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Serbian Chemical Society

58. Savetovanje Srpskog hemijskog društva

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Ova knjiga sadrži kratke izvode
četiri plenarna predavanja (PP),
dva predavanja dobitnika Medalje SHD (MP),
četiri predavanja po pozivu (PPP),
sto četrnaest saopštenja (obima jedna stranica) i
osam radova (obima od najmanje četiri stranice),
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This book contains abstracts of
four plenary lectures (PP),
two lectures of SCS Medal awardees (MP),
four invited lectures (PPP),
one hundred and fourteen abstracts and
eight papers accepted for presentation at
the 58th Meeting of the Serbian Chemical Society.

SADRŽAJ/CONTENTS

Plenarna predavanja
Plenary lectures

Predavanja dobitnika Medalje SHD
Lectures of SCS Medal awardees

Predavanja po pozivu
Invited lectures

Saopštenja

Contributions

Analitička hemija/Analytical Chemistry

Biohemija/Biochemistry

Elektrohemija/Electrochemistry

Zelena hemija/Green Chemistry

Medicinska hemija/Medicinal Chemistry

Nastava i istorija hemije/Education in and History of Chemistry

Nauka o materijalima/Material Science

Neorganska hemija/Inorganic Chemistry

Organska hemija/ Organic Chemistry

Tekstilno inženjerstvo/Textile Engineering

Teorijska hemija/Theoretical Chemistry

Fizička hemija/Physical Chemistry

Hemija životne sredine/Environmental Chemistry

Hemija i tehnologija makromolekula/Chemistry and Technology of Macromolecules

Hemija i tehnologija hrane/Chemistry and Technology of Food

Hemijsko inženjerstvo/Chemical Engineering

Knjiga radova/Proceedings

Analitička hemija/Analytical Chemistry

Elektrohemija/Electrochemistry

Hemijsko inženjerstvo/Chemical Engineering

Tekstilno inženjerstvo/Textile Engineering

Hemija životne sredine/Environmental Chemistry

KRATKI IZVODI RADOVA

Short abstracts

Plenarna predavanja

Plenary Lectures

PP-1

ТОПОЛОШКИ ИНДЕКСИ

Иван Гутман
Природно-математички факултет, Универзитет у Крагујевцу, Радоја Домановића 12, Крагујевац

Према IUPAC-овој дефиницији [Pure Appl. Chem. 69 (1997) 1137]:

Тополошки индекс је бројчана вредност придружена хемијској конституцији (која служи) за корелацију хемијске структуре са различитим физичким особинама, хемијској реактивности или биолошкој активности.

У савременој математичкој хемији постоје два основна правца истраживања везана за тополошке индексе

– одређивање њихових математичких особина и математичких веза међу њима, и

– тестирање њихове применљивости за предвиђање физичко-хемијских, фармаколошких, токсиколошких и других особина појединих класа једињења.

У предавању ће бити описани основни појмови у вези тополошких индекса, са нагласком на њиховој примени. На почетку ћемо се подсетити на постојање и примене индекса у најразличитијим областима људске делатности, и на разлоге зашто се они употребљавају.

Тополошки индекси се конструишу применом математичке теорије графова, конкретно преко такозваног „молекулског графа“. Биће укратко изложени неопходни појмови о графовима, а затим приказани неки најпопуларнији тополошки индекси. У оквиру тога биће поменути и неки од предавачевих доприноса.

На крају ће бити укратко описане технике помоћу којих се тополошки индекси примењују при решавању конкретних проблема, а биће наведени и неки комерцијано значајни резултати.

PP-2

Electrolyte solutions: the case of ionic liquids

Marija Bešter-Rogač
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Electrolyte solutions are ubiquitous and solvated ions have great influence on many (naturally) occurring processes. Charged species also affect the mechanism and thus the kinetics of many chemical reactions. Therefore, ionic systems are still the subject of many experimental and theoretical studies.

In recent decades, ionic liquids (ILs) have attracted attention due to their suitability as systems for a variety of applications. However, the growing number of studies dealing with the physicochemical properties of ILs in their pure state has been extended to investigations of their mixtures with molecular co-solvents. It turned out that ILs in solutions can serve as excellent (electrolytes) model systems because they exist in a variety of structures and many of them are fully miscible with different solvents, while the solubility of "classical" electrolytes is limited. However, the structures of ions also play a very important role in solutions, since a wide variety of interactions between ions and solvents can occur [1].

Theories for concentrated electrolyte solutions are still lacking. While for "classical" electrolytes the limited solubility could be the reason for the lower effort in studying concentrated solutions, for ILs the whole concentration range from pure solvent to pure electrolyte can be covered. Despite many studies, the observed maximum in electrical conductivity [2] is still not well described and remains a challenge for the future.

Therefore, ILs can serve as excellent model systems for the study of ionic interactions, hydrophobic effects, and specific ion effects and help us to extend and deepen the knowledge of electrolytes and surfactants in aqueous and non-aqueous solutions.

1. M. Bešter-Rogač, M.V. Fedotova, S.E. Kruchinin, M. Klähn. Phys. Chem. Chem. Phys. 2016, 18, 28594.

2. M. Bešter-Rogač, Acta Chim. Slov. 2020, 67, 1.

PP-3

125 година Српског хемијског друштва

Снежана Бојовић
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Српско хемијско друштво основао је Марко Леко са још десет београдских хемичара 1897. године. До Првог светског рата Друштво је било најактивније у првих десет година, док је на његовом челу био Марко Леко који је организовао састанке и уређивао први часопис „Записници Српског хемијског друштва“. Касније се број састанака проредио а рат је прекинуо рад Друштва.

Друштво је обновило рад 1927. године под именом **Хемијско друштво Краљевине Срба, Хрвата и Словенаца**. Поред редовних једномесечних састанака једанпут годишње држана је Главна годишња скупштина на којој је подношен извештај о раду Друштва. Године 1930. почео је да излази часопис Друштва *Гласник Хемијског друштва Краљевине Југославије.*

После Другог светског рата друштво је 1945. г**о**дине обновило рад под именом **Српско хемијско друштво**. Од педесетих година 20. века Друштво оснива подружнице у већим градовима, секције за различите обалласти хемије и саветовања која представљају преглед научне и стручне активности у свим гранама хемије.

Поред *Гласника,* који од 1984. излази на енглеском језику, *Journal of the Serbian Chemical Society*, од 1950. године излази стручни часопис *Хемјски преглед.*

За протеклих 125 година Друштво није променило најважније задатке и циљеве зацртане 1897. године, али је развило многе нове делатности из којих се може сагледати развој и значај Српског хемијског друштва.

Кључне речи: Српско хемијско друштво, Марко Леко, Гласник Српског хемијског друштва, Хемијски преглед

125 years of Serbian Chemical Society

Snežana Bojović
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The **Serbian Chemical Society** was founded in 1897 by Marko Leko and ten chemists from Belgrade. The Society was very active in the first decade after the establishment, while led by Marko Leko, who was organizing meetings and editing the first magazine “*Serbian Chemical Society Chronicles*”. In the following period the number of meetings

decreased and the Society stopped working with the commencement of the First World War.

The Society re-launched activities in 1927 under the new name – ***The Kingdom of Serbs, Croats and Slovenes Chemical Society***. Beside regular monthly meetings, the General Assembly meeting was organised once a year, with the aim of presenting the report on the activities of the Society. In 1930 the magazine "*Journal of the Kingdom of Yugoslavia Chemical Society*" was published.

After the Second World War, in 1945, the Society reactivated its work once again, under the name ***Serbian Chemical Society***. Starting in 1950', branch offices were being established in big cities, with sections from different chemistry and consulting fields, presenting reviews of scientific and expert activities in all chemistry branches.

Starting from 1984, "*Journal of the Serbian Chemical Society*" was being issued in English, while in 1950 another professional journal, "*Chemical review",* was published.
During 125 years of existence, the Society maintained all main activities and goals set in 1897, but extended its scope of work in order to better present the development and importance of the Serbian Chemical Society.

PP-4

"Anti-aging" efekti vodonik sulfida: da li fontana mladosti miriše na sumpor

Miloš R. Filipović
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Za održavanje života, priroda koristi limitarani set hemijskih reakcija od kojih je hemija sumpora posebno zastupljena u kontroli ununtarćelijskih redoks procesa. Vodonik sulfid (H_2S) je jedan od najjednostavnijih molekula koji sadrže sumpor, a koji je nađen u ćelijama. Od kako je prvi put prijavljena njegova potencijalna fiziološka uloga, literatura koja se bavi biološkim ulogama H_2S vrtoglavo raste. Vrlo brzo se H_2S pridružio azot monoksidu i ugljen monoksidu kao treći gasni transmitter. Nedavno je H_2S-u pripisana i uloga u prevenciji starenja. Međutim, mehanistička objašnjenja za sve ove biološke uloge vodonik sulfida su još uvek predmet aktivnog istraživanja. U ovom predavanju će akcenat biti na tri različite reakcije kojima H_2S kontroliše ćelijsku funkciju: (i) reakcija sa reaktivnim kiseoničnim i azotovim vrstama, (ii) reakcija sa metalnim centrima i verovatno najbitnija (iii) reakcija sa proteinima, zvana persulfidacija. Iako sadrže samo jedan sumporov atom više od klasičnih tiola, persulfidi su mnogo reaktivniji i nije ih lako selektivno obeležiti. Nove metode za obeležavanje, razvijene u našoj laboratoriji, pomogle su rasvetljavanju fizioloških uloga H_2S. Persulfidacija je evolutivno konzervirana posttranslaciona modifikacija koju ćelije koriste kao zaštitni mehanizam od hiperoksidacije cisteinskih ostataka. Sa starenjem, ćelijski kapacitet da proizvodi persulfide opada kod svih bioloških vrsta, ali to se može predupreditи farmakološkim donorima H_2S ili kalorijskom restrikcijom, što za rezultat ima produžetak života i bolju rezistentnost organizma na oksidativni stress.

Anti-aging effects of hydrogen sulfide: does the fountain of youth stink of sulfur

Milos R. Filipovic
Leibniz Institute for Analytical Sciences, ISAS, e.V., Dortmund, Germany

In order to maintain life, nature actually uses limited number of chemical reactions, one of which is sulfur-based chemistry, mainly exploited for the control of intracellular redox homeostasis and redox-based signalling. Hydrogen sulfide (H_2S) is one of the simplest sulfur-containing molecules found in the cells and since the first report of its potential physiological role, there has been a growing literature on the subject of H_2S signalling. Very fast, H_2S joined the other two gases, NO and CO, as the third gasotransmitter. Recently, H_2S emerged as an anti-aging molecule with strong therapeutic potential. However, the mechanistic explanations for such plethora of biological effects are lacking. This talk will discuss three main reactions through which H_2S controls cellular functions: (i) reaction with/scavenging of reactive oxygen and reactive nitrogen species, (ii) binding to and/or subsequent redox reactions with metal centers and (iii) reaction with proteins, called persulfidation. Being "one sulfur away" from thiols, persulfides are not easy to

monitor. However, recent developments of persulfide labelling techniques have started unravelling the role of this modification in (patho)physiology. Persulfidation is an evolutionarily conserved modification and employed by cells to prevent irreversible cysteine overoxidation preserving protein function. However, an age-associated decline in persulfidation is conserved across evolutionary boundaries. Accordingly, dietary or pharmacological interventions to increase persulfidation associate with increased longevity and improved capacity to cope with stress stimuli.

Predavanja dobitnika Medalje SHD

Lectures of SCS Medal awardees

Selektivno transformisanje amidne veze: specifičnosti i značaj

Slobodan D. Petrović

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Prikazane su različite mogućnosti transformisanja amidne veze. Postupak selektivnog transformisanja amidne veze može biti od velike važnosti pri konverziji prirodnog u polusintetske peniciline ili pri sintezi komercijalno važnih viših supstituisanih analoga amida. Ovo poslednje je značajno za sintetičko dobijanje raznih pesticidnih jedinjenja. Uspešna primena ovih transformacija zahteva seletivno alkilovanje amidne veze koje se može izvesti na N- ili O-atomu. Izloženi su efekti primene različitih agenasa za direktno ili selektivno alkilovanje amidne veze, posebno kod odgovarajućih N-monosupstituisanih amida kao model supstance kao i kod prirodnog benzilpenicilina. Analizirane su reakcije alkilovanja pri neutralnim, baznim i uslovima međufazne katalize.

Selective transformation of the amide bond: specificity and importance

Slobodan D. Petrović

University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

The different possibilities for the amide bond transformation were reviewed. The procedure of the selective transformation of the amide bond can be of a great importance in the conversion of natural into semisynthetic penicillins or in the synthesis of commercially important higher substituted analogs of amides. The latter is significant for the synthetic preparation of various pesticide compounds. The successful application of these transformations requires selective alkylation attack of amide bond, which can be done at the N- or O-atom. The effects of application of different agents for the direct or selective alkylation of the amide bond, especially on the corresponding N-monosubstituted amides as model substances, as well as natural benzylpenicillin are also discussed. The alkylation reactions under neutral basic and phase-transfer conditions were analyzed.

MP-2

Primenjena spektroskopija

Vlatka E. Vajs
Univerzitet u Beogradu, Hemijski fakultet, IHTM, Beograd, Srbja

Tema ovog predavanja je primena spektroskopije kroz primere iz prakse Centra za instrumentalnu analizu (Hemijski fakultet, Beograd i Centar za hemiju, IHTM Beograd).

Centar za instrumentalnu analizu (CIA) jedinstven je u ovom delu Evrope po opremljenosti i kadrovima. Raspolaže aparatima, za snimanje NMR, MS, IR, UV-Vis spektara, tečnim i gasnim hromatografima, kao i elementarnom mikroanalizom, na kojima rade i interpretiraju rezultate veoma stručni operateri.

Tokom dugogodišnjeg rada u nauci i nastavi, kao i kroz saradnju sa drugim institucijama i privredom (MUP-om , Agencijom za lekove, Hemofarmom, Galenikom, Organizacijom za zabranu hemijskog oružja itd.), analizirani su mnogobrojni uzorci.

Za ovo predavanje izabrani su najinteresantniji primeri, koji pokazuju kako se kombinacijom hromatografskih i spektroskopskih metoda mogu dešifrovati uzorci nepoznatog sastava.

Analize sirovih ekstrakata endemskog i lekovitog bilja, lažnih lekova kao i OPCW testovi bojnih otrova, pokazuju na koji način se pomoću spektara dolazi do dragocenih, široko primenjivih rezultata.

Applied spectroscopy

Vlatka E. Vajs
University of Belgrade Faculty for Chemistry, ICTM , Belgrade, Serbia

This lecture is concerned with the application of spectroscopy through examples from the Center for instrumental analysis (Faculty for Chemistry, Belgrade and Center for Chemistry ICTM Belgrade).

Center for instrumental analysis (CIA) is unique in this part of Europe with its sophisticated equipment (IR, NMR, MS, LC/ESI MS TOF, GC/MS and microanalysis) operated by highly trained staff.

A variety of samples have been analysed during a long standing scientific work and through collaboration with other institutions and industry (Ministry for home affairs, Drug agency, OPCW, Hemofarm, Galenika..).

The examples have been chosen to illustrate and explain how to solve, decode, unknown samples using combination of chromatographic and spectroscopic methods.
Analysis of endemic and medicinal plant crude extracts, drugs, false drugs as well as OPCW tests of chemical weapons, have been selected as examples to demonstrate how by interpretation of spectra one can reach valuable and widely applicable results.

Predavanja po pozivu

Invited Lectures

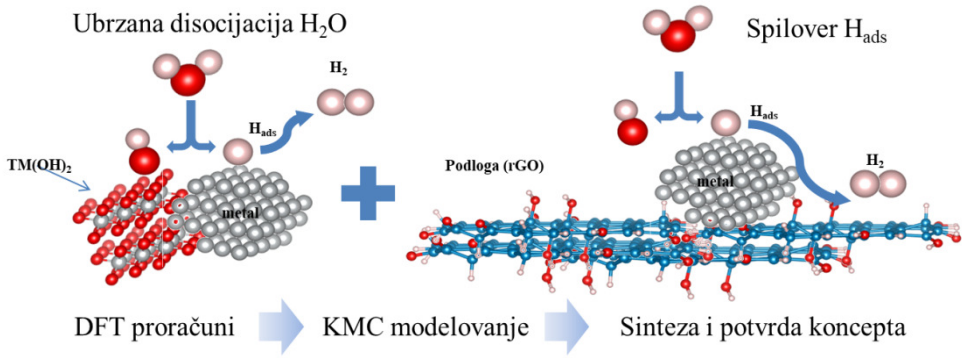
PPP-1

Sinergija teorije i eksperimenta u razvoju novih materijala za energetske izazove budućnosti

Igor A. Pašti[1]

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

Razvoj efikasnih tehnologija za konverziju i skladištenje energije jedno je od gorućih pitanja savremenog društva. Podsticaj za prelazak sa tehnologija zavisnih od fosilnih goriva na nove održive je veoma snažan, ali u ovoj tranziciji ne postoji jedinstveno rešenje. Očekuje se da će elektrohemija i nauka o materijalima igrati ključnu ulogu u ovom procesu nudeći različita rešenja – baterije, gorivne ćelije, superkondenzatore, fotonaponske uređaje i druga. Nema sumnje da su zadaci sa kojima se naučna zajednica suočava veoma teški. Međutim, novi alati, poput teorijskih i računskih metoda razvijenih u poslednje dve decenije, praćeni povećanjem snage računara, mogli bi biti od velike pomoći u potrazi za novim materijalima za konverziju energije. Navešćemo nekoliko primera uspešnog razvoja novih elektrokatalitičkih materijala za proizvodnju zelenog vodonika – jednog od stubova tranzicije ka zelenoj energiji. Posebno ćemo se usredsrediti na racionalni dizajn novih elektroda za evoluciju vodonika korišćenjem tandemskih procesa na kompleksnim višefaznim elektrodama. Istraživanje kombinuje proračune na bazi teorije funkcionala gustine i kinetičko Monte Karlo modeliranje sa rigoroznom elektrohemijskom sintezom i testiranjem novih elektrokatalizatora za proizvodnju vodonika u procesu alkalne elektrolize – strategiju razvijenu u okviru projekta RatioCAT (Slika 1). Ovaj pristup ne samo da predstavlja novu paradigmu u proizvodnji vodonika, već nudi i nove materijale sa superiornim performansama i značajno smanjuje troškove proizvodnje zelenog vodonika.



Slika 1. Koncept projekta RatioCAT: ubrzanje disocijacije H_2O i spilovera vodonika za efikasnu proizvodnju H_2.

The synergy of theory and experiment in the development of new materials for the energy challenges of the future

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The development of efficient energy conversion and storage technologies is one of the burning issues of modern society. The impetus to switch from fossil fuel-dependent technologies to new sustainable ones is very strong but there is no single solution in this transition. Electrochemistry and Materials Science are expected to play key roles in this process offering various solutions – batteries, fuel cells, supercapacitors, photovoltaics, and others. There is no doubt that the tasks the scientific community is facing are very difficult. However, new tools, like theoretical and computational methods developed in the last two decades, and followed by the increase in computer power, could be of great help in the search for new materials for energy conversion. We shall provide several examples of the successful development of novel electrocatalytic materials for green hydrogen production – one of the pillars of the green energy transition. In particular, we shall focus on the rational design of new electrodes for hydrogen evolution, employing a tandem interfacial process at complex electrode interfaces. The work combines Density Functional Theory calculations and Kinetic Monte Carlo modelling with rigorous electrochemical synthesis and testing of novel electrocatalysts for hydrogen production in the alkaline electrolysis process – the strategy developed within the RatioCAT project (Figure 1). This approach not only shifts the current paradigm in hydrogen production but also offers novel materials with superior performance and significantly lowers green hydrogen production costs.

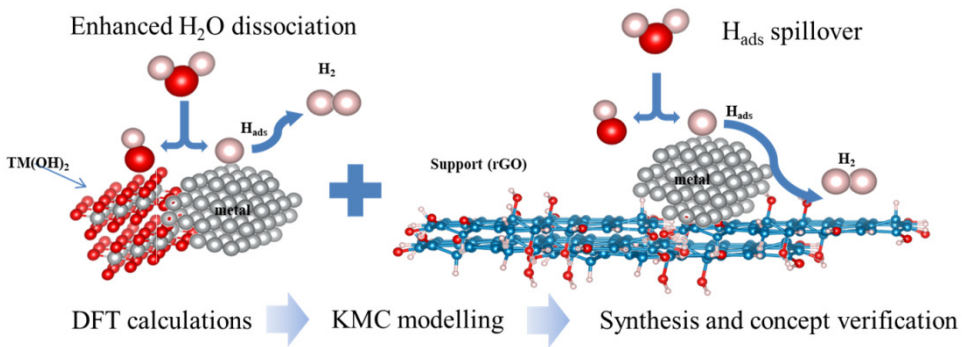

Figure 1. RatioCAT project concept: boosting H_2O dissociation and H_{ads} spillover for superior H_2 production

Acknowledgment: Presented work is financially supported by the Science Fund of the Republic of Serbia through the project RatioCAT (PROMIS programme).

PPP-2

Izazovi i potencijali nanoinženjerstva u oblasti tekstila

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Nanotehnologije su gotovo dve decenije u fokusu istraživača ali i tekstilne industrije koja čini napore da dostignuća u ovoj oblasti implementira u svojoj praksi. Modifikovanjem tekstila nanočesticama metala i oksida metala (Ag, TiO_2, Cu, Cu_2O i CuO) mogu se postići izvanredna antimikrobna svojstva, UV zaštita i efekat samočišćenja. Međutim, imobilizacija nanočestica posebno na hidrofobnim tekstilnim materijalima nije jednostavna i zahteva prethodnu aktivaciju površine vlakana koja se ostvaruje obradom plazmom, modifikovanjem polimerima ili oksidacijom površine hemijskim putem. Danas se sve češće vrši *in situ* sinteza nanočestica na bazi bakra i srebra na tekstilu. Posebna pažnja se poklanja zelenim redukcionim sredstvima uključujući i poljoprivredni otpad. Kako se ovakvi materijali mogu primeniti u medicini i zaštiti zdravlja, veliki je izazov ustanoviti optimalne uslove koji istovremeno pružaju maksimalnu antimikrobnu aktivnost prema širokom spektru mikroorganizama i nizak nivo citotoksičnosti. U poslednje vreme takođe je od velikog značaja i tehnologija naslojavanja nanofilmova koja tekstilu obezbeđuje multifunkcionalnost i posebno važnu zaštitu od zapaljivosti.

Challenges and potentials of nano-engineering in textiles

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Nanotechnologies are almost two decades in the focus of researchers and textile industry, which makes efforts to implement the achievements in this field in practice. Modification of textiles with metal and metal oxide nanoparticles (Ag, TiO_2, Cu, Cu_2O and CuO) provides extraordinary antimicrobial, UV protective and self-cleaning properties. However, immobilization of nanoparticles particularly on hydrophobic textiles is not easy and it demands previous activation of fiber surfaces. This is obtained by plasma treatment, modification with polymers or chemical oxidation of fibers. In situ syntheses of copper- and silver-based nanoparticles are currently more often exploited on textiles. Special attention is paid to green reducing agents including the agricultural waste. Since such textiles are applicable to medical and healthcare purposes, a big challenge is to optimize the conditions that can provide maximum antimicrobial activity against wide spectra of microorganisms and low level of cytotoxicity. Recently, particularly important became the technology based on the coating with nanofilms i.e. layer-by-layer deposition that can impart multifunctionality to textiles and crucially important flame protection.

Acknowledgment: This research was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No.451-03-68/2022-14/200135).

PPP-3

Indolski alkaloidi: totalna sinteza alstoskolarisina A i alstonlarsina A

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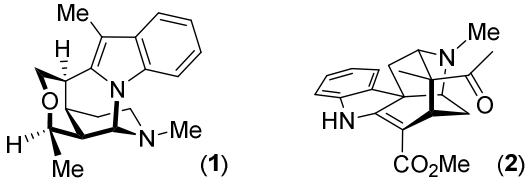
Indolski alkaloidi čine jednu od najvećih klasa alkaloida, a odlikuje ih raznovrsna i izražena biološka aktivnost: neuroaktivnost, antitumorska aktivnost, antiinflamatorna aktivnost, antimalarijska aktivnost, itd. Izražena bioaktivnost, u kombinaciji sa često specifičnim i topološki kompleksnim strukturama, čine indolske alkaloide izazovnim metama u organskoj sintezi. Njihova strukturna kompleksnost neretko iziskuje neefikasne sintetičke puteve, sa velikim brojem reakcionih koraka. Jedan od pristupa za ostvarivanje efikasnih sinteza zasniva se na primeni domino-reakcija – ovakav pristup omogućava brzo i dramatično povećanje kompleksnosti molekula u samo jednom sintetičkom koraku. U okviru ovog predavanja, biće prikazane totalne sinteze dva indolska alkaloida (alstoskolarisina A (**1**) i alstonlarsina A (**2**), Slika 1), ostvarene u našim laboratorijama, a u kojima su domino-reakcije iskorišćene u ključnim fazama sinteze.



*Slika 1. Strukture alstoskolarisina A (**1**) i alstonlarsina A (**2**).*

Indole alkaloids: total synthesis of alstoscholarisine A and alstonlarsine A

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Indole alkaloids comprise a large group of alkaloids, possessing diverse and pronounced bioactivities – neuroactivity, antitumor activity, anti-inflammatory activity and antimalarial activity among others. Out of this reason, combined with their specific and topologically complex (often unique) chemical architecture, indole alkaloids represent attractive synthetic targets. However, their intricate structural complexity often results in ineffective synthetic approaches, involving many reaction steps. One approach to increasing the synthetic efficiency, consequently leading to the significantly shorter syntheses, is by utilizing domino reactions in the planning tactic – such approach results in a rapid and dramatic increase of a molecular complexity in a single reaction step. Our achieved total syntheses of two indole alkaloids – alstoscholarisine A (**1**) and alstonlarsine A (**2**) – relied on domino sequences for the efficient formation of the polycyclic cores.

PPP-4

Развој иминошећера као анти-ковид-19 агенаса

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Пандемија ковида-19 подстакла је велики број истраживања усмерених ка развоју нових и пренаменовању постојећих лекова за терапију ове болести. Наш приступ обухвата примену иминошећера као потенцијалних терапеутских агенаса и заснива се на чињеници да вируси не могу сами синтетисати протеине, већ се за то служе ћелијама домаћина. Стога би привремена инхибиција процесирања гликопротеина дејством иминошећера могла имати терапеутску перспективу. Интердисциплинарним приступом, који обухвата рачунарско моделовање, органску синтезу, биохемијске пробе и биолошке тестове, дошли смо до једињења која имају потенцијал за даљи развој и могућу терапеутску примену. Овај приступ није ограничен на SARS-CoV-2, већ се може применити и у борби против других вируса.

The development of iminosugars as anti-COVID-19 agents

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The COVID-19 pandemics instigated extensive research directed towards the development of new and repurposing of existing drugs against the disease. Our approach involves the application of iminosugars as potential therapeutic agents, and relies on the fact that viruses cannot synthesize proteins on their own, but rely on the host's cells. Therefore, temporary inhibition of glycoprotein processing by iminosugars might have a therapeutic perspective. An interdisciplinary approach, encompassing computational modeling, organic synthesis, biochemical assays and biological tests brought about compounds endowed with a potential for further development and possible therapeutic application. This approach is not limited to SARS-CoV-2, but can also be applied against other viruses.

Saopštenja / Contributions

Analitička hemija

Analytical Chemistry

AH-1

Optimizacija i validacija metode za određivanje etilen-oksida i 2-hlor-etanola u uzorcima susama primenom gasne hromatografije i masene spektrometrije

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Etilen-oksid (EO) se zbog fizičkohemijskih svojstava i snažnog antimikrobnog delovanja koristi kao fumigans. Evropska Unija zabranjuje njegovu upotrebu u prezerviranju žitarica i prehrambenih proizvoda, a maksimalno dozvoljena koncentracija u susamu je 0,05 mg/kg. Metode za određivanje EO i njegovog primarnog metabolita - 2-hloretanola (2-CE) zasnivaju se na ekstrakciji umereno polarnim rastvaračima, uklanjanju lipida i direktnoj analizi ekstrakta primenom gasne hromatografije. U ovom radu, primenom Plaket-Burmanovog dizajna ispitan je uticaj jedanaest faktora tokom pripreme uzorka susama na analitički prinos EO i 2-CE. Od toga, tri faktora, ključna za uklanjanje lipida, su pokazala statističku značajnost i dalje su optimizovana primenom Boks-Benkenovog dizajna i metode površine odgovora. Za optimalne uslove rada određena je tačnost (84% - iskazana kao analitički prinos), dok je ponovljivost iznosila RSD_r = 7%, a unutarlaboratorijska reproduktivnost RSD_{Rw} = 9,8%.

Optimization and method validation for the determination of ethylene oxide and 2-chloroethanol in sesame seed using gas chromatography coupled with mass spectrometry

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Ethylene oxide (EO) is used as a fumigant due to its good physicochemical properties and strong antimicrobial action. The European Union bans its use for preservation of cereals and food products, and the maximum allowed concentration in sesame is 0.05 mg/kg. Methods for the determination of EO and its primary metabolite - 2-chloroethanol (2-CE) are based on analyte extraction with moderately polar solvents, followed by removal of lipids and direct analysis of the extract using gas chromatography. In this paper, the effect of eleven factors during the preparation of sesame seeds on the analytical yield of EO and 2-CE was investigated using the Plaket-Burman design. Of these, three factors, crucial for lipid removal, showed statistical significance and were further optimized using the Box-Benken design and response surface method. Method accuracy was determined for optimal operating conditions (84% - expressed as analytical yield), while repeatability was RSD_r = 7%, and intermediate reproducibility RSD_{Rw} = 9.8%.

AH-2

Optimizacija ultrazvučne ekstrakcije polifenola iz listova zelenog čaja (*Camellia sinensis*) primenom tankoslojne hromatografije, analize slike i višekriterijumskog odlučivanja

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Zeleni čaj je odličan izvor polifenola, a koristi se u ishrani, zdravstvu i kozmetici. Ograničavajući faktori za dobijanje ekstrakta optimalnog sastava su izbor ekstrakcionog sredstva odgovarajuće polarnosti i optimalno trajanje ekstrakcije. Visokoefikasna tankoslojna hromatografija (HPTLC) zajedno sa analizom slike korišćena je za analizu polifenolnih profila ekstrakata dobijenih pod različitim uslovima. Optimalani sastav vodeno-acetonske smeše i trajanje ultrazvučne ekstrakcije određeni su primenom centralnog kompozitnog dizajna, metoda površine odgovora i četiri različita algoritma višekriterijumske optimizacije: Derindžerovog pristupa poželjnosti, PROMETHEE-II, TOPSIS i SRD. Prva tri algoritma su usaglašena i ukazuju da se optimalan ekstrakt dobija primenom 73 - 74% acetonsko-vodenog rastvora nakon 40 minuta ekstrakcije. SRD algoritam značajno odstupa u rangiranju optimalnih rešenja.

HPTLC-guided optimization of ultrasound assisted extraction of polyphenols from green tea leaves (*Camellia sinensis*) using image analysis and multicriteria optimization

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Green tea is a great source of polyphenols. It is used in nutrition, healthcare, and cosmetics. Key factors for obtaining optimal extracts are selection of solvents of adequate polarity, and optimal duration of extraction. High performance thin-layer chromatography (HPTLC) coupled with image analysis was used to map the polyphenolic profiles of extracts obtained under different conditions. The central composite design and response surface methodology were used to model the effect of the composition of acetone-water mixtures, and duration of the ultrasonic assisted extraction on the chromatographic profiles of extracts. Four different multiobjective optimization algorithms: Derringer's approach, PROMETHEE-II, TOPSIS and SRD were compared. The first three algorithms were coherent indicating 73 - 74% acetone-aqueous solution and 40 minutes of extraction as optimal. The SRD deviated significantly in the ranking of optimal solutions.

AH-3

Ispitivanje potencijala 18 lekovitih biljaka iz Srbije na proces usporavanja starenja kože

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Višak slobodnih radikala u koži uzrokuje oksidativni proces, što dovodi do starenja kože i stvaranja staračkih pega. Enzim tirozinaza je odgovoran za navedeni proces. Usporavanje ovog „neželjenog procesa" predstavlja jedan od izazova savremene nauke. S tim u vezi, cilj navedenog istraživanja je ispitivanje potencijala određenih biljnih ekstrakata na sprečavanje oksidativnog stresa i pojavu hiperpigmentacije. Ekstrakti su hemijski okarakterisani primenom visoko-efikasne tankoslojne hromatografije i visoko-efikasne tečne hromatografije kuplovane sa masenom spektrometrijom. Određena je antioksidativna aktivnost ekstrakata kao i inhibitorni efekat na enzim tirozinazu. Devetnaest fenolnih jedinjenja je kvantifikovano u ispitivanim ekstraktima. Dobijeni rezultati izdvajaju ekstrakte *Morus alba (92%), Rubus (86%)* i *Agrimona eupatoria (84%)* kao najefikasnije inhibitore. Ekstrakti *Teucrium chamaedrys* i *Agrimona eupatoria* su pokazali visoke vrednosti antioksidativne aktivnosti. Navedeni uzorci su komercijalni.

Skin anti-ageing potential of 18 medicinal herbs collected from Serbia

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Excess of free radicals in skin causes oxidative stress, which results to skin aging and appearance of age spots. The enzyme tyrosinase is responsible for mentioned process. Slowing down of this unwanted process is one of the challenges of modern science. Thus, the aim of this study is to examine the potential of selected plant extracts to reduce oxidation stress and the appearance of hyperpigmentation. The extracts were characterized by the use of high-performance thin-layer chromatography and high-performance liquid chromatography coupled with mass spectrometry. The antioxidant activity of the extracts and potential for the inhibition of tyrosinase enzyme were determined. Nineteen phenolic compounds were quantificated in the tested extracts. The obtained results demonstrate that the extracts of *Morus alba (92%), Rubus (86%)* and *Agrimona eupatoria (84%)* are the most effective inhibitors. The *Teucrium chamaedrys* and *Agrimona eupatoria* showed high values of antioxidant activity. The listed samples are commercial.

AH-4

Procena autentičnosti medljikovca na osnovu fitohemijskog profila

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Uzimajući u obzir činjenicu da je u bazi podataka kojom se definišu parametri kvaliteta najzastupljenijih evropskih medova, medljikovac, specifična vrsta meda koja nastaje prikupljanjem biljnih sokova i sokova koje izlučuju biljne vaši, naveden kao jedinstvena grupa bez definisanog biljnog porekla, cilj ovog rada je definisanje kriterijuma za diferencijaciju i klasifikaciju četiri biljne vrste medljikovca. U cilju procene autentičnosti analiziranisu fenolni profil i antioksidativna aktivnost medljikovaca primenom visoko-efikasne tankoslojne hromatografije u kombinaciji sa obradom slike i hemometrijom. Rezultati potvrđuju mogućnost procene botaničkog porekla medljikovca na osnovu karakterističnih hemijskih profila pojedinih biljnih vrsta, kao i prednost primene multivarijantne obrade podataka dobijenih metodom 'otiska prsta'.

Authenticity assessment of honeydew honey based on phytochemical profile

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Considering the fact that the database of the quality parameters of the most common European honeys define honeydew honey, a specific type of honey produced by collecting plant secretions and excretions of plant-sucking insects, as a unique group without defined its plant origin, the aim of this paper is to define criteria for the differentiation and classification of four varieties of honeydew honey. In order to assess the authenticity, the phenolic profile and antioxidant activity of honeydew honey were analyzed using high-performance thin-layer chromatography in combination with image processing and chemometrics. The results confirm the possibility of assessing the botanical origin of honeydew honey based on the characteristic chemical profiles of individual plant species, as well as the advantage of multivariate data processing in fingerprint analysis.

AH-5

Protočno injekcioni sistem za određivanje aksorbinske kiseline na modifikovanoj elektrodi od ugljenične paste

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U ovom radu je optimizovan jednostavan FIA sistem sa amperometrijskom detekcijom askorbinske kiseline na modifikovanoj elektrodi od ugljenične paste. Ugljenična pasta je pripremljena mešanjem grafita i kompleksa Šifove baze sa bakrom [Cu(phacac$_2$en)] [1]. Pod optimalnim FIA uslovima (0,6 V *vs.* Ag/AgCl, 50 µl za petlju za uzorak i 100 µl za reakcionu petlju i 0,04 mol/L BRP (pH 5) kao reagens), dobijena je linearna zavisnost odgovora amperometrijskog detektora u odnosu na koncentraciju u opsegu od 0 do 75 µmol/L, sa jednačinom prave, I = 0,0198c + 0,0102 (r^2 0,998) i granicom detekcija (3σ/s) od 3,5 µmol/L. Protočno injekcioni sistem je uspešno primenjen na određivanje askorbinske kiseline u uzorcima pića.

Flow injection system for ascorbic acid determination on modified carbon paste electrode

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A simple flow injection system for ascorbic acid determination on modified carbon paste electrode was optimised. The carbon paste electrode was prepared by mixing of carbon powder with Schiff base complex with copper [Cu(phacac$_2$en)]. Under the optimal FIA conditions (0.6 V *vs.* Ag/AgCl, 50 µl injection volume, 100 µl for reaction coil and 0.04 mol/L BRB (pH 5) as reagent) linear response of amperometric detector in the concentration range from 0 to 75 µmol/L for ascorbic acid was obtained. Corresponding equation was I = 0.0198c + 0.0102 (r^2 0.998), calculated limit of detection (3σ/s) was 3.5 µmol/L of ascorbic acid. The FIA system was successfully applied on determination of ascorbic acid in beverages.

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AH-6

Zeleni analitički pristup za ekstrakciju i hemijsko profilisanje fenolnih jedinjenja iz prirodnih proizvoda na primeru biljke podubice (*Teucrium chamaedrys* L.)

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Jedan od glavnih ciljeva zelene analitičke hemije je eliminisanje ili smanjenje upotrebe organskih rastvarača i reagenasa i zbog toga je primena prirodnih eutektičkih smeša (NADES -natural deep eutectic solvents) kao medijuma za ekstrakciju uzoraka prepoznata kao zelena alternativa. U ovom radu je primenjeno 19 različitih prirodnih eutektičkih smeša za ekstrakciju fenolnih jedinjenja iz biljke podubice. Za hemijsko profilisanje ekstrakata korišćena je visoko-efikasna tankoslojna hromatografija (HPTLC – High-performance thin-layer chromatography) koja predstavlja zelenu tehniku zbog istovremene analize velikog broja uzoraka, uz upotrebu male količine ekstrakata i minimalnih količina rastvarača. Ekološka prihvatljivost predložene metodologije procenjena jeprimenom Nacionalnog indeksa uticaja metode na životnu sredinu i eko-skale.

Green analytical approach for extraction and chemical profiling of phenolic compounds from natural products: A case study of *Teucriumchamaedrys*L.

Mila Č.Lazović[1], Milica S. Jankov[1], Jelena Đ.Trifković[2], Ilija N.Cvijetić[2], Petar M. Ristivojević[2], Dušanka M. Milojković Opsenica[2]

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One of the main principles of green analytical chemistry is to eliminate or reduce the use of organic solvents and reagents, and therefore use of Natural Deep Eutectic Solvents (NADES) as medium in sample extraction was recognized as green alternative to conventional one. In this paper, 19 different natural deep eutectic solventswere used for the extraction of phenolic compounds from *Teucriumchamaedrys* L. Chemical profiles of the extracts were obtained by applying high-performance thin-layer chromatography (HPTLC), which is a green technique due to the simultaneous analysis of a large number of samples, using small amounts of extracts and minimal amounts of solvents. Greenness of proposed methodology was estimated by NEMI pictogram and analytical eco-scale.

AH-7

Protočno injekcioni sistem za određivanje kofeina na modifikovanoj elektrodi od staklastog ugljenika

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U ovom radu je optimizovan jednostavan protočno injekcioni sistem za određivanje kofeina na elektrodi od staklastog ugljenika modifikovanoj nanočesticama $MnCo_2O_4$ [1] i nafiona. Cikličnom voltametrijom je poređena osetljivost oksidacije kofeina na nemodifikovanoj i modifikovanoj elektrodi. Pod optimalnim FIA uslovima (1,5 V *vs.* Ag/AgCl, 50 µl za petlju za uzorak i 100 µl za reakcionu petlju i 0,1 mol/L H_2SO_4 kao reagens), dobijena je linearna zavisnost odgovora amperometrijskog detektora u odnosu na koncentraciju kofeina u opsegu od 0 do 75 µmol/L, sa jednačinom prave, I = 0,0856c + 0,0423 (r^2 0,9996) i granicom detekcija (3σ/s) od 1,5 µmol/L kofeina. Protočno injekcioni sistem je uspešno primenjen na određivanje kofeina u različitim napitcima.

Flow injection system for caffeine determination on modified glassy carbon electrode

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In this work a simple flow injection system for caffeine determination on modified glassy carbon electrode was optimised. The electrode was modified with $MnCo_2O_4$ nanoparticles and nafion [1]. Cyclic voltammetry was used for comparison of the caffeine oxidation on bare and modified electrode. Under the optimal FIA conditions (1.5 V *vs*. Ag/AgCl, 50 µl injection volume, 100 µl for reaction coil and 0.1 mol/L H_2SO_4 as reagent), a linear response of amperometric detector in the concentration range of 0 - 75 µmol/L for caffeine was obtained. Corresponding equation was I = 0.0856c + 0.0423 (r^2 0.9996), calculated limit of detection (3σ/s) was 1.5 µmol/L of caffeine. The FIA system was successfully applied on caffeine determination in different beverages.

