Michael tandem reakcija

Jovica B. Branković, Milena D. Vukić, Vladimir P. Petrović
Univerzitet u Kragujevcu, Prirodno-matematički fakultet , Institut za hemiju, Kragujevac, Srbija
vladimir.petrovic@pmf.kg.ac.rs

U ovom radu prikazana je sinteza odabranih bis-pirazolskih derivata primenom bazno-katalizovanih tandem Knoevenagel–Michael reakcija.[1,2] Ciljni proizvodi dobijeni su u dobrom do odličnom prinosu, pod umerenim reakcionim uslovima i jednostavnom obradom reakcione smeše. Strukture sintetisanih jedinjenja potvrđene su primenom NMR i IR spektroskopskih metoda. Potencijal dobijenih proizvoda ogleda se u mogućnosti daljih sintetičkih transformacija i evaluaciji njihovih bioaktivnih svojstava.

Synthesis of selected bis-pyrazoles *via* a Knoevenagel–Michael tandem reactions

Jovica B. Branković, Milena D. Vukić, Vladimir P. Petrović
University of Kragujevac, Faculty of Science, Department of Chemistry, Kragujevac, Serbia
vladimir.petrovic@pmf.kg.ac.rs

This work describes the synthesis of selected bis-pyrazole derivatives *via* base-catalyzed tandem Knoevenagel–Michael reactions.[1,2] The target compounds were obtained in good to excellent yield, under moderate reaction conditions, and with straightforward reaction work-up. The structures of the synthesized compounds were confirmed by NMR and IR spectroscopic methods. The obtained compounds possess valuable potential as scaffolds for further synthetic transformations and candidates for bioactivity screening.

References

1. J. Branković, V. M. Milovanović, D. Simijonović, S. Novaković, Z. D. Petrović, S. S. Trifunović, G. A. Bogdanović, V. P. Petrović, *RSC Adv.*, **2022**, 12, 16054.
2. J. Branković, V. M. Milovanović, Z. D. Petrović, D. Simijonović, V. P. Petrović, *RSC Adv.*, **2023**, 13, 2884.

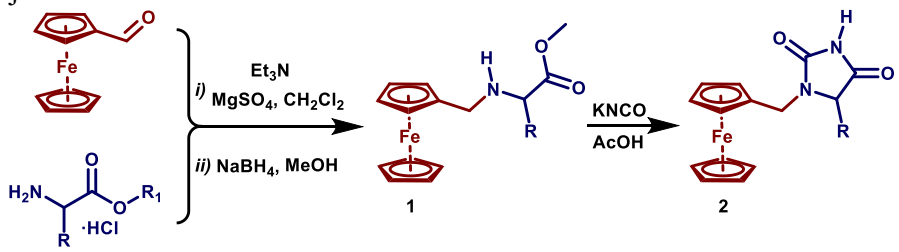
Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-34/2026-03/ 200122 and 451-03-33/2026-03/ 200122).

P-OH-5

Sinteza ferocenskih hidantoina

Dragana D. Stevanović, Marko S. Pešić, Jovana P. Bugarinović, Ivan S. Damljanović
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija
dragana.stevanovic@pmf.kg.ac.rs

Razvoj novih farmaceutskih proizvoda sve više je usmeren na dizajn i sintezu hibridnih molekula koji kombinuju biološki aktivne farmakofore. Integracija ferocenske jedinice i hidantoinskog jezgra može značajno uticati na biološku aktivnost obe farmakofore [1]. Stoga, ovaj rad opisuje sintezu novih hidantoina sa ferocenskim jezgrom **2** (Shema 1). Sintetički pristup uključuje pripremu ferocenskih *N*-supstituisanih derivata amino kiselina **1** pogodnih za dobijanje hidantoina uz pomoć cijanata.



Shema 1. Sinteza ferocenskih hidantoina

Synthesis of ferrocene-hybrid hydantoins

Dragana D. Stevanović, Marko S. Pešić, Jovana P. Bugarinović, Ivan S. Damljanović
University of Kragujevac, Faculty of Science, Kragujevac, Serbia
dragana.stevanovic@pmf.kg.ac.rs

The development of novel pharmaceuticals is increasingly focused on the design and synthesis of hybrid molecules that combine multiple biologically active pharmacophores. The integration of the ferrocene unit and the hydantoin core can affect the biological activity of both pharmacophores [1]. The present report describes the synthesis of new ferrocene-based hydantoin derivatives **2** (Scheme 1). The synthetic approach involves the preparation of ferrocene-containing *N*-substituted amino acid derivatives **1**, which serve as suitable precursors for cyanate-assisted hydantoin synthesis.

1. O. Payen *et al.*, *J. Med. Chem.* **2008**, *51*, 1791–1799.

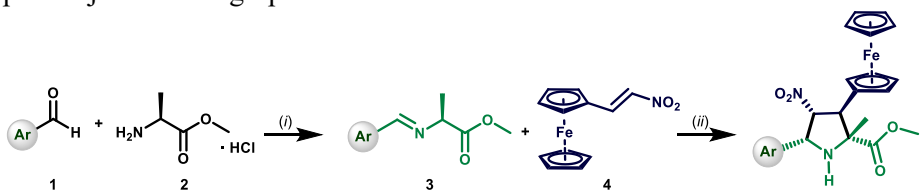
Acknowledgements: Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant Nos 451-03-34/2026-03/ 200122 and 51-03-33/2026-03/ 200122).

