Srpsko hemijsko društvo

Serbian Chemical Society

59. Savetovanje
Srpskog hemijskog društva

KRATKI IZVODI RADOVA

KNJIGA RADOVA

59th Meeting of the Serbian Chemical Society

Book of Abstracts
Proceedings

Novi Sad 1. i 2. jun 2023. godine
Novi Sad, Serbia, June 1-2, 2023

CIP- Каталогизација у публикацији
Народна библиотека Србије, Београд

59. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA,
Novi Sad, 1. i 2. jun 2023.
KRATKI IZVODI RADOVA/KNJIGA RADOVA
59th MEETING OF THE SERBIAN CHEMICAL SOCIETY
Novi Sad, Serbia, 1-2 June 2023
BOOK OF ABSTRACTS/PROCEEDINGS

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

Glavni i odgovorni urednik/ Editor
Daniela Šojić Merkulov
Uređivački odbor/Editorial Board
Suzana Jovanović-Šanta, Stanislava Olić Ninković, Ksenija Pavlović, Aleksandar Oklješa

Priprema za štampu i štampa/Prepress and printing
Razvojno-istraživački centar grafičkog inženjerstva Tehnološko-metalurškog fakulteta, Beograd / Research and Development Centre of Printing Engineering, Belgrade

Tiraž/ Circulation
30 primeraka/ 30 copies printing

ISBN 978-86-7132-081-8

Naučni odbor

Scientific Committee

Daniela Šojić Merkulov, predsednik/chair

Dušan Sladić
Vesna Mišković Stanković
Olgica Nedić
Dragica Trivić
Slađana Alagić
Snežana Rajković
Aleksandar Bojić
Dušanka Milojković Opsenica
Dejan Opsenica
Maja Radetić
Branka Petković
Ljiljana Vojinović Ješić
Igor Opsenica
Milan Vraneš
Biljana Šmit
Sanja Panić
Jovana Francuz
Ivan Ristić
Milena Krstić
Vesna Despotović
Dragana Tomašević Pilipović
Marija Nikolić
Branislav Šojić
Tamara Premović

Organizacioni odbor

Organising Committee

Suzana Jovanović-Šanta, predsednik/chair

Srđan Miletić
Zorica Stojanović
Bojana Srećo Zelenović
Ksenija Pavlović
Aleksandar Oklješa
Mirjana Radanović
Tamara Ivetić
Stanislava Olić Ninković
Danica Jović
Mirjana Petronijević
Ružica Ždero Pavlović
Sofija Bekić
Snežana Papović
Jelena Bajac
Ana Đurović
Tatjana Jurić
Tatjana Majkić
Jelena Tanasić
Tijana Marjanović
Marija Kostić

Savetovanje je podržalo /*Supported by*

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

Ova knjiga sadrži kratke izvode
četiri plenarna predavanja (PP),
dva predavanja dobitnika Medalje SHD (MP),
tri predavanja po pozivu (PPP),
devedeset šest saopštenja (obima jedne stranice) i
pet radova (obima od najmanje četiri stranice),
prihvaćenih za prezentovanje na
59. Savetovanju Srpskog hemijskog društva.

This book contains abstracts of
four plenary lectures (PP),
two lectures of SCS Medal awardees (MP),
three invited lectures (PPP),
ninety-six abstracts and
five papers accepted for presentation at
the 59th Meeting of the Serbian Chemical Society.

SADRŽAJ/CONTENTS

Plenarna predavanja
Plenary lectures

Predavanja po pozivu
Invited lectures

Predavanja dobitnika medalje SHD za pregalaštvo i uspeh u nauci

Lectures by the winners of the SCS medal for achievement and success in science

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

Neorganska hemija/Inorganic Chemistry

Organska hemija/ Organic Chemistry

Teorijska hemija/Theoretical Chemistry

Fizička hemija/Physical Chemistry

Hemija životne sredine/Environmental Chemistry

Hemijsko inženjerstvo/Chemical Engineering

Hemija i tehnologija materijala/Chemistry and Technology of Materials

Hemija i tehnologija hrane/Chemistry and Technology of Food

Knjiga radova/Proceedings

Analitička hemija/Analytical Chemistry

Hemija životne sredine/Environmental Chemistry

Hemijsko inženjerstvo/Chemical Engineering

Hemija i tehnologija materijala/Chemistry and Technology of Materials

KRATKI IZVODI RADOVA

Short abstracts

Plenarna predavanja

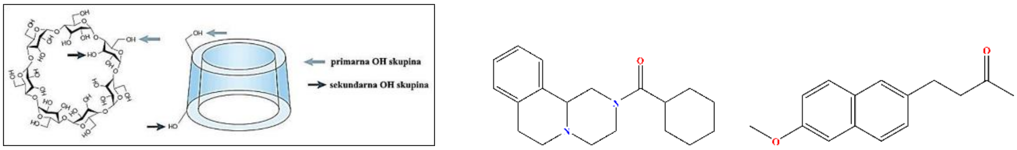
Plenary Lectures

PP-1

Drug/cyclodextrin supramolecular complexes with enhanced functionality

Nives Galić
University of Zagreb - Department of Chemistry, Faculty of Science, Zagreb, Croatia

To be pharmacologically active, all drugs must be soluble in water to some extent, and most of them should be lipophilic to penetrate biological membranes. The water solubility depends on the drug structure, but also on the drug formulation. Different technologies and methods are continuously developed to improve the solubility of poorly soluble drugs, including drugs into macrocycles such as cyclodextrins (CDs).[1] CDs are cyclic oligomers composed of glucopyranose units connected through glycosidic α-1,4 bonds. Their structures resemble a truncated cone having a narrow rim, a wide rim and a cavity (Figure 1). Praziquantel (PZQ) and nabumetone (NAB) are, according to a biopharmaceutical classification system (BCS) class II drugs which are characterized by good permeability and poor solubility. Due to their low aqueous solubility, large oral doses are required, which can be efficiently solved by complexation of drugs with (CDs).



β-cyclodextrin praziquantel nabumetone

Figure 1. Chemical structures ofβ-cyclodextrin and poorly soluble drugs

The investigation of drug/cyclodextrin complexes was conducted using UV-Vis spectroscopy, spectrofluorimetry, calorimetry, LC-HRMS/MS, NMR spectroscopy and molecular modelling. The results obtained for PZQ and NAB complexes with β-cyclodextrin and its derivatives, namely hydroxypropyl-β-CD (HPβCD), sulfobutylether-β-CD (SBEβCD) and randomly methylated β-cyclodextrin (RMβCD) are presented. The enhancement of the aqueous solubility of both drugs was achieved. HRMS, NMR and molecular modelling confirmed the formation of 1:1 inclusion complex. Furthermore, the influence of CDs on PZQ stability was investigated in solution (HCl, NaOH, H_2O_2) and the solid state (accelerated degradation, photostability) by UPLC-DAD/MS.

1. T. Kezele Špehar, M. Pocrnić, D. Klarić, B. Bertoša, A. Čikoš, M. Jug, J. Padovan, S. Dragojević, N. Galić, Investigation of praziquantel/cyclodextrin inclusion complexation by NMR and LC-HRMS/MS: mechanism, solubility, chemical stability and degradation products, *Mol. Pharm.* **2021**, 18, 4210.