1. V. Antunović, M. Ilić, R. Baošić, D. Jelić, A. Lolić, *PLOS One*. **2019**, *14(2)*, e0210904

AH-8

Proučavanje ravnoteža u heterogenim sistemima tricikličnog antidepresiva amitriptilina

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Cilj ovog rada bio je proučavanje ravnoteža u heterogenim sistemima tricikličnog antidepresiva amitriptilina (Am) koji sadrže hloride i/ili fosfate. Rastvorljivost Am u uslovima povećane jonske sile određena je pH–*Ramp shake–flask* metodom.[1, 2] Veća rastvorljivost Am u kiseloj sredini od očekivane, posledica je agregacije – analiza eksperimentalnih podataka pomoću programa *p*DISOL–X^{TM} ukazuje na verovatno građenje pentamera $Am_5H_5^{5+}$. Kritična micelarna koncentracija i stepen disocijacije agregata određeni su primenom konduktometrijskih titracija. U baznoj sredini primećena je delimična degradacija Am. Eksperimentalno dobijeni podaci o rastvorljivosti biološki aktivnih supstanci i postojećim ravnotežama u heterogenim sistemima važni su u svim fazama dizajna i razvoja lekova.

Study of equilibria in heterogeneous systems of tricyclic antidepressant amitriptyline

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The aim of this work was to study the equilibria in tricyclic antidepressant amitriptyline (Am) heterogeneous systems containing chloride and/or phosphate ions. Solubility of Am in high ionic strength conditions was determined using pH–*Ramp shake–flask* method.[1, 2] Higher solubility of Am than expected in an acidic media is a consequence of self-aggregation – pentamer formation ($Am_5H_5^{5+}$) according to *p*DISOL–X^{TM} analysis. Critical micelle concentration and the degree of the aggregate dissociation were determined by conductometric titrations. Partial degradation of Am in alkaline suspensions was observed. Experimental studies of solubility as well as the existing equilibria in heterogeneous systems of biologically active compounds are important at all stages of drug design and development.

1. O. Marković, M. Pešić, A. Shah, A. Serajuddin, T. Verbić, A. Avdeef, *Eur. J. Pharm. Sci*. **2019**, *133*, 264.
2. O. Marković, N. Patel, A. Serajuddin, A. Avdeef, T. Verbić, *Mol. Pharmaceutics*. **2022**, *19*, 710.
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AH-9

Sadržaj esencijalnih i toksičnih elemenata u lekovitoj biljci *Capsella bursa-pastoris* (L.) Medic. i njenim ekstraktima

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Zbog svojih antiinflamatornih i antibakterijskih svojstva *Capsella bursa-pastoris* (L.) Medic., vekovima je smatrana lekovitom biljkom, i stoga se često koristi za pripremanje čajeva i lekovitih tinktura. U ovom istraživanju prikupljeni su uzorci ove lekovite biljke, u Beogradu, Boru, Vršcu i Sremskoj Mitrovici u Srbiji, tokom proleća 2021 godine. Ovom studijom određeni su nivoi toksičnih i esencijalnih elemenata koji se akumuliraju u nadzemnom delu biljke i korenu, kao i njihov sadržaj u biljnim infuzijama, i etanolnim ekstraktima nadzemnog dela. Koncentracija elemenata: As, Ba, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Se, Zn, S, P, Mg, K i Ca određena je indukovano spregnutom plazmom optički emisionom spektroskopijom (ICP-OES). Translokacioni faktori su izračunati za svako mesto uzorkovanja, praćeni korelacionom analizom, kako bi se istražili nivoi ekstrakcije i distribucije elemenata.

Essential and toxic elements content in the medicinal plant *Capsella bursa-pastoris* (L.) Medic. and its extracts

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Due to its anti-inflammatory and antibacterial properties, *Capsella bursa-pastoris* (L.) Medic., has been considered a medicinal plant, and hence, it is frequently used for teas and tincture preparation. In this research, samples of this medicinal plant were collected in Belgrade, Bor, Vršac, and Sremska Mitrovica in Serbia, during the spring of 2021. This study assessed the levels of toxic and essential elements accumulated in theabove-ground parts of a plant, and herbal infusions, and ethanolic extracts prepared of same aerial parts of plant. The concentration of elements: As, Ba, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Se, Zn, S, P, Mg, K, and Ca was determined by inductively coupled plasma optical emission spectroscopy (ICP-OES). Translocation factors were calculated for each sampling site, followed by correlation analysis, in order to investigate elements distribution and extraction levels.

AH-10

Spektrofotometrijsko određivanje sadržaja ukupnih fenola i antioksidativnog kapaciteta ekstrakata lista čuvarkuće (*Sempervivum tectorum* L.) i fenolni profil

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List čuvarkuće (*Sempervivum tectorum* L.) ima široku primenu u narodnoj medicini za lečenje promena na koži. Dvadeset različitih ekstrakata lista čuvarkuće je okarakterisano primenom spektrofotometrije i visokoefikasne tankoslojne hromatografije (HPTLC). Antioksidativni kapacitet ekstrakata određen je primenom četiri spektrofotometrijska testa, dok je sadržaj ukupnih fenola određen Folin-Ciocalteu metodom. Analiza glavnih komponenti (PCA) je primenjena na rezultate spektrofotometrijskih testova u cilju grupisanja uzoraka prema intenzitetu ispoljavanja antioksidativne aktivnosti. Uzorci su raspoređeni u dve grupe, osim tri uzorka koji se izdvajaju. Uočava se sličan fenolni profil ekstrakata lista *S. tectorum* koji je dobijen primenom HPTLC metode. Kaemferol i kaemferol 3-*O*-glukozid, galna i kofeinska kiselina kao i kvercetin 3-*O*-glukozid su identifikovani u ekstraktima listova čuvarkuće.

Spectrophotometric determination of total phenolic content and antioxidant capacity of houseleek leaf extracts (*Sempervivum tectorum* L.) and phenolic profile

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Houseleek leaves (*Sempervivum tectorum* L.) has a wide application in folk medicine for treating skin changes. Twenty different extracts of houseleek leaves were characterized by spectrophotometry and high-performance thin-layer chromatography (HPTLC). The antioxidant capacity of the extracts was determined using four spectrophotometric assays, while the content of total phenols was determined by the Folin-Ciocalteu's method. The principal component analysis (PCA) was applied to the results obtained by spectrophotometric assays in order to group the samples according to the intensity of antioxidant activity. The samples were divided into two clusters, except for three separated samples. A similar phenolic profile of *S. tectorum* leaves extracts obtained by HPTLC was observed. Kaempferol and kaempferol 3-*O*-glucoside, gallic and caffeic acids as well as the quercetin 3-*O*-glucoside have been identified in houseleek leaves extracts.

AH-11

Validacija metode za određivanje sadržaja citrata u bagremovom medu jonskom hromatografijom

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Sadržaj limunske kiseline u medu može da pruži informacije za procenu autentičnosti meda. Međutim, važeći *Codexalimentarius* kao i *Pravilnik o kvalitetu meda* ne pružaju informacije o sadržaju limunske kiseline u medu. Imajući to u vidu, predmet ovog rada je razvoj i validacija metode za određivanje citrata u medu. Analiza citrata urađena je primenom jonske hromatografijesa konduktometrijskom detekcijom na DIONEX AS 15 analitičkoj koloni uz upotrebu 30 mM kalijum-hidroksida kao mobilne faze.Validovana metoda se može primeniti za određivanje sadržaja citrata u medu u intervalu 1 – 100 mg/kg s agranicom detekcije od 0,36 mg/kg igranicomkvantifikacije 1,20 mg/kg.Tačnost metode je proverena testom obogaćenja (95 – 101%), a preciznost ponovljenim analizama u toku više dana. Metoda je proverena analizom 25 uzoraka bagremovog meda pri čemu je sadržaj citrata bio u opsegu 10,82 – 55,74 mg/kg. Parametri validacije metode potvrđuju mogućnost primene jonskehromatografije sa konduktometrijskom detekcijom za brzo i tačno određivanje citrata u uzorcima bagremovog meda.

Method validation for determining the citrate content in acacia honey by ion chromatography

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The citric acid content can give useful information about honey authenticity. However, *Codex Alimentarius* and the *Serbian regulation* do not provide information on the content of citric acid in honey. Hence,the object of this paper is the method development and validation for the determination of citrate content in honey. The concentration of citrate in honey was determined by ion chromatography with conductivity detection on DIONEX AS 15 column and 30 mM potassium-hydroxide as mobile phase. The method validation revealed that method can be used for determination of citrate in acaciahoney from 1 to100 mg/kg. The limit of detection was 0.36 mg/kg and limit of quantification 1.20 mg/kg. The accuracy was determined with recovery test (95–101%), and precision with repeat analysis during few days. Analysis of 25 acacia honey samples confirmed applicability of method and revealed that amount of citrate was10.82 – 55.74 mg/kg. The statistical parameters of method validation pointed out that the ion chromatography with conductometry detection enabled rapid and accurate determination of citrate in acacia honey.

AH-12

Application of donepezil-imprinted polymers for controlled drug release

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Molecularly imprinted polymers (MIPs) are smart materials with predetermined selectivity and binding capacity for particular molecule - template. MIPs for donepezil were prepared using methacrylic acid as the functional monomer and divinylbenzene, trimethylolpropane trimethacrylateorethylene glycol dimethacrylate as crosslinker. Obtained polymers werecharacterized by FTIR spectroscopy, scanning electron microscopy and adsorption isotherms. Based on the re-binding of the template to the obtained imprinted and non-imprinted polymers, it was determined that the imprinting was successful. Adsorption isotherms confirmed the presence of highly specific binding sites. MIPs were subjected to physiological-like conditions to test theability to release donepezil in a controlled manner. This experiment showed that under conditions of low pH, donepezil is released very quickly, in just a few hours. At physiological pH (7.40) the release occurs in small doses and lasts for days, indicating that these polymers may be a potentially useful way to dose this drug if they are protected from low gastric pH when administered orally.
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Primena donepezilom obeleženih polimera kao sistema za kontrolisano otpuštanje

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Molekulski obeleženi polimeri (MOPi) predstavljaju pametne materijale sa predodređenom selektivnošću i kapacitetom vezivanja za izabrani molekul - templat. MOPi za donepezil su dobijeni koristeći metakrilnu kiselinu kao funkcionalni monomer i divinilbenzen, trimetilolpropan-trimetakrilatietilen-glikol-dimetakrilat kao umreživače. Dobijeni polimeri su karakterisani pomoću infracrvene spektroskopije, skenirajuće elektronske mikroskopije i pomoću adsorpcionih izotermi. Na osnovu rezultata dobijenih ponovnim vezivanjem templata za neobeležene i obeležene polimere, zaključeno je da je proces obeležavanja uspešno izveden. Pomoću adsorpcionih izotermi utvđeno je prisustvo visoko specifičnih mesta za vezivanje donepezila. MOPi su podvrgnuti uslovima sličnim fiziološkim u cilju ispitivanja mogućnosti primene za kontrolisano otpuštanje donepezila. U kiselim uslovima, do otpuštanja donepezila dolazi brzo, tokom nekoliko sati. Pri fiziološkim uslovima (pH 7,40) otpuštanje donepezila se dešava u malim količinama tokom nekoliko dana, ukazujući na mogućnost primene MOPa za kontrolisano otpuštanje.

Biohemija

Biochemistry

BH-1

Ekotoksikološka analiza proizvoda elektrohemijske degradacije Reactive black 5 boje pomoću MFC kao izvora električne energije

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Koncept mikrobnih gorivnih ćelija, poznat još sa početka 18og veka, svoje mesto našao je u potencijalnoj primeni među alternativnim izvorima energije. Koristeći mikroorganizme, uspešno dolazi do konvertovanja hemijske energije u električnu energiju. Nastala energija, ima mogućnosti da se iskoristi za napajanje malih potrošača, kao što je sistem elektroda za elektrohemijsku degradaciju boja.

Vodeni rastvor boje (100 mL) RB5 od 25 mg/L i 1 mM H_2O_2 elektrohemijski je tretiran, koristeći Pt i Fe elektrodu. MFC ćelija se koristila kao izvor struje za degradaciju. Ekotoksikološka analiza pomoću bakterije *Vibrio fisheri* je pokazala da najveću toksičnost ima polazna boja RB5 (EC_{20} 8,17%), dok nastali degradacioni proizvod nakon 6 h tretiranja strujom dobijenom preko MFC sistema ima najmanju toksičnost na spomenutu bakteriju (EC_{20} 33,05%).

Ecotoxicity of degradation product from dye Reactive Black 5 by electrochemical degradation products using MFC as a source of electricity

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The concept of microbial fuel cells, known since the beginning of the 18th century, has found its place in potential application among alternative energy sources. Using microorganisms, chemical energy is successfully converted into electricity. The resulting energy has the potential to be used to power small consumers, such as an electrode system for electrochemical color degradation.

Aqueous dye solution (100 mL) RB5 of 25 mg / L and 1 mM H_2O_2 was electrochemically treated, using Pt and Fe electrode. The MFC cell was used as a current source for degradation. Ecotoxicological analysis using *Vibrio fisheri* showed that the highest toxicity is the RB5 dye (EC_{20} 8.17%), while the resulting degradation product after 6 h of treatment with electricity obtained through the MFC system has the lowest toxicity to this bacterium (EC_{20} 33.05%).

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BH-2

In vitro analiza amiloidogeneze pod uticajem teških metala primenom biofizičkih metoda

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Pod specifičnim uslovima, proteini zauzimaju nenativnu, izuzetno stabilnu, visoko-uređenu strukturu – amiloidne fibrile, koji su povezani sa mnogim neurodegenerativnim oboljenjima. Pojava amiloidnih plaka u tkivima je korelisana sa prisustvom jona teških metala, mada sam mehanizam njihovog uticaja nije razjašnjen. Cilj ovog rada je opisivanje uticaja teških metala, konkretno olova i kadmijuma, na amiloidnu agregaciju ovalbumina *in vitro* primenom ThT fluorescencije, ATR-FTIR spektroskopije, i mikroskopskih tehnika. Dobijeni rezultati ukazuju da ispitivani joni teških metala pokazuju nedvosmisleno pozitivan, međusobno nezavisan, aditivan efekat na klasterovanje amiloidnih fibrila u kompleksne makromolekulske agregate.

An *in vitro* analysis of heavy metal-influenced amyloidogenesis using biophysical methods

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Under specific conditions, exceptionally stable, highly-ordered protein structures may form – amyloid fibrils, which have been linked to many neurodegenerative diseases. The formation of amyloid plaques in tissues has been correlated to the presence of heavy metal ions, although the precise mechanism has not been described yet. The effect of these metals, specifically lead and cadmium, on *in vitro* ovalbumin amyloid aggregation has been monitored via ThT fluorescence, ATR-FTIR spectroscopy, as well as microscopic techniques. The results obtained show a clear positive, independent, and additive effect of investigated heavy metal ions on the clustering of amyloid fibrils into complex macromolecular aggregates.

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BH-3

Fikocijanin iz mikroalge Spiruline: prečišćavanje i vezivanje odabranih (poli)fenola

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Stabilizacija živopisnih boja fikobilinskih proteina mikro/makroalgi preduslov je za njihovo veće korišćenje u industriji hrane. Fikocijanin (C-PC) je prečišćen iz sirovog ekstrakta cijanobakterije Spirulina (*Arthrospira*) Pacifica, taloženjem proteina amonijum-sulfatom i anjonskom jonoizmenjivačkom hromatografijom. Čistoća je potvrđena elektroforetski (SDS-PAGE). Vezivanje deset odabranih bioaktivnih polifenola za C-PC (uključujući kvarcetin, koenzim Q10, galnu kiselinu, vanilinsku kiselinu i resveratrol) ispitano je standardnim spektroskopskim metodama. Kvarcetin je pokazao najjače vezivanje (K_a~3x10^5 M^{-1}), uz stabilizaciju sekundarne strukture proteina pod fiziološkim uslovima.

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Phycocyanin from microalgae Spirulina: purification and binding of selected (poly)phenols

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Stabilization of the vivid colors of phycobiliproteins of micro/macroalgae is a prerequisite for their greater use in the food industry. Phycocyanin (C-PC) was purified from cyanobacteria Spirulina (*Arthrospira*) Pacifica raw extract by ammonium sulfate protein precipitation and anion ion-exchange chromatography. Purity was confirmed electrophoretically (SDS-PAGE). The binding of ten selected bioactive polyphenols to C-PC (including quercetin, coenzyme Q10, gallic acid, vanillic acid, and resveratrol) was examined by standard spectroscopic methods. Quercetin is shown to have the strongest binding (K_a~3x10^5 M^{-1}), with stabilization of the secondary protein structure under physiological conditions.

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BH-4

Protein interactions of six tea plant extracts

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Polyphenols are a large group of natural organic compounds mainly found in plants, in whom they have diverse protective and metabolic functions. It's also known that phenolic compounds, especially tannins, interact with proteins in various significant and distinct ways. Tannins also complex proteins[1], which generally precipitates them and it's their most important industrially utilised characteristic. This study, which was a continuation of our previous work, focused on interactions of aqueous tea plant extracts with laccase from *Trametes 63ersicolour* and β-amylase from *Ipomoea batatas*. Tea plants used in this study were*Saturejamontana*, *Menthapiperita*, *Salvia officinalis*, *Matricariachamomilla*, *Camellia cinensis* and *Arctostaphylosuva-ursi*. Total phenolic content was determined using Folin-Ciocalteu reagent, which showed us that chosen plants vary considerably in their total phenolic content and the highest concentration was found to be in *Arctostaphylosuva-ursi*. Protein interactions between tea plant extracts were measured using spectrophotometric, spectrofluorimetric and electrophoretic methods. These methods showed that tea plant extracts lead to various structural changes within the protein, nature of which require further research. Finally, it was also found that all tea plant extracts, except *Matricariachamomilla*extract, reversibly precipitate β-amylase – whilst retaining most of its enzymatic activity after dissolving.Best results were obtained using *Arctostaphylosuva-ursi*extract, which precipitated the highest quantity of β-amylase, with highest activity retention. Although being an interesting phenomenon, furtherresearch is necessary to determine the nature andimportance of reversible tannic enzyme precipitation.

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BH-5

Optimizacija ekstrakcije tropomiozina gambora i njegova kvantifikacija upotrebom razvijene ELISA metode

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Tropomiozin (TPM) se smatra glavnim alergenom morskih plodova. Razvoj metoda za kvantifikaciju TPM-a u prehrambenim proizvodima je ključan za alergične osobe. Nekoliko pufera za ekstrakciju je upoređeno u pogledu efikasnosti ekstrakcije protein iz sveže zamrznutih i kuvanih gambora, tokom 2 i 24 časa. Sadržaj proteina u solubilnim ekstraktima je određen Bredfordovom metodom. Proteinski profil ekstrakata je analiziran SDS-PAGE metodom. Za kvantifikaciju TPM-a je razvijena sendvič ELISA metoda. Nijedan puffer nije pokazao značajnu razliku u količini ekstrahovanih protein nakon 2 i 24 časa ekstrakcije. U poređenju sa sirovim, značajno manje proteina je ekstrahovano iz kuvanih gambora. Kvantifikacija TPM-a ELISA metodom je pokazala da se fosfatom puferisanim fiziološkim rastvorom (PBS) koji sadrži 1 M NaCl (PBSN) i karbonatnim puferom, pH 10, ekstrahuje oko 6 puta više TPM-a u poređenju sa PBS-om. Ovo ukazuje na značaj odabira adekvatnog pufera za ekstrakciju TPM-a, jer se upotrebom tradicionalno korišćenih pufera može potceniti koncentracija TPM-a u gamborima.

Optimization of extraction conditions of tropomyosin from razor mud shrimp and its quantification by developed ELISA

Tropomyosin (TPM) is considered as a major allergen among different shellfish species. Therefore, the development of methods for quantifying TPM in food products iscrucial for allergic persons. Several extraction buffers were tested for their efficiency in recovering proteins from fresh frozen and cooked razor mud shrimp during 2 and 24 hours of extraction. The protein content was quantified using the Bradford protein assay. SDS-PAGE was used for protein profiling of soluble extracts. Sandwich ELISA was developed and used to quantify TPM content. None of the extraction buffers showed a significant difference in total protein content between 2 and 24 hours of extraction. Significantly fewer proteins were extracted from cooked shrimp compared to the raw shrimp. ELISA quantification showed that phosphate-buffered saline (PBS) containing 1 M NaCl (PBSN) and carbonate buffer, pH 10, extracted approximately 6 times higher amount of tropomyosin in comparison to PBS, highlighting the importance of choosing the appropriate extraction buffer for the precise quantification of TPM. Traditionally used extraction buffer PBS could significantly underestimate shrimp TPM content.

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BH-6

Razvoj sendvič ELISA testa specifičnog za SARS-CoV-2 N-protein

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Tačna dijagnoza ljudi sa sumnjom na infekciju SARS-CoV-2 je od suštinskog značaja za suzbijanje globalnog širenja COVID-19. Prisustvo SARS-CoV-2 može se otkriti RT-PCR-om (otkriva RNK virusa) ili detekcijom prisustva virusnih antigena u biološkim tečnostima ELISA-om ili sličnom tehnikom koje koriste antitela razvijena u životinjama. Cilj studije je bio uspostavljanje kvantitativnog testa koji se zasniva na korišćenju poliklonskih seruma za rutinsko određivanje koncentracije SARS-CoV-2 nukleokapsidnog proteina merenjam apsorbancije u standardnoj mikrotitarskoj pločici sa 96 bunara. Za potrebe razvoja testa proizveden je rekombinantni N-protein i korišćen za proizvodnju antiseruma u miševima i zečevima. Proizvedeni antiserumi su prečišćeni i određen im je titar. Poliklonskiantiserumi visokog afiniteta specifični za N-protein korišćeni su za razvoj ELISA testa specifičnog za ovaj protein. Test se zasniva na korišćenju poliklonskih seruma miševa koji su adherirani na dno bunara mikrotitarske pločice za hvatanje N-proteina iz uzorka. Različite koncentracije rekombinantnog N-proteina su korišćene za standardnu krivu za kvantifikaciju proteina. N-protein vezan za antitela miševa je detektovan zečjim poliklonskim serumom i anti-zečjim antitelom povezanim sa enzimom koji obezbeđuje spektrofotometrijsko merenje. Uspešno smo razvili prototip ELISA testa za kvantifikaciju N-proteina sa granicom detekcije u opsegu od ng/mL. Prosečna vrednost LOD za prototip ELISA testa za detekciju N-proteina je 9,2 ng/mL, dok je prosečna vrednost LOQ 10,2 ng/mL. Pokazali smo da su proizvedeni poliklonski antiserumi pogodni za detekciju N-proteina sa sličnim ili boljim afinitetom i specifičnošću od komercijalnih antitela. Štaviše, prototip ELISA testa se može koristiti sa zadovoljavajućom pouzdanošću za kvantifikaciju N-proteina u uzorcima bogatim proteinima, poput ljudskih seruma.

Development of SARS-CoV-2 N-protein specific capture ELISA

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The accurate diagnosis of people with suspected infection with the SARS-CoV-2 is essential to curb the global spread of COVID-19. The presence of SARS-CoV-2 can be detected by RT-PCR (it detects RNA of the virus) or by the presence of viral antigens in biological fluids in ELISA or similar techniques using antibodies developed in animals. The aim of the study was the establishment of a quantitative polyclonal sera-based test for routine measurement of the concentration of SARS CoV-2 nucleocapsid protein using absorbance measurement in a standard 96-well microtiter plate. For the purposes of the test development, recombinant N protein was produced and used for the production of mice and rabbit antisera. Produced antisera were purified and titer was determined. High-affinity polyclonal N-protein specific antisera were used for N-protein specific ELISA test development. The test is based on mice polyclonal sera adhered to microtiter plate bottom for the capture of the N protein from the specimen. Various concentrations of the recombinant N-protein were used to generate a standard curve for protein quantification. The N-protein bound to the mice antibodies was detected with rabbit polyclonal sera and anti-rabbit antibody coupled to an enzyme that provides spectrophotometric measurement. We have successfully developed the prototype ELISA for the quantification of N-protein with the detection limit being in the range of ng/mL. The average LOD value for the prototype ELISA was determined to be 9.2 ng/mL, while the average LOQ value was 10.2 ng/mL. We have demonstrated that produced polyclonal antisera are suitable for the detection of N-protein with affinity and specificity similar to, or better than commercial antibodies. Furthermore, the prototype ELISA can be used with satisfactory confidence for quantification of the N-protein in protein-rich samples, similar to human sera.

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ВН-7

Селективност везивања EcSSB за хомополимерне олигонуклеотиде

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Једноланчани ДНК-везујући протеин *E. coli* (EcSSB) игра кључну улогу у савијању ДНК и заштити на високој температури, делује као пратилац[1]. EcSSB је такође атрактиван кандидат за афинитетно пречишћавање једноланчане ДНК која је неспецифична за секвенцу. У овом раду описујемо принцип пречишћавања једноланчане ДНК засноване на EcSSB. Наши резултати показују да EcSSB има различит афинитет према синтетичким једноланчаним полинуклеотидима који се разликују по дужини и садржају нуклеотида. Поред тога, само dT_5-dT_{25} се може елуирати са колоне повећањем јонске снаге. Други хомополимери би могли да се одвоје од EcSSB само у присуству хаотропних реагенаса, који развијају EcSSB.
Разлог за такву селективност према хомополимерној ссДНК се проучава.

Binding selectivity of EcSSB to homopolymericoligonucleotides

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The *E. coli*single-stranded DNA-binding protein(EcSSB)plays a key role in DNA folding and protection at high temperature, act as chaperones[1].EcSSB is also attractive candidate for affinity purification of single-stranded DNA that is nonspecific to the sequence. In the current work, we describethe principle of single-stranded DNA purification based on EcSSB. Our resultsshow that EcSSB has different affinity to synthetic single-stranded polynucleotidesthat vary in length and nucleotide content. In addition,only dT_5-dT_{25} could be eluted from the column by increasingtheionic strength. Other homopolymers could be dissociated from EcSSB only in the presence of chaotropic reagents, that unfold EcSSB.
The reason for such selectivity to homopolymeric ssDNA is under study.

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BH-8

Kloniranje i ekspresija fluorescentno obeleženog α-sinukleina u bakteriji *Escherichia coli*

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Fluorescentno obeleženi proteini su neprocenjivi alati u laboratorijskoj praksi za *in vivo* lokalizovanje i ispitivanje interakcija proteina. Dizajnirali smo vektor za ekspresiju mCerulean3 sa N-terminalnim heksahistidinskim obeleživačem fuzionisanim preko poliasparaginskog linkera i proteolitičkog mesta za proteazu virusa graviranosti duvana (TEV) sa α-sinukleinom. Ovaj konstrukt može se upotrebiti za proizvodnju α-sinukleina nativne sekvence nakon proteolize TEV proteazom. Gen za mCerulean3 je nizom lančanih reakcija polimeraze (SOEing PCR) fuzionisan sa genom za α-sinuklein i nakon amplifikacije ukloniran u plazmid pDUET-1. *Escherichia coli* BL21(DE3) je, nakon transformacije ovim konstruktom, upotrebljena za proizvodnju himernog proteina koji je zadržao fluorescentna svojstva sa prinosom od ~2 mg po litru medijuma nakon prečišćavanja imobilizovanom metal-afinitetnom hromatografijom (elektroforetska čistoća: ~80%). Ovaj himerni protein je uspešno proteolizovan TEV proteazom.

Cloning and expression of fluorescently labeled α-synuclein in *Eschierichia coli*

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Fluorescently labeled proteins are invaluable tools in laboratory practice to assess the *in vivo* localization and the interactions of proteins. Here we have designed an expression vector with an N-terminal hexahistidine-tagged mCerulean3 fused through a polyasparagine linker and the proteolytic site of tobacco etch virus protease (TEV) to α-synuclein. This construct can be used to produce α-synuclein of a native sequence after proteolysis with TEV protease. After fusion of the genes for mCerulean3 and α-synuclein through a series of polymerase chain reactions (SOEing PCR), the resulting gene for the chimeric protein was cloned into the pDUET-1 plasmid. *Escherichia coli* BL21(DE3), upon transformation with this construct, can be used to produce the chimeric protein that retained the fluorescent properties of mCerulean3, with a yield of ~2 mg per liter of medium after purification by immobilized metal-affinity chromatography (electrophoretic purity: ~80%). This chimeric protein was successfully proteolyzed by TEV protease.
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Elektrohemija

Electrochemistry

EH-1

Potencijal otvorenog kola različitih referentnih elektroda u etalinu

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Eutektičke smeše su od početka 21. veka dobile veliku pažnju hemičara i našle primenu u različitim oblastima, npr. kao elektroliti za elektrohemijsko taloženje. Kod primene ovih smeša u elektrohemiji veoma je važno odabrati adekvatnu referentnu elektrodu pomoću koje se može tačno meriti elektrodni potencijal radne elektrode tokom vremena. Cilj ovog rada je bio da se ispita stabilnost različitih komercijalnih referentnih elektroda (kalomelova-ZKE, srebro-srerbo hloridna i metalna) u eutektičkoj smeši holin hlorida i etilenglikola – etalinu. Tokom dužeg vremena praćen je elektrodni potencijal sedam elektroda i pokazano je da ZKE ima veoma nestabilan elektrodni potencijal u etalinu. Kao najstabilnije elektrode u etalinu su se pokazale metalne elektrode, odnosno srebrna i platinska žica.

Open circuit potential of various reference electrodes in ethaline

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Deep eutectic mixtures (DES) have received great attention since the beginning of the 21st century and have been used in various fields, such as electrolytes for electrochemical deposition. In DES application in electrochemistry, it is very important to choose an adequate reference electrode (RE) that can accurately measure the electrode potential of the working electrode over time. The aim of this study was to examine the stability of various commercial REs (calomel-SCE, silver-silver chloride and metal) in mixture of choline chloride and ethylene glycol – ethaline. The electrode potential of seven RE was monitored over time and it was shown that SCE has an unstable electrode potential in ethaline. Metal electrodes, the silver and platinum wire, proved to be the most stable electrodes in ethaline.

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EH-2

Kompozitne bioaktivne prevlake sa gentamicinom elektroforetski taložene na titanu

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Multifunkcionalni i višekomponentni biomaterijali se često primenjuju u rekonstruktivnoj hirurgiji zbog sposobnosti da pospešuju osteointegraciju, istovremeno omogućavajući primenu antibakterijskih agenasa direktno na mestu intervencije. Primenom elektroforetskog taloženja, iz četvorokomponentne vodene suspenzije (hidroksiapatit, poli(vinilalkohol), hitozan i gentamicin) dobijene su, u jednom koraku, bioaktivne i antibakterijske kompozitne prevlake na titanu. Karakterizacija prevlaka je izvršena primenom rendgenske difrakcione analize (XRD), infracrvene spektroskopije sa Furijeovom transformacijom (FTIR) i skenirajuće elektronske mikroskopije (SEM). Praćenjem kinetike antibakterijske aktivnosti u suspenziji potvrđena je antibakterijska efikasnost prevlake sa gentamicinom. Prema dobijenim rezultatima moguće je zaključiti da dobijene kompozitne prevlake sa gentamicinom predstavljaju uspešan biomaterijal za potencijalnu primenu u biomedicini.

Composite bioactive coatings loaded with gentamicin electrophoretically deposited on titanium

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Multifunctional and multicomponent biomaterials are very often the material of choice in reconstructive surgery, having the ability to promote osteointegration, allowing the antibacterial agents application directly at the site of intervention. Single-step electrophoretic deposition was employed to assemble bioactive and antibacterial composite coatings on titanium, from a four-component aqueous suspension (hydroxyapatite, poly(vinyl alcohol), chitosan and gentamicin). Physico-chemical characterization of the coatings was performed using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). Antibacterial activity of gentamicin loaded coating was confirmed by antibacterial activity kinetics in suspension. According to the obtained results, it can be concluded that composite coating loaded with gentamicin represents a successful biomaterial for possible application in biomedicine.

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EH-3

Elektroforetski taložene kompozitne prevlake kao nosači lekova

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Metoda elektroforetskog taloženja (EPD)se koristi za sintezu biokompatibilnih kompozitnih materijala za medicinsku primenu kao antibakterijske prevlake za koštane implantate. Taloženjem pri konstantnom naponu je uspešno dobijena kompozitna prevlaka hidroksiapatit/hitozan/poli(vinilalkohol) (HAP/CS/PVA) koja sadrži gentamicin (Gent). Bioaktivnost prevlake je dokazana formiranjem novonastalog apatitnog sloja u simuliranoj telesnoj tečnosti i karakterisana primenom skenirajuće elektronske mikroskopije (SEM) I infracrvene spektroskopije sa Furijeovom transformacijom (FTIR). Sposobnost oseointegracije dalje je potvrđena merenjem aktivnosti alkalne fosfataze (ALP), što ukazuje na povoljna oseopromotivna svojstva taloženih prevlaka. Kada su testirane humane i mišje fibroblastne ćelijske linije (MRC-5 i L929), kompozitne prevlake nisu pokazale citotoksični efekat.

Electrophoretically deposited composite coatings as drug carriers

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The electrophoretic deposition (EPD) method isused for the synthesis of biocompatible composite materials for medical use as antibacterial coatings for bone implants. Deposition at the constant voltage yielded composite coating hydroxyapatite/chitosan/poly(vinyl alcohol)(HAP/CS/PVA) loaded with gentamicin (Gent). Bioactivity of the coating was proved by a newly formed apatite layer in simulated body fluid and characterized usingscanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). The osseointegration ability was validated by measuring the alkaline phosphatase activity (ALP) indicating the favorable osseopromotive properties of deposited coatings. When tested against human and mice fibroblast cells lines (MRC-5 and L929), composite coatings did not exhibit cytotoxic effect.

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EH-4

Bakterijska nanoceluloza kao nosač metalnih nanočestica za efektivnu oksidaciju metanola

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Bakterijska nanoceluloza (BNC) privlači sve veću pažnju istraživanja zahvaljujući svojoj održivosti, biodegradabilnosti, obnovljivosti, nanometarskim dimenzijama, razvijenoj površini, jedinstvenim optičkim i mehaničkim svojstvima, itd. Pored toga što je primena BNC prepoznata u različitim oblastima: kao ambalažni materijal za hranu, biomedicini, farmaciji, tretmanu vode, elektronici, biosenzorima, BNC ima veliki potencijal kao "zeleni" nosač metalnih čestica sa superiornim katalitičkim svojstvima. Cilj ove studije je razvoj platinski nanočestica na BNC kao "zelenom" nosaču, Pt-BNC. Novi Pt-BNC katalizator je uspešno sintetisan metodom mikrotalasne iradijacije, što je potvrđeno infracrvenom spektroskopijom sa Furijevom transformacijom (FTIR), termogravimetrijskom analizom (TGA), mikroskopijom atomskih sila (AFM), transmisionom elektronskom mikroskopijom (TEM), dok je željena elektrokatalitička aktivnost povrđena u reakciji oksidacije metanola.

Bacterial nanocellulose as metalic nanoparticles carrier for effective methanol oxidation

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Bacterial nanocellulose (BNC) has attained an extensive research attention due to its sustainability, biodegradability, renewability, nanoscale dimensions, large surface area, unique optical and mechanical performance, etc. Besides the application of BNC has been recognized in various fields: food packaging, biomedical, pharmaceutical, water treatment, electronics, biosensors, BNC has a great potential as a green support for metalic nanoparticles with superior catalytic properties. The aim of this study was development of platinum supported nanoparticles on BNC as a green carrier, Pt-BNC. The new Pt-BNC catalyst was succesfully synthesized applying microwave assisted irradiation method, which was confirmed by Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), atomic force microscopy (AFM), and transmission-electron microscopy (TEM), while the desirable electrocatalytic activity was confirmed in methanol oxidation reaction.

EH-5

Kompozit polipirol/srebro-hlorid kao katodni materijal za punjive magnezijumske baterije

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U radu je ispitivano elektrohemijsko ponašanje elektrode na bazi polipirola (PPy) kao katodnog materijala u magnezijumskim punjivim ćelijama. PPy je sintetisan galvanostatski na ugljeničnoj tkanini (CF). Potom je na CF/PPy nanet AgCl primenom modifikovane metode sukcesivne jonske adsorpcije i reakcije (SILAR) [1]. Primenom ciklične voltametrije i galavnostatskog punjenja/pražnjenja pokazano je veoma dobro elektrohemijsko ponašanje kompozitnog materijala CF/PPy-AgCl. Za punjivu magnezijumsku ćeliju na bazi vodenog elektrolita: AZ63 | 3.5% NaCl | CF/PPy-AgCl, primenom specifičnih struja u opsegu od 135 do 1350 A g^{-1} dobijene su vrednosti specifične energije u opsegu 42-25 Wh kg^{-1}, specifične snage 100 – 1600 W kg^{-1}, specifičnog kapaciteta 35-25 Ah kg^{-1}. Takođe, ispitivana je i ciklična stabilnost.

[1] Grgur, B.N., Gojgić, J., Petrović, M., J. Power Sources, **2021**, *490*, 229549

Polypyrol/silver chloride composite as cathodic material for rechargeable magnesium batteries

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The electrochemical behavior of an electrode based on polypyrrole (PPy) as a cathode material in rechargeable aqueous-based magnesium cells was investigated. PPy was synthesized galvanostatically on carbon felt (CF). AgCl was then applied to CF / PPy using the modified successive ionic adsorption and reaction method (SILAR) [1]. The application of cyclic voltammetry and galvanostatic charge/discharge showed very good electrochemical behavior of the composite material CF/PPy-AgCl. For rechargeable magnesium cell based on water electrolyte: AZ63 | 3.5% NaCl | CF/PPy-AgCl, using specific currents in the range from 135 to 1350 A g^{-1}, the values of specific energy of 42-25 Wh kg^{-1}, specific power 100 - 1600 W kg^{-1}, and specific capacity 35-25 Ah kg^{-1} were obtained. Cyclic stability was also examined.
[1] Grgur, B.N., Gojgić, J., Petrović, M., J. Power Sources, **2021**, *490*, 229549

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EH-6

Etarsko ulje *Picea omorika* kao zeleni inhibitor korozije mekog čelika u 1M rastvoru HCl

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Etarska ulja i ekstrakti biljaka spadaju u zelene inhibitore korozije jer su ekološki prihvatljivi, jeftini, netoksični po ljude i poseduju veliku efikasnost inhibicije korozije. U našem istraživanju proučavali smo etarsko ulje *Picea omorika* (Pančić) Purk., kao zelenog inhibitora korozije na čeliku u 1M HCl. Etarko ulje je dobijeno hidrodestilacijom svežih iglica korišćenjem aparature po Klevendžeru. Inhibitorska efikasnost je određena za različite koncentracije inhibitora, tokom različitog vremena delovanja agensa korozije. Koroziona stabilnost inhibitora je određena elektrohemijskim metodama, spektroskopijom elektrohemijske impedancije (EIS) i polarizacionim merenjima. Pokazano je da se optimalna efikasnost inhibicije korozije od 92% postiže sa 200 ppm ulja Pančiceve omorike nakon četiri sata.

Picea omorika essential oil as a green corrosion inhibitor for mild steel in 1M HCl solution

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Essential oils and extracts of plants are green corrosion inhibitors because there are environmentally friendly, non-toxic, inexpensive, not harmful to human health, and they possessing high corrosion inhibition efficiency. In our research, we studied the essential oil of *Picea omorika* (Pančić) Purk. as a green corrosion inhibitor on steel in 1M HCl. Essential oil of fresh dried needles was obtained by hydrodistillation using the Clevenger-type apparatus. IE was determined for different concentrations of inhibitors, as well as for different times of immersion in HCl. Electrochemical Impedance Spectroscopy (EIS) and Polarization Measurements were utilised to estimate the IE of the oil. Our results showed that the optimal concentration of 200 ppm *P. omorika* essential oil providing 92% inhibition efficiency after four hours.

EH-7

Zeleni čaj kao inhibitor korozije čelika u rastvoru veštačke krvne plazme

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Ekstrakt zelenog čaja ispitivan je kao potencijalni inhibitor korozije čelika u rastvoru veštačke krvne plazme. Na osnovu potenciodinamičkih polarizacionih merenja u osnovnom rastvoru i uz dodatak inhibitora, uočeno je da u prisustvu ekstrakta zelenog čaja dolazi do pomeranja korozionog potencijala ka pozitivnijim vrednostima i do smanjenja korozione gustine struje, što ukazuje da dolazi do usporavanja anodnog korozionog procesa. Pored toga, uočeno je da povećanje masenog udela ekstrakta zelenog čaja u rastvoru veštačke krvne plazme dovodi do povećanja efikasnosti inhibicije. Najveći stepen efikasnosti (89,2%) postignut je pri masenom udelu inhibitora od 40%. Takođe, na osnovu rezultata ciklične voltametrije uočeno je da se sa povećanjem masenog udela inhibitora smanjuje brzina oksidacije čelika.

Green tea as an inhibitor of steel corrosion in artificial blood plasma solution

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Green tea extract has been investigated as a potential inhibitor of steel corrosion in artificial blood plasma solution. According to the potentiodynamic polarization measurements in blank solution and in the presence of inhibitor, it was observed that the addition of green tea extract shifted the corrosion potential to more positive values and reduced the corrosion current density. This behavior indicates that the anodic corrosion process is slowed down. In addition, it has been observed that increasing the mass fraction of green tea extract in artificial blood plasma solution leads to increased inhibition efficiency. The highest degree of efficiency (89.2%) was achieved with a mass fraction of green tea extract of 40%. Also, based on the results of cyclic voltammetry, it was observed that the rate of oxidation of steel decreases with increasing mass fraction of inhibitor.

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Zelena hemija

Green Chemistry

GC-1

Adsorpcija i desorpcija potencijalno toksičnih metala na mehanohemijski modifikovanom pirofilitu

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Uklanjanje potencijalno toksičnih metala iz otpadnih voda primenom adsorpcije na prirodnom materijalu kao što su gline predstavlja efikasan, jeftin i ekološki prihvatljiv postupak u očuvanju životne sredine. Pirofilit je prirodni mineral aluminijum-silikatne gline sa visokom tačkom topljenja i stabilnim hemijskim svojstvima. Cilj ovog rada je ispitivanje sorpcionih svojstava mehanički aktiviranog pirofilita za uklanjanje dvovalentnih potencijalno toksičnih metala (Me(II): Zn, Cd, Pb, Cu i Ni). Utvrđeno je da su manje čestice pirofilita efikasnije za uklanjanje Me(II) zbog veće površine adsorbenta i veće dostupnosti aktivnih mesta za adsorpciju. Sorpcija odabranih jona metala na pirofilitu opada sledećim redosledom (Cu ≈ Pb > Cd > Zn > Ni). Takođe, Me(II) koji se najbrže i najviše adsorbuju na pirofilit (Cu i Pb) se najmanje desorbuju. Rezultati su pokazali da manipulacijom eksperimentalnih uslova moguće ukloniti > 99% Me(II).