P-OH-6

Sinteza ferocenil pirolidina iz azometin-ilida

Dragana D. Stevanović, Marko S. Pešić, Jovana P. Bugarinović, Ivan S. Damljanović
Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija
dragana.stevanovic@pmf.kg.ac.rs

Sintetisana je nova serija ferocen-supstituisanih pirolidina putem stereoselektivne [3+2] dipolarne cikloadicije azometin-ilida sa 1-ferocenil-2-nitroetenom u blagim reakcionim uslovima [1]. Azometin-ilidi su generisani *in situ* iz α-imino estara dobijenih od metil-estra L-alanina i različitih aromatičnih aldehida, u prisustvu srebro(I)-acetata i DBU baze (Shema 1). Dobijena jedinjenja su okarakterisana IR, ^{1}H i ^{13}C NMR spektroskopijom, kao i rendgenskom strukturnom analizom monokristala. Spektroskopski podaci potvrdili su formiranje pirolidinskog prstena i karakterističan obrazac supstitucije ferocenil grupom.



(*i*) Et_3N, Na_2SO_4, DCM, 20 h at RT; (*ii*) AgOAc, DBU, ACN, 45 min at RT

Shema 1. Sintetički put za dobijanje ferocen-supstituisanih pirolidina.

Azomethine ylide approach to ferrocenyl pyrrolidines

Dragana D. Stevanović, Marko S. Pešić, Jovana P. Bugarinović, Ivan S. Damljanović
University of Kragujevac, Faculty of Science, Kragujevac, Serbia
dragana.stevanovic@pmf.kg.ac.rs

A new series of ferrocene-substituted pyrrolidines was synthesized through stereoselective [3+2] dipolar cycloaddition reactions of azomethine ylides with 1-ferrocenyl-2-nitroethene under mild reaction conditions [1]. The azomethine ylides were generated *in situ* from α-imino esters derived from L-alanine methyl ester and various aromatic aldehydes, in the presence of silver(I) acetate and DBU. The obtained compounds were fully characterized by IR, ^{1}H and ^{13}C NMR spectroscopy, and single-crystal X-ray diffraction. Spectroscopic data confirmed the formation of the pyrrolidine framework and the characteristic ferrocenyl substitution pattern.

1. M. Pešić *et al.*, *Polyhedron,* **2026**, *286,* 117951.

Acknowledgements: Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No 451-03-34/2026-03/ 200122 and 51-03-33/2026-03/ 200122).

P-OH-7

Multikomponentni, kaskadni proces A^3 kuplovanje/*5-endo dig* ciklizacija katalizovan metalima u sintezi derivata pirazola

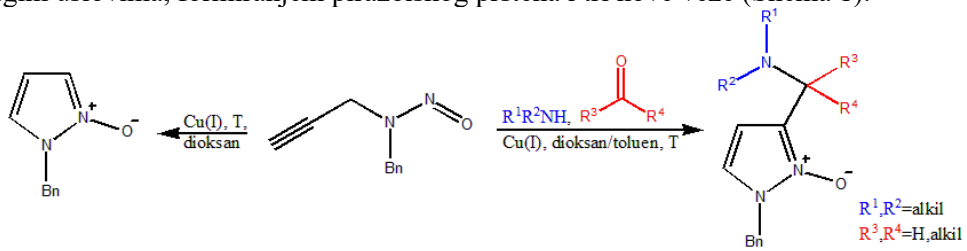
Nikola M. Mitrović[1], Branislav Z. Kokić[1], Predrag M. Jovanović[1], Milena R. Simić[1], Gordana D. Tasić[1], Veselin R. Maslak[2], Vladimir M. Savić[1]

[1]*Univerzitet u Beogradu - Farmaceutski fakultet, Katedra za organsku hemiju, Vojvode Stepe 450, 11221 Beograd, Srbija*

[2] *Univerzitet u Beogradu - Hemijski fakultet, Katedra za organsku hemiju, Studentski trg 12-16, 11000 Beograd, Srbija*

gordanat@pharmacy.bg.ac.rs

Propargilni derivati koji poseduju proksimalnu *N*-nitrozil grupu su proučavani kao polazna jedinjenja za dobijanje kako nesupstituisanih tako i supstituisanih derivata pirazol-*N*-oksida[1]. Primena CuI kao katalizatora omogućila je inkorporiranje A^3 transformacije[2] u proces rezultujući, pod blagim uslovima, formiranjem pirazolskog prstena i tri nove veze (Shema 1).



Shema 1. Ciklizacija i tandem A^3 kuplovanje/5-endo dig ciklizacija.

Metal-catalyzed multicomponent, cascade A^3 coupling/5-*endo dig* cyclization process in the synthesis of pyrazole derivatives

Nikola M. Mitrović[1], Branislav Z. Kokić[1], Predrag M. Jovanović[1], Milena R. Simić[1], Gordana D. Tasić[1], Veselin R. Maslak[2], Vladimir M. Savić[1]

[1]*University of Belgrade - Faculty of Pharmacy, Department of Organic Chemistry, Vojvode Stepe 450, 11221 Belgrade, Serbia*

[2]*University of Belgrade - Faculty of Chemistry, Department of Organic Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia*

gordanat@pharmacy.bg.ac.rs

Propargyl derivatives possessing a proximal *N*-nitrosyl group have been studied as starting compounds for the preparation of both unsubstituted and substituted pyrazole-*N*-oxide derivatives[1]. The use of CuI as a catalyst enabled the incorporation of the A^3 coupling[2] into the process resulting, under mild conditions, in the formation of a pyrazole ring and three new bonds (Scheme 1).