PP-2

IR laser-induced ablative deposition of polymer composites

Jadranka Blazhevska Gilev

Faculty of Technology and Metallurgy, Ss. Cyril and Methodius University in Skopje,
Rugjer Boskovic 16, 1000 Skopje, R.n. Macedonia

Polymer composite films have attracted much attention because of their widespread applications. IR laser-induced ablative deposition are promising in view of the fabrication of polymers containing polar groups that can serve as protective layers to different nano-bodies (metals, metal chalcogenide's, conductive polymer nanocomposites carbon-based nanofillers, such as graphene, carbon nanotubes and carbon nanoribbons. This specific process occurs within a temperature jump and is controlled by kinetic rather than thermodynamic polymer degradation. It is feasible through multiple-photon absorption of energy-poor infrared photons, which leads to high vibrational excitation density in the polymer and high heating and cooling rates (respectively, $\sim 10^{6-11}$ and $\sim 10^{3-6} Ks^{-1}$). We have examined IR laser-induced ablative deposition with poly (vinyl acetate) (PVAc), poly(vinyl chloride) (PVC), poly(vinyl chloride-co-vinyl acetate) P(VC/VAc), poly(vinyl acetate) loaded with Fe and Cu particles, poly(ethylene-co-acrylic acid)zinc salt (PEAZn), poly(phenylene ether-sulfone) (PES) to establish its specific features and differences from conventional pyrolysis. It was of interest to us to continue our previous effort on pulsed laser ablation of polymer composites and we focused on nanocomposites from graphene incorporated into acrylic/methacrylic matrices.

Nanocomposites based on poly (butylacrylate-co-methyl methacrylate) and graphene were ablated with IR CO_2 laser using an incident fluence of up to 7 Jcm^{-2}. This resulted in the deposition of thin composite films with graphene sheets that were very well distributed in the polymer matrix. Graphene/noble metal substrates for surface enhanced RAMAN scattering (SERS) possess synergistically improved performance, due to the strong chemical enhancement mechanism accounted to graphene and the electromagnetic mechanism raised from the metal nanoparticles. In attempts to bring light to the effect of the quality of graphene on the effect of noble metal nanoparticles characteristics on the SERS performance, in this work, two different graphene oxides were selected, slightly oxidized GOS (20%) with low aspect ratio (1000) and highly oxidized (50%) GOG with a high aspect ratio (14,000). GO and precursors for noble metal nanoparticles (NP) simultaneously were reduced, resulting in rGO decorated with AgNPs and AuNPs. The graphene characteristics affected the size, shape, and packing of nanoparticles. The oxygen functionalities actuated as nucleation sites for AgNPs, thus GOG was decorated with a higher number and smaller size AgNPs than GOS. Oppositely, AuNPs preferred bare graphene surface, thus GOS was covered with smaller size, densely packed nanoparticles, resulting in the best SERS performance. Fluorescein in a concentration of 10^{-7} M was detected with enhancement factor of 82×10^4. This work demonstrates that the selection of graphene is an additional tool toward powerful SERS substrates.

PP-3

Modern chemical and biochemical approaches towards identification of anticancer and drug resistance preventing steroidal agents

Erzsébet Mernyák[1], Rebeka Jójárt[1], Henrietta Ágoston[1], Tamás Hlogyik[1], Zita Tamási[1], Csilla Laczka[2], Réka Rigó[2], Vivien Resch[3], Gábor Paragi[4,5], Renáta Minorics[6], István Zupkó[6], Tea Lanisnik-Rizner[7]

[1]Department of Inorganic, Organic and Analitical Chemistry, University of Szeged, Dóm tér 8, H-6720 Szeged, Hungary
[2]Drug resistance research group, Institute of Enzymology, Research Centre for Natural Sciences, Magyar tudósok körútja 2, H-1117 Budapest, Hungary
[3]Department of Medicinal Chemistry, University of Szeged, Dóm tér 8, H-6720 Szeged, Hungary
[4]Institute of Physics, University of Pécs, Ifjúság útja 6, H-7625, Pécs, Hungary; paragi@sol.cc.u-szeged.hu
[5]Department of Theoretical Physics, University of Szeged, Tisza Lajos krt. 84-86, H-6720, Szeged, Hungary
[6]Institute of Pharmacodynamics and Biopharmacy, University of Szeged, Eötvös u. 6, H-6720 Szeged, Hungary
[7]Institute of Biochemistry and Molecular Genetics, Faculty of Medicine, University of Ljubljana, 1000 Ljubljana, Slovenia

Modern transition metal-catalyzed synthetic methodologies revolutionized organic chemistry. Utilization of these innovative approaches in drug design might lead to novel drug candidates with special biological activities. We have recently described halogenations and microwave-assisted Pd-catalyzed cross couplings at the A-ring of the hormonally inactive 13α-estrone. Additionally, chelation-directed ortho or meta functionalizations were performed. The majority of our recently synthesized A-ring modified 13α-estrone derivatives proved to be biologically active. Certain potent inhibitors of established anticancer drug targets, namely 17β-hydroxysteroid dehydrogenase 1 (17β-HSD1), steroid sulfatase (STS), OATP2B1 or AKR1C1–3 have been identified, and important structure-activity results appeared. Highly desirable red-emitting fluorophores, amenable for biomolecule labeling have also been synthesized. We suppose that development of novel fluorescent labeled derivatives will provide valuable information concerning the biological behavior of the compounds.

This work was supported by the National Research, Development and Innovation Office-NKFIH through projects OTKA SNN 124329 and OTKA139323 to E.M. and projects N1-0066 and N1-0234 from the Slovenian Research Agency to T.L.R.

PP-4

Cholinesterase inhibitors as drugs for Alzheimer's disease

Anita Bosak
Institute for medical research and occupational health, Zagreb, Croatia

Alzheimer's disease (AD) is a neurodegenerative disease with a complex pathophysiology, which despite the significant progress in the field, remains unclear. During the years, a few hypotheses to explain the disease’s progress were developed. The most widespread is cholinergic hypothesis, which assumes that memory impairments in AD are associated with decreased brain levels of the neurotransmitter acetylcholine leading to decline in memory, problems with communication, memory, orientation and judgment. In line with this hypothesis, the inhibition of enzymes involved in acetylcholine breakdown, acetylcholinesterase and butyrylcholinesterase, represents the mainstream in treatment of neurodegenerative diseases associated with declined levels of acetylcholine. Although the complex and multi-layered pathophysiology of AD led to redirecting the ‘magic bullet’ concept of treatment strategy toward the „multi-target-directed ligands“ concept, cholinesterase inhibition remains the most desirable trait of any potential drug candidate. Compounds based on a quinoline structure and compounds with carbamate functionality represent a very promising structural base for development of MTDL compounds due to their high inhibition potency towards human cholinesterases, and ability to act as metal chelators and inhibitors of beta secretase 1 as an additional beneficial activity.

Acknowledgment: Supported by the CSF grant No. IP-2020-02-9343 and by MSTDI of RS Contract No. 451-03-47/2023-01/200026.

Predavanja po pozivu

Invited Lectures

PPP-1

Novi izazovi u modernoj teoriji hemijske veze

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

Hemijska veza predstavlja jedan od centralnih pojmova u hemiji. Teorija hemijske veze se i dalje aktivno razvija, iako je Luis (Lewis) pre više od jednog veka postavio osnove modernog opisa hemijske veze. U uvodnom delu izlaganja biće predstavljeni osnovni koncepti klasične teorije valentne veze (valence bond, VB). Na primeru serije MX (M = Cu, Ag, Au; X = F, Cl, Br) biće prikazano koji su izazovi u opisu hemijskog vezivanje u okviru VB teorije. Naše istraživanje je pokazalo da vezivanje u MX sistemima dominantno dolazi od σ veze, koja pokazuje značajan karakter vezivanja putem pomaka naelektrisanje (Charge-Shift Bonding, CSB). Nađeni CSB karakter se javlja kao posledica odbojih interakcija između *m*p slobodnih elektronskih parova na atomima halogena i popunjenih (*n*-1) d orbitala na atomima metala. Dobijeni rezultati pokazuju da između atoma u MX molekulima postoji i značajno π vezivanje, koje se javlja kao posledica dativne π veze nastale doniranjem elektrona iz *m*p slobodnih elektronskih parova na atomima halogena u nepopunjene *n*p orbitale atoma metala.