Adsorption and desorption properties of potentially toxic metals by mechanochemically activated pyrophyllite

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Removal of potentially toxic metals from wastewater using adsorption by natural materials such as clays is an efficient, inexpensive and environmentally friendly process. Pyrophyllite is a natural mineral of aluminum silicate clay with a high melting point and stable chemical properties. This paper aims to investigate the sorption properties of mechanically activated pyrophyllite for the removal of divalent potentially toxic metals (Me (II): Zn, Cd, Pb, Cu and Ni). Smaller pyrophyllite particles are more efficient for the removal of Me(II) due to the increased adsorbent surface area and enhanced availability of more active sites for the adsorption. Sorption of selected metal ions on pyrophyllite decreases in the following order (Cu ≈ Pb> Cd> Zn> Ni). Also, Cu(II) and Pb(II), which are the fastest and most adsorbed on pyrophyllite, are desorbed in a very low percentage. The results showed higher than 99% of Me(II) could be removed by manipulating the experimental conditions.

GC-2

Procena ekološke prihvatljivosti separacione metode na bazi jonskih tečnosti za određivanje Cd(II) i Pb(II)

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Vodeni dvofazni sistemi (DVS) na bazi jonskih tečnosti (DVS-JT) predstavljaju novi pravac u razvoju separacionih metoda zasnovanih na principima zelene hemije. U ovom radu razvijena je metoda pripreme uzorka sa funkcionalizovanom JT (1-butil-3-metilimidazolijum 2-merkaptobenzotiazolom) za direktnu ekstrakciju Cd(II) i Pb(II) iz sedimenta reke Save. Zelenost predložene metode je procenjena korišćenjem sledećih kompjuterskih alata: NEMI (Environmental Methods Index, 2007), GAPI (Green Analytical Procedure Index, 2018), AGREE (Analytical GREEnness Metric Approach and Software, 2020) i AGREEprep (Analytical greenness metric for sample preparation, 2022). Kriterijumi za ocenjivanje zelenosti su zanovani na proncipima zelene hemije i transformisani su u skalu od 0–1. Predložena metoda ima skor zelenosti od 0.7 što je svrstava u zelene metode.

Evaluation of the environmental acceptability of the separation method based on ionic liquid for Cd(II) and Pb(II) determination

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Aqueous two-phase systems (ABS) based on ionic liquids (ABS-IL) represent a new direction in the development of separation methods based on the principles of green chemistry. In this work, a sample preparation method with functionalized IL (1-butyl-3-methylimidazolium 2-mercaptobenzothiazole) for direct extraction of Cd(II) and Pb(II) from the solid sample (sediment of the Sava River) was developed. The greenness of the proposed method was evaluated using tools like NEMI (National Environmental Methods Index, 2007), GAPI (Green Analytical Procedure Index, 2018), AGREE (Analytical GREEnness Metric Approach and Software, 2020) and AGREEprep (Analytical greenness metric for sample preparation, 2022). The assessment criteria are taken from the principles of green chemistry and transformed into a unified 0–1 scale. The method proposed in this paper has a greenness score of 0.7 which classifies it as a green method.

GC-3

Ispitivanje interakcija u vodenim rastvorima novosintetisane jonske tečnosti tetrabutilfosfonijum-nikotinata

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Cilj ovog rada je sinteza i ispitivanje solvatacionih svojstava herbicidne jonske tečnosti na bazi tetrabutilfosfonijum katjona ($[tbP]^+$), tipičnog predstavnika herbicidnih jona, dok je anjon nikotinska kiselina ($[Nic]^-$). Uspešnost sinteze je potvrđena IR i NMR merenjima. Ispitivane su interakcije ove jonske tečnosti sa vodom, osnovnim medijumom u kom se odvijaju biohemijski procesi. Merenja gustina, viskoznosti, indeksa refrakcije i prostiranja brzine zvuka kroz vodene rastvore [tbP][Nic] urađena su u temperaturnom opsegu od 293,15 do 313,15 K. Izračunate su privdne molarne zapremine koje su fitovane *Masson*-ovom jednačinom iz koje dobijeni nagib (S_v) ukazuje na jake interkacije između jona, dok *Hepler*-ov koeficijent ukazuje na *structure making* svojstva [tbP][Nic]. Dobijene vrednosti koeficijenta *B* iz *Jones-Dole*-ove jednačine i njegova promena sa temperaturom potvrđuju *structure making* osobine jonske tečnosti [tbP][Nic].

Investigation of interactions in aqueous solutions of newly synthesized ionic liquid tetrabutylphosphonium nicotinate

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The aim of this work is the synthesis and solvation properties investigation of herbicidal ionic liquid based on tetrabutylphosphonium cation ($[tbP]^+$), a typical herbicidal ion, while the anion is nicotinic acid ($[Nic]^-$). The success of the synthesis was confirmed by IR and NMR measurements. The interactions of this ionic liquid with water, the essential medium for biochemical processes, were investigated. Measurements of density, viscosity, refractive index and speed of sound for [tbP][Nic] aqueous solutions were made in the temperature range from 293.15 to 313.15 K. The slope (S_v) indicates strong interactions between ions, while the *Hepler* coefficient indicates the *structure making* properties of the [tbP][Nic]. The obtained coefficient *B* values from the *Jones-Dole* equation and its change with temperature confirm the *structure making* properties of the ionic liquid [tbP][Nic].

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GC-4

Biokataliza u mikroreaktoru: enzimsko obezbojavanje tekstilne boje

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Uklanjanje boja iz otpadnih voda je jedan od glavnih interesovanja naučne zajednice koja se bavi zaštitom životne sredine. U ekološko prihvatljive metode za prečišćavanje otpadnih voda spadaju i enzimski tretmani, među kojima je i oksidacija boja peroksidazom. Visoka tržišna cena prečišćenih enzima dovela je do izolovanja enzima iz jeftinih izvora i do primene enzima u obliku sirovog ekstrakta. Izvođenje kontinualnog sistema doprinosi povećanoj efikasnosti procesa. U ovom radu, izolovana je peroksidaza iz otpadnog materijala – krompirovih ljuski za obezbojavanje boje Acid Violet 109. Uklanjanje je izvršeno u kontinualnom mikroreaktoru. Optimizovani su glavni procesni parametri: vreme zadržavanja, aktivnost enzima, koncentracija vodonik-peroksida i boje, kao i prečnik i dužina reaktora. Nakon vremena zadržavanja od 3 min u mikroreaktoru prečnika 0,5 mm i dužine 6m, procenat obezbojavanje je iznosio 76%.

Continuous flowbiocatalysis: enzymatic decolorization of textile dye

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Dye removal from wastewater is one of the major interests of the scientific community dealing with environmental protection. Among available techniques for wastewater decolorization is dye oxidation using peroxidase. Taking into consideration the high market price of purified enzymes, the isolation of enzymes from cheap sources and the potential use of crude enzyme extractscontributes to the sustainabilityof the treatment. Furthermore, introducing continuous flow systems enhances the process's productivity and efficiency. In this study, peroxidase was isolated from waste material –potato peel and used for removal of anthraquinone dye Acid Violet 109 in a continuous flow. The main process parameters were optimized: residence time, enzyme activity, hydrogen peroxide and dye concentration, as well as the reactor's length and diameter. After 3min of residence time, in a microreactor with 0.5 mm diameter and 6m length, the decolorization rate was 76%.

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GC-5

Fizičko-hemijska svojstva i antifungalna aktivnost novosintetisanih jonskih tečnosti na bazi imidazola sa homologim nizom hloridnih oksianjona

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Cilj ovog rada je ispitivanje fizičko-hemijskih svojstava i antifungalne aktivnosti jonskih tečnosti na bazi 1-butil-3-metilimidazolijum katjona ($[Bmim]^+$) sa hloridnim oksianjonima slabe kiseline ($HClO_2$) i jakih kiselina ($HClO_3$ i $HClO_4$) u homologom nizu. Sintetisane su tri jonske tečnosti: $[Bmim][ClO_2]$, $[Bmim][ClO_3]$ i $[Bmim][ClO_4]$. Merenja gustina, viskoznosti i električne provodljivosti urađena su u temperaturnom opsegu od 293,15 do 323,15 K. Izračunate su vrednosti energije aktivacije viskoznog toka i molarne provodljivosti. Vrednosti stepena jonizacije dobijene iz *Walden*-ovog zakona ukazuju da su jonske tečnosti $[Bmim][ClO_3]$ i $[Bmim][ClO_4]$ skoro potpuno disosovane. Nasuprot njima, $[Bmim][ClO_2]$, spada u "poor ionic liquids" što ukazuje na postojanje značajne asocijacije u ovoj jonskoj tečnosti. Antifungalna aktivnost jonskih tečnosti ispitana je na većem broju gljiva iz soja *Fusarium*.

Physicochemical properties and antifungal activity of newly synthesized imidazole-based ionic liquids with homologous series of chlorine oxyanions

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This paper investigates the physicochemical properties and antifungal activity of 1-butyl-3-methylimidazolium ($[Bmim]^+$) based ionic liquids with chlorine oxyanions of a weak acid ($HClO_2$) and strong acids ($HClO_3$ and $HClO_4$) in a homologous series. Three ionic liquids were synthesized: $[Bmim][ClO_2]$, $[Bmim][ClO_3]$ and $[Bmim][ClO_4]$. Measurements of density, viscosity and electrical conductivity were performed in the temperature range from 293.15 to 323.15 K. The values of activation energy of viscous flow and molar conductivity were calculated. The values of the ionicity obtained from Walden's law indicate that the ionic liquids $[Bmim][ClO_3]$ and $[Bmim][ClO_4]$ are almost completely dissociated. In contrast, $[Bmim][ClO_2]$ belongs to the "poor ionic liquids" and indicates a significant association in this ionic liquid. The antifungal activities of ionic liquids against several *Fusarium* strains were examined.

Acknowledgment: This Project is supported by Provincial Secretariat for Higher Education and Scientific Research, grant number: 142-451-2545/2021-01.

Medicinska hemija

Medicinal Chemistry

MH-1

In silico ispitivanje interakcija Ru(II) kompleksa sa DNK i humanim serum albuminom

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Glavni cilj u otkriću novih lekova na bazi jona metala predstavlja razvoj i implementacija inovativnih terapija povećane efikasnosti i tolerancije.[1] Kompleksi rutenijuma u okviru ovih istraživanja pokazali su obećavajuće rezultate kao potencijalni antikancerogeni agensi, što je posledica njihovih jedinstvenih osobina.[2] Da bi se razumeo mehanizam delovanja Ru(II) kompleksa, neohodno je poznavati agens/DNK i agens/protein interakcije. U okviru ovog istraživanja izučavane su interakcije novih Ru(II) kompleksa (opšte formule *mer*-[Ru(tpy)(N-N)Cl]Cl, gde je N-N *o*-benzohinondiamin (**1**) i 2,3-naftohinondiamin (**2**)) sa DNK i humanim serum albuminom (HSA) primenom simulacije molekulskog dokinga. Kompleks **2**, usled prisustva dodatne fenil grupe, pokazao je bolje rezultate u interakcijama sa DNK, interkalacijom i vezivanjem za mali žljeb, kao i bolje rezultate u interakcijama sa HSA molekulom.

In silico investigation of the interactions of Ru(II) complexes with DNA and human serum albumin

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The major goal in the discovery of new metallodrugs is to develop and implement innovative therapies with increased effectiveness and tolerability.[1] Ruthenium-based drugs have achieved promising results as potential anticancer agents due to their unique properties.[2] To reveal the mechanism of action of Ru(II)-based drugs, it is essential to understand both drug/DNA and drug/protein interactions. Within this paper are presented the results of the *in silico* investigation of the interactions of Ru(II) complexes (with general formula *mer*-[Ru(tpy)(N-N)Cl]Cl, where N-N is *o*-benzoquinonediimine and 2,3-naphthoquinonediimine) with DNA and human serum albumin (HSA) by applying a molecular docking simulation. Complex **2,** due to the presence of additional phenyl group, has exhibit better results in the interactions with DNA, by intercalation and by minor groove binding, as well as better results in the interactions with HSA.

1.T. Lazarević, A. Rilak, Ž. D. Bugarčić, *Eur. J. Med. Chem.*, **2017**, 142, 8 -31.
2.A. Rilak Simović, R. Masnikosa, I. Bratsos, E. Alessio, *Coord. Chem. Rev.*, **2019**, 398, 113011.

MH-2

Sinteza i antiproliferativna aktivnost (+)-protulaktona A i njegovih analoga

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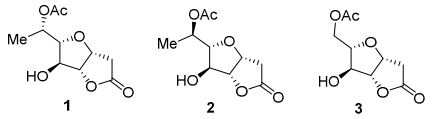
U ovom radu će biti prikazana sinteza, antiproliferativna i antimikrobna aktivnost prirodnog proizvoda (+)-protulaktona A (**1**), njegovog C-7 epimera (**2**) i nor-analoga (**3**), prikazanih na Shemi 1. Struktura prirodnog proizvoda **1** je potvrđena rendgenostrukturnom analizom. Biće razmatrana i veza odabranih strukturnih karakteristika i antiproliferativne aktivnosti (SAR analiza).



*Shema 1. Strukture (+)-protulaktona A (**1**) i njegovih analoga **2** i **3**.*

Synthesis and antiproliferative activity of (+)-protulactone A and its analogues

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This paper will present the synthesis, antiproliferative and antimicrobial activity of the natural product (+)-protulactone A (**1**), its C-7 epimer (**2**), and nor analogue (**3**), shown in Scheme 1. The structure of natural product **1** was confirmed by X-ray analysis. In addition, the relationship between selected structural features and antiproliferative activity (SAR analysis) will be considered.

Acknowledgment to financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-68/2022-14/200125) and (in part) research projects from the Serbian Academy of Sciences and Arts (Grant No. 01-2019-F6501-2019-F65 and F-130).

MH-3

Kreiranje QSAR modela humanog CYP17A1

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Cilj u razvoju lekova za androgen-zavisne bolesti je inhibicija enzima CYP17A1. *In vitro* skrining velikih baza radi otkrivanja vodećih jedinjenja je veoma zahtevno, pa je potrebno kreirati kompjuterski model za predviđanje potencijalnih liganada ovog enzima. Razvili smo QSAR model, zasnovan na *in vitro* dobijenim IC_{50} vrednostima jedinjenja (244 liganada CYP17A1: 135 aktivni i 109 neaktivnih), selekcijom među derivatima androstana i žučnih kiselina pomoću Random Forest classifier. Na osnovu razvijenog modela, 75% svih jedinjenja koja se nalaze u domenu primenljivosti modela, je tačno klasifikovano, pa da se dobijeni model može koristiti za virtuelni skrining novih liganada humanog CYP17A1 enzima.

Creation of the QSAR model of human CYP17A1

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One of the main targets in the development of efficient drugs for the treatment of androgen-dependent cancer is human cytochrome P450 17A1 enzyme. *In vitro* screening of a huge library of substances for the identification of lead compound is time- and resource-consuming, so the creation of a computational model for the prediction of the perspective molecules for further experimental evaluation is of high importance. In the present study QSAR model, based on Random Forest classifier was developed and evaluated using the database of the modified androstanes and bile acids, where a database was created on the basis of the *in vitro* obtained IC_{50} values of the compounds (244 CYP17A1 ligands: 135 active, 109 inactive). 1D and 2D descriptors were calculated using PaDEL-Descriptor software. The best parameters of the model were identified using a grid search approach with k-fold cross-validation (k=8) and applicability domain based on the Local Outlier Factor was calculated. Based on the developed model, 75% of all compounds that are in the applicability domain of the model were classified correctly, so obtained model can be used for the virtual screening of novel ligands of human CYP17A1 enzyme.

Results are obtained in the frame of Belarus-Serbia bilateral projects (X18SRBG-002/51-03-003036/2017-09/02 and X20SRBG-004/337-00-00612/2019-09/04)

MH-4

QSAR analiza inhibitora karboanhidraze: Slučaj GABA konjugata aromatičnih/heterocikličnih sulfonamida

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Aromatični/heterociklični sulfonamidni lekovi su poznati po inhibiciji enzima karboanhidraze koji učestvuju u različitim fiziološkim procesima. Sulfonamidi se uspešno koriste u lečenju periodične i prolazne slabosti koja često prati hiperkalemijsku periodičnu paralizu, kongenitalnu paramiotoniju i Bekerovu mišićnu distrofiju. Modelovanje kvantitativnog odnosa strukture i aktivnosti (QSAR) moćna je metoda kompjuterske medicinske hemije. QSAR analiza serije aromatičnih/heterocikličnih sulfonamida sa fragmentom γ-aminobuterne kiseline (GABA), sprovedena je da bi se odredili topološki i fizičko-hemijski parametri odgovorni za inhibitornu aktivnost sulfonamida prema izoformama karboanhidraze (CA) II i IV. Dobijeni QSAR modeli su omogućili utvrđivanje ključnih strukturnih karakteristika sulfonamida, značajnih za njihovo vezivanje za ispitane CA izoforme. Rezultati ove studije mogu pomoći u dizajniranju snažnijih inhibitora karboanhidraze, koji se mogu potencijalno koristiti u lečenju hiperkalemijske periodične paralize.

QSAR analysis of carbonic anhydrase inhibitors: A case of GABA conjugates of aromatic/heterocyclic sulfonamides

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Aromatic/heterocyclic sulfonamide drugs are clinically known for inhibiting carbonic anhydrase enzymes involved in different physiological functions. Sulfonamides are successfully used to resolve episodic and transient weakness that frequently accompanies hyperkalemic periodic paralysis, paramyotonia congenita, and Becker disease. Quantitative structure-activity relationship (QSAR) modeling is a powerful computational tool employed in medicinal chemistry. A QSAR study on a series of aromatic/heterocyclic sulfonamides, incorporating γ-aminobutyric acid (GABA) moiety, was performed to explore the topological and physicochemical parameters responsible for their inhibitory activity toward carbonic anhydrase (CA) II and IV isoforms. The derived QSAR models allowed us to put forth structural features that played a crucial role in the binding affinity of sulfonamides versus the two CA isoforms. The results of the present study may be helpful in the design of more potent carbonic anhydrase inhibitors for hyperkalemic periodic paralysis treatment.

Acknowledgment: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2022-14/200113)

MH-5

Sinteza i citotoksičnost novog butanolida

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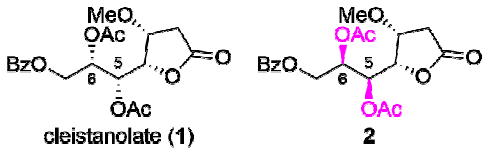
Nyandoro i saradnici[1] su 2017. godine izolovali prirodni kleistanolat (**1**) iz metanolnog ekstrakta listova *Cleistochlamys Kirkii*. U ovom radu prikazana je višefazna sinteza novog analoga kleinstanolata **2** (*Scheme 1*) polazeći iz D-ksiloze. Antiproliferativna aktivnost jedinjenja **2**, kao i uticaj stereohemije na C-5 i/ili C-6 na citotoksičnost detaljno će biti prezentovani.



*Scheme 1. Structures of cleistanolate (**1**) and its novel analogue **2**.*

Synthesis and citotoxicity of novel butanolide

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In 2017, Nyadoro and coworkers[1] has isolated natural cleistanolate (**1**) from methanol extract of leaves of *Cleistochlamys Kirkii*. In this report is presented synthesis of novel cleistanolate analogue **2** (*Scheme 1.*) starting from D-xylose. Antiproliferative activity of compound **2**, as well as influence of stereochemistry at C-5 and/or C-6 on citotoxic activity will be presented in details.

Acknowledgment to financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-68/2022-14/200125) and (in part) research projects from the Serbian Academy of Sciences and Arts (Grant No. 01-2019-F6501-2019-F65 and F-130).

[1] S. S. Nyandoro, J. J. E. Munissi, A. Gruhonjic, S. Duffy, F. Pan, R. Puttreddy, J. P. Holleran, P. A. Fitzpatrick, J. Pelletier, V. M. Avery, K. Rissanen, M. Erdélyi, *J. Nat. Prod.* **2017**, *80*, 114–125.

MH-6

Uticaj kompleksa Ru(II) na moguće puteve apoptoze u K562 ćelijama leukemije

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U cilju pronalaženja adekvatne terapije u lečenju maligniteta kompleksi rutenijuma pokazali su zavidan potencijal. Kompleksi Ru(II) sa *N*-alkilfenotiazinima, hlorpromazinom, trifluoperazinom i tioridazinom, korišćeni su u ispitivanju mogućih puteva apoptoze u K562 ćelijama. Ispitivana je spektrofotometrijski ekstracelularna LDH, ekspresija COX-2, t-JNK, p-JNK i β-aktina imunohemijski nakon SDS elektroforeze. Kompleks Ru(II) sa trifluoperazinom u koncentraciji od 10 μM smanjuje ekspresiju t-JNK, inhibira COX-2 oko 42%, značajno povećava količinu ekstracelularne LDH u odnosu na netretirane K562 ćelije i time potvrdjuje apoptozu ovih ćelija.

Influence of Ru(II) complex on possible pathways of apoptosis in K562 leukemia cells

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[1] Faculty of Veterinary Medicine, University of Belgrade, Bulevar oslobodjenja 18, 11000 Belgrade, Serbia, [2]Institute for Medical Research, P.O. Box 102, 11129 Belgrade, Serbia, [3]Faculty of Chemistry, University of Belgrade, P.O. Box 158, 11001 Belgrade, Serbia

Ruthenium complexes are of significant interest in the treatment of malignancies. Ru(II) complexes with *N*-alkylphenothiazines (chlorpromazine, trifluoperazine, and thioridazine) were used in the study of possible apoptosis pathways in K562 cells. Spectrophotometrically extracellular LDH was quantified and immunochemical expression of COX-2, t-JNK, p-JNK and β-actin after SDS electrophoresis was determined. The Ru(II) complex with trifluoperazine at a concentration of 10 μM reduced t-JNK expression, inhibited COX-2 by about 42%, significantly increased the amount of extracellular LDH compared to the untreated K562 cells and thus confirmed apoptosis.

Acknowledgements: The study was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract number 451-03-68/2022-14/200143).

MH-7

Sinteza i ispitivanje biološke aktivnosti ariltio i aralkiltio derivata 2-*terc*-butil-1,4-benzohinona

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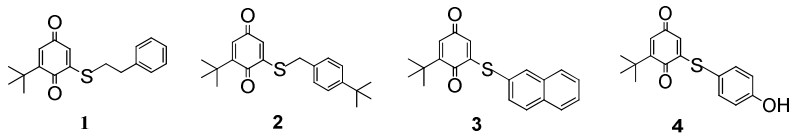
Sintetisana su dva ariltio i dva aralkiltio derivata 2-*terc*-butil-1,4-benzohinona reakcijom Michael-ove adicije tiola na hinonsko jezgro u etanolu (Slika 1).



Slika 1. Sintetisani derivati 2-*terc*-butil-1,4-benzohinona.

Dobijenim derivatima je ispitana antimikrobna i antioksidativna aktivnost, kao i toksičnost na račiće *Artemia salina.* Najjaču antimikrobnu aktivnost je pokazao derivat **4**, najveću antioksidativnu aktivnost je imao derivat **2** (IC_{50}=0,0526 mM), dok je toksičnost prema račićima ispoljio samo derivat **4** (LC_{50}=0,032 mM).

Synthesis and investigation of biological activity of arylthio and aralkylthio derivatives of 2-*tert*-butyl-1.4-benzoquinone

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Two arylthio and aralkylthio derivatives of 2-*tert*-butyl-1.4-benzoquinone were synthesized by Michael addition of thiols on quionone moiety in ethanol (Figure 1).

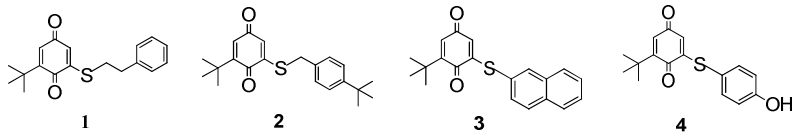

Figure 1. Synthesized derivatives of 2-*tert*-butyl-1.4-benzoquinone.

For all compounds antimicrobial and antioxidant activity was investigated, as well as toxicity towards nauplii of *Artemia salina.* Derivative **4** showed the strongest antimicrobial activity, derivative **2** showed the most intense antioxidant activity (IC_{50}=0.0526 mM), while only derivative **4** showed toxicity against nauplii of *A. salina* (LC_{50}=0.032 mM).

MH-8

Interakcija novih androstanskih derivata i receptora steroidnih hormona

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U ovom radu je ispitan afinitet novosintetizovanih steroidnih derivata za ligand-vezujuće domene estrogenih receptora α i β (ERα i ERβ), kao i androgenog receptora (AR) fluorescentnim testom u kvascu [1,2]. Naši rezultati su pokazali da nekoliko testiranih jedinjenja ispoljava značajan afinitet prema izoformama estrogenog receptora, pri čemu se jedan androstanski derivat vezao približno jednako jako kao prirodni ligand, estron. Testirana jedinjenja nisu ispoljila androgena svojstva.

Interaction of new androstane derivatives with steroid hormone receptors

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In the present study, newly synthesized steroid derivatives were tested for affinity to the ligand-binding domains (LBDs) of estrogen receptors α and β (ERα and ERβ), as well as androgen receptor (AR) using a fluorescent assay in yeast [1,2]. Several of the test compounds exhibited significant binding affinity for estrogen receptor isoforms, while one androstane derivative was found to bind as strongly as thenatural ER ligand estrone. None of the test compounds displayed an affinity for the AR.

1. S. Bekić, M. Marinović, E. Petri, M. Sakač, A. Nikolić, V. Kojić, A. Ćelić, *Steroids*. **2018**, *130*, 22-30.

2. M. Savić, J. Ajduković, J. Plavša, S. Bekić, A. Ćelić, O. Klisurić, D. Jakimov, E. Petri, E. Djurendić, *MedChemComm*. **2018**, *9*, 969-981.

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MH-9

Synthesis and antitumour activity of two novel (–)-goniofufurone analogues

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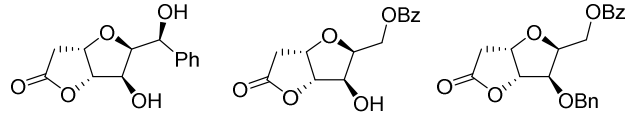
(–)-Goniofufurone (**1**) is a synthetic lactone, which is the opposite enantiomer of naturally occurring (+)-goniofufurone, that exhibited a significant antitumour activity. Novel (–)-goniofufurone analogues, **2** and **3** (*Scheme 1*), with benzoyl group at the C-7 position were prepared from L-xylose. Their synthesis and *in vitro* antitumour activity against a panel of human tumour cell lines and single normal cell line (MRC-5) will be presented.



*Scheme 1. Structures of (–)-goniofufurone (**1**) and novel analogues **2** and **3**.*

Sinteza i antitumorska aktivnost dva nova analoga (–)-goniofufurona

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(–)-Goniofufuron (**1**) je enantiomer prirodnog proizvoda (+)-goniofufurona, koji pokazuje značajnu antitumorsku aktivnost. U ovom radu je ostvarena sinteza dva nova analoga (–)-goniofufurona, **2** i **3** (*Scheme 1*), sa benzoil grupom u položaju C-7 polazeći od L-ksiloze. Pored sinteze, u okviru ovog rada biće predstavljena *in vitro* antitumorska aktivnost na nekoliko ćelijskih linija tumora i jednoj normalnoj ćelijskoj liniji (MRC-5).

Acknowledgment to financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-68/2022-14/200125) and (in part) research projects from the Serbian Academy of Sciences and Arts (Grant No. 01-2019-F6501-2019-F65 and F-130).

MH-10

Citotoksičnost novog steroidnog bis(karbazatnog) estra

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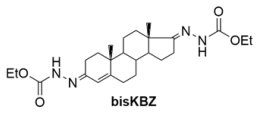
Usled stalne potrebe za novim antitumorskim lekovima, počevši od androstanskog bis(semikarbazona), sintetisan je novi bis(karbazatni) estar (**bisKBZ**) za koji je određena antimikrobna aktivnost, citotoksična aktivnost na tri maligne ćelijske linije, i urađen je *brine shrimp* test toksičnosti. Novo jedinjenje se nije pokazalo kao dobar antimikrobni agens, ispoljilo je umerenu citotoksičnost prema testiranim ćelijskim linijama i pokazalo se kao pet puta manje toksično od cisplatina za račiće *Artemia salina* što je u dobroj korelaciji sa citotoksičnošću prema HeLa ćelijskoj liniji.

Tabela 1. Citotoksičnost i brine shrimp toksičnost novog bis(karbazatnog) estra, ***bisKBZ***



bisKBZ

Jedinjenje	**IC_{50} ± SD (μM)**	**LC_{50} (mM)**
bisKBZ	32 ± 4	0.029
cisplatin	4.60 ± 0.07	0.006

Cytotoxicity of a new steroidal bis(carbazate) ester

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Due to the constant need for new antitumor drugs, starting from androstane bis(semicarbazone), a new bis(carbazate) ester (**bis-KBZ**) was synthesized; antimicrobial activity and cytotoxicity against three malignant cell lines were determined, and the brine shrimp toxicity test was performed. The new compound did not prove to be a good antimicrobial agent, it showed moderate cytotoxicity to the tested cell lines, and proved to be five times less toxic than cisplatin to *Artemia salina*, which correlates well with the cytotoxicity to HeLa cell line.

1. M. Živković, Irena T. Novaković, Ivana Z. Matić, Dušan M. Sladić, Natalija M. Krstić, *Steroids*, **2019**, 148, 36.

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Nastava i istorija hemije

Education in and History of Chemistry

NIH-1

Ostvarenost standarda postignuća o ugljenim hidratima kod brucoša kao indikator efektivnosti srednjoškolske nastave hemije tokom pandemije COVID-19

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Cilj ovog rada bio je ispitivanje nivoa ostvarenosti obrazovnih standarda o ugljenim hidratima za nastavni predmet Hemija, kod studenata prve godine studija hemije. Istraživanje je realizovano tokom proleća 2022. godine. Uzorak istraživanja činilo je ukupno 54 studenta I godine Departmana za hemiju, biohemiju i zaštitu životne sredine (PMF, Novi Sad). Uzorak je činilo 13,46 % ispitanika muškog i 86,54 % ženskog pola, čija je prosečna ocena iz hemije u srednjoj školi, iznosila 4,84. Za potrebe istraživanja konstruisan je test znanja sa 18 pitanja. Prosečni rezultat koji su ostvarili studenti iznosio je 8,82 bodova, odnosno 49 %. Osnovni nivo u ispitivanoj oblasti dostiglo je 65 % studenata, srednji nivo 70 %, a napredni nivo 40 %. Spirmanov koeficijent korelacije ostvarenih rezultata sa ocenom iz hemije (-0,12) ukazuje na nerealne ocene iz hemije na kraju srednje škole. Međutim, u proceni efekata srednjoškolskog obrazovanja važno je da se uzmu u obzir uslovi rada tokom pandemije Kovid-19, odnosno onlajn i kombinovana nastava, što je otežavalo izučavanje kompleksnih sadržaja biohemije.

Achieving educational standards on carbohydrates in freshmen students as an indicator of the effectiveness of secondary school chemistry during the COVID-19 pandemic

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The aim of this paper was to examine the level of achievement of educational standards on carbohydrates in Chemistry in freshmen chemistry students. The research was realized during the spring of 2022. The research sample consisted of a total of 54 first-year students enrolled into the Department of Chemistry, Biochemistry and Environmental Protection (PMF, Novi Sad). The sample consisted of 13.46 % of male and 86.54 % of female respondents, and their average grade in chemistry was 4.84. For the purpose of the research, a knowledge test with 18 questions was constructed. The average score was 8.82 points, or 49 %. The basic level in the field of Carbohydrates reached 65% students, the intermediate level in 70%, and the advanced level in 40%. Spearman's coefficient of correlation of the achieved results with the grade in chemistry (-0.12) indicates unrealistic grades in chemistry at the end of high school. However, in assessing the effects of secondary education, it is important to take into account the working conditions during the Covid-19 pandemic, ie online or blended teaching content online or combined, which made it difficult to study complex biochemistry.

NIH-2

Asinhrono i sinhrono onlajn učenje iz ugla nastavnika hemije

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Dva načina onlajn učenja, asinhrono i sinhrono, iskustveno su poznata većini nastavnika hemije od početka pandemije izazvane korona virusom. Cilj sprovedenog istraživanja je da se ispita da li su nastavnici hemije upoznati sa karakteristikama ovih pristupa nastavi/učenju i kakav stav imaju u vezi sa njihovom primenom u školskoj praksi. U istraživanju je učestvovalo ukupno 98 nastavnika hemije iz Republike Srbije. Podaci su prikupljeni pomoću onlajn upitnika. Rezultati pokazuju da 40,8 % nastavnika delimično poznaje značenje pojmova asinhrono i sinhrono onlajn učenje. Kao važne karakteristike asinhronog onlajn učenja većina njih identifikuje prilagođenost tempu usvajanja znanja učenika i to što nije vremenski definisano. Najvažnija odlika sinhronog onlajn učenja po njihovom mišljenju je pedagoška interakcija između nastavnika i učenika, kao i samih učenika. Ipak smatraju da je najefektivniji pristup za nastavu/učenje hemije uobičajeni, koji se odvija u školskoj sredini uz istovremeno prisustvo nastavnika i učenika.

Zahvalnica: Rad je deo istraživanja u okviru projekta sa evidencionim brojem 451-03-68/2022-14/200168 koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije

Asynchronous and synchronous online learning from the point of view of chemistry teachers

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Two ways of online learning, asynchronous and synchronous, have been familiar to most chemistry teachers since the beginning of the coronavirus pandemic. The aim of the research is to examine whether chemistry teachers are familiar with the characteristics of this teaching/learning approaches and what is attitude of teachers regarding their application in school practice. The 98 chemistry teachers from the Republic of Serbia participated in the research. Data were collected using an online questionnaire. The results show that 40.8 % of teachers partially know the meaning of the terms asynchronous and synchronous online learning. Most of them as significant characteristics of asynchronous online learning identify the adaptation to the pace of students' knowledge acquisition and the fact that it is not defined in time. In their opinion, the most significant feature of synchronous online learning is the pedagogical interaction between teachers and students, and the students themselves.

Nauka o materijalima

Material Science

NM-1

Kinetika procesa oksidacije Sb_2S_3 u atmosferi vazduha u izotermskim uslovima

Nada D. Štrbac[1], Aleksandra M. Mitovski[1], Kristina N. Božinović[1], Milan D. Gorgievski[1], Vesna J. Grekulović[1], Miljan S. Marković[1], Marina Z. Berkenječević[1]

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Veliki problem poslednjih nekoliko decenija je iscrpljivanje bogatih ruda obojenih metala i prerada koncentrata sa visokim sadržajem primesa. Ponašanje onečišćujućih komponenti je predmet istraživanja ne samo zbog ekoloških razloga i zaštite životne sredine, već i zbog toga što ove primese mogu imati negativan uticaj na kvalitet dobijenog metala [1]. Pošto je Sb jedan od čestih primesa u sulfidnim koncentratima obojenih metala i važi za jednu od najštetnijih komponenti, zajedno sa olovom, arsenom i bizmutom, ispitivano je ponašanje Sb_2S_3 na povišenim temperaturama. U ovom radu je proučavana kinetika procesa oksidacije Sb_2S_3 u atmosferi vazduha u izotermskim uslovima.

1. R.Padilla, A. Aracena,&M. C. Ruiz, *J. Min. Metall. B: Metall.***2014**, *50(2)*, 127-127.

Kinetics of Sb_2S_3 isothermal oxidation process in air atmosphere

Nada D. Štrbac[1], Aleksandra M. Mitovski[1], Kristina N. Božinović[1], Milan D. Gorgievski[1], Vesna J. Grekulović[1], Miljan S. Marković[1], Marina Z. Berkenječević[1]

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A major problem of the last few decades is the depletion of rich non-ferrous metal ores and the processing of concentrates with a high content of impurities. The behavior of minor elements has been the subject of industrial concern not just for environmental reasons, but also because these impurities can have a negative impact on the quality of the final metal [1]. Since Sb is one of the frequent contaminants insulfide concentrates of non-ferrous metals and is considered as one of the most harmful components, together with lead, arsenic and bismuth, the behavior of Sb_2S_3 at elevated temperatures was investigated. In this paper, the kinetics of isothermal oxidation of Sb_2S_3 in air atmosphere was studied.

1. R.Padilla, A. Aracena,&M. C. Ruiz, *J. Min. Metall. B: Metall.***2014**, *50(2)*, 127-127.

Acknowledgment: The research presented in this paper was done with the financial support of the Ministry of Education, Science and Technological Development of theRepublic of Serbia, within the funding of the scientific research work at the University ofBelgrade, Technical Faculty in Bor, according to the contract with registration number451-03-68/2022-14/200131.

NM-2

Elektrohemijske osobine i rastvorljivost metanofulerena i derivata C_{60} sa dihidrofuranskim prstenom

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Zbog velikog afiniteta prema elektronima, fuleren se u fotonaponskim uređajima predstavlja kao elektron-akceptor. Stoga je do danas testirano mnoštvo različitih materijala odnosno uređaja, koji sadrže polimer kao donor i derivat fulerena kao akceptor. Cilj našeg istraživanja bio je da se ispitaju elektrohemijska svojstva i rastvorljivost različitih metanofulerena i derivata C_{60} sa dihidrofuranskim prstenom kako bismo dizajnirali nove materijale. Elektrohemijska svojstva reprezentativnih proizvoda ispitana su cikličnom voltametrijom (CV). Ovi proizvodi pokazuju dobru rastvorljivost u uobičajenim organskim rastvaračima kao što su toluen, dihlorometan i hloroform. Derivati C_{60} sa dihidrofuranskim prstenom mogu biti dobri kandidati za akceptorsku komponentu u organskim fotonaponskim uređajima na osnovu vrednosti za prvi pik redukcije, kao i zbog njihove poboljšane rastvorljivosti i stabilnosti što je razjašnjeno DFT proračunima.

Electrochemical properties and solubility of metanofullerenes and dihydrofuran-fused C_{60} derivatives

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Due to its high affinity for electron, fullerene is presented as an electron acceptor in photovoltaic devices. Therefore, to date, many different materials or devices have been tested, which contain a polymer as a donor and a fullerene derivative as an acceptor. The aim of our research was to investigate the electrochemical properties and solubility of different metanofullerenes and dihydrofuran-fused C_{60} derivatives to design new materials. Electrochemical properties of the representative products were investigated by cyclic voltammetry (CV). These products show good solubility in common organic solvents such as toluene, dichloromethane and chloroform. Dihydrofuran-fused fullerenes could make good candidates for acceptor component in organic photovoltaic devices based on values for the first reduction peak as well owing to their improved solubility and stability as rationalized by DFT calculations.

1. J. Jakšić, A. Mitrović, Z. Tokić Vujošević, M. Milčić, V. Maslak, *RSC Adv.*, **2021**, *11*, 29426-29432.

Acknowledgment: Ministry of Education, Science and Technological Development of Republic of Serbia (451-03-68/2022-14/200168)

NM-3

Ispitivanje površinskih interakcija indola i mezoporoznih silikata metodama FTIR spektroskopije i hiperspektralnog snimanja

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2 Univerzitet u Novom Sadu, Institut Biosens, Novi Sad, Srbija

U ovom radu ispitivana je adsorpcija indola na mezoporoznom silikatu iz rastvora CCl_4. Promene u adsorpcionom kapacitetu indola potiču od adsorpcije vlage na površini mezoporoznh silikata. Spektralne promene (nove trake) u opsegu N-H vibracionih i deformacionih traka uočene su kako u srednjoj IR oblasti (FTIR tehnikom) tako i u bliskoj NIR oblasti (hiperspektralnom tehnikom). Promene uočene u FTIR i hiperspektralnim odgovorima mogu biti od značajne praktične koristi za razvoj senzora za male biomolekule kao što je indol.

Investigation of the surface interactions of indole with mesoporous silica using FTIR spectroscopy and hyperspectral imaging

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[1] University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia
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The adsorption of indole from carbon tetrachloride on mesoporous silicate nanomaterial MSN was investigated in this study. Changes in the adsorption capacity of indole originate from the adsorption of moisture on the surface of mesoporous silicates. Spectral changes in the range of N-H vibration and deformation bands were observed both in the middle IR region (FTIR technique) and in the near NIR region (hyperspectral technique). The changes observed in the FTIR and hyperspectral responses can be of significant practical use for the development of new qualitative sensors for small bioactive molecules such as indole

B. Jović, M. Panić, N. Radnović, K. Zivojević, M. Mladenović, V. Crnojević,,N. Knežević. *J. ofMol. Struc,***2020***, 1219*,128562

Istraživanja je finansiralo Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije (Ev.br. 451-03-68/2022-14/200125)

NM-4

Abnormalni rast zrna u toku medjužarenja u Al-Mg legurama

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U završnoj fazi prerade Al-Mg legura, pojava abnormalnih zrna (AGG) u strukturi je nepoželjna, jer dovodi do pogoršanja mehaničkih osobina. Medjutim, postoji veliki interes za proučavanjem uticaja AGG, koja nastaju u toku medjužarenja, na razvoj mikrostrukture i teksture tokom dalje prerade. Naime, odredjene teksturne komponente i tipovi granica zrna imaju pozitivan uticaj na deformaciono i koroziono ponašanje.U ovom radu je opisan efekat uslova medjužarenja i hemijskog sastava na mikrostrukturu Al-Mg legura. Uzorci, izohrono žareni na temperaturama 350-550°C,ili tretirani na 520°C pri različitim vremenima, su ispitivani optičkom mikroskopijom u polarizovanom svetlu. Utvrdjeno je da je AGG ograničen na pojas u blizini ivice uzorka. Abnormalna zrna poseduju visok stepen anizotropije, a inicijalno brz rast stagnira sa produžetkom žarenja. Uticaj hemijskog sastava na pojavu AGG je ispitivan u slučaju četiri legure i rezultati su pokazali da niži sadržaj legirajućih elemenata pospešuje AGG.