1. R. Unnava, A.K. Saikia, *ChemistrySelect*. **2016**, *1*, 1816-1823.
2. H. Ohno, Y. Ohta et al., Angew. Chem. Int. Ed. **2007**, 46, 2295-2298.

Acknowledgements: Ministry of Science, Technological Development, and Innovation of the Republic of Serbia through two grant agreements with the University of Belgrade – Faculty of Pharmacy (Nos. 451-03-33/2026-03/200161 and 451-03-34/2026-03/200161).

P-OH-8

Sinteza i spektralna karakterizacija novih derivata tiabendazola koji sadrže vanilinski fragment

Tamara Todorović[1], Jovana Muškinja[1], Violeta Marković[2]

[1]*Univerzitet u Kragujevcu, Institut za informacione tehnologije, Departman za prirodno-matematičke nauke, Liceja Kneževine Srbije 1A, 34 000 Kragujevac, Srbija*

[2]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, R. Domanovića 12, 34 000 Kragujevac, Srbija*

tamara.todorovic@uni.kg.ac.rs

Tiabendazol i derivati benzimidazola predstavljaju značajnu klasu jedinjenja zbog širokog spektra bioloških aktivnosti, dok vanilin i njegovi derivati pokazuju različite farmakološke efekte. U cilju poboljšanja biološke aktivnosti, sintetizovano je šest novih jedinjenja koja sadrže obe farmakofore. U prvom koraku sinteze izvršeno je alkilovanje NH grupe tiabendazola pomoću etil-bromacetata, a potom je formirani estar preveden u karbohidrazid reakcijom sa hidrazin monohidratom. Dobijeni karbohidrazid je dalje funkcionalizovan reakcijom sa O-alkilovanim derivatima vanilinske kiseline. Struktura sintetizovanih jedinjenja potvrđena je primenom NMR spektroskopije.

Synthesis and spectral characterization of novel thiabendazole derivatives containing a vanillin moiety

Tamara Todorović[1], Jovana Muškinja[1], Violeta Marković[2]

[1]*University of Kragujevac, Institute for Information Technologies, Department of Science, Liceja Kneževine Srbije 1A, 34 000 Kragujevac, Serbia*

[2]*University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34 000 Kragujevac, Serbia*

tamara.todorovic@uni.kg.ac.rs

Thiabendazole and benzimidazole derivatives represent an important class of compounds due to their broad spectrum of biological activities, while vanillin derivatives exhibit various pharmacological effects. With the aim of enhancing biological activity, six novel compounds containing both pharmacophores were synthesized. In the first step of the synthesis, the NH group of thiabendazole was alkylated using ethyl bromoacetate, after which the obtained ester was converted into the corresponding carbohydrazide by reaction with hydrazine monohydrate. The resulting carbohydrazide was further functionalized by reaction with *O*-alkylated derivatives of vanillic acid. The structures of the synthesized compounds were confirmed by NMR spectroscopy.

This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-33/2026-03/200378 and 451-03-34/2026-03/200122).

P-OH-9

Proučavanje odnosa strukture i svojstava fotoaktivnih tečnih kristala savijene molekulske geometrije

Nemanja Trišović[1], Kristina Gak Simić[2], Ivana Đorđević[3], Paulina Rybak[4], Damian Pociecha[4], Raquel Giménez[5,6], Maria Blanca Ros[5,6]

[1]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[3]*Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Srbija*
[4]*Hemijski fakultet, Univerzitet u Varšavi, Varšava, Poljska*
[5]*Institut za nauku o nanomaterijalima Aragona, CSIC-Univerzitet u Saragosi, Saragosa, Španija*
[6]*Prirodno-matematički fakultet, Univerzitet u Saragosi, Saragosa, Španija*
ntrisovic@tmf.bg.ac.rs

U ovom radu ispitan je uticaj strukture π-sistema na tečnokristalna i fotofizička svojstva novosintetisane serije molekula savijene geometrije. Jedinjenje na bazi azobenzena gradi enantiotropnu B_7 fazu, dok jedinjenja koja sadrže (cijano)stilbensku jedinicu formiraju monotropnu B_{1Rev} fazu. Jedinjenja na bazi cijanostilbena pokazuju pojačanu emisiju usled agregacije i reverzibilno mehanofluorohromno ponašanje. U sprezi sa kvantno-hemijskim proračunima, dobijeni rezultati pružaju smernice za razvoj novih samoorganizujućih materijala osetljivih na spoljašnje stimuluse.

Structure–property relationship of photoactive bent-core liquid crystals

Nemanja Trišović[1], Kristina Gak Simić[2], Ivana Đorđević[3], Paulina Rybak[4], Damian Pociecha[4], Raquel Giménez[5,6], Maria Blanca Ros[5,6]

[1]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia.*
[3]*University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia*
[4]*Faculty of Chemistry, University of Warsaw, Warsaw, Poland*
[5]*Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain*
[6]*Facultad de Ciencias, Universidad de Zaragoza, Zaragoza, Spain*
ntrisovic@tmf.bg.ac.rs

The influence of the π-system structure on liquid crystalline and photophysical properties of a newly synthesized series of bent-core molecules was investigated. The azobenzene-based compound exhibited an enantiotropic B_7 phase, whereas those with a (cyano)stilbene unit formed a monotropic B_{1Rev} phase. The cyanostilbene-based compounds showed aggregation-induced emission enhancement, and reversible mechanofluorochromic behaviour. Coupled with quantum-chemical calculations, the obtained results offer guidelines for the development of new stimuli-responsive self-assembled materials.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/200026, 451-03-34/2026-03/200135 and 451-03-33/2026-03/200287), the Spanish project PID2021−122882NB-I00 financed by MCIN/AEI/10.13039/ 501100011033/and by "ERDF A way of making Europe".

P-OH-10

Sinteza triarilmetana na bazi antipirina primenom mikrotalasnog zračenja

Anita Lazić[1], Jelena Lađarević[2], Nemanja Trišović[2], Marija Dimitrijević[2], Aleksandra Mašulović[1], Luka Matović[1], Dušan Mijin[2]

[1]*Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
ntrisovic@tmf.bg.ac.rs

Najjednostavniji način dobijanja triarilmetana podrazumeva Bajerovu kondenzaciju. U ovom radu prikazana je sinteza osam triarilmetana polazeći od različitih aromatičnih aldehida i antipirina (2,3-dimetil-1-fenil-3-pirazolon-5-ona) u prisustvu *p*-toluensulfonske kiseline kao katalizatora primenom mikrotalasnog zračenja u odsustvu rastvarača. Sintetički protokol je optimizovan koristeći *p*-*N*,*N*-dimetilaminobenzaldehid, pri čemu su sistematski ispitani uticaji odnosa reaktanata, vremena reakcije i temperature. Reakcije su izvođene u mikrotalasnom reaktoru na 100 °C u trajanju od 1 minuta i odnosu reaktanata 2:1 (antipirin:aldehid). Strukture svih dobijenih jedinjenja potvrđene su različitim spektroskopskim tehnikama.

Microwave-assisted preparation of antipyrine-based triarylmethanes

Anita Lazić[1], Jelena Lađarević[2], Nemanja Trišović[2], Marija Dimitrijević[2], Aleksandra Mašulović[1], Luka Matović[1], Dušan Mijin[2]

[1]*Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
ntrisovic@tmf.bg.ac.rs

The simplest method for the synthesis of triarylmethanes is the Baeyer condensation. In this work, a microwave-assisted, solvent-free approach for the synthesis of eight triarylmethanes from aromatic aldehydes and antipyrine (2,3-dimethyl-1-phenyl-3-pyrazoline-5-one) in the presence of *p*-toluenesulfonic acid as a catalyst is reported. The synthetic protocol was optimized using *p*-*N*,*N*-dimethylaminobenzaldehyde, while the effects of reactant ratios, reaction time, and temperature were systematically investigated. The reactions were performed in a microwave reactor at 100 °C for 1 min with antypirine:aldehyde ratio 2:1. The structures of all obtained compounds were confirmed by various spectroscopic techniques.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Grants No. 451-03-34/2026-03/200135 and 451-03-33/2026-03/200287).

Teorijska hemija

Theoretical Chemistry

P-TH-1

Ispitivanje aromatičnosti u organometalnim polusendvič-jedinjenjima sa π-akceptorskim ligandima

Milenko M. Bunović[1,2], Katarina A. Ćeranić[2], Slađana Đorđević[3], Dušan P. Malenov[1]
[1]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
[2]*Inovacioni centar Hemijskog fakulteta u Beogradu, Beograd, Srbija*
[3]*Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Kragujevac, Srbija*
katarina_ceranic@chem.bg.ac.rs

Aromatičnost arenskih liganada u polusendvič-jedinjenjima sa π-akceptorima ispitivana je na osnovu dva deskriptora: elektronske gustine delokalizovanih veza (EDDB) i gustine magnetno indukovanih struja (MICD). Optimizacijom molekula na B3PW91/def2-TZVP nivou teorije, praćeno računanjem EDDB indeksa, kao i MICD u programu SYSMOIC, utvrđeno je da benzen i ciklopentadienil kao ligandi imaju smanjen aromatičan karakter u odnosu na nekoordinovani benzen. Pokazano je da vrednosti jačina struja kroz veze zavise od položaja i jačine π-akceptora. Takođe, utvrđeno je da se u svakoj seriji ispitivanih kompleksa zapaža povećanje elektronske delokalizacije u arenskim prstenovima idući od 3d- ka 5d-metalima.