New challenges in modern chemical bonding theory

Slavko Radenković[1]
[1] *University of Kragujevac, Faculty of Science, Kragujevac, Republic of Serbia*

The chemical bond is a cornerstone concept in chemistry. The theory of the chemical bond is still an evolving field, although the foundation of modern understanding of the chemical bonding was put forward by Lewis more than 100 years ago. A brief overview of the basic concepts of classical valence bond (VB) theory will be presented. A series of coinage-metal halides (MX, M = Cu, Ag, Au; X = F, Cl, Br) was selected as the study case showing all challenges in understanding the nature of chemical bond within the modern VB theory. It was shown that the bonding in coinage-metal halides is dominated by σ bond, which exhibits a significant Charge-Shift Bond (CSB) character. This CSB character originates from the repulsion between the *m*p lone pairs of the halogen atom and the filled semi-core (*n*-1) d pairs of the metal. In addition, our analysis revealed that all MX dimers display secondary though significant π bonding character, which comes from a dative π bond created by donation of a *m*p lone pair of the halogen atom into a vacant *n*p valence orbital of the metal.

Acknowledgment: Authors thanks the Ministry of Education, Science and Technological Development of the Republic of Serbia (Agreement No. 451-03-47/2023-01/200122).

PPP-2

Biopolimeri iz obnovljivih izvora – hemijska modifikacija i primena

Milica P. Rančić
[1] *Univerzitet u Beogradu – Šumarski fakultet, Beograd, Srbija*

Sve veća zabritutost za ekologiju i ekonomiju, zajedno sa ograničenim petrohemijskim resursima, izazvala je nagli porast istraživanja i razvoja biopolimera kako bi se sadašnja ekonomija zasnovana na fosilnim resursima zamenila održivijom zasnovanom na obnovljivim izvorima. Implementacija sistema cirkularne ekonomije i sve veći fokus na minimiziranju odlaganja ne-biorazgradivih materijala doprinose očuvanju životne sredine. Kompoziti na bazi lignoceluloznih materijala dobijaju veliku pažnju poslednjih godina jer su obnovljivi, biorazgradivi i često ekološki prihvatljivi u poređenju sa sintetičkim materijalima. Uspešno uvođenje celuloze ili lignina u proizvodnju novih biomaterijala u velikoj meri zavisi od njihove strukture i čistoće, odnosno načina izolovanja. Njihova primena je klasifikovana u dve grupe: (i) bez hemijskih modifikacija, direktno ugrađivanje u polimernu matricu radi dobijanja kompozita novih ili poboljšanih svojstava, i (ii) sa hemijskom modifikacijom za pripremu širokog spektra hemikalija, gradivnih blokova-monomera i polimera. Brojne mogućnosti hemijske modifikacije/funkcionalizacije da bi se poboljšala interakcija između punila i polimernog matriksa daju širok spektar primena u ekološki prihvatljivim materijalima –zelenim kompozitima sa poboljšanim karakteristikama.

Biopolymers from renewable resources – chemical modification and application

Milica P. Rančić
[1] *University of Belgrade – Faculty of Forestry, Belgrade, Serbia*

Growing environmental and economic concerns, along with the finite petrochemical resources, have caused a rapid increase in the research and development of bio-based polymers to replace the current fossil-based economy with a more sustainable one based on renewable resources. The implementation of circular economy systems and the increasing focus on minimizing the disposal of non-biodegradable materials deliver significant environmental benefits. Lignocellulosic-based composites have received great attention recently because they are renewable, biodegradable, and often eco-friendly compared to synthetic materials. The successful introduction of cellulose or lignin in producing new biobased materials is highly dependent on its structure and purity, that is, the isolation method. The main uses have been classified into two groups: (i) without chemical modification, direct incorporation into a polymer matrix to give new or improved properties, and (ii) with chemical modification to prepare an extensive range of chemicals, building blocks, and polymers. The considerable potential for chemical modification to improve the interfacial interaction/reactivity between filler and polymer matrix gives a broad range of opportunities for application in ecologically benign green composites with improved characteristics.

PPP-3

Prirodne eutektičke smeše – rastvarači budućnosti

Boris M. Popović, Tatjana Jurić, Ružica Ždero Pavlović, Denis Uka
Univerzitet u Novom Sadu - Poljoprivredni fakultet, Laboratorija za hemiju i biohemiju, Trg Dositeja Obradovića 8, Novi Sad, Srbija

Dizajn zelenih i održivih metoda ekstrakcije prirodnih proizvoda trenutno je vrlo aktuelna tema istraživanja u primenjenoj hemiji i tehnologiji. NADES sistemi (Natural Deep Eutectic Solvents) su potklasa šire klase rastvarača pod nazivom eutektičke smeše u kojima sastojci ne moraju biti prirodna jedinjenja. Približno 40% odobrenih lekova i 90% lekova u razvoju je slabo rastvorljivo u vodi, što dovodi do njihove niske biorasploživosti. Stoga je poboljšanje biodostupnosti bioaktivnih jedinjenja i postojećih lekova trenutno jedan od glavnih ciljeva farmaceutske industrije. Rastvaranjem aktivnih farmaceutskih sastojaka (API) u NADES sistemima dobijaju se takozvani APIDES sistemi (Active Pharmaceutical Ingredient Deep Eutectic Solvents). Upotrebom NADES-a rastvorljivost API-ja može da se poveća stotinama pa i hiljadama puta tako da je velika perspektiva APIDES-a u sistemima za dostavu lekova.

Natural deep eutectic solvents – the solvents of the future

Boris M. Popović, Tatjana Jurić, Ružica Ždero Pavlović, Denis Uka
University of Novi Sad - Faculty of Agriculture, Chemistry & Biochemistry Laboratory, Trg Dositeja Obradovića 8, Novi Sad, Serbia

The design of green and sustainable extraction methods of natural products is currently a hot research topic in the multidisciplinary area of applied chemistry and technology. NADES systems are a subclass of a wider class of solvents named Deep Eutectic Solvents (DES) in which the ingredients do not have to be natural compounds. Approximately 40% of approved drugs and 90% of drugs under development are poorly water-soluble, which leads to low bioavailability. Therefore, improving the bioavailability of bioactive compounds and existing drugs is currently one of the major goals of the pharmaceutical industry. By dissolving Active Pharmaceutical Ingredients (APIs) in NADES systems, the so-called APIDES systems are obtained (Active Pharmaceutical Ingredient Deep Eutectic Solvents). Using NADES, the solubility of APIs can increase hundreds and thousands of times, so there is a great perspective of APIDES systems as vehicles for drug delivery.

Predavanja dobitnika medalje SHD za pregalaštvo i uspeh u nauci

Lectures by the winners of the SCS medal for achievement and success in science

MP-1

Novi standard za visokoefikasnu pretragu biokatalizatora: unapređenje termalne stabilinosti lipaze

Xinge Diana Zhang[1], Anqi Chen[1], David A. Weitz[1-3], Karla Ilić Đurđić[1,3,4]
[1]Škola za inženjering i primenjene nauke, Harvard Univerzitet, Kembridž, MA 02138, SAD
[2]Departman za fiziku, Harvard Univerzitet, Kembridž, MA02138, SAD
[3] Wyss Institut za biološki inspirisan inženjering, Harvard Univerzitet 3 Blackfan Circle, Boston, MA, 02115, SAD
[4] Univerzitet u Beogradu-Hemijski fakultet, Studentski trg 12-16, 11000, Belgrad Srbja

Enzimi su visokospecifični biokatalizatori primenjeni u velikom broju industrijskih procesa. Međutim, enzimi pronađeni u prirodi moraju biti optimizovani da bi mogli da funkcionišu u industrijskim uslovima. Ovo se najčeće postiže primenom dirigovane evolucije. Ovaj metod limitira istraživanje odnosa sekvence i funkcije proteina na isključivo evolutivno favorizovane amino kiseline. Mi smo razvili novi metod za pripremu biblioteka gena kako bismo uveli sve moguće mutacije na svakoj poziciji. Dok visokoefikasne metode za pretragu biokatalizatora omogućavaja pretragu od oko jednog miliona varijanti i limitirane su brzinom sortiranja, naše metode se zansnivaju na *in vitro* ekspresiji mutanata enzima i uzastopnom sortiranju primenom mikrofluidike, i omogućavaju pretragu triliona mutiranih varijanti enzima. Kombinacija metoda za pripremu biblioteka gena i visokoefikasnu pretragu biokatalizatora dovela je do izolovanja variajnti lipaze sa značajno unapređenom termalnom stabilnošću u samo jednom koraku.

A new standard for ultrahigh throughput functional screens: Thermally stable lipases

Xinge Diana Zhang[1], Anqi Chen[1], David A. Weitz[1-3], Karla Ilić Đurđić[1,3,4]
[1] School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA
[2] Department of Physics, Harvard University, Cambridge, MA 02138, USA
[3] Wyss Institute for Biologically Inspired Engineering, Harvard University, 3 Blackfan Circle, Boston, MA, 02115, USA
[4] University of Belgrade-Faculty of Chemistry, Studentski trg 12-16, 11000, Belgrade, Serbia

Enzymes are highly specific catalysts delivering improved drugs and greener industrial processes. Naturally occurring enzymes must be optimized which is often accomplished through directed evolution. However, this method limits exploration of fitness landscape to only evolutionary favored amino acid substitutions. We developed a new library preparation method to enable introduction of all possible substitutions at each position with highly controllable mutation rates. While highest throughput methods for screening of enzyme libraries are limited by throughput of microfluidic devices to 10^6 variants, we leverage *in vitro* transcription and translation in a combination with multiplexed consecutive microfluidics-based sorting to screen libraries with more than 10^{12} variants. We combined new library preparation and screening methods to improve thermal stability of lipase in a single mutagenesis step.

MP-2

Sinteza i biološka aktivnost odabranih heterocikličnih farmakofora

Nenad Janković
Univerzitet u Kragujevcu, Institut za informacione tehnologije Kragujevac, Kragujevac, Srbija

Sintetička hemija se iz godine u godinu sve više okreće novim-starim trendovima koji omogućavaju pristup velikom broju različitih heterociklčinih molekula. Zahvaljujući mogućnosti sinteze u jednom koraku, uz poštovanje zelenih principa, multikomponentne reakcije predstavljaju najproučavanije i najkorisnije sintetičke pristupe današnjice. Jedna od najviše proučavanih multikomponentnih reakcija je Biđinelijeva sinteza. Ova reakcija omogućava sintezu značajnog broja derivata polazeći od aktivnih metilenskih jedinjenja, različitih karbonila i (tio)uree. Zbog svojih svojstava, molekulske raznolikosti, kao i mogućnosti za dalju derivatizaciju tetra(di)hidropirimidini koji nastaju kao proizvodi ove reakcije nalaze veliku primenu u hemiji materijala i farmaciji. Potencijal koji imaju ovi molekuli za retrovirusne terapije je nemerljiv, ali se poslednjih godina sve više posvećuje pažnja njihovom antitumorskom delovanju.

Synthesis and biological activity of selected heterocyclic pharmacophores

Nenad Janković
University of Kragujevac, Institute for Information Technologies Kragujevac, Kragujevac, Serbia

Synthetic chemistry takes more and more attention to new-old fashion that allow access to a large number of different heterocyclic molecules. Giving the possibility for synthesis in one step and respecting green principles, multicomponent reactions represent the most useful synthetic approaches. One of the most studied multicomponent reactions is the Biginelli synthesis. This reaction enables the synthesis of a significant number of derivatives starting from active methylene compounds, various carbonyls and (thio)urea. Due to their properties and the possibility for further derivatization, the tetra(di)hydropyrimidines that are formed as products of this reaction, are widely used in material chemistry and pharmacy. The potential of these molecules for retroviral therapies is immeasurable, therefore in recent years so much attention has been paid to their antitumor activity.

Acknowledgment: Author acknowledges the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (451-03-68/2023-14/200378).

Saopštenja / Contributions

Analitička hemija

Analytical Chemistry

AH-1

Razvoj voltametrijske metode za određivanje avobenzona u uzorku bazenske vode

Jasmina S. Anojčić, Sanja D. Mutić, Milan B. Vraneš, Jovana J. Panić, Snežana M. Papović

Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija

Organski UV filteri su klasa jedinjenja prisutna u sredstvima za zaštitu od sunca i pokazuju tendenciju da se akumuliraju u životnoj sredini. Cilj ovog rada je bio razviti visokoosetljivu, selektivnu i jednostavnu voltametrijsku metodu za određivanje UV filtera avobenzona (AVO). Kao radna elektroda primenjena je elektroda od ugljenične paste modifikovana 1-butil-3-metilpiridinijum-hloridom. Optimizovana je količina modifikatora, pH vrednost pomoćnog elektrolita, kao i parametri adsorptivne voltametrijske metode sa pravougaonim talasima. Linearnost kalibracione krive je postignuta u opsegu koncentracija AVO od 0,05 µg mL^{-1} do 1,77 µg mL^{-1} pri pH 12 (E_{acc} = 0,2 V, t_{acc} = 100 s), dok je granica detekcije iznosila 0,015 µg mL^{-1}. Razvijena metoda je uspešno primenjena za kvantifikaciju AVO u matriksu bazenske vode sa odličnim prinosom i ponovljivošću merenja.

Development of a voltammetric method for the determination of avobenzone in a swimming pool water sample

Jasmina S. Anojčić, Sanja D. Mutić, Milan B. Vraneš, Jovana J. Panić, Snežana M. Papović

University of Novi Sad - Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

Organic UV filters are a class of compounds present in sunscreen agents and show a tendency to accumulate in the environment. The aim of this work was to develop a highly sensitive, selective and simple voltammetric method for the determination of the UV filter avobenzone (AVO). A carbon paste electrode modified with 1-butyl-3-methylpyridinium chloride was used as the working electrode. The amount of modifier, the pH of the supporting electrolyte, as well as the parameters of the square-wave adsorptive stripping voltammetric method were optimized. The linearity of the calibration curve was achieved in the AVO concentration range from 0.05 µg mL^{-1} to 1.77 µg mL^{-1} at pH 12 (E_{acc} = 0.2 V, t_{acc} = 100 s), while the limit of detection was 0.015 µg mL^{-1}. The developed method was successfully applied for the quantification of AVO in the swimming pool water matrix with excellent recovery and reproducibility of measurements.

Acknowledgment: The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125) and the Provincial Secretariat for Higher Education and Scientific Research (Grant No. 142-451-3167/2020-03).

AH-2

Uticaj odabranog aditiva na bazi salicilata na rastvorljivost i strukturnu organizaciju kofeina u vodi

Teona Teodora V. Borović, Snežana M. Papović, Jovana J. Panić, Slobodan B. Gadžurić, Sanja D. Belić, Nikolett A. Cako Bagány, Milan B. Vraneš
Univerzitet u Novom Sadu - Departman za hemiju, biohemiju i zaštitu životne sredine, Prirodno-matematički fakultet, Novom Sadu, Srbija

Kofein, najčešće konzumirana psihoaktivna supstanca, pripada grupi ksantinskih alkaloida. Rastvorljivost kofeina u vodi je relativno niska (~ 16 $\mathrm{mg \cdot mL^{-1}}$ na sobnoj temperaturi), što je jedan od ključnih problema, posebno u preparatima koji se konzumiraju ili čuvaju na niskim temperaturama, kao što su neka pića, suplementi, farmaceutski i kozmetički proizvodi. Smatra se ograničeno rastvorljivim u vodi zbog samoagregacije izazvanom hidrofobnim interakcijama. Povećanje rastvorljivosti i ograničavanje agregacije postiže se dodavanjem biokompatibilnih aditiva. Cilj rada je ispitivanje fizičko-hemijskih svojstava iz volumetrijskih, viskozimetrijskih merenja i računarskih simulacija da bi se razumela svojstva hidratacije i agregacije kofeina u 0,1 $\mathrm{mol \cdot kg^{-1}}$ vodenom rastvoru natrijum salicilata. Natrijum salicilat smanjuje gorak ukus i povećava rastvorljivost kofeina u vodi. Rezultati dobijeni volumetrijskim i viskozimetrijskim merenjima ukazuju da natrijum salicilat pospešuje samoagregaciju kofeina u vodi.