Abnormal grain growth during intermediate annealing of Al-Mg alloys

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During final annealing of Al-Mg alloys, abnormal grain growth (AGG) is undesirableasit deteriorates mechanical properties. However, there is interest to investigate how the introduction of the AGG during intermediate annealing affects microstructure and texture development upon further processing.It is known that certain texture components and grain boundary types can affect formabilityand IGC susceptibility. In this study, the effect of intermediate annealing conditions andchemical composition on the microstructure of of Al-Mg alloysis reported. The specimens,annealed isochronally at temperatures of 350-550°C or isothermally at 520°C for various times, were examined by optical microscopy in polarized light. It is found that the AGG is confined to a band near the surface.There is astrong anisotropy in grains shape and initially rapid grain growth stagnates with furtherannealing. The influence of the chemical composition on the AGG was investigated in four alloys and the results showed that the decrease in the alloying elementscontent promoted AGG.

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2022-14/200135).

NM-5

Toplotna provodnost i mikrostruktura Bi-Cu legura

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

Toplotne transportne osobine čvrstih Bi-Cu legura su proučavane u širokom opsegu koncentracija i temperaturnom opsegu od 25 do 250 °C. Toplotna difuzivnost je merena primenom fleš metoda. Utvrđeno je da toplotna difuzivnost kontinualno opada sa porastom sadržaja bizmuta i temperature. Gustine Bi-Cu legura na 25 °C merene su Arhimedovom metodom. Toplotna provodnost je određena na osnovu merenih vrednosti toplotne difuzivnosti i gustine kao i na bazi proračunatih specifičnih toplotnih kapaciteta. Saglasno toplotnoj difuzivnosti, toplotna provodnost proučavanih Bi-Cu legura se snižava sa porastom sadržaja bizmuta i temperature. Mikrostruktura i interval topljenja Bi-Cu legura su proučavani primenom skenirajuće elektronske mikroskopije (SEM) sa energo-disperzivnom spektrometrijom (EDS) i diferencijalno skenirajuće kalorimetrije (DSC).

Thermal conductivity and microstructure of the Bi-Cu alloys

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Thermal transport properties of solid Bi-Cu alloys were studied in a wide composition range and the temperature range from 25 up to 250 °C. Thermal diffusivity was measured using the flash method. It was found that the thermal diffusivity continuously decreases with increasing bismuth content and temperature. The density of the Bi-Cu alloys at 25 °C was measured using the indirect Archimedean method. Thermal conductivity was determined based on measured diffusivity and density of alloys, as well as based on calculated specific heat capacity. Analogous to the thermal diffusivity, the thermal conductivity of the studied Bi-Cu alloys decreases with increasing bismuth content and temperature.

The microstructure and melting interval of the Bi-Cu alloys were analyzed using scanning electron microscopy (SEM) with energy dispersive X-ray spectrometry (EDS) and differential scanning calorimetry (DSC).

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NM-6

Nanokompoziti TiO_2/PANI za primenu u fotokatalizi

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Poznato je da je titan-dioksid, kao netoksičan, stabilan i ekonomičan materijal, jedan od najčešće korišćenih fotokatalizatora. S druge strane, elektroprovodni polianilin (PANI) je takođe pogodan kandidat za primenu u fotokatalizi. Cilj ovog rada bio je dobijanje nanokompozita TiO_2/PANI sa boljom fotokatalitičkom aktivnošću u odnosu na TiO_2. U cilju optimizacije sadržaja polimera sintetisano je 4 uzorka TiO_2/*x*%PANI (*x* = 0, 1, 3 i 5 mas.%), koji su okarakterisani XRD i TG/DTA metodama, dok je fotokatalitička aktivnost ispitana kroz razgradnju toksične tekstilne boje RO16. Pokazano je da su svi kompoziti fotokatalitički aktivniji od TiO_2, i da optimalan sadržaj polianilina iznosi 3 mas.%. Naime, uzorak TiO_2/3%PANI je, nakon 60 minuta, razgradio 95 % boje, što je za 17 % više u odnosu na TiO_2, dok je nakon 120 minuta fotorazgradnja boje potpuna. Pored toga, ovaj uzorak je pokazao čak 14 puta izraženiju adsorpciju od TiO_2. Efikasnost TiO_2/5%PANI je slična TiO_2/3%PANI, ali sa slabije izraženim adsorpcionim svojstvima, dok je efikasnost TiO_2/1%PANI bliska TiO_2.

TiO_2/PANI nanocomposites for photocatalytic application

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It is well known that the non-toxic, stable and economical titanium dioxide is one of the most commonly used photocatalysts. On the other hand, the conductive polyaniline (PANI) is also suitable candidate for photocatalytic application. The aim of this work was to obtain the TiO_2/PANI nanocomposites with increased photocatalytic activity comparing to TiO_2. In order to determine the optimal PANI content, four TiO_2/*x*%PANI samples (*x* = 0, 1, 3 and 5 wt.%) were synthesized and characterized by XRD and TG/DTA analysis. The photocatalytic activity was tested on the toxic textile RO16 dye. It is shown that all the composites exhibited better photocatalytic performances than TiO_2 and that the optimal PANI content amounted 3 wt.%. Namely, the TiO_2/3%PANI degraded 95 % of the dye within 60 minutes, which is for 17 % better comparing to TiO_2. The full photodegradation was reached in 120 min. This sample showed even 14 times better adsorption than TiO_2. The efficiency of TiO_2/5%PANI was similar to TiO_2/3%PANI, but with poorer adsorption, while the efficiency of TiO_2/1%PANI was close to TiO_2.

NM-7

Fotokatalizatori na bazi TiO_2 za redukciju Cr(VI)

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Fotokatalizatori za redukciju Cr(VI) sintetisani su deponovanjem nanočestica CdS i/ili Cu na TiO_2. Redukcijom Cu^{2+} jona ekstraktom lišća hrasta u prisustvu TiO_2 sintetisan je Cu-TiO_2, a Cu-TiO_2-CdS reakcijom kadmijum-acetata i tiouree u prisustvu Cu-TiO_2. Redukcija Cr(VI) je ispitivana pod dejstvom simuliranog vidljivog zračenja, na pH=3 i pH=6. DRS je pokazala da fotokatalizatori apsorbuju u vidljivom delu spektra. Cu-TiO_2-CdS pokazuje dve granice apsorpcije, za TiO_2 i za CdS. Cu-TiO_2 je imao užu zabranjenu zonu u odnosu na TiO_2 i dodatnu apsorpciju u vidljivoj oblasti. Oba fotokatalizatora, a posebno Cu-TiO_2-CdS, su pokazala znatno veću efikasnost od čistog TiO_2. Određivanjem sadržaja Cd^{2+} jona u rastvoru i ispitivanjem mogućnosti ponovne upotrebe fotokatalizatora, utvrđeno je da dolazi do korozije Cu-TiO_2-CdS pri pH=3. Korozija je značajno smanjena pri pH=6, ali je i fotokatalitička efikasnost bila manja.

Photocatalysts based on TiO_2 for the reduction of Cr(VI)

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Photocatalysts for the reduction of Cr(VI) were synthesized by depositing CdS and/or Cu nanoparticles on TiO_2. Cu-TiO_2 was synthesized by the reduction of Cu^{2+} ions with oak leaf extract in the presence of TiO_2, and Cu-TiO_2-CdS by the reaction of cadmium acetate and thiourea in the presence of Cu-TiO_2. The reduction of Cr(VI) was tested under simulated visible irradiation, at pH=3 or pH=6. DRS has shown that the photocatalysts absorb in the visible part of the spectrum. Cu-TiO_2-CdS showed two absorption edges, one for TiO_2 and the other for CdS. The Cu-TiO_2 sample had a narrower band gap than TiO_2 and additional absorption in the visible region. Both photocatalysts, especially Cu-TiO_2-CdS, showed significantly higher efficiency than pure TiO_2. Based on determining the content of Cd^{2+} ions in the solution and examining the possibility of reusing photocatalysts, it was determined that Cu-TiO_2-CdS corrosion occurs at pH=3. Corrosion was significantly reduced at pH=6, but the photocatalytic efficiency was also lower.

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NM-8

Perovskitne solarne ćelije – organski mezoporozni slojevi na delu

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Perovskitne solarne ćelije su jedna od najinteresantnijih tema pošto su ispoljile ogroman potencijal dostizanja visokih efikasnosti konverzije solarne u električnu energiju. Zajedno sa činjenicom da su cene materijala, sinteze i procesiranja veoma niske, jasno je zašto ove ćelije privlače toliku pažnju. U ovom radu, nov organski mezoporozni sloj je procesiran na ekološki prihvatljiv način čineći sistem obećavajućom alternativom etabliranim neorganskim slojevima. Stoga, perovskit efikasno prodire u mezoporoznu strukturu i sa poboljšanim kvašenjem površine perovskit drastično povećava homogenost što doprinosi porastu efikasnosti konverzije kao i termalnoj stabilnosti. Osim gornje elektrode, svi slojevi su procesirani iz tečne faze.

Perovskite solar cells – organic mesoporous layers at work

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Perovskite solar cells have been one of the hottest topics as they have shown enormous potential for reaching high power convertion efficiency. Coupled with the fact that the costs of the materials, synthesis and processing are very low, it is clear why these cells attract huge interest. In this work, a novel organic-based mesoporous interfacial layer was produced in an ecofriendly way making it a promising alternative to established inorganic interfaces. Thusly, the perovskite effectively infiltrates into this mesoporous structure, and with enhanced wetting of the surface, the perovskite dramatically increases its homogeneity, leading to efficiency enhancement and thermal stability. Excluding the top electrode, all layers were processed entirely from liquid phase.

NM-9

Dobijanje poroznih 3D biaoaktivnih fosfatnih staklokeramičkih nosača

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Staklokeramički nosači koji oponašaju strukturu kostiju dobijeni su korišćenjem poliuretanske (PU) pene i polifosfatnog stakla u prahu. Osnovno staklo je pripremljeno standardnom tehnikom izlivanja rastopa i njegovog hlađenja na sobnoj temperaturi. Kocke pene su potapane u koloidni rastvor stakla, presovane i osušene. PU pena obložena staklenim česticama je termički obrađena i staklo je sinterovano 3 h na 620 ^{0}C. Mikrostruktura, morfologija i fazni sastav pripremljenih staklokeramičkih nosača ispitivani su metodama skenirajuće elektronske mikroskopije i rendgenske difrakcije. Dobijeni su 3D porozni staklokeramički nosači koji sadrže bioaktivne kristalne faze β-$Ca_3(PO_4)_2$ i β-$Ca_2P_2O_7$. Struktura sinterovanih nosača je veoma porozna, a stubovi između pora su dobro sinterovani. Dobijeni fazni sastav i mikrostruktura nosača ukazuju na mogućnost njihove primene kao bioaktivnih materijala za inženjering koštanih tkiva.

Fabrication of porous 3D bioactive phosphate glass-ceramic scaffolds

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Glass-ceramic scaffolds mimicking the bone structure were obtained by the foam replica technique using a polyurethane (PU) foam and powdered polyphosphate glass. The parent glass was prepared by the standard melt-quenching technique. The foam cubes were soaked into the glass slurry, compressed, and dried. PU foam coated with glass particles was thermally treated and the glass was sintered for 3h at 620 ^{0}C. The microstructure, morphology, and phase composition of the as-prepared glass-ceramic scaffolds were investigated using scanning electron microscopy and x-ray diffraction methods. 3D porous glass-ceramic scaffold containing bioactive β-$Ca_3(PO_4)_2$ and β-$Ca_2P_2O_7$ crystalline phases was fabricated. The morphology of the sintered scaffold was highly porous and the pore struts were well sintered. The obtained phase composition and the microstructure of the as-prepared scaffold indicated its possible application as a bioactive material for bone tissue engineering.

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Neorganska hemija

Inorganic Chemistry

NH-1

Bakar(II) i srebro(I) kompleksi sa dimetil 6-(pirazin-2-il)piridin-3,4-dikarboksilatom: antimikrobna aktivnost i DNA/BSA interakcije

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Dimetil 6-(pirazin-2-il)piridin-3,4-dikarboksilat (py-2pz) korišćen je kao ligand za sintezu novih kompleksa bakra(II) i srebra(I).[1] Sintetisani kompleksi, $[CuCl_2(py\text{-}2pz)]_2$ (**1**), $[Cu(CF_3SO_3)(H_2O)(py\text{-}2pz)_2]CF_3SO_3{\cdot}2H_2O$ (**2**), $[Ag(py\text{-}2pz)_2]PF_6$ (**3**) i $[Ag(NO_3)(py\text{-}2pz)]_n$ (**4**) okarakterisani su primenom različitih spektroskopskih metoda i rendgenske strukturne analize. Ispitivana je antimikrobna aktivnost sintetisanih kompleksa prema mikroorganizmima koji mogu biti uzročnici različitih infekcija, kao i njihove interakcije sa DNA i BSA.

Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate: antimicrobial activity and DNA/BSA interactions

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Dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz) was used as a ligand for the synthesis of new copper(II) and silver(I) complexes.[1] The synthesized complexes, $[CuCl_2(py\text{-}2pz)]_2$ (**1**), $[Cu(CF_3SO_3)(H_2O)(py\text{-}2pz)_2]CF_3SO_3{\cdot}2H_2O$ (**2**), $[Ag(py\text{-}2pz)_2]PF_6$ (**3**) and $[Ag(NO_3)(py\text{-}2pz)]_n$ (**4**) were characterized by spectroscopy and X-ray crystallography. The antimicrobial activity of the synthesized complexes was evaluated against microorganisms that can cause different infections, as well as their interactions with DNA and BSA.

1. T. P. Andrejević, I. Aleksic, J. Kljun, B. V. Pantović, D. Milivojevic, I. Turel, M. I. Djuran, B. Đ. Glišić, *Manuscript in preparation*

NH-2

Kompleksi Zn(II) sa tiazolil-hidrazonima: struktura, fotofizička svojstva i antiproliferativna aktivnost

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Netoksični kompleksi na bazi Zn(II) privlače pažnju kao obećavajući kandidati za različite primene. U ovom radu je sintetisano i strukturno okarakterisano šest kompleksa Zn(II) (**1–3-NO$_3$** i **1–3-Cl**) sa tiazolil-hidrazonskim ligandima na bazi piridina, koji se razlikuju po prirodi supstituenata na periferiji liganda, tipu anjona i geometriji oko jona metala. Simetrični kompleksi **2-Cl** i **3-Cl**, gde se atomi cinka nalaze na osi rotacije 2, ne pokazuju fotofizička svojstva, za razliku od drugih sintetisanih asimetričnih kompleksa. Poreklo fotoluminiscentnih svojstava je razjašnjeno korišćenjem DFT i TD-DFT proračuna. Antiproliferativna aktivnost kompleksa je bila u nanomolarnom opsegu na nekim od ispitivanih ćelijskih linija raka. Ukupni rezultati ukazuju na to da kompleksi Zn(II) sa tiazoil-hidrazonima imaju značajan potencijal kao multifunkcionalni materijali.

Zn(II) complexes with thyazolyl-hydrazones: structure, photophysical properties, and antiproliferative activity

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Non-toxic Zn-based complexes are drawing attention as promising candidates for various applications. In this study we report six Zn(II) complexes (**1–3-NO$_3$** and **1–3-Cl**) with pyridyl-based thiazolyl-hydrazone ligands, which differ in the nature of substituents at the ligands' periphery, anion type, and geometry around the metal ion. The symmetrical complexes **2-Cl** and **3-Cl**, where zinc atoms are located at a two-fold axis, do not exhibit photophysical properties, unlike other synthetized asymmetrical complexes. The origin of photoluminescent properties have been elucidated using DFT and TD-DFT calculations. Antiproliferative activity of the complexes was in the nanomolar range on some of the investigated cancer cell lines. The overall results suggest that Zn(II) thiazoyl-hydrazone complexes have considerable potential as multifunctional materials.

NH-3

Sinteza i strukturna karakterizacija kompleksa kobalta(II) i magnezijuma(II) sa 2,2-diMe-1,3-pdta

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Sintetisani su i primenom spektroskopije i kristalografije okarakterisani kompleksi kobalta(II) i magnezijuma(II) sa 2,2-dimetil-1,3-propandiamin-*N,N,N',N'*-tetraacetato ligandom, $[Co(H_2O)_5Co(2,2\text{-diMe-}1,3\text{-pdta})]\cdot H_2O$ i $[Mg(H_2O)_5Mg(2,2\text{-diMe-}1,3\text{-pdta})]\cdot 1{,}5H_2O$.[1] U ovim kompleksima je 2,2-diMe-1,3-pdta heksadentatno koordinovan za Co(II) i Mg(II) jone preko 2N i 4O atoma, formirajući $[M(H_2O)_5M'(2,2\text{-diMe-}1,3\text{-pdta})]$ kompleksnu jedinicu koja sadrži $[M'(2,2\text{-diMe-}1,3\text{-pdta})]^{2-}$ i $[M(H_2O)_5O]^{2+}$ oktaedre međusobno povezane preko kiseonikovog atoma iz jedne aksijalne karboksilne grupe.

Synthesis and structural characterization of cobalt(II) and magnesium(II) complexes with 2,2-diMe-1,3-pdta

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Cobalt(II) and magnesium(II) complexes with 2,2-dimethyl-1,3-propanediamine-*N,N,N',N'*-tetraacetato ligand, $[Co(H_2O)_5Co(2,2\text{-diMe-}1,3\text{-pdta})]\cdot H_2O$ and $[Mg(H_2O)_5Mg(2,2\text{-diMe-}1,3\text{-pdta})]\cdot 1.5H_2O$, were synthesized and characterized by spectroscopy and single-crystal X-ray diffraction analysis.[1] In these complexes 2,2-diMe-1,3-pdta ligand is hexadentately coordinated to the metal ion through 2N and 4O atoms forming $[M(H_2O)_5M'(2,2\text{-diMe-}1,3\text{-pdta})]$ complex unit, which is composed of $[M'(2,2\text{-diMe-}1,3\text{-pdta})]^{2-}$ and $[M(H_2O)_5O]^{2+}$ octahedra bridged together by one of the axial carboxylate groups.

1. J. Gitarić et al, *submitted for publication*

NH-4

Ispitivanje koordinacionih sposobnosti NNO i NNS Šifovih baza kao liganada u kompleksima Co(III)

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Kompleks $[Co(\mathbf{L}^1)_2]BF_4 \cdot H_2O$ (**1**) dobijen je u reakciji $Co(BF_4)_2 \cdot 6H_2O$ sa kondenzacionim proizvodom tiosemikarbazida i 2-acetiltiazola ($\mathbf{HL}^1$), dok je kompleks $[Co(\mathbf{L}^2)(N_3)_3]$ (**2**) dobijen u reakciji iste soli sa kondenzacionim proizvodom 2-acetilpiridina i Žirarovog P reagensa ($\mathbf{HL}^2Cl$). Oba kompleksa su okarakterisana elementalnom analizom, IC i NMR spektroskopijom i rendgenskom strukturnom analizom. Kod kompleksa Co(III) sa $\mathbf{HL}^1$ uočena je bis oktaedarska geometrija. Hidrazonski ligand ($\mathbf{L}^2$) je za centralni metalni jon kompleksa **2** koordinovan tridentatno preko NNO seta atoma i tri meridijalno koordinovana azido anjona, pri čemu se formira monokis oktaedarska geometrija. DFT proračunima određena je termodinamička stabilnost kompleksa.

Coordination preferences of NNO and NNS Schiff base ligands with Co(III) complexes

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Two Co(III) complexes $[Co(\mathbf{L}^1)_2]BF_4 \cdot H_2O$ (**1**), and $[Co(\mathbf{L}^2)(N_3)_3]$ (**2**) with condensation product of thiosemicarbazide and 2-acetylthiazole ($\mathbf{HL}^1$) and the condensation product of 2-acetylpyridine and Girard's P reagent ($\mathbf{HL}^2Cl$) and $Co(BF_4)_2 \cdot 6H_2O$ have been synthesized. Complexes were characterized by elemental analysis, IR and NMR spectroscopy and X-ray crystallographic analysis. Cobalt(III) complex with $H\mathbf{L}^1$ ligand forms a bis octahedral complex. The hydrazone ligand ($\mathbf{L}^2$) is coordinated to Co(III) ion with tridentate NNO set of donor atoms and the other three coordination sites of a monokis octahedron are occupied by meridionally coordinated azide anions. DFT calculations revealed the thermodynamical stability of obtained complexes.

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NH-5

Sinteza i karakterizacija kompleksa trifenilkalaja(IV) sa 2-(4-hidroksi-2-oksohinolinil)etanskom kiselinom

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U datom radu opisana je sinteza 2-(4-hidroksi-2-oksohinolinil)etanske kiseline i njenog kompleksa trifenilkalaja(IV). Ligand je dobijen hidrolizom metil-estra sintetisanog u reakciji između4-hidroksi-2-hinolona i metil-2-bromoetanoata. U reakciji deprotonovanog liganda i ekvimolarne količine Ph_3SnCl dobijen je kompleks u obliku belog taloga. Sintetisana jedinjenja su okarakterisana standardnim analitičkim metodama. Naredna istraživanja sintetisanih jedinjenja biće usmerena ka ispitivanju antitumorske aktivnosti prema raznim ćelijskim linijama karcinoma.

Synthesis and characterization of novel triphenyltin(IV) complex with 2-(4-hydroxy-2-oxoquinolinyl)ethanoic acid

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Synthesis of 2-(4-methyl-2-oxoquinolinyl)ethanoic acid and its triphenyltin(IV) complex has been performed. The ligand has been obtained by the hydrolysis of methyl ester synthesized in the reaction between 4-hydroxy-2-quinolone and methyl 2-bromoethanoate. In the reaction of deprotonated ligand with equimolar amount of Ph_3SnCl, the desired complex was precipitated as a white solid. The synthesized compounds have been characterized using standard analytical methods. The following research of synthesized compounds will be focused on examining their antitumor activity against various cancer cell lines.

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NH-6

Adsorpcija boje indocijanin zeleno na površini nanočestica srebra i zlata

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U poslednje vreme intenzivno se ispituju nanočestice metala za primenu u medicini kao nosači lekova i drugih biološki važnih molekula, koji bi poboljšali stabilnost leka i terapeutsku efikasnost. U ovom radu je ispitana adsorpcija fluorescentne boje indocijanin zeleno (ICG) na površini nanočestica srebra i zlata. Nanočestice srebra i zlata dobijene su zelenom sintezom u prisustvu aminokiseline L-metionina kao redukcionog i stabilizacionog sredstva. Dobijene su nanočestice sfernog oblika, negativno naelektrisane, sa adsorbovanim molekulima L-metionina. Primena ove boje kao kontrastnog agensa u medicinskoj dijagnostici je odobrena od agencije za hranu i lekove. Nanočestice zlata i srebra su služile kao nosači molekula ove boje, a kako je razblaženi vodeni rastvor ICG nestabilan i podleže fotodegradaciji, na taj način se i stabilišu molekuli boje u vodenom rastvoru.

Indocyanine green dye adsorption on the surface of silver and gold nanoparticles

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Recently, metal nanoparticles (NPs) were intensively studied for medical application as carriers for drugs and other biologically important molecules to improve drugs' stability and therapeutic efficiency. In this work we studied the adsorption of a fluorescent dye Indocyanine green (ICG) on the surface of gold and silver NPs. Silver and gold NPs were synthesized by a green method in the presence of amino acid L-methionine as a reducing and stabilizing agent. The obtained L-methionine capped NPs were spherical in shape and with a negative charge. The application of ICG for human medical imaging and diagnosis is approved by the Food and Drug Administration. Since an aqueous solution of ICG is unstable and undergoes photodegradation, gold and silver NPs served here as carriers of ICG molecules andstabilized dye molecules in aqueous solution.

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NH-7

Стекинг метилованих циклопентадиенилних лиганада у кристалним структурама комплекса прелазних метала

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Кристалне структуре метилованих (Me) циклопентадиенилних (Cp) комплекса су систематски анализиране претрагом Кембричке базе структурних података (CSD) и описани су преовлађујући положаји метилованих Cp лиганада у стекинг оријентацији. Стекинг контакти Me_5Cp комплекса су далеко најучесталији (3632 контакта), а затим следе MeCp (446) и Me_4Cp (151). Контакти у највећој мери садрже симултане паралелно-померене стекинг интеракције и CH/π интеракције, али се јављају и саме паралелно-померене стекинг интеракције и стекинг интеракције са великим хоризонталним померањима. Са повећањем броја метил-супституената опада заступљеност стекинга на великим померањима (48,4% за MeCp, 28,5% за Me_4Cp, 3,8% за Me_5Cp), пошто CH/π интеракције стабилизују геометрије на мањим померањима. Различити типови интеракција се могу објаснити на основу мапа електростатичких потенцијала испитиваних комплекса.

Stacking of the methylated cyclopentadienyl ligands in crystal structures of transition metal complexes

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Crystal structures of the methylated cyclopentadienyl (Cp) complexes are systematically analysed by searching the Cambridge Structural Database (CSD) and the preferred positions of the stacked methylated Cp ligands are described. The stacking contacts of the Me_5Cp complexes are by far the most frequently found in the CSD (3632 contacts), followed by MeCp (446) and Me_4Cp (151). These contacts mostly correspond to simultaneous parallel-displaced stacking and CH/π interactions, as well as parallel-displaced stacking and stacking interactions at large horizontal displacements. With increasing the number of methyl substituents the occurrence of stacking with large displacements decreases (48.4% for MeCp, 28.5% for Me_4Cp, 3.8% for Me_5Cp), because CH/π interactions stabilize geometries with smaller displacements. Different interaction types can be explained by the electrostatic potential maps of the studied complexes.

NH-8

Sinteza, karakterizacija i citotoksičnost kompleksa Cu(II) sa *O,O'*-dietil estrom (*S,S*)-etilendiamin-*N,N'*-di-2-(4-metil)-pentanske kiseline

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Bakar(II) ima važnu biološku ulogu u svim živim sistemima kao esencijalni element u tragovima. Cu(II) kompleksi sa organskim ligandima su korišćeni kao analgetički, antipiretički i antiinflamatorni agensi. Imaju antioksidativno kao i antitumorsko dejstvo. U ovom radu sintetisan je kompleks bakra(II) sa bidentatnim *N,N'*-ligandom, *O,O'*-dietil estrom (*S,S*)-etilendiamin-*N,N'*-di-2-(4-metil) pentanske kiseline. Struktura izolovanog kompleksa predložena je na osnovu elementalne mikroanalize i infracrvenog spektra. *In vitro* antitumorska aktivnost sintetisanog liganda i bakra(II) kompleksa ispitana je na HT-29, PC3, MCF-7, B16F1 tumorskim ćelijskim linijama koristeći kristal violet (CV) i MTT test, a kao kontrola korišćena je cisplatina. Bakar(II) kompleks pokazao je dva do tri puta veću aktivnost od polaznog liganda.

Synthesis, characterization and cytotoxicity of Cu(II) complex with *O,O'*-diethyl ester of (*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)-pentanoic acid

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Copper(II) has an important biological role in all living systems as an essential trace element. The Cu(II) complexes with organic ligands have been used as analgesic, antipyretic and anti-inflammatory agents. They have antioxidant and antitumor activity. Copper(II) complex with bidentate *N,N'*-ligand, *O,O'*-diethyl ester of (*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)pentanoic acid was prepared.The structure of the isolated complex is proposed on the basis of elemental microanalysis and infrared spectra. The ligand and its complex were tested for their *in vitro* cytotoxic activity against HT-29, PC-3, MCF-7 and B16F1 cell line, using crystal violet (CV) and MTT assay with the aim of assessing *in vitro* antitumoral activity and compared with cisplatin as control. Copper(II) complex shows two to three times higher cytotoxicity than ligand precursor.

NH-9

Ru(II) bipiridinski kompleksi sa analozima acetilpiridina: spektralna i elektrohemijska karakterizacija

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Raznovrsna hemija kompleksa rutenijuma obuhvata hiljade jedinjenja namenjenih za različite primene, npr. homogenu katalizu, terapiju kancera, dijagnozu tumora i moderne materijale.[1] S tim u vezi se opisuje sinteza i kompletna (elektro)hemijska karakterizacija tri nova Ru(II) kompleksa sa acetilpiridinskim ligandom (acpy). Kompleksi su dobijeni reakcijom tri ekvivalenta liganda (2-, 3-, i 4-acpy) sa ekvimolarnom količinom prekursora metala, $[RuCl_2(bpy)_2]$ u metanolu. Nakon refluksa preko noći, reakciona smeša je ostavljena da se ohladi kad je dodata ekvimolarna količina NH_4PF_6. Produkti su izolovani u obliku tamnocrvenog praha. Kompleksi su okarakterisani IC, NMR i MS pokazujući bidentatnu koordinaciju 2-acpy i monodentatno vezivanje 3- i 4-acpy. Njihov elektrohemijski profil je ispitan cikličnom voltametrijom koja je potvrdila bogatu redoks hemiju.

Ru(II) bipyridine complexes with acetylpyridine analogues: spectral and electrochemical characterization

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The versatile chemistry of ruthenium complexes involves thousands of compounds aimed for different applications related to e.g. homogenous catalysis, cancer therapy, tumor diagnosis, and advanced materials.[1] Thus, the synthesis and full (electro)chemical characterization of three new Ru(II) complexes carrying acetylpyridine (acpy) ligand unitis is described. The complexes were obtained via reaction of three ligand equivalents (2-, 3-, and 4-acpy) with an equimolar amount of metal precursor, $[RuCl_2(bpy)_2]$ in methanol. After the overnight reflux, the reaction mixture was left to cool when equimolar amount of NH_4PF_6 was added. The products were isolated in a form of dark red powder. The complexes were characterized by IR, NMR and MS revealing bidentate coordination of 2-acpy and monodentate binding of 3- and 4-acpy. Their electrochemical profile was studied by cyclic voltammetry which confirmed rich redox chemistry.

1. I. Dragutan, V. Dragutan, A. Demonceau, *Molecules*. **2015**, *20*, 17244.
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NH-10

Ispitivanje uticaja pH i granulacije na početnu brzinu rastvaranja fosfatnog stakla

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Fosfatna stakla imaju jedinstveno svojstvo da se mogu potpuno rastvoriti u vodenim rastvorima, a brzina rastvaranja može da se kontroliše. Proces rastvaranja stakla počinje razmenom katjona sa površine stakla sa protonima iz rastvora (H^+ ili H_3O^+) i hidratacijom staklene mreže. Početna brzina rastvaranja je osnovna karakteristika rastvaranja stakla. Analiza početnih brzina rastvaranja fosfatnog stakla, koje je dobijeno topljenjem, pokazuje da su brzine značajno veće u kiseloj sredini u odnosu na brzine rastvaranja u neutralnoj. Granulacija uzorka ima veći uticaj na početne brzine u neutralnoj sredini. Granulacija uzorka ne utiče na vrednost energije aktivacija početnih brzina rastvaranja u obe sredine. U neutralnoj sredini temperatura manje utiče na hidrolizu, a više na difuziju katjona, dok je u kiseloj sredini suprotno.

Investigation of the influence of pH and granulation on the initial dissolution rate of phosphate glass

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Phosphate glasses have the unique property that they can be completely dissolved in aqueous solutions, and the dissolution rate can be controlled. The process of dissolving glass begins by exchanging cations from the glass surface with protons from solution (H^+ or H_3O^+) and hidratation of the glass network. The initial dissolution rate is the basic characteristic of glass dissolution. Analysis of the initial dissolution rates of phosphate glass, which was obtained by melting, shows that the rates are significantly higher in an acidic environment compared to the dissolution rates in a neutral one. Sample granulation has a greater effect on initial rates in a neutral medium. The granulation of the sample does not affect the value of the activation energy of the initial dissolution rates in both media. In a neutral medium, the temperature has less effect on hydrolysis and more on the diffusion of cations, while the opposite stands for an acid. *This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2022-14/200023 and Contract No. 451-03-68/2022-14/200135) .*

NH-11

Sinteza, karakterizacija i antimikrobna aktivnost kompleksa Cu(II) sa kondenzacionim derivatom 2-acetilpiridina i dihidrazida malonske kiseline

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Kompleks Cu(II) sa kondenzacionim derivatom 2-acetilpiridina i dihidrazida malonske kiseline (H_2L) je dobijen direktnom sintezom. Prekristalizacijom je dobijen monokristalni proizvod te je struktura kompleksa rešena primenom rendgenske strukturne analize. U unutrašnjoj sferi binuklearnog simetričnog kompleksa, sa distorgovanom oktaedarskom geometrijom oko jona Cu(II), jedan molekul liganda je koordinovan u anjonskom, a drugi u neutralnom obliku, oba *bis*-tridentatno preko *N,N,O* seta donorskih atoma. U spoljašnjoj sferi kompleksa se nalaze perhloratni joni i molekuli vode. Kompleks je pokazao antimikrobnu aktivnost u niskom mikromolarnom opsegu na svim testiranim mikroorganizmima.

Synthesis, characterization and antimicrobial activity of Cu(II) complex with condensation derivative of 2-acetylpyridine and malonic acid dihydrazide

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The Cu(II) complex with the ligand H_2L, which is a condensation derivative of 2-acetylpyridine and malonic acid dihydrazide, was obtained by direct synthesis. Recrystallization gave a single crystal product, and the structure of the complex was solved by X-ray structural analysis. In the inner sphere of the binuclear symmetrical complex, with distorted octahedral geometry around Cu(II) ions, one ligand molecule is coordinated in anionic and the other in neutral form, both *bis*-tridentaly *via* the *N, N, O* set of donor atoms. Perchlorate ions and water molecules are located in the outer sphere of the complex. The complex showed antimicrobial activity in the low micromolar range on all tested microorganisms.

NH-12

Novi dinuklearni Au(III) kompleks: Sinteza, karkterizacija i ispitivanje interakcija sa DNK

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S obzirom da su kompleksi zlata(III) izoelektronski i izostrukturni sa kompleksima platine(II), sinteza i biološka aktivnost ovih jedinjenja su predmet intenzivnih izučavanja poslednjih godina.[1] U okviru ovog istraživanja sintetisan je novi dinuklearni kompleks zlata(III) sa 1,5-naftiridinom kao mostnim ligandom. Struktura kompleksa okarakterisana je različitim analitičkim metodama (IR, UV-Vis, ^{1}H NMR, ESI-MS, konduktometrija). Ispitivane su interakcije kompleksa sa DNK pomoću UV-Vis spektrofotometrije, merenjem fluorescencije i merenjem viskoznosti. Na osnovu UV-Vis spektrofotometrije potvrđeno je da se kompleks vezuje za DNK, dok je na osnovu rezultata dobijenih spektrofluorimetrijom i merenjem viskoznosti potvrđeno da se kompleks kovalentno vezuje sa molekul DNK.

New dinuclear Au(III) complex: Synthesis, characterization and study of the interections with DNA

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Considering that gold(III) complexes are isostructural and isoelectronic with platinum(II) complexes, the synthesis, characterization and study of their biological activity were very common in the last few years. We have synthesized new dinuclear gold(III) complex with 1.5-naphtiridine as bridging ligand. The structure of this complex was confirmed by different analytical methods (IR, UV-Vis,^{1}H NMR, mass analysis, conductometry). The study of the interactions between complex and DNA was performed by UV-Vis spectrofotometry, fluorescence spectroscopy and viscosity measurement. Based on the results of UV-Vis spectrofotometry can be concluded that complex binds to DNA. According to the results obtained by fluorescence spectroscopy and by viscosity measurement, the covalent binding mode between complex and DNA was confirmed.

1. M. Cini, T. D. Bradshaw, S. Woodward, *Chem. Soc. Rev.*, **2017**, 46, 1040.

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NH-13

Синтеза и структурна карактеризација комплекса Cu(II) са бис(салицилалдехид)-2,2′-диаминобифенил-4,4′-дикарбоксилном киселином

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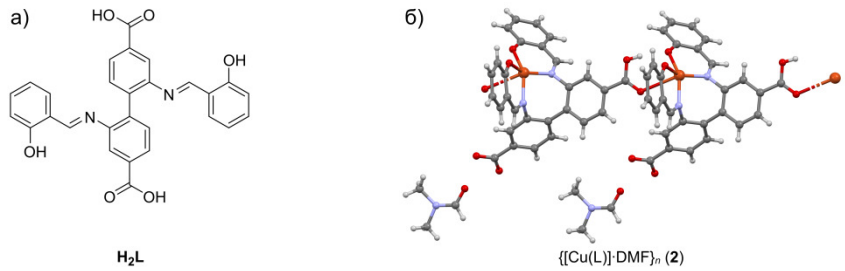
Лиганд (**H_2L**) синтетисан у кондензационој реакцији салицилалдехида и 2,2′-диаминобифенил-4,4′-дикарбоксилне киселине приказан је на слици 1а. У реакцији лиганда са $Cu(OAc)_2 \cdot H_2O$ у метанолном раствору добијен је полимерни комплекс $\{[Cu(L)] \cdot MeOH\}_n$ (**1**), док се други полимерни комплекс, $\{[Cu(L)] \cdot DMF\}_n$ (**2**), добија када се реакција изводи у DMF у присуству мрављe киселине. Лиганд и комплекси су окарактерисани FTIR спектроскопијом и термичком анализом, а кристалне структуре су одређене дифракцијом рендгенских зрака на монокристалу (слика 1б).



*Слика 1. Хемијска формула H_2L и молекулска структура комплекса (**2**).*

Synthesis and structural characterization of Cu(II) complexes with bis(salicylaldehyde)-2,2′-diaminobiphenyl-4,4′-dicarboxylic acid

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Ligand (**H_2L**) was synthesized by the condensation reaction of salicylaldehyde and 2,2′-diaminobiphenyl-4,4′-dicarboxylic acid. Reaction of the ligand with $Cu(OAc)_2 \cdot H_2O$ in methanolic solution yields polymeric complexes $\{[Cu(L)] \cdot MeOH\}_n$ (**1**), while in DMF solution, in presence of formic acid, polymeric $\{[Cu(L)] \cdot DMF\}_n$ (**2**) complex was obtained. The ligand and complexes are characterized by FTIR spectroscopy and thermal analysis, while their crystal structures were determined by single crystal X-ray crystallography.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, PROMIS, #6066708, CASCH-MOF

NH-14

Ispitivanje interakcija dinuklearnih kompleksa platine(II) sa serum albuminom

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Ispitivanje interakcija kompleksa prelaznih metala sa serum albuminima poslednjih godina predmet su mnogih istraživanja. Humani serum albumin (HSA) je jedan od osnovnih proteina u krvnoj plazmi, koji ima važnu ulogu u transportu mnogih lekova. U ovom radu ispitivane su interakcije tri dinuklearna kompleksa platine(II), $[\{Pt(en)Cl\}_2(\mu\text{-}qx)]Cl_2 \cdot 2H_2O$, $[\{Pt(en)Cl\}_2(\mu\text{-phtz})]Cl_2 \cdot 4H_2Oi$ $[\{Pt(en)Cl\}_2(\mu\text{-qz})](ClO_4)_2$, (en je bidentatno koordinovani etilendiamin, dok su hinoksalin (qx), hinazolin (qz) i ftalazin (phtz) mostni ligandi) sa serum albuminom, koji je izolovan iz krvi goveda (BSA), primenom UV-Vis i fluorescentne spektroskopije. Rezultati ispitivanja su pokazali da dinuklearni kompleksi platine(II) ostvaruju nekovalentne interakcije sa BSA i da se na taj način mogu transportovatido ćelije.

Investigation of the interactions of dinuclear platinum(II) complexes with serum albumin

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The interactions of transition metal complexes with serum albumins have been extensively investigated in recent years. Human serum albumin (HSA), one of the vital proteins in drug delivery system in the body, was used as a target protein. In the present study, the interactions of three dinuclear platinum(II) complexes, $[\{Pt(en)Cl\}_2(\mu\text{-qx})]Cl_2 \cdot 2H_2O$, $[\{Pt(en)Cl\}_2(\mu\text{-phtz})]Cl_2 \cdot 4H_2O$ and $[\{Pt(en)Cl\}_2(\mu\text{-qz})](ClO_4)_2$ (en is bidentate coordinated ethylenediamine, while quinoxaline (qx), phthalazine (phtz) and quinazoline (qz) are bridging ligands) with bovine serum albumin (BSA) were investigated by UV**-**Visand fluorescence spectroscopy. The obtained results showed that these dinuclear platinum(II) complexes achieve noncovalent interactions with BSAandcan be transported to the cell in this way.

Acknowledgmentt: This work funded in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Agreement No. 451-03-68/2022-14/200122)

NH-15

Multifunkcionalni koordinacioni polimeri Ag(I) sa ditopnim ligandima

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Sintetisano je i strukturno okarakterisano devet koordinacionih polimera Ag(I) sa ditopnim ligandima: 2-piridintiocijanatom, tiomorfolin-4-karbonitrilom i piperazin-1,4-dikarbonitrilom, kao i ko-ligandima na bazi polioksokiselina. Osam novosintetisanih koordinacionih polimera ima uporedivu ili veću fotokatalitičku aktivnost od standarda TiO_2. Ispitivanje mehanizma razgradnje azo-boje mordant 9 plava je pokazalo da se fotokatalitički procesi dešavaju stvaranjem fotoekscitovanih elektrona ili superoksidnih jona kao reaktivnih vrsta. Dva koordinaciona polimera koja sadrže ko-ligand ispoljavaju fotoluminescentna svojstva, čije je poreklo razjašnjeno pomoću DFT i TD-DFT proračuna. Rezultati ove studije mogu doprineti kako racionalnom dizajnu novih koordinacionih polimera Ag(I), tako i proceni njihove potencijalne primene kao efikasnih fotokatalizatora i OLED materijala.