A study on aromaticity in organometallic half-sandwich compounds with π-acceptor ligands

Milenko M. Bunović[1,2], Katarina A. Ćeranić[2], Slađana Đorđević[3], Dušan P. Malenov[1]
[1]*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
[2]*Innovative Centre of the Faculty of Chemistry in Belgrade, Belgrade, Serbia*
[3] *University of Kragujevac, Faculty of Science, Kragujevac, Serbia*
katarina_ceranic@chem.bg.ac.rs

Aromaticity of arene ligands in half-sandwich compounds with π-acceptor ligands was studied using two descriptors: the electron density of delocalized bonds (EDDB), as well as the magnetically induced current densities (MICD). Optimizing the molecules on the B3PW91/def2-TZVP level of theory, followed by calculating the EDDB values, as well as the MICD values in the SYSMOIC program, it was determined that benzene and cyclopentadienyl ligands have reduced aromatic character compared to uncoordinated benzene. It was shown that the values of current strengths through bonds depend on the position and strength of π-acceptors. Also, it was determined that each series of studied complexes has an increase in electron delocalization in arene rings going from 3d to 5d metals.

Acknowledgment: Supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia, contracts: 451-03-33/2026-03/200288, 451-03-33/2026-03/200168 and 451-03-34/2026-03/200122.

P-TH-2

Indenilni kompleks gvožđa(II) kao veoma efikasan receptor za katjone – računarsko ispitivanje

Katarina A. Ćeranić[1,2], Snežana D. Zarić[3], Dušan P. Malenov[3]
[1]*Inovacioni centar Hemijskog fakulteta u Beogradu, Beograd, Srbija*
[2]*Univerzitet u Beogradu, Fakultet za fizičnu hemiju, Beograd, Srbija*
[3]*Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*
katarina_ceranic@chem.bg.ac.rs

Jačina katjon-π interakcija se može značajno povećati ako se aromatičan prsten koordinuje za prelazne metale.[1] U ovom radu analizirali smo katjon-π interakcije između katjona alkalnih i zemnoalkalnih metala sa sendvič-jedinjenjem [FeCpInd], kako bismo detaljnije procenili uticaj koordinacije na katjon-π interakciju, s obzirom da je indenil-ligand (Ind) jednim prstenom koordinovan za prelazni metal, dok je drugi prsten nekoordinovan. Proračuni na B3LYP-D3/def2-TZVP nivou teorije pokazali su da se kod ovog sistema katjon-π interakcija može formirati sa svim aromatičnim prstenovima gotovo jednakom jačinom, osim u slučaju kada katjon istovremeno interaguje i sa nekoordinovanim prstenom indenila i sa prelaznim metalom u sendvič-jedinjenju.

Indenyl complex of iron(II) as a very efficient cation receptor – a computational study

Katarina A. Ćeranić[1,2], Snežana D. Zarić[3], Dušan P. Malenov[3]
[1] *Innovative Centre of the Faculty of Chemistry in Belgrade, Belgrade, Serbia*
[2]*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*
[3]*University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
katarina_ceranic@chem.bg.ac.rs

The strength of cation-π interactions can significantly increase if the aromatic ring is coordinated to transition metals.[1] In this study we have analyzed the cation-π interactions between alkali and alkaline earth cations with the sandwich compound [FeCpInd], in order to assess the influence of coordination more thoroughly, considering that indenyl ligand (Ind) has one ring coordinated to the transition metal, while the other ring is not. The B3LYP-D3/def2-TZVP calculations have shown that in this system cation-π interaction can be formed with all aromatic rings with very similar intensities, with the exception of simultaneous interaction with uncoordinated indenyl ring and the transition metal in the sandwich compound.

1. K. Ćeranić, S. Zarić, D. Malenov, *Dalton Trans*. **2025**, 54, 7700.

Acknowledgment: This work is supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (contracts number: 451-03-33/2026-03/200168 and 451-03-33/2026-03/200288).

Zelena hemija

Green Chemistry

P-ZH-1

Membranski potpomognuta ekstrakcija i stabilizacija parthenolida iz *Tanacetum parthenium* primenom PPG400

Jelena Jovanović[1], Dajana Lazarević[1], Nada Ćujić Nikolić[2], Katarina Šavikin[2], Predrag Petrović[3], Goran Vladisavljević[4] and Tatjana Trtić-Petrović[1]

[1]*Laboratorija za fiziku, Vinča Institut za nuklearne nauke – Nacionalni Institut Republike Srbije, Univerzitet u Beogradu Mike Petrovića Alasa 12-14, 11001 Beograd, Srbija*

[2]*Instut za proučavanje lekovitog bilja, Dr Josif Pančić, Beograd, Srbija*

[3]*Inovacioni centar Tehnološko-metalurškog fakulteta, Univerzitet u Beogradu, Karnegijeva 4, 11000 Beograde, Srbija*

[4]*Departman za hemijsko inženjerstvo, Univerzitet Loughborough, Loughborough, Leicestershire, UK*

jelena.jovanovic@vin.bg.ac.rs.

Parthenolid (PAR), glavno bioaktivno jedinjenje biljke *Tanacetum parthenium* L., pokazuje antiinflamatorna i antimigrenska svojstva, ali je njegova primena ograničena slabom rastvorljivošću i niskom stabilnošću. U ovom radu ispitivana je primena polipropilen-glikola 400 (PPG400) za ekstrakciju i stabilizaciju PAR-a iz biomase buhača. Ispitivan je uticaj veličine čestica biomase, odnosa čvrsto–tečno i koncentracije PPG400 na prinos PAR-a i ukupnih fenolnih jedinjenja (TPC). Povećanje koncentracije PPG400 poboljšalo je ekstrakciju PAR-a i TPC, pri čemu su najbolji rezultati dobijeni sa 15% PPG400. Ispitivanja stabilnosti pokazala su veću stabilnost PAR-a u sistemima sa PPG400. Dobijeni rezultati ukazuju da PPG400 predstavlja perspektivan zeleni pristup za ekstrakciju i stabilizaciju bioaktivnih jedinjenja biljnog porekla.

Membrane-assisted extraction and stabilization of parthenolide from *Tanacetum parthenium* using PPG400

Jelena Jovanović[1], Dajana Lazarević[1], Nada Ćujić Nikolić[2], Katarina Šavikin[2], Predrag Petrović[3], Goran Vladisavljević[4] and Tatjana Trtić-Petrović[1]

[1]*Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11001 Belgrade, Serbia*

[2]*Institute for Medicinal Plant Research, Dr Josif Pančić, Belgrade, Serbia*

[3]*Innovation Centre of Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia*

[4]*Chemical Engineering Department, Loughborough University, Loughborough, Leicestershire, UK*

jelena.jovanovic@vin.bg.ac.rs.

Parthenolide (PAR), the primary bioactive compound of *Tanacetum parthenium* L., exhibits anti-inflammatory and anti-migraine properties; however, its application is limited by poor solubility and low stability. In this study, polypropylene glycol 400 (PPG400) was investigated for extraction and stabilization of PAR from feverfew biomass. The effects of biomass particle size, solid-to-liquid ratio and PPG400 concentration on PAR yield and total phenolic content (TPC) were evaluated. Increasing the PPG400 concentration improved PAR and TPC extraction, with optimal results obtained using a 15% PPG400 solution. Stability studies showed enhanced PAR preservation in PPG400 systems. The obtained results indicate that PPG400 represents a promising green approach for the extraction and stabilization of plant-derived bioactive compounds.

Acknowledgement: This research was supported by the Science Fund of the Republic of Serbia, Grant No 17475, Green Innovation: Unlocking the Bioactive Potential of Biomass for Enhanced Pharmaceuticals and Foods through Eco-Friendly Sustainable Technologies – VIVE

Indeks autora / Author Index

I

J

K

L

M

N

O

P

R

S

Z

Ž

ORCID

Autor	ORCID
Acković, Jovana S.	0000-0002-4355-923X
Agbaba, Jasmina R.	0000-0002-9915-2885
Ajdačić, Vladimir	0000-0002-3423-0862
Ajduković, Jovana J.	0000-0003-0218-3640
Andrejević, Tina P.	0000-0002-9537-5926
Andrijević, Ana	0000-0003-3818-8208
Ašanin, Darko P.	0000-0003-1098-400X
Bajat, Jelena B.	0000-0003-0742-8176
Balula, Salete S.	0000-0002-8984-0473
Beara, Ivana	0000-0002-7587-957X
Bekić, Sofija S.	0000-0002-9020-698X
Benedeković, Goran	0000-0002-4752-7569
Bihelović, Filip J.	0000-0002-7654-3189
Bjedov, Srđan	0000-0002-9630-5831
Bogojeski, Jovana	0000-0002-3433-7774
Branković, Jovica B.	0000-0003-1635-4519
Bugarinović, Jovana P.	0000-0002-3561-6732
Bulatović, Sandra S.	0000-0002-7861-4489
Bunović, Milenko M.	0009-0006-8119-5103
Çobanoğlu, Duygu Nur	0000-0002-8583-8114
Cunha-Silva, Luís	0000-0001-9229-1412
Cvijić, Sergej	0009-0006-2473-0536
Ćelić, Anđelka S.	0000-0002-1058-6872
Ćeranić, Katarina A.	0009-0000-1688-5972
Ćirković Veličković, Tanja	0000-0003-2559-5234
Ćoćić, Dušan S.	0000-0002-8008-7876
Ćujić Nikolić, Nada	0000-0002-6736-3637
Damljanović, Ivan S.	0000-0001-5687-2885
Dapčević, Aleksandra H.	0000-0001-7650-7156
de Azambuja, Francisco	0000-0002-5537-5411
Declerck, Kilian	0000-0003-3711-7344
Despotović, Vesna N.	0000-0003-4113-6724
Dikić, Jelena K.	0000-0002-3454-735X

Dimitrijević, Marija	0000-0002-4999-1664
Dinkova-Kostova, Albena	0000-0003-0316-9859
Djošić, Marija	0000-0002-0869-2182
Djuran, Miloš I.	0000-0003-2763-2852
Drašković, Nenad S.	0000-0002-3455-1033
Dupé, Antoine	0000-0001-7781-0771
Duzdaban, Piroz	0000-0002-4686-9030
Dzichenka, Yaraslau U.	0000-0002-8655-8704
Đokić, Sanja M.	0000-0003-0448-6282
Đorđević, Aleksandar M.	0000-0002-0350-5368
Đorđević, Ivana	0000-0001-5981-9385
Đorđević, Slađana	0000-0003-0194-3927
Felek, Ikranur	0000-0001-9503-5772
Francuz, Jovana	0000-0002-4330-8561
Franich, Anđela A.	0000-0003-1904-9368
Gak Simić, Kristina	0000-0003-3928-9967
Gašić, Uroš	0000-0001-5384-8396
Gazikalović, Ivana V.	0000-0002-6481-8966
Gigić, Andrija D.	0009-0000-3242-0657
Giménez, Raquel	0000-0002-7854-6316
Glišić, Biljana Đ.	0000-0002-6343-8611
Grgurić-Šipka, Sanja	0000-0003-1906-535X
Gutman, Ivan	0000-0001-9681-1550
Ilić, Budimir, S.	0000-0002-2808-3501
Jakimov, Dimitar S.	0000-0002-1747-4718
Janaćković, Đorđe	0000-0002-8291-4345
Janković, Ana	0000-0002-5605-3297
Janković, Đorđe D.	0009-0001-0628-1435
Jeremić, Nevena S.	0000-0002-5284-8180
Jerosimić, Stanka V.	0000-0001-5873-0477
Joksimović, Nenad M.	0000-0003-3365-6762
Jovanović, Jelena	0009-0009-5706-771X
Jovanović, Predrag M.	0000-0001-9002-2796
Jovanović-Šanta, Suzana	0000-0002-4579-5762
Kalagasidis Krušić, Melina T.	0000-0003-0517-1952

Kandić, Ana	0009-0002-4709-5628
Katanić Stanković, Jelena S.	0000-0002-2997-9588
Kesić, Ana	0000-0002-8729-8748
Kilibarda, Sofija	0000-0001-9634-8359
Kljun, Jakob	0000-0002-1986-4840
Knežević-Jugović, Zorica D.	0000-0003-3009-1698
Kokanović, Andreja P.	0009-0007-3428-5947
Kokić, Branislav Z.	0000-0002-4821-2884
Koračak, Ljiljana	0000-0003-4892-1290
Kostić, Aleksandar Ž.	0000-0002-1012-4029
Košević, Milica G.	0000-0002-2105-4425
Kuč, Marija Z.	0009-0007-4538-9602
Kuzminac, Ivana Z.	0000-0001-8045-3568
Laban, Bojana B.	0000-0002-7758-445X
Lađarević, Jelena	0000-0002-5554-7295
Lazarević, Dajana	0000-0002-5200-9512
Lazarević, Slavica S.	0000-0002-9748-9353
Lazić, Anita	0000-0003-4855-3782
Leskovac, Andreja	0000-0002-6293-5237
Levovnik, Bojan D.	0009-0000-4953-2663
Lović, Jelena D.	0000-0001-5956-8571
Lučić-Škorić, Marija Lj.	0000-0003-1667-9436
Lupšić, Ema	0000-0001-7824-1689
Majkić, Tatjana	0000-0002-2384-5546
Maksimović, Jelena P.	0000-0001-7138-6666
Malenov, Dušan P.	0000-0002-3060-3377
Maletić, Snežana P.	0000-0002-5026-3365
Marinković, Dragana	0000-0002-6017-2109
Marinović, Maja A.	0000-0001-8696-7148
Marjanović Srebro, Tijana M.	0009-0006-9886-6516
Marković, Bojana M.	0000-0001-7608-8289
Marković, Maja D.	0000-0002-9739-2957
Marković, Violeta R.	0000-0001-5561-0672
Maslak, Veselin R.	0000-0002-5735-3953
Mašulović, Aleksandra	0000-0002-5279-7694

Matić, Sanja Lj.	0000-0003-4570-4370
Matović, Luka	0000-0003-4945-7776
Međedović-Stefanović, Milica G.	0000-0002-2024-2344
Micić, Ružica J.	0000-0003-3295-3159
Mihailović, Nevena	0000-0002-9105-7680
Mihailović, Vladimir B.	0000-0003-4113-6804
Mihajlović, Ljiljana E.	0000-0003-4802-432X
Mijin , Dušan, Ž.	0000-0001-5691-2971
Milašinović, Nikola Z.	0000-0002-2744-4002
Milinčić, Danijel D.	0000-0002-2476-9426
Milojković, Natalija D.	0000-0002-6112-6219
Milović, Emilija	0000-0002-4242-1562
Miljković, Đorđe	0000-0002-5613-9306
Mišić, Danijela	0000-0003-4116-3474
Mišković Stanković, Vesna B.	0000-0001-6525-9820
Mitrović, Nikola M.	0000-0002-0882-7307
Mladenović, Milan P.	0000-0002-6556-8778
Mojsilović, Kristina	0000-0003-1424-3225
Molnar Jazić, Jelena J.	0000-0002-8696-7647
Muškinja, Jovana	0000-0002-0638-3423
Nastasović, Aleksandra B.	0000-0002-8589-6437
Nedeljkov, Tanja, M.	0009-0007-6159-6943
Nedić, Natalija Ž.	0009-0002-5621-9223
Nikolić, Andrea M.	0000-0003-1907-1565
Nikolić, Nebojša D.	0000-0002-6385-5714
Nikolić, Stefan R.	0000-0002-0164-134X
Novaković, Miroslav	0000-0002-4984-041X
Opsenica, Igor M.	0000-0003-4942-4042
Pagnacco, Maja C.	0000-0002-1299-7974
Pajović, Milica	0000-0001-7312-0861
Panić, Vesna V.	0000-0003-3617-1533
Pantelić, Nebojša Đ.	0000-0003-1843-9890
Pantić, Olga J.	0000-0003-4667-2585
Pantović, Bojana V.	0000-0003-1997-625X
Parac-Vogt, Tatjana N.	0000-0002-6188-3957

Pašti, Igor A.	0000-0002-1000-9784
Pavlović, Radoslav Z.	0000-0003-1216-3950
Pešić, Marko S.	0000-0002-3871-5795
Pešić, Milica	0000-0002-9045-8239
Pešić, Mirjana B.	0000-0001-9779-1686
Petković, Sofija	0009-0001-5593-0630
Petri, Edward T.	0000-0002-3650-1523
Petrović, Biljana V.	0000-0001-7914-6026
Petrović, Jana Lj.	0009-0004-7543-7589
Petrović, Predrag	0000-0002-1967-8298
Petrović, Rada	0000-0001-9511-5633
Petrović, Sandra	0000-0003-0930-6455
Petrović, Tamara A.	0000-0003-1818-8710
Petrović, Vladimir P.	0000-0002-1904-368X
Pociecha, Damian	0000-0001-7734-3181
Počkaj, Marta	0000-0002-6306-1631
Podolski Renić, Ana	0000-0001-7412-3685
Polović, Natalija Đ.	0000-0002-9127-2014
Poljarević, Jelena M.	0000-0002-6706-0281
Popsavin, Mirjana	0000-0002-0924-1041
Popsavin, Velimir	0000-0001-9910-2987
Postolović, Katarina S.	0000-0002-6383-1659
Prekodravac Filipović, Jovana R.	0000-0002-5692-0119
Radenković, Slavko	0000-0002-1928-5494
Radinović, Kristina	0000-0003-3404-5760
Radovanović, Lidija D.	0000-0002-7505-6290
Rajić, Vladimir	0000-0001-7053-572X
Rajković, Snežana	0000-0002-7135-4063
Ralević, Uroš	0009-0005-7717-3000
Rilak Simović, Ana M.	0000-0001-8731-3605
Ros, Maria Blanca	0000-0003-4416-1036
Rybak, Paulina	0000-0002-6445-2765
Sakač, Marija N.	0000-0002-2796-1296
Santos, Diogo M. F.	0000-0002-7920-2638
Savic, Nada D.	0000-0002-6593-3499

Savić, Marina P.	0000-0002-1019-3673
Savić, Sanja I.	0000-0001-7021-9508
Savić, Vladimir M.	0000-0002-0033-1390
Selaković, Milica	0000-0001-5606-2401
Senćanski, Jelena V.	0000-0002-2020-0435
Simetić, Tajana M.	0000-0002-0923-7034
Simić, Milena R.	0000-0002-0865-5509
Simms, Charlotte	0000-0002-9334-9476
Simović, Anđela R.	0000-0003-4026-5647
Simović, Bojana M.	0000-0002-9407-155X
Spasojević, Pavle M.	0000-0001-8903-2102
Spasojević-Savković, Milica M.	0000-0001-9134-6637
Srećković, Nikola	0000-0002-0216-5816
Srećo Zelenović, Bojana	0000-0003-0216-2583
Stanić, Petar B.	0000-0002-3655-6452
Stanić, Zorka D.	0000-0002-4813-9808
Stanisavljević, Slađana	0000-0002-4766-9137
Stepanović, Ana	0000-0003-3006-3902
Stevanović, Dragana D.	0000-0003-3199-0775
Stevanović, Milena	0000-0002-8083-3787
Stevanović, Milica Z.	0000-0003-1961-737X
Stevanović, Nevena Lj.	0000-0003-3261-478X
Stojanović, Snežana R.	0000-0003-0894-2118
Stojković, Pavle	0000-0002-4660-5537
Svirčev, Miloš M.	0000-0003-1808-1315
Swinnen, Siene	0000-0002-7089-8173
Šavikin, Katarina	0000-0002-2086-9593
Šekuljica, Nataša, Ž.	0000-0001-8260-6556
Šljukić, Biljana	0000-0003-0203-4012
Šmit, Biljana M.	0000-0001-9799-4723
Tadić, Jelena	0000-0001-9407-0568
Tadić, Tamara T.	0000-0003-4484-1568
Tancić, Pavle I.	0000-0002-4024-710X
Tasić, Gordana D.	0000-0003-4784-9581
Terzić Jovanović, Nataša	0000-0002-4127-525X

Thi Ly, Hong Giang	0000-0003-4783-7417
Timotijević, Jana	0009-0001-3602-3955
Todorović, Tamara	0000-0002-7740-3639
Tomašević, Nevena M.	0000-0001-5218-8293
Tot, Nataša, J.	0009-0009-8041-859X
Trišović, Nemanja	0000-0002-9231-4810
Trtić-Petrović, Tatjana	0000-0002-0817-8343
Tubić, Aleksandra M.	0000-0001-7503-7754
Vasilić Rastko	0000-0003-2476-7516
Vasiljević, Bojana, R.	0000-0002-0335-1987
Viana Alexandre	0000-0002-4472-5834
Vladisavljević, Goran	0000-0002-8894-975X
Vujačić Nikezić, Ana	0000-0002-0843-6840
Vukić, Milena D.	0000-0001-7222-7245
Vuković, Nenad	0000-0003-4382-9743
Vuković, Sandra	0000-0001-8633-8237
Zarić, Snežana D.	0000-0002-6067-2349
Zlatović, Mario	0000-0003-4311-1731
Živković, Marija	0000-0001-6887-9566