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Ova knjiga sadrži kratke izvode
dva plenarna predavanja (PP),
šest predavanja po pozivu (PPP),
jedno predavanja dobitnika Medalje SHD (MP),
deset usmenih saopštenja (US) i
osamdeset dva saopštenja (obima jedne stranice)
prihvaćenih za prezentovanje na
60. Savetovanju Srpskog hemijskog društva.

This book contains abstracts of
two plenary lectures (PP),
six invited lectures (PPP),
lecture of SCS Medal awardee (MP),
ten oral presentations (US), and
eighty-two abstracts
accepted for presentation at
the 60th Meeting of the Serbian Chemical Society.

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Tekstilno inženjerstvo / Textile Engineering

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KRATKI IZVODI RADOVA

Short abstracts

Plenarna predavanja

Plenary Lectures

PP-1

Transformations and applications of biomass-derived C5 and C6-furanic platform chemicals

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Institute of Organic Chemistry with Centre of Phytochemistry – BAS, Sofia, Bulgaria

Nowadays, biorefinery is considered the most promising approach that may gradually replace current dependence on fossil resources, which although cheap and easy to obtain, lack any sustainability. The C5 and C6-furanics gain their moment as primary biorefinery feedstock due to the accessibility from the largest pool of biorenewable carbon, namely lignocellulose. Over the last decade, many obstacles have been overcome that have hampered their industrial applications. However, many challenges concerning the production chain from the preparation to the downstream synthetic processing still have to be addressed. This talk will cover some major directions in the transformations and applications of the two major pillars of biomass-derived C5 and C6-furanics, namely 5-hydroxymethyl furfural and furfural. It will provide a historical perspective of the developments in this area from our research group. Our recent works that provided advancements in the interface between organic synthesis, transition metal catalysis, and biorenewbales will be highlighted. The report will also share future development directions and general considerations.

PP-2

Recent advances in stereodynamics and conformational analysis of new functional materials by dynamic NMR and theoretical calculations

Nikolay G. Vassilev

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Dynamic NMR spectroscopy can determine energy barriers due to internal motion over the range of about 4.5–23 kcal/mol. Conformational analysis of the frozen conformations can be simulated and interpreted by reliable theoretical calculations based mainly on density functional theory (DFT). The same calculations can identify transition states and predict the values of energy barriers involved in stereodynamic processes. These calculations can predict the populations of conformers or chemical shifts of the nuclei in exchanging sites, which helps in assignment of these sites. Theoretical calculations can also answer the fundamental question of the origin of studied stereodynamic processes.

Recent advances in the experimental and theoretical approaches used in the field of the stereodynamic analysis are reviewed and examples include fluxional Pd(II) NHC complexes,[1-4] OLED relevant 1,3,5-triazine derivatives,[5] molecules related to the design of molecular machines[6] and 2,4-dihalogeno substituted synthetic analogues of the natural compound carvacrol.[7]

1. M. Dangalov, M. Stoyanova, P. Petrov, M. Putala, N. G. Vassilev *J. Organomet. Chem.* **2016**, *817*, 1.
2. M. Dangalov, P. Petrov, N. Vassilev *J. Organomet. Chem.* **2016**, *824*, 104.
3. R. Lyapchev, P. Petrov, M. Dangalov, N. Vassilev *J. Organomet. Chem.* **2017**, *851*, 194.
4. M. Dangalov, P. Petrov and N. G. Vassilev *J. Mol. Struct*. **2021**, *1230*, 129944.
5. G. M. Dobrikov, Y. Nikolova, I. Slavchev, M. Dangalov, V. Deneva, L. Antonov, N. G. Vassilev *Molecules*, **2023**, *28(3)*, 1248.
6. N. G. Vassilev, I. C. Ivanov, *Molecules*, **2023**, *28(24)*, 8004.
7. M. Đorđević Zlatković, N. Radulović, M. Dangalov, N. G. Vassilev *Molecules*, **2024**, *29(9)*, 1962.

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Predavanja po pozivu

Invited Lectures

PPP-1

O konfiguraciji prirodnih 2,6-ciklokuparan-3-ola: konačno razrešenje sporne situacije

Dragan B. Zlatković, Miljana R. Đorđević Zlatković, Niko S. Radulović
Univerzitet u Nišu, Prirodno-matematički fakultet u Nišu, Niš, Srbija

2,6-Ciklokuparan-3-oli su hemijski markeri i najzastupljenija isparljiva jedinjenja nekoliko vrsta jetrenjača. U literaturi se mogu naći međusodno suprotstavljene informacije o strukturama ciklokuparanola – različite istraživačke grupe su dodelile iste spektralne podatke različitim strukturama. Ove nedoslednosti nikada nisu razmatrane, a kamoli objašnjene na zadovoljavajući način. Sva četiri dijastereoizomerna ciklokuparanola su izolovana iz jetrenjače *Marchantia polymorpha*, njihove relativne i apsolutne konfiguracije su detaljno proučavane hemijskim i spektroskopskim metodama, a zatim su predložene definitivne stereostrukture.

On the configuration and occurrence of 2,6-cyclocuparan-3-ols: resolving a lasting discrepancy

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2,6-Cyclocuparan-3-ols are chemical markers and major volatiles of several liverwort species. Conflicting reports on the structures of these cyclocuparanols can be found in the literature–different research groups assigned the same spectral data to different structures, yet these inconsistencies were never addressed, let alone satisfactorily explained. Following the isolation of all four diastereoisomeric cyclocuparanols from *Marchantia polymorpha*, their relative and absolute configurations were extensively studied by chemical and spectroscopic methods and definite stereostructures were proposed.

1. D.B. Zlatković, M.R. Đorđević Zlatković, N.S. Radulović *Phytochemistry*. **2023**, *207*, 113566.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract Numbers 451-03-66/2024-03/200124 and 451-03-65/2024-03/200124).

PPP-2

Hybrid organic-inorganic perovskites: synthesis and spectroscopic properties

Miha Bukleski, Mihail Trajkov, Darko Stojchev, Sandra Dimitrovska-Lazova, Slobotka Aleksovska

Ss Cyril and Methodius University, Faculty of Natural Sciences and Mathematics, Institute of Chemistry, Skopje, RN Macedonia

The quest for finding new materials with enhanced optoelectronic properties and their potential application in the design of diodes, photosensors, and photovoltaic cells has spurred numerous research groups to focus their attention on hybrid organic-inorganic perovskites (HOIPs). Since the synthesis and design of the first perovskite containing an organic cation in the A position, research in this field has significantly expanded. The relatively low band-gap of the methylammonium lead iodide $(CH_3NH_3)PbI_3$ has opened a new field in solar cell research, reaching efficiency of nearly 30% which is comparable to metal-semiconductor sandwich cells.

The synthesis pathway of HOIPs plays an important role in obtaining the desired material. Low content of water in the system can lead to crystalohydrates with different properties. In this work, several different approaches for the synthetic procedure will be discussed in more detail. The synthesis can be carried out as a one stage process where all reactants are mixed in an exact stoichiometric ratio. The next step involves refluxing or reducing the solvent temperature. After refluxing, depending on the HOIP in question, various strategies can be employed. One such strategy is employing the anti-solvent approach, which results in larger crystals. In addition to the one-stage synthesis, a two-stage synthesis involves obtaining the A cation in the desired form and then combining it with the metal halide, which will later form the corresponding octahedra in the 3D perovskite structure. All of the described methods lead to obtaining larger monocrystals suitable for single-crystal XRD measurements.

The obtained compounds are investigated by single crystal XRD and vibrational spectroscopy techniques (IR and Raman) in a wide temperature range[1,2] (liquid nitrogen temperature to +200 °C), in order to gain information of the phases that are stabile at different temperatures. Vibrational spectroscopy techniques remain among the leading affordable methods capable of describing and explaining material behavior, especially when hydrogen bonding is present.

1. M. Bukleski, S. Dimitrovska Lazova, S. Aleksovska, *Spectrochim. Acta A.* **2022**, *266*, 120462.

2. K. Gjorgjevikj, M. Bukleski, S. Dimitrovska-Lazova, S. Aleksovska, *J. Mol. Struct*. **2023**, *1293*, 136236.

PPP-3

Zelene ekstrakcione metode: progres i izazovi

Tatjana M. Trtić-Petrović
Univerzitet u Beogradu, Institut za nuklearne nauke "Vinča", Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Srbija

Zelene ekstrakcione metode obuhvataju različite savremene pristupe koji se odlikuju smanjenjem negativnog uticaja na životnu sredinu. Ovo se postiže ili zamenom tradicionalnih organskih rastvarača netoksičnim alternativama poput vode, jonskih tečnosti, dubokih eutektičkih smeša, superkritičnih rastvora, ili značajnim smanjenjem upotrebe rastvarača i ekstragenasa. Cilj ovog rada je razvoj zelenih ektrakcionih metoda sa novim, netoksičnim rastvaračima i ekstragensima, kao i razvoj održivih ekstrakcionih metoda sa malom potrošnjom organskih rastvarača (membranska ekstrakcija). Biće prikazani odabrani primeri zelenih metoda na bazi jonskih tečnosti i membranskih procesa za ekstrakciju organskih i neorganskih zagađivača, kao i prirodnih jedinjenja uz evaluaciju njihovog zelenog indeksa i doprinosa cirkularnoj ekonomiji.

Green extraction methods: progress and challenges

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Green extraction methods encompass various modern approaches aimed at reducing the negative impact on the environment. This is achieved either by replacing traditional organic solvents with non-toxic alternatives such as ionic liquids, deep eutectic solvents, water, or supercritical solvents, or by reducing the use of solvents and extractants. The focus of these studies is on the development of green extraction methods that replace toxic solvents with ionic liquids and on the development of sustainable extraction methods with low consumption of organic solvents, such as membrane extraction. Selected examples of green methods based on ionic liquids and membrane processes for the extraction of organic and inorganic pollutants, as well as natural compounds, will be presented, along with an evaluation of their green index and contribution to the circular economy.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation, Republic of Serbia (contract number 451-03-66/2024-03/200017).

PPP-4

Koordinaciona hemija Šifovih baza - primena u solarnim tehnologijama

Mirjana M. Radanović
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Zahvaljujući jednostavnoj sintezi, raznolikim koordinacionim svojstvima, strukturnim karakteristikama dobijenih kompleksa, te mogućnosti raznovrsne primene, Šifove baze su široko proučavana grupa organskih jedinjenja. Osim obećavajućih bioloških svojstava, u novije vreme sve se više ispituju optička svojstva kompleksa sa ovom vrstom liganada, a radi primene solarnim tehnologijama. Sa ciljem boljeg razumevanja povezanosti strukture i svojstava kompleksa, kao i rasta interesa za primenu koordinacionih jedinjenja u ovoj oblasti, ovde dajemo pregled najvažnijih rezultata istraživanja mogućnosti primene kompleksa metala sa Šifovim bazama kao fotosenziterima u bojom senzibilizovanim solarnim ćelijama (DSSC), kao i mogućnost poboljšanja performansi danas najpopularnijih perovskitskih solarnih ćelija (PSC).

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Schiff Bases Coordination Chemistry - Application in Solar Technologies

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Schiff bases are intriguing due to their easy synthesis, versatile coordination modes, and unique structural properties. In addition to their well-documented biological activities, their high photoluminescence makes them promising for optical materials and solar cells. Here, we aim to pique the curiosity of coordination chemists by highlighting key findings that help understand the structure-property relationships, thus enabling the design of new materials with improved characteristics. The results of investigations into the use of Schiff bases and their metal complexes in the field of dye-sensitized solar cells (DSSC), as well as the currently popular perovskite solar cells (PSC), will be discussed (Figure 1).

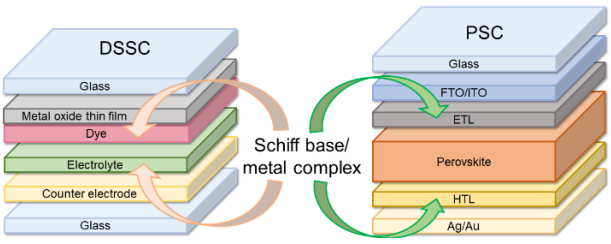

Figure 1. Potential use of Schiff base derivatives in solar cells

PPP-5

Ftalati: izvori, migracija, određivanje i štetno dejstvo

Tatjana D. Anđelković
Univerzitet u Nišu, Prirodno-matematički fakultet u Nišu, Niš, Srbija

Ftalati su sveprisutne zagađujuće supstance životne sredine usled njihovog lakog oslobađanja iz plastike u vodu, zemljište, vazduh i hranu [1]. Ftalati su grupa diestara *orto*-ftalne kiseline (dialkil- ili alkilaril-estri 1,2-benzendikarboksilne kiseline). Ftalati veće molekulske težine, kao što je "di-(2-etilheksil)-ftalat" (DEHP), koriste se kao plastifikatori za omekšavanje proizvoda od polivinil-hlorida (PVC), dok ftalati niže molekulske težine, kao što je di-*n*-butil-ftalat (DBP) ili butil-benzil-ftalat (BBzP), koriste se kao rastvarači za zadržavanje boje i mirisa u proizvodima. Mogu se naći u većini proizvoda koji imaju kontakt sa plastikom tokom proizvodnje, pakovanja ili isporuke. Pošto je hrana glavni izvor izloženosti ljudi ftalatima, informacije o nivoima ftalata u hrani su važne za procenu izloženosti ljudi. Migracija ftalata iz različitih materijala za pakovanje hrane, proizvoda za široku potrošnju i ličnu i medicinsku negu je česta pri nepravilnom skladištenju ovih proizvoda izloženim određenim spoljašnjim faktorima (temperatura, UV zračenje) i u slučaju duže ekspozicije plastike ovim faktorima.

Phthalates: sources, migration, determination and health impact

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Phthalates are ubiquitous environmental contaminants due to their easy release from plastics into water, soil, air, and food [1]. Phthalates are a group of diesters of *ortho*-phthalic acid (dialkyl or alkyl aryl esters of 1,2-benzenedicarboxylic acid). Higher-molecular-weight phthalates, such as di-2-ethylhexyl phthalate (DEHP), are used as plasticizers for softening polyvinyl chloride (PVC) products, while lower-molecular-weight phthalates, such as di-*n*-butyl phthalate (DBP) and butyl benzyl phthalate (BBzP), are widely used as solvents to hold color and scent in various products. Phthalates can be found in most products that come into contact with plastics during production, packaging, or delivery. Since foods are the major source of exposure to phthalates, information on phthalate levels in foods is important for human exposure assessment. The migration of phthalates from different materials used in food packaging, consumer products, and personal and medical care is common during improper storage of these products when exposed to certain external factors (temperature, UV radiation), and in cases of prolonged exposure of plastic to these factors.

1. T. Andjelković, D. Bogdanović, I. Kostić, G. Kocić, G. Nikolić, R. Pavlović, *Environ. Sci. Pollut. Res*. **2021**, *28*, 31380.

Acknowledgment: Supported by Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract No. 451-03-66/2024-03/200124).

PPP-6

Višestruki pokazatelji učeničkih postignuća u hemiji

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Ocena učeničkih postignuća u hemiji tradicionalno se oslanja na merenje performansi poput rezultata na kontrolnim zadacima. Iako ovaj pokazatelj pruža korisne uvide u savladavanje gradiva, on često ne daje informaciju o samim učeničkim iskustvima u toku učenja. Da bi se prevazišla ova ograničenja, istraživači u oblasti hemijskog obrazovanja sve više se okreću primeni dodatnih mera koje dublje istražuju kognitivne procese i ponašanje učenika. Analiza mentalnog napora pruža uvid u kognitivno opterećenje koje učenici doživljavaju tokom učenja ili rešavanja zadataka. Slično tome, analiza praćenja pogleda pruža uvid u obrasce vizuelne pažnje učenika, otkrivajući kako oni interaguju sa vizuelnim stimulansima i kako raspoređuju pažnju tokom aktivnosti učenja. U ovom apstraktu istražujemo integraciju inovativnih pokazatelja, uključujući analizu mentalnog napora i tehnologiju praćenja pogleda, uz tradicionalne metričke pokazatelje. U okviru prezentacije biće prikazane metodologije, rezultati i implikacije integrisanja ovih pokazatelja za procenu učeničkih postignuća u hemiji. Prihvatajući holistički pristup oceni postignuća, cilj nam je da podstaknemo sveobuhvatnije razumevanje procesa učenja.

Multiple metrics of students' achievements in chemistry

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The assessment of students' achievements in chemistry has traditionally relied on performance metrics such as exam scores. While these metrics offer valuable insights into content mastery, they often fall short of capturing the full spectrum of student learning experiences. To address this limitation, educators and researchers are increasingly turning to supplementary measures that probe deeper into cognitive processes and learning behaviors. Mental effort analysis provides a glimpse into the cognitive load students experience during learning and problem-solving. Similarly, eye-tracking analysis offers insight into students' visual attention patterns, revealing how they interact with visual stimuli and allocate their attention during learning activities. In this abstract, we explore the integration of innovative measures, including mental effort analysis and eye-tracking technology, alongside traditional assessment metrics. This presentation will showcase the methodologies, findings, and implications of these measures in assessing student achievements in chemistry. By embracing a holistic approach to assessment, we aim to foster a more comprehensive understanding of student learning processes.

Predavanje dobitnika medalje SHD za pregalaštvo i uspeh u nauci

Lecture by the winner of the SCS medal for achievement and success in science

MP-1

Primena UHPLC Q-ToF MS za analizu bioaktivnih jedinjenja u hrani

Danijel D. Milinčić, Aleksandar Ž. Kostić, Slađana P. Stanojević, Mirjana B. Pešić
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Ultra efikasna tečna hromatografija kombinovana sa kvadrupol-vreme leta masenom spektrometrijom (UHPLC/Q-ToF/MS) je napredna tehnika koja se koristi u analizi različitih bioaktivnih jedinjenja. Kombinacija kvadrupol i ToF masenih analizatora daje jedinstvene karakteristike Q-ToF detektora (brza akvizicija, širok opseg mase i visoka pokretljivost jona), što omogućava primenu u analizi poznatih i nepoznatih biomolekula. Ova tehnika se može uspešno primeniti za identifikaciju biomolekula i njihovih struktura, zbog UHPLC sposobnost razdvajanja i Q-ToF/MS podata (*m/z* tačna masa i MS fragmentacija). U ovom pregledu su sumirane sve specifičnosti i aspekti primene UHPLC/Q-ToF/MS tehnike za identifikaciju različitih bioaktivnih jedinjenja: fenolna jedinjenja, fenilamidi, glukozinolati i saponini dobijeni iz biljnog materijala ili hrane. Razmatrano je i korišćenje ove tehnike u analizi metabolita nastalih tokom prerade i digestije hrane. Ovaj pregled ukazuje na prednosti i ograničenja UHPLC/Q-ToF/MS tehnike i podstiče njenu primenu u analizi bioaktivnih jedinjenja.

Application of UHPLC Q-ToF MS for analysis of bioactive compounds in food

Danijel D. Milinčić, Aleksandar Ž. Kostić, Slađana P. Stanojević, Mirjana B. Pešić
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Ultra-high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (UHPLC/Q-ToF/MS) is an advanced technique that has been used in the analysis of various bioactive compounds. The combination of quadrupole and ToF mass analyzers gives unique characteristics of Q-ToF detector (fast acquisition, wide mass range, and high ion mobility), which enables its application for target and untarget analysis of biomolecules. This technique can be a powerful tool for identification and structure elucidation of various biomolecules, due to separation ability of UHPLC and Q-ToF/MS data (*m/z* exact mass and MS fragmentation). In this review all the specifics and aspects of the application of UHPLC/Q-ToF/MS technique for identification of various bioactive compounds: phenolic compounds, phenylamides, glucosinolates, derived from plant materials or food were summarized. The analysis of metabolites formed during food processing and digestion by this technique is also considered. This review points out advantages and limitations of UHPLC/Q-ToF/MS technique and encourages its application in analysis of bioactive compounds.

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Usmena Saopštenja

Oral Presentations

US-1

„U labu” – naučno-popularni podkast

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Podkast „U labu“ / „LABkast“ (www.ulabu.org) je inicijativa trojice profesora hemije/biohemije sa Prirodno-matematičkog fakulteta u Novom Sadu – Srđana Bjedova, Branislava Jovića i Miloša Svirčeva – koji kroz neformalne razgovore i širok spektar tema pokušava da popularizuje nauku. Proces naučne komunikacije, koji je suštinski za premošćavanje jaza između naučne zajednice i šire javnosti, ključan je element ovog podkasta. Cilj podkasta je promocija naučne pismenosti, omogućavanje informisanog donošenja odluka i podrška naučnom napretku kroz pristupačno predstavljanje kompleksnih tema. Saopštavanjem naučnih informacija na razumljiv način, podkast ne samo da demistifikuje nauku, već i promoviše kritičko mišljenje i donošenje odluka zasnovano na dokazima. Ovakav pristup doprinosi dubljem razumevanju i uvažavanju nauke u društvu, podstiče radoznalost i inspiriše buduće generacije naučnika. Na Savetovanju će biti predstavljeno iskustvo autora u realizaciji podkasta, izbor tema, metodologija komunikacije, interakcija sa slušaocima, kao i izazovi i budući planovi.

“U labu” – a popular science podcast

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The podcast "U labu" / “LABkast” (www.ulabu.org) is an initiative of three chemistry/biochemistry professors from the Faculty of Sciences in Novi Sad – Srđan Bjedov, Branislav Jović, and Miloš Svirčev – which attempts to popularize science through informal conversations and a wide range of topics. The process of scientific communication, which is essential for bridging the gap between the scientific community and the general audience, is a key element of this podcast. The goal of the podcast is to promote scientific literacy, enable informed decision-making, and support scientific progress through an accessible presentation of complex topics. By understandably conveying scientific information, the podcast not only demystifies science but also promotes critical thinking and evidence-based decision-making. This approach contributes to a deeper understanding and appreciation of science in society, encourages curiosity, and inspires future scientists. At the Conference, the authors' experience in podcast implementation, topic selection, communication methodology, interaction with listeners, challenges, and plans will be presented.

*Acknowledgment: “**LABkast**” is a project realized by the team of the podcast “U labu“, in collaboration with the **Scientific Club Novi Sad** and supported by the **Center for the Promotion of Science** through a Public Call for Support for Projects of Science Promotion and Popularization.*

US-2

Strukturna zavisnost energije tripletnih stanja u konjugovanim molekulima

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U ovom istraživanju smo pokazali da se efekat benzo-anelacije može primeniti za predviđanje energije tripletnih stanja derivata antracena, fluorantena i bifenilena. Razvijen je kvantitativni model zasnovan na broju angularno, linearno i geminalno aneliranih benzenovih prstena, koji veoma tačno predviđa energije tripletnih stanja ispitivanih molekula. Pokazali smo i da je energija tripletnih stanja povezana sa indeksima aromatičnosti centralnih prstenova u singletnom stanju proučavanih sistema. (Anti)aromatični karakter ovih molekula je procenjen uz pomoć energetskog efekta (ef), HOMA indeksa, multicentričnog delokalizacionog indeksa (MCI), gustine magnetno indukovanih struja (MICD) i indeksa NICS.

Revealing structural dependence of the triplet state excitation energies in conjugated molecules

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In this study we showed that the effect of benzo-annelation can be used to predict the triplet state excitation energies of anthracene, fluoranthene and biphenylene derivatives. A quantitative model based only on the number of angularly, linearly, and geminally annelated benzene rings was established, being able to accurately predict the triplet state excitation energies of the studied molecules. In addition, we showed that the triplet state excitation energy is correlated with the aromaticity indices of the central ring in the singlet state of the studied systems. The (anti)aromatic character of the examined molecules was studied using the energy effect (ef), harmonic oscillator model of aromaticity (HOMA), multicentre delocalization indices (MCI), magnetically induced current densities (MICDs) and nucleus independent chemical shifts (NICS).

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US-3

Priroda jon-π interakcija (polu)sendvič-jedinjenja – XEDA studija

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Aromatični sistemi formiraju veoma jake jon-π interakcije ukoliko se koordinuju za prelazne metale.[1,2] Kako bi se ispitala priroda ovih interakcija, urađena je Xiamen dekompozicija energije (XEDA) anjon-π i katjon-π interakcija na modelima organometalnih jedinjenja. XEDA rezultati ukazuju na to da su elektrostatičke sile dominantne u anjon-π interakcijama između polusendvič-jedinjenja i halogenidnih anjona. S druge strane, polarizacija nadjačava elektrostatičke efekte u katjon-π dimerima sendvič-jedinjenja, naročito sa malim katjonima alkalnih metala. Oba tipa jon-π interakcija su jača kod (polu)sendvič-jedinjenja nego kod organskih aromatičnih jedinjenja primarno usled pojačanih polarizacionih efekata.

The nature of ion-π interactions of (half-)sandwich compounds – a XEDA study

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Aromatic systems form very strong ion-π interactions upon coordination to transition metals.[1,2] To study the nature of these interactions, we have performed Xiamen Energy Decomposition Analysis (XEDA) of anion-π and cation-π interactions of model organometallic compounds. The XEDA results indicate that anion-π interactions between half-sandwich compounds and halide anions are dominated by electrostatic forces. On the other hand, polarization prevails over electrostatic effects in cation-π dimers of sandwich compounds, particularly with small alkali cations. Both types of interactions are stronger in (half-)sandwich than in organic aromatic compounds primarily due to increased polarization effects.

1. D. P. Malenov, S. D. Zarić, *Chem. Eur. J.* **2021**, *27*, 17862.
2. K. A. Ćeranić, S. D. Zarić, D. P. Malenov, **2024**, *manuscript in preparation*.

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US-4

Kristalna struktura novog hibrida ferocena i tiazolo[3,4-*a*]pirazin-5,8-diona

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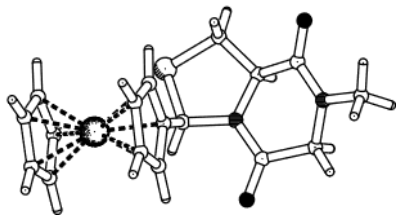
Kristalna i molekulska struktura jedinjenja je određena rendgenskom difrakcijom na monokristalu (slika 1). Apsolutna struktura je utvrđena na osnovu efekta rezonantnog rasejanja analizom Bajfutovih parova. Utvrđeno je da tiazolski prsten zauzima uvijenu konformaciju, dok se pirazinski prsten nalazi u konformaciji deformisane lađe. U kristalnoj strukturi je svaki molekul okružen sa 16 suseda. Šest molekula koji su raspoređeni kvazi-heksagonalno u kristalografskoj *bc* ravni gradi najjače interakcije (tri nezavisna para), te je ova diperiodična mreža – sloj – osnovna gradivna jedinica kristalne strukture. U ovim interakcijama dominira disperzioni tip privlačenja. Ostale interakcije su dvostruko i više slabije i deluju između slojeva.



Slika 1. Molekulska struktura jedinjenja

Crystal structure the new ferrocene – thiazol[3,4-*a*]pyrazin-5,8-dione hybride

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The crystal and molecular structure of the compound was elucidated through X-ray diffraction analysis on a single crystal (Figure 1). The absolute structure was determined utilizing the resonance scattering effect, employing analysis of Bijvoet pairs. Our findings reveal that the thiazole ring adopts a twisted conformation, while the pyrazine ring exhibits a deformed boat conformation. Within the crystal structure, each molecule is surrounded by 16 neighbors. Notably, six molecules arranged quasi-hexagonally in the crystallographic *bc* plane form the strongest interactions. This diperiodic network, or layer, serves as the fundamental building unit of the crystal structure. These interactions are primarily governed by a dispersion-type attraction. Additionally, weaker interactions occur between layers, approximately half the strength of the intra-layer interactions.

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US-5

Simultano određivanje dopamina, serotonina, askorbinske kiseline i nitritnog jona primenom modifikovane GCE

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Dopamin, serotonin, askorbinska kiselina i nitritni jon su uključeni u različite fiziološke procese u metabolizmu.[1] U ovom radu je razvijen senzor za simultano određivanje navedenih komponenti, primenom adsorptivne SWV. Staklasti ugljenik je modifikovan polielektrolitnim kompleksom hitozana i alginata, uz dodatak elektrohemijski redukovanog grafen-oksida. Prisustvo polisaharida poboljšalo je adsoprciju analita na površini elektrode, dok je redukovani grafen-oksid značajno povećao električnu provodljivost. Primenom modifikovane elektrode optimizovanog sastava, uz optimalne eksperimentalne uslove (pH vrednost, potencijal i vreme akumulacije, SWV parametri), dobijena je linearna zavisnost anodne struje od koncentracije svih ispitivanih analita. Niski limiti detekcije analita, stabilnost senzora, selektivnost, mogućnost regenerisanja površine elektrode, ukazuju na značajan potencijal primene razvijenog senzora za određivanje ispitivanih analita u biološkim uzorcima i farmaceutskim formulacijama.

Simultaneous determination of dopamine, serotonin, ascorbic acid and nitrite ion using modified GCE

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Dopamine, serotonin, ascorbic acid, and nitrite ions play crucial roles in various physiological metabolic processes.[1] In this study, we developed a new sensor capable of simultaneously determining these components using adsorptive square wave voltammetry (SWV). The glassy carbon electrode was modified with a polyelectrolyte complex of chitosan and alginate, supplemented with electrochemically reduced graphene oxide. The presence of polysaccharides enhanced the adsorption of analytes on the electrode surface, while reduced graphene oxide significantly increased electrical conductivity. By employing the modified electrode with optimized composition and under optimal experimental conditions (including pH, accumulation potential and time, and SWV parameters), we observed a linear dependence of the anodic current on the concentration of all tested analytes. The sensor exhibited low limits of detection for the analytes, demonstrated stability, selectivity, and the possibility of electrode surface renewal. These characteristics indicate significant potential for the application of the developed sensor in determining target analytes in biological samples and pharmaceutical formulations.

1. C.H. Su, C.L. Sun, Y.C. Liao, *ACS Omega*. **2017**, *2*, 4245–4252.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No: 451-03-66/2024-03/200122).

US-6

Inhibicija aktivnosti butirilholinesteraze od strane abamektina i boskalida: kompjuterska i *in vitro* proučavanja

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Rastući trend za poljoprivrednim proizvodima doveo je do pogrešne upotrebe pesticida. Butirilholinesteraza (BChE) sprečava određene pesticide da nepovratno inhibiraju acetilholinesterazu (AChE), drugi enzim ključan za neurotransmisiju. Za naša istraživanja smo izabrali često korišćene pesticide abamektin i boskalid. Naša *in silico* i *in vitro* istraživanja su pokazala da BChE iz *Homo sapiens-a* nije meta za abamektine B1A i B1B. Boskalid je pokazao gori Glide score (-6.88 kcal/mol) nego potvrđeni inhibitor BChE (2-((1-(benzensulfonil)-1*H*-indol-4-il)oksi)etil)(benzil)amin sa IC_{50}=0.473 μM (Glide score = -8.64 kcal/mol), tako da nije iznenađujuće da je njegov IC_{50} značajno viši. Ova studija naglašava zaštitnu ulogu BChE protiv određenih pesticida.

Inhibition of butyrylcholinesterase activity by abamectin and boscalid: computational and *in vitro* studies

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The growing demand for agricultural products has led to the misuse of pesticides. Butyrylcholinesterase (BChE) prevents some pesticides from irreversibly inhibiting acetylcholinesterase (AChE), another enzyme crucial for neurotransmission. For our studies, we choose commonly used pesticides abamectin and boscalid. The *Homo sapiens* BChE was shown not to be a target for abamectins B1A and B1B either *in silico* or *in vitro*. Boscalid showed a worse Glide score (-6.88 kcal/mol) than the approved BChE inhibitor (2-((1-(benzenesulfonyl)-1*H*-indol-4-yl)oxy)ethyl)(benzyl)amine with an IC_{50} value of 0.473 μM (Glide score=-8.64 kcal/mol), so it is not surprising that its IC_{50} is significantly higher. This study highlights the protective role of BChE against certain pesticides.

US-7

Uticaj estarskih grupa na biološku aktivnost analoga kleistanolata

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Prirodni proizvodi, njihovi analozi i derivati, a takođe i jedinjenja koja sadrže farmakoforu prirodnog proizvoda predstavljaju jedan od vodećih izvora u pronalaženju novih lekova.[1] U ovom radu će biti opisana sinteza novih analoga kleistanolata, sa jednom i više estarskih funkcija, kao i ispitivanje njihove biološke aktivnosti. U okviru rezultata, detaljno će biti diskutovana antiproliferativna aktivnost, kao i uticaj strukture na aktivnost ispitivanih jedinjenja (SAR). Dodatno, biće prikazani rezultati preliminarnog ispitivanja inhibicije humanih holinesteraza analozima kleistanolata.

Influence of ester groups to biological activity of cleistanolate analogues

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Natural products, their analogs and derivatives, as well as compounds that contain the corresponding pharmacophore represent one of the important class of compounds for drug discovery.[1] Herein, we describe the synthesis of novel cleistanolate analogues with one or more ester-groups. Their antiproliferative activity and SAR analysis will be discussed in detail. Additionally, the results of preliminary investigations of cleistanolate analogues as human cholinesterase inhibitors will be also presented.

1. D. J. Newman, G. N. Cragg, *J. Nat. Prod*. **2020**, *83*, 770.

Acknowledgment: The work was supported by a grant from Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-66/2024-03/ 200125 & 451-03-65/2024-03/200125), by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130), and by the project of Croatian Science Foundation (Grant No. HrZZ-IP-2020-02-9343).

US-8

Antimikrobna aktivnost salvipizona: *in silico* i *in vitro* ispitivanja

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Metodom molekulskog dokinga određena je termodinamička stabilnost kompleksa nagrađenog između enzima giraze Gram(-) bakterije *E. coli* (PDB ID: 3NUH) i enzima giraze Gram(+) bakterije *S. aureus* (PDB ID: 6FQS), sa enolnim i keto-oblikom abietanskog diterpena salvipizona i gepotidacinom (JHN, poznati inhibitor) kao ligandima. Primenjena *in silico* analiza je pokazala da enolni oblik salvipizona inhibira 3NUH protein čak uspešnije nego JHN, pri čemu je bolji inhibitor 6FQS proteina keto-oblik salvipizona. Značajna inhibitorska aktivnost salvipizona prema ispitivanim girazama posledica je brojnih vodoničnih veza i interakcija koje uključuju π-elektrone u nagrađenim protein-ligand kompleksima. Dobijeni rezultati saglasni su sa eksperimentalnim rezultatima dobijenim primenom *in vitro* metode mikrodilucije za procenu uticaja salvipizona na rast odabranih bakterijskih sojeva.

In silico and *in vitro* investigation of the antimicrobial activity of salvipisone

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Molecular docking analysis was used to determine the thermodynamic stability of the complexes formed between the gyrase enzyme of Gram-negative bacteria *E. coli* (PDB ID: 3NUH) and the gyrase enzyme of Gram-positive bacteria *S. aureus* (PDB ID: 6FQS) with the enol and keto forms of the abietane diterpene salvipisone and gepotidacin (JHN, a known inhibitor) as ligands. The applied *in silico* analysis showed that the enol form of salvipisone inhibits the 3NUH protein even more successfully than JHN, while the keto form of salvipisone is a better inhibitor of the 6FQS protein. The significant inhibitory activity of salvipisone against the investigated gyrases is a consequence of numerous hydrogen bonds and interactions involving π-electrons in the protein-ligand complexes. These results are in agreement with experimental results obtained using the *in vitro* microdilution method to evaluate the effect of salvipisone on the growth of selected bacterial strains.

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US-9

Novi steroidni karbamati kao potencijalni ligandi za estrogene receptore

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Estrogeni receptor alfa (ERα) je eksprimiran u oko 75% slučajeva tumora dojke i jedan je od najvažnijih prognostičkih faktora koji određuju lečenje ovog tipa kancera. S druge strane, efekti estrogenog receptora beta (ERβ) se suprotstavljaju proliferativnim efektima ERα u progresiji tumorskih ćelija. Endokrine terapije koje ometaju signalizaciju estrogena su osnova za lečenje kancera dojke kod kojih je utvrđena ekspresija ER. Karbamati predstavljaju važan strukturni motiv mnogih lekova koji se koriste u terapiji bolesti kao što su kancer, Alchajmerova bolest itd. Stoga smo sintetizovali nove androstanske derivate karbamata i testirali *in vitro* njihov relativni afinitet vezivanja za ligand-vezujuće domene ERα i ERβ, praćeno *in silico* studijama.

New steroid carbamates as potential ligands for estrogen receptors

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Estrogen receptor alpha (ERα) is expressed in ~75% of breast tumors and is one of the most important prognostic factors determining breast cancer treatment. On the other hand, estrogen receptor beta (ERβ) can counteract the proliferative effects of ERα in cancer progression. Endocrine therapies that target estrogen signaling are the basis for trearment of ER-positive breast cancer. Carbamates represent an important structural motif of many drugs used to treat various diseases such as cancer, Alzheimer's disease, etc. Considering these facts, we have synthesized new androstane carbamate derivatives and tested *in vitro* their relative binding affinities for the ligand-binding domains of ERα and ERβ, followed by *in silico* studies.

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US-10

Halogenovani tiazolni furo-dioksolani i *in silico* pretraga za njihovim potencijalnim metama

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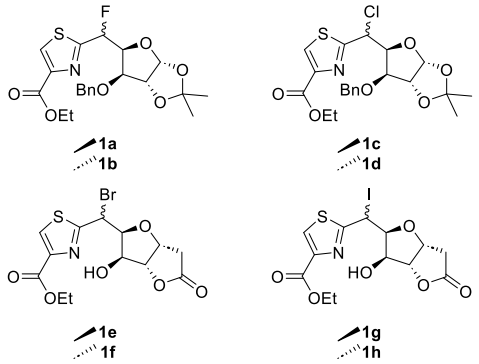
Serija od osam halogenovanih tiazolnih furo-dioksolana (**1a-h**, Šema 1), prekursora planiranih furofuranona, ispitana je pomoću nekoliko strategija/servera za inverzni *in silico* dizajn lekova, odnosno pretragu baza podataka sa potencijalnim metama. Rezultati svake pretrage su dodatno ispitani dokovanjem pomoću alata AutoDock Vina, i biće tabelarno i grafički predstavljeni, upoređeni i iskombinovani. Sinteza prikazanih furo-dioksolanskih prekursora, finalnih furofuranona, kao i ispitivanje njihovih antiproliferativnih aktivnosti prema odabranim ćelijama kancera, je u toku.



*Šema 1. Ispitana jedinjenja **1a-h***

Halogenated thiazole furano-dioxolanes and *in silico* search for their potential targets

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A series of eight halogenated thiazole furo-dioxolanes (**1a-h**, Scheme 1), precursors of the planned furofuranones, were examined using several strategies/servers for inverse in silico drug design, i.e., database search for potential targets. The results of each search were further examined by docking using the AutoDock Vina tool and will be presented in tables and graphs, compared, and combined. The synthesis of the presented furo-dioxolane precursors, the final furofuranones, as well as the examination of their antiproliferative activities against selected cancer cells, is underway.

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).

Saopštenja / Contributions

Analitička hemija

Analytical Chemistry

AH-1

Određivanje makro- i mikroelemenata u uzorcima *Rosa agrestis* Savi. primenom optimizovane i validirane ICP AES metode

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Optimizovana i validirana metoda atomske emisione spektroskopije sa indukovano spregnutom plazmom (ICP AES) je primenjena za određivanje makro- i mikroelemenata u uzorcima vrste *Rosa agrestis* Savi. Praćenjem odnosa linija Mg II (280,270 nm)/Mg I (285,213 nm) pri aksijalnom i radijalnom režimu posmatranja plazme, robusni uslovi plazme su postignuti pri RF snazi od 1150 W i protoku raspršivačkog gasa od 0,5 l/min. Kalibracione prave za sve elemente imaju dobru linearnost, sa koeficijentima korelacije većim od 0,999. Tačnost metode je ispitana primenom standardnog referentnog materijala (CRM-LGC7162) i računanjem „*recovery"* vrednosti, dok je preciznost metode data kao relativna standardna devijacija (RSD, n=3). Najzastupljeniji makroelement je K, a zatim slede Ca, P, Mg i Na. Među mikroelementima, najzastupljeniji su: Mn, Fe, Zn, Si i Cu. Sadržaji toksičnih elemenata (Cd i Pb) su ispod vrednosti EU regulative za voće, dok As nije nađen.

Macro and microelements determination in *Rosa agrestis* Savi. samples by an optimized and validated ICP AES method

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The optimized and validated inductively coupled plasma atomic emission spectroscopy (ICP AES) method was used to determine macro and microelements in *Rosa agrestis* Savi samples. Using the Mg II (280.270 nm)/Mg I (285.213 nm) line ratios for axial and radial observation modes, robust plasma conditions were achieved at an RF power of 1150 W and a nebulizer gas flow rate of 0.5 L/min. Calibration curves for all elements exhibited good linearity, with correlation coefficients higher than 0.999. The accuracy of the method was evaluated using Certified Reference Material (CRM-LGC7162) and calculating recovery values, while the precision of the method was expressed as relative standard deviation (RSD, n=3). The most abundant macroelement is K, followed by Ca, P, Mg, and Na. Among the microelements, Mn, Fe, Zn, Si, and Cu are present in the highest concentrations. The contents of toxic elements (Cd and Pb) are below the values set for fruits by the EU Commission Regulation. As was not detected.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development, and Innovation of Republic of Serbia (Contracts No. 451-03-47/2023-01/200124, 451-03-65/2024-03/200124 and 451-03-66/2024-03/200124).

AH-2

Lipofilnost i retenciono ponašanje derivata ariliden-2-tiohidantoina na F5 koloni primenom HPLC tehnike

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Hidrantoini su heterociklična jedinjenja poznata po svojim biološkim aktivnostima, kao što su antikancerogena, antimikrobna, antikonvulzivna i antiinflamatorna svojstva, i njihovoj primeni u medicini i industriji. Ovaj rad ispituje retenciono ponašanje 13 derivata ariliden-2-tiohidantoina korišćenjem HPLC. Retencioni parametar logk_0 je korišćen da bi se aproksimirala lipofilnost jedinjenja. Korišćene su F5 kolona i mobilna faza metanol-voda (MeOH-V), sa povećanjem metanola sa 45% na 75% u koracima od 5%. Retencioni parametri log$k$ su izračunati i fitovani sa φ u parabole. Odsečci (logk_0) su upoređeni sa koeficijentom lipofilnosti log$P$, pokazujući linearno uklapanje sa R^2 = 0,94829. Parametar logk_0 pokazao je potencijal kao deskriptor lipofilnosti.

Lipophilicity and retention behavior of arylidene 2-thiohydantoin derivatives on the F5 column by HPLC

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Hydantoins are heterocyclic compounds known for their biological activities, such as anticancer, antimicrobial, anticonvulsant, and anti-inflammatory properties, and their applications in medicine and industry. This paper examines the retention behavior of 13 arylidene 2-thiohydantoin derivatives using HPLC. The retention parameter logk_0 was evaluated to approximate the lipophilicity of the compounds. An F5 column and a methanol-water (MeOH-W) mobile phase, with methanol increasing from 45% to 75% in 5% increments, were used. Retention coefficients log$k$ were calculated and fitted with φ into parables. Intercepts (logk_0) were compared to the lipophilicity coefficient log$P$, showing a linear fit with R^2 = 0.94829. The logk_0 parameter demonstrated potential as a lipophilicity descriptor.

AH-3

Procena pogodnosti podzemnih voda za piće i navodnjavanje u dolini reke Jadar

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Podzemne vode su ključan izvor slatke vode neophodan za regionalni razvoj i očuvanje ekologije, što čini bezbednost njihovog korišćenja od presudnog značaja za dobrobit ljudi. U ovom radu je ispitivana pogodnost podzemnih voda za piće i navodnjavanje u dolini reke Jadar. Pogodnost podzemnih voda za piće procenjivana je korišćenjem entropijskog indeksa kvaliteta vode (EWQI), dok je pogodnost podzemnih voda za navodnjavanje procenjena korišćenjem koeficijenta adsorpcije natrijuma (SAR) i procenta natrijuma (%Na). Rezultati su pokazali da je 13,6% uzoraka imalo EWQI vrednost nižu od 100, što su podzemne vode pogodne za piće. Proračunate SAR i %Na vrednosti kretale su se u rasponu 0,2–744 i 4%–99,5%, pri čemu je većina uzoraka pripala kategorijama odličnog do dobrog kvaliteta vode. Voda najlošijeg kvaliteta primećena je u centralnom delu istraživanja područja, dok se kretajući ka obodu njen kvalitet poboljšavao.

Assessment of groundwater suitability for drinking and irrigation in the Jadar river valley

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Groundwater is a vital freshwater resource crucial for regional development and ecological preservation, making its safety imperative for human well-being. This study investigated the suitability of groundwater for drinking and irrigation purposes in the Jadar River valley. The suitability of groundwater for drinking was assessed using the entropy-weighted water quality index (EWQI), while the suitability of groundwater for irrigation was evaluated using the sodium adsorption ratio (SAR) and sodium percentage (%Na) indices. The results showed that 13.6% of the samples exhibited an EWQI value below 100, suggesting groundwater suitable for drinking. The SAR and %Na of the samples ranged from 0.2 to 744 and 4% to 99.5%, respectively, with the majority of the samples falling within the excellent to good water quality categories. The central portion of the study area exhibited the poorest water quality, which gradually improved towards the periphery.

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AH-4

Efikasnost adsorpcije-desorpcije i ponovna upotreba modifikovanog letećeg pepela u uklanjanju azo-boja

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Efikasnost modifikovanog letećeg pepela za uklanjanje azo-boja i mogućnost njegove ponovne upotrebe utvrđeni su kroz cikluse adsorpcije i desorpcije. Adsorbenti su okarakterisani standardnim metodama, FTIR i SEM. Ispitivanje efikasnosti adsorpcije pokazalo je da su modifikovani materijali efikasniji u uklanjanju metilen plavog, kristalno ljubičastog i briljantno zelenog u poređenju sa sirovim letećim pepelom. Desorpcija metilenskog plavog sa materijala nakon adsorpcije ispitivana je korišćenjem različitih organskih rastvarača (metanol, etanol, etil-acetat), pri čemu je etanol izabran kao najefikasniji. Ponovna upotreba modifikovanog letećeg pepela ispitana je u tri ciklusa procesa adsorpcije i desorpcije. Utvrđeno je da se termički modifikovana smeša letećeg pepela i NaOH može koristiti kao efikasan adsorbent za uklanjanje odabranih azo-boja.

Adsorption-desorption efficiency and reusability of modified fly ash in removing azo dyes

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The efficiency of modified fly ash for the removal of azo dyes and its reuse cycles were determined through adsorption-desorption tests. The adsorbents were characterized using standard methods, FTIR, and SEM. The adsorption test showed that the modified materials were more effective in removing methylene blue, crystal violet, and brilliant green compared to raw fly ash. The desorption of methylene blue from the material was investigated using different organic solvents (methanol, ethanol, ethyl acetate), with ethanol being the most effective. The reuse of modified fly ash was investigated over three cycles of adsorption and desorption processes. It was found that a thermally modified mixture of fly ash and NaOH can be used as an effective adsorbent for the removal of selected azo dyes.

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AH-5

Toksični elementi u uzorcima biljne vrste *Symphytum officinale* L. sa planine Golije, Novi Pazar, Srbija

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Gavez (*Symphytum officinale* L.) je u tradicionalnoj medicini poznat kao biljka koja ima lekovita svojsta i koristi se u vidu krema kod preloma kostiju, radi zarastanja. Cilj ovog istraživanja je bio da se utvrdi potencijalno prisustvo toksičnih elemenata (Al, As, Ba, Be, Pb i Hg) u ovoj biljnoj vrsti, metodom ICP OES. Analizirani su delovi biljke: cvet (F), list (L), stablo (S), koren (R), kao i zemljište (O) na kome je rasla biljka. Primenom metode suve mineralizacije uzoraka, potvrđeno je odsustvo Hg u svim ispitivanim uzorcima. Koncentracije Al i Be - osim u korenu, imale su manje vrednosti kada je primenjivana metoda mineralizacije uzoraka mokrim postupkom. Ovom metodom As je detektovan samo u korenu biljke. Koncentracije ispitivanih elemenata bile su znatno više u zemljištu na kome je biljka rasla nego u ispitivanim delovima biljke.

Toxic elements in samples of the plant species *Symphytum officinale* L. from the mountain Golija, Novi Pazar, Serbia

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In traditional medicine, comfrey (*Symphytum officinale* L.) is used as a medicinal plant and in creams to treat bone fractures and promote recovery. The aim of this study was to identify potentially toxic elements (Al, As, Ba, Be, Pb, and Hg) in the selected plant species using the ICP OES method. The analyzed parts of the plant were: flower (F), leaf (L), stem (S), roots (R), and the soil (O) where the plant grew. Applying the method of dry mineralization to the samples, the absence of Hg was confirmed in all tested samples. Applying the method of wet mineralization to the samples resulted in lower concentrations of Al and Be, except in the roots. With this method, As was detected only in the roots of the plant. Concentrations of the tested elements were significantly higher in the soil where the plant grew than in the tested parts of the plant.

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AH-6

Upoređivanje različitih protokola za ekstrakciju lipida iz uzoraka humane plazme i seruma

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Upoređeni su različiti protokoli za ekstrakciju (fosfo)lipida iz četiri tipa humanih uzoraka dobijenih iz krvi: plazme, seruma, liofilizovane plazme i liofilizovanog seruma koristeći devet eksperimentalnih protokola, zasnovanih na tri metode ekstrakcije (*Folch*, *Matyash*, *Alshehry*) izvedene na tri različite temperature. Analiziran je uticaj liofilizacije i kombinacije metoda-temperatura na prinos ekstrakcije različitih klasa (fosfo)lipida koji je procenjen tankoslojnom hromatografijom. Pokazana je uspešna ekstrakcija liofilizovanih uzoraka, što je važno zbog njihovog lakšeg čuvanja (na 4-8 °C umesto na -80 °C) i transporta. Temperatura je pokazala značajan uticaj jedino na uspešnost ekstrakcije po *Matyash*-u, koja je na 25 °C i 40 °C bila veća nego na 4 °C. Upotrebom metode po *Matyash*-u i *Folch*-u zabeležen je veći prinos (fosfo)lipida u odnosu na *Alshehry*.

Comparing different protocols for lipid extraction from samples of human plasma and serum

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Nine experimental protocols for (phospho)lipid extraction were designed as combinations of three common extraction methods (Folch, Matyash, Alshehry) and three different temperatures. These protocols were applied to four types of human samples: plasma, serum, lyophilized plasma, and lyophilized serum. The respective yields of specific (phospho)lipid classes were analyzed by thin-layer chromatography and compared. The effect of lyophilization and the method-temperature combination on the yields were evaluated. We demonstrated the successful utilization of lyophilized samples in the tested protocols, which is important for convenient sample storage (at 4-8 °C instead of -80 °C) and transport. The temperature affected only the Matyash method, where the yields were better at 25 °C and 40 °C than at 4 °C. The Matyash and Folch methods exhibited higher extraction efficiency of (phospho)lipids compared to the Alshehry method.

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AH-7

Procena ekološkog rizika deponovanja letećeg pepela

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Deponovanje letećeg pepela, kao jednog od osnovnih produkata sagorevanja uglja u termoelektranama, može izazvati brojne negativne ekološke posledice. U sastav letećeg pepela, pored osnovnih mineralnih materija (SiO_2, Fe_2O_3 i Al_2O_3), ulaze u manjoj ili većoj meri i toksični elementi kao što su: Cd, Co, Cr, Cu, Mn, Ni, Pb, Zn, As i Hg. U okviru ovog istraživanja izvršena je procena ekološkog rizika na osnovu kvantitativnih faktora – ekološkog faktora rizika (ER) i indeksa rizika (RI) u sedam različitih uzoraka letećeg pepela prikupljenih iz termoelektrane Nikola Tesla. Uzorci su pripremani metodom mikrotalasne digestije smešom koncentrovanih mineralnih kiselina HNO_3/HCl/HF, dok su koncentracije izluženih metala određene tehnikom ICP-OES. Rezultati su pokazali da pet uzoraka letećeg pepela pokazuje veoma visok nivo rizika, dok ostala dva uzorka pokazuju visok nivo rizika. Elementi koji su pokazali najveći nivo rizika po životnu sredinu su Cd, As i Hg.

Assessment of Environmental Risk of Fly Ash Disposal

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The deposition of fly ash, a primary byproduct of coal combustion in thermal power plants, can lead to numerous negative environmental consequences. Apart from its basic mineral components (SiO_2, Fe_2O_3, and Al_2O_3), fly ash may contain toxic elements such as Cd, Co, Cr, Cu, Mn, Ni, Pb, Zn, As, and Hg. In this study, ecological risk was assessed using quantitative factors - ecological risk factor (ER) and risk index (RI) - across seven different samples of fly ash collected from the Nikola Tesla thermal power plant. The samples were prepared using the microwave digestion method with a mixture of concentrated mineral acids (HNO_3/HCl/HF), and the concentrations of leached metals were measured using the ICP-OES technique. The results indicate that five ash samples exhibit a very high level of risk, while the remaining two samples show only a high level of risk. Elements posing the highest environmental risk include Cd, As, and Hg.

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AH-8

Ispitivanje uticaja koncentracije suspenzije na širinu $pH_{max} - pH_{min}$ opsega tokom određivanja rastvorljivosti

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Cilj ovog rada bio je ispitivanje uticaja koncentracije suspenzije na širinu $pH_{max} - pH_{min}$ opsega tokom određivanja rastvorljivosti pH-*Ramp shake-flask* metodom. Kao model jedinjenja izabrani su nortriptilin-hidrohlorid i atorvastatin-kalcijum. Rezultati su pokazali da sa porastom koncentracije suspenzije dolazi do širenja opsega $pH_{max} - pH_{min}$, a ovakva proučavanja mogu značajno doprineti optimizaciji formulacije u procesu dizajna i razvoja lekova.

The influence of suspension concentration on the $pH_{max} - pH_{min}$ range during the solubility determination

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The solubility profile of a drug typically consists of two independent curves that intersect at a specific point called pH_{max}. At pH_{max}, both salt and base coexist as solid phases. While two solids coexist, pH and solubility in the heterogeneous system remain constant (according to the Gibbs Phase Rule).[1,2] Recent studies, however, have shown that pH and solubility might change during the salt-to-free-base transformation. This pH range, containing two solids, is termed the $pH_{max} - pH_{min}$ range. pH_{max} refers to the pH value at the maximum solubility of a eutectic mixture, whereas pH_{min} represents the pH value at the minimum solubility of the eutectic mixture. The objective of this study was to investigate the influence of suspension concentration (the ratio of drug mass to suspension volume) on the $pH_{max} - pH_{min}$ range during solubility determination using the pH-*Ramp shake-flask* method. Nortriptyline hydrochloride (Nor, monoprotic base) and atorvastatin calcium (At, monoprotic acid) were employed as model compounds. Results indicate that the $pH_{max} - pH_{min}$ range increases as suspension concentration rises (for 20.10 mg NorHCl/mL: pHmax=3.55, ΔpH=0; for 59.82 mg NorHCl/mL: $pH_{max} - pH_{min}$= 3.56 – 4.52, ΔpH=0.96). Understanding the details of the $pH_{max} - pH_{min}$ range could significantly impact product formulation optimization in drug research.

1. A. Avdeef, *Mol. Pharmaceutics*. **2021**, *18*, 2724.
2. O. Marković *et al*, *Mol. Pharmaceutics*. **2022**, *19*, 710.

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AH-9

Bioaktivnost kompozitnih biokeramičkih prevlaka i otpuštanje gentamicina – *in vitro* ispitivanja

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Površine titanskih implantata se mogu unaprediti primenom biokeramičkih, multifunkcionalnih prevlaka koristeći proces elektroforetskog taloženja (EPD) u cilju sprečavanja korozije, poboljšanja biokompatibilnosti i antibakterijske aktivnosti, kao i unapređenja osteointegracije. Materijali poput hidroksiapatita (HAP), hitozana (CS), poli(vinil-alkohola) (PVA) i antibiotika gentamicina (Gent) su korišćeni u ovom procesu kako bi se razvile poboljšane antibakterijske kompozitne prevlake. Nakon taloženja, prevlake su potapane u simuliranu telesnu tečnost (SBF) na 37 °C, a zatim je izvršena karakterizacija skenirajućom elektronskom mikroskopijom sa emisijom polja (FE-SEM) i rendgenskom difrakcionom analizom (XRD). Bioaktivnost istaloženih prevlaka je pokazana i analizom aktivnosti alkalne fosfataze prema MRC-5 i L929 ćelijskim linijama. Koncentracija otpuštenog gentamicina je određena korišćenjem tečne hromatografije visokih performansi (HPLC) sa masenom detekcijom (MS).

Bioactivity of Composite Bioceramic Coatings and Gentamicin Release - *in vitro* Studies

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Titanium implant surfaces can be enhanced by applying bioceramic multifunctional coatings using the electrophoretic deposition process (EPD). This method helps prevent corrosion, enhance biocompatibility, combat bacterial growth, and promote osseointegration. Materials such as hydroxyapatite (HAP), chitosan (CS), poly(vinyl alcohol) (PVA), and the antibiotic gentamicin (Gent) were utilized to develop advanced antibacterial composite coatings. Following deposition, the coatings undergo immersion in simulated body fluid (SBF) at 37°C. Characterization involves scanning electron microscopy with field emission (FE-SEM) and X-ray diffraction (XRD) analysis. The bioactivity of the deposited coatings was demonstrated by analyzing alkaline phosphatase activity towards MRC-5 and L929 cell lines. Quantification of gentamicin release was achieved through high-performance liquid chromatography (HPLC) coupled with a mass selective detector (MS).

AH-10

Sinteza elektrohemijskog PPy-MWCNT-GCE MOP senzora za osetljivu detekciju ciprofloksacina

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Senzori sa molekulski obeleženim polimerima (MOP) su efikasne i ekološki prihvatljive platforme za detekciju farmaceutika.[1,2] Ovo istraživanje je imalo za cilj sintezu ekološki prihvatljivog MOP senzora za osetljivu i selektivnu elektrohemijsku detekciju antibiotika ciprofloksacina (CIP). Elektroda od staklastog ugljenika (GCE) je modifikovana sa višeslojnim ugljeničnim nanocevima (MWCNT), a MOP-polipirol (PPy) film je elektrohemijski sintetisan hronoamperometrijski na konstantnom potencijalu od +0,80 V u odnosu na Ag/AgCl tokom 150 s. Dobijeni senzor, označen sa PPy-MWCNT-GCE, pokazao je linearni odgovor u dva koncentraciona opsega: 0,01 - 1,00 μM ($I(\mu A) = 2{,}4695c + 0{,}5160$, $R^2 = 0{,}995$) i 5,00 - 50,00 μM ($I(\mu A) = 0{,}1984c + 7{,}9660$, $R^2 = 0{,}993$). Izračunata granica detekcije za MOP senzor ($3\sigma/s$) iznosi 0,09 μM u nižem linearnom opsegu. Ovaj senzor će biti korišćen za pouzdanu i selektivnu detekciju i praćenje ciprofloksacina u kompleksnim matricama kao što su biološki uzorci, gradska otpadna voda i prehrambeni proizvodi.

Synthesis of electrochemical PPy-MWCNT-GCE MIP sensor for the sensitive ciprofloxacin detection

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Molecularly imprinted polymers (MIP) sensors are effective and environmentally friendly platforms for detecting pharmaceuticals.[1,2] This study aimed to synthesize an eco-friendly MIP sensor for sensitive and selective electrochemical detection of ciprofloxacin (CIP), an antibiotic. The glassy carbon electrode (GCE) was modified with multi-walled carbon nanotubes (MWCNT), and the MIP polypyrrole (PPy) film was electrochemically synthesized chronoamperometrically at a constant potential of +0.80 V vs. Ag/AgCl for 150 s. The resulting sensor, designated as PPy-MWCNT-GCE, exhibited a linear response in two concentration ranges: 0.01 - 1.00 μM ($I(\mu A) = 2.4695c + 0.5160$, $R^2 = 0.995$) and 5.00 - 50.00 μM ($I(\mu A) = 0.1984c + 7.9660$, $R^2 = 0.993$). The calculated detection limit for the MIP sensor ($3\sigma/s$) is 0.09 μM in the lower linear range. This sensor will be utilized for reliable and selective detection and monitoring of ciprofloxacin in complex matrices such as biological samples, urban wastewater, and food products.

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AH-11

Određivanje mineralnog sastava tri lekovite gljive koje rastu na bukvi na teritoriji Srbije

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Cilj ovog istraživanja bio je da se ispita mineralni sastav tri vrste gljiva koje uspevaju na bukvi. Razlike u sadržaju makroelemenata i mikroelemenata, kao i potencijalno toksičnih elemenata zavise u manjoj ili većoj meri od porekla, spoljašnjih uticaja i antropogenih aktivnosti, koncentracije elemenata u zemljištu i mogu varirati u širokom opsegu. Uzorci koji su korišćeni za istraživanje bili su osušeni uzorci tri vrste gljiva sa bukve (*Fomes fomentarius, Ganoderma lucidum* i *Trametes versicolor*). Uzorci su pripremljeni mikrotalasnom digestijom smešom mineralnih kiselina. Sadržaj 20 elemenata prisutnih u plodnom telu gljiva je određen metodom induktivno spregnute plazme sa optičkom emisionom spektroskopijom (ICP-OES). Dobijeni rezultati treba da ukažu na mogućnost bezbedne primene ovih vrsta lekovitih gljiva sa područja Srbije koje imaju veoma izraženo antioksidativno i antikancer dejstvo u medicini, farmaceutskoj i kozmetičkoj industriji.

Mineral composition of three medical beech mushrooms from Serbia

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The goal of this research was to analyze the mineral composition of three types of mushrooms growing on beech trees. Differences in macro and microelement content, as well as potentially toxic elements, vary depending on origin, external influences, anthropogenic activities, and soil element concentrations. The research utilized dried samples of three mushrooms—*Fomes fomentarius, Ganoderma lucidum*, and *Trametes versicolor*—prepared through microwave digestion with mineral acid mixtures. The ICP-OES method determined the presence of 20 elements in the mushroom fruiting body. The results suggest the safe application of these medicinal mushrooms from Serbia, known for their antioxidant and anticancer effects, in medical, pharmaceutical, and cosmetic industries.

Biohemija

Biochemistry

BH-1

Dizajn bočno usmerene mutageneze za dobijanje polimorfnih oblika LacI proteina

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Usmerena evolucija enzima ključna je za stvaranje novih enzima sa željenim osobinama. Bakterijske ćelije često se koriste za selekciju varijanti proteina. Šema za usmerenu mutagenezu proteina LacI osmišljena je na osnovu modeliranja farmakofore i strukturne analize podataka iz proteinske baze podataka. Rezultati su ukazali na specifične aminokiseline koje su uključene u vezivanje liganda i interakcije sa domenima. Identifikovani su i hidrofobne ostaci koji formiraju šupljinu, kao i stabilizujući ostaci, zajedno sa onima koji su uključeni u interfejs domena i fleksibilne delove linkera. Imajući u vidu ove rezultate i željenu upotrebu za selekciju steroidnih molekula, neophodna je usmerena mutageneza koja cilja aminokiseline koje vezuju ligand, udaljene od interfejsa domena, koristeći tehniku "bump-and-hole".

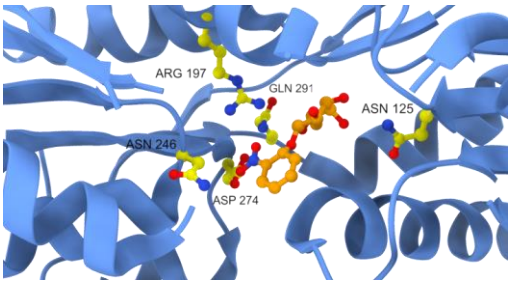

Figure 1. Fragment of LacI structure in complex with inducer IPTG with amino acid residues that will be changed

Design of side-directed mutagenesis scheme for obtaining of LacI protein polymorphic forms

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Directed enzyme evolution is crucial for creating new enzymes with desired properties. Bacterial cells are commonly used to select protein variants. A scheme for side-directed mutagenesis of the LacI protein was devised based on pharmacophore modeling and structural analysis from the Protein Data Bank. Results identified specific amino acids involved in ligand binding and domain interactions. Hydrophobic cavity-forming residues and stabilizing residues were identified, along with those involved in domain interface and flexible linker regions. Considering these findings and the intended use for selecting steroidal molecules, side-directed mutagenesis targeting ligand-binding amino acids distant from domain interfaces is necessary, utilizing the "bump-and-hole" technique.

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BH-2

Soft i hard korona mikroplastike u interakciji sa alergenom β-laktoglobulinom kravljeg mleka

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Interakcija mikroplastike (MP) s proteinima stvara kompleks poznat kao proteinska korona. U okviru korone, MP dobija nove biološke osobine, uključujući izbegavanje imunog sistema, dugotrajnije zadržavanje u cirkulaciji i ometanje ćelijskih procesa. Formiranje biofilma na površini MP je višestepeni proces, gde se nakon prvobitnog vezivanja molekula s visokim afinitetom i formiranja čvrste korone, može razviti i labavija korona u kasnijim fazama. β-laktoglobulin (BLG), glavni protein u surutki kravljeg mleka, često korišćen u hrani, može izazvati značajne zdravstvene probleme kod osoba alergičnih na mleko. Ovo istraživanje je imalo za cilj da pruži bolji uvid u interakcije između BLG kao alergena hrane i odabranih MP (polietilen-tereftalat, PET, <80μm; polipropilen, PP, 63-180μm). Izolovani nepasterizovani/pasterizovani BLG je inkubiran s PP i PET *in vitro*, u simuliranim fiziološkim tečnostima, a formirane korone su analizirane SDSPAGE elektroforezom pod redukujućim uslovima i denzitometrijom. Rezultati pokazuju da BLG slabo vezuje za obe MP. Postoji razlika u proteinima čvrstih korona između pasterizovanog i nepasterizovanog BLG, kao i u proteinskom profilu korona PP i PET inkubiranih s pasterizovanim ili nepasterizovanim BLG. Naši rezultati ukazuju da prisustvo MP može uticati na biodostupnost i alergene osobine i pasterizovanog i nepasterizovanog BLG.

Soft and hard corona of microplastics interacted with allergenic bovine milk β-lactoglobulin

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Microplastics (MPs) interact with proteins, forming a complex called a protein corona. This corona alters the biological identity and properties of MPs, enabling them to evade the immune system, persist longer in circulation, and disrupt cellular and molecular processes. Biofilm formation on MPs occurs in several steps, starting with initial binding of molecules to form a hard corona, followed by the formation of a soft corona. β-Lactoglobulin (BLG), a major whey protein in bovine milk, is highly valued as a food ingredient but poses significant health risks to milk-allergic individuals. This study aimed to understand BLG's interactions with selected MPs (polyethylene terephthalate, PET, <80μm; polypropylene, PP, 63-180μm). BLG, isolated from unpasteurized/pasteurized milk, was incubated with PP and PET in simulated physiological fluids. The resulting coronas were analyzed using reduced SDS-PAGE electrophoresis and densitometry. BLG exhibited low binding to both MPs, with pasteurized BLG showing the lowest binding to PP (less than 1% of control in its soft corona). There were differences in the protein content of hard coronas between pasteurized and unpasteurized BLG, with a slightly higher percentage of bound proteins in the hard corona of unpasteurized BLG. Additionally, the protein profile of hard coronas differed between PET and PP incubated with pasteurized BLG compared to those with unpasteurized BLG. These findings suggest that the presence of MPs may affect the bioavailability and allergenic properties of both pasteurized and unpasteurized BLG.

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Elektrohemija

Electrochemistry

EH-1

Elektrohemijska aktivnost perovskitskog oksida $Ca_{0,9}Er_{0,1}MnO_3$

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Oksid perovskitske strukture, $Ca_{0.9}Er_{0.1}MnO_3$, sintetisan je metodom saharoza-nitrat (SNP). Ovom metodom dgovarajuće nitratne soli su zagrevane u čvrstom stanju, a kao gorivo korišćena je saharoza $C_{12}H_{22}O_{11}$. Odgovarajući metalni nitrati i saharoza su kombinovani u izračunatim stehiometrijskim odnosima kako bi se dobio perovskit odgovarajuće strukture. Pripremljen prah je žaren na temperaturama od 800-1000 °C u temperaturnom intervalu od 15 minuta. Nanostrukturni prah perovskitske strukture $Ca_{0.9}Er_{0.1}MnO_3$ okarakterisan je primenom DTA, XRD, FTIR i FESEM. EIS ispitivanja i ciklični voltamogrami su pokazali da provodljivost i elektrohemijska aktivnost ispitivanog nanostrukturisanog oksida, ugrađenog u elektrodu od ugljenične paste, raste sa porastom temperature žarenja oksida u toku priprme (800, 900 i 1000 °C), i znatno je bolja od nemodifikovane CPE, što $Ca_{0.9}Er_{0.1}MnO_3$ čini obećavajućim materijalom za modifikaciju elektrohemijskih senzora.

Electrochemical activity of perovskite oxide $Ca_{0.9}Er_{0.1}MnO_3$

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An oxide with the perovskite structure $Ca_{0.9}Er_{0.1}MnO_3$ was synthesized by the sucrose-nitrate process (SNP). The suitable nitrate salts were mixed in this burning method, and sucrose $C_{12}H_{22}O_{11}$ was used as fuel. These metal nitrates and sucrose are combined in appropriate stoichiometric ratios to produce a perovskite of the appropriate structure. The obtained powder was heated at temperature intervals of 800-1000 °C for 15 minutes. DTA, XRD, FTIR, and FESEM were used to characterize the nanostructured $Ca_{0.9}Er_{0.1}MnO_3$. EIS tests and cyclic voltammograms showed that the conductivity and electrochemical activity of the examined nanostructured oxide embedded in the carbon paste electrode increases with the increase in the annealing temperature of the oxide during preparation (800, 900 and 1000 °C), and is significantly better than unmodified CPE, which makes $Ca_{0.9}Er_{0.1}MnO_3$ a promising material for the modification of electrochemical sensors.

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EH-2

Aktivnost elektrohemijski taloženih nanosfera Pd u reakcijama oksidacije metanola i etanola u alkalnim rastvorima

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Racionalno projektovanje materijala na bazi plemenitih metala je od velikog interesa za njihovu primenu u oblasti elektrokatalize. U ovom radu prikazana je galvanostatska priprema Pd iz rastvora bez surfaktanata. Analiza skenirajuće elektronske mikroskopije pokazala je nanosfere Pd veličine do 300 nm. Uporednim ispitivanjem oksidacije metanola i etanola utvrđena je veća aktivnost katalizatora u rastvoru LiOH u odnosu na rastvor NaOH usled formiranja klastera OH_{ad} – katjona. Naime, nekovalentna interakcija i formiranje OH_{ad} – katjonskih klastera određuju interakciju alkoholne OH grupe sa OH grupom na površini Pd, i posledično određuju aktivnost Pd u ispitivanim reakcijama. Može se zaključiti da izbor katjona alkalnih metala reguliše elektrokatalitičku aktivnost i da se može smatrati jednim od bitnih parametara u elektrokatalizi.

Activity of electrodeposited Pd nanospheres in methanol and ethanol oxidation in alkaline solutions

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Rationally designing of noble metal materials are of great interest for supporting their applications in the field of electrocatalysis. In this contribution, we demonstrated the galvanostatic preparation of Pd from surfactant free solution. Scanning electron microscopy analysis revealed Pd nanospheres of up to 300 nm. Comparative study of methanol and ethanol electrochemical oxidation reveals higher catalyst activity in LiOH solution in regard to NaOH solution due to the formation of OH_{ad} – cation clusters. Namely non-covalent interaction and formation of OH_{ad} – cation clusters govern the interaction of the alcohol OH group with the OH group on the Pd surface, and in turn determined its electrooxidation activity on Pd. It was pointed out that the choice of alkali metal cations regulate the electrocatalytic activity and can be considered as one of the tuning parameter in electrocatalysis.

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EH-3

Sinergetski efekat Co i RE-kompleksa u prevlakama Zn za zaštitu čelika od korozije

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Prevlake cinka se često legiraju radi povećanja otpornosti na koroziju. Pored legirajućeg elementa (Co, Ni, Fe) u poslednje vreme se prevlakama cinka dodaju razni inhibitori korozije, od kojih su najpoznatiji lantanoidi (RE). U radu su ispitivane elektrohemijski taložene prevlake Zn i Zn-Co legura dopirane česticama na bazi Ce. Ispitivan je uticaj izvora Ce: CeO_2, $CeCl_3$ ili sintetisani kompleks Ce-tioglikolat. Hemijski sastav prevlaka je određen EDS metodom, morfologija SEM a koroziona stabilnost spektroskopijom elektrohemijske impedancije (EIS). Diskutovan je mehanizam zaštite koji pruža različit izvor Ce, kao i razlike u korozionoj stabilnosti svih zaštitnih sistema.

The synergistic effect of Co and RE-complex in Zn coatings for steel corrosion protection

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The protective properties of zinc coatings are often improved by alloying. Besides alloying elements (Ni, Co, Fe) the addition of inhibitors has recently been analyzed, particularly rare earth (RE) elements. The electrochemically deposited Zn and Zn-Co alloy coatings were studied in this work, dopped with Ce-based particles: CeO_2, $CeCl_3$ or synthesized complex Ce-thioglycolate. The chemical content of the coatings was determined by EDS, morphology by EDS and corrosion stability by EIS. The influence of Ce source was discussed, as well as differences observed in corrosion stability provided by different protective systems.

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EH-4

Polimer/hidroksiapatit kompozitne prevlake na površini implantata dobijene elektroforetskim taloženjem

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U cilju poboljšanja bioaktivnosti i antibakterijskih svojstava metalnog implantata (titana), primenom elektroforetskog taloženja u jednom stupnju, iz četvorokomponentne vodene suspenzije dobijene su biokeramičke, kompozitne miltifunkcionalne prevlake na bazi hidroksiapatita, poli(vinil alkohola) i hitozana uz dodatak antibakterijskog agensa, antibiotika gentamicina. Na osnovu rezultata dobijenih FTIR, XRD i TG analizom pokazano je prisustvo karbonatno-supstituisanog hidroksiapatita (prisutnog i u prirodnom koštanom tkivu) i potvrđena je uspešna inkorporacija gentamicina u prevlaku, što ovu kompozitnu prevlaku čini pogodnom za potencijalnu primenu u biomedicini.

Polymer/hydroxyapatite composite coatings on implant's surface obtained by electrophoretic deposition

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In order to improve the bioactivity and antibacterial properties of a metal implant (titanium), single step electrophoretic deposition from a four-component aqueous suspension was employed to produce composite multifunctional coatings based on hydroxyapatite, poly(vinyl alcohol) and chitosan with the addition of an antibacterial agent, the antibiotic gentamicin. Based on the results obtained by FTIR, XRD and TG analysis, the presence of carbonate-substituted hydroxyapatite (main mineral component in natural bone tissue) was confirmed, along with successful incorporation of gentamicin into the coating, which makes this composite coating suitable for potential application in biomedicine.

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Fizička hemija

Physical Chemistry

FH-1

Sinteza i karakterizacija soli heteropoli kiseline dopirane Zn^{2+} jonima

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Heteropoli kiseline i soli heteropoli kiselina su interesantne za izučavanje jer se mogu strukturno modifikovati u fosfat volframovu bronzu termičkim tretmanom na oko 600 °C. U ovom radu sintetisali smo 12-volfram fosfornu kiselinu, $H_3PW_{12}O_{40} \times nH_2O$ - (PWA). Sinteza soli je obavljena jonskom izmenom dodavanjem ekvimolarnih količina $ZnCl_2$ u rastvor heteropoli kiseline. Karakterizacija je izvršena korišćenjem infracrvene spektroskopije Furijeove transformacije (FTIR), difrakcije rendgenskih zraka na prahu (XRPD) skenirajuće elektronske mikroskopije (SEM) i ciklične voltametrije. Dobijeni rezultati otvaraju nove pravce istraživanja Zn-PWA kao potencijalni elektrodni materijal.

Synthesis and characterization of heteropoly acid salts doped with Zn^{2+} ions

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Heteropoly acids and salts of heteropoly acids are interesting for study because they can be structurally modified into phosphate tungsten bronze by thermal treatment at eye 600 °C. In this work, we synthesized 12-tungsten phosphoric acid, of $H_3PW_{12}O_{40} \times nH_2O$ - (PWA) are obtained. Salt synthesis was performed by ion exchange by adding equimolar amounts of $ZnCl_2$ to a heteropoly acid solution. Characterization was performed using Fourier transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRPD), scanning electron microscopy (SEM) and cyclic voltammetry. The obtained results open new directions of Zn-PWA research as a potential electrode material.

FH-2

Uticaj veštačkih zaslađivača natrijum-saharina i kalijum-acesulfama na hidrataciona svojstva, ukus i rastvorljivost kofeina

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Kofein ulazi u sastav velikog broja proizvoda (kafa, energetski napici, suplementi, farmaceutski i kozmetički proizvodi itd.) i time je najšire korišćena psihoaktivna supstanca. Veštački zaslađivači poseduju viši stepen slatkoće i nižu kalorijsku vrednost od uobičajenih zaslađivača. Zahvaljujući ovim osobinama, nalaze sve širu primenu u svakodnevnom životu i privredi kao zamena za uobičajene zaslađivače. Cilj ovog rada je ispitivanje svojstva hidratacije, ukusa, rastvorljivosti i agragacije kofeina u prisustvu veštačkih zaslađivača natrijum saharina i kalijum acesulfama iz volumetrijskih, akustičnih i viskozimetrijskih merenja uz prateće računarske simulacije. Rezultati dobijeni ukazuju da oba veštačka zaslađivača dovode do smanjenja gorčine kofeina, potspešuju samoagregaciju i povećavaju rastvorljivost kofeina.

Influence of artificial sweeteners sodium saccharin and acesulfame potassium on the hydration properties, taste behavior and solubility of caffeine

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Caffeine is an ingredient of a wide range of products (coffee, energy drinks, supplements, pharmaceuticals, cosmetics, etc.) and is therefore the most widely used psychoactive substance. Artificial sweeteners possess higher sweetness and lower caloric value than regular sweeteners. Due to these characteristics their use as replacements for traditional sweeteners in various industries and everyday life is growing. The purpose of this work is the investigation of hydration, taste, solubility and aggregation properties of caffeine in the presence of artificial sweeteners sodium saccharin and acesulfame potassium by volumetric, acoustic and viscosimetric measurements along with accompanying computer simulations. The received results indicate that both artificial sweeteners reduce the bitterness of caffeine, promote self-aggregation and increase caffeine solubility.

Hemijsko inženjerstvo

Chemical Engineering

HI-1

Ekstrakcija polifenola iz kore nara u sistemu sa pakovanim slojem i recirkulacijom tečne faze

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Kora nara se često odbacuje i tretira kao otpad. Međutim kora nara ima visok sadržaj polifenola. Sa ciljem da se kora nara koristi za proizvodnju ukupnih i određenih polifenola, urađena je ekstrakcija kore nara u kome su zrna kore nara postavljena u pakovanom sloju kroz koji recirkuliše pogodan rastvarač. Prečnik kolone u kojoj je rađena ekstrakcija je 40mm, srednji prečnik zrna kore nara je 2mm. Eksperimentalna aparatura poseduje grejač i regulaciju temperature, pomoću koje se temperatura u sistemu menja. Korišćeni su sledeći rastvarači: voda, vodeni rastvor etanola od 50vol% i 96vol% etanola. Prikazane su zavisnosti koncentracije ukupnih polifenola u funkciji vremena za tri različite temperature i tri različita rastvarača. Pokazan je uticaj temperature i izbora rastvarača na prinos ekstrakcije. Utvrđeni su optimalni uslovi rada sa tendencijom razvijanja jednačina koje opisuju ekstrakciju u ovom sistemu.

Extraction polyphenols from pomegranate peel in packed bed systems and by recirculation of the liquid phase

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Pomegranate peel is often discarded and is treated as waste. However, pomegranate peel has a high content of polyphenols. With the aim of pomegranate peel for the production of total and certain polyphenols, it is done extraction pomegranate peel in which they are grains of pomegranate peel in packed bed through which it recirculates suitable solvent. Column diameter in which the extraction was carried out is 40mm, mean diameter grains pomegranate peel is 2mm. The experimental apparatus is equipped with a heater and temperature regulation, which is used to change the temperature in the system. The following solvents were used: water, aqueous solution ethanol of the 50vol% i 96vol% ethanol. The dependencies of the concentration of total polyphenols as a function of times for three different temperature and three different solvents are shown. The influence of the temperature and the choice of solvent on the yield of the extraction is shown. Optimal working conditions were determined with a tendency to develop equations that describe the extraction in this system.

HI-2

Eksperimentalno ispitivanje pada pritiska u modifikovanom fontanskom sloju

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Jedan od najvažnijih projektnih parametara nekog kontaktora čestice-fluid je pritisak. U ovom radu su dati rezultati eksperimentalnog ispitivanja uticaja različitih parametara sistema na padove pritiska u fontanskom sloju sa cevnim umetkom. U eksperimentima su korišćene čestice stakla prečnika 1 mm, 2 mm i 3 mm dok je vazduh, kao agens fontanovanja, uvođen na dno kolone i u anularni prostor. Određivani su pritisci duž centralne cevi i u anularnom prostoru za: različite protoke kroz centralnu cev i anularni prostor, različite prečnike centralne cevi i različita rastojanja centralne cevi od dna kolone. Prikazane su dobijene zavisnosti pada pritiska kroz centralnu cev i anularni prostor od protoka fluida, prečnika i rastojanja centralne cevi od dna kolone i dobijeni rezultati su upoređeni sa podacima iz dostupne literature.

Experimental investigation of the pressure drop in the modified spouted bed

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One of the most important design parameters of a fluid-particle contactor is the pressure. This paper presents the results of an experimental investigation of the influence of various system parameters on the pressure drop in the spout-fluid bed with draft tube. In the experiments, glass particles with a diameter of 1 mm, 2 mm and 3 mm were used, while air was introduced as a fountaining agent, was introduced to the bottom of the column and into the annulus. The pressures along the central tubes and in the annulus were determined for: different flows through the draft tube and the annulus, different diameters of the draft tube and different distances of the draft tube from the bottom of the column. The obtained dependencies of the pressure drop through the central tube and the annulus on the fluid flow, the diameter and the distance of the central tube from the bottom of the column are shown, and the obtained results are compared with data from the available literature.

Hemija i tehnologija hrane

Chemistry and Technology of Food

HTH-1

UV-VIS metoda za kontrolu sadržaja prolina u uzorcima meda

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Prolin se koristi za procenu autentičnosti meda. Minimalan sadržaj prolina u prirodnom medu ne sme biti manji od 180 mg/kg meda. Cilj našeg istraživanja je bio razvoj jeftine i brze metode za određivanje sadržaja prolina u industrijskim laboratorijama. Kao razvijači u prvoj dimenziji 2D papirne hromatografije korišćeni su rastvori kiselina (galne, salicilne, benzoeve), kao i smeša fenol:voda=4:1. Smeša *n*-butanol:sirćetna kiselina:voda=4:1:5 je korišćena u svim slučajevima kao razvijač u drugoj dimenziji 2D papirne hromatografije. Rastvor galne kiseline (0.04 g/mL) je dao najbolje rezultate. Apsorbancu kompleksa prolina sa ninhidrinom smo određivali na talasnoj dužini od 356 nm. Količina prolina je određena na osnovu kalibracione prave dobijene od rastvora prolina u vodi različitih koncentracija, i izražena u mg/kg meda. Razvijena brza, jednostavna i repetabilna UV-VIS spektrofotometrijska metoda za određivanje sadržaja prolina u medu pokazala se podobnom za procenu autentičnosti uzoraka meda, koja može da se izvede u industrijskoj laboratoriji za kontrolu ulaznih sirovina.

UV-VIS method for the control of proline content in honey samples

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Proline is used for the estimation of the authenticity of honey. The minimum content of proline in natural honey must not be less than 180 mg/kg of honey. The aim of our study was the development of a cheap and fast method for the determination of proline content in industrial laboratories. The solutions of acids (gallic, salicylic, benzoic) and the mixture phenol:water=4:1 were used in the first dimension of 2D paper chromatography. The mixture *n*-butanol:acetic acid:water=4:1:5 was used in all cases as the mobile phase in the second dimension of 2D paper chromatography. Gallic acid solution (0.04 g/mL) gave the best results. The absorbance of proline complex with ninhydrin was measured at 356 nm. Proline quantity was determined based on the calibration curve obtained using the proline solutions of different concentrations in water, and expressed in mg/kg of honey. Developed fast, simple and repeatable UV-VIS spectrophotometric method for the determination of proline content in honey was shown as suitable for the estimation of the authenticity of honey samples, which can be applied in the industrial laboratories for the control of raw materials.

HTH-2

Multielementarna analiza flaširanih voda pomoću tehnike ICP-AES

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Zna se da je tokom poslednjih nekoliko decenija flaširana voda veoma tražen i komercijalno važan prehrambeni proizvod [1]. Prosečni potrošač obično razlikuje dve glavne vrste flaširanih voda: negazirane vode i gazirane vode. Ipak, prema preciznijoj klasifikaciji, flaširane vode se razlikuju prema poreklu i pripremi i to su: (i) prirodne izvorske vode, (ii) prirodne mineralne vode, (iii) stone vode.

U kontekstu našeg interesovanja za multielementarnu analizu vode [2] provedena je analiza uzoraka flaširanih voda različitih marki. Merenja su provedena tehnikom atomske emisione spektrometrije sa induktivno spregnutom plazmom (ICP-AES). Analizovane vode potiču iz nekoliko različitih evropskih zemalja, ali na posteru – gde će rezultati analize većeg broja odabranih metala i metaloida biti prezentovani − marke će biti anonimizovane.

Multi-element analysis of bottled waters by means of ICP-AES

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It is well known that, during the last few decades, bottled water has become a much requested and commercially important food product.[1] From the point of view of average consumers, there are two main types of bottled waters: still waters and sparkling waters. More precise classification differentiates bottled waters according to their origin and preparation: (i) natural spring waters, (ii) natural mineral waters, and (iii) table waters.

In the context of our interest in multi-elemental analysis of waters,[2] samples of several different still water brands were analyzed by using inductively coupled plasma – atomic emission spectrometry (ICP-AES). The analyzed water samples originate from various European countries, but in the communication the brands will be anonymized. Results of determination of selected metals and metalloids will be presented.

1. M. Diduch, Ż. Polkowska, J. Namieśnik, *J. Food Sci.* **2011**, *76*, R178.
2. V. Roje, P. Šutalo, *J. Geochem. Explor.* **2019**, *201*, 79.

HTH-3

Proteinski profil liofilisanog praha kozijeg mleka obogaćenog ekstraktom *Agrocybe aegerita* (V. Brig.) Singer

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Cilj ove studije je bio elektroforetska analiza polipeptidnog profila liofilisanog obezmašćenog kozije mleko (MP) obogaćenog vodenim ekstraktom *Agrocybe aegerita* (ME), optimizovanog primenom centralnog kompozitnog dizajna. Na elektroforegramu kontrolnog praha kozijeg mleka su detektovane trake proteina kozijeg mleka, koje pripadaju kazeinima i serum proteinima. Na elektroforegramu MP/ME uzorka, pored proteinskih traka mleka je uočeno pet novih (nekarakterističnih) polipeptidnih traka koje nisu detektovane na kontrolnom MP uzorku. Na istom elektroforegramu se može primetiti smanjen intenzitet trake koje pripadaju β-CN i potpuno odsustvo trake koja pripada k-CN. Dobijeni rezultati ukazuju na proteolitičku aktivnosti specifičnih enzima pečurke, koji selektivno hodrolizuju kazeine kozijeg mleka. Dobijen MP/ME prah ima izmenjen polipeptidni sastav, što može uticati na njegova funkcionalna svojstva.

Protein profile of freeze-dried goat milk powder mushroom enriched with *Agrocybe aegerita* (V. Brig.) Singer extract

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The aim of this study was the electrophoretic analyses of the polypeptide profile of freeze-dried goat skimmed milk powder (MP) enriched with an aqueous extract of *A. aegerita* mushroom (ME), optimized by Central Composite Design. On the electrophoretic pattern of MP sample protein bands of goat milk corresponding to caseins and whey proteins were detected. On the MP/ME electrophoretic pattern, however, five new (uncharacteristic) polypeptide bands were observed, apart from milk protein bands, which were not detected on the control sample. Moreover, on the same electrophoretic pattern, a reduced intensity of the band corresponding to β-CN and a complete absence of the k-CN band were observed. The results indicate the proteolytic activity of specific mushroom enzymes, that are able to selectively cleave goat's milk caseins. The formulated MP/ME powder has a modified polypeptide composition, which could have an impact on its functional properties.

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Hemija i tehnologija materijala

Chemistry and Technology of Materials

HTM-1

Ekološki prihvatljivo rešenje za zagađenje vode: hidrogelovi hitozana

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Zagađenje vode izazvano bojama iz veš mašina predstavlja važan ekološki problem zbog čega se poslednjih godina stavlja akcenat na istraživanja o sorbentima na bazi prirodnih polimera, kao što je hitozan. Jedan od rešenja ovog problema je priprema hidrogel-kuglica pomoću hitozana modifikovanog različitim jedinjenjima. Dobijeni sorbenti su testirani prema protokolu Međunarodne asocijacije za sapune, detergente i proizvode za održavanje (A.I.S.E.). Efikasnost pripremljenih sorbenata ispitana je korišćenjem pamučnih tkanina različitih boja i pomoću C.I. Acid Orange 7 kao model boje. Rezultati ukazuju da sintetisani sorbenti imaju potencijal da deluju kao hvatači boje za pranje veša. Ovo istraživanje otvara prostor za jednostavno i ekološki prihvatljivo rešenje za problem otpadnih voda iz veš mašine.

Eco-friendly solution for water treatment: Chitosan hydrogels as color catchers

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The dye pollution from washing machines presents a significant environmental concern, therefore research about natural-based polymer sorbents, such as chitosan, is performed. One of the solutions to this problem is the preparation of hydrogel beads using chitosan modified with various compounds. The obtained sorbents were tested according to the protocol of the International Association for Soaps, Detergents, and Maintenance Products. The efficiency of prepared sorbents was evaluated using differently colored cotton fabrics and C.I. Acid Orange 7 as a dye model. The results indicate the potential of the synthetized sorbents to act as a color catcher for laundry machine-washing. Overall, this research highlights a practical and eco-friendly solution to address dye pollution in wastewater from washing machines, contributing to the broader efforts in environmental sustainability.

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HTM-2

Zeleni hidrogelovi na bazi polisaharida za remedijaciju otpadnih voda

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Zaštita životne sredine i remedijacija voda predstavljaju važne teme današnjice, s toga istraživanja u oblasti polisaharidnih hidrogelova za uklanjanje zagađujućih materija iz otpadnih voda privlače pažnju naučnika. Polisaharidi, kao što su natrijum-karboksimetilceluloza (CMC) i natrijum-alginat (SA) su biokompatibilni, biorazgradivi, netoksični i jeftini, ali poseduju nedostatke koje je potrebno prevazići. Efikasan metod za poboljšanje učinka i svojstava CMC/SA hidrogelova je proces umrežavanja. Taninska kiselina zajedno sa $ZnCl_2$ korišćena je u dvostepenom procesu umrežavanja za proizvodnju zelenih CMC/SA hidrogelova. Tema ovog istraživanja je sinteza zelenih i održivih CMC/SA hidrogelova i njihova sorpcija zagađujućih materija iz otpadnih voda. Različiti parametri praćeni su tokom procesa sorpcije. Ekološki prihvatljivi zeleni CMC/SA hidrogelovi dobijeni dvostepenom sintezom pokazali su odličnu moć sorpcije zagađujućih materija.

Green polysaccharide hydrogels for wastewater remediation

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In light of environmental protection and water remediation as important topics nowadays, research in the field of polysaccharide hydrogels as wastewater pollutant sorbents attracts the attention of scientists. Polysaccharides, such as sodium carboxymethylcellulose (CMC) and sodium alginate (SA) are biocompatible, biodegradable, non-toxic, and low-cost but have some drawbacks that should be overcome. An effective method to improve the performance and physical properties of CMC/SA hydrogels is a crosslinking process. Tannic acid together with $ZnCl_2$ is used in a two-step crosslinking process for green CMC/SA hydrogel production. The topic of this work is the synthesis of green and sustainable CMC/SA hydrogels and their sorption of pollutants from wastewater. Different parameters were monitored during the sorption process. The eco-friendly green CMC/SA hydrogels obtained by two-step synthesis have excellent sorption properties of the pollutants.

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HTM-3

Modeli otpuštanja leka iz hidrogela poli(vinil alkohol)/hitozan/gentamicin (PVA/CHI/Gent)

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Hidrogel poli(vinil alkohol)/hitozan/gentamicin (PVA/CHI/Gent) pripremljen je fizičkim umrežavanjem disperzije poli(vinil alkohola)/hitozana i namenjen je za upotrebu kao materijal za medicinske obloge dubokih nekrotičnih rana kao što su dekubitusi. Ispitivane su fizičko-hemijske (FTIR, SEM), mehaničke i biološke (citotoksičnost, antibakterijska aktivnost) osobine. Mehanizam difuzije gentamicina iz hidrogela PVA/CHI/Gent proučavan je upoređivanjem novog dvo-kompartmentskog modela sa opštim frakcionim izvodima (GFD) i Korsmajer-Pepas, Makoid-Banakar i Kopča difuzionih modela. GFD model bolje se poklapao sa eksperimentalnim podacima od drugih modela i takođe je omogućio određivanje koeficijenta difuzije gentamicina tokom celog proučavanog vremenskog perioda.

Drug release models from poly (vinyl alcohol)/chitosan/gentamicin (PVA/CHI/Gent) hydrogel

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The poly (vinyl alcohol)/chitosan/gentamicin (PVA/CHI/Gent) hydrogel was prepared by physical cross-linking of poly(vinyl alcohol)/chitosan dispersion and intended for wound dressing material in medical treatment of deep necrotic wounds such as pressure ulcers. Physico-chemical (FTIR, SEM), mechanical and biological (cytotoxicity, antibacterial activity) properties were determined. Diffusion mechanism of gentamicin release from PVA/CHI/Gent hydrogel was studied by comparison of novel two compartmental models with General fractional derivative (GFD) and Korsmeyer-Peppas, Makoid-Banakar and Kopcha diffusion models. GFD model better fitted the experimental data than other models, and also allowed for the determination of the diffusion coefficient of gentamicin over the entire time period studied.

Hemija životne sredine

Environmental Chemistry

HŽS-1

Fotodegradacija ciprofloksacina sa Fe-modifikovanim TiO_2

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Zagađenje vodene sredine antibioticima izaziva veliku zabrinutost širom sveta, a jedan od najčešće detektovanih antibiotika jeste ciprofloksacin. Ciprofloksacin je sintetički derivat fluorokinolona sa širokom upotrebom za lečenje upalnih oboljenja kod životinja i ljudi. Kako se *UV* fotodegradacija sa nanomaterijalima na bazi poluprovodnika pokazala kao obećavajuća metoda za uklanjanje antibiotika, u ovom istraživanju smo sintetisali TiO_2 modifikovan sa Fe u tri različita molarna odnosa (0,5, 1 i 2 %) i primenili za fotodegradaciju rastvora ciprofloksacina za infuziju. Proces fotodegradacije je praćen *UV-Vis* spektroskopijom tokom 240 minuta. Rezultati pokazuju da se povećanjem molarnog udela gvožđa u fotkatalizatoru, povećava i efikasnost degradacije.

Photodegradation of ciprofloxacin with Fe-modified TiO_2

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The pollution of the water environment with antibiotics is a major concern worldwide. One of the most detected antibiotics in the treated wastewater is ciprofloxacin. Ciprofloxacin is a synthetic fluoroquinolone derivative with a large usage scale for inflammatory treatment for animals and humans. As UV-based photodegradation with semiconductor-based nanomaterials has shown promising results for antibiotic removal, in this research, we synthesized TiO_2 modified with Fe in three different molar ratios (0.5, 1 and 2 %) and applied it to the photodegradation of the ciprofloxacin infusion solution. The photodegradation process was monitored by UV-Vis spectroscopy for 240 minutes. The results indicate that increasing the molar ratio of iron in the photocatalyst increases the degradation efficiency.

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HŽS-2

Odnos između unutrašnjeg i spoljašnjeg aerozagađenja u školi

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Loš kvalitet vazduha negativno utiče na kognitivne sposobnosti i zdravlje učenika. Cilj ovog istraživanja bio je da se proceni odnos između unutrašnjeg i spoljašnjeg aerozagađenja u školi. Određivane su koncentracije ugljen-dioksida (CO_2), formaldehida (HCOH), čestica ($PM_{2,5}$) i ukupnih isparljivih organskih jedinjenja (TVOC), tokom dve nedelje u februaru 2024. godine, u školi u centru Beograda. Prosečne koncentracije CO_2 (586±200 prema 450±37 ppm) i HCOH (26,9±17,2 prema 7,7±5,6 μg/m^{-3}) u unutrašnjem prostoru bile su veće nego u spoljašnjoj sredini. Suprotno, prosečne koncentracije $PM_{2,5}$ (15,6±9,6 prema 36,1±33,3 μg/m^{-3}) i TVOC (8,4±26,6 prema 28,7±44,7 μg/m^{-3}) u unutrašnjem prostoru bile su niže od spoljašnjih. Dobijeni rezultati pokazuju značajne razlike između koncentracija zagađujućih supstanci vazduha u unutrašnjoj i spoljašnjoj sredini, ukazujući da CO_2 i HCOH dominantno potiču iz unutrašnje, dok $PM_{2,5}$ i TVOC potiču iz spoljašnje sredine.

The relationship between indoor and outdoor air pollution in school

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Poor air quality adversely affects the cognitive abilities and health of students. The aim of this study was to assess link between indoor and outdoor air pollution in school. The concentrations of carbon dioxide (CO_2), formaldehyde (HCOH), particulate matter ($PM_{2.5}$) and total volatile organic compound (TVOC) were determined for two weeks of February 2024 in school, centrally located in Belgrade. The average concentrations of CO_2 (586±200 vs 450±37 ppm) and HCOH (26.9±17.2 vs 7.7±5.6 μg/m^{-3}) indoor were higher than outdoor. Contrary, the average concentrations of $PM_{2.5}$ (15.6±9.6 vs 36.1±33.3 μg/m^{-3}) and TVOC (8.4±26.6 vs 28.7±44.7 μg/m^{-3}) indoor were lower than outdoor. These findings revealed significant differences between indoor and outdoor concentrations of air pollutants, suggesting that CO_2 and HCOH predominantly originate from indoor, while $PM_{2.5}$ and TVOC come from external sources.

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HŽS-3

Per- i polifluoralkil supstance u Srbiji – prisustvo, sudbina i kruženje u vodenim sredinama

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Per i polifluoralkil supstance (PFAS) su toksične hemikalije antropogenog porekla, otporne na razgradnju u prirodi. Bioakumulaciona svojstva omogućavaju da se PFAS akumuliraju u jetri, krvi i bubrezima, a dugoročno izlaganje čoveka može dovesti do razvoja kancera i hormonskih poremećaja. Stoga je važno produbiti znanje o prisustvu i inkorporaciji PFAS-a u niže trofičke nivoe, koji su baza za dalji transport i bioakumulaciju do viših organizama, uključujući i čoveka. Kombinovanjem rezultata monitoringa PFAS-a u površinskim vodama, sedimentu i planktonu sa rezultatima inkubacionog eksperimenta gde će se izlaganjem algi raznim dozama PFAS-a izučavati njihova inkorporacija u ćeliju, dobićemo uvid u afinitet i kompeticiju različitih PFAS-a u zavisnosti od njihove strukture, kao i u potencijalni mehanizam inkorporacije ovih jedinjenja u ćelije organizama široko prisutnih u životnoj sredini Srbije.

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Per- and polyfluoroalkyl substances in Serbia – occurrence, fate and cycling in aquatic environments

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Per- and polyfluoroalkyl substances (PFAS) are toxic chemicals of anthropogenic origin, resistant to environmental degradation. PFAS accumulate in the liver, blood and kidneys, and long exposure to these chemicals may cause cancer and endocrine disruption. Therefore, it is important to deepen the knowledge on PFAS occurrence and incorporation in lower trophic level organisms, responsible for further transport, and bioaccumulation to higher organisms, including humans. Combining the monitoring data on PFAS in surface waters, sediment and plankton with the results obtained through a series of exposure experiments where PFAS affinity to algal cells will be studied, we will gain insight into the affinity and competition of different PFAS as well as understanding of a potential mechanism for incorporation of these compounds into cells of organisms widely spread in Serbian environment.

HŽS-4

Uklanjanje fenola iz vode primenom biouglja dobijenog iz različitih vrsta lignocelulozne biomase

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Biougalj je ugljenični materijal koji se proizvodi procesom pirolize iz različitih vrsta biomase. Zbog svojih specifičnih karakteristika pokazao se kao dobar adsorbens za uklanjanje različitih organskih polutanata iz vode. U ovom radu ispitana je efikasnost primene biouglja dobijenog iz različitih vrsta otpadne lignocelulozne biomase za uklanjanje fenola iz vode procesom adsorpcije. Ispitani uzorcibiouglja dobijeni su iz slame ječma, slame soje, klipova kukuruza i iz piljevine bukve pirolizom na temperaturi od 700 °C u trajanju od 3 h. Primenom ispitivanih uzoraka biouglja u koncentraciji od 8,0 g/l efikasnost uklanjanja fenola se kretala u opsegu 33-77% nakon 2 h trajanja adsorpcije. Najbolji rezultati su postignuti primenom biouglja dobijenog iz otpadne drvne biomase.

Phenol removal from water using biochar derived from different types of lignocellulose biomass

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Biochar is carbon material produced by the pyrolysis of different types of biomass. Due to some specific characteristics, it proved to be good adsorbent for removing various organic pollutants from water. In the present study, the effectiveness of the application of biochar obtained from different types of waste lignocellulose biomass for the removal of phenol from water by the adsorption process was examined. Samples of biochar were obtained from barley straw, soybean straw, corn cobs, and beech sawdust by pyrolysis at a temperature of 700 °C for 3 h. Utilizing the investigated biochar samples in a concentration of 8.0 g/L, the removal efficiency of phenol was in the range of 33-77% after 2 h of adsorption. The best results were achieved using biochar obtained from waste woody biomass.

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HŽS-5

Primena pikosekundnog i nanosekundnog impulsnog laserskog zračenja u predtretmanu TiO_2 za primene u fotokatalizi

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Ultrakratki laserski impulsi (pikosekundni ili nanosekundni) mogu se koristiti za tretiranje i poboljšanje površinskih svojstava metala. Promena parametara laserskog zračenja omogućava dobijanje optimalnih strukturnih i morfoloških promena ozračenog materijala od titanijuma.[1] U cilju precizne površinske obrade, titanijumske mete biće ozračene primenom pikosekundnog i nanosekundnog laserskog zračenja. Ozračene titanijumske mete biće okarakterisane naprednim mikroskopskim tehnikama u cilju utvrđivanja morfoloških karakteristika.

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Application of picosecond and nanosecond pulsed laser irradiation in the pretreatment of TiO_2 for applications in photocatalysis

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Ultrashort laser pulses (picosecond or nanosecond) can be used to treat and improve the surface properties of metals. Changing the parameters of laser irradiation allows optimal structural and morphological changes in the irradiated titanium material.[1] In order to achieve precise surface treatment, titanium targets will be irradiated using picosecond and nanosecond laser irradiation. The irradiated titanium targets will be characterized by advanced microscopic techniques in order to determine their morphological characteristics.

1. S. Laketić, M. Rakin, M. Momčilović, J. Ciganović, Đ. Veljović, I. Cvijović-Alagić, *Surface and Coatings Technology*. **2018**, *418*, 127255.

HŽS-6

Distribucija metala u tragovima u zemljištu u blizini termoelektrana i procena statusa zagađenja

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Ovo istraživanje sprovedeno je u Braničevskom okrugu, koji se nalazi na desnoj obali reke Dunav u severoistočnom delu Srbije. Uzimajući u obzir istorijske i sadašnje aktivnosti korišćenja zemljišta u području ispitivanja, a koje uključuju poljoprivredu, arheologiju, rudarstvo, industrijalizaciju, urbanizaciju i deponije, ovim istraživanjem se pretpostavlja da ispitivano zemljište može biti kontaminirano potencijalno toksičnim elementima, što predstavlja rastuću zabrinutost za životnu sredinu. Ispitivan je uticaj i akumulacija sadržaja teških metal(oid)a, kao i status zagađenja zemljišta u blizini termoelektrana, rudnika uglja (lignita) i deponija letećeg pepela. Ukupno 23 uzorka površinskog sloja zemljišta (0-30 cm) različitih namena prikupljena su sa odabranih lokacija u jesen 2023. godine.

Zahvalnica: Autori se zahvaljuju MNTRI Republike Srbije za finansijsku podršku istraživanju kroz institucionalno finansiranje (Broj ugovora 451-03-66/2024-03/200017, 451-03-66/2024-03/200287).

Distribution of trace metals in soils adjacent to a thermal power plants and assessment of pollution status

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This investigation is conducted in the Braničevo District, located on the right bank of the Danube River in the northeastern part of Serbia. Considering the historical and present land use activities in the study area, which encompass agriculture, archeology, mining, industrialization, urbanization, and landfills, this research hypothesizes that the examined soil could be contaminated with potentially hazardous elements, presenting a growing environmental concern. The impact and accumulation of heavy metal(oid)s content, as well as the pollution status of soil in the vicinity of thermal power plants, coal (lignite) mine, and fly ash landfills were examined. A total of 23 topsoil samples (0-30 cm) of different land uses were collected from selected locations in autumn 2023.

HŽS-7

Adsorpcija mezotriona iz vodenih rastvora korišćenjem aktiviranog ugljeničnog materijala agroindustrijskog otpada suncokreta

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U ovom radu za uklanjanje mezotriona iz vodenih rastvora korišćen je aktivirani ugljenični materijal dobijen karbonizacijom, a zatim i hemijskom aktivacijom agroindustrijskog otpada suncokreta. Karbonizacija, a zatim i hemijska aktivacija sprovedene su na temperaturi od 900ºC, u struji azota sa brzinom zagrevanja od 5ºC/min. Adsorpcija pesticida kao i optimizacija uslova adsorpcije korišćenjem sintetizovanog materijala određena je pomoću *UV-Vis* spektroskopije. Na osnovu dobijenih rezultata utvrđeno je da se sintetisani aktivirani ugljenični materijal može efikasno primeniti za svrhu uklanjanja mezotriona iz vodenih rastvora.

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Adsorption of mesotrione from aqueous solutions using activated carbon material of sunflower agro-industrial waste

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In this work, activated carbon material obtained by carbonization and then chemical activation of sunflower agro-industrial waste was used for the removal of mesotrione from aqueous solutions. Carbonization and chemical activation were carried out at a temperature of 900ºC, in a stream of nitrogen with a heating rate of 5ºC/min. Adsorption of pesticides as well as the optimization of adsorption conditions using the synthesized material was determined by UV-VIS spectroscopy. Based on the obtained results, it was determined that the synthesized activated carbon material can be effectively applied for the purpose of removing mesotrione from aqueous solutions.

HŽS-8

Sadržaj toksičnih elemenata u zemljištu sa dečjih igrališta urbanog područja Beograda

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Za zemljišta urbanih gradskih područja se očekuje da budu zagađena potencijalno toksičnim elementima (PTE), zbog saobraćaja, urbanizacije i industralizacij. Budući da deca provode dosta vremena na igralištima, igrajući se zemljom, njihova izloženost ovim elementima i potencijalni štetni efekti na zdravlje su poslednjih godina postala vrlo značajna tema. [1-2] Cilj ovog rada je bio određivanje sadržaja arsena (As), kadmijuma (Cd), olova (Pb), nikla (Ni), hroma (Cr), bakra (Cu) i cinka (Zn) u 17 uzoraka zemljišta sa različitih dečjih igrališta u urbanoj zoni Beograda. Uzorci su pripremani kiselom mikrotalasnom digestijom, a sadržaj elemenata je određivan metodom induktivno spregnute plazme optičke emisione spektroskopije (ISP-OES). Tačnost metode je procenjena upotrebom sertifikovanog referentnog materijala NIST 2711a, i dobijene su vrednosti u opsegu 80-120%. Prosečna koncentracija ispitivanih PTE sledi navedeni niz: Zn (68,24 mg/kg) > Ni (60,99 mg/kg) > Cr (51,685 mg/kg) > Pb (21,615 mg/kg) > Cu (19,785 mg/kg) > As (8,1125 mg/kg) > Cd (0,1566 mg/kg). Koncentracije svih ispitivanih PTE su u saglasnosti sa legislativma Republike Srbije, Evropske unije (EU) i Svetske zdravstvene organizacije (SZO). S obzirom na potencijal PTE za bioakumulaciju i uključivanje u lanac ishran, vrlo je važno njihovo konstantno praćenje, a u tom smislu ovaj rad može imati doprinos u očuvanju urbane sredine.

Toxic Elements in Soil of Children's Playgrounds in the Belgrade Urban Area

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Soils in the urban area are suspected to be contaminated with potentially toxic elements (PTEs), due to traffic, urbanisation, and industrialization. The possibility of adverse health effects and the exposure of children who spend a lot of time in playgrounds and playing with soil, has attracted a lot of attention in recent years, especially with regard to the potential risk to children's health. [1-2] The aim of this study was to determine the levels of arsenic (As), cadmium (Cd), lead (Pb), nickel (Ni), chromium (Cr), copper (Cu), and zinc (Zn) in 17 soil samples from different children's playgrounds in the city of Belgrade. The samples were prepared by acid assisted microwave digestion and the concentrations of elements were determined by inductively coupled plasma optical emission spectroscopy (ICP-OES). Accuracy was assessed using the certified reference material NIST 2711a, and recoveries obtained were in the range of 80-120%. The average concentration of PTEs followed the following order: Zn (68.24 mg/kg) > Ni (60.99 mg/kg) > Cr (51.685 mg/kg) > Pb (21.615 mg/kg) > Cu (19.785 mg/kg) > As (8.1125 mg/kg) > Cd (0.1566 mg/kg). The average concentration of all metals in soil did not exceed the permissible limits according to the guidelines of Serbian legislation, the European Union (EU), and the World Health Organization (WHO). Since these PTEs can bioaccumulate and biomagnify in the food chain, their concentration in soil should be continuously monitored so this study should contribute to rising awareness for the protection of the urban environment.

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HŽS-9

Materijali na bazi geopolimera za adsorpciju fenola iz otpadnih voda

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Geo-polimeri su pokazali značajne performanse u cilju poboljšanja kvaliteta vode kao kombinovani i napredni sistemi za adsorpciju sa standardnim tehnologijama tretmana kao što su aeracija, sedimentacija, filtracija i oksidacioni procesi. Ovi materijali, nano i milimetarske granulacije, imaju veliki kapacitet uklanjanja teških metala i metaloida u odnosu na konvencionalne, kao što su aktivni ugalj, oksidi grafena i ugljenične nanocevi. Proizvodnja biofunkcionalizovanih (bio-vezanih) kompozitnih materijala na bazi magnetitnih nanočestica (MNP), geopolimera i biljnih ekstrakata (geo-MNP kompoziti), predstavlja inovativni pristup za dobijanje kompozitnog adsorbenta u procesu tretmana vode. Preliminarni rezultati pokazuju da je prirodni i sintetički alofan nanostrukture materijal koji ima kapacitet visoke adsorpcione moći i dalja ispitivanja će biti sprovedena kako bi se sa laboratorijskog nivoa skaliralo na nivo pilot istraživanja i na taj način definisale performanse uređaja za uklanjanje fenola iz otpadnih voda.

Geo-polymer based materials for phenol adsorption from wastewater

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Geo-polymers have demonstrated significant promise in enhancing water quality as combined and advanced adsorption system coupled with standard pretreatment technologies e.g. aeration, sedimentation, filtration and oxidation. These materials (nano- to mm - scale) show great removal capacity for heavy metals and metalloids over conventional ones such as activated carbon, graphene oxides and carbon nanotubes. The production of bio-functionalized (bio-linked) composite materials based on magnetite nanoparticles (MNPs), geo-polymers and plant extracts (geo-MNP composites), represents an innovative approach for the production of adsorbent in water treatment. Preliminary results show that natural and synthetic allophane of nano- structure is promising material and further testing will be conducted in order to ensure the high adsorption cost-effective performance for phenols removal from ground- and wastewater.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7464, Novel Bio-linked Magnetite/geopolymer Composites in Phenol-containing Wastewater Treatment: Toward Zero-waste Technology – BioCompWaterClean.

Medicinska hemija

Medicinal Chemistry

MH-1

Simulacije molekularne dinamike vezivanja 7,8-dihidroksiflavona za TrkB receptor: uvidi u agonistički mehanizam

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Ova studija koristi simulacije molekularne dinamike za istraživanje interakcije između 7,8-dihidroksiflavona (7,8-DHF) i tropomiozin receptora kinaze B (TrkB). 7,8-DHF je snažan TrkB agonist poznat po svojim neuroprotektivnim svojstvima[1,2]. Simulacije pružaju detaljne uvide u afinitet vezivanja i konformacione promene koje 7,8-DHF izaziva na TrkB receptoru. Ključne interakcije vezivanja i stabilnost kompleksa liganda i receptora analizirane su kako bi se razumela molekularna osnova agonističke aktivnosti 7,8-DHF. Rezultati ukazuju na značajne aminokiselinske ostatke uključene u proces aktivacije, nudeći potencijalne mete za poboljšanje terapeutske efikasnosti u lečenju neuroloških poremećaja.

Molecular dynamics simulations of 7,8-dihydroxyflavone binding to TrkB receptor: Insights into agonistic mechanism

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This study employs molecular dynamics simulations to explore the interaction between 7,8-dihydroxyflavone (7,8-DHF) and the tropomyosin receptor kinase B (TrkB). 7,8-DHF is a potent TrkB agonist known for its neuroprotective properties[1,2]. The simulations provide detailed insights into the binding affinity and conformational changes induced by 7,8-DHF on TrkB. Key binding interactions and stability of the ligand-receptor complex are analyzed to understand the molecular basis of the agonistic activity of 7,8-DHF. The results suggest critical amino acid residues involved in the activation process, offering potential targets for enhancing therapeutic efficacy in treating neurological disorders.

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MH-2

Novi steroidni NRF2 aktivatori. Sinteza i biološka aktivnost

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Nuklearni faktor poput eritroidnog faktora 2 (NRF2) je transkripcioni faktor ključan za ćelijsku odbranu od oksidativnog stresa i upale, što ga čini ključnom metom za lečenje nezaraznih bolesti. Ursodeoksiholna kiselina je lek odobren od strane FDA koji aktivira NRF2 signalni put i ukazuije na terapeutski potencijal steroidnih NRF2 aktivatora. Naše istraživanje je fokusirano na sintezu novih NRF2 aktivatora baziranih na žučnim kiselinama. Antioksidativna svojstva ovih jedinjenja su ispitana merenjem ekspresije NRF2 ciljnih gena kvantitativnim PCR-om. Jedinjenja SB140 i SB141 su pokazala snažnu pozitivnu regulaciju gena, što ukazuje na efikasnu aktivaciju NRF2 signalnog puta kao i potencijal za lečenje bolesti povezanih sa oksidativnim stresom. Prezentacija će pokriti sintezu i antioksidativne efekte ovih jedinjenja, podržavajući dalje istraživanje steroidnih aktivatora NRF2 za kliničku upotrebu.

New steroidal NRF2 activators. Synthesis and biological activity

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Nuclear factor like erythroid factor 2 (NRF2) is a transcription factor crucial for cellular defense against oxidative stress and inflammation, making it a key target for treating non-communicable diseases. Ursodeoxycholic acid is also an FDA-approved drug that activates the NRF2 signaling pathway highlighting the therapeutic potential of steroidal NRF2 activators. Our research is focused on synthesizing new NRF2 activators based on bile acids. The antioxidant properties of these compounds were tested by measuring the expression of NRF2 target genes using quantitative PCR. Compounds SB140 and SB141 showed strong positive regulation of genes, indicating effective activation of the NRF2 signaling pathway and potential for treating diseases associated with oxidative stress. The presentation will cover the synthesis and antioxidant effects of these compounds, supporting further research into steroid NRF2 activators for clinical use.

MH-3

Tiazolo[3,4-*a*]pirazin-5,8-dioni sa ferocenskim i hinolinskim motivima kao obećavajući antimikrobni agensi

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U ovom radu je ispitana *in vitro* antimikrobna aktivnost 11 novih 3-feroceniltetrahitro-3*H*-tiazolo[3,4-a]pirazin-5,8-diona kod kojih su u položaju N-7 uvedene različite alkil- ili alkil-aril-grupe. Najaktivnijim su bili hibridi sa 4-amino-7-hlorhinolinskom farmakoforom. Posebno se izdvojilo jedinjenje sa linkerom od 3 C-atoma koje je pokazalo jak i selektivan efekat na rast 2 Gram-pozitivne bakterije: *Staphylococcus aureus* i *Bacillus cereus*. Hlorohin i analogni derivat bez hinolinskog jezgra inhibirali su rast ova 2 soja pri znatno višim koncentracijama. Stoga, uočena antimikrobna aktivnost može predstavljati rezultat sintergističkog delovanja 3 farmakofore: ferocena, 4-amino-7-hlorhinolina i tiazolo[3,4-*a*]pirazin-5,8-diona, koje su objedinjene u ovom molekulu.

Thiazolo[3,4-*a*]pyrazine-5,8-diones tethered with ferrocene and quinoline motifs as promising antimicrobial agents

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Herein, 11 new 3-ferrocenyltetrahydro-3*H*-thiazolo[3,4-*a*]pyrazine-5,8-diones with different alkyl or alkyl-aryl groups on N-7 were evaluated for their *in vitro* antimicrobial potential. The most efficient were those containing the 4-amino-7-chloroquinoline pharmacophore, especially the one with a 3 C-atom linker. This compound showed strong and selective action against 2 Gram-positive bacteria, *Staphylococcus aureus* and *Bacillus cereus*. Chloroquine and an analogous derivative lacking the quinoline scaffold inhibited the growth of these 2 strains at much higher MICs. Hence, the observed antimicrobial effect may result from the combined action of 3 pharmacophores: ferrocene, 4-amino-7-chloroquinoline, and thiazolo[3,4-*a*]pyrazine-5,8-dione, integrated into this molecule.

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MH-4

Potencijal nanočestica zlata i srebra u inhibiciji oralnih patogena

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Nanočestice zlata i srebra sintetisane su metodom pulsne laserske ablacije ispitivanja njihovog antibakterijskog potencijala na bakterijskim izolatima *Streptococcus* spp. od značaja za etiologiju karijesa (*S. mutans, S. sanguinis, S. mitis, S. gordonii*), upotrebom mikrodilucionog testa. Testirane nanočestice ispoljile su primetan antimikrobni potencijal, minimalne inhibitorne koncentracije i minimalne baktericidne koncentracije kretale su se od 5 μg/mL do 71 μg/mL.

Antibacterial potential of the gold and silver nanoparticles against oral pathogens

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Gold and silver nanoparticles were synthetized by pulsed laser ablation aiming to test the antimicrobial potential towards *Streptococcus* spp. isolates relevant to tooth caries (*S.* mutans, *S. sanguinis, S. mitis, S. gordonii*), using the microdilution test. Tested nanoparticles achieved noticeable antimicrobial activity, with minimal inhibitory concentrations and minimal bactericidal concentrations ranging from 5 μg/mL to 71 μg/mL.

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MH-5

Uticaj uvođenja Zr jona na stabilnost, lipofilnost i mogućnosti prolaska krvno-moždane barijere polioksometalata

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Alchajmerova bolest (AB) je neurodegenerativno oboljenje sa kompleksnom patofiziologijom koja zahteva primenu koncepta "višenamenskog" leka. Polioksometalati (POM) su klasa negativno naelektrisanih jedinjenja koja ispoljavaju značajnu antiviralnu, antibakterijsku i anticancer aktivnost. Poslednjih godina, zbog svoje sposobnosti da inhibiraju holinergičke enzyme kao i agregaciju β-amiloida, mogućnost primene POMova u AB je takođe u žiži interesovanja naučnika. Međutim, pored značajne biološke aktivnosti koju predloženi lek za AB poseduje, često se dešava da poseduje neadekvatnu stabilnost, lipofilnost i da ne može preći krvno-moždanu barijeru (KMB). Ovim radom je ispitan uticaj uvođenja Zr jona u Keginovu strukturu POMa na njihovu stabilnost, lipofilnost i sposobnost prelaska krvno-moždane-barijere.

Influence of Zr ion on polyoxometalates' stability, lipophilicity, and ability to cross blood-brain-barrier

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Alzheimer's disease is a neurodegenerative disease with a complex pathophysiology, which requires the implementation of the concept of "multi-target-directed ligands" (MTDL). Polyoxometalates (POMs) are a class of negatively charged inorganic compounds that possess pronounced antiviral, antibacterial and anticancer properties. In recent years, due to the ability to inhibit cholinergic enzymes as well as amyloid aggregation, POMs have been investigated as effective agents in the combat against AD. However, in addition to the significant biological activity of the newly proposed drug, it often suffers from inappropriate lipophilicity and the inability to cross blood-brain-barrier (BBB). This work reveals the influence of the introduction of Zr^{4+} ion(s) into POM's Keggin structure on their stability, lipophilicity, and ability to cross BBB.

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MH-6

Sinteza, *in vitro* i *in silico* ispitivanja novog analoga (–)-murikatacina

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(–)-Murikatacin (**1**) je prirodni γ-lakton, prvi put izolovan iz biljke *Annona* Muricata,[1] koji pokazuje značajnu antitumorsku aktivnost.[2] U ovom radu će biti predstavljena sinteza novog analoga (–)-muricatacina (**2**) polazeći od L-ksiloze, kao i rezultati ispitivanja njegove citotoksične aktivnosti. Takođe, upotrebom *SwissTargetPrediction* web alata postavljena je hipoteza o potencijalnom ciljnom molekulu pa će biti prikazani rezultati molekulskog dokovanja enzima i analoga **2**.

Synthesis, *in vitro* and *in silico* studies of a new (–)-muricatacin analogue

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(–)-Muricatacin (**1**) is a natural γ-lactone, first isolated from *Annona* Muricata,[1] which exhibits significant antitumor activity.[2] The synthesis of novel (–)-muricatacin analogue (**2**) starting from L-xylose will be presented, along with the results of the cytotoxic activity of compound **2**. Additionally, using the *SwissTargetPrediction* web tool, a potential target molecule has been determined, and the results of molecular docking of the potential target enzyme and the new molecule will be presented.

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MH-7

Sinteza i *in silico* analiza dva nova bromovana furodioksolna epimera

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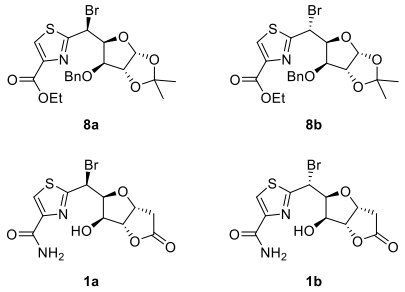
Prikazana je sedmofazna sinteza dva bromovana derivata D-glukoze (**8a** i **8b**), koji predstavljaju intermedijere na putu dobijanja bromovanih hibrida sintetskog *C*-nukleozida tiazofurina i prirodnog stiril-laktona (+)-goniofufurona (**1a** i **1b**, Šema 1). Urađena je *in silico* analiza pomoću servera Pharmmapper pomoću kog su dobijene potencijalne mete novosintetisanih jedinjenja, nakon čega su jedinjenja dokovana na dobijene mete pomoću alata AutoDock Vina.



*Šema 1. Dobijena jedinjenja **8a** i **8b** i ciljana jedinjenja **1a** i **1b***

Synthesis and *in silico* analysis of two new brominated furodioxol epimers

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We present the seven-step synthesis of two brominated derivates of D-glucose (**8a** and **8b**), which serve as intermediates on the path to obtaining brominated hybrids of the synthetic C-nucleoside tiazofurin and the natural styryl-lactone (+)-goniofufurone (**1a** and **1b**, Scheme 1). An *in silico* analysis was performed using the Pharmmapper server which provided potential targets for newly synthesized compounds, after which the compounds were docked to the obtained targets using the AutoDock Vina tool.

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Neorganska hemija

Inorganic Chemistry

NH-1

Sinteza i strukturna karakterizacija kompleksa galijuma(III) sa 1,3-propandiamin-*N,N*'-diacetatom

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U ovom radu, 1,3-pdda (1,3-propandiamin-*N,N*'-diacetat) je korišćen kao ligand za sintezu dinuklearnog galijum(III) kompleksa, $[\{Ga(1,3\text{-pdda})(\mu\text{-OH})\}_2]\cdot H_2O$. Kompleks je okarakterisan pomoću IR i NMR (^1H i ^{13}C) spektroskopije, dok je njegova kristalna struktura određena metodom difrakcije X-zraka sa monokristala. U ovom kompleksu, Ga(III) joni imaju oktaedarsku geometriju, pri čemu su za svaki Ga(III) jon koordinovana dva atoma azota i dva atoma kiseonika iz 1,3-pdda liganda, kao i dva atoma kiseonika iz mostno koordinovanih hidroksilnih grupa.

Synthesis and structural characterization of gallium(III) complex with 1,3-propanediamine-*N,N*'-diacetate

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In this study, 1,3-pdda (1,3-propanediamine-*N,N*'-diacetate) was used as a ligand for the synthesis of a new dinuclear gallium(III) complex, $[\{Ga(1,3\text{-pdda})(\mu\text{-OH})\}_2]\cdot H_2O$. This complex was characterized by IR and NMR (^1H and ^{13}C) spectroscopy, while its crystal structure was determined by single-crystal X-ray diffraction analysis. In this complex, both Ga(III) ions have octahedral geometry, whereas each Ga(III) ion is coordinated by two nitrogen and two oxygen atoms of 1,3-pdda ligand, as well as two oxygen atoms of the bridging hydroxyl groups.

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NH-2

Katalitička aktivnost kompleksa bakra(II) sa dimetil-6-(pirazin-2-il)piridin-3,4-dikarboksilatom u oksidaciji 3,5-di-*terc*-butilkatehola

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Bakar, kao esencijalni element, ulazi u sastav brojnih enzima, neophodnih za normalno funkcionisanje mnogih procesa u organizmu, dok se njegova uloga kao aktivnog centra zasniva na redoks procesima. Jedan od glavnih enzima bakra je katehol oksidaza, koja katalizuje aerobnu reakciju oksidacije katehola do odgovarajućih hinona. U cilju ispitivanja potencijalne sposobnosti kompleksa bakra(II), $[CuCl_2(py\text{-}2pz)]_2$, (py-2pz je dimetil-6-(pirazin-2-il)piridin-3,4-dikarboksilat), da oponaša aktivnost ovog enzima, ispitivana je kinetika njegove redoks reakcije sa 3,5-di-*tert*-butilkateholom.[1]

Catalytic activity of copper(II) complex with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate in oxidation of 3,5-di-*tert*-butylcatechol

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Copper, as an essential element, is included in the numerous enzymes, necessary for the normal functioning of many processes in the body, while its role as an active center is based on redox processes. One of the main copper enzymes is catechol oxidase, which catalyzes the aerobic reaction of catechol oxidation to the corresponding quinones. The kinetics of catechol oxidase biomimetic catalytic activity of the copper(II) complex, $[CuCl_2(py\text{-}2pz)]_2$, (py-2pz is dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate) was investigated using 3,5-di-*terc*-butylcatechol as a substrate in the redox reaction.[1]

1. T. P. Andrejević, I. Aleksic, J. Kljun, M. Počkaj, M. Zlatar, S. Vojnovic, J. Nikodinovic-Runic, I. Turel, M. I. Djuran, B. Đ. Glišić *RSC Adv*. **2023**, *13*, 4376.

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NH-3

Ispitivanje BSA interakcija kompleksa zlata(III) sa azolima

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Ispitivane su interakcije mononuklearnih kompleksa zlata(III) opšte formule [$AuCl_3$(azol)], gde azol predstavlja ekonazol, tiokonazol, vorikonazol i mikonazol, sa goveđim serum albuminom (BSA) u prisustvu markera eozina Y i ibuprofena. Goveđi serum albumin se sastoji od tri strukturno slična domena (I, II i III) koji su podeljeni na poddomene A i B. Markeri su korišćeni radi dobijanja boljeg uvida u vezujuće mesto kompleksa za molekul BSA, pri čemu eozin Y predstavlja marker za domen I i poddomen IIA, dok ibuprofen marker za domen II i poddomen IIIA. Dobijene vrednosti konstanti vezivanja K_A ispitivanih kompleksa su manje u prisustvu eozina Y što ukazuje na to da se ispitivani kompleksi vezuju za domen I i poddomen IIA u BSA molekulu.

Investigation of the BSA interactions of gold(III) complexes with azoles

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The interactions of mononuclear gold(III) complexes of the general formula [$AuCl_3$(azole)], where azole is econazole, tioconazole, voriconazole and miconazole, with bovine serum albumin (BSA) were investigated in the presence of site markers eosin Y and ibuprofen. Bovine serum albumin consists of three structurally similar domains (I, II and III) that are divided into subdomains A and B. The site markers were used to get a better insight into the binding site in the BSA, whereby eosin Y is a marker for domain I and subdomain IIA, while ibuprofen is a marker for domain II and subdomain IIIA. The obtained values of the binding constants K_A for the investigated complexes are lower in the presence of eosin Y, indicating their BSA binding to domain I and subdomain IIA.

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NH-4

Evaluacija biološke aktivnosti hidrazonskih kompleksa cinka

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Tri nova kompleksa Zn(II) sa (*E*)-2-(2-(1-(6-brompiridin-2-il)etiliden)hidrazinil)-*N*,*N*,*N*-trimetil-2-oksoetan-1-aminijum hloridom **HL**Cl su sintetisana i okarakterisana u čvrstom stanju i u rastvoru različitim metodama. Kompleks **1** formira oktaedarsku geometriju, dok kompleksi **2** i **3** formiraju iskrivljenu trigonalno bipiramidalnu geometriju. Biološka aktivnost ovih kompleksa je testirana na panelu gram-negativnih i gram-pozitivnih bakterija, dva soja gljivica i jedan soj kvasca. Doking analiza je predvidela da je geranilgeranil-pirofosfat sintaza, enzim neophodan za biosintezu sterola, najverovatnija meta za inhibiciju testiranih kompleksa.

Evaluation of the biological activity of zinc(II) hydrazone complexes

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Three new Zn(II) complexes with (*E*)-2-(2-(1-(6-bromopyridin-2-yl)ethylidene)hydrazinyl)-*N*,*N*,*N*-trimethyl-2-oxoethan-1-aminium chloride (**HL**Cl) have been synthesized and characterized in the solid state and in solution by different methods. Complex **1** forms an octahedral geometry, while complexes **2** and **3** form distorted trigonal bipyramidal geometry. The biological activity of these complexes was tested against a panel of Gram-negative and Gram-positive bacteria, two fungal strains, and a yeast strain. Molecular docking analysis predicted that geranylgeranyl pyrophosphate synthase, an enzyme essential for sterol biosynthesis is the most likely target for inhibition by the tested complexes.

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NH-5

Sinteza i stabilnost hidrazonskih kompleksa Zn(II)

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Kondenzacionom reakcijom 2-acetil-6-brompiridina sa Žirarovim T reagensom dobijen je ligand **HL**Cl *(E)*-2-(2-(1-(6-brompiridin-2-il)etiliden)hidrazinil)-*N*,*N*,*N*- trimetil-2-oksoetan-1-aminijum hlorid. Oktaedarski kompleks **1**, opšte formule $[Zn\mathbf{L}_2](BF_4)_2$ koji sadrži dva koordinovana liganda, dobijen je u reakciji liganda sa $Zn(BF_4)_2$ i NaN_3 u molarnom odnosu 1:1:4. Kompleks **2** je dobijen pod istim reakcionim uslovima kao i kompleks **1** pri čemu je Zn(II) pentakoordinovan preko NNO seta atoma jednog molekula liganda i dva NCO^- liganda. Međutim, reakcijom **HL**Cl sa $Zn(BF_4)_2$ i NaN_3 u višku (1:1:12) formiran je kompleks **3**, opšte formule $[Zn\mathbf{L}(N_3)_2]$. DFT proračuni su izvedeni da bi se poboljšalo razumevanje struktura kompleksa i potvrdila njihova struktura u rastvoru.

Synthesis and stability of Zn(II) hydrazone complexes

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The condensation of 2-acetyl-6-bromopyridine with Girard's T reagent produced the ligand **HL**Cl (*E*)-2-(2-(1-(6-bromopyridin-2-yl)ethylidene)hydrazinyl)-*N*,*N*,*N*-trimethyl-2-oxoethan-1-aminium chloride. Complex **1**, an octahedral complex containing two molecules of the coordinated ligand, was obtained when the ligand reacted with $Zn(BF_4)_2{\cdot}6H_2O$ and NaN_3 in molar ratio 1:1:4. Complex **2**, was obtained under the same reaction conditions as complex **1** where Zn(II) is pentacoordinated via one ligand molecule through NNO set of atoms and two NCO^- ligands. However, by reacting **HL**Cl with $Zn(BF_4)_2{\cdot}6H_2O$ and NaN_3 in excess (1:1:12) complex **3** with different composition, $[Zn\mathbf{L}(N_3)_2]$, was formed. Density functional theory (**DFT**) calculations were performed to enhance our understanding of the structures of the complexes in the solution.

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NH-6

DFT ispitivanje dimerizacije Ni(II) kompleksa

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Sintetizovali smo seriju Ni kompleksa koristeći različite donorske ligande na bazi NNO hidrazona i azidne anjone. Tri kompleksa su kristalizovala kao dvonuklearna, Ni(II) jona su koordinovani sa NNO ligandom i tri azidna liganda (dva mostna). U četvrtom kompleksu, Ni (II) je koordinovan sa dva NNO liganda. Da bismo razumeli ove različite ishode, izračunali smo ΔG energije za dimerizaciju i formiranje kompleksa sa dva NNO liganda, iz mononuklearnih kompleksa. Energije su izračunate koristeći M06-2X metodu sa Grimeovom D3 disperzionom korekcijom i def2-TZVP bazisom. Iako je dimerizacija povoljnija u svim slučajevima, ΔG energetska razlika je samo 1,7 kcal/mol za četvrti kompleks. Ova mala razlika se može prevazići energijama interakcije sa rastvorom ili u kristalnim strukturama. ΔG energetske razlike u drugim kompleksima su od 5 kcal/mol do 15 kcal/mol.

DFT study of the dimerization of Ni (II) complexes

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We have synthesized a series of a Ni complex using different NNO hydrazone-based donor ligands and azide anions. Three complexes crystallized as dinuclear, Ni(II) ions are coordinated with NNO ligand and three azide ligands (two bridging). In the fourth complex, Ni(II) is coordinated with two NNO ligands. To understand these different outcomes, we calculated the ΔG energies for dimerization and formation of complexes with two NNO ligands, from mononuclear complexes. The energies are calculated using the M06-2X method with Grimmes D3 dispersion correction and def2-TZVP basis. Aldo the dimerization is more favorable in all cases, the ΔG energy difference is only 1.7 kcal/mole for the fourth complex. This small difference could be overcome by the interaction energies with the solution or in the crystal structures. The ΔG energy differences in other complexes are from 5 kcal/mol to 15 kcal/mol.

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Nastava i istorija hemije

Education in and History of Chemistry

NIH-1

Kako učenici sedmog razreda u Srbiji prepoznaju i analiziraju probleme u životnoj sredini?

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Koristeći međunarodni upitnik za ispitivanje ekološke pismenosti (MSELS), utvrđen je nivo kognitivnih veština učenika sedmog razreda osnovne škole u Srbiji (n=877). Maksimalni skor na skali kognitivnih veština je iznosio 60 poena, a učenici su prosečno osvojili 25,97 poena. Na različitim vrstama zadataka postignuti su podjednaki rezultati: zadaci koji mere prepoznavanje problema (8,27), analiza problema (8,96), kao i planiranje aktivnosti za rešavanje problema (8,74). Kao način da se kognitivne veštine učenika podstaknu, u radu je predstavljen primer zadatka kojim se zahteva od učenika da analiziraju opisani problem zagađenja reke i da koncipiraju strategije za njegovo rešenje.

How 7th-grade students in Serbia identify and analyze environmental issues?

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Using the international environmental literacy survey (MSELS), the level of cognitive skills of seventh-grade elementary school students in Serbia (n=877) was determined. The maximum score on the cognitive skills scale was 60 points, and the students scored an average of 25.97 points. Students performed similarly on all task types: tasks that measure issue identification (8.27), issue analysis (8.96), as well as planning activities to solve issues (8.74). As a way to encourage students' cognitive skills, the paper presents an example of a task that requires students to analyze the specific problem of river pollution and to devise strategies for its solution.

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NIH-2

Poređenje Fenske-Holovog metoda i metoda Teorije funkcionala gustine za razjašnjavanje koncepta molekulskih orbitala u kompleksima prelaznih metala

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Razumevanje koncepta molekulskih orbitala se pokazalo kao veoma zahtevno za studente osnovnih studija. Ovo je posebno problematično u slučaju kompleksa prelaznih metala. Jedan od pristupa za rešavanje ovog problema je primena tehnika računarske hemije za računanje osobina molekulskih orbitala. U ovom radu smo primenili Fenski-Hol (FH) i proračune zasnovane na Teoriji funkcionala gustine (DFT) na odabrane komplekse prelaznih metala. Rezultati su pokazali da je FH metoda znatno brža od DFT metoda, i da oba pristupa daju slične rezultate prilikom računanja oblika molekulskih orbitala i atomskih doprinosa.

Comparison of Fenske-Hall and Density Functional Theory methods for clarification of the concept of molecular orbitals in transition metal complexes

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The understanding of the molecular orbital concept is very challenging for undergraduate students.[1] This is especially difficult in the case of transition metal complexes. One of the approaches to address this issue is utilization of computational chemistry techniques for calculation of the properties of molecular orbitals. In this work, we have performed Fenske-Hall (FH) and Density Functional Theory (DFT) calculations on selected transition metal complexes to compare efficiency and quality of the results of molecular orbital calculations for selected transition metal complexes. The results showed that FH method is significantly faster compared to DFT methods, and that both approaches provide similar results in terms of shape of molecular orbitals and atomic contributions.

1. G. Tsaparlis, *Research in Science Education*. **1997**, *27(2)*, *271.*

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NIH-3

Učeničko tumačenje reprezentacija iz udžbenika hemije pre i tokom pandemije COVID-19

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Reprezentacije u udžbenicima hemije trebalo bi da podrže formiranje pojmova kod učenika. Cilj istraživanja je bio da se uradi komparativna analiza učeničkih interpretacija reprezentacija makroskopskog, submikroskopskog i simboličkog nivoa u udžbenicima hemije, a koje se odnose na hemijsku vezu, u uslovima učenja pre i tokom pandemije COVID-19. U istraživanju je učestvovalo ukupno 422 učenika prvog i drugog razreda gimnazije (242 učenika je učestvovalo uživo pre pandemije i 180 učenika onlajn tokom pandemije). Za potrebe istraživanja kreiran je test sa šest zadataka, među kojima su bili i višeslojni zadaci za proveru sigurnosti učenika u pružene odgovore, kao i upitnik. Učesnici istraživanja tokom pandemije ostvarili su slabija postignuća, ali su izrazili veću sigurnost u pružene odgovore u odnosu na učesnike istraživanja pre pandemije. Ipak, ispitanici u vreme pandemije su na onlajn upitniku niže procenili sopstveno razumevanje ilustracija iz udžbenika nego učenici koji su upitnik popunjavali uživo, pre pandemije.

Zahvalnica: Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije Evidencioni broj:451-03-66/2024-03/200168

Students' interpretation of representations from chemistry textbooks before and during the COVID-19 pandemic

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Representations in chemistry textbooks should support students' concept formation. This research aimed to conduct a comparative analysis of students' interpretations of macroscopic, submicroscopic, and symbolic representations related to chemical bonding in chemistry textbooks. The study researched learning conditions before and during the COVID-19 pandemic. A total of 422 first and second-year grammar school students participated in the research, with 242 students participating in person before the pandemic and 180 students participating online during the pandemic. The study utilized a test consisting of six tasks, including multi-tiered tasks to assess students' confidence in their answers, along with a questionnaire. Results indicated that participants during the pandemic exhibited lower achievements but expressed greater confidence in their answers compared to those before the pandemic. However, respondents during the pandemic rated their understanding of textbook illustrations lower on the online questionnaire compared to students who completed the questionnaire in person before the pandemic.

Organska hemija

Organic Chemistry

OH-1

Antitumorska aktivnost novih proizvoda dearomatizacije estradiola

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Derivati prirodnih steroidnih hormona su pokazali značajnu antitumorsku aktivnost. Stoga su u ovom radu izvršene reakcije dearomatizacije estradiola u cilju dobijanja 10-alkoksi-1,4-dien-3-on sistema u steroidnom jezgru. Novosintetisana jedinjenja su testirana *in silico* radi utvrđivanja njihovih ADME svojstava, kao i *in vitro* citotoksičnosti. *In vitro* ispitivanja su vršena na četiri humane ćelijske linije kancera: HCT116, Huh7, MCF-7 i MDA-MB-231. Najaktivnijim su se pokazali 10-butoksi i 10-propargiloksi derivati.

Antitumor activity of novel products of estradiol dearomatization

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Derivatives of natural steroid hormones have shown significant antitumor activity and therefore, in this work, the dearomatization of estradiol was carried out in order to obtain a 10-alkoxy-1,4-dien-3-one system in the steroid core. Newly synthesized compounds were tested *in silico* to provide their ADME profile, as well as *in vitro* for their cytotoxicity. *In vitro* testing was conducted against four human cancer cell lines HCT116, Huh7, MCF7, and MDA-MB-231. 10-Buthoxy and 10-propargyloxy derivatives have shown to be the most active.

Acknowledgment: The authors acknowledge the financial support of the Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina [Project No. 142-451-3463/2023-01] and The Ministry of Science, Technological Development and Innovation of the Republic of Serbia and Austria's Agency for Education and Internalisation (OeAD) for the financial support of bilateral cooperation between the Republic of Austria and the Republic of Serbia [Project No. 337-00-577/2021-09/27 and OeAD RS15/2022].

OH-2

In silico dizajn i ispitivanje odabranih eutektičkih rastvarača na bazi holin-hlorida

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Eutektički rastvarači (DESs) predstavljaju novu klasu "zelenih" reakcionih medijuma poznatih po svojim brojnim korisnim karakteristikama, kao što su prilagodljivost, rasnovrsnost u primeni, jednostavna priprema, obnovljivost i biodegradabilnost. U ovom radu izvršen je *in silico* dizajn i optimizacija nekoliko eutektičkih sistema holin hlorida sa različitim donorima vodonične veze, primenom metoda teorije funkcionala gustine (DFT). Dobijeni rezultati pružili su uvid u strukturna i termodinamička svojstva ispitivanih DES-ova, što bi moglo poslužiti kao osnova za ispitivanje njihove potencijalne primene u sintezi različitih organskih jedinjenja od biološkog značaja.

In silico design and investigation of the selected choline chloride-based deep eutectic solvents

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Deep eutectic solvents (DESs) represent an uprising class of "green" reaction mediums known for their multiple beneficial features, such as high tunability, versatility, feasible preparation, renewability, and biodegradability. In this work, several choline chloride-based DESs with diverse hydrogen bond donors were designed and optimized *in silico* employing density functional theory (DFT). The obtained results provided valuable insight into the structural and thermodynamic properties of investigated DESs, which could serve as a basis for their potential implementation in synthesizing diverse organic compounds of biological interest.

This research was funded by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Agreements No. 451-03-66/2024-03/200122, 451-03-65/2024-03/200122 and 451-03-66/2024-03/200378), University of Kragujevac and SASA (GreenBICH project).

OH-3

Prva totalna sinteza (+)- i (–)-asperilaktona B

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(+)-Asperilakton B (**1**) je furano-lakton koji je izolovan iz endofitne gljivice *Aspergillus nidulans* početkom 2024. godine.[1] U ovom radu će biti prikazana prva višefazna totalna sinteza (+)-asperilaktona B (**1**), zasnovana na D-glukozi, kao hiralnom prekursoru (Shema 1). Pored toga, ostvarena je sinteza enantiomernog (–)-asperilaktona B (*ent*-**1**), u samo jednom sintetskom koraku, polazeći iz L-ramnoze (Shema 1). Struktura i stereohemija sintetizovanih jedinjenja su potvrđene rendgeno-strukturnom analizom.

The first total synthesis of (+)-and (–)-asperilactones B

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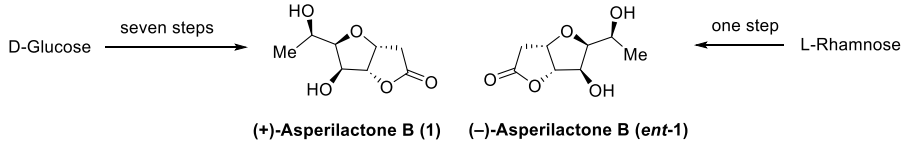
(+)-Asperilactone B (**1**) is a furano-lactone that was isolated from the endophytic fungus *Aspergillus nidulans* at the beginning of 2024.[1] Herein we present the first multi-step total synthesis of (+)-asperilactone B (**1**) based on D-glucose as a chiral precursor (Scheme 1). In addition, the synthesis of enantiomeric (–)-asperilactone B (*ent*-**1**) was achieved in just one synthetic step, starting from L-rhamnose (Scheme 1). The structure and stereochemistry of the synthesized compounds was confirmed by X-ray analysis.



Scheme 1. Synthetic approach to enantiomeric (+)- *and* (–)*-asperilactones B (**1** and ent-**1**).*

1. Q. Li, A. Fu, J. Dong, Y. Xiao, B. Dai, M. Wei, Z. Huang, J. Liu, C. Chen, H. Zhu, Y. Lu, D. Li, Y. Zhang, *Fitoterapia*. **2024**, *173*, 105790.

Acknowledgment: The work was supported by a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-65/2024-03/200125 & 451-03-66/2024-03/200125), and by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

OH-4

Hemijski sastav odbrambenog sekreta stonoge *Megaphyllum erythronotum* (Latzel, 1884) (Diplopoda, Julida)

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Sastav odbrambenog sekreta vrste *Megaphyllum erythronotum* (Latzel, 1884) (Diplopoda, Julida) je određen korišćenjem podataka dobijenih primenom gasne hromatografije-masene spektrometrije (GC-MS), sintezom odabranih sastojaka i hemijskom transformacijom ekstrakta sekreta. Identifikovano je više od 70 sastojaka (hinona, estara i ugljovodonika). Najzastupljeniji sastojci u odbrambenom sekretu su estri zasićenih i nezasićenih (*n*- i račvastih) karboksilnih kiselina. Dobiveni rezultati su pokazali da 14 od identifikovana 52 estra predstavlja nove prirodne proizvode, kao i da molekulski diverzitet analiziranih ekstrakata odbrambenog sekreta predstavlja potencijalno značajan hemotaksonomski karakter ove vrste stonoga.

Chemical composition of the defensive secretion of the millipede *Megaphyllum erythronotum* (Latzel, 1884) (Diplopoda, Julida)

Bojan S. Ilić[1], Marko Z. Mladenović[2], Jelena Z. Milovanović[1], Mirko M. Šević[1], Zvezdana S. Jovanović[1], Dalibor Z. Stojanović[1], Niko S. Radulović[2], Slobodan E. Makarov[1]

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The composition of the defensive secretion of *Megaphyllum erythronotum* (Latzel, 1884) (Diplopoda, Julida) was analyzed using data obtained by gas chromatography-mass spectrometry (GC-MS), synthesis, and chemical transformations of crude defensive secretion extracts. The data revealed the presence of more than 70 compounds (quinones, esters and hydrocarbons) in the analyzed extracts. The most abundant compounds in the defensive secretion are esters of long-chain (*n*- and branched) saturated and unsaturated carboxylic acids. Out of 52 identified esters, 14 represent new natural products and the molecular diversity of the analyzed defensive secretion extracts potentially represent an important chemotaxonomic marker for the millipede species in question.

OH-5

Dizajn, sinteza i spektralna karakterizacija novih kumarin-halkonskih derivata

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Sintetski hibridni molekuli, u kojima su integrisane kumarinske i halkonske farmakofore, poseduju značajnu fiziološku aktivnost. Imajući ovo u vidu, sintetisana je i u potpunosti spektralno okarakterisana serija novih kumarin-halkon konjugovanih proizvoda. Sinteza je ostvarena u dva reakciona koraka: prvo je sintetisan 3-acetil-4-hidroksikumarin, acetilovanjem 4-hidroksikumarina, a zatim, Claisen-Schmidt-ovim kondenzovanjem, iz 3-acetil-4-hidroksikumarina i različito supstituisanih aromatičnih aldehida nagrađeni su finalni produkti. Dobijeni proizvodi su potpuno spektralno okarakterisani pomoću HRMS-EI, IR, 1D i 2D NMR spektroskopije.

Design, synthesis and spectral characterization of novel coumarin-chalcone derivatives

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Synthetic hybrid molecules, in which coumarin and chalcone pharmacophores are integrated, possess significant physiological activity. Bearing this in mind, a series of new coumarin-chalcone conjugated products were synthesized and spectrally characterized. The synthesis was accomplished in two reaction steps: first, 3-acetyl-4-hydroxycoumarin was synthesized by acetylation of 4-hydroxycoumarin, and then, by Claisen-Schmidt condensation, from 3-acetyl-4-hydroxycoumarin and variously substituted aromatic aldehydes, the final products. The obtained products were fully spectrally characterized by HRMS-EI, IR, 1D, and 2D NMR spectroscopy.

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OH-6

Sinteza benzimidazola primenom DES-a

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Eutektički rastvarači (DES) predstavljaju klasu jonskih tečnosti koje se sastoje od dve ili više komponenti. Oni se ponašaju kao katalizatori i rastvarači i idealni su za sintezu biloški aktivnih heterocikličnih jedinjenja. Benzimidazol je važno aromatično, azotno heterociklično jedinjenje, a molekuli koji sadrže ovaj prsten u svojoj strukturi poseduju mnoge biološke osobine. U ovom radu, izvršena je optimizacija uslova za sintezu DES, pri čemu je kao akceptor vodonične veze korišćen holin-hlorid, a kao donori vodonične veze su korišćene različite organske kiseline, glicerol i *o*-fenilendiamin. Formirani DES su testirani na model reakciji sinteze benzimidazola iz acetofenona i *o*-fenilendiamina.

Synthesis of benzimidazole using DESs

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Eutectic solvents (DESs) represent a class of ionic liquids consisting of two or more components. They act as catalysts and solvents and are ideal for the synthesis of biologically active heterocyclic compounds. Benzimidazole is an important aromatic, nitrogenous heterocyclic compound, and molecules that possess this ring in their structure contain many biological properties. In this work, the reaction conditions for the synthesis of DESs were optimized, where choline chloride was used as a hydrogen bond acceptor, and various organic acids, glycerol, and *o*-phenylenediamine were used as hydrogen bond donors. The formed DESs were tested on the model reaction of benzimidazole synthesis from acetophenone and *o*-phenylenediamine.

Acknowledgement: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-66/2024-03/200122, 451-03-65/2024-03/200122 and 451-03-66/2024-03/200378), University of Kragujevac and SASA (GreenBICH project).

OH-7

Intramolekulska kooperativno katalizovana Cuđi-Trostova reakcija kao nova metoda za sintezu spirobicikličnih jedinjenja

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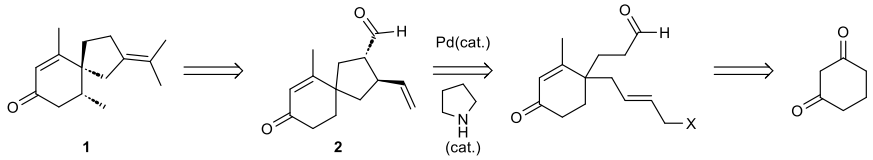
Vetispiranski tip seskviterpenoida čine jedinjenja sa karakterističnim spiro[4,5]-dekanskim skeletom, kao što je *β*-vetivon **1** (Slika 1). Ova jedinjenja predstavljaju važnu klasu sekundarnih metabolita sa širokim spektrom bioloških aktivnosti.[1] Naš pristup vetispiranskom sistemu zasnovan je na primeni kooperativne katalize – kombinacije organokatalize i katalize prelaznim metalima – kao ključne reakcije za formiranje funkcionalizovanog spiro[4,5]-dekanskog skeleta. Biciklični proizvodi tipa **2** predstavljaju dobru osnovu za sintezu prirodnih vetispirana i njihovih sintetičkih analoga.



Slika 1. Retrosintetička analiza β-vetivona.

Intramolecular cooperatively catalysed Tsuji-Trost reaction as a new method for synthesis of spiro-bicyclic compounds

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Vetispirane-type sesquiterpenoids, such as *β*-vetivone **1**, are natural products which possess spiro[4.5]-decane skeleton, and a wide range of biological activities.[1] Our approach to vetispirane core is based on dual catalysis – the combination of organocatalysis and transition metal catalysis – as a key reaction to form the functionalized spiro[4.5]-decane skeleton. Bicyclic products of type **2** are a good starting point for the synthesis of natural vetispiranes and their synthetic analogs.

1. X. Yin, Y. Liu, J. Pan, H.-L. Ye, Y. Sun, D.-Y. Zhao, H.-X. Kuang, B.-Y. Yang *J. Nat. Prod.* **2019**, *82*, 3242.

OH-8

Novi estri iz etarskog ulja *Pelargonium* sp. (Geraniaceae)

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Etarska ulja biljnih vrsta iz roda *Pelargonium* se koriste širom sveta u parfimeriji i narodnoj medicini.[1] Međutim, hemijski sastav etarskih ulja je nedovoljno ispitan. GC-MS analizom komercijalno dostupnog etarskog ulja, proizvedenog u Srbiji, utvrđeno je, pored više od 230 identifikovanih sastojaka, prisustvo 7 jedinjenja, za koja je, na osnovu analize masenih spektara, pretpostavljeno da su to (*Z*)-heks-3-en-1-il-, citronelil-, neril- i geranil-estri 3-metilpentanske, undekanske, tridekanske i/ili pentadekanske kiseline. Da bi se potvrdilo prisustvo ovih sastojaka u ulju, sintetisana su 23 (od kojih 15 potpuno novih) estra. Sva sintetisana jedinjenja su spektralno okarakterisana (MS, IR, NMR). GC-MS koinjekcijom uzorka etarskog ulja sa sintetisanim standardima je potvrđena identifikacija pomenutih sastojaka etarskog ulja.

New esters from the essential oil of *Pelargonium* sp. (Geraniaceae)

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University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry, Niš, Serbia

Essential oils of *Pelargonium* taxa are widely used as fragrant components in perfumery, and also in ethnomedicine.[1] However, the chemical composition of the oils has not been investigated in detail. A GC-MS analysis of a commercially available essential oil produced in Serbia revealed, among more than 230 identified constituents, the presence of 7 compounds that were, according to their mass spectra, tentatively identified as (*Z*)-hex-3-en-1-yl, citronellyl, neryl, and geranyl esters of 3-methylpentanoic, undecanoic, tridecanoic and/or pentadecanoic acids. Henceforth, to determine the presence of these minor essential-oil constituents, 23 (15 completely new) esters were synthesized. All synthesized compounds were spectrally characterized by MS, IR, and NMR. GC-MS co-injection of the essential-oil sample with the synthesized standards confirmed the identity of the mentioned essential-oil constituents.

1. F. Bakker, A. Culham, P. Hettiarachi, T. Touloumenidou, M. Gibby, *Taxon*. **2004**, *53*, 17.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (grant No. 451-03-66/2024-03/200124 and 451-03-65/2024-03/200124).

OH-9

Nova reakcija tioestara sa stabilizovanim karbenima: dobijanje α-tioketona

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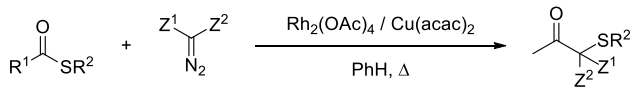
U sprovedenom istraživanju je opisana nova reakcija između tioestara i stabilizovanih karbena kojom nastaju funkcionalizovani α-tioketoni (Slika 1). Eksperimentalni podaci ukazuju na to da reakcija započinje generisanjem karbenoida i građenjem intermedijernog ilida reakcijom sa tioestarskim sumporom. Formirani ilid podleže [1,4]-acilnom transferu, pri čemu nastaje intermedijer koji se potom termički premešta u proizvod formalne 1,2-insercije (1,2-acil transfer). Nakon optimizacije reakcionih uslova, ispitani su dometi i ograničenja reakcije, kao i neke od mogućih transformacija dobijenih visokofunkcionalizovanih proizvoda.



Slika 1. Reakciona shema.

A new reaction of thioesters with stabilized carbenes: preparation of α-thioketones

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A new reaction between thioesters and stabilized carbenes for preparation of functionalized α-thioketones is reported (Figure 1). Experimental data indicate that the reaction commences with the generation of carbenoid, followed by the reaction with the thioester sulfur atom, to form an intermediate ylide. The formed ylide undergoes [1,4]-acyl transfer to produce intermediate which under thermal conditions rearranges itself into the product of a formal 1,2-insertion (1,2-acyl transfer). After optimizing the reaction conditions, scope and limitations of the reaction were investigated, as well as some of the possible transformations of the obtained functionalized products.

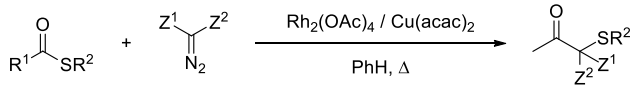

Figure 1. Reaction sheme.

Acknowledgment: This research was supported by the Science fund of the Republic of Serbia, Grant Number: 7750119, project acronym – New SMART Synthesis.

OH-10

Konformaciona analiza na osnovu analize konstanti sprezanja u ^{1}H NMR spektru salvipizona

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U ^{1}H NMR spektru abietanskog diterpena salvipizona uočen je multiplet AA′XX′-tipa umesto očekivanog 1:2:1 tripleta. Detaljnom analizom uočenog multipleta određene su konstante kuplovanja koje su omogućile određivanje relativnog odnosa *anti*, *gauche* i *gauche′* konformera (u odnosu na C12–C13 vezu) koji je iznosio 80:4:16.[1] Dobijeni rezultati potvrđeni su simulacijom uočenog multipleta u programu WinDNMR-Pro. Nakon određivanja relativne zastupljenosti najstabilnijih konformacionih izomera salvipizona izvršena je konformaciona analiza korišćenjem programa Chem3D, pri čemu je određena njihova konformaciona energija. Uočena razlika u odgovarajućim energetskim minimumima jasno ukazuje na razlog neravnomerne zastupljenosti dva *gauche* konformera.

Conformational analysis of salvipisone on the basis of ^{1}H NMR higher-order spin-spin interactions

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An analysis of the ^{1}H NMR spectrum of a abietane diterpene salvipisone revealed the presence of a higher-order AA′XX′-type multiplet with centrosymmetric patterns instead of the expected first-order 1:2:1 triplet. A closer examination of the observed higher-order spin-spin interactions, following the methodology outlined by Liu *et al.*, provided insight into the relative populations of the three staggered conformers.[1] The population ratio was determined to be 80:4:16 for the *anti*, *gauche*, and *gauche′*-conformers (relative to the C12–C13 bond). The observed higher-order couplings were further confirmed through simulation of a higher-order multiplet using the WinDNMR-Pro program. Additionally, an investigation into the energy differences and relative stabilities of staggered conformers was conducted. The observed energy difference in the rotation-energy diagram strongly suggests the cause of the uneven population of the two *gauche* conformers.

1. T. Liu, I. Abrahams, T. J. S. J. Dennis, *J. Phys. Chem. Lett.* **2020**, *11*, 5397.

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OH-11

Potencijalni nosioci antioksidativne aktivnosti gljive *Hericium erinaceus*: uvid iz (q)NMR analize

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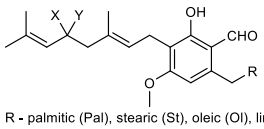
Hericium erinaceus (Bull.) Pers., lavlja griva, jestiva je gljiva poznata po širokom spektru bioloških aktivnosti. U cilju utvrđivanja nosioca antioksidativne aktivnosti ove gljive, etanolni ekstrakt gljive podvrgnut je NMR analizi. Preliminarnom NMR analizom ekstrakta utvrđeno je prisustvo hericena i hericenona (slika 1), dok je naknadnom kvantitativnom NMR (qNMR) analizom određeno da ukupan sadržaj ovih jedinjenja iznosi 0,43% (*w/w*), izraženo kao sadržaj hericenona C u ekstraktu. Imajući u vidu strukturne karakteristike pomenutih jedinjenja, antioksidativna aktivnost gljive se, barem delimično, može objasniti njihovim prisustvom.



Hericene	A	B	C	D	E	F	G	H
X	H	H	H	H	H	H	H	H
Y	H	H	H	H	Pal	Lin	Ol	Lin
R	Pal	Ol	St	Lin	Pal	Pal	Pal	St

5-Hydroxy hericene	A	B	C	D
X	H	H	H	H
Y	OH	OH	OH	OH
R	Pal	Ol	St	Lin

Hericenone	C	D	E
X, Y	=O	=O	=O
R	Pal	St	Lin

R - palmitic (Pal), stearic (St), oleic (Ol), linoleic (Lin) moiety

Slika 1.

Strukture hericena i hericenona prisutnih u H. erinaceus.

Unveiling antioxidant-active compounds in *Hericium erinaceus*: Insights from (q)NMR analysis

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Hericium erinaceus (Bull.) Pers., commonly known as Lion's Mane, is a culinary fungus renowned for its array of biological activities, notably its antioxidant potential. To identify the chemical constituents responsible for its antioxidant activity, the ethanolic extract of this fungus underwent NMR analysis, complemented by quantitative NMR (qNMR) for their quantification. Initial NMR analysis unveiled the presence of hericenes and hericenones (Figure 1) within the extract. Subsequent qNMR analysis provided their total content, quantified at 0.43% (*w/w*), expressed as the relative content of hericenone C within the extract. Given the structural characteristics, it is plausible that the mentioned compounds contribute to the antioxidant activity of *H. erinaceus*.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of RS (Contract Nos. 451-03-66/2024-03/200148, 451-03-65/2024-03/200124, 451-03-66/2024-03/200124, 451-03-47/2024-01/200287)

OH-12

Fotokatalitičko fluorovanje neaktiviranih C-H veza u mikrofluidnim reaktorima

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Uvođenje fluora u biološki aktivne molekule široko se koristi kao taktika u medicinskoj hemiji. Zamena vodonika fluorom može poboljšati osobine potencijalnog leka poput blokiranja neželjenog metabolizma na specifičnim mestima, povećavajući lipofilnost ili afinitet vezivanja, ili menjajući karakteristike apsorpcije, distribucije ili izlučivanja. U razvoju reakcije fluorovanja iskoristili smo fotoaktivnost aromatičnih ketone kao organskih fotokatalizatora u cilju postizanja selektivne apstrakcije C−H veza. Reakcije fluorovanja smo sproveli na seriji bioaktivnih molekula i procenili selektivnost i reaktivnost različitih fotokatalizatora i fluorujućih reagensa (NFSI, Selectfluor I, Selectfluor II). Nakon optimizacije u balonu, protokoli su preneti u mikrofluidne reaktore. Karakteristike ovih sistema koje uključuju bolje iskorišćenje svetlosti, poboljšan transfer toplote i mase omogućile su poboljšane prinose i selektivnost reakcija u odnosu na reakcije u balonu.

Photocatalytic fluorination of unactivated C-H bonds under microfluidic conditions

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Introducing a fluorine atom into a biologically active molecules is a widely employed tactic in medicinal chemistry. Often, substituting a single hydrogen with fluorine enhances the drug's properties by preventing unwanted metabolism at specific sites, increasing its lipophilicity or binding affinity, or altering its absorption, distribution, or excretion characteristics. We used the reactivity of photoactive ketones as photo catalysts to achieve selective C−H abstraction. We targeted the weakly activated benzylic position, ideal for strategic fluorination in medicinal chemistry due to metabolic considerations. We performed fluorination reactions on a series of bioactive molecules and assessed chemoselectivity and reactivity of different organic photocatalysts and fluorinating reagents (NFSI, Selectfluor I, Selectfluor II). Upon batch optimization, fluorination protocols were assessed in custom made microfluidic reactors.

OH-13

Hidroalkilovanje vinil-sulfona alkoholima pomoću vidljive svetlosti bez upotrebe fotokatalizatora

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Fotokataliza pomoću vidljive svetlosti je moćan alat za selektivnu aktivaciju malih organskih molekula i stvaranje novih veza. Tokom godina, upotrebljavani su različiti tipovi fotokatalizatora poput (skupih) kompleksa prelaznih metala, organskih fotoredoks-katalizatora i heterogenih fotokatalizatora. Ipak, razvoj procesa koji se odigravaju bez upotrebe fotokatalizatora je preporučljiv sa stanovišta održivog razvoja. U ovom radu, opisano je hidroalkilovanje vinil-sulfona pomoću alkohola pod dejstvom vidljive svetlosti. Reakcija se odigrava pod blagim uslovima, bez dodatka fotokatalizatora, metala ili spoljašnjeg redoks-reagensa. I primarni i sekundarni alkoholi reaguju, a mehanističke studije ukazuju na to da reakcija ima indukcioni period. Pored toga što se može primeniti za funkcionalizaciju u kasnoj fazi sinteze, opisani protokol omogućuje pristup γ-hidroksi-sulfonima, korisnoj grupi sintetičkih gradivnih jedinica.

Photocatalyst-free, visible light-induced hydroalkylation of vinylsulfones with alcohols

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Visible-light photocatalysis is a powerful tool for selective activation of small organic molecules and formation of new chemical bonds. Different types of photocatalysts like (expensive) transition metal complexes, organophotoredox catalysts, heterogeneous photocatalysts, have emerged over the years. However, the development of new processes under photocatalyst-free conditions are preferable from the viewpoint of sustainable development. Herein, we report a visible light-induced protocol for the hydroalkylation of vinyl sulfones using alcohols. The reaction occurs under mild conditions free of a photocatalyst, metal or external redox agents. Both primary and secondary alcohols are reactive, and preliminary mechanistic experiments indicate that reaction has an induction period. In addition to late-stage applicability, this operationally simple protocol offers convenient approach to γ-hydroxy sulfones, a valuable class of building blocks for synthesis.

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OH-14

Proizvodnja i karakterizacija nanočestica poli(etilen-tereftalata): sinteza, određivanje veličine i kontrola sastava

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Predstavljena je procedura za pripremu nanočestica poli(etilen-tereftalata) (nanoPET) primenom jonskog surfaktanta natarijum-dodecil sulfata (SDS), polazeći od tri različita materijala. Dva su bila lako dostupna, dok je treći morao biti sintetisan. Sintetisani proizvod je okarakterisan ^{1}H NMR spektroskopijom. Razvijena je metoda za proizvodnju nanoPET čestica koja uključuje detaljne korake za pouzdanost i ponovljivost postupka. Veličina dobijenih nanočestica određena je korišćenjem dinamičkog rasipanja svetlosti (DLS), što je omogućilo merenje raspodele veličine čestica u vodenim suspenzijama. Ovaj korak je bio ključan za potvrdu da nanočestice ispunjavaju željene kriterijume u pogledu veličine i uniformnosti. Dodatno, sprovedena su testiranja na prisustvo potencijalno toksičnih supstanci u cilju kontrole bezbednosti za buduće primene. Provera prisustva SDS-a izvršena je primenom ^{1}H NMR spektroskopije. Takođe, sadržaj antimona kvanitifikovan je pomoću ICP-OES-a.

Preparation and characterization of poly(ethylene terephthalate) nanoparticles: synthesis, size determination, and control of composition

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The procedure for the preparation of poly(ethylene terephthalate) nanoparticles (nanoPET) was developed using ionic surfactant sodium dodecyl sulphate with different starting materials. Two of the starting materials were readily available, while the third required synthesis. The synthesized product was characterized using ^{1}H NMR spectroscopy. A method for preparing nanoPET particles was developed with detailed steps to ensure consistency and reliability. The size of the resulting nanoparticles was determined using dynamic light scattering (DLS), providing measurements of particle size distribution in aqueous suspensions, verifying they met the desired specifications. To ensure the nanoparticles' safety for future applications, we tested for potentially toxic substances. Presence of residual SDS was confirmed using ^{1}H NMR spectroscopy. Additionally, antimony was quantified using ICP-OES, verifying the nanoparticles did not contain hazardous levels.

Acknowledgment: This project has received funding from the European Union, H2020-EU.3.1.1. Grant agreement n° 965173.

OH-15

Potpuna spektralna karakterizacija preizokalamendiola izolovanog iz etarskog ulja biljne vrste *Acorus calamus* L.

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Etarsko ulje iđirota (*Acorus calamus* L.), akorenonskog tipa, podvrgnuto je *dry-flash* hromatografiji, a zatim hromatografiji na koloni silika-gela, čime je izolovano nekoliko čistih seskviterpena. Među njima je bio i preizokalamendiol, što je inicijalno pretpostavljeno na osnovu masenog spektra i retencionog indeksa, a potvrda da se radi o njemu dobijena je detaljnom analizom 1D i 2D-NMR spektara ovog jedinjenja snimljenih u $CDCl_3$. Takođe, izvršena je potpuna spinska simulacija ^{1}H-NMR spektara, što je omogućilo dobijanje svih relevantnih NMR podataka (^{1}H-NMR hemijska pomeranja, ^{1}H-^{1}H konstante kuplovanja) po prvi put. Ovo je rezultiralo potvrdom njegove relativne konfiguracije, kao i određivanjem najstabilnije konformacije preizokalamendiola. Pored toga, dato je i poređenje ovako dobijenih podataka sa vrlo oskudnim i nepotpunim podacima iz literature.

Complete spectral characterization of preisocalamendiol isolated from the essential oil of the plant species *Acorus calamus* L.

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The acorenone-type essential oil of *Acorus calamus* L. underwent silica-gel dry-flash and subsequent column chromatographies, leading to the isolation of several pure sesquiterpenoids, including preisocalamendiol, one of the most abundant components. Identification of preisocalamendiol was initially tentative, based on mass spectrum and retention index comparison with literature data, and later confirmed through complete assignment of its ^{1}H and ^{13}C NMR spectra, recorded in $CDCl_3$ (1D and 2D NMR). Spin simulation of the ^{1}H NMR spectra was also conducted, providing all relevant NMR data (^{1}H NMR chemical shifts, ^{1}H-^{1}H coupling constants) for the first time. This allowed for confirmation of its relative configuration and determination of the most stable conformation of preisocalamendiol. Additionally, comparison of the obtained data with previously reported, incomplete data was organized into tables for clarity.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (No. contract 451-03-66/2024-03/200124 and 451-03-65/2024-03/200124).

Teorijska hemija

Theoretical Chemistry

TH-1

Tautomerne preferencije derivata 5-benzilidenbarbiturne kiseline: eksperimentalno i kvantnohemijsko proučavanje

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Barbiturna kiselina i njeni sintetički derivati privlače veliku pažnju zbog svojih jedinstvenih strukturnih svojstava i značajne tehnološke i farmaceutske upotrebe. Spektrofotometrijskom titracijom u vodenom rastvoru određene su p*K*a vrednosti derivata 5-benzilidenbarbiturne kiseline (5-BBA) sa najjačim elektron-donorskim supstituentom u ispitivanoj seriji. Primetno visoka vrednost pK_{a3} (12,27±0,02) sugeriše da u rastvoru preovlađuje triketo oblik. Osim toga, ^{13}C NMR analiza u DMSO-*d6* potvrdila je triketo oblik kao dominantnu tautomernu vrstu. Kvantno hemijski proračuni korišćenjem MP2/6-311G(d,p) metode potvrdili su da je triketo oblik najstabilniji tautomer 5-BBA. Proračuni su takođe pokazali da su diketo i monoketo tautomeri destabilizovani za 15,4-20,6 kcal/mol i 32,5-35,8 kcal/mol, respektivno.

The tautomeric preferences of 5-benzylidenebarbituric acid derivatives: experimental and quantum chemical studies

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Barbituric acid and its synthetic derivatives are garnering major attention due to their unique structural properties and significant technological and pharmaceutical uses. The p*K*a values of 5-benzylidenebarbituric acid (5-BBA) derivative with the strongest electron-donating substituent in the series were determined by spectrophotometric titration in an aqueous solution. The notably high pK_{a3} value (12.27±0.02) suggests that triketo form predominates in solution. Furthermore, ^{13}C NMR analysis in DMSO-d_6 confirmed the triketo form as the dominant tautomeric species. Quantum chemical calculations using the MP2/6-311G(d,p) method confirmed the triketo form as the most stable tautomer of 5-BBA. The calculations also showed that the diketo and monoketo tautomers are destabilized by 15.4-20.6 kcal/mol and 32.5-35.8 kcal/mol, respectively.

Acknowledgment: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract number: 451-03-65/2024/03 and 451-03-66/2024-03/200168).

TH-2

Mehanizmi supstitucije halogena tetrazolatnim jonom

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Reakcije nukleofilne aromatične supstitucije (S_NAr), zbog njihove široke primene, su predmet istraživanja više od jednog veka. Dugi niz godina, najprihvaćenije mišljenje je bilo da se većina ovih reakcija odigrava iz dva koraka, preko nearomatičnog Majzenhajmerovog kompleksa. Zadnjih godina publikovano je više radova u kojima su navedeni primeri reakcija koje se najverovatnije odigravaju po koncertovanom mehanizmu (cS_NAr) i na taj način je dovedena u pitanje ranija tvrdnja da „koncertovane reakcije predstavljaju izuzetak a ne pravilo“.[1] U ovom radu analizirani su mehanizmi reakcije 5-brom-2-nitrobenzotrifluorida i kalijumove soli 5-metil-1*H*-tetrazola. Geometrije stacionarnih tačaka, termohemijske korekcije kao i solvatacione korekcije su određene primenom ωB97X-D4 hibridnog funkcionala gustine uz upotrebu def2-TZVP(-f) bazisnog skupa. Energije stacionarnih tačaka su izračunate upotrebom DLPNO-CCSD(T) metode.

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Mechanisms of halogen substitution by a tetrazolate ion

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Nucleophilic aromatic substitutions (S_NAr) have been an attractive research field for over a century due to their wide applications. The long-accepted mechanism involved a two-stage process that featured a non-aromatic Meisenheimer complex. In recent years, several papers have been published in which examples of reactions that proceed in a concerted manner (cS_NAr) have been presented. Hence, the previous claim that "concerted reactions are the exception rather than the rule" has been challenged.[1] Herein, mechanisms of the reaction between 5-bromo-2-nitrobenzotrifluoride and a potassium salt of 5-methyl-1*H*-tetrazole have been studied. Geometries of the stationary points were optimized at ωB97X-D4/def2-TZVP(-f) level of theory. Thermochemical and solvation corrections were obtained at the same level of theory. Single-point energies of the stationary points were calculated by using the DLPNO-CCSD(T) method.

1. S. Rohrbach, A.J. Smith, J.H. Pang, D.L. Poole, T. Tuttle, S. Chiba, J.A. Murphy *Angew. Chem. Int. Ed.* **2019**, *58*, 16368.

Tekstilno inženjerstvo

Textile Engineering

TI-1

Uspostavljanje nove metode za merenje jačine i izduženja spiralno obmotanih elastomernih pređa

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Cilj ovog istraživanja je da uspostavi novu metodu za merenje prekidne sile i izduženja spiralno obmotanih elastomernih pređa. Standardna metoda za merenje mehaničkih karakteristika nije primenljiva na ovu vrstu pređa. Glavni razlog je to što je poliamid namotan na elastomer poput opruge, i u slučaju istezanja, elastičnost celog sistema je na nivou elastičnosti elastomera. Porastom sile istezanja smanjuje se prečnik spirale poliamidnog filamenta, stoga na elastomer deluju dve sile, sila istezanja i sila pritiska poliamida. Da bi se isključila ova mogućnost, merenja su rađena uz primenu nekoliko različitih sila predzatezanja, većih nego kod standardne metode. Ustanovljeno je da je odnos finoće formirane hibridne elastomer/poliamid pređe obrnuto srazmeran potrebnoj sili predzatezanja. Predložena metoda bi trebalo da se dodatno razvije u smeru određivanja tačne korelacije odnosa finoće elastomer/poliamid pređe i sile predzatezanja.

Development and validation of a new method for measuring mechanical strength and elongation of spirally covered elastomeric yarns

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The aim of this study was to highlight the possibility of using a new method for measuring mechanical strength and elongation of spirally covered elastomer/polyamide hybrid yarns. A standard approach to measuring mechanical characteristics cannot be applied to this type of yarn blend. The main reason is that polyamide filament in hybrid yarn behaves like a spring, with an elasticity that can be as high as the one of elastomer fiber. In addition, the diameter of the polyamide spiral is inversely proportional to the tension force. Consequently, two forces act simultaneously on elastomer fibers with the growth of tension force: a tension force and a pressure force from polyamide filament. To exclude this effect, measurements were done with several pretension forces, higher than standard ones. It was determined that the linear density ratio of polyamide/elastomer and pretension force are inversely proportional. The proposed method for measuring mechanical strengths and elongation of spirally covered elastomer/polyamide hybrid yarn must be further developed to provide a clearer correlation between the pretension force and linear density of the polyamide/elastomer yarn.

Zelena hemija

Green Chemistry

ZH-1

Optimalno dobijanje bioaktivnih ekstrakata iz otpadnog materijala vrsta roda *Mentha* natkritičnom ekstrakcijom

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Mentha piperita L. među mnogobrojnim biljkama predstavlja najzastupljeniju na Balkanskim prostorima, stoga je od interesa definisati optimalne uslove dobijanja bioaktivnih ekstrakata pri uslovima zelene hemije, natkritičnim ugljenik(IV)-oksidom sa prednošću dobijanja čistih ekstrakata. Kako se seme mente podrazumeva kao otpad u agroindustriji, iskoristivost lako dostupnog materijala kao značajne sirovine bioaktivnih komponenata još uvek neistraženo je od bitnog značaja. U cilju optimizacije dobijanja ekstrakata bogatih komponentama od značajne bioaktivnosti, natkritična ekstrakcija je primenjena pri više procesnih uslova od 10 MPa do 30MPa i od 40 do 50°C. Poređenje postignutih prinosa i sastava bioaktivnih komponenata u dobijenim ekstraktima pri različitim procesnim uslovima, omogućilo je definisanje opitmalnih uslova za dobijanje maksimalnih prinosa sa maksimalnim sadržajem biaoktivnih komponenti.

Achieving bioactive extracts from *Mentha* waste obtaining optimal conditions by SFE

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Among cultivate medicinal and aromatic herbs (*Mentha piperita* L.) is one of the most often grown herb in the Balkan region. Almost all part of the plant is used as a source of bioactive compounds, while seeds are excluded as agro-industrial waste and represent potential low cost material and an unvestigated source of bioactive compounds. Therefore, pepermint seeds are investgated in bioactive content by green solvent technology, supercritical CO_2 extraction. Supercritical CO_2 extraction reveal the most promising technique with the advantages to obtain extract free of organic solvents, much faster without necessity to employ the steps of further purification. In aim to enable extracts rich in bioactive compounds from peppermint seed waste, supercritical extraction was applied in several process conditions in range from 10MPa to 30 MPa and 40 to 50°C. The yields of extract as well as its composition were determined and analyzed at different process conditions of pressure and temperature following kinetics and mechanism of extraction. Optimization was obtained to define optimal conditions for maximal yield and most significant content of bioactive compounds.

ZH-2

Zeleni pristup za diverzifikaciju bakterijskih prirodnih proizvoda

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Bakterijski prirodni proizvodi (BPP) su od ključnog značaja u savremenoj medicini zahvaljujući svojoj efikasnosti i širokoj kliničkoj primeni, a pored toga imaju veliki potencijal i kao kandidati za razvoj novih lekova i za hemijske inovacije. Perspektiva korišćenja biokatalize za diverzifikaciju BPP-a predstavlja privlačnu alternativu totalnoj hemijskoj sintezi. Uprkos sve većem prihvatanju biokatalize kao ekološki prihvatljivog pristupa, značajan deo sekvenciranih genoma, povezanih sa metaboličkim putevima za biosintezu BNP-a i njihovim modifikacijskim enzimima, a kojima funkcija nije ispitana, ostaje uglavnom neiskorišćen. Ova studija ističe ispitivanje zelenih biotransformacija 1-hidroksifenazina i aktinomicina D, što može pomoći u pronalaženju novih strukturnih optimizacija bioaktivnih molekula i unapređenju razvoja lekova.

Green chemistry approaches for late-stage diversification of bacterial natural products

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Bacterial natural products (BNPs) are crucial in modern medicine due to their effectiveness and diverse applications, as evidenced by their extensive clinical use, and also as potential drug leads and for chemical innovation. The prospect of employing biocatalysis for late-stage diversification of BNPs presents an appealing alternative to total chemical synthesis. Despite the growing acceptance of biocatalysis as an environmentally friendly approach, a significant portion of orphan sequenced genomic data associated with metabolic pathways for BNP biosynthesis and their modifying enzymes remains largely untapped. This study highlights an examination of the green biotransformations to of 1-hydroxyphenazine and actinomycin D, which may aid in identifying novel structural optimizations of bioactive molecules and ultimately advancing drug development.

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ZH-3

Ambrosia artemisiifolia – biosorbent za sintetičke organske boje

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Ambrosia artemisiifolia je invazivna, korovska biljka, poznata po sposobnosti da izazove alergijske reakcije kod ljudi. Prema trenutno dostupnim podacima, koncentracija polena ambrozije u Srbiji 2022. bila je 9476 pz/m^3, čineći je dominantnom u poređenju sa ostalim alergenima. Zbog svoje rasprostranjenosti i štetnih uticaja, kontrolisanje ove biljke je od suštinskog značaja za smanjenje medicinskih, ekoloških i agronomskih problema. Cilj ovog istraživanja bio je ispitivanje efikasnosti ambrozije, kao biosorbenta, za sorpciju sintetičkih organskih boja Kongo crveno (KR), Brilijant Krezol plavo (BKP) i Toluidin plavo (TP) iz vodenih rastvora. Pri početnoj koncentraciji boje od 25 mg/L i kontaktnim vremenom od 1 h, određen je kapacitet sorpcije biosorbenta. Ispitivani biosorbent se pokazao kao efikasan u sorpciji boja KR, BKP i TP sa kapacitetom sorpcije od 4,0 mg/g, 4,24 mg/g i 44,1 mg/g. Za određivanje koncentracije boja korišćena je UV/Vis spektroskopija (NOVEL-102S, COLOLab Experts, Slovenia).

Ambrosia artemisiifolia – biosorbent for synthetic organic dyes

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Ambrosia artemisiifolia is an invasive weed known for its ability to trigger allergic reactions in humans. According to the currently available data, the concentration of Ambrosia pollen in Serbia in 2022 was 9476 grain/m^3, making it dominant compared to other allergens. Because of its prevalence and adverse effects, controlling this plant is essential to reduce medical, ecological, and agronomic problems. The objective of this research was to investigate the effectiveness of using Ambrosia as a biosorbent for the sorption of synthetic organic dyes Congo red (CR), Brilliant Cresyl blue (BCB) and Toluidine blue (TB) from aqueous solutions. At an initial dye concentration of 25 mg/L and a contact time of 1 h, the sorption capacity of the biosorbent was determined. The tested biosorbent proved to be effective in the sorption of CR, BCB and TB dyes with a sorption capacity of 4.0 mg/g, 4.24 mg/g and 44.1 mg/g. UV/Vis spectroscopy (NOVEL-102S, COLOLab Experts, Slovenia) was used to determine the dye concentrations.

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ZH-4

Optimizacija procesa umrežavanja ekološki prihvatljive nezasićene poliestarske smole

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Ekološki prihvatljive nezasićene poliestarske smole sa svojstvima sličnim komercijalnim smolama dobijenim iz petrohemijskih sirovina u fokusu su novijih istraživanja zasnovanih na principima održivog razvoja. Jedan od glavnih izazova pri umreževanju je pravilan izbor inicijator/aktivator sistema za reakciju umrežavanja. U ovom radu je ispitan uticaj odnosa metil etil keton peroksida kao inicijatora i kobalt oktoata kao aktivatora na svojstva sintetisane nezasićene poliestarske smole na bazi itakonata. Utvrđen je optimalan sastav sistema inicijator/aktivator od 1,5:1,0 mas.%, pri kom je umrežena smola najveće zatezne čvrstoće i stepena umreženja. Pokazano je da povećanjem udela inicijatora u datom sistemu inicijator/aktivator od samo 4 puta dolazi do desetostrukog povećanja vrednosti zatezne čvrstoće.

The curing process optimization of an eco-friendly unsaturated polyester resin

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Novel research guided by sustainable development principles aims to generate eco-friendly unsaturated polyester resins with comparable properties to commercial petroleum-based resins. One of the main challenges encountered is the proper selection of the initiator/activator system for the crosslinking reaction. In this research, the influence of the ratio of methyl ethyl ketone peroxide as an initiator and cobalt octoate as an activator on the properties of the synthesized itaconate based unsaturated polyester resin was studied. The optimal composition of the initiator/activator system was found to be 1.5:1.0 wt.%, at which the cured resin showed the highest tensile strength and degree of crosslinking. It was further shown that a fourfold increase of initiator in a given initiator/activator system resulted in increased value of tensile strength by an order of magnitude.

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ZH-5

Antimikrobna aktivnost novosintetisanih jonskih tečnosti sa karboksilatnim anjonima

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COVID-19 pandemija je ukazala na nedostatke postojećih metoda za dezinfekciju i sanitarnu zaštitu. Zbog toga je dizajniranje novih jedinjenja sa antibakterijskim delovanjem postalo izuzetno važno. Poznato je da jonske tečnosti pokazuju dobra antibakterijska svojstva i da one koje sadrže imidazolijum katjon poseduju jaču antimikrobnu aktivnost od ostalih. U ovom radu sintetisane su jonske tečnosti koje kao katjon sadrže 1-butil-3-metilimidazolijum jon i različite karboksilatne anjone: fenilacetat, benzoat i 4-metoksifenilacetat. Interakcije između katjona i anjona i fizičko-hemijska svojstva su razmatrani na osnovu izmerene gustine, viskoznosti i električne provodljivosti. Potom je ispitivana njihova antimikrobna aktivnost, kako bi razmotrili sinergističko delovanje između katjona i odabranih anjona, kao i povećanje antimikrobne aktivnosti u odnosu na čiste komponente.

Antimicrobial activity of newly synthesized ionic liquids with carboxylate anions

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The outbreak of the COVID-19 pandemic reinforced the importance of the synthesis and characterization of new antimicrobial substances. Designing new compounds, such as ionic liquids (ILs), that show antibacterial activities is very important. Most of the ILs show good antibacterial properties, but ILs that consist of the imidazolium cation were even more antibacterial than those in the positive control. In this work, ionic liquids were synthesized, formed by the combination of cation (1-butyl-3-methylimidazolium) and various carboxylate anions (phenylacetate, benzoate, and 4-methoxyphenylacetate). Interactions between cations and anions were discussed based on the measured density, viscosity, and electrical conductivity. The antimicrobial activity of ionic liquids based on 1-butyl-3-methylimidazolium cation and selected anions was tested for synergistic action and improved antimicrobial activity compared to pure components.

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ZH-6

Inhibicija korozije ugljeničnog čelika u 1 M HCl pomoću ekološki prihvatljivog inhibitora (Pančićeva omorika): kombinovanje eksperimentalnih i teorijskih metoda

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Etarsko ulje Pančićeve omorike analizirano je gasnom hromatografijom u kombinaciji sa masenom spektrometrijom (GC/MS). Eektrohemijska merenja su pokazala da u koncentaciji od 200 ppm ovaj zeleni inhibitor smanjuje brzinu korozije čelika sa značajnom efikasnošću od 93 % nakon 4 h. Polarizaciona mjerenja su pokazala da je etarsko ulje inhibitor mešovitog tipa. Inhibirana i neinhibirana površina čelika je analizirana skenirajućom elektronskom mikroskopijom (SEM), i merenjem kontaktnog ugla. Adsorpcija organskih aktivnih supstanci na površini čelika prati Lengmirovu adsorpcionu izotermu i rendgenska fotoelektronska spektroskopija (XPS) je pružila dublji uvid u mehanizam inhibicije korozije. Eksperimentalne studije su upotpunjene teorijskim proračunima.

Corrosion inhibition of carbon steel in 1 M HCl via environmentally friendly inhibitor (*Picea omorika*): Combining experimental and theoretical methods

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Picea omorika essential oil was analyzed by gas chromatography combined with mass spectrometry (GC/MS). Electrochemical measurements showed that this green inhibitor reduces the corrosion rate of steel with a significant efficiency of 93% after 4 h at a concentration of 200 ppm. Polarization measurements showed that the essential oil is a mixed type inhibitor. The inhibited and non-inhibited surface of the steel was analyzed by scanning electron microscopy (SEM) and contact angle measurements. X-ray photoelectron spectroscopy (XPS) provided a deeper insight into the mechanism of corrosion inhibition. The adsorption of organic active substances on the steel surface follows the Langmire adsorption isotherm. Experimental studies were completed with the theoretical studies.

ZH-7

Ispitivanje vodenih rastvora novosintetisane jonske tečnosti 1-butil-3-metilimidazolijum-2-hidroksi-2-fenilacetata

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Jedna od najperspektivnijih oblasti istraživanja novih zelenih tehnologija je primena zelenih rastvarača, jonskih tečnosti. One su neisparljive, nezapaljive i termički stabilne, dobro rastvaraju veliki broj organskih i neorganskih supstanci i relativno su zahvalne za proizvodnju. Zbog svojih jedinstvenih svojstava, primenjuju se u mnogim oblastima hemije, tehnologije i farmaceutske industrije. U ovom radu je sintetisana jonska tečnost 1-butil-3-metilimidazolijum-2-hidroksi-2-fenilacetat. Za sintezu je korišćena bademova kiselina koja ima bakteriostatičko dejstvo. Fizičko-hemijska svojstva vodenih rastvora ove jonske tečnosti su razmatrana na osnovu izmerene gustine i viskoznosti. Potom je ispitivana i antimikrobna aktivnost tih rastvora.

Examination of aqueous solutions of the newly synthesized ionic liquid 1-butyl-3-methylimidazolium 2-hydroxy-2-phenylacetate

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One of the most promising areas of research into new green technologies is the application of green solvents, like ionic liquids. These are non-volatile, non-flammable, and thermally stable, which dissolve well a large number of organic and inorganic substances and are relatively easy to produce. Due to their unique properties, these liquids are used in many fields of chemistry, technology, and pharmaceutical industry. In this work, the ionic liquid 1-butyl-3-methylimidazolium 2-hydroxy-2-phenylacetate was synthesized. Mandelic acid, which has bacteriostatic properties, was used for the synthesis. The physicochemical properties of aqueous solution of the ionic liquid were discussed based on the measured density and viscosity. The antimicrobial activity of the ionic liquid was investigated.

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ZH-8

PdZn-ZnO bimetalni katalizator sintetisan u gasovitoj fazi u jednom koraku za redukciju nitroarenskih zagađivača

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Nitroareni su grupa jedinjenja koja se frekventno koristi u različitim industrijama. Kada se nađu u prirodi, predstavljaju veoma toksične i izdržljive zagađivače. U okviru ovog istraživanja, predstavljamo novu metodu, zasnovanu na sintezi u gasovitoj fazi, u jednom koraku, nazvanu sinteza putem organo-metalnih para, kojom je sintetisan PdZn-ZnO bimetalni katalizator. Bez postsintetskih obrada, PdZn-ZnO katalizator je iskorišćen za redukciju nitroarenskih zagađivača, transformišući ih u manje toksične aniline, koji pronalaze naširoku upotrebu u hemijskoj industriji. Svi supstrati su prevedeni u proizvode u visokim prinosima i pokazana je odlična mogućnost reciklaže u osam uzastopnih katalitičkih ciklusa.

One-step gas-phase synthesis of PdZn-ZnO bimetallic catalyst for reduction of nitroarene pollutants

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Nitroarenes are a group of compounds which is frequently used in various industries. When found in the environment, they present a group of persistent and highly toxic pollutants. In this contribution, we present a novel, one-step gas phase-based method, namely metal-organic chemical vapor synthesis (MOCVS), by which a PdZn-ZnO bimetallic catalytic system was synthesized. The as-synthesized PdZn-ZnO catalyst was utilized for the reduction of nitroarene pollutants, converting them into less toxic anilines, which find broad industrial application. All of the substrates were converted in high yields and excellent recyclability potential was shown, in eight consecutive catalytic cycles.

ZH-9

Zelena hemija: trendovi u Srbiji (2014-2024)

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Zelena hemija je postala značajno polje nauke usled ekoloških izazova, potrebe za smanjenjem zdravstvenih rizika od opasnih hemikalija, regulatornog pritiska i ekonomskih benefita. Ovaj rad analizira trend naučnih publikacija iz zelene hemije u Srbiji u poslednjih 10 godina. Podaci su prikupljeni sa platforme Scopus za period 2014.-2024. godine, za Srbiju. Ukupno je prikupljeno 96 zapisa. Rezultati ukazuju da zelena hemija sve više dobija značaj u različitim oblastima znanja u Srbiji, sa najvećim procentima u hemiji (22,1%), biohemiji, genetici i molekularnoj biologiji (19,1%) i životnoj sredini (13,6%). Broj publikacija je dostigao prvi pik 2018. godine, zatim opao u narednim godinama verovatno zbog pandemije COVID-19, i ponovo dostigao još viši pik 2022. godine. Što se tiče vrsta publikacija, većinu čine članci (90,6%) i pregledni radovi (7,3%), pri čemu je više od polovine povezano sa Univerzitetom u Beogradu (56 zapisa). Dobijeni rezultati ukazuju da zelena hemija u Srbiji postaje sve prepoznatljivija među istraživačima poslednjih godina, i može se pretpostaviti da će ovaj trend nastaviti da raste.

Green chemistry: trends in Serbia (2014-2024)

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Green chemistry has emerged as a significant field in science in recent years due to environmental concerns, the need to mitigate chemicals health hazards, regulatory pressure, and economic benefits. This paper analyzes the trend of scientific publications on green chemistry in Serbia over the last 10 years. For this purpose, data were retrieved from the Scopus through a search for the study period, 2014-2024, limited to Serbia. In total, 96 records were retrieved. The results showed that green chemistry is increasingly prevalent in different fields of knowledge in Serbia, with the highest percentages in chemistry (22.1%), biochemistry, genetics, and molecular biology (19.1%), environmental science (13.6%), The number of publications first peaked in 2018, decreasing in subsequent years probably due to the COVID-19 pandemic, and then peaking again even more in 2022. Concerning the type of publication, most publications are Articles (90.6%) and Reviews (7.3%), with more than half affiliated with the University of Belgrade (56 documents). The obtained results indicate that the green chemistry in Serbia is becoming more recognizable among researchers in recent years, and it can be assumed that this interest will continue to trend upwards.

ZH-10

Zelena ekstrakcija: termoreverzibilni vodeni dvofazni sistemi za direktno izolovanje partenolida iz biomase

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Termoreverzibilni vodeni bifazni sistemi (VBS) predstavljaju jedinstvene sisteme za ekstrakciju i prečišćavanje osetljivih biomolekula. Fokus ovog istraživanja je na razvoju i optimizaciji zelene metode ekstrakcije visoko potentnog bioaktivnog jedineja – partenolida iz biomase. Zelena ekstrakciona metoda je zasnovana na termoreverzibilnim VBS koji se sastoje od biokompatibilnih materijala: holinijumskih jonskih tečnosti i kopolimera Pluronic 17R4. Uticaj temperature na ponašanje VBS je proučavan u cilju optimizovanja ekstrakcionih parametera, a radi dobijanja visokih stepena ekstrakcije sa minimalnom potrošnjom ektragenasa. Takođe ispitan je i uticaj VBS-a na veličinu formiranih polimernih micela u toku ekstrakcije. Pokazan je potencijal VBS-a kao ekološki prihvatljive zamene za toksične organske rastvarače za izolovanje bioaktivnih jedinjenja iz biomase.

Green extraction: thermoreversible aqueous two-phase systems for direct isolation of parthenolide from biomass

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Thermoreversible aqueous biphasic systems (ABS) represent unique systems for the extraction and purification of sensitive biomolecules. The focus of this research is on the development and optimization of a green extraction method for the highly potent bioactive compound – parthenolide from biomass. The green extraction method is based on thermoreversible ABS consisting of biocompatible materials: cholinium ionic liquids and Pluronic 17R4 copolymers. The influence of temperature on the behavior of ABS was studied to optimize extraction parameters, aiming to achieve high extraction yields with minimal extragens consumption. Additionally, the effect of ABS on the size of formed polymer micelles during extraction was investigated. The potential of VBS as an environmentally acceptable substitute for toxic organic solvents for the isolation of bioactive compounds from biomass has been demonstrated.

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Jednostavna sinteza različito supstituisanih 2-piridona u čvrstoj fazi

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U ovom radu, predstavljamo jednostavan metod za sintezu različito supstituisanih 2-piridona polazeći iz lako dostupnih materijala **1** i **2**, na (15% Cs_2CO_3) silika-gelu kao čvrstoj fazi i u maloj reakcionoj bočici kao jedinoj aparaturi. Metod karakteriše nekorišćenje rastvarača i drugih reagenasa, lako praćenje standardnim analitičkim tehnikama, visoka ekonomičnost atoma, ekološki neškodljiv EtOH kao jedini sporedni proizvod, ušteda električne energije jer se zagrevanje, ako je potrebno, obavlja u laboratorijskoj sušnici, tolerancija različitih funkcionalnih grupa, sintetički korisni konjugovani dieni **3** kao jedini intermedijeri, i sinteza na gramskoj skali.

Simple, solid-state synthesis of variously substituted 2-pyridones

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We present a simple method for the synthesis of variously substituted 2-pyridones starting from readily available materials **1** and **2**, using (15% Cs_2CO_3) silica gel as a solid phase, and a small reaction vial as the only equipment. The method features no use of solvents and other reagents, easy monitoring by standard analytical techniques, high atom economy, environmentally friendly EtOH as the only by-product, no additional energy consumption since heating, if necessary, is done in a laboratory oven, different functional group tolerance, synthetically useful conjugated dienes **3** as only intermediates, and gram-scale synthesis.

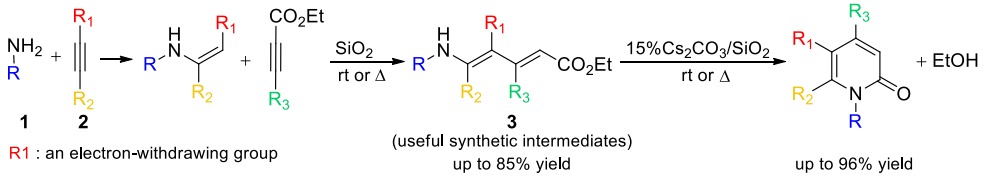

Figure 1. Synthesis of variously substituted 2-pyridones

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Zelena ekstrakcija bioaktivnih pigmenata iz spiruline primenom prirodnih eutektičkih smeša

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Prirodni pigmenti dobijeni iz alge Spirulina su jedinjenja sa visokom antioksidativnom i antiinflamatornim dejstvom i imaju značajnu primenu u prehrambenoj, farmaceutskoj i kozmetčkoj industriji. Tradicionalne metode ekstrakcije koje se koriste za izolovanje ovih pigmenata uključuju upotrebu organskih rastvarača koji imaju negativan uticaj na životnu sredinu. Cilj ovog rada je izolovanje pigmenata iz spiruline primenom prirodnih eutektičkih smeša (NADES) u cilju zamene tokičnih organskih rastvarača sa alternativnim zelenim rastvaračima. Sintetisano je 10 NADESa baziranih holinijum-hloridu, betainu, glicerolu, i šećerima. Antioksidativni kapacitet ekstraktovanih pigmenata je procenjen korišćenjem DPPH testa. Najviši antioksidativni kapacitet pigmenata ekstraktovanih iz spiruline dobijen je primenom NADES na bazi betaina i glicerola.

Green extraction of bioactive pigments from spirulina using natural deep eutectic solvents

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Natural pigments derived from the alga Spirulina are compounds with high antioxidant and anti-inflammatory effects, and they have significant applications in the food, pharmaceutical, and cosmetic industries. Traditional extraction methods used to isolate these pigments involve the use of organic solvents, which have a negative impact on the environment. The aim of this study is to isolate pigments from Spirulina using natural deep eutectic solvents (NADES) to replace toxic organic solvents with alternative green solvents. Ten NADESs were synthesized based on choline chloride, betaine, glycerol and sugars. The antioxidant capacity of extracted pigments was evaluated using DPPH test. The highest antioxidative capacity of pigments extracted from spirulina was obtained using NADES based on betaine and glycerol.