Multifunctional Ag(I) coordination polymers with ditopic ligands

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Nine Ag (I) coordination polymers with ditopic ligands: 2-pyridinthiocyanate, thiomorpholine-4-carbonitrile, piperazine-1,4-dicarbonitrile, and polyoxoacids as co-ligands, were synthesized and structurally characterized. Eight coordination polymers have comparable or higher photocatalytic activity than TiO_2 standard. Investigation of the azo-dye mordant 9 blue degradation mechanism has shown that photocatalytic processes occur by forming photoexcited electrons or superoxide ions as reactive species. Two coordination polymers containing co-ligands exhibit photoluminescent properties, the origin of which has been elucidated using DFT and TD-DFT calculations. The results of this study can contribute to the rational design of new Ag(I) coordination polymers and the assessment of their potential application as efficient photocatalysts and OLED materials.

NH-16

Prvi kompleks vanadijuma sa Šifovom bazom aminogvanidina i 2,4-dihidroksibenzaldehida

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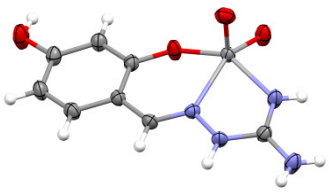
Reakcijom amonijum-metavanadata sa Šifovom bazom, kondenzacionim proizvodom aminogvanidina i 2,4-dihidroksibenzaldehida, u molskom odnosu 1:1, u amonijaku uz refluks, dobijeni su monokristali kompleksa formule $[VO_2(L)]$, gde je L – monoanjon Šifove baze. Kompleks je slabo rastvoran u vodi, alkoholima i acetonu, a dobro rastvoran u DMF. Ligand je koordinovan na tridentatni ONN način i to preko atoma kiseonika hidroksilne grupe iz položaja 2, atoma azota azometinske i imino grupe aminogvanidinskog fragmenta. Vanadijum je smešten u kvadratno-piramidalno okruženje tri donorna atoma helatnog liganda i jednog oksido liganda u ekvatorijalnoj ravni i drugog oksido liganda u apikalnom položaju (slika 1).



Slika 1. Molekulska struktura kopmpleksa

The first vanadium complex with Schiff base of aminoguanidine and 2,4-dihydroxybenzaldehyde

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Ljiljana S. Vojinović Ješić, Svetlana Belošević, Vukadin M. Leovac.
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The reaction of ammonium-metavanadate with the aminoguanidinium-2,4-dihydroxybenzaldehyde chloride in molar ratio 1:1, in ammonia under reflux, yielded in formation of single crystals of the complex $[VO_2(L)]$, L – monoanion of the Schiff base. The complex is poorly soluble in water, alcohols and acetone, and well soluble in DMF. The ligand is coordinated in ONN manner, through oxygen atom of the hydroxy-group in position 2, azomethine and nitrogen atom of imino group of aminoguanidine residue. Vanadium atom is situated in square-pyramidal environment formed by three ligators of the chelating ligand, one oxido-ligand in basal plane, and the other oxido-ligand in the apical position.

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NH-17

Sinteza i karakterizacija kompleksa Fe(III) i Mn(II) sa kondenzacionim proizvodom tiosemikarbazida i 2-acetiltiazola

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Ligand (**HL**) sintetisan je u reakciji tiosemikarbazida i 2-acetiltiazola u molarnom odnosu 1 : 1 u vodi, u kiseloj sredini. Kompleks $[Fe(\mathbf{L})_2]BF_4 \cdot H_2O$ (**1**) dobijen je u reakciji liganda i $Fe(BF_4)_2 \cdot 6H_2O$ u metanolu i nakon potpunog rastvaranja Fe(II) soli dodat je NaN_3 u višku (1 : 1 : 4). U reakciji liganda (**HL**), $MnCl_2 \cdot 4H_2O$ i NaN_3 u molarnom odnosu 1 : 1 : 4, dobijen je kompleks Mn(II), $[Mn(\mathbf{L})_2]$ (**2**). Kompleksi **1** i **2** okarakterisani su elementalnom analizom, IC spektroskopijom, UV/Vis spektroskopijom i rendgenskom strukturnom analizom. Kod oba kompleksa **1** i **2** dolazi do forimiranja bis oktaedarske geometrije tako što se za centralni metalni jon koordinuju dva deprotonovana liganda preko dva NNS donorska seta atoma u mer okruženju. Do koordinacije liganda za centralni metalni jon, kako Fe(III), tako i Mn(II), dolazi preko dva azota, od kojih jedan potiče iz tiazola, a drugi iz iminske grupe, kao i preko sumpora iz tioenolatne grupe.

Synthesis and characterization of Fe(III) i Mn(II) complexes with condensation product of thiosemicarbazide and 2-acetylthiazole

Milica Savić[a], Nevena Stevanović[b], Mima Jevtović[c], Maja Gruden[b], Katarina Anđelković[b], Božidar Čobeljić[b], Matija Zlatar[a]

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The **HL** ligand was synthetized in the reaction of thiosemicarbazide and 2-acetylthiazole in molar ratio 1:1 in water, with 3 drops of 2M HCl. Complex $[Fe(\mathbf{L})_2]BF_4 \cdot H_2O$ (**1**) was synthetized in reaction of ligand and $Fe(BF_4)_6 \cdot 6H_2O$ in MeOH, after complete dissolution of $Fe(BF_4)_2 \cdot 6H_2O$ in the reaction mixture, NaN_3 was added. In the reaction of ligand (**HL**), $MnCl_2 \cdot 4H_2O$ and NaN_3, in molar rotio 1 : 1 : 4, Mn(II) complex (**2**) was obtained. Complexes **1** and **2** were characterized by elemental analysis, IR and UV/Vis spectroscopy and X-ray crystallographic analysis. Both complexes **1** and **2** with **HL** ligand are bis octahedral complexes in which two deprotonated ligand molecules coordinate in a *mer* arrangement through two NNS sets of donor atoms, through thiazole and imine nitrogens and thioenolate sulfur.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes – TMMagCat.

NH-18

Hidrazonski kompleksi Cu(II), Mn(II) i Zn(II) sa kvaternernim amonijum fragmentom: sinteza, karakterizacija i DFT proračuni

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U reakciji liganda **HL**Cl sa solima metala $Cu(BF_4)_2 \cdot 6H_2O$ / $MnCl_2 \cdot 4H_2O$ / $Zn(BF_4)_2 \cdot 6H_2O$ i NaN_3 u metanolu, dobijeni su mononuklearni kompleksi koordinacionog broja pet: $[Cu\mathbf{L}(N_3)(CH_3OH)]BF_4$ (**1**) i $[Zn\mathbf{L}(N_3)_2]$ (**2**) i dinuklearni kompleks $[Mn_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]\cdot 2CH_3OH$ (**3**). Kompleksi **1**, **2** i **3** okarakterisani su elementalnom analizom, IC spektroskopijom, rendgenskom stukturnom analizom i DFT proračunima. U sva tri kompleksa ligand (**L**) se koordinuje u deprotonovanom obliku preko NNO donorskog seta atoma. DTF proračuni su pokazali da je kompleks Cu(II) u DMSO-u najstabilniji u obliku kvadratno-planarne geometrije. U istom rastvoru kompleks Mn(II) se nalazi kao smeša kompleksa $[Mn\mathbf{L}(N_3)_2]$ i $[Mn_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]$.

Cu(II), Mn(II) and Zn(II) complexes of hydrazones with quaternary ammonium moiety: Synthesis, characterization and DFT calculation

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The **HL**Cl ligand with metal salts $Cu(BF_4)_2 \cdot 6H_2O$ / $MnCl_2 \cdot 4H_2O$ / $Zn(BF_4)_2 \cdot 6H_2O$ and NaN_3, in methanol form mononuclear penta-coordinated complexes $[Cu\mathbf{L}(N_3)(CH_3OH)]BF_4$ (**1**) and $[Zn\mathbf{L}(N_3)_2]$ (**2**) and binuclear $[Mn_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]\cdot 2CH_3OH$ (**3**) complex. Complexes **1**, **2** and **3** were characterized by elemental analysis, IR spectroscopy, single-crystal X-ray diffraction, and DFT calculations. In all three complexes ligand ($\mathbf{L}^1$) is coordinated in deprotonated formally neutral form *via* NNO donor set atoms. According to the DFT studies, Cu(II) complex is the most stable in square-planar geometry, while in the same DMSO solution, Mn(II) complex is the mixture of $[Mn\mathbf{L}(N_3)_2]$ and $[Mn_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]$ complexes.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes – TMMagCat.

NH-19

Sinteza, karakterizacija i antimikrobna aktivnost kompleksa srebra(I) i zlata(III) sa antifungalnim agensom mikonazolom

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Sintetisani su kompleksi srebra(I) i zlata(III) sa antifungalnim agensom mikonazolom (mcz), $[Ag(mcz)_2]NO_3$ (**1**) i $[AuCl_3(mcz)]$ (**2**).[1] Kompleksi su okarakterisani primenom spektroskopskih metoda, dok je kristalna struktura kompleksa **1** određena metodom difrakcije rendgenskih zraka sa monokristala. Ispitivana je antimikrobna aktivnost kompleksa **1** i **2** prema različitim sojevima bakterija i gljivica, kao i njihova citotoksična aktivnost prema normalnoj ćelijskoj liniji fibroblasta pluća (MRC-5). Za kompleks **2** ispitivane su interakcije sa DNK i albuminom goveđeg seruma primenom fluorescentne spektroskopije.

Synthesis, characterization and antimicrobial activity of silver(I) and gold(III) complexes with the antifungal agent miconazole

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Silver(I) and gold(III) complexes with the antifungal agent miconazole (mcz), $[Ag(mcz)_2]NO_3$ (**1**) and $[AuCl_3(mcz)]$ (**2**) were synthesized.[1] These complexes were characterized by spectroscopic methods, while the structure of complex **1** was determined by a single-crystal X-ray diffraction analysis. The antimicrobial activity of complexes **1** and **2** was investigated against different bacterial and fungal strains, as well as their cytotoxic activity on the normal human lung fibroblast cell line (MRC-5). The interactions of complex **2** with DNA and bovine serum albumin were studied by fluorescence spectroscopy.

1. N. Lj. Stevanović, J. Kljun, M. Stankovic, S. Skaro-Bogojevic, J. Lazic, I. Turel, M. I. Djuran, B. Đ. Glišić, *Manuscript in preparation*

Organska hemija

Organic Chemistry

OH-1

Sinteza novih tetrazola kao potencijalnih antiandrogena

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Kancer prostate (KP) je složena bolest koja pogađa milione muškaraca svake godine. Pošto je preko 80% KP androgen-zavisno, lijekovi koji sprečavaju biosintezu androgena i/ili blokiraju dejstvo androgenih receptora (AR), u mnogim slučajevima mogu da inhibiraju rast kancera. Nesteroidna jedinjenja kao što su flutamid i nilutamid suprotstavljaju se dejstvu androgena vezivanjem za AR. Oni su čisti antiandrogeni bez androgenih svojstava, što ih čini pogodnim za upotrebu u liječenju KP.[1] Prisustvo elektron-akceptorskih grupa (npr. nitro-, trifluormetil-, nitrilna) u aromatičnom prstenu važno je za antiandrogenu aktivnost flutamida i njegovih derivata.[2] Jedinjenja koja sadrže tetrazolski prsten ispoljavaju različite biološke aktivnosti. Ovdje prijavljujemo sintezu novih *N*-aril-tetrazola čiji fenil-supstituenti sadrže dvije elektron-akceptorske grupe.

Synthesis of novel tetrazoles as potential antiandrogens

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Prostate cancer (PC) is a complex disease that affects millions of men each year. Since over 80% of PC is androgen-dependent, drugs that prevent the biosynthesis of androgens and/or block the action of androgen receptors (AR), can in many cases inhibit cancer growth. Nonsteroidal compounds such as flutamide and nilutamide antagonize the actions of androgens by competing for AR binding site. They are pure antiandrogens without androgenic properties, which makes them suitable for use in the treatment of PC.[1] The presence of electron-withdrawing substituents (e.g., nitro, trifluoromethyl, nitrile) in the aromatic ring is important for the antiandrogenic activity of flutamide and its derivatives.[2] Compounds containing a tetrazole moiety exhibit diverse biological activities. Herein, we report a synthesis of novel *N*-aryl tetrazole derivatives with a phenyl substituent that bears two electron-withdrawing groups.

1. M. Tan, J. Li, H. Xu, K. Melcher, E. Yong, *Acta Pharmacol. Sin.* **2015**, *36*, 3.
2. S. Singh, S. Gauthier, F. Labrie, *Curr. Med. Chem.* **2000**, *7*, 211.

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OH-2

Sinteza i karakterizacija gradivnih blokova poli(etilen-tereftalata)

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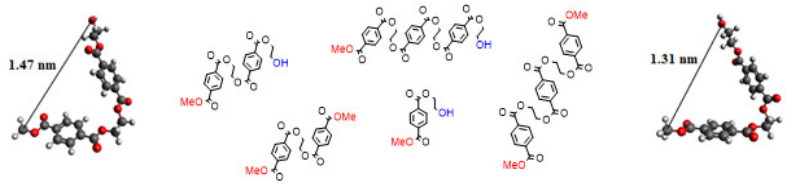
U radu je predstavljena „*bottom-up*" metodologija sinteze oligomera poli(etilen-tereftalata), polazeći od relativno jednostavnih i jeftinih reaktanata: etilen-glikola i tereftalne kiseline. Serija različito funkcionalizovanih PET oligoestara je sintetisana primenom *Steglich-ovog* esterifikacionog protokola i *Schotten-Baumann-ove* reakcije acilovanja na ortogonalno zaštićenim reaktantima. Primenom računskih metoda procenjena je veličina sintetisanih molekula koja se nalazi u nano- skali (1-3 nm). Dodatno, sprovedeni su i VPO (*eng. vapor pressure osmometry*) ekseperimenti koji ukazuju da sintetisani molekuli u rastvoru ispoljavaju sklonost ka građenju većih agregata.



Slika 1. Sturkture sintetisanih PET oligoestara sa izdvojenim konformerima PET dimera

Synthesis and characterization of poly(ethylene-terephthalate) building blocks

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The paper presents a „*bottom-up*" methodology for the synthesis of poly(ethylene-terephthalate) oligomers, starting from relatively simple and cheap reactants: ethylene glycol and terephthalic acid. A series of differently functionalized PET oligoesters was synthesized using the *Steglich* esterification protocol and the *Schotten-Baumann* acylation reaction on orthogonally protected reactants. The size of the synthesized molecules in the nanoscale (1-3 nm) was estimated using computer methods. In addition, VPO experiments were performed, which indicate that the synthesized molecules in solution show a tendency to build larger aggregates.

Acknowledgment: This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 870292 (BioICEP).

OH-3

Sinteza, karakterizacija i antioksidativna aktivnost 1,3-dihidro-3-[4-supstituisanih-(fenilmetil)imino]-2*H*-indol-2-ona

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Izvršena je sinteza četiri 1,3-dihidro-3-[4-supstituisanih-(fenilmetil)imino]-2*H*-indol-2-ona i to: 1,3-dihidro-3-[(fenilmetil)imino]-2*H*-indol-2-ona, 1,3-dihidro-3-[4-brom-(fenilmetil)imino]-2*H*-indol-2-ona, 1,3-dihidro-3-[4-hidroksi-(fenilmetil) imino]-2*H*-indol-2-ona, 1,3-dihidro-3-[4-metoksi-(fenilmetil)imino]-2*H*-indol-2-ona, kao i jedinjenja slične strukture, 1,3-dihidro-3-[(2-feniletil)imino]-2*H*-indol-2-ona. Urađena je karakterizacija sintetisanih jedinjenja primenom FTIR spektroskopije, određivanjem temperature topljenja i elementalnom analizom, nakon čega je izvršeno ispitivanje antioksidativne aktivnosti svih pet jedinjenja. Antioksidativna aktivnost je određena primenom DPPH (1,1-difenil-2-pikril-hidrazil radikal) metode, u cilju određivanja najefikasinijeg jedinjenja od značaja za dalje istraživanje.

Synthesis, characterization and antioxidative activity of 1,3-dihydro-3-[4-substituted-(phenylmethyl)imino]-2*H*-indole-2-ones

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The synthesis of 1,3-dihydro-3-[4-substituted-(phenylmethyl)imino]-2*H*-indole-2-ones: 1,3-dihydro-3-[(phenylmethyl)imino]-2*H*-indol-2-one, 1,3-dihydro-3-[4-bromo-(phenylmethyl)imino]-2*H*-indol-2-one, 1,3-dihydro-3-[4-hydroxy-phenyl-methyl)imino]-2*H*-indol-2-one, 1,3-dihydro-3-[4-methoxy-(phenylmethyl)imino]-2*H*-indol-2-one, as well as of the compound of similar structure, 1,3-dihydro-3-[(2-phenylethyl)imino]-2*H*-indol-2-one, was performed. The characterization of the obtained five compounds was carried out using FTIR, melting points and elemental analysis. Their antioxydative activity was then tested by DPPH (2,2-diphenyl-1-picrylhydrazyl radical) method and the results were compared in order to determine the most efficient compound, significant for further research.

OH-4

Insercija bakar-karbenoida/Horner-Wadsworth-Emmons-ova reakcija kao nova metoda za sintezu tricikličnog jezgra (+)-alstonlarsina A

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Jedan od ključnih koraka u okviru planirane totalne sinteze (+)-alstonlarsina A[1] je intramolekulska Horner-Wadsworth-Emmons-ova (HWE) reakcija za zatvaranje cikloheptenskog prstena. Nedavno izolovani monoterpenski indolski alkaloid (+)-alstonlarsin A poseduje jedinstvenu kavezastu strukturu, kao i biološki interesantnu osobinu da se ponaša kao inhibitor DRAK2 enzima. Stoga je razvijena nova metodologija za funkcionalizaciju indola u položaju 2, kako bi se sintetisao odgovarajući 2-fosfonoacetatni indolski prekursor. Ova metodologija se zasniva na efikasnoj intramolekulskoj bakar-karbenoidnoj inserciji, čime je omogućena kasnija HWE reakcija i dobijanje kondenzovanih indolskih derivata sa kondenzovanim petočlanim, šestočlanim, sedmočlanim i osmočlanim prstenom.

A copper carbenoid insertion/Horner-Wadsworth-Emmons reaction as a new method for the synthesis (+)-alstonlarsine A tricyclic core

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One of the key steps in our efforts toward the total synthesis of (+)-alstonlarsine A[1] – a recently isolated monoterpenoid indole alkaloid possessing a unique cage-shaped structure and acting as Drak2 inhibitor – was an intramolecular Horner-Wadsworth-Emmons (HWE) reaction for the formation of the cycloheptene ring. To achieve this transformation, a new methodology for indole C-2 functionalization was developed aiming to synthesize the 2-phosphonoacetate indole precursor. The represented methodology relied on an efficient intermolecular copper carbenoid insertion, thus allowing a subsequent formation of indole derivatives with condensed 5-, 6-, 7- and 8-membered rings *via* HWE reaction.

1. X.-X. Zhu, Y.-Y. Fan, L. Xu, Q.-F. Liu, J.-P. Wu, J.-Y. Li, J. Li, K. Gao, J.-M. Yue, *Org. Lett.*, **2019**, *21*, 1471.

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

OH-5

Sintetičke studije za dobijanje (+)-rauvomina B i drugih članova makrolinske/sarpaginske grupe alkaloida

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Indolski alkaloid (+)-rauvomin B[1] u svojoj strukturi ima ciklopropanski prsten inkorporiran u jedinstven 6/5/6/6/3/5 heksaciklični skelet sa 6 stereocentara, zbog čega ovaj molekul predstavlja ozbiljan sintetički izazov.
Naša strategija za totalnu sintezu (+)-rauvomina B obuhvata sintezu tetracikličnog indolskog derivata, kao jednog od ključnih intermedijera. Ovaj molekul se može dobiti u 4 koraka, iz komercijalno dostupnog N-Boc-(*S*)-triptofana, sledećim nizom reakcija: 1) homologizacija do homotriptofana 2) aldolna reakcija 3) Pictet-Spengler-ova reakcija 4) eliminacija. Takodje, nekoliko drugih članova klase makrolinskih/sarpaginskih alkaloida se mogu dobiti iz ovog zajedničkog intermedijera, omogućavajući objedinjenu sintezu ovih prirodnih proizvoda.

Synthetic studies towards (+)-rauvomine B and other macroline/sarpagine alkaloids

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University of Belgrade – Faculty of Chemistry, Belgrade, Serbia
2

Indole alkaloid (+)-rauvomine B[1] contains cyclopropane ring incorporated in the unprecedented 6/5/6/6/3/5 hexacyclic structure ornate with six stereocenters, making this compound a challenging synthetic task.

Our strategy for (+)-rauvomine B total synthesis proceeds *via* a key tetracyclic intermediate, which could be efficiently prepared from commercially available *N*-Boc-(*S*)-tryptophan in 4 steps: 1) homologization to homotryptophan 2) aldol reaction 3) Pictet-Spengler reaction 4) elimination. This efficient route also enabled several other members of macroline/sarpagine indole alkaloids to be synthesized from this common intermediate, *via* unified strategy.

1. J. Zeng, D.-B. Zhang, P.-P. Zhou, Q.-L. Zhang, L. Zhao, J.-J. Chen, K. Gao, *Org. Lett.* **2017**, *19*, 3998

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

OH-6

Fotoredoks funkcionalizacija N-aril-tetrahidroizohinolina u mikrofluidnim uređajima

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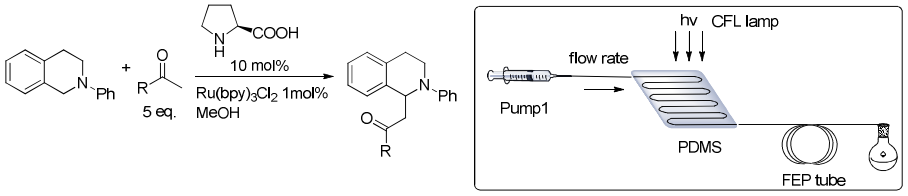
Primena mikrofluidnih uređaja u direktnoj funkcionalizaciji biološki aktivnih N-aril-tetrahidroizohinolina, u prisustvu fotokatalizatora $Ru(bpy)_3Cl_2$, ukazuje na superiornost ove eksperimentalne tehnike u odnosu na konvencionalne reaktore. Mikrofluidni uređaji su primenjeni za ispitivanje Manihove reakcije, Štrekerove reakcije i reakcije alkinilovanja. Kako je za reoksidaciju fotokatalizatora neophodan kiseonik, mikroreaktor od PDMS-a koji je porozan za gasove omogućio je najefikasniju oksidaciju u poređenju sa drugim ispitivanim mikroreaktorima.



Slika 1. Manihova reakcija N-aril-tetrahidroizohinolina u mikrofluidnom uređaju.

Visible Light Promoted Cross-Dehydrogenative Coupling Reactions (CDC) of N-Aryl- tetrahydroisoquinolines in Flow

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

Application of microfluidic devices in the visible light promoted cross-dehydrogenative coupling reactions (CDC) of N-aryl-tetrahydroisoquinolines (THIQs), priviledged, biologically active structures, using $Ru(bpy)_3Cl_2$ complexes as photosenzitizers proved as a very efficient strategy for C-1 functionalization of THIQs including Mannich reaction, Strecker reaction, and alkynylation reaction setups. The use of a gas porous PDMS microreactor proved to be crucial regarding the C–H oxidation step. Based on our results the utilization of microreactors in CDC coupling reactions has great perspective and has high importance in the functionalization of biologically active structures such as THIQs.[1]

1. References: A. Filipović, Z. Džambaski, D. Vasiljević-Radović, and B. P. Bondžić, *Org. Biomol. Chem.*, 2021, 19, 2668–2675

Acknowledgement: This work was supported by Ministry of Education, Science and Technological development (Project No 451-03-68/2022-14/200026)

OH-7

Oksidativna fragmentacija i dekarbonilativno acilovanje

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Oksidativno raskidanje veze karbonilnog ugljenika sa C_α atomom je intrigantna reakcija koja je privukla pažnju hemičara u protekloj deceniji jer se odvija pod relativno blagim uslovima koji zadovoljavaju principe zelene hemije. Razvijena je jednostavna procedura za efikasno izvodjenje oksidativne fragmentacije na aldehidima. Optimizovana je one-pot varijanta konsekutivnog alfa-arilovanja i oksidativne fragmentacije. Ukupna transformacija (dekarbonilativno acilovanje) je primenljiva na supstrate sa različitim elektronskim efektima i koliko je nama poznato, nije do sada prijavljena u literaturi.

Oxidative fragmentation and decarbonylative acylation

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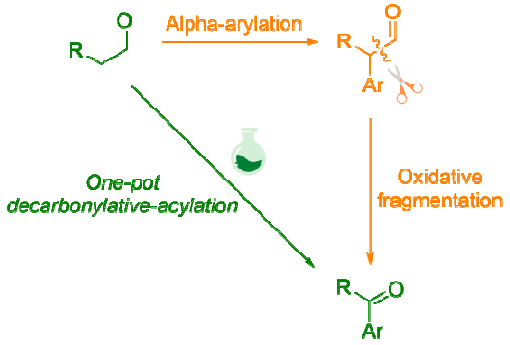
[2] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

An oxidative cleavage of a bond between carbonyl carbon and C_α carbon atom is an intriguing reaction which has attracted interest of chemists in the last decade because of mild and green conditions needed for the transformation. A simple procedure for oxidative fragmentation of aldehydes is developed. A conditions for one-pot consecutive alpha-arylation and oxidative fragmentation have been optimized (Scheme 1). An overall transformation (decarbonylative acylation) is applicable to supstrates that differ in electronic effects and to our knowledge, it hasn't been reported so far in the literature.



Scheme 1. Alpha-arylation, oxidative fragmentation and a one-pot combination of the two

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OH-8

Sinteza, biološka ispitivanja i *in silico* testiranje 17α-(piridin-2-il)-estra-1,3,5(10)-trien derivata

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Uvođenjem heteroatoma ili heterocikla u strukturu steroidnog skeleta često dolazi do promena u njegovim biološkim i/ili farmakološkim aktivnostima. S obzirom na ovo, sintetisani su 17-(piridin-2-il) derivati estra-1,3,5(10)-triena, polazeći od estrona i njegovih C3 analoga. Za sva sintetisana jedinjenja ispitana su *in silico* ADMET svojstva koristeći online web alate. U cilju utvrđivanja proteina za koje će se sintetizovana jedinjenja potencijalno vezati izvršen je virtuelni skrining dobijenih jedinjenja. U okviru *in vitro* testova ispitan je relativni afinitet vezivanja za ligand-vezujuće domene estrogenih receptora α i β, kao i androgenih receptora.

Synthesis, biological investigation and *in silico* studies of 17α-(pyridin-2-yl)-estra-1,3,5(10)-triene derivatives

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Introduction of a heteroatom or a heterocycle into steroid compounds often results in alteration of their biological and/or pharmacological activities. Considering this, 17-(pyridin-2-yl) derivates of estra-1,3,5(10)-triene were synthesized, starting from estrone and its C3 analogs. For all synthesized compounds, *in silico* ADMET properties were calculated using online web tools. Furthermore, virtual screening was performed in order to predict potential protein targets for the newly synthesized compounds. Relative binding affinities to the ligand-binding domains of estrogen receptors α and β and androgen receptors were measured using *in vitro* assays.

Acknowledgements: The authors acknowledge the financial support of Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina [Project: New steroid derivatives - potential chemotherapeutics, No. 142-451-2667/2021].

OH-9

Proučavanje konformacije i kristalne strukture odabranih derivata cikloheksan-5-spirohidantoina

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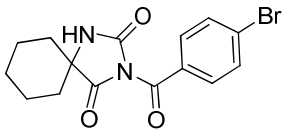
Derivat cikloheksan-5-spirohidantoina (Slika 1) je sintetisan, određena je njegova kristalna struktura i urađena kvantno-hemijska analiza. Kristalno pakovanje grade mreže supramolekulskih $R_6^4(32)$ prstenova postavljenih međusobno paralelno, pri čemu se formiraju linearni kanali. Određene su vrednosti energije intermolekulskih interakcija za različite dimerne motive dobijene iz kristalne strukture. Uzimajući u razmatranje prethodno strukturno okarakterisane srodne spirohidantoine [1], dobijena je serija jedinjenja koja je omogućila procenu uticaja supstituenata na njihovu molekulsku i kristalnu strukturu.



Slika 1. 3-(4-Brombenzoil)-1,3- diazaspiro[4.5]dekan-2,4-dion.
Figure 1. 3-(4-Bromobenzoyl)-1,3- diazaspiro[4.5]decane-2,4-dione.

Insights into conformational and cristal structure features of selected cyclohexane-5-spirohydantoin derivatives

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A spirohydantoin derivative (Figure 1) was synthesized and its crystal structure was determined by single crystal X-ray diffraction and analysed by DFT calculations. The crystal packing is made of supramolecular nets of $R_6^4(32)$ rings linked together to form stacks that enclose linear channels. The intermolecular interaction energies are quantified for various dimeric motifs. By including the previously reported structurally-related spirohydantoins [1], we created a set of compounds that enabled us to evaluate substituent effects on both molecular and crystal structures.

1. K. Gak Simić, I. Đorđević, A. Lazić, L. Radovanović, M. Petković-Benazzouz, J. Rogan, N. Trišović, G. Janjić, *CrystEngComm* **2021**, *23*, 2606.

OH-10

Sinteza, UV-Vis spektrofotometrijska titracija i teorijski proračuni 6-hidroksi-4-metl-3-(piridinijum-1-il)-2-piridona

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U ovom radu prikazana je sinteza i karakterizacija 6-hidroksi-4-metil-3-(piridinijum-1-il)-2-piridona. Sintetisano jedinjenje dobijeno je u obliku dipol-jona. Spektrofotometrijskom titracijom u rastvoru etanola ispitan je uticaj pH vrijednosti na strukturu jedinjenja. Kako bi se detaljno opisala struktura derivata 2-piridona, eksperimentalno dobijene vrijednosti dobijenih apsorpcionih maksimuma upoređeni su sa kvantno-hemijskim proračunima optimizovanih geometrija i teorijskih UV-Vis spektara pri različitim pH vrijednostima.

Synthesis, UV-Vis spectrophotometric titration and theoretical calculations of 6-hydroxy-4-methyl-3--(pyridinium-1-yl)-2-pyridone

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In this research, synthesis and characterization of 6-hydroxy-4-methyl-3-(pyridinium-1-yl)-2-piridone was shown. Synthesized compound was achieved in the zwitterionic form. UV-Vis spectrophotometric titration was performed in order to examine the influence of pH values on the structure of the compound. For the purpose of detail characterization of 2-pyridone derivative, experimentally obtained results were compared to quantum-chemical calculations of optimized geometries and theoretical UV-Vis spectra of solution for different pH values.

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OH-11

Sinteza, karakterizacija i antioksidativna aktivnost proizvoda aminolize Hančovih dihidropiridina

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Supstituisani estri 1,4-dihidropiridina (1,4-DHP) nastaju u reakciji etil-acetoacetata i odgovarajućih supstituisanih aldehida u prisustvu amonijaka. Nastali estri sa primarnim aminima formiraju amide. Serija amida nastalih od navednih jedinjenja je sintetisana sa namerom da se ispitaju njihove karakteristike i antioksidativna aktivnost. U ovde prikazanom istraživanju za aminolizu upotrebljen je 2-aminotiazol. Antioksidativna aktivnost je ispitivana DPPH (2,2-difenil-1-pikrilhidrazil-radikal) i ABTS (2,2'-azino-bis(3-etilbenzotiazolin-6-sulfonska kiselina)) metodama, a pored toga određene su tačke topljenje, snimljeni IR spektri i izvršena je elementalna analiza.

Synthesis, characterization and antioxidative activity of aminolysis products of Hantzsch dihydropyridines

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The substituted esters of 1,4-dihydropyirdines (1,4-DHP) are formed in the reaction of ethyl acetoacetate and corresponding substituted aldehydes in the presence of ammonia. Amides form from esters of substituted 1,4-DHP by aminolysis employing primary amines. A series of amides of the mentioned compounds was synthesized with the aim to analyze their chemical properties and antioxidative activity. The amine used in the present research was 2-aminothiazole. The antioxidative activity was determined by DPPH (2,2-diphenyl-1-picrylhydrazyl radical) and ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) methods; melting points and IR were measured and elemental analysis was performed.

OH-12

Hemijski raznoliki, visoko nezasićeni estri i laktoni iz biljne vrste *Bupleurum veronense* Turra (Apiaceae)

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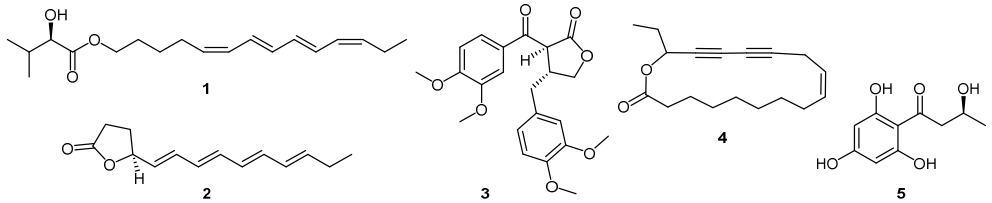
Hromatografsko razdvajanje etarskog ekstrakta biljne vrste *Bupleurum veronense* Turra (Apiaceae) rezultovalo je izolovanjem 5 novih prirodnih proizvoda (Slika 1): estar tetradeka-5,7,9,11-tetraen-1-ola (**1**), tetranezasićeni γ-tetradekalakton (**2**), dibenzilbutirolaktonski lignan (**3**), 17-očlanog makrolida (**4**) sa konjugovanim diinskim sistemom i acilfloroglucinolski derivat (**5**). Jedinjenja su u potpunosti spektralno okarakterisana (NMR, IR, UV, MS), određena je optička rotacija, a apsolutna konfiguracija jedinjenja **1**, **2** i **5** određena je na osnovu hemijskih korelacija i NMR analize Mošerovih estara. Jedinjenje **4** verovatno predstavlja nedostajući biosintetski intermedijer koji povezuje krepeninsku kiselinu i derivate falkarinola.



*Slika 1. Strukture izolovanih jedinjenja **1-5**.*

Chemically diverse, highly unsaturated esters and lactones from *Bupleurum veronense* Turra (Apiaceae)

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Chromatographical separations of diethyl-ether extracts of *Bupleurum veronense* Turra (Apiaceae) yielded 5 new natural products (Figure 1): an ester of tetradeca-5,7,9,11-tetraen-1-ol (**1**), a tetraunsaturated γ-tetradecalactone (**2**), a diphenylbutyrolactone lignan (**3**), a 17-membered macrolide (**4**) possessing a conjugated diyne-system, and an acylphloroglucinol derivative (**5**). All compounds were fully characterized by NMR, IR, UV, MS, and optical rotation, whereas the absolute configurations of **1**, **2**, and **5** were determined via chemical correlations and NMR analysis of Mosher's esters. Compound **4** might represent a missing link in the biosynthetic pathway from crepenynic acid to falcarinol derivatives.

OH-13

Antimikrobna aktivnost novih mešovitih azina kumarina i heteroaril-aldehida

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Azinska funkcionalna grupa ulazi u sastav mnogih jedinjenja koja ispoljavaju širok spektar farmakoloških aktivnosti. Kao deo naših istraživanja biološki aktivnih jedinjenja, dizajnirali smo, sintetisali i spektralno okarakterisali seriju mešovitih azina sa kumarinskim i još jednim heterocikličnim jezgrom. Antimikrobna aktivnost sintetisanih derivata ispitana je metodom mikrodilucije prema pet sojeva mikroorganizama i to prema Gram-pozitivnim bakterijama (*Staphylococcus aureus* i *Bacillus cereus*), Gram-negativnim bakterijama (*Escherichia coli* i *Salmonella enteritidis*) i jednom soju kvasca (*Candida albicans*). Ispitivana jedinjenja pokazala su veću inhibitornu aktivnost prema Gram-negativnim bakterijama, sa najvećom osetljivošću *E. coli* prema derivatima sa pirolskim fragmentom. Sojevi *B. cereus* i *C. albicans* pokazali su najveću rezistenciju prema testiranim jedinjenjima.

Antimicrobial activity of new mixed azines of coumarins and heteroaryl aldehydes

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The azine functional group is a part of numerous compounds exhibiting a range of pharmacological activities. As part of our continuous search for new pharmacologically active compounds, we designed, synthesized, and spectrally characterized a series of mixed azines containing coumarin and another heterocyclic moiety. Antimicrobial activity of the synthesized compounds was evaluated by a microdilution assay against five different microorganisms, namely Gram-positive bacteria (*Staphylococcus aureus* and *Bacillus cereus*), Gram-negative bacteria (*Escherichia coli* and *Salmonella enteritidis*), and one yeast (*Candida albicans*). It was found that the tested compounds showed higher inhibitory activity against Gram-negative bacteria, with the greatest sensitivity of *E. coli* to the derivatives with a pyrrole fragment. *B. cereus* and *C. albicans* were the most resistant strains to the tested compounds.

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OH-14

Triterpeni biljne vrste *Euphorbia palustris*

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Biljne vrste roda *Euphorbia* imaju važno mesto u tradicionalnoj medicini zahvaljujući sekundarnim metabolitima koje proizvode. Najznačajniji metaboliti pripadaju klasama diterpena i triterpena. Istraživanja su pokazala da ova jedinjenja imaju antitumorska, antivirusna, antibakterijska, antiinflamatorna i druga svojstva. Cilj ovog istraživanja bio je ispitivanje triterpenskog sastava biljne vrste *Euphorbia palustris*. Primenom hromatografskih tehnika iz biljnog materijala izolovana su četiri triterpenska derivata i to:(+)-tirukalol (1), lanosterol (2), 27-nor-3β-hidroksicikloart-23-en-25-on (3) i (+)-obtusifoliol (4). U nastavku istraživanja biće ispitane njihove biološke aktivnosti.

Triterpene composition of the plant species *Euphorbia palustris*

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Plant species of the genus *Euphorbia* have an important place in the traditional medicine due to the secondary metabolites which they produce. The most important metabolites come from the classes of diterpenes and triterpenes. The studies have shown that these compounds can have antitumour, antiviral, antibacterial, anti-inflammatory and other properties. The aim of the research was to investigatethe triterpene composition of *Euphorbia palustris*. Using chromatographic techniques, four triterpene derivatives were isolated from the plant material, as follows: (+)-tirucallol (1), lanosterol (2), 27-nor-3β-hydroxycycloart-23-en-25-one (3) and (+)-obtusifoliol (4). In the continuation of the research, their biological activities will be examined.

Acknowledgment. This work was financially supported by the Serbian Academy of Sciences and Arts (Strategic Project MilkIng, No. 01-2022), and by Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract Nos: 451-03-68/2022-14/200168 and 451-03-68/2022-14/200026).

OH-15

HPLC profil metanolnog ekstrakta biljne mešavine korišćene na Balkanu za eliminisanje kamena u bubregu*

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Po prvi put je određen HPLC profil metanolnog ekstrakta biljne mešavine sastavljene od bobica *Juniperus oxycedrus* L. (JO), zrna *Avena sativa* L. (AS) i potkore *Betula pendula* Roth. (BP) koja se koristi na Balkanskom poluostrvu za uklanjanje kamena u bubregu. Hemijski sastav metanolnih ekstrakata pojedinačnih komponenata biljne mešavine određen je takođe HPLC-UV analizom. Konstituenti zastupljeni preko 1000 μg po gramu suvog metanolnog ekstrakta biljne mešavine su: galna kiselina, protokatehinska kiselina i amentoflavon. Najzastupljenije komponente metanolnog ekstrakta uzorka JO su protokatehinska kiselina, amentoflavon i kupresoflavon dok su kemferol-3-*O*-glukozid i galna kiselina najzastupljeniji u uzorku AS. Siringiska kiselina, praćena derivatima katehina i epikatehina su identifikovani u uzorku BP.

HPLC profile of methanol extracts of the herbal mixture used in Balkan penisula to eliminate the kidney stones*

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This is a first report of HPLC profile of methanol extract of herbal mixture made of *Juniperus oxycedrus* L. berries (JO), *Avena sativa* L. grains (AS) and inner bark of *Betula pendula* Roth. (BP) used in Balkan peninsula to eliminate the kidney stones. Also, composition of methanol extracts of individual mixture components was determined. Constituents represented by over 1000 μg per g of herbal mixture dry methanol extract were: gallic acid, protocatechuic acid and amentoflavone. Protocatechuic acid, amentoflavone and cupressoflavone were the most abundant components of JO sample while kaempferol-3-*O*-glycoside and gallic acid were the main compounds of AS sample. Syringic acid accompanied with catechin and epicatechin derivatives were identified in BP sample.

Acknowledgment: This research was supported by the Ministry of Education, Science and Technological Development of Serbia (Project No. 451-03-9/2022-4-200124).

*The results presented here are the part of the submitted manuscript (NPX-22-0001).

Tekstilno inženjerstvo

Textile Engineering

TI-1

Antimikrobna aktivnost viskozne tkanine modifikovane hitozanom i nanočesticama Ag

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Potrebe za medicinskim tekstilom koji poseduje antimikrobna svojstva kontinualno rastu. U poslednje vreme se čine napori da se sinteza nanočestica Ag ostvari upotrebom zelenih redukcionih sredstava, a pre svega biljnih ekstrakta. U ovom radu su nanočestice Ag sintetisane na viskoznoj tkanini modifikovanoj biopolimerom hitozanom sa i bez prisustva umreživača 1,2,3,4-butantetrakarboksilne kiseline primenom ekstrakta kore nara kao redukcionog sredstva. Uprkos razlici u sadržaju i veličini nanočestica Ag, oba uzorka pokazuju odličnu antibakterijsku aktivnost prema bakterijama*S. aureus*i *E. coli*, a još bolju antifungalnu aktivnost prema kvascu *C. albicans*. Pri tome je citotoksičnost ovih uzoraka prema ćelijama keratinocita ljudske kože niska.

Antimicrobial activity of viscose rayon fabric modified with chitosan and Ag nanoparticles

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The needs for medical textiles with antimicrobial properties are continually growing. Recently many efforts have been made to synthesize Ag nanoparticles using green reducing agents, in particular plant extracts. In this study Ag nanoparticles were synthesized on viscose rayon fabric modified with biopolymer chitosan with or without crosslinker 1,2,3,4-tetrabutanecarboxylic acid by applying pomegranate peel extract as a reducing agent. Despite the difference in content andsize of Ag nanoparticles both samples showed excellent antibacterial activity against bacteria *S. aureus* and *E. coli* and even better against yeast *C. albicans*. The cytotoxicity of these samples onhuman keratinocyte cellswas low.

Acknowledgment: This study was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No.451-03-68/2022-14/200135 and 451-03-68/2022-14/200287).

TI-2

Aksijalna deformacija konoplja/filament hibridnih pređa

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Deformaciono ponašanje tekstilnog materijala tokom istezanja, savijanja, kompresije i smicanja uslovljava njegov taktilni komfor. Veća sposobnost istezanja materijala i relaksacije po prestanku dejstva opterećenja podrazumevaju bolji taktilni komfor. Sposobnost aksijalne deformacije i relaksacije pređe predstavlja najvažniji faktor deformacionog ponašanja tkanine ili pletenine prilikom istezanja. Tekstilni materijali od konoplje se odlikuju dobrim termofiziološkim svojstvima, ali imaju određena ograničenja u pogledu taktilnog komfora usled smanjene istegljivosti vlakana. U okviru ovog istraživanja ponuđeno je rešenje problema formiranjem kompleksnih hibridnih pređa metodom končanja jednožične konopljine pređe sa glatkim viskoznim ili teksturiranim poliamidnim filamentom. Pređe su podvrgnute istezanju do kidanja, i istezanju i relaksaciji pri 25% i 50% od prekidnog opterećenja. Na osnovu utvrđenih komponenata aksijalne deformacije (elastična, viskoelastična i plastična), kao i udela relativnih komponenata deformacije u ukupnoj deformaciji pređe, može se zaključiti da predloženo rešenje predstavlja efikasno sredstvo za unapređenje deformacionih svojstava pređa na bazi konoplje.

Axial deformation of hemp/filament hybrid yarns

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The deformation behavior of textile material during stretching, bending, compression and shearing is responsible for tactile comfort. The tensile behavior of textile fabric is highly correlated with its comfort in such a way that higher extensibility and tensile recovery of the fabric signify better tactile comfort. Among the factors influencing the tensile behavior of textile material, the extensibility and relaxation ability of the constituent yarn are the most important. Hemp textile fabrics are physiological-friendly textiles, but they have some limitations in terms of tactile comfort due to the limited extensibility of hemp fibers. In this study, the limitation of hemp was overcome by developing complex hemp-based yarns containing stretchable filament as a component. The folding technique was used to combine the single hemp yarn with viscose filament or polyamide textured filament. The hemp/filament yarns were subjected to axial stress and relaxation under various test conditions (breaking load, 25% and 50% of the breaking strength). Determined deformation components at extension (elastic, viscoelastic and plastic), as well as the share of the relative deformation components in the total elongation, indicated the proposed solution as an effective means for improving the deformation properties of hemp based yarns.

Teorijska hemija

Theoretical Chemistry

TH-1

Magnetno indukovane gustine struja u singuletnim i tripletnim disk-klasterima bora

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Struktura klasteri bora čija geometrija podseća na disk duže vreme fasciniraju i privlače pažnju hemičara. Raspodela molekulskih orbitala u ovim sistemima se može opisati jednostavnim modelom „čestice u prstenu“. Po ovom modelu molekulske orbitale se javljaju u degenerisanim parovima, sa izuzetkom za m = 0 (bez angularne čvorne površine). Magnetno indukovane gustine struje su pokazale da disk-klasteri bora sa konfiguracijom zatvorene ljuske u svom osnovnom singuletnom stanju pokazuju aromatični karakter. Nađeno je da disk klasteri bora koji su aromatični u singuletnom stanju zadržavaju aromatični karakter i u tripletnom stanju, kada im se oduzmu ili dodaju dva elektrona. Aromatičnost disk klastera bora u njihovim singletnim i tripletnim stanjima, sa izuzetkom tripletnog $^3B_{19}^-$, može se uspešno predvideti pomoću Hückelovog i Bairdovog pravila.

Magnetically induced current densities in singlet and triplet disk-like boron clusters

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The disk-like boron clusters are among the most alluring boron cluster forms. Molecular orbital distribution in these clusters can be rationalized by means of the simple particle-on-a-disk model. In this model, the molecular orbitals come by pairs except for m = 0 (no angular nodes). The calculated magnetically induced current densities revealed that the disk-like boron clusters in their singlet ground state with closed-shell configuration are aromatic. It was found that the disk-like boron clusters that are aromatic in their ground states remain aromatic in their lowest-lying triplet states when the number of valence electrons is increased or reduced by two electrons. In addition, if the lowest-lying triplet state in disk-like boron clusters is aromatic, this triplet state is the ground state for these species. Aromaticity of the studied disk-like boron clusters in their lowest-lying singlet and triplet state, with the exception of triplet $^3B_{19}^-$ can be predicted based on Hückel and Baird's rules.

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TH-2

Procena efikasnosti *push-pull* elektronskih sistema sa barbiturnom kiselinom

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Derivati barbiturne kiseline imaju široku primenu u dizajnu organskih nelinearnih optičkih (NLO) materijala, organskih svetlećih dioda (OLED), solarnih ćelija sa fotoosetljivim pigmentom (DSSC), kolorimetrijskih pH senzora i jonskih detektora. *Push-pull* karakter *para*-supstituisanih derivata 5-benzilidenbarbiturne kiseline ispitivan je na osnovu razlike vrednosti hemijskih pomeranja u ^{13}C NMR spektrima, Mayer-ovom analizom prirode hemijske veze, "*hole-electron*" analizom procesa pobuđivanja elektrona i izračunavanjem CT indeksa. Rezultati pokazuju da u kompleksu sa jakim elektron-donorskim grupama, barbiturna kiselina ima ulogu elektron-akceptora, dok kuplovana sa jakim elektron-akceptorima barbiturna kiselina ima ulogu slabog donora elektrona u *push-pull* elektronskim sistemima.

Assessing the efficiency of *push-pull* electronic systems with barbituric acid

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Barbituric acid derivatives have a broad range of applications in the design of organic nonlinear optic (NLO) materials, organic light-emitting diodes (OLEDs), dye-sensitized solar cells (DSSCs), colorimetric pH sensors, and ion detection. ^{13}C NMR chemical shift differences, Mayer π bond order analysis, "*hole-electron"* analysis, and calculations of CT indices for investigation of the efficiency *push-pull* character of *para*-substituted 5-benzylidenebarbituric acid derivatives were used. The results indicate that in the complex with strong electron-donor groups, barbituric acid can act as the electron-acceptor, while when coupled with a strong electron-acceptor in *push-pull* electronic system, barbituric acid can act as the weak electron-donor.

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ТН-3

Нитро-ацетилацетонато комплекси као нова класа високоенергетских материјала: синтеза, карактеризација и квантнохемијска проучавања

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Хелатна координациона једињења представљају нову класу високоенергетских материјала са унапређеним перформансама и стабилношћу. У овом раду користили смо квантнохемијске прорачуне да предвидимо детонационе карактеристике одабраних нитро-ацетилацетонатних комплекса прелазних метала. Мапе електростатичког потенцијала и енергије дисоцијације C-NO_2 веза су израчунате за ове комплексе и анализиране. Одабрани нитро-ацетилацетонато комплекси су синтетисани и окарактерисани помоћу УВ/ВИС спектроскопије. Резултати тестова у отвореном пламену су показали да нитро-ацетилацетонато комплекси горе приликом паљења и да ови молекули могу да се употребе као нова група високоенергетских материјала.

Nitro-acetylacetonato complexes as a new class of highly energetic materials: synthesis, characterization and quantum chemical studies

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Chelate coordination compounds represent a new class of promising highly energetic materials with improved performance and stability. In this work, we used quantum chemical calculations to predict detonation characteristics of selected nitro-acetylacetonato complexes of transition metals. Electrostatic potential maps and bond dissociation energies of C-NO_2 bonds were calculated for these complexes and analyzed. Selected nitro-acetylacetonato complexes were prepared and characterized by UV/VIS spectroscopy. The results of the open-flame tests showed that nitro-acetylacetonato complexes burn upon ignition and that these molecules could be used as a new class of highly energetic materials.

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TH-4

Teorijsko proučavanje uticaja veličine aromatičnog sistema na osetljivost nitroaromatičnih eksploziva

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Jedna od ključnih osobina eksploziva koja utiče na njihovu osetljivost ka detonaciji jeste postojanje pozitivnog naelektrisanja u centralnom regionu molekula. Mape elektrostatičkih potencijala tetranitro derivata benzena, naftalena, antracena, tetracena i pentacena izračunate na PBE/6-311G** nivou teorije ukazuju da produženje aromatičnog niza dovodi do smanjenja pozitivnih vrednosti naelektrisanja u centralnim delovima ispitivanih molekula.[1] Rezultati dobijeni analizom energija disocijacije hemijske veze su u skladu sa izračunatim mapama elektrostatičkog potencijala i ukazuju da se veličina aromaticnog sistema može upotrebiti za modifikaciju osetljivosti nitroaromatičnih eksploziva ka detonaciji.

Theoretical study of the influence of aromatic system size on the sensitivity of nitroaromatic explosives

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One of the key properties of explosives that makes them prone to detonation is a positive charge above the central regions of the molecular surface. Electrostatic potential maps were calculated for tetranitro-derivatives of benzene, naphthalene, anthracene, tetracene, and pentacene. Results of calculations performed at PBE/6-311G** level show that with the increase in the number of condensed aromatic rings positive values of electrostatic potentials in the central regions of studied nitroaromatic molecules decreases.[1] Results obtained by bond dissociation energy analysis are consistent with the calculated electrostatic potential maps indicating that aromatic system size could be used as a tool to modify the sensitivity toward detonation of nitroaromatic explosives.

1. I. Veljković, J. Radovanović, D. Veljković, *RSC Adv*. **2021**, *11*, 31933.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, PROMIS, #6066886, CD-HEM

TH-5

Magnetna anizotropija u pentagonalno bipiramidalnim kompleksima prve serije prelaznih metala

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U ovom radu prikazana je validaciona studija u cilju preciznog izračunavanja magnetne anizotropije primenom teorije funkcionala gustine (DFT). Analizirana su 26 sedmo-koordinovana visoko-spinska kompleksa prve serije prelaznih metala, upotrebom dve DFT metode (CP-DFT i LF-DFT), a dobijeni rezultati upoređeni sa eksperimentalnim. U potrazi za najtačnijim teorijskim opisom magnetne anizotropije, testirali smo različite tipove aproksimacija funkcionala gustine kako za izračunavanje precizne geometrije, tako i za tačan opis magnetne anizotropije.

Slika 1. Geometrija prve koordinacione sfere ispitivanih kompleksa

Magnetic anisotropy in pentagonal bipyramidal complexes of first-row transition metal ions

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We present a validation study that aims to accurately describe magnetic anisotropy using the density functional theory (DFT) approach. We have examined 26 seven-coordinate high-spin first-row transition metal complexes with two DFT methods (CP-DFT and LF-DFT) and compared the result with available experimental data. We have tested various DFT flavors in search of the best geometrical optimization conditions and the most accurate theoretical description of magnetic anisotropy.

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TH-6

Uticaj koordinacije na jačinu NH···O interakcije

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Uticaj koordinacije aminskih liganada na jačinu NH/O interakcije upoređivan je za etilendiamin (*en*) i četiri aminokiseline (Gly, Cis, Phe, Ser). Prethodni rezultati pretrage banke kristalografskih podataka (CSD) su pokazala da se koordinovanjem *en* dužina d_{NO} smanjuje, a α uglovi postaju linearniji. Ovaj trend je takođe opažen u proračunima, jer koordinovani *en* ima višestruko jaču energiju interakcije (-28,0 kcal/mol) od nekoordinovanog *en* (-2,3 kcal/mol). Uzimajući u obzir da slobodne aminokiseline u kristalnim strukturama imaju pozitivno naelektrisanu NH_3 grupu, u ovom slučaju, koordinacijom se ne menja značajno jačina interakcije. Pretraga banke podataka je pokazala da nekoordinovane naelektrisane aminokiseline imaju kraća d_{NO} rastojanja od koordinovanih aminokiselina. Energija interakcije za nekoordinovane aminokiseline (Gly^{1+}; -17,4 kcal/mol) je slična sa energijom za koordinovane aminokiseline ($[Co(H_2O)_4Gly]^{2+}$; -16,9 kcal/mol).

The influence of coordination on NH···O bond strength

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The influence of coordination of ammino ligands on NH/O bond strength has been studied for ethylenediamine (*en*) and four amino acids (Gly, Cis, Phe, Ser). The previous results from the Cambridge Crystallographic Database (CSD) search have shown that with coordination of *en*, the d_{NO} distance becomes shorter while α angles become more linear. This trend is also observed in calculations, where coordinated *en* has stronger interaction energies (-28.0 kcal/mol) than noncoordinated *en* (-2.3 kcal/mol). Considering that free amino acids have a positively charged NH_3 group, in this case, coordination does not influence hydrogen bond strength significantly. The results of CSD search have shown that noncoordinated amino acids have shorter d_{NO} distances than coordinated amino acids. The interaction energy for noncoordinated amino acids (Gly^{1+}; -17.4 kcal/mol) is similar to the interaction energy for coordinated amino acids ($[Co(H_2O)_4Gly]^{2+}$; -16.9 kcal/mol).

Fizička hemija

Physical Chemistry

FH-1

Dobijanje i karakterizacija fosfatvolframove bronze dopirane gvožđem iz heteropolisoli kao prekursora

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Хетерополи киселине и соли хетерополи киселина се могу користити као полазни материјали за добијање волфрамових бронзи. Због своје јонске и електронске проводљивости и других корисних својстава хетерополи једињења имају широку примену: као нови материјали, суперјонски проводници, у биологији, фармацији и медицини. Ове бронзе имају специфичну структуру која настаје рушењем Кегиновог анјона на температури од 602 ^{0}C. Та структура је слојевита и састоји се од међусобно повезаних PO_4 тетраедара и WO_6 октаедара, са пентагоналним и хексагоналним отворима (шупљине, канали) у којима долази до измене у потпуности или делимично H јона у WPA. У овом раду је синтетисана 12-волфрамфосфорна киселина, из које је јонском изменом добијена со прелазног метала ($FePW_{12}O_{40} \cdot nH_2O$). Термијском анализом одређена је температура фазног прелаза (температура на којој долази до нарушавања структуре Кегиновог анјона) (око 600^{0}C) и прелаза у фосфатволфрамове бронзе допиране гвожђем. За карактеризацију материјала коришћене су физичко-хемијске методе IR, XRPD и SEM.

Preparation and characterization of phosphatetungsten bronze doped with iron from heteropoly salts as precursors

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Heteropoly acids and salts can also be used as starting materials for the production of tungsten bronzes. Due to their ionic and electronic conductivity and other useful properties, heteropoly compounds are widely used: as new materials, superionic conductors, in biology, pharmacy and medicine. These bronzes have a specific structure that results from the collapse of the Kegin anion at a temperature of 602 ^{o}C. This structure is layered and consists of interconnected PO_4 tetrahedra and WO6 octahedra. In such a structure, pentagonal and hexagonal openings (cavities, channels) are formed, exchanging completely or partially H ions in WPA. In this work, 12-tungsten phosphoric acid were synthesized, ion exchange gave 12-tungsten phosphoric acid of the transition metal ($FePW_{12}O_{40} \cdot nH_2O$). Thermal analysis determined the temperature of the phase transition (the temperature at which the structure of the Kegin anion is collapsed) to the temperature (around 600^{o}C), which yields phosphate tungsten bronzes doped with iron. Physico-chemical methods IR, XRPD and SEM were used to characterize the material.

FH-2

Fotokatalitička primena laserski sintetisanih nanočestica

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U ovom radu ispitivana je mogućnost primene nanočestica ZnO za fotokatalitičku degradaciju boje bromkrezol zeleno i komercijalno dostupne boje za bojenje tekstila. Vodena suspenzija nanočestica ZnO dobijena je laserskom ablacijom [1]. Koncentracija nanočestica određena je metodom ISP-OES. Rastvori boje sa različitim količinama nanočestica izlagani su dejstvu UVC zračenja i to u intervalima od 5 minuta u ukupnom trajanju od sat vremena. Degradacija boja u toku ozračivanja utvrđena je merenjem apsorbancije UV-VIS spektrometrijom pre, tokom i nakon ozračivanja. Preliminarni rezultati potvrdili su početnu pretpostavku da se nanočestice dobijene laserskom sintezom mogu koristiti za degradaciju boja.

Photocatalytic application of laser synthesized nanoparticles

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In this paper, the possible use of ZnO nanoparticles for photocatalytic degradation of dyes, in particular bromocresol green and commercial textile dyes, was examined. A water suspension of ZnO nanoparticles was prepared by laser ablation. Concentration of nanoparticles was measured by ICP-OES technique. Dyes solutions with different amounts of nanoparticles were exposed to UVC irradiation at 5 minute intervals for a total period of 1 hour. Degradation of dyes during irradiation was determined by UV-VIS spectroscopy by measuring solution absorbance before, during, and after exposition. Preliminary results confirmed the initial assumption that laser synthesized nanoparticles could be used for dye degradation.

[1] D. Blažeka, J. Car, N. Klobučar, A. Jurov, J. Zavašnik, A. Jagodar, E. Kovačević, N. Krstulović, *Materials (Basel).,* (2020), *13*, 1–15.

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FH-3

Uticaj vode na metalo-organske umrežene strukture na bazi cirkonijuma postmodifikovane Šifovim bazama

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Metalo-organske umrežene strukture (MOF) su zbog svoje poroznosti u kristalnoj strukturi pokazale veliku adsorpcionu moć, ali njihova najveća slabost je mala otpornost na vodu koja urušava njihovu strukturu. Kako bi se utvrdio uticaj vode, ispitana je hidroliza odabranog postmodifikovanih MOF-ova u vodi. UV-VIS spektrofotometar je korišćen da bi se pratila promena koncentracije aldehida koji je korišćen za postmodifikaciju u zavisnosti od vremena. Razlike u strukturi pre i posle izlaganja vodi potvrđene su i korišćenjem FT-IR spektroskopije i difrakcije rendgenskih zraka na prahu.

Influence of water on Schiff base postmodified zirconium-based metal-organic frameworks

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Metal-organic frameworks (MOF) have shown great adsorption power due to their porosity in the crystal structure, one of their weaknesses is the lack of resistance to water that results the collapse in their structure. To determine the effect of water, the hydrolysis of selected postmodified MOFs in water was investigated. UV-VIS spectrophotometer was used to monitor the change in concentration of the aldehyde used for postmodification over time. Differences in structures before and after exposure to water were also confirmed using FT-IR spectroscopy and X-ray powder diffraction.

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Hemija životne sredine

Environmental Chemistry

HŽS-1

Razvoj sopstvene radne procedure za analizu odabranih lekova u vodi

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Prikazana je interna validacija GC/MS metode za određivanje ibuprofena (IB), kofeina (CF) i diklofenaka (DCF) u vodi, a nakon čvrsto-tečne ekstrakcije (SPE Oasis® HLB, 60 mg) i trimetilsililovanja. Iako su dobijene zadovoljavajuće performanse, metilen-hlorid (DCM) je pokazao nisku efikasnost ekstrakcije za DCF (19%), dok je za IB i CF ona bila 101% i 94%, redom. Nakon 3 meseca ponovljen je eksperiment i rezultati za efikasnost ekstrakcije su bili 15%, 79% i 92% za DCF, IB i CF, redom. Produženje vremena kontakta DCM i čvrste faze za 20 min nije poboljšalo rezultate. Međutim, etil-acetat se pokazao efikasnijim za DCF (101%), te će ova modifikacija metode biti validovana u budućem radu, uz čestu verifikaciju ne samo kalibracije, nego i efikasnosti ekstrakcije.

Operational procedure development for analysis of selected pharmaceuticals in water

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Internal GC/MS method validation is presented for analysis of ibuprofen (IB), caffeine (CF) and diclofenac (DCF) in water after solid-phase extraction (SPE, Oasis® HLB, 60 mg) and trimethylsilylation. The method performance was satisfactory even though methylene chloride (DCM) achieved low extraction efficiency for DCF (19%) in comparison to IB (101%) and CF (94%). Repetition, after three months showed extraction efficiency of 15%, 79% and 92% for DCF, IB and CF, respectively. Prolongation of DCM and solid phase contact time for 20 minutes did not improve extraction. However, ethyl acetate improved result for DCF (101%). This method modification will be further validated with frequent not only calibration, but also extraction efficiency verification.

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HŽS-2

Nanočestice magnetita prevučene poli(etilen glikolom) kao nosač za imobilizaciju peroksidaze

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Cilj ovog rada bio je ispitivanje mogućnosti primene modifikovanih nanočestica magnetita (Fe_3O_4) kao nosača za imobilizaciju peroksidaze iz rena. Određivani su optimalni uslovi aktivnosti imobilisanog enzima na različitim temperaturama (10-80°C) i pH (4-10) vrednostima, mogućnost njegove ponovne primene i stabilnost skladištenja (4 i 25°C) u periodu od mesec dana. Nanočestice magnetita su sintetisane iz Fe(II) i Fe(III) sulfatnih soli metodom koprecipitacije u prisustvu 5% poli(etilen glikola). Enzim je kovalentno vezan za modifikovane Fe_3O_4 nanočestice preko glutaraldehida kao vezujućeg agensa. Nakon imobilizacije, peroksidaza je pokazala visoku aktivnost (29,1 U/g). Enzim je pokazao najveću aktivnost na 40°C pri pH 7,0. Posle mesec dana čuvanja imobilizovanog enzima (4°C i 25°C) njegova aktivnost je bila 58% i 3%, redom, u poređenju sa početnom vrednošću. Enzim zadržava oko 50% svoje aktivnosti nakon četiri uzastopna ciklusa ispiranja, što ukazuje na mogućnost njegove ponovne upotrebe.

Poly(ethylene glycol) -coated magnetite nanoparticles as support for peroxidase immobilization

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The aim of this work was to determine eligibility of modified magnetite nanoparticles (MNPs) as a support for immobilization of horseradish peroxidase. The optimum conditions for immobilized enzyme activity at different temperatures (10-80°C) and pH (4-10) values, reusability and storage stability (4 and 25°C) over a period of one month were investigated. MNPs were synthesized from Fe(II) and Fe(III) sulphate salts by co-precipitation method in the presence of 5% poly(ethylene glycol). The enzyme was covalently bound onto modified MNPs via glutaraldehyde as a cross-linker. After immobilization, peroxidase showed high activity (29.1 U/g). The enzyme showed the highest activity at 40°C and pH 7.0. After one month of storage of the immobilized enzyme (4°C and 25°C) its activity was 58% and 3%, respectively, compared to the initial value. The enzyme retains about 50% of its activity after four consecutive washing cycles, which indicates the possibility of its reuse.

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HŽS-3

Procena efikasnosti uklanjanja teških metala iz vodenih rastvora i industrijske otpadne vode korišćenjem suncokretove ljuske kao biosorbenta

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U ovom radu korišćena je ljuska suncokreta za procenu efikasnosti uklanjanja teških metala iz vodenih rastvora. Na samom početku optimizovani su uslovi maksimalne adsorpcije teških metala u funkciji pH rastvora i vremena kontakta. Nakon toga, određena je efikasnost uklanjanja Ni iz uzorka otpadne vode korišćenjem suncokretove ljuske kao biosorbenta spektroskopijom laserski indukovane plazme (LIBS) i standardnom spektrohemijskom ICP-OES metodom. Rezultati su upoređeni, a dobijene vrednosti su u opsegu granica nesigurnosti LIBS metode.

Evaluation of heavy metal removal efficiency from aqueous solutions and industrial wastewater using sunflower seed husk as a biosorbent

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In this work, the sunflower husk was used to evaluate the removal efficiency of heavy metals from an aqueous solution. Firstly, the condition for maximum adsorption of heavy metals is optimized as a function of pH and contact time. Thereafter, the removal efficiency of Ni from the industrial wastewater by the usage of the sunflower husk as a biosorbent was evaluated by laser-induced breakdown spectroscopy (LIBS), and by the standard spectrochemical ICP-OES method. The values obtained by these two methods were compared and the results are within the uncertainty of the LIBS method.

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HŽS-4

Elektrohemijska degradacija *Reactive Black 5* pomoću čeličnih elektroda modifikovanih PbO_2 i grafitnim ugljen-nitridom

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Elektrode modifikovane kompozitom PbO_2 sa grafitnim ugljen-nitridom (GCN) upotrebljene su za elekrohemijsku degradaciju tekstilne boje *Reactive Black 5*. Modifikovana čelična elektroda je korišćena kao anoda, a kao katoda čista čelična elektroda. Ispitan je uticaj strukture PbO_2 na elektrokatalitičke karakteristike elektroda. Morfologija materijala je ispitana SEM-om, TEM-om i XRD-om, dok su elektrohemijske osobine ispitane uz pomoć CV i EIS merenja. Efikasnost degradacije je praćena UV-Vis spektrofotometrijom i tečnom hromatografijom. Pri optimalnim parametrima pH, koncentracije pomoćnog elektrolita, jačine struje i koncentracije ispitivane boje, najbolji rezultati su dobijeni sa elektrodom gde je cetiltrimetilamonijum-bromid (CTAB) korišćen kao templat za sintezu PbO_2. Pod ovim uslovima je postignuta potpuna degradacija nakon 60 min tretmana, a proizvodi degradacije su određeni korišćenjem HPLC-MS/MS metode.

Electrochemical degradation of *Reactive Black 5* using $PbO_2$and graphite carbon nitride modified steel electrodes

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Electrodes modified by PbO_2 and graphite carbon nitride (GCN) composite were used for electrochemical degradation of *Reactive Black 5* textile dye. A modified steel electrode was used as the anode, while a pure steel electrode was used as the cathode. The influence of PbO_2 structre on electrocatalytic characteristics of electrodes was investigated. The morphology of the material was examined by SEM, TEM and XRD, while the electrochemical properties were analyzed using means of CV and EIS measurements. The degradation efficiency was monitored by UV-Vis spectrophotometry and liquid chromatography. At optimal pH parameters, supporting electrolyte concentration, current strength and test dye concentration, the best results were obtained with an electrode where cetyl trimethyl ammonium bromide (CTAB) was used as a template for PbO_2 synthesis. Under these conditions, complete degradation was achieved after 60 min of treatment, and degradation products were determined using the HPLC-MS/MS method.

HŽS-5

Monitoring polihlorovanih bifenila u uzorcima zemljišta u Crnoj Gori

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U radu je prikazan monitoring zemljišta na 40 selektovanih kritičnih lokacija u Crnoj Gori, gde su detektovane koncentracije 7 EPA kongenera polihlorovanih bifenila (PCB). Nakon mlevenja zemljišta, PCB su ekstrahovani pomoću heksana i dihlormetana (1:1). Ekstrakti su prečišćavani natrijum sulfatom, nakon uparavanja u struji azota eluirani heksanom (2mL) i analizirani na gasnom hromatografu sa masenim spektrometrom u Centru za ekotoksikološka ispitivanja u Podgorici. Zemljište je bilo ugroženo PCB kongenerima u opštinama Nikšić, Tivat, Podgorica i Berane, dok u ostalim gradovima rezultati analize PCB-a nisu prelazili maksimalno dozvoljene koncentracije od 0,004 mg/kg zemljišta. Rezultati su pokazali da uzorci zemljišta imaju najviše koncentracije PCB kongenera u blizini deponije Željezara Nikšić (0,253 mg/kg), kao i na nekoliko lokacija blizu trafostanica i u blizini aerodroma Tivat i Podgorica.

Monitoring of polychlorinated biphenyls in the soil samples in Montenegro

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The paper presents monitoring of soil samples at 40 selected critical locations in Montenegro, where the concentrations of 7 EPA congeners of polychlorinated biphenyls (PCBs) were detected. PCBs were extracted with hexane and dichloromethane (1:1). The extracts were purified by sodium sulfate, eluted with hexane (2mL) after evaporation under a stream of nitrogen and analyzed using gas chromatograph with a mass spectrometer at the Center for Ecotoxicological Research in Podgorica. Soil was endangered by PCB congeners in the municipalities of Nikšić, Tivat, Podgorica and Berane, while in other cities the results of PCB concentrations didn't exceed the maximum allowable concentration of 0.004 mg/kg. The results showed that soil samples have the highest concentrations of PCB congeners near the Niksić landfill (0.253 mg/kg), as well as within several locations near transformer stations and near Tivat and Podgorica airports.

HŽS-6

Fotokatalitička efikasnost novosintetisanih nanoprahova na bazi ZnO u prisustvu simuliranog sunčevog zračenja

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Cilj ovoga rada je bio ispitivanje fotokatalitičke aktivnosti novosintetisanih nanoprahova na bazi ZnO za uklanjanje herbicida klomazona iz vodene sredine primenom simuliranog sunčevog zračenja. Isto tako, ispitan je uticaj količine katalizatora, kao i uticaj pH-vrednosti suspenzije na efikasnost fotorazgradnje supstrata. Fotokatalizatori: ZnO/ZrO_2, ZnO/CeO_2 i ZnO/MgO su pripremljeni mehanohemijskom metodom u molskom odnosu 2:1. Rezultati su pokazali da se bolja efikasnost uklanjanja klomazona postiže primenom ZnO/ZrO_2 kao fotokatalizatora u poređenju sa ZnO/CeO_2 i ZnO/MgO.

Photocatalytic efficiency of newly synthesized ZnO based nanopowders in the presence of simulated solar irradiation

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The aim of this study was to investigate the photocatalytic activity of newly synthesized ZnO based nanopowders for the removal of herbicide clomazone from aqueous media using simulated solar irradiation. Also, the influence of the catalyst loading, as well as the effect of the pH value of the suspension on the efficiency of clomazone photodegradation was investigated. Photocatalysts: ZnO/ZrO_2, ZnO/CeO_2 and ZnO/MgO were prepared by mechanochemical method in a molar ratio of 2:1. The results showed that better efficiency of clomazone removal is achieved by using ZnO/ZrO_2 as a photocatalyst compared to ZnO/CeO_2 and ZnO/MgO.

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Hemija i tehnologija makromolekula

Chemistry and Technology of Macromolecules

HTM-1

Ultrazvučna ekstrakcija pektina iz otpadne jabučne kaše primenom eutektičkih rastvarača na bazi holin hlorida

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Pektin i pektinski oligosaharidi mogu se dobiti iz otpadne jabučne kaše. Ovaj prirodni polimer ima široku primenu u industriji. Tradicionalna metoda za ekstrakciju pektina podrazumeva tretman razblaženim mineralnim kiselinama na povišenoj temperaturi, pri čemu se prinosi ostvaruju od oko 10 do 15%. Kao alternativa tradicionalnim rastvaračima sve češće se koriste i eutektički rastvarači, koje odlikuju daleko superiornija svojstva kada je reč o ciljanoj ekstrakciji određenih komponenti iz biomase. Cilj ovog rada je ultrazvučna ekstrakcija pektina primenom eutektičkih rastvarača na bazi holin hlorida i mlečne kiseline. Svojstva ekstrahovanog proizvoda ispitana su primenom FTIR spektroskopije i diferencijalne skenirajuće kalorimetrije.

Ultrasound assisted extraction of pectin from waste apple pomace using choline chloride based eutectic solvents

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Pectin and pectin derived oligosaccharides can be obtained from waste apple pomace (biomass). Traditional method for pectin extraction involves use of diluted mineral acids at elevated temperatures, with yields of about 10 to 15%. As an alternative to conventional methods, the use of eutectic solvents is increasing because of their superior properties when it comes to targeted extraction of certain components from biomass. The aim of this paper is ultrasound assisted extraction of pectin from waste apple pomace using choline chloride based eutectic solvents and lactic acid. Properties of extracted products were examined using FTIR spectroscopy and differential scanning calorimetry.

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HTM-2

Priprema i karakterizacija kompozita poli(mlečne kiseline) i zeolita modifikovanog benzalkonijum-hloridom

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Poli(mlečna kiselina), PLA, je jedan od najistaknutijih predstavnika biodegradabilnih sintetskih polimera. Ovaj polimer ima i dodatnu prednost u tome što se dobija iz obnovljivih izvora. Radi povećanja upotrebne vrednosti PLA, svojstva joj se mogu modifikovati i poboljšati različitim puniocima mikro i nano dimenzija. U okviru ovog rada pripremljena je serija kompozita sa PLA kao matricom i puniocem prirodnog porekla, zeolitom (1, 3, 5 mas.%) modifikovanim benzalkonijum-hloridom. TG analizom je ispitana termooksidativna stabilnost kompozita koja se nije umanjila dodatkom punioca. DSC analizom je određen stepen kristaliničnosti PLA matrice koji pokazuje nešto veće vrednosti pri najvećem sadržaju zeolita, uz skoro nepromenjenu temperaturu topljenja. Dinamičko-mehaničkim merenjima je pokazano da je dodatak punioca uticao na poboljšanje mehaničkih svojstava matrice, posebno u gumolikom stanju. U testovima alkalne hidrolize je utvrđeno da se degradabilnost kompozita povećava sa povećanjem sadržaja modifikovanog zeolita.

Preparation and characterization of composites based on poly(lactic acid) and benzalkonium chloride modified zeolite

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Poly(lactic acid), PLA, is one of the most prominent member of biodegradable synthetic polymers. PLA is obtained from renewable sources, which is an additional advantage of this polyester. In order to expand its application window, properties of PLA could be further improved by composite preparation. In this work, composites of PLA with benzalkonium chloride-modified zeolite (1, 3, 5 wt%), as a filler of natural origin, were prepared by solution casting. Thermal stability of PLA was preserved after the addition of zeolite, as determined by TG analysis. DSC measurements showed that degree of crystallinity was slightly higher for the composite with the highest amount of zeolite, with unaltered melting temperature. Mechanical properties were improved, especially in the rubbery state, evidenced from dynamic mechanical analysis. In alkaline hydrolysis tests composites showed trend of increased degradability with higher amount of zeolite.

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Hemija i tehnologija hrane

Chemistry and Technology of Food

HTH-1

Izolovanje RuBisCO proteina iz lišća bundeve ultrazvučno potpomognutim procesom ekstrakcije

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Proteini životinjskog i biljnog porekla čine osnovne namirnice ljudske ishrane. Prema konceptu zelene biorafinerije, izolovanje RuBisCO proteina (ribuloza-1,5-bisfosfat karboksilaza/oksigenaze) iz zelene biomase kakva je lišće bundeve, nusproizvod industrije prerade uljarica, je obećavajući pristup za dobijanje proteina sa visokom nutritivnom vrednošću koje je moguće koristiti kao zamenu za proteine životinjskog porekla. U ovom radu, ultrazvučno potpomognutim procesom ekstrakcije izolovani su proteini iz lišća bundeve. Ultrazvučni proces ekstrakcije RuBisCO proteina optimizovan je variranjem odnosa rastvarač-uzorak, pH rastvarača, vremena trajanja i amplitude ultrazvuka. Ultrazvuk je ispoljio veliki pozitivan efekat na izolovanje RuBisCO proteina iz lišća bundeve, na šta je u najvećoj meri tokom optimizacije procesa uticao odnos rastvarač-uzorak, kao i amplituda i vreme ultrazvuka.

Ultrasound-assisted extraction process for recovery of RuBisCO proteins from pumpkin leaves

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Proteins are an essential component of the human diet and effectively are provided from both animal and plant sources. Sourcing ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO) from green biomass such as pumpkin leaves, a by-product of the oil industry, is a promising tool for obtaining protein with an excellent nutritional profile under the green biorafinery concept, that can be used as a substitute for animal proteins. This study provides the results regarding the implementation of ultrasound-assisted processing (UAP) in the protein extraction from pumpkin leaves. UAP for recovery of RuBisCO proteins was optimized by varing the solvent-to-sample ratio, solvent pH, ultrasound amplitudes and time. UAP appears to have a strong potential for recovering RuBisCO protein from pumpkin leaves, as it was highly influenced by the solvent-to-sample ratio along with UAP amplitude and time.

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HTH-2

Poboljšanje antioksidativnih svojstava čajnog peciva sa dodatkom praha cvekle

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Zbog porasta bolesti povezanih sa oksidativnim stresom, kao što su dijabetes, kardiovaskularne bolesti i kancer, proizvođači hrane razvijaju funkcionalne proizvode obogaćene antioksidantima. Antioksidanti imaju ulogu da inhibiraju ili odlažu oksidaciju biološki važnih molekula gašenjem slobodnih radikala, i na taj način štite ćelije od oksidativnog stresa. U ovom radu je ispitan efekat zamene speltinog brašna prahom cvekle (do 50 %) na antioksidativna svojstva proizvoda tipa čajnog peciva. Na početku skladištenja, kao i nakon 3 i 6 meseci, ispitan je sadržaj betalaina, ukupnih polifenola i flavonoida, kao i kapacitet za uklanjanje DPPH radikala. Svi navedeni parametri su rasli sa povećanjem udela praha cvekle u pecivu i opadali sa vremenom skladištenja. Tokom skladištenja je dolazilo do tamnjenja boje peciva. Čajno pecivo sa cveklom je pokazalo značajno poboljšana antioksidativna svojstva u poređenju sa kontrolnim uzorkom bez cvekle.

Improving the antioxidant properties of biscuits with the addition of beetroot powder

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Due to the increase in diseases related to oxidative stress, such as diabetes, cardiovascular diseases, and cancer, food producers are developing functional products enriched with antioxidants. Antioxidants can inhibit or delay the oxidation of biologically essential molecules by quenching free radicals, thus protecting cells from oxidative stress. In this work, the effect of replacing spelt flour with beetroot powder (up to 50 %) on the antioxidant properties of biscuits was investigated. At the beginning of storage and after 3 and 6 months, the content of betalains, total polyphenols, and flavonoids and the capacity to remove DPPH radicals were examined. All the mentioned parameters increased with the content of beetroot powder in the biscuit and decreased with the rise of the storage time. During storage, the biscuit color turned brown. The biscuits with the beetroot showed significantly improved antioxidant properties compared to the control sample without beetroot.

HTH-3

Polifenolni profil i antioksidativna aktivnost vina od domaćih sorti vinove loze Crna tamjanika i Frankovka

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Polifenolna jedinjenja, zahvaljujući svojoj hemijskoj strukturi i funkcionalnim svojstvima, doprinose finalnoj kompleksnosti i senzorskim karakteristikama vina i veoma često se koriste za njihovu diferencijaciju i klasifikaciju.

U radu je HPLC metodomispitan sastav polifenolnih jedinjenja u vinima domaćih sorti Crna tamjanika i Frankovka. Takođe, primenom spektrofotometrijskih testova određena je i antioksidativna aktivnost vina navedenih sorti na 2,2-difenil-1-pikrilhidrazil radikale ($DPPH^{\bullet}$), kao i njihova redukciona sposobnost (RP). U ispitivanim uzorcima vina utvrđeno je da se od detektovanih polifenola po koncentraciji ističu: antocijani, kumarinska, *p*-hidroksibenzoeva i galna kiselina. Vrednosti parametra antioksidativne aktivnosti uzoraka vina na $DPPH^{\bullet}$ bile su u granicama od 243,83 do 798,84 mmol TE/100 mL, dok su vrednosti RP bile u intervalu od 202,33 do 1480,02 mmolTE/100 mL. Visok stepen korelacije,iskazan preko korelacionog faktora R^2, utvrđen je između rezultata DPPH testa i sadržaja ferulne kiseline (0,80), kao i zbira sadržaja svih polifenola (0,75), ali i za rezultate RP i sadržaja *p*-hidroksibenzoeve kiseline (0,94).

Polyphenol profile and antioxidant activity of wines from domestic grape varieties Crna tamjanika and Frankovka

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Due to their chemical structure and functional properties, polyphenolic compounds contribute to the complexity and sensory characteristics of wine and these compounds are very often used for their differentiation and classification.

In this paper,using HPLC methodthe polyphenol profile of wines from domesticgrape varietiesCrna tamjanika and Frankovka was investigated. Their antioxidant activity was determined using spectrophotometric DPPH (2,2-diphenyl-1-picrylhydrazyl)assay and reducing power (RP). HPLC analysis revealed higher concentrations of anthocyanins, coumaric, *p*-hydroxybezoic and gallic acid among polyphenolic compounds determined in wine samples. Antioxidant activity of wine samples expressed by DPPH assay ranged from 243.83 to 798.84 mmol TE/100 mL, while RP values ranged from 202.33 to 1480.02 mmol TE/100 mL. A high level of correlation, expressed through the correlation factor R^2, was determined between antioxidative activity on $DPPH^{\bullet}$and ferulic acid content (0.80) and the sum of polyphenols (0.75), as well as between RP values and *p*-hydroxybenzoic acidcontent (0.94).

HTH-4

Uticaj temperature sušenja na sadržaj ukupnih karotenoida i β-karotena u šipurku (*Rosa canina* L.)

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Karotenoidi predstavljaju veliku grupu prirodnih metabolita odgovornih za crvenu, narandžastu i žutu boju voća. Učestvuju u regulaciji mnogih metaboličkih procesa i blagotvorno utiču na zdravlje ljudi [1]. Šipurak je 'lažni' plod pasje ruže (*Rosa canina* L.) I upotrebljava se za pripremu voćnih infuzija – tisane [2]. Sveži plodovi sušeni su u eksperimentalnoj sušari pri protoku vazduha od 2 m/s i na različitim temperaturama (40, 50 i 60°C), a zatim je određivan sadržaj ukupnih karotenoida i β-karotena. Rezultati su pokazali da je najveći sadržaj ukupnih karotenoida (40,95 μg/g) i β-karotena (28,84 μg/g) izmeren u šipurku sušenom na najvišoj primenjenoj temperaturi, 60 ^{o}C.

Influence of drying temperature on the content of total carotenoids and β-carotene in rosehip (*Rosa canina* L.)

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Carotenoids represent a large group of natural metabolites responsible for red, orange, and yellow color of fruits. They are involved in regulation of many metabolic processes and have beneficial effects on human health [1]. Rosehip is a pseudo-fruit of the dog rose (*Rosa canina* L.)and is used for preparation of fruit infusions-tisanes[2]. Fresh fruits were dried in an experimental dryer at the air flow rate of 2 m/s and different temperatures (40, 50 and 60°C), followed by the measurement of total carotenoids and β-carotene. The results indicated that the highest content of total carotenoids and β-carotene (40.95 and 28.84 μg/g, respectively) was found in rosehips dried at the highest applied temperature, 60 ^{o}C.

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[2] I. Pećinar, Dj. Krstić, G. Caruso, J.B. Popović-Djordjević,*Roy Soc Open Sci,***2021**,8,202064.

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Hemijsko inženjerstvo

Chemical Engineering

HI-1

Određivanje optimalne poroznosti u fluidizovanom sloju korišćenjem tehnike merenja intenziteta zvuka

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U ovom radu korišćena je tehnika merenja intenziteta zvuka zaodređivanje optimalne poroznosti fluidizovanog sloja na osnovu frekvencije sudara čestica. Optimalna poroznost sloja je poroznost pri kojoj je intenzitet međučestičnih sudara i sudara čestica sa zidom maksimalan a samim tim i najefikasniji prenos količine kretanja, mase i toplote. Eksperimentalna merenja intenziteta zvuka rađenasu u dve 2D kolone (kvadratnog poprečnog preseka) dimenzija 160 x 10 mm i 190 x 13 mm kao i u cilindričnoj koloni prečnika $Dc=62$ mm i visine $H=$ 65 cm. U eksperimentima su korišćene staklene sferične čestice prečnika d_p=3.0 mm i d_p=4.0 mm i gustine ρ_p= 2550 kg/m^3. Intenzitet zvuka meren je uređajem **EXTECH 407760** za više različitih poroznosti sloja. Pokazano je da se optimalna poroznost sloja dobija za vrednosti $\varepsilon_{opt} \approx 0.7$, što je u saglasnosti sa literaturnim podacima.

Determination of the optimal porosity in a fluidized bed using the sound intensity measurement technique

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In this study, the sound intensity measurement technique was used to determine the optimal porosity in a fluidized bed, based on particle collision frequency. The optimal bed porosity is the porosity at which the intensity of interparticle collisions and collisions of particles with the wall is maximal and therefore the momentum, mass and heat transfer are the most efficient. Sound intensity measurements were performed in two 2D columns (square cross-section), D=160x10mm and D=190x13mm as well in the cylindrical column Dc = 62 mm in dia. and H = 650mm in height. In the experiments glass spheresof d_p=3.0 mm and d_p=4.0 mm (ρ_p= 2550 kg/m^3 in density) were used.Sound intensity measurements were done for several different bed porosities using the **EXTECH 407760** device. It was shown that the optimal bed porosity is$\varepsilon_{opt} \approx 0.7$,that is in agreement with the literature data.

HI-2

Prenos mase u inverzno fluidizovanim slojevima

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Inverzna fluidizacija se ostvaruje u kontaktorima u kojima je gustina medijuma kojim se vrši fluidizacija veća od gustine čestica. U ovim radu su prikazani rezultati eksperimentalnih ispitivanja prenosa mase fluid-zid u prisustvu inverzno fluidizovanih čestica. Korišćena je adsorpciona metoda. Kao čvrste čestice korišćene su sferične i nesferične čestice polipropilena i polietilena. Fluidizacioni medijum je razblaženi rastvor metilenskog plavog u vodi. Ovaj rastvor je ujedno i rastvor adsorbata koji se adsorbovao na zid kolone presvučene silikagelom. Izvršeno je poređenje rezultata dobijenih u ovom radu sa podacima za prenos mase u jednofaznom toku i konvencionalno fluidizovanim slojevima. Na osnovu analize uveden je koncept tretiranja inverzno fluidizovanog sloja kao pseudofluida.

Ključne reči: Inverzna fluidizacija, prenos mase, adsorpcija fluid-zid, pseudofluid

Mass transfer in inverse fluidized beds

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Inverse fluidization is realized in contactors when the density of the fluidizing medium (fluid) is higher than the density of the particles. This paper presents the results of experimental investigations of fluid-wall mass transfer in the presence of inversely fluidized particles. The adsorption method was used. Spherical and non-spherical particles of polypropylene and polyethylene were used as solid particles. A dilute solution of methylene blue in water was used as the fluidization medium. This solution is also an adsorbate solution that was adsorbed on the wall of the column coated with silica gel. A comparison of the results obtained in this paper with the data for mass transfer in single - phase flow and conventional fluidized beds was performed. Based on the analysis, the concept of treating the inverse fluidized bed as a pseudofluid was introduced.

Keywords: Inverse fluidization, mass transfer, fluid-wall adsorption, pseudofluid

HI-3

Izolovanje etarskog ulja ploda kleke (*Juniperus communis* L.) hidrodestilacijom pod sniženim pritiskom

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Etarsko ulje ploda kleke (*Juniperus communis* L.) sastoji se od isparljivih bioaktivnih jedinjenja, koja pokazuju različita fiziološka svojstva i kao takva nalaze primenu u medicini, farmaciji, veterini, prehrambenoj i kozmetičkoj industriji. Cilj ovog rada je poređenje prinosa etarskog ulja kleke dobijenog destilacijom vodom mokro mlevenih bobica kleke na pritiscima u opsegu od 50 kPa do atmosferskog pritiska, kao i ispitivanje uticaja pritiska na sastav etarskog ulja. Etarsko ulje bobica kleke dobijeno vakuum hidrodestilacijom (50 kPa) sadrži 52,63% monoterpena, od kojih dominiraju α-pinen (21,08%) i β-mircen (16,72%), 3,51% oksidovanih monoterpena gde dominira terpinen-4-ol (3,06%) i 42,85% seskviterpena sa dominantnim sadržajem germakrena D (19,81%). Hidrodestilacijom na atmosferskom pritisku izoluje se etarsko ulje kleke sa 82,08% monoterpena (24,26% α-pinen i 19,79% β-mircen), 3,98% oksidovanih monoterpena (3,01% terpinen-4-ol) i 13,20% seskviterpena (7,78% germakren D).

Isolation of juniper berry essential oil (*Juniperus communis* L.) by vacuum hydrodistillation

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Juniper berry essential oil (*Juniperus communis* L.) consist of volatile bioactive compounds having different physiological properties, thus being suitable for application in a food, medicine, pharmacy, cosmetics and veterinary industry. The aim of this study is to compare the yield of juniper berry essential oil obtained by hydrodistillation of wet milled fruits at pressures ranging from 50 kPa to atmospheric pressure, and to examine the effect of the pressure on the oils' composition. Juniper berry essential oil obtained by vacuum distillation (50 kPa) contained 52.63% of monoterpenes, where dominant components were α-pinene (21.08%) and β-myrcene (16.72%), 3.51% of oxidized monoterpenes, with the highest level of terpinen-4-ol (3.06%) and 42.85% was the sesquiterpene's fraction with a dominant content of germacrene D (19.81%). Hydrodistillation at atmospheric pressure enabled isolation of essential oil with 82.08% monoterpenes (24.26% α-pinene and 19.79% β-myrcene), 3.98% oxidized monoterpenes (3.01% terpinen-4-ol) and 13.20 % sesquiterpenes (7.78% germacrene D).

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HI-4

Ekspanzija sloja i kretanje čestica u inverzno fluidizovanim slojevima

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Dva važnaparametraza projektovanje sistema sa fluidizovanim slojem čestica su ekspanzija sloja i kretanje čestica. U ovom radu su predstavljeni eksperimentalno dobijeni rezultati u inverzno fluidizovanom sloju u cilindričnoj koloni prečnika 45 mm i koloni pravougaonog poprečnog preseka dimenzija 138 x10 mm. Kao čvrste čestice korišćene su čestice polipropilena, polietilena i polistirena, a kao fluidizacioni medijum korišćena je voda i vodeni rastvor glicerina. Prikazane su dobijene zavisnosti poroznosti sloja od površinske brzine fluida, postavljene su korelacije ekspanzije inverzno fluidizovanog sloja i data su poređenja sa korelacijom Richardson-Zaki u konvencionalno fluidizovanom sloju. U radu su prikazani rezultati koji pokazuju kretanje čestice u sloju, njenu srednju brzinu, kao i uticaj viskoznosti sloja i gustine čestica na njeno kretanje.

Bed expansion and particle motion in inverse fluidized beds

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Bed expansion and particle motion are two important parameters for designing a fluidized bed system. This paper presents the experimentally obtained results in an inverse fluidized bed in a cylindrical column with a diameter of 45 mm and a column with a rectangular cross section of138 x 10 mm. Particles ofpolypropylene, polyethylene and polystyrene were used as solid particles, and water and an aqueous solution of glycerin were used as the fluidizing medium. The obtained dependences of the bed porosity on the fluid surface velocity are presented, the correlations of the expansion of the inverse fluidized bed are set and comparisons with the Richardson-Zaki correlation in the conventional fluidized bed are given. The presented results show the particle motion in the bed, its meanvelocity,as well as the influence of the bed viscosity and particle density on its motion.

KNJIGA RADOVA

Proceedings

Analitička hemija

Analytical Chemistry

R-AH-1

Procena ekotoksikološkog rizika veštačkih zaslađivača saharina i sukraloze u rečnoj vodi na teritoriji Beograda

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Veštački zaslađivači saharin i sukraloza predstavljaju emergentne zagađujuće materije čije prisustvo u akvatičnim ekosistemima može negativno uticati na osetljive organizme. Veoma su postojani u životnoj sredini, a posebno je zabrinjavajuće njihovo toksično dejstvo na planktonske vrste. U ovom radu je izvršena HPLC–MS/MS analiza tragova saharina i sukraloze u pet uzoraka rečne vode iz Save i Dunava na teritoriji Beograda radi procene prisustva i određivanja ekotoksikološkog rizika. Rezultati su pokazali da detektovane koncentracije ovih zaslađivača u reci Dunav (do 396 ng L^{-1} za saharin i do 349 ng L^{-1} za sukralozu) pokazuju nizak ekotoksikološki rizik za vodene organizme, ali zbog "koktel efekta" njihov kumulativni doprinos može predstavljati veći rizik po vodeni svet.

Uvod

Saharin i sukraloza su široko zastupljeni veštački zaslađivači u hrani i piću, čija je moć zaslađivanja nekoliko stotina puta veća od običnog šećera. Pošto se ne metabolišu u ljudskom telu, putem kanalizacije dospevaju nepromenjeni u akvatične ekosisteme. Postojani su u životnoj sredini, posebno sukraloza, što ih čini idealnim indikatorima zagađenja komunalnim otpadnim vodama [1]. Ubrajaju se u emergentne zagađujuće materije čije se prisustvo može detektovati u životnoj sredini, ali koje nisu uključene u programe monitoringa voda i čiji toksični efekti još uvek nisu dovoljno istraženi [1]. Nekoliko toksikoloških studija je pokazalo da ove supstance mogu da imaju štetne efekte po živi svet u vodi utičući na ponašanje i reprodukciju kod ispitivanih vrsta [2]. Takođe, zabrinjavajuća je činjenica da prisustvo sukraloze može ometati proces fotosinteze, naročito kod algi.

U ovom radu je opisana analiza tragova saharina i sukraloze u uzorcima reka Save i Dunava na teritoriji Beograda, kao i procena ekotoksikološkog uticaja na vodene organizme. Ekotoksikološki rizik je određen na osnovu eksperimentalnih PNEC (eng. predicted no-effect concentration) vrednosti dobijenih iz NORMAN-ove (eng. Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances) ekotoksikološke baze podataka. Uzorci vode su analizirani metodom tečne hromatografije visokih performansi u sprezi sa tandem masenom spektrometrijom (eng. high performance liquid chromatography–tandem mass spectrometry, HPLC–MS/MS).

Eksperimentalni deo

Analitički standard saharina i sukraloze su nabavljeni od proizvođača Sigma-Aldrich (Sent Luis, SAD). Metanol (HPLC čistoće) je nabavljen od proizvođača J.T. Baker (Glivice, Poljska). Amonijum-acetat je kupljen od proizvođača Fisher Chemical (Lafboro, Velika Britanija). Za podešavanje pH vrednosti tokom pripreme uzoraka vode korišćena je sirćetna kiselina analitičke čistoće.

Uzorci rečne vode su sakupljeni na teritoriji Beograda: dva iz reke Save (SAVA1, SAVA2) i tri iz reke Dunav (DUNAV1, DUNAV2 i DUNAV3). Uzorci su čuvani u plastičnim bocama od 1 L, u zamrzivaču, bez dodatka konzervansa, do analize. Za izolovanje i koncentrovanje veštačkih zaslađivača korišćena je metoda ekstrakcije na čvrstoj fazi (eng. solid-phase extraction, SPE) uz upotrebu Oasis HLB kertridža kao adsorbensa. Pre SPE procedure, uzorci su odmrznuti i filtrirani kroz filtere od staklenih vlakana, veličine pora 1–3 μm. Na pakovanje SPE kolone je nanošeno 50 mL uzorka rečne vode sa podešenom pH vrednošću na 3,0. Zaslađivači su eluirani sa adsorbensa pomoću 10 mL metanola, a zatim su dobijeni ekstrakti uparavani do zapremine od 1 mL.

HPLC–MS/MS analiza zaslađivača saharina i sukraloze je izvršena na Dionex UltiMate® 3000 HPLC sistemu u sprezi sa LTQ XL linearnim jonskim trapom kao masenim analizatorom, proizvođača Thermo Fisher Scientific (Voltam, SAD). Kao jonizaciona tehnika je korišćena elektrosprej jonizacija u negativnom režimu rada. Za hromatografsko razdvajanje zaslađivača korišćena je reverzno-fazna kolona Luna C8 (3,0 mm × 150 mm × 3 μm), proizvođača Phenomenex (Torans, SAD). Kao rastvarači u mobilnoj fazi korišćeni su metanol i voda, uz dodatak 0,1 mol L^{-1} rastvora amonijum-acetata kao aditiva. U maseno-spektrometrijskoj analizi korišćene su karakteristične reakcije fragmentacije za kvantitativno određivanje saharina i sukraloze, kao i za potvrdu prisustva ovih analita u rečnoj vodi, koje su odabrane u prethodnom istraživanju [3].

Procena ekotoksikološkog rizika je izvršena izračunavanjem koeficijenta rizika (eng. risk quotient, RQ) za detektovane zaslađivače deljenjem detektovanih koncentracija u rečnoj vodi sa odgovarajućom PNEC vrednošću za odabrani zaslađivač iz NORMAN-ove ekotoksikološke baze podataka [4], koja pokazuje graničnu vrednost koja ne izaziva ekotoksične efekte kod slatkovodnih organizama.

Rezultati i diskusija

HPLC–MS/MS analizom uzoraka rečne vode iz Save i Dunava utvrđeno je prisustvo sukraloze u svim uzorcima, kao i saharina u tri uzorka. Koncentracije detektovanih zaslađivača su prikazane u tabeli 1.

Tabela 1. Koncentracije detektovanih veštačkih zaslađivača saharina i sukraloze u rečnoj vodi (ng L^{-1}) i koeficijenti rizika (RQ) za slatkovodne organizme.

Uzorci	Saharin	RQ	Sukraloza	RQ
Reka Sava				
SAVA1	104 ± 19	0,003	111 ± 23	0,004
SAVA2	–	–	68 ± 7	0,002
Reka Dunav				
DUNAV1	92 ± 19	0,002	89 ± 9	0,003
DUNAV2	396 ± 37	0,011	206 ± 18	0,007
DUNAV3	–	–	349 ± 36	0,012

Uzimajući u obzir PNEC vrednost za saharin dobijenu iz NORMAN-ove ekotoksikološke baze podataka (35,9 µg L^{-1}), utvrđeno je da pri detektovanim koncentracijama u reci Savi ne postoji rizik za akvatične organizme (RQ manji od 0,01), dok u Dunavu (DUNAV2) registrovan nivo saharina pokazuje nizak ekotoksikološki rizik (RQ između 0,01 i 0,1). Takođe, na osnovu eksperimentalno ustanovljenih PNEC vrednosti za sukralozu (29,7 µg L^{-1}), u reci Savi nisu zabeležene koncentracije koje mogu da izazovu toksične efekte. S druge strane, u Dunavu (DUNAV3) detektovan nivo sukraloze od 349 ng L^{-1} ukazuje na nizak ekotoksikološki rizik (RQ između 0,01 i 0,1).

Povišene koncentracije na lokalitetima na Dunavu (DUNAV2 i DUNAV3) se mogu objasniti pozicijom nizvodno od velikih gradskih kanalizacionih ispusta iz kojih se u reku direktno ispušta netretirana komunalna voda. Iako detektovane koncentracije zaslađivača predstavljaju nizak rizik po vodene organizme, postoji mogućnost povećanja ekotoksikološkog rizika tokom letnjeg perioda kada se pri visokim dnevnim temperaturama i nižim vodostajima mogu detektovati visoke koncentracije, što je primećeno kod velikog broja evropskih reka (do 1 µg L^{-1}) [5]. Dodatno, niske koncentracije pojedinačnih zaslađivača sumarno doprinose povećanju ekotoksikološkog rizika zbog tzv. „koktel efekta“ [6].

Zaključak

HPLC–MS/MS analizom uzoraka rečne vode potvrđeno je prisustvo saharina i sukraloze u Savi i Dunavu (do 396 ng L^{-1} za saharin i do 349 ng L^{-1} za sukralozu), kao rezultat konstantnog ispuštanja netretiranih komunalnih voda u reke. Na osnovu izmerenih koncentracija zaslađivača u reci Savi nije utvrđen ekotoksikološki rizik, dok je u Dunavu zabeležen nizak rizik za oba zaslađivača. Uzimajući u obzir povećanje koncentracija zaslađivača u letnjem periodu, kao i njihov zbirni doprinos, postoji mogućnost povećanja ekotoksikološkog rizika po živi svet u rečnoj vodi.

Ecotoxicological risk assessment of artificial sweeteners saccharin and sucralose in the river water in Belgrade

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Artificial sweeteners saccharin and sucralose are emerging pollutants whose presence in aquatic ecosystems can adversely affect sensitive organisms. They are very persistent in the environment, and their toxic effect on planktonic species is of particular concern. In this paper, HPLC–MS/MS analysis of saccharin and sucralose traces in five samples of river water from the Sava and Danube in the territory of Belgrade was performed to assess the presence and determine ecotoxicological risk. The results showed that the detected concentrations of these sweeteners in the Danube (up to 396 ng L^{-1} for saccharin and up to 349 ng L^{-1} for sucralose) show low ecotoxicological risk for aquatic organisms, but due to the "cocktail effect" their cumulative contribution may pose a higher risk to aquatic wildlife.

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Zahvalnica

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R-AH-2

Comparison of nitric acid and *aqua regia* as extractants for heavy metals in soil samples

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Abstract

A comparison of extraction abilities of nitric acid alone (HNO_3) and *aqua regia* in one-step microwave enhanced digestion procedure is presented in this communication. The certified reference material for soil Metranal^{TM} 33 (Analytika, Czech Republic) as a model soil sample was used. The measurements of the selected elements were done by means of ICP-AES. The results obtained in this research suggest that both tested reagents display similar extraction abilities toward heavy metals that are usually analyzed in soils.

Introduction

A large number of various analytical methods of quantitative analysis of metals and metalloids in soil samples (and similar samples from the Environment) has been described in the scientific literature [1,2]. Most of those methods consist of quantification by some of the spectrometric techniques (*e.g.* AES, AAS, ICP-MS) that require a transformation of a solid sample into solution state. Therefore, the first step of such an analytical procedure, when applied to soil samples, a complete digestion of samples or extraction of the analytes into water solution usually is. Consequently, in the context of the elemental characterisation of soils, methods of preparation of the samples are subject of researchers' attention worldwide. A selection of a digestion/extraction method primarily depends on aims and scopes of the research. Thus, if one wants to know a total content of an element in soil, method of choice for total digestion of samples should contain hydrofluoric acid [3]. On the other hand, in order to assess bioavailable fraction of so-called 'heavy metals' in soil, research have to employ less strong (even mild) extraction media and conditions [2]. Even though *aqua regia* is quite strong, it is set as a referent digestion reagent for quantification (and comparison with maximum allowable mass fractions) of hazardous chemical elements in soils in many countries [4-7].

This research was conducted in the context of our interests in the field of multi-element analysis of soils and testings of various extraction media [8, 9]. Its main aim is to compare the extraction abilities of concentrated nitric acid and *aqua regia* toward heavy metals that are usually analyzed in soil samples; namely the metals and metalloids that are commonly considered as elements that easily enter in the environment as a consequence of various human activities [10].

Results and Discussion

The results of the analyses are presented in Table 1 and Figure 1.

Table 1. Mass fraction values (mg/kg) of the selected metals in the soil certified reference material Metranal™ 33 obtained after digestion with concentrated nitric acid (HNO_3) or *aqua regia*

	Cert. tot. content	**Found after digestion with conc. HNO_3**		**Found after digestion with *aqua regia***	
	mg/kg	Av. ± Std.dev. (mg/kg)	RSD (%)	Av. ± Std.dev. (mg/kg)	RSD (%)
Al	65015	41000 ± 3940	10	38750 ± 1240	3
As	16.7	5.59 ± 0.70	13	18.9 ± 2.5	13
Ba	495	254 ± 27	11	250 ± 4	2
Be	2.18±0.16	1.34 ± 0.63	47	1.54 ± 0.42	27
Cd	0.32±0.04	< 0.12	n.d.	0.548 ± 0.080	15
Cr	79.8±6.7	81.4 ± 17.7	22	50.1 ± 6.7	13
Fe	29026	31460 ± 5070	16	30030 ± 790	3
Mn	600±37	658 ± 110	17	632 ± 16	3
Ni	31.3±1.5	34.7 ± 6.7	19	34.7 ± 4.2	12
Pb	33.5±2.4	25.5 ± 3.8	15	26.3 ± 2.3	9
Zn	81.0±7.6	79.8 ± 11.1	14	75.3 ± 4.8	6
Ca	9862	10380 ± 1580	15	9309 ± 407	4
K	18346	7981 ± 809	10	9069 ± 201	2
Mg	6151	6053 ± 900	15	5745 ± 175	3
Na	5490	200 ± 21	11	456 ± 121	27

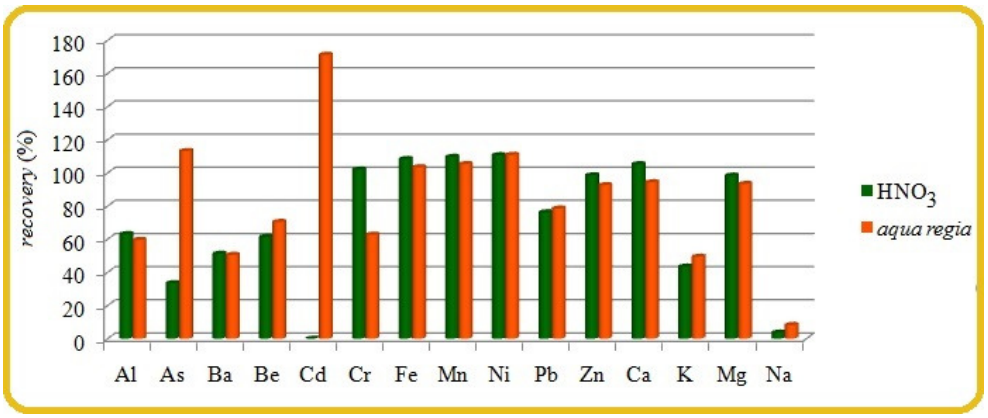

Figure 1. Comparison of the recoveries of the analyzed elements in Metranal™ 33 obtained with two different digestion reagents

The recoveries ($w_{found}/w_{total,\ certified}$) displayed in Fig. 1 suggest that most of the elements – namely, Al, Ba, Be, Fe, Mn, Ni, Pb, Zn, K, and Na – were extracted in similar proportions, both by HNO_3 and *aqua regia*. Such findings are consistent with previously obtained results in similar testings that were made on an other soil CRM [11]. The mass fraction values obtained herein for Fe, Mn, Ni, and Ca are slighlty higher than the certified ones, for unknown reasons. It was not possible to quantify Cd in the HNO_3-digestates, because it was present in the quantities that were found to be below its detection limit value, while in the digestates prepared by *aqua regia* this element was over-quantified. Usually, it is not possible to accurately and precisely quantify this element in clean soil samples by such a method (which is consisted by direct measurement of the analyte in digestate) due to its (i) low concentration, and (ii) relatively low sensitivity of the ICP-AES toward Cd [12]. Similar problem is also known in the case of As [12].

Experimental

Chemicals

Certified reference material (CRM) for soil Metranal™ 33 (produced by Analytika Ltd, Prague, Czeck Republic) was used as a model soil sample. It is a clay loam soil, with normal levels of the analytes.

Nitric acid (HNO_3, *p.a.*, 65 %) and hydrochloric acid (HCl, *p.a.*, 36 %), both produced by Carlo Erba, Italija were used for microwave enhanced digestion.

Multi-element ICP-Standard-Solution ROTI®STAR, ROTH (Carl Roth GmbH & Co., Karlsruhe, Deutchland) was used for preparation of the series of the standard solutions for external calibration of atomic emission spectrometer. Also, *Multielement standard solution III for ICP* TraceCERT® (Fluka, Switzerland) was used for calibration of Ca, K, Mg, and Na, after 1000-fold dilution.

Nitric acid of the *supra pur* grade (HNO_3, 65 %, *supra pur*, Fluka) was used for acidification of the standard solutions (instrumental blank solution included); its final percentage was set as *v/v* 1%.

All dilution procedures were made by using ultrapure water (Siemens Ultra clear, 0.055 μS/cm).

Soil samples preparation and spectrometric quantification of the analytes

The samples of the CRM were weighted (~0.1000 g each) and mixed with 10 mL of an acidic reagent (nitric acid alone or *aqua regia* which was being prepared *in sitū*) in the teflon vessels. The CRM samples were subjected to microwave enhanced wet digestion procedure that was performed using *Anton Paar MW-3000* microwave digestion system. The main parameters of the digestion procedures were set as follows: t_{max} = 200 °C; P_{max} = 1200W; p_{max} = 60 bar; τ(ramp) = 20 min, τ(heating at max. temperature) = 20 min, τ(cooling) = 20 min. Other parameters of the digestion procedure as well as of the digestate preparation can be found elsewhere [12].

Quantification of the selected metals and metalloids in the prepared solutions was made by means of atomic emission spectrometer with inductively coupled plasma, ICP-AES (*Thermo Fischer iCAP6300 Duo*) [12].

Apstrakt

U ovom istraživanju napravljeno je poređenje ekstrakcijskih moći koncentrovane azotne kiseline (HNO_3) i carske vode u mikrovalno potpomognutoj proceduri u jednom koraku. Kao model zemljišta korišćen je sertifikovani referentni materijal Metranal^{TM} 33 (Analytika, Czech Republic). Određivanje odabranih elemenata obavljeno je tehnikom ICP-AES. Rezultati dobiveni u ovom radu sugerišu da oba ispitivana reagensa pokazuju međusobno slične ekstrakcijske moći prema teškim metalima koji se uobičajeno analizuju u uzorcima zemljišta. Vrednosti dobivene u ovom radu mogu služiti kao orijentacione vrednosti u eventualnim budućim upotrebama ovog referentnog materijala, u metodološki sličnim analizama.

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Elektrohemija

Electrochemistry

R-EH-1

Synergistic effect of Neodymium and Cysteine as inhibitors for AA7075 alloy in NaCl solution

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Abstract

The synergistic effect of neodymium chloride and cysteine in NaCl solution was investigated. The concentration ratio of these two inhibitors was 1: 3 (neodymium: cysteine). The corrosion resistance of AA7075 alloy was tested electrochemically using electrochemical impedance spectroscopy (EIS). Significantly higher polaryzation resistance in inhibitor containing solution, along with phase angle peak shift to more negative values, indicate good corrosion inhibition by Nd-cysteine. The morphology, analyzed by scanning electron microscopy (SEM/EDS), shown that the surface of the AA7075 alloy was wholly protected from corrosion after 24h in NaCl solution.

Introduction

Aluminum alloy AA7075 belongs to alloys that have extremely high strength, and are used in various industries, mostly in the aircraft industry. However, in the presence of chloride ions it is prone to corrosion, which is one of its main disadvantages [1,2]. The simplest and most economical way of its protection is by inhibitors. The most effective inhibitors were chromates, but due to their harmfulness and carcinogenicity, they were banned by European regulations [3]. Recently, so-called green or eco-friendly inhibitors have been used as not harmful ones to humans and nature. Lanthanides, either alone or in combination with organic compounds, are good inhibitors in NaCl solution [4].

The aim of this paper is to analyse the combination of cysteine and neodymium, as green corrosion inhibitors, for AA7075 alloy. Inhibitory behavior was evaluated by electrochemical impedance spectroscopy (EIS), and the surface of the specimens before and after the experiments was examined using a scanning electron microscopy (SEM / EDS).

Materials and methods

The chemical composition of AA7075 alloy, determined by XRF method (Olympus Vanta C Series Handheld XRF Analyzer) is shown in Table 1. For electrochemical testing the specimens were mechanically polished with SiC paper up to 1200 grit, and for SEM /EDS analysis, they were additionally polished by water based Al_2O_3 suspension (5 μm and 1 μm). The following chemicals were used for the preparation of the solutions: 0.1M NaCl (p.a. grade, Sigma Aldrich), 0.3mM cysteine (≥98%, Sigma Aldrich), 0.1mM $NdCl_3$ (99 %, Across Organics), high-purity water (Millipore, 18 MΩ cm resistance, using Milli-Q Water Purification Systems).

Table 1. Chemical composition of AA7075 alloy, wt.%

Zn	Mg	Cu	Mn	Cr	Si	Fe	Al
6.90	2.64	1.62	0.27	0.24	0.20	0.09	Rest

The EIS measurements were carried out by GAMRY Reference 1010E Potentiostat/Galvanostat/ZRA in a standard three-electrode cell setup. The working electrode was the aluminum alloy, the counter electrode was Pt mesh, and the reference electrode was saturated calomel electrode (SCE). Measurements were performed in triplicate at the corrosion potential over the frequency range: 100 kHz – 10 mHz, ±10 mV amplitude of the sinusoidal voltage.

Microstructural analyses of samples before and after corrosion measurements were performed using field emission scanning electron microscopy (FE-SEM) JEOL JSM-6610LV, 20 kV working voltage, with Energy Dispersive X-Ray Spectroscopy (EDS).

Results and Discussion

SEM/EDS analysis- The surface morphology and chemical composition of polished, bare AA7075 specimen were analyzed by SEM-EDS technique (Fig. 1).

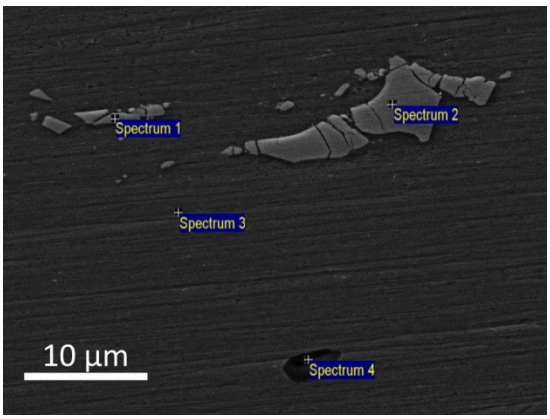

Figure 1. SEM microphotograph of AA7075 alloy

AA7075 alloy contains intermetallic particles (IMP) of micrometer dimensions, which can be anodic or cathodic. IMPs containing Mg, Zn, and Si are of an anodic character, they dissolve in the initial period of the corrosion process but they do not significantly deteriorate the corrosion properties of aluminum alloy, and they are darker than matrix (Fig. 1, Spectrum 4: 6.8 % Zn, 12.6 % Mg, 1.5 % Cu, 12.8 % Si). IMPs containing Fe and Cu are cathodic and lighter than matrix, as shown in Fig. 1 by Spectrums 1 (2.1 % Zn, 3.8 % Cu, 4.5 % Si, 16.4 % Fe, 5.7 % Mn) and 2 (2.7 % Zn, 0.2 % Mg, 3.5 % Cu, 4.3 % Si, 15.8 % Fe, 5.1 % Mn). A cathodic oxygen reduction reaction occurs on the surface of cathodic IMPs during the corrosion process in neutral chloride solutions. As a result, these particles significantly deteriorate the corrosion properties of AA7075 alloy. In Fig. 1, Spectrum 3 refers to an aluminium matrix.

Bode-Phase diagrams for AA7075 alloy obtained in NaCl solution without and in the presence of Nd-cysteine inhibitor are shown in Figure 2. A significant increase in the polarization resistance in inhibitor containing solution was obtained. The phase angle peak in the presence of Nd-cysteine shifts to more negative values (Figure 2b), and it is expanded over greater frequency range as compared with the inhibitor-free NaCl solution.

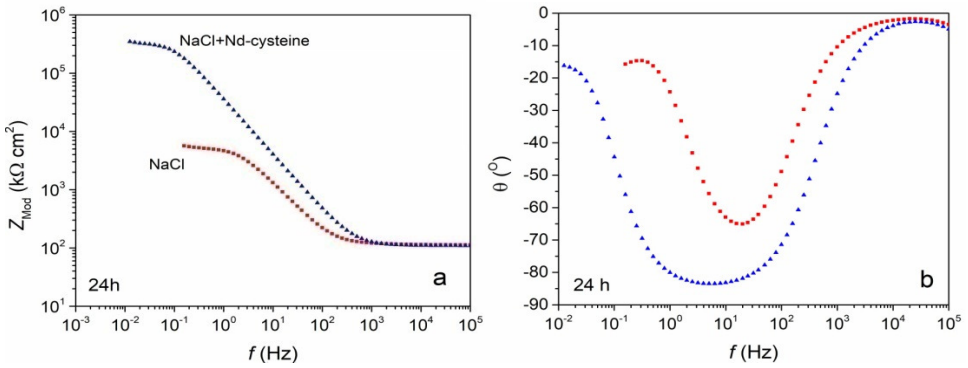

Figure 2. a) Bode modulus and b) Bode phase diagram for AA7075 alloy in NaCl solution without and in presence of Nd-cysteine.

After immersing the specimens in the inhibitor-free NaCl solution, trenches along cathodic IMPs edges were formed (Figure 3a), denoting a form of pitting corrosion of AA7075 alloy. SEM micrograph of the AA7075 alloy surface after immersion for 24 h in the inhibitory solution is shown in Figure 3b. Figure 3b, unlike Figure 3a, does not show any trenches or other corrosion damage around the IMPs. The surface of the AA7075 alloy is protected against corrosion when an inhibitor is present.

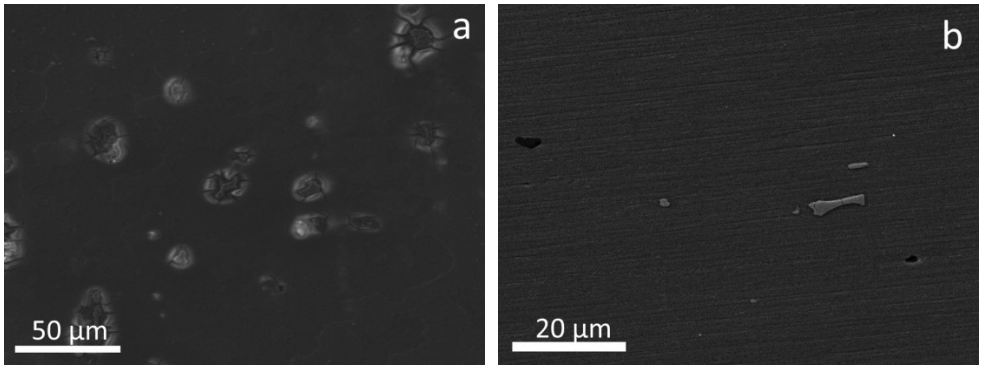

Figure 3. SEM micrograph of the surface AA7075 alloy after immersion for 24 h in: a) NaCl solution, b) NaCl solution + inhibitor.

Conclusion

Electrochemical measurements have shown that $NdCl_3$ in combination with cysteine, acting in synergy, plays a significant role in protecting the AA7075 alloy in 0.1M NaCl solution. Bode phase diagrams confirmed that the synergetic effect of cysteine and $NdCl_3$ showed good inhibitor protection. SEM analysis confirmed that tested corrosion inhibitors provide satisfying corrosion protection in NaCl solution after 24h, compared to inhibitor-free NaCl solution.

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Sinergetsko dejstvo neodimijuma i cisteina na leguri AA7075 u rastvoru NaCl

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Ispitano je sinergetsko dejstvo neodijumhlorida i cisteina u rastvoru NaCl. Odnos koncentracija ova dva inhibitora je bio 1:3 (neodijum:cistein). Otpornost na koroziju legure AA7075 ispitana je elektrohemijski pomoću spektroskopije elektrohemijske impendancije (EIS). Znatno veća otpornost u rastvoru inhibitora i manje vrednosti faznog ugla ukazuju na dobro inhibitorsko dejstvo neodimijuma i cisteina. Analiza površina uzoraka pre i posle korozionih ispitivanja, snimljenih pomoću skenirajuće elektronske mikroskopije (SEM/EDS), pokazuje da se posle 24h delovanja agensa korozije ne javljaju oštećenja AA7075 legure, što potvrđuje dobru zaštitu postignutu ispitivanim inhibitorima.

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Hemijsko inženjerstvo

Chemical Engineering

R-HI-1

Thermodynamic and transport properties of binary system of biomass-derived chemicals: eugenol + 4-propylguaiacol

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Abstract

Biomass has attracted a great deal of attention as a cheap and widespread renewable substitute for fossil fuels, the processing of which, in addition to biofuels, can provide various biomaterials and biochemicals. For successful design of biomass valorisation process, it is necessary to develop microkinetic models, which requires knowledge of thermodynamic and transport properties of all compounds involved in the process.[1]

Eugenol and 4-propylguaiacol are platform compounds that can be obtained from biomass and are widely used.[2] The densities of pure eugenol and 4-propyl guaiacol as well as their mixtures were measured at temperatures (293.15 – 413.15) K and pressures up to 60 MPa. The viscosities of the mentioned mixtures were measured at temperatures (288.15 - 373.15) K and atmospheric pressure. The obtained results showed that the behaviour of the mixtures did not differ significantly from that expected for ideal mixtures, which may be the result of a similar structure of the components of the mixture.

Introduction

It has long been known that the use of fossil fuels has a negative impact on the environment. In addition, problem isalso their limited sources, so all this together encouraged researchers to find an adequate replacement for fossil fuels. Biomass has attracted a lot of attention as a cheap and widespread renewable energy source that can be used in production of various biofuels, biomaterials and biochemicals. Bio-oils obtained by processing biomass are not at the same energy level as fossil fuels due to the higher share of oxidized functional groups. In order to increase their energy density, it is necessary to reduce the oxidized functional groups, which is done, for example by hydrodeoxygenation process.[1] In order for biomass valorisation to be effective, it is necessary to develop accurate microkinetic models that include all the phenomena that take place in the process of biomass valorisation. Evidently, the biomass processing design is impossible without knowledge of the thermodynamic and transport properties under different conditions of all compounds and mixtures that participate in it.

Eugenol and 4-propyl guaiacol are platform compounds that can be obtained from biomass and further converted to various added-value compounds.[2]The densities of pure eugenol and 4-propyl guaiacol as well as their mixtures were measured at temperatures (293.15 – 413.15) K and pressures up to 60 MPa. The viscosities of the mentioned mixtures were measured at temperatures (288.15 - 373.15) K and atmospheric pressure. The influence of

temperature, pressure and composition on the thermodynamic behaviour of the studied mixtures was analysed.

Results and Discussion

Viscosity of eugenol, 4-propylguaiacol and their binary mixtures (eugenol (1) + 4-propylguaiacol) was measured at temperatures (288.15 – 373.15) K and atmospheric pressure. The results showed expected dependence, viscosity decreases as temperature rises. Eugenol exhibited lower viscosity than 4-propylguaiacol and the mixture's viscosity exponentially decreases with the increase in the eugenol fraction in the mixture (Fig. 1).

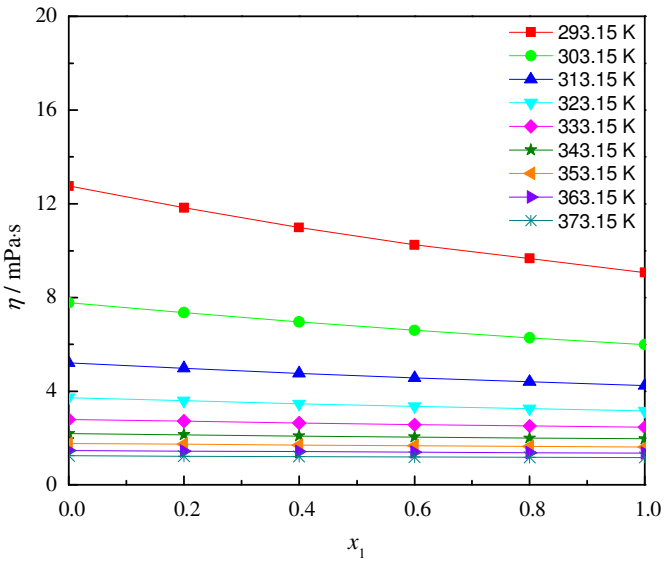

Figure 1. The dependence of viscosity of the mixtures eugenol (1) + 4-propylguaiacol on their composition at atmospheric pressure and various temperatures

Density of eugenol, 4-propylguaiacol and their binary mixtures (eugenol (1) + 4-propylguaiacol) was measured at temperatures (293.15 – 413.15) K and pressures up to60 MPa. As expected, the density increases with the increase in pressure and the decrease in temperature. Eugenol was denser than 4-propylguaiacol and consequently density of the studied mixture increased linearly with the rise of eugenol fraction in the mixture (Fig.2).

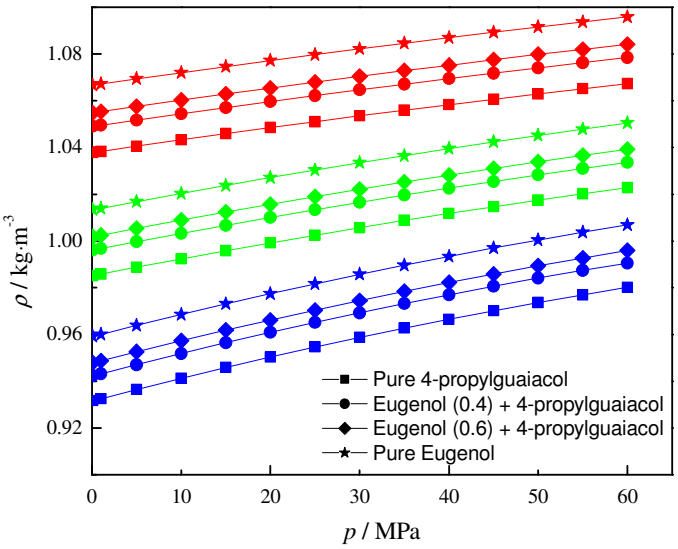

Figure 2. The dependence of density on pressure for pure eugenol, pure 4-propylguaiacol and their mixtures at temperatures: ***293.15 K, 353.15 K****, and* ***413.15 K***

The obtained results showed that the analysed behaviour of the mixtures was quite similar to that expected for ideal mixtures. The reason for this could be the similar structure of the studiedcompounds, unsaturated allyl group opposite to propyl group in 4-propylguaiacol.

Experimental Part

Eugenol and 4-propylguaiacol of high purity (> 99wt. %) were supplied by Sigma-Aldrich.

All mixtures were prepared using a Mettler Toledo AG 204 mass balance with the precision $1 \cdot 10^{-7}$ kg. The estimated standard uncertainty, u, in mole fraction, x, was less than $\pm 1 \cdot 10^{-4}$.

Dynamic viscosity(η) was measured using Stabinger viscometer SVM 3000/G2. The viscosity measurement is based on the measurement of torque and speed of the rotor immersed in the sample. In addition to the cylinder for measuring the dynamic viscosity, the device also has an oscillating U-tube for density measurement.Besides dynamic viscosity in the range (0.2 – 20000) mPa·s, this device also measures kinematic viscosity in the range (0.2 – 20000) $mm^2 \cdot s^{-1}$ and density within (0.65 – 3) $g \cdot cm^{-3}$, at temperatures starting from 20 K below room temperature to 378.15 K.[3]

Density at pressures(p) up to 60 MPa and temperatures (T) in the range (293.15 – 413.15) K were experimentally determined on Anton Paar digital vibrating tube density meter DMA HP.Since DMA HP measuring cell does not have a screen, density meter DMA 5000

was used to adjust and monitor its operating conditions. The cell temperature was controlled by an integrated Peltier thermostat and pressure was generated and controlled with a Pressure Generator model 50-6-15, High Pressure Equipment Co. Since The classic calibration procedure with one reference fluid, proposed by Comuñas et al. was applied.[4]

Termodinamička i transportna svojstva binarnog sistema komponenti dobijenih iz biomase: eugenol + 4-propilgvajakol

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Biomasa je privukla ogromnu pažnju kao jeftina i široko rasprostranjena obnovljiva zamena za fosilna goriva čijom preradom se, pored biogoriva, mogu dobiti različiti biomaterijali i biohemikalije. Za uspešno projektovanje procesa valorizacije biomase neophodno je razviti mikrokinetičke modele što zahteva i poznavanje termodinamičkih itransportnih svojstava svih jedinjenja koja učestvuju u procesu.[1]

Eugenol i 4-propilgvajakol su platformna jedinjenja koja se mogu dobiti iz biomase iimaju široku upotrebu.[2] Gustine čistih eugenola i 4-propilgvajakola kao i njihovih smeša su merene na temperaturama (293.15 – 413.15) K i pritiscima do 60 MPa. Viskoznosti pomenutih smeša su merene na temperaturama (288.15 – 373.15) K i atmosferskom pritisku. Dobijeni rezultati su pokazali da se ponašanje smeša ne razlikuje značajno od onog očekivanog za idealne smeše, što može biti rezultat slične strukture komponenti smeše.

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Application of predictive group contribution models on estimating viscosity of binary acetate + alcohol mixtures

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Abstract

Experimental data for viscosity of eight binary mixtures consisting of acetate and alcohol is used to test predictive models to calculate this transport property. Group contribution models UNIFAC-VISCO and ASOG-VISCO were tested and calculated viscosity values were compared with the measured ones though the values of the percentage deviations. The results showed very good agreement for the systems with ethyl acetate, with values for the percentage deviations below 3% for some temperatures. For systems with isoamyl acetate, percentage deviations vary greatly for different temperatures and go from 3% up to 25%.

Introduction

In order to design and develop the appropriate equipment or numerical calculations, it is necessary to have accurate and reliable data on chemical, physical and transport properties of pure solvents and their binary mixtures with other substances. Viscosity is one of the most important properties used in numerous chemical-engineering correlations for fluid flow analysis and mass and heat transfer calculations. These calculations should be based on reliable experimental data for a needed mixture, at a given temperature, pressure and composition. However, these data are often not available, so various models for calculating viscosity are used.

When modeling viscosity, it is important to take into account the limitations associated with individual approaches. The significance of the predictive approach is that the viscosity of the mixture can be calculated from a limited amount of data; data for pure components and interaction parameters between functional groups present in component molecules.

Predictive UNIFAC-VISCO [1,2] and ASOG-VISCO [3] models were tested to calculate viscosity of eight binary mixtures consisting of acetate and alcohol: ethyl acetate + 1-propanol, ethyl acetate + 1-butanol, isoamyl acetate + 1-propanol, isoamyl acetate + 1-butanol, isoamyl acetate + 1-hexanol, isoamyl acetate + isobutanol, isoamyl acetate + isopentanol and isoamyl acetate + terc-butanol.

Approach and models used

The advantage of using predictive models is that the viscosity of mixtures can be calculated based on knowledge of the viscosity of pure components and the contribution of the corresponding functional groups. The disadvantage of this approach is that the

contributions of individual groups must be very precisely determined in order to obtain satisfactory results. They are suitable for use under different conditions of temperature, pressure and composition. However, there is a possibility that the interaction parameters of certain groups present in the tested mixtures are not known. These parameters can be determined by using a number of similar systems and certain optimization techniques, which allows them later to be applied as purely predictive.

Group contribution models view fluid as a solution of the functional groups that the molecules of the mixture components consist of. The basic property of the group contribution model is additivity; it is considered that some physical property of the compound is the sum of the contributions of the functional groups that make it up. The contribution of one group is considered independent of the contribution of the other group, i.e. the place where the given group is in the molecule is neglected. The advantage of these models is that there are significantly fewer functional groups in the mixtures used in industry than the components of the mixtures.

The division of molecules into functional groups is different in different group contribution models. The accuracy of prediction increases with decreasing number of groups into which the molecule is divided and is greatest when the whole molecule is viewed as one functional group. In this way, the total number of groups grows, and if the whole molecule is viewed as one group, the group contribution model loses its meaning. Therefore, when dividing molecules into functional groups, it is necessary to find a balance between several requirements, and above all between the requirements for model accuracy and the requirements for the existence of a relatively small number of groups. The best-known group contribution models developed to predict viscosity are UNIFAC-VISCO [1,2] and ASOG-VISCO [3].

Modeling results

The quality of the models used in this paper to predict the viscosity of investigated binary systems was estimated by calculating the percentage deviation (*PD*) by the equation:

$$PD(\eta) = \frac{100}{m}\sum_{i=1}^{m}\left|\frac{\eta_{exp} - \eta_{cal}}{\eta_{exp}}\right|_i \qquad (1)$$

where η_{exp} and η_{cal} are the experimental and calculated viscosity values.

The percentage deviation values for both models at each temperature are given in Table 1.

Table 1. Viscosity prediction results for binary mixtures acetate (1) + alcohol (2) by UNIFAC-VISCO (U-V) and ASOG-VISCO (A-V) models.

T/(K)	*PD*/(%)							
	ethyl acetate + 1-propanol		ethyl acetate + 1-butanol		isoamyl acetate + 1-propanol		isoamyl acetate + 1-butanol	
	U-V	A-V	U-V	A-V	U-V	A-V	U-V	A-V

288.15	5.43	15.82	3.88	14.37	14.44	15.84	15.84	17.41
293.15	4.64	7.90	2.88	6.88	13.83	5.90	15.03	7.91
298.15	4.04	4.17	2.48	3.58	13.11	2.68	14.49	3.29
303.15	3.36	3.78	2.04	2.81	12.48	3.87	13.91	3.31
308.15	3.06	4.73	1.74	3.36	11.73	4.66	13.19	4.02
313.15	2.65	6.64	1.37	4.95	11.15	5.08	12.52	4.93
318.15	2.46	10.11	1.31	7.80	10.39	6.22	11.84	6.74
323.15	2.24	15.22	1.71	11.65	9.81	9.71	11.15	10.43

	isoamyl acetate + 1-hexanol		isoamyl acetate + isobutanol		isoamyl acetate + isopentanol		isoamyl acetate + terc-butanol	
	U-V	A-V	U-V	A-V	U-V	A-V	U-V	A-V
288.15	15.85	16.69	20.57	23.98	14.41	19.66		
293.15	15.06	8.45	19.23	14.03	13.27	10.52		
298.15	14.72	4.34	17.25	7.92	12.51	5.88		
303.15	14.39	3.18	15.82	5.80	11.75	4.69	25.24	11.85
308.15	13.81	3.50	14.69	6.02	10.76	4.97	21.97	9.74
313.15	13.12	4.42	13.75	7.20	9.80	5.86	19.01	9.38
318.15	12.73	6.47	13.12	9.70	8.80	7.59	16.48	10.51
323.15	12.16	9.74	11.99	13.36	7.84	10.80	14.20	13.29
328.15							12.21	18.57
333.15							9.39	25.26

UNIFAC-VISCO and ASOG-VISCO models were used in this paper as purely predictive models, since the interaction parameters between the groups present in the investigated substances can be found in the literature. Parameters are taken either from the original papers [1-3] or have been determined in our previous works [4,5].

Predictive models generally give poorer results in viscosity modeling, comparing to correlative models, which can be observed in our systems as well. For the tested systems with ethyl acetate, UNIFAC-VISCO gives much better results than ASOG-VISCO. For the mixtures with isoamyl acetate the *PD* values obtained with the UNIFAC-VISCO model are very high and this model cannot be used to calculate the viscosity of these systems.

Noticeable is the different behavior of percentage deviation with the temperature between two models. For the UNIFAC-VISCO model *PD* values decrease with the increase of the temperature, while for the ASOG-VISCO model the lowest values are present for the middle temperatures of the investigated temperature range. Although for the first and last temperature *PD* values are either similar or smaller for the UNIFAC-VISCO model, for the middle temperatures big differences are noticeable in favor of ASOG-VISCO model.

For the systems with isoamyl acetate values of percentage deviations are increasing with the increase of the chain length and branching of the alcohol molecule.

A comparison of the experimental and calculated values of the dynamic viscosity of the binary systems ethyl acetate + 1-propanol and isoamyl acetate + 1-hexanol is shown in Figure 1.

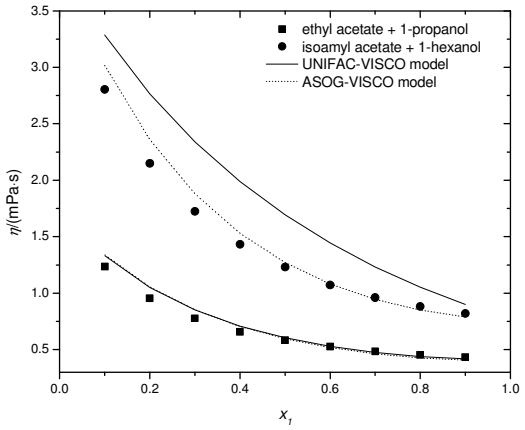

Figure 1. Comparison of experimental and calculated values of dynamic viscosity for systems ethyl acetate + 1-propanol and isoamyl acetate + 1-hexanol at 303.15 K.

Primena prediktivnih modela doprinosa grupa za izračunavanje viskoznosti binarnih smeša acetat + alkohol

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Eksperimentalni podaci za viskoznost osam binarnih smeša koje se sastoje od acetata i alkohola iskorišćeni su za testiranje prediktivnih modela za izračunavanje ovog transportnog svojstva. Ispitani su modeli doprinosa grupa UNIFAC-VISCO i ASOG-VISCO i izračunate vrednosti viskoziteta su upoređene sa izmerenim preko vrednosti procentualnih odstupanja. Rezultati su pokazali veoma dobro slaganje za sisteme sa etil acetatom, sa vrednostima procentualnih odstupanja ispod 3% za neke temperature. Za sisteme sa izoamil acetatom, procentualna odstupanja se veoma razlikuju po temperaturama i kreću se od 3% do 25%.

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Tekstilno inženjerstvo

Textile Engineering

R-TI-1

Adsorption of Congo Red as an indicator for the oxidized jute fabric's sorption properties

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This work aims to obtain jute fabrics with improved sorption properties that could be used as a novel solution for biodegraded land rehabilitation. For that purpose, raw jute fabric was oxidized with 0.4% sodium periodate ($NaIO_4$), while the adsorption of textile dye Congo Red (CR) was used as an indicator for fabrics' sorption properties. The kinetic study revealed that fabric oxidized for 60 min reached equilibrium dye adsorption after 270 min, while in the case of jute oxidized for 120 min, the equilibrium was attained 30 min faster. This behavior is ascribed to the better availability and higher content of functional groups (capable of binding CR) within fabric oxidized for 120 min than within those oxidized for 60 min. The above-mentioned could be also used as an explanation for the 35 and 50% higher adsorption capacities of fabrics oxidized for 60 and 120 min compared to the raw fabric, respectively. With increasing the initial concentration of CR from 25 up to 100 mg L^{-1}, the equilibrium adsorption increased up to 2.6 times.

Introduction

Over 40% of terrestrial ecosystems worldwide suffer from land degradation, a natural or human-influenced process that affects the functionality of the land. Biocrust carpet engineering has been proposed to fight land degradation and cyanobacteria as primary colonizers have been introduced as a potential solution. However, the rehabilitation takes a long time due to the lack of moisture during the initial phase. In this paper we prepared jute-based supports to provide the necessary water for the growth of the microbiota and to promote a sustainable relationship between microbiota and abiotic constituents in the degraded land surface. Namely, raw jute fabric was oxidized with 0.4% sodium periodate ($NaIO_4$) for 60 or 120 min to improve fabric sorption properties, whereby the adsorption of CR was used as an indicator. This selective oxidation agent lead to the conversion of cellulose hydroxyl groups on C2 and C3 atoms to aldehydes, wherein the ring cleavage occurred and 2,3-dialdehyde cellulose was formed [1].

Results and Discussion

Content of carboxyl (COOH) and aldehyde (CHO) groups in the jute fabrics

The oxidation of raw jute fabric with 0.4% $NaIO_4$ for different times was performed to introduce new functional groups, and hence, to improve the fabric sorption properties. The

results listed in Table 1 indicated that oxidations for 60 and 120 min (fabrics JO60 and JO120) led to an increase in the aldehyde group content by 1.8 and 2.1 times, respectively. On the other hand, applied periodate oxidations did not affect the content of COOH groups, Table 1. Considering the increased total content of COOH and CHO groups after oxidations, it is reasonable to assume that oxidized jute fabrics have improved sorption properties. In light of that, adsorption of CR was used to evaluate the sorption properties of jute fabrics.

Table 1. Content of functional groups within the jute fabric

	RJ	JO60	JO120
COOH	0.169	0.171	0.173
CHO	0.185	0.326	0.397
COOH + CHO	0.354	0.497	0.570

Effect of contact time on the adsorption of CR

A kinetic study was performed having in mind that, from the economic point of view, the contact time is the most important adsorption variable. According to the results presented in Figure 1, among all fabrics, RJ possessed the lowest adsorption capacity independently of the contact time, which is ascribed to the lowest availability and content of functional groups capable of binding CR, Table 1. After the oxidation with $NaIO_4$, the content of COOH and CHO groups increased, and therefore, the adsorption of CR increased. Fabric JO60 reached equilibrium adsorption of 4.05 mg g^{-1} after 270 min of contact time, while 30 min shorter adsorption time resulted in the highest adsorption (4.47 mg g^{-1}) of CR onto JO120.

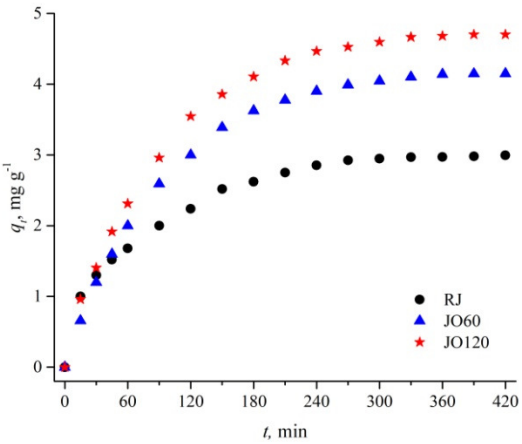

Figure 1. Effect of contact time on the CR adsorption onto jute fabric.

The influence of initial CR concentration on the fabric adsorption efficiency

The initial dye concentration in the solution plays an important role in the content of dye adsorbed per gram adsorbent. The adsorption capacity of differently treated fabric samples for CR present at different initial concentrations (25-100 mg L^{-1}) was investigated after a contact time of 270 min. From the results presented in Figure 2, it is evident that with increasing the initial concentration of CR from 25 to 100 mg L^{-1}, the equilibrium adsorption (q_e) increased by maximum of 2.6 times (JO120).

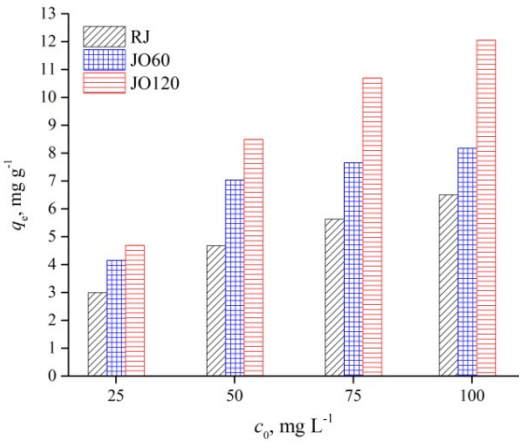

Figure 2. Effect of initial CR concentration on its adsorption onto jute fabrics.

Experimental Part

Adsorbents' Preparation and Characterization

The raw jute fabric (RJ) was oxidized with 0.4% sodium periodate ($NaIO_4$) solution for 60 or 120 min (oxidized fabrics' codes: JO60 and JO120, respectively) according to the procedure given in the literature [1]. The content of carboxyl (COOH) and aldehyde groups (CHO) was determined using the calcium-acetate method previously described by Ivanovska et al. [2].

Adsorption of CR

The adsorption experiments were carried out at a pH of 10.00 by varying the contact time and initial dye concentration at room temperature. A specimen of jute fabric (0.5 g) was immersed in 100 ml of CR solution containing 15 g L^{-1} NaCl and constantly shaken. The concentration of CR in aqueous solution was determined based on the UV-Vis (Shimadzu 1700 spectrophotometer) absorbance spectra at λ_{max} = 486 nm.

Adsorpcija Kongo crvenog kao indikatora sorpcionih svojstava oksidisane tkanine od jute

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Cilj ovog rada je dobijanje tkanine od jute sa poboljšanim sorpcionim svojstvima koja će se koristititi za rehabilitaciju degradiranog zemljišta. U tu svrhu, sirova tkanina jute oksidisana je 0,4% rastvora natrijum-perjodata ($NaIO_4$), dok je adsorpcija tekstilne boje Kongo crvenog (CR) korišćena kao indikator sorpcionih svojstava. Kinetička istraživanja pokazala su da je tkanina oksidisana tokom 60 minuta dostigla ravnotežnu adsorpciju boje nakon 270 minuta, dok je u slučaju tkanine od jute oksidisane tokom 120 minuta ravnoteža postignuta 30 minuta brže. Ovakvo ponašanje posledica je bolje dostupnosti i većeg sadržaja funkcionalnih grupa (sposobnih da vežu CR) unutar tkanine oksidisane tokom 120 minuta u odnosu na tkaninu oksidisanu tokom 60 minuta. Navedeno bi se moglo koristiti i kao objašnjenje za 35 i 50% veće adsorpcione kapacitete uzoraka tkanine oksidisanih tokom 60 i 120 minuta u poređenju sa sirovom tkaninom, redosledno . Sa povećanjem početne koncentracije CR sa 25 na 100 mg L^{-1}, ravnotežna adsorpcija se povećava do 2,6 puta.

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Hemija životne sredine

Environmental Chemistry

R-HŽS-1

Modifikovana otpadna prediva pamuka i pamuk/poliestra kao adsorbenti za uklanjanje organskih boja iz otpadnih voda

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U cilju dobijanja adsorbenata za uklanjanje organskih boja iz otpadnih voda, u okviru ovog rada su primenjene dve vrste industrijskih otpadnih materijala. Otpadna prediva pamuka i mešavine pamuk/poliestar modifikovana su korišćenjem smeše natrijum karboksimetil celuloze i letećeg pepela. Karakterizacija polaznih i modifikovanih prediva izvršena je skenirajućom elektronskom mikroskopijom i infracrvenom spektroskopijom sa Furijeovom transformacijom, dok je adsorpcija metilensko plavog i metil oranža primenjena za ispitivanje efikasnosti uklanjanja. Svi ispitivani uzorci pokazuju bolju efikasnost u uklanjanju metilensko plavog, a primenjena modifikacija povećava adsorpcionu efikasnost skoro dva puta. Pokazano je da se kombinovanjem dve vrste otpada, pamučnog prediva i letećeg pepela, dobijaju visoko efikasni adsorbenti za uklanjanje metilensko plavog iz vode.

Uvod

Organske boje predstavljaju jednu od najčešće detektovanih zagađujućih materija u industrijskim otpadnim vodama (iz tekstilne industrije, industrije kože, kozmetičke industrije i industrije papira). Neke od organskih boja pokazuju visok nivo biotoksičnosti, i mogu negativno uticati na zdravlje ljudi. Stoga je, od suštinskog značaja, uklanjanje boja iz otpadnih voda pre ispuštanja u recipijente [1,2]. Među standardnim metodama koje se koriste za prečišćavanje vode, jedna od najefikasnijih, a uz to i najjednostavnijih i najjeftinijih, je adsorpcija. Kao specifičan vid reciklaže, poslednjih godina se različiti, jeftini i lako dostupni otpadni materijali koriste za dobijanje adsorbenata. Ovakva ponovna primena otpadnih materijala dovodi do smanjenja troškova odlaganja otpada, uz istovremeno ispunjenje zahteva cirkularne ekonomije, održivog razvoja i očuvanja životne sredine. Stoga je u ovom radu ispitana mogućnost dobijanja efikasnih adsorbenata za uklanjanje boja iz vode, polazeći od otpadnih materijala dostupnih u Srbiji u velikim količinama. Leteći pepeo, dobijen iz termoelektrana kao sporedni proizvod, korišćen je za modifikaciju i poboljšanje adsorpcione efikasnosti prediva pamuka i mešavine pamuka i poliestra, koja su dobijena kao otpad iz tekstilne industrije. Metilensko plavo (MB) i metil oranž (MO) su primenjeni kao modeli katjonske i anjonske boje za ispitivanje adsorpcione efikasnosti nemodifikovanih i modifikovanih prediva. Takođe, ispitan je uticaj prisustva poliestarske komponente i primenjene modifikacije na adsorpcionu efikasnost.

Materijal i metode

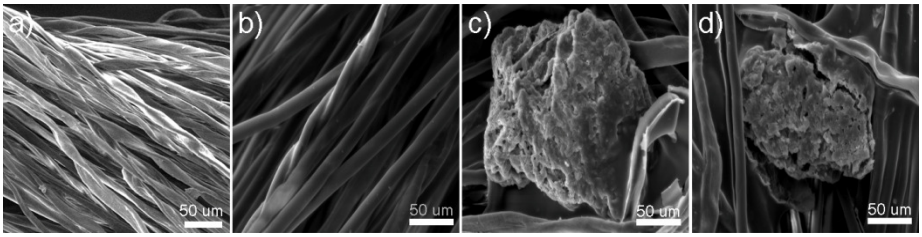
Otpadno pamučno predivo (P) i otpadna mešavina pamuk/poliestar (50 % pamuk-50 % poliestar) (P/PES) dobijeni su iz proizvodnih procesa tekstilne fabrike SIMPO Dekor (Vranje, Srbija). Modifikacija prediva (0,1 g) izvršena je u dva ciklusa. Odmereno predivo potopljeno je u 4 ml smeše 0,5 % vodenog rastvora natrijum karboksimetil celuloze i 0,1 g letećeg pepela, i nakon 10 minuta potapanja, predivo je sušeno 1h na 60 ^{o}C. Posle drugog ciklusa modifikacije, prediva su sušena na 60 ^{o}C, preko noći, a modifikovana prediva su obeležena kao P_{mod} i P/PES_{mod}, za modifikovani pamuk i pamuk/poliestar, redom. Morfološke karakteristike površine polaznih i modifikovanih uzoraka ispitane su skenirajućim elektronskim mikroskopom (SEM). Ispitivanje sadržaja funkcionalnih grupa na površini uzoraka prediva, izvršeno je metodom infracrvene spektrometrije sa Furijeovom transformacijom (FTIR). FTIR spektri uzoraka su snimljeni u opsegu talasnih brojeva 400–4000 cm^{-1}, sa rezolucijom 4 cm^{-1}. U cilju ispitivanja adsorpcione efikasnosti nemodifikovanih i modifikovanih prediva, izvršena je adsorpcija MB i MO. Uzorak prediva, mase 0,02 g, potopljen je u 20 ml vodenog rastvora boje, koncentracije 10 mg/dm^3. Adsorpcija je vršena u šaržnom sistemu, na sobnoj temperaturi uz konstantno mešanje (150 o/min) u trajanju od 3 h. Koncentracija boje nakon adsorpcije merena je korišćenjem spektrofotometra za vidljivu oblast. Efikasnost adsorpcije (AE, %) ispitivanih prediva u uklanjanju organskih boja izračunata je primenom sledeće jednačine:

$$AE = 100 - \frac{C_e \cdot 100}{C_0}$$

gde su C_e i C_0 ravnotežna, odnosno početna koncentracija boje u mg/dm^3.

Rezultati i diskusija

Morfologija i struktura ispitivanih uzoraka prikazane su na Slici 1. Primećuje se spiralna uvijenost pamučnih vlakana, kao i nehomogenost i hrapavost njihove površine (Slika 1a).



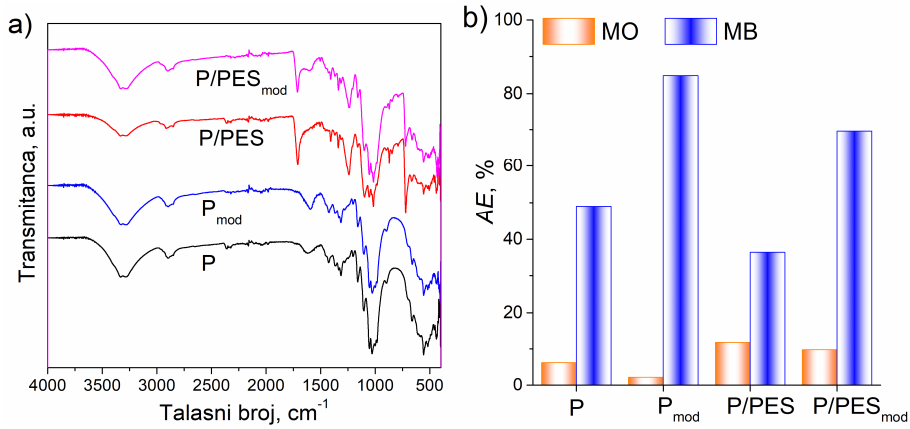
Slika 1. SEM fotografije a) P, b) P/PES, c) P_{mod} i d) P/PES_{mod}

Na Slici 1b, koja pokazuje nemodifikovano predivo pamuk/poliestar, pored pamučne komponente uočava se prisustvo i poliestarskih vlakana sa jednoličnom cevastom strukturom i glatkom površinom. Leteći pepeo je isprepletan između vlakana prediva (Slika 1c i 1d) i vezan za njih zahvaljujući dodatku natrijum karboksimetil celuloze.

FTIR spektri (Slika 2a), prikazuju sadržaj funkcionalnih grupa koje mogu predstavljati aktivna mesta za adsorpciju na površini ispitivanih uzoraka. Prisustvo široke trake u

opsegu 3350-3250 cm^{-1} kod svih uzoraka, potiče od vibracija istezanja O-H veze u hidroksilnoj grupi. Dva pika na oko 2900 cm^{-1} i 2850 cm^{-1} potiču od asimetričnih i simetričnih vibracija C-H veze u metil ili metilenskoj grupi molekula celuloze [3]. Karakteristične trake na spektru nemodifikovanih i modifikovanih uzoraka, koje se nalaze na oko 1600 cm^{-1} i u opsegu 1000-1160 cm^{-1} mogu biti posledica vibracija istezanja C=O i C-O veza u celulozi iz pamučne komponente [3]. FTIR spektri prediva P/PES i P/PES_{mod} imaju, u odnosu na spektre pamučnih prediva, dodatne pikove na 1710 cm^{-1} i 1240 cm^{-1} što ukazuje na prisustvo estarske grupe, dok pik na 1505 cm^{-1} potiče od vibracija aromatičnih prstenova u poliestarskim lancima [4]. Može se primetiti da primenjena modifikacija ne dovodi do promena u sadržaju grupa.

Efikasnost ispitivanih uzoraka u uklanjanju MO i MB iz vodenih rastvora prikazana je na Slici 2b. Svi ispitivani materijali pokazuju bolju adsorpcionu efikasnost u uklanjanju katjonske boje, zahvaljujući prisustvu hidroksilnih i karboksilnih grupa na površini pamučnih vlakana. Takođe, prisustvo poliestarske komponente ima negativan uticaj na efikasnost adsorpcije katjonske boje, dok neznatno povećava adsorpciju anjonske boje. Dobijeni rezultati ukazuju da primenjena modifikacija povećava efikasnost materijala za adsorpciju katjonske boje (MB), dok se efikasnost adsorpcije anjonske boje (MO) smanjuje.



Slika 2. FTIR spektri (a) i adsorpciona efikasnost (b) ispitivanih uzoraka

Zaključak

Modifikacijom prediva pamuka i mešavine pamuk/poliestar u prisustvu smeše natrijum karboksimetil celuloze i letećeg pepela dobijeni su efikasni adsorbenti za uklanjanje katjonske boje iz vodenog rastvora. Veća efikasnost u uklanjanju katjonske boje, i kod nemodifikovanih i kod modifikovanih uzoraka, može biti posledica prisustva hidroksilnih i karboksilnih grupa na površini pamučne komponente, dok prisustvo estarskih grupa na površini poliestarske komponente doprinosi neznatnom povećanju efikasnosti adsorpcije anjonske boje. Adsorpciona efikasnost, od preko 80 % za uklanjanje metilensko plavog, dobijena za modifikovano otpadno pamučno predivo, ukazuje da se, polazeći od dve različite vrste industrijskih otpadnih materija, mogu dobiti efikasni adsorbenti za uklanjanje katjonskih boja iz otpadnih voda.

Modified waste cotton and cotton/polyester yarns as adsorbents for removal of organic dyes from wastewater

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In order to obtain adsorbents for the removal of organic dyes from wastewater, two types of industrial waste materials were used in this study. Waste cotton and cotton/polyester yarns were modified using a mixture of sodium carboxymethyl cellulose and fly ash. Characterization of the unmodified and modified yarns was performed by scanning electron microscopy and infrared spectroscopy with Fourier transform, while the adsorption of methylene blue and methyl orange was used to examine the removal efficiency. All tested samples show better efficiency in removing methylene blue, and applied modification increase the adsorption efficiency almost twice. It has been shown that by combining waste cotton yarn and fly ash, highly efficient adsorbents for removal of methylene blue from water can be obtained.

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R-HŽS-2

Adsorption of selected pharmaceuticals on LDPE, PA, and PET microplastics

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Unappropriated disposing of unused drugs leads to an increase in their concentration in the environment. Furthermore, wastewater treatment plants are not sufficient to prevent the transport of drugs. Microplastics (MPs), which are also recognized as important pollutants, can be divided into primary and secondary. The primary MPs are produced for commercial purposes, while the secondary MPs are formed by the decomposition of plastic residues. The hydrophobic nature and large specific surface area of MPs facilitate pollutants binding. Animals misunderstand MPs for food and consume it, which could have harmful health impacts because both MPs and adsorbed pollutants are ingested. In this paper, the adsorption of the selected drugs - azithromycin, carbamazepine, sulfamethoxazole, and diclofenac on low-density polyethylene (LDPE), polyamide (PA), and poly(ethylene terephthalate) (PET) microplastics are presented. The experiment showed that drugs bind best to PA and that azithromycin has the highest binding affinity.

Adsorpcija odabranih lekova na LDPE, PA i PET mikroplastici

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Neadekvatno odlaganje neiskorišćenih lekova dovodi do povećanja njihove koncentracije u životnoj sredini. Pored toga, postrojenja za prečišćavanje otpadnih voda nisu dovoljna barijera za sprečavanje transporta lekova. Mikroplastika (MP), koja je takođe detektovana kao bitan polutant, može se podeliti na primarnu i sekundarnu. Primarna se proizvodi za komercijalne svrhe, a sekundarna nastaje razgradnjom plastičnih ostataka. Hidrofobna priroda i velika specifična površina MP olakšava adsorpciju polutanata na ove materijale. Životinje mešaju MP sa hranom i unose je u svoj organizam, što može imati negativni uticaj na njihovo zdravlje, jer se tako unose i MP i adsorbovani polutanti. U ovom radu je prikazana adsorpcija odabranih lekova - azitromicina, karbamazepina, sulfametoksazola i diklofenaka na sledećim vrstama mikroplastike - polietilenu niske gustine (LDPE), poliamidu (PA) i poli(etilen tereftalatu) (PET). Eksperiment je pokazao da se lekovi najbolje vezuju za PA, kao i da azitromicin ima najveći afinitet vezivanja.

Uvod

Prema najnovijim istraživanjima mikroplastika (MP) je označena kao polutant čije prisustvo u životnoj sredini intenzivno raste. MP je pronađena u zemljištu, površinskim vodama, lagunama i estuarima, priobalnim regionima mora, arktičkoj slatkoj vodi, ledu i okeanima [1]. Svaki komad plastike prečnika od 100 nm do 5 mm definiše se kao MP [2]. Ona se u životnoj sredini može naći u raznolikim oblicima npr. u obliku kuglica, nepravilnih fragmenata ili vlakana [3]. Sintetički plastični peleti, perle, vlakna i praškovi proizvedeni u komercijalne svrhe poznati su kao primarna MP [4]. Sekundarna MP nastala je razgradnjom plastičnih ostataka pod dejstvom različitih fizičkih, hemijskih i bioloških faktora kao što je UV zračenje, degradacija mikrobima, mehanička abrazija, rad talasa i slično. Zahvaljujući hidrofobnoj prirodi i velikoj specifičnoj površini MP može vezati i transportovati organske zagađujuće materije u vodenoj sredini. Akumulacija lekova na MP, koju životinje unose zajedno sa hranom, može da ima negativan uticaj na živi svet [5].

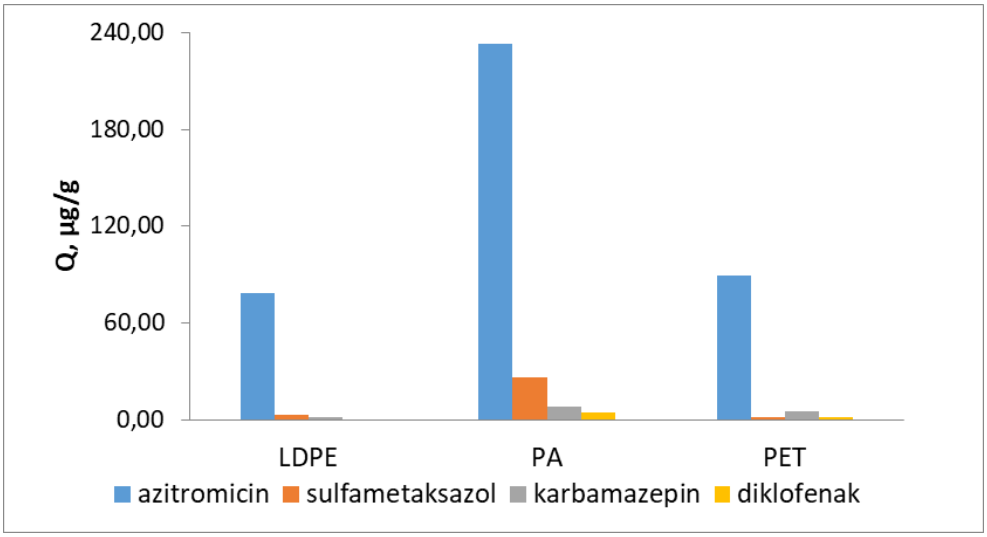
U ovom radu ispitivana je adsorpcija odabranih lekova na MP. Tipovi MP koji su korišćeni su poli(etilen tereftalat) (PET), polietilen niske gustine (LDPE) i poliamid (PA). Odabrani lekovi su antiepileptik karbamazepin, antibiotici sulfametoksazol i azitromicin i analgetik diklofenak. Karbamazepin je jedan od najčešće detektovanih lekova u akvatičnoj sredini [6]. Azitromicin i diklofenak su se nalazili na prethodnim verzijama tzv. "liste posmatranja" (Watch List under the European Water Framework Directive), a sulfametoksazol se nalazi na trenutnoj verziji liste. Azitromicin je široko korišćen kao dopunska terapija u lečenju obolelih od virusa COVID-19 [7], pa je njegovo prisustvo u životnoj sredini povećano i iz tog razloga je izabran za analizu.

Eksperimentalni deo

Efikasnost adsorpcije odabranih polutanata ispitivana je u šaržnom sistemu sa konstantnim mešanjem od 150 o/min tokom 48 h. Mase čestica MP su bile 0,1167 g, 0,0398 g, 0,1106 g za LDPE, PA i PET respektivno. One su potopljene u vodene rastvore smeše lekova zapremine 20 ml, koncentracije 500 ppb i pH ≈ 6. Nakon adsorpcije, svi uzorci su profiltrirani kroz PVDF filtere, 0,45 mm. Koncentracija ispitivanih lekova je analizirana metodom tečne hromatografije u sprezi sa tandem-masenom spektrometrijom (LC-MS/MS) - Dionex UltiMate 3000® LC system u sprezi sa LTQ XL linearnim jonskim trapom (Thermo Fisher Scientific, Waltham, MA, USA). Korišćena je kolona Zorbax Eclipse XDB-C18, (75 mm × 4,6 mm × 3,5 μm), Agilent Technologies, USA. Mobilna faza se sastojala od 75% metanola i 25% mravlje kiseline (0,1% vodenog rastvora) protoka 0,3 ml/min. Metoda je bila izokratska. Jonizacija elektrosprejom se koristila u pozitivnom režimu. Za svaki analit praćena je odgovarajuća reakcija fragmentacije protonovanog molekulskog jona - azitromicin (749→591), sulfametoksazol (254→188), karbamazepin (237→194) i diklofenak (296→278).

Rezultati i diskusija

Rezultati, prikazani na slici 1, pokazuju da PA ima izrazito veći kapacitet sorpcije odabranih lekova u poređenju sa LDPE i PET. Razlog tome može biti to što on jedini poseduje amidnu grupu (donor protona), koja omogućava formiranje vodoničnih veza sa karbonilnom grupom lekova (akceptor protona) [8]. Takođe, poroznost ove vrste plastike može uticati na adsorpciju što je pokazano u ekperimentima pronađenim u literaturi [9].



Slika 1. Adsorpcija lekova na MP

Tabela 1. Fizičko-hemijski parametri odabranih lekova

Naziv leka	Mr	logKow	pKa
azitromicin	749	4,02	8,50
sulfametoksazol	253	0,89	1,83
karbamazepin	236	2,45	13,90
diklofenak	295	4,51	4,15

Među odabranim lekovima azitromicin ima najveći afinitet vezivanja za mikroplastiku, što je u skladu sa visokom vrednošću logKow (tabela 1) i pretpostavkom da je hidrofobnost organskih polutanata bitan faktor koji utiče na stepen adsorpcije na MP. Sa druge strane, hidrofobnost ne objašnjava u potpunosti razlike u kapacitetima adsorpcije ostalih lekova. Na primer, primećeno je da se diklofenak slabo vezuje za MP i pored visoke vrednosti logKow. Pored hidrofobnosti, elektrostatička privlačenja/odbijanja mogu imati bitnu ulogu

pri adsorpciji. Za većinu plastičnih materijala tačka nultog naelektrisanja (pH_{PZC}) je oko 4 [8], tako da je površina MP pri odabranim uslovima negativno naelektrisana. U zavisnosti od eksperimentalne vrednosti pH, lekovi mogu biti prisutni u različitim oblicima: kao katjoni, zwitter-joni ili anjoni. Na pH vrednosti ~ 6 diklofenak je prisutan u anjonskom obliku i najverovatnije dolazi do elektrostatičkog odbijanja sa MP.

Zaključak

Mikroplastika je prepoznata kao nosilac različitih organskih kontaminanata i raste zabrinutost obzirom na njihov loš potencijalni uticaj na ekosistem i ljudsko zdravlje. U ovom radu ispitivana je adsorpcija četiri vrste lekova na tri vrste mikroplastike. Rezultati su pokazali da se stepen adsorpcije lekova razlikuje na različitim vrstama mikroplastike. Svi ispitivani lekovi su imali najveći afinitet prema PA, verovatno zbog formiranja vodoničnih veza. Azitromicin je imao najveći afinitet vezivanja, što se može pripisati njegovoj visokoj vrednosti koeficijenta logKow. Međutim, iako takođe ima visoku vrednost koeficijenta logKow, diklofenak se veoma slabo vezao za MP, što implicira da i elektrostatičke interakcije imaju ulogu u adsorpciji lekova na MP.

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