The influence of selected salicylate-based additive on the solubility and structural organization of caffeine in water

Teona Teodora V. Borović, Snežana M. Papović, Jovana J. Panić, Slobodan B. Gadžurić, Sanja D. Belić, Nikolett A. Cako Bagány, Milan B. Vraneš
University of Novi Sad - Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, Novi Sad, Serbia

Caffeine, the most widely used psychoactive substance, belongs to the group of xanthine alkaloids. Caffeine solubility in water is relatively low (~ 16 $\mathrm{mg \cdot mL^{-1}}$ at room temperature), which is one of the crucial problems, especially in preparations consumed or stored at low temperatures, such as some drinks, supplements, pharmaceuticals and cosmetic industries. Caffeine is considered limitedly soluble in water due to self-association and aggregation of caffeine molecules by hydrophobic interactions. Solution for increasing solubility and limiting aggregation is to add biocompatible additives. The present study analyzed experimental data from volumetric, viscosimetric measurements and computational simulations to understand caffeine hydration and aggregation properties in 0.1 $\mathrm{mol \cdot kg^{-1}}$ sodium salicylate aqueous solution. Sodium salicylate reduces the bitter taste and increases the solubility of caffeine in water. Results noted in volumetric and viscosimetric measurements indicate that sodium salicylate promotes the self-aggregation of caffeine in water.

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

AH-3

Kinetika fotorazgradnje ciprofloksacina i identifikacija intermedijera fotokatalitičke razgradnje primenom LC–ESI–MS/MS

Dušica K. Jovanović, Dejan Z. Orčić, Daniela V. Šojić Merkulov, Vesna N. Despotović, Szabolcs I. Bognár, Nina L. Finčur
Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija

U ovom radu ispitivana je kinetika uklanjanja fluorohinolonskog antibiotika ciprofloksacina, aktivne komponente leka Ciprocinal®, iz vodene sredine primenom simuliranog sunčevog zračenja. Ispitana je efikasnost indirektne fotolize ciprofloksacina u prisustvu H_2O_2 i $KBrO_3$, kao i heterogene fotokatalize primenom ZnO kao fotokatalizatora. Primenom heterogene fotokatalize uklonjeno je 94,2% ciprofloksacina nakon 60 min procesa. Pored toga, identifikacija devet intermedijera nastalih u toku procesa heterogene fotokatalize ciprofloksacina izvedena je primenom LC–ESI–MS/MS tehnike.

Kinetics of ciprofloxacin photodegradation and LC–ESI–MS/MS identification of photocatalytic degradation intermediates

Dušica K. Jovanović, Dejan Z. Orčić, Daniela V. Šojić Merkulov, Vesna N. Despotović, Szabolcs I. Bognár, Nina L. Finčur
University of Novi Sad Faculty of Sciences - Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

This study was concerned with the investigation of the removal kinetics of the fluoroquinolone antibiotic ciprofloxacin, the active compound of the Ciprocinal® drug, from the aqueous environment utilizing simulated sunlight. The efficacy of indirect photolysis of ciprofloxacin in the presence of H_2O_2 and $KBrO_3$, as well as heterogeneous photocatalysis using ZnO as a photocatalyst, was examined. Using heterogeneous photocatalysis, 94.2% of ciprofloxacin was removed after 60 min of process. Besides, the identification of nine intermediates, formed during the process of heterogeneous photocatalysis of ciprofloxacin was performed using the LC–ESI–MS/MS technique.

Acknowledgment: This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125) and by the Science Fund of the Republic of Serbia (Grant No 7747845, In situ pollutants removal from waters by sustainable green nanotechnologies-CleanNanoCatalyze).

AH-4

Fenolni profil i *in vitro* citotoksični efekat odabranih biljaka sa potencijalom za usporavanje starenja kože

Đurđa D. Ivković[1], Olga M. Trifunović[2], Filip Lj. Andrić[2], Maja V. Krstić Ristivojević[2], Petar M. Ristivojević[2]
[1] Univerzitet u Beogradu - Inovacioni centar Hemijskog fakulteta d.o.o., Beograd, Srbija
[2] Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija

Najnovije studije pokazuju da UV i plava svetlost, koju emituju ekrani elektronskih uređaja, usporavaju proliferaciju keratinocita i stvaraju slobodne radikale koji dovode do starenja kože[1]. Polifenoli, jedinjenja koja se nalaze u biljkama, mogu sprečiti oštećenja kože izazvana zračenjem. Stoga, postoji potreba za dobijanjem biljnih formulacija sa protektivnim efektima od kojih bi se izrađivali kozmetički preparati. Primenom masene spektrometrije identifikovana su i kvantifikovana fenolna jedinjenja u ekstraktima iz 18 biljaka gajenih u istočnoj Srbiji. Ispitana je citotoksičnost ekstrakata na HaCaT ćelijama (humani keratinociti) i određene su IC_{50} vrednosti. Dobijeni ekstrakti su bogate mešavine fenolnih jedinjenja koje se moraju pravilno dozirati jer u većim koncentracijama oštećuju ćelije kože.

Phenolic profile and *in vitro* cytotoxic effects of selected herbs with potential skin anti-ageing properties

Đurđa D. Ivković[1], Olga M. Trifunović[2], Filip Lj. Andrić[2], Maja V. Krstić Ristivojević[2], Petar M. Ristivojević[2]
[1] University of Belgrade - Innovative Centre of the Faculty of Chemistry, Belgrade, Serbia
[2] University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

The latest studies show that UV and blue light, emitted by electronic devices with screens, slows the proliferation of the keratinocytes and generates free radicals leading to skin ageing[1]. Polyphenols, a compounds found in plants, can prevent light-induced damage to the skin. A constant screening of plant extracts is requisite in order to discern light-protective formulations to constitute cosmetic products. Using mass spectrometry, phenolic compounds were identified and quantified in plant extracts from 18 plants grown in Eastern Serbia. The cytotoxicity of the obtained extracts was tested on HaCaT cells (immortalized human keratinocytes) and IC_{50} values were determined. The obtained extracts are rich mixtures of phenolic compounds that must be dosed appropriately since they also damage skin cells at larger concentrations.

1. Nakashima Y, et al., *Free Radic. Biol. Med.* **2017**, 108, 300–310.

Acknowledgment: This work was supported by The Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Program, No.6389927, Ministry of Science, Technological Development and Innovation of Republic of Serbia Contract numbers 451-03-47/2023-01/200168 and 451-03-47/2023-01/200288.

AH-5

Hromatografski parametri u proceni lipofilnosti i ekotoksičnosti derivata hloroacetamida

Dragana C. Mekić, Đenđi Đ. Vaštag, Suzana Lj. Apostolov
Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija

Lipofilnost je usko povezana sa bioraspoloživošću odnosno potencijalnom biološkom aktivnošću jedinjenja. Ovaj važan fizičko-hemijski parametar je za derivate hloroacetamida određen eksperimentalnim putem, primenom reverzno-fazne tankoslojne hromatografije, RPTLC C18/UV_{254s} u smeši vode i dva organska modifikatora, ponaosob, kao i računskim putem primenom softverskih paketa. Zavisnost između hromatografskih parametara (R_M^0 i m) i softverski dobijenih vrednosti standardnog merila lipofilnosti ($\log P$), ali i odabranih parametara ekotoksičnosti je ispitana primenom metode linearne regresije. Dobijeni matematički modeli ukazuju na pouzdanost primene hromatografskih parametara, R_M^0 i m u proceni lipofilnosti i ekotoksičnosti proučavanih derivata hloroacetamida.

Chromatographic parameters in the assessment of chloroacetamide derivatives’ lipophilicity and ecotoxicity

Dragana C. Mekić, Đenđi Đ. Vaštag, Suzana Lj. Apostolov
University of Novi Sad - Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia

Lipophilicity is closely related to the bioavailability or potential biological activity of the compound. For chloroacetamides this important physicochemical parameter derivatives was determined experimentally, by using reversed-phase thin-layer chromatography, RPTLC C18/UV_{254s} in the mixtures of water and two organic modifiers, separately, as well as computationally by using software packages. The dependence between the chromatographic parameters (R_M^0 and m) and the software-derived values of the standard measure of lipophilicity ($\log P$), as well as the selected ecotoxicity parameters, was examined by applying linear regression analysis. The obtained mathematical models indicate the reliable application of the chromatographic parameters, R_M^0 and m in the assessment of the studied chloroacetamide derivatives’ lipophilicity and ecotoxicity.

AH-6

Primena modifikovane ugljenične paste za određivanje antiinflamatornog leka diklofenaka

Katarina S. Postolović, Zorka D. Stanić

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

Diklofenak pripada grupi nesteroidnih antiinflamatornih lekova [1]. U ovom radu je primenjen novi, efektivni elektrohemijski senzor za određivanje diklofenaka, modifikovanjem elektrode na bazi ugljenične paste. Elektroda je modifikovana hitozanom, biopolimerom sa odličnim adsorptivnim svojstvima i nanočesticama TiO_2, katalitički aktivnim materijalom. Modifikovanje elektrode je omogućilo veću aktivnu površinu, kao i veću električnu provodljivost, što je uticalo na poboljšanje elektrohemijske detekcije diklofenaka na pH vrednosti 5.0, primenom adsorptivne diferencijalne pulsne voltametrije. Postignuta je linearna zavisnost anodne struje od koncentracije diklofenaka u dva različita opsega, 0.2–10 μM i 10–100 μM, sa limitom detekcije od 0.013 μM. Razvijen senzor je uspešno primenjen i za određivanje diklofenaka u sintetičkom urinu i komercijalnim tabletama. Postignuti limit detekcije, stabilnost elektrode, selektivnost, kao i dobra reproduktivnost rezultata ukazuju na značajan potencijal ovog senzora za određivanje diklofenaka u različitim uzorcima.

Application of modified carbon paste electrode for determination of diclofenac as an anti-inflammatory drug

Katarina S. Postolović, Zorka D. Stanić

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

Diclofenac belongs to the group of non-steroidal anti-inflammatory drugs [1]. In this paper, a new and effective electrochemical sensor was developed for the determination of diclofenac by modifying the carbon paste electrode. The electrode was modified with chitosan, a biopolymer with excellent adsorptive properties, and TiO_2 nanoparticles, a catalytically active material. The electrode modification provided a larger surface area and improved electrical conductivity, leading to enhanced electrochemical detection of diclofenac at a pH of 5.0 using adsorptive differential pulse voltammetry. A linear response of the anodic current on the diclofenac concentration was observed in two different ranges, 0.2–10 μM and 10–100 μM, with a detection limit of 0.013 μM. The developed sensor was successfully applied to determine diclofenac in synthetic urine and commercial tablets. The obtained detection limit, electrode stability, selectivity, and good reproducibility of results indicate the significant potential of this sensor for diclofenac determination in various samples.

1. A. Afkhami, A. Bahiraei, T. Madrakian, *Mater. Sci. Eng. C.* **2016**, *59*, 168.

Acknowledgment: This work was financially supported by the Serbian Ministry of Education, Science and Technological Development (Grant No: 451-03-47/2023-01/200122).

AH-7

Fenolni profil i antioksidativni potencijal sedamnaest ekstrakata cvetnih latica

Đurđa D. Ivković[1], Milica Z. Topić[2], Jelena Đ. Trifković[2], Maja Krstić Ristivojević[2], Petar M. Ristivojević[2]

[1] Univerzitet u Beogradu - Inovacioni centar Hemijskog fakulteta, Beograd, Srbija
[2] Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija

Zbog snažnog antioksidativnog potencijala, latice cveća se smatraju važnim sirovina za razvoj kozmetičkih proizvoda[1]. Ova studija je ispitivala fenolni profil i antioksidativni potencijal 17 različitih latica cveća i njihovu potencijalnu primenu u kozmetičkoj industriji. Fenolni profil ispitivanih ekstrakata određen je Visoko-Efikasnom Tankoslojnom Hromatografijom (HPTLC). Antioksidativna aktivnost estrakata je procenjena primenom ABTS i DPPH spektrofotometrijskih testova, kao i sadržaj ukupnih fenola. DPPH-HPTLC je primenjen za identifikaciju jedinjenja sa najvećom antioksidativnom aktivnošću. Pet polifenola je identifikovano u ispitivanim ekstraktima. Na osnovu antioksidativnih testova, *Paeonia lactifora*, *Paeonia decora*, *Rosa istriaca* i *Pelargonium peltatum* su prepoznati kao ekstrakti sa najvećim antioksidativnim potencijalom, dok je galna kiselina je izdvojena kao najsnažniji antioksidans.

The phenolic profile and antioxidative activity of seventeen flower petals extracts

Đurđa D. Ivković[1], Milica Z. Topić[2], Jelena Đ. Trifković[2], Maja Krstić Ristivojević[2], Petar M. Ristivojević[2]

[1] University of Belgrade - Inovative centre of Faculty of Chemistry, Belgrade, Serbia
[2] University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

Due to their strong antioxidative potential, flower petals are considered important starting materials for the development of cosmetic products[1]. Present study explored phenolic profile and antioxidative potential of 17 flower petals and their potential application in the cosmetics industry. The phenolic profile of investigated extracts was determined using High-Performance Thin Layer Chromatography (HPTLC). The antioxidative potential was assessed using both ABTS and DPPH spectrophotometric tests, and total phenol content. DPPH-HPTLC assay was applied to identify compounds with the highest antioxidative activity. Five phenols were identified in the investigated extracts. Based on radical antioxidative tests, *Paeonia lactifora*, *Paeonia decora*, *Rosa istriaca* and *Pelargonium peltatum* were identified as species with the highest antioxidative potential, while gallic acid was recognized as the strongest antioxidants.

1. D. F. Hernandez et all, *Crit. Rev. Food. Sci. Nutr,* **2021**, 61, 3740-3755.

Acknowledgement: This work was supported by The *Science Fund* of the *Republic of Serbia, Serbian Science and Diaspora Collaboration Program, No.6389927.*

AH-8

Rastvor Melih-3 (*Mehlich-3)* kao ekstraktant za multielementarnu analizu uzoraka zemljišta

Vibor Roje, Robert Potočnjak, Mario Sladin, Ivan Perković, Darko Bakšić
Sveučilište u Zagrebu - Fakultet šumarstva i drvne tehnologije, Svetošimunska 23,
HR-10002 Zagreb, Croatia

Rastvor Melih-3 (*Mehlich-3*) među mnogobrojnim je reagensima i metodama za ekstrakciju metala, metaloida i nemetala iz uzoraka zemljišta koji su opisani u naučnoj literaturi ili se koriste u praksi [1]. Ovo istraživanje urađeno je u kontekstu našeg interesa u području multielementarne analize uzoraka zemljišta i testiranja različitih medijuma za ekstrakciju [2]. Upoređene su ekstrakcione moći otopine Melih-3 sa dva ekstraktanta koji su mnogo češće korišćeni i citirani u literaturi, a to su carska voda i deionizovana voda. Rezultati pokazuju da je, uprkos slabijoj ekstrakcionoj moći otopine Melih-3 u poređenju sa carskom vodom, mikronutrijente Ca, Cu, Fe, K, Mg, Mn, Na, P, S i Zn u takvim ekstraktima moguće pouzdano kvantifikovati tehnikom atomske emisione spektrometrije sa induktivno spregnutom plazmom (ICP-AES).

Mehlich-3 solution as an extractant for multi-element analysis of soil samples

Vibor Roje, Robert Potočnjak, Mario Sladin, Ivan Perković, Darko Bakšić
University of Zagreb - Faculty of Forestry and Wood Technology, Svetošimunska 23,
HR-10002 Zagreb, Croatia

Amongst numerous reagents and methods for extraction of metals, metalloids and non-metals from soil samples described in the scientific literature and/or applied in practice is the Mehlich-3 solution [1]. This research was conducted in the context of our interests in the multi-element analysis of soils and tests of various extraction media [2]. The extraction ability of the Mehlich-3 solution was compared to other extraction reagents (*aqua regia* and deionized water) that are more commonly used and cited in the literature. The results show that, despite the weaker extraction power of the Mehlich-3 solution in comparison to *aqua regia*, the micronutrients Ca, Cu, Fe, K, Mg, Mn, Na, P, S, and Zn in such extracts can be reliably quantified using inductively coupled plasma-atomic emission spectrometry (ICP-AES).

[1] A. Mehlich, *Commun. Soil Sci. Plan. Anal.* **1984**, *15,* 1409.

[2] V. Roje, D. Buršić, I. Košutić, Comparison of nitric acid and *aqua regia* as extractants for heavy metals in soil samples in B. Šolaja (ed.), 58th Meeting of the Serbian chemical society, Belgrade, Serbia, 9-10 June **2022**, Book of Abstracts/Proceedings, R-AH-2, 190-194.

AH-9

Analiza sadržaja mikroelemenata i elemenata u tragovima u letećem pepelu uglja primenom različitih metoda digestije

Dragana Z. Živojinović, Sanja S. Vučić, Dušan V. Trajković, Maja B. Đolić, Mirjana Đ. Ristić, Aleksandra A. Perić Grujić
Univerzitet u Beogradu - Tehnološko-metalurški fakultet, Beograd, Srbija

Sagorevanjem uglja u termoelektranama u Republici Srbiji svakodnevno se izdvaja velika količina letećeg pepela, kao otpadnog materijala, Ovaj otpad, pored toga što sadrži zagađujuće materije, kao što su teški metali i toksični elementi (olovo, arsen, kadmijum, živa), sadrži i retke elemente zemlje, koji su danas prepoznati kao strateški elementi. U ovom radu ispitane su dve metode pripreme uzoraka i efekat koji način pripreme ima na ekstrakciju elemenata iz pepela i njihove konačne koncentracije. Uzorci letećeg pepela uzorkovani su u termoelektranama Nikola Tesla blokovi A i B. Uzorci su tretirani na dva načina: digestijom mineralnim kiselinama $HNO_3/HClO_4/HCl$ i digestijom smešom kiselina HNO_3/H_2SO_4 uz V_2O_5 kao katalizator. Ekstrahovani elementi određeni su metodom indukovane spregnute plazme sa optičkim emisionim detektorom, ICP-OES. Rezultati ispitivanja pokazali su da način pripreme uzorka, s obzirom na kompleksnost matrice, ima veliki uticaj na dobijene koncentracije izluženih elemenata.

Microelement and trace element analysis in coal fly ash using different digestion procedures

Dragana Z. Živojinović, Sanja S. Vučić, Dušan V. Trajković, Maja B. Đolić, Mirjana Đ. Ristić, Aleksandra A. Perić Grujić
University of Belgrade - Faculty of Technology and Metallurgy, Belgrade, Serbia

A large amount of coal fly ash is generated as waste material from thermal power plants in Serbia. It is well known that fly ash contains pollutants such as heavy metals and toxic elements (lead, cadmium, arsenic, mercury), as well as rare earth elements, nowadays recognized as strategic elements. In this research, two sample preparation methods have been examined to determine the effect of the digestion method on the extraction efficiency. The coal fly ash was sampled from Nikola Tesla thermal power plant, blocks A and B. Ash samples were prepared using two digestion procedures: 1) with mineral acids mixture $HNO_3/HClO_4/HCl$, and 2) with a mixture of acids HNO_3/H_2SO_4 with V_2O_5 as a catalyst. Extracted elements are determined using the ICP-OES technique. Considering the matrix complexity, it has been shown that the sample preparation method greatly impacts the obtained results.

Zahvalnica: Istraživanje u okviru ovog rada sprovedeno je uz podršku Fonda za nauku Republike Srbije, Projekat iz programa IDEJE 7743343, Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants – SIW4SE.

AH-10

Detekcija antibakterijskih jedinjenja u tinkturama biljaka iz familije *Asteraceae* primenom HPTLC-bioautografije

Jelena Đ. Trifković[1], Petar M. Ristivojević[1], Vukosava M. Živković-Radovanović[1], Marko D. Jović[2]

[1] Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija
[2] Univerzitet u Beogradu - Inovacioni centar Hemijskog fakulteta Beograd, Srbija

Farmakološka ispitivanja biljaka iz familije *Asteraceae* potvrđuju njihova mnogobrojna lekovita svojstva, poput antimikrobne, antiinflamatorne, antikancerogene i antioksidativne aktivnosti. Cilj ovog rada je bio razvoj jednostavne i brze procedure za detekciju antibakterijskih jedinjenja u tinkturama 14 nazličitih vrsta biljaka iz ove familije. Metaboliti su razdvojeni primenom visoko-efikasne tankoslojne hromatografije (HPTLC), a bioautografski eseji su optimizovani za nekoliko sojeva gram-pozitivnih i gram-negativnih bakterija, koje su česti uzročnici respiratornih i urinarnih infekcija. Dobijeni rezultati ukazuju na prisustvo većeg broja aktivnih jedinjenja, karakterističnih za pojedine biljne vrste. U poređenju sa drugim konvencionalnim *in vitro* metodama, HPTLC-bioutografija pruža mogućnost brze i jeftine analize lekovitog bilja, a zatim i selekcije one vrste sa najvećim antibakterijskim potencijalom za dalja ispitivanja.

Detection of antibacterial compounds in tinctures of plants from the *Asteraceae* family using HPTLC-bioautography

Jelena Đ. Trifković[1], Petar M. Ristivojević[1], Vukosava M. Živković-Radovanović[1], Marko D. Jović[2]

[1] University of Belgrade - Faculty of Chemistry, Belgrade, Serbia
[2] University of Belgrade - Innovative Centre of the Faculty of Chemistry, Belgrade, Serbia

Pharmacological investigations on plants belonging to the *Asteraceae* family have confirmed their multiple therapeutic properties, including antimicrobial, anti-inflammatory, anti-cancer, and antioxidant activities. In this study, we aimed to develop a rapid and simple method for detecting antibacterial compounds in tinctures of 14 different types of plants from this family. Metabolites were separated using high-performance thin-layer chromatography (HPTLC), and bioautographic assays were optimized for several strains of gram-positive and gram-negative bacteria that frequently cause respiratory and urinary infections. The results obtained suggest the presence of a high number of active compounds specific to certain plant species. Compared to conventional *in vitro* methods, HPTLC-bioautography enables time-saving and economical analysis of medicinal plants, allowing the selection of species with the highest antibacterial potential for further investigation.

Acknowledgment: This work has been supported by the Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Program, No 6389927.

AH-11

Procena kvaliteta podzemnih voda u Banatu korišćenjem entropijskog indeksa kvaliteta vode (EWQI)

Jelena B. Vesković[1,2], Andrijana N. Miletić[2], Slavica S. Ražić[1], Antonije E. Onjia[2]
[1] *Univerzitet u Beogradu, - Farmaceutski fakultet, Vojvode Stepe 450, Beograd, Srbija*
[2] *Univerzitet u Beogradu - Tehnološko-metalurški fakultet, Karnegijeva 4, Beograd, Srbija*

Kvalitet podzemnih voda je jako bitan, budući da utiče na mogućnost njihovog korišćenja. U ovom radu je ispitan kvalitet podzemnih voda Banata. Analiziran je veliki broj uzoraka podzemne vode na sadržaj zagađujućih supstanci. U cilju određivanja prihvatljivosti podzemne vode kao pijaće vode, primenjena je metoda entropijskog indeksa kvaliteta vode (EWQI). Izračunate vrednosti EWQI varirale su između 7,0 i 326, sa srednjom vrednošću od 66,9. Na osnovu EWQI, vode su razvrstane tako da je 25,0%, 30,6%, 22,2%, 13,0% i 9,3% uzoraka podzemnih voda „odličnog", „dobrog", „srednjeg", „lošeg" i „ekstremno lošeg" kvaliteta, redom. U južnom Banatu prisutne su vode „odličnog" i „dobrog" kvaliteta, dok su na severu istraživanog područja prisutne vode „srednjeg", „lošeg" i „ekstremno lošeg" kvaliteta.

Quality assessment of groundwater in Banat plain using entropy-weighted water quality index (EWQI)

Jelena B. Vesković[1,2], Andrijana N. Miletić[2], Slavica S. Ražić[1], Antonije E. Onjia[2]
[1] *University of Belgrade - Faculty of Pharmacy, Vojvode Stepe 450, Belgrade, Serbia*
[2] *University of Belgrade - Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia*

The quality of groundwater is of crucial importance, as it determines its usability. In this paper, the quality of groundwater in Banat is investigated. A number of groundwater samples were analyzed for the presence of contaminants. The entropy-weighted water quality index (EWQI) method was used to determine the acceptability of groundwater as a drinking water source. The calculated EWQI ranged from 7.0 to 326, with a mean value of 66.9. According to the EWQI, 25.0%, 30.6%, 22.2%, 13.0%, and 9.3% of the groundwater samples were of "excellent", "good", "moderate", "poor", and "extremely poor" quality, respectively. In the southern Banat, there are waters of "excellent" and "good" quality, while in the northern part of the study area there is water of "moderate", "poor", and "extremely poor" quality.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation, Republic of Serbia (Grants 451-03-47/2023-01/200161 and 451-03-47/2023-01/200135).

Biohemija

Biochemistry

BH-1

Modelovanje farmakofora zasnovano na ligandima za LacI protein

Yaraslau U. Dzichenka[1], Michail A. Shapira[1], Suzana S. Jovanović-Šanta[2]
[1] Institute of Bioorganic Chemistry of National Academy of Sciences, Minsk, Belarus
[2] PMF Univerziteta u Novom Sadu, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija

Usmerena evolucija enzima se koristi za kreiranje novih enzima sa određenim svojstvima, pri čemu su jako važni genetska raznovrsnost, metoda skrininga i selekcija. Za selekciju polimorfnih varijanti proteina često se koriste ćelije bakterija. Najčešće se selekcija zasniva na promenama koje su veštački napravljene u strukturi komponenti bakterijskog operona. U ovom radu su napravljena 2 modela farmakofora za usmerenu evoluciju LacI proteina (laktoza operon represor) za jedinjenja predstavljena u PDB (ID: 1EFA, 4RZT, 2PE5, 2P9H) da bi se identifikovale ključne aminokiseline koje interaguju sa malim molekulima. Za svako jedinjenje je identifikovan skup farmakofornih karakteristika na osnovu biblioteke RDKit (v. 2022.09.4) za Pithon (v. 3.7.13): donori i akceptori vodonične veze i u manjoj meri aromatični i hidrofobni fragmenti. Lokalizacija karakteristika odgovara atomima kiseonika molekula šećera, dok su za molekule represora važne i hidrofobne interakcije bočnih grupa.

Ligand-based pharmacophore modeling for the LacI protein

Yaraslau U. Dzichenka[1], Michail A. Shapira[1], Suzana S. Jovanović-Šanta[2]
[1] Institute of Bioorganic Chemistry of National Academy of Sciences, Minsk, Belarus
[2] University of Novi Sad Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental protection, Novi Sad, Serbia

Directed enzyme evolution is widely used for the creation of novel enzymes with desired properties, where genetic diversity, high throughput screening and selection methods are very important. Bacterial cells are often used for the selection of polymorphic variants of proteins. The most prominent way of selection is based on the changes artificially made in the structure of components of bacterial operon. Here 2 pharmacophore models were built for LacI protein (lactose operon repressor) ligands in order to identify key amino acids which interact with small molecules for the compounds presented in PDB (IDs: 1EFA, 4RZT, 2PE5, 2P9H). For each compound a set of pharmacophore features was identified using functionality of RDKit library (v. 2022.09.4) for Python (v. 3.7.13): H bond donors and acceptors, while aromatic and hydrophobic fragments were less presented. Localization of the features corresponds to the oxygen atoms of a sugar molecule, while for repressor molecules hydrophobic interactions of side groups are also important.

Acknowledgment: Results are obtained in the frame of Belarus-Serbia bilateral project (X22SRBG-009 and 337-00-00230/2022-09/09)

BH-2

Ekspresija JNK kinaza u THP-1 celijama tretiranim Ru(II) kompleksima

Milena P. Krstić[1], Juan Francisco Santibanez[2], Jelena Poljarević[3], Sanja R. Grgurić-Šipka[3], Sunčica Z. Borozan[1]

[1]Fakultet veterinarske medicine, Univerzitet u Beogradu, Bulevar oslobodjenja 18, 11000 Beograd, Srbija, [2] Institut za medicinska istraživanja, poštanski fah 102, 11129 Beograd, Srbija, [3]Hemijski fakultet, Univerzitet u Beogradu, poštanski fah 158, 11001 Beograd, Srbija

C-Jun N-terminalne kinaze (JNK) spadaju u mitogen-aktivirane protein kinaze (MAPK) i imaju važnu ulogu u kontroli niza ćelijskih procesa uključujući proliferaciju, kancerogenezu i apoptozu. Kompleksi rutenijuma pokazali su izuzetan potencijal kao mogući citostatici. Upravo iz ovih razloga ispitivan je mehanizam delovanja kompleksa Ru(II) sa *N*-alkilfenotiazinima (hlorpromazinom, trifluoperazinom i tioridazinom) na signalne parametre (t-JNK, p-JNK i β-aktin) u THP-1 ćelijama humane leukemije. U ćelijama tretiranim kompleksom sa fluoperazinom u koncentraciji od 10 μM (IC_{50} je 10,5 μM) ekspresija t-JNK povećana je za 47,45%, dok je ekspresija p-JNK dvostruko veća u poređenju sa netretiranim ćelijama, što sugeriše da su t-JNK i p-JNK uključeni u apoptozu ovih ćelija.

Expression of JNK kinases in THP-1 cells treated with Ru(II) complexes

Milena P. Krstić[1], Juan Francisco Santibanez[2], Jelena Poljarević[3], Sanja R. Grgurić-Šipka[3], Sunčica Z. Borozan[1]

[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

The c-Jun N-terminal kinase (JNK) belongs to the family of mitogen-activated protein kinases (MAPKs) that play an important role in the control of a number of celular processes, including proliferation, cancerogenesis and apoptosis. Ruthenium complexes have shown remarkable potential as possible cytostatics. Precisely for these reasons, the mechanism of action of Ru(II) complexes with *N*-alkylphenothiazines (chlorpromazine, trifluoperazine, and thioridazine) on signalling parameters (t-JNK, p-JNK and β-actin) in THP-1 human leucemic cells was investigated. In cells treated with fluoperazine complex at a concentration of 10 μM (IC_{50} is 10.5 μM), an increased expression of t-JNK by 47.45% was found while the expression of p-JNK was twice higher compared to untreated cells, suggesting that t-JNK and p-JNK are involved in the apoptosis of these cells.

Acknowledgements: The study was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract number 451-03-47/2023-01/200143).

BH-3

Uticaj modernih tehnologija sušenja na biološku aktivnost ekstrakata ploda zove

Tatjana M. Majkić[1], Jelena D. Bajac[2], Vladimir S. Filipović[2], Ivana N. Beara[1], Marija M. Radojković[1], Ljiljana S. Milovanović[1], Milena D. Terzić[2].
[1] *Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Trg Dositeja Obradovića 3, Novi Sad, Srbija*
[2] *Univerzitet u Novom Sadu - Tehnološki fakultet Novi Sad, Bulevar cara Lazara 1, Novi Sad, Srbija*

Zova (*Sambucus nigra* L.) je samonikla biljna vrsta izuzetno bogata polifenolnim jedinjenjima. Primena savremenih tehnologija omogućila je efikasniju izolaciju bioaktivnih jedinjenja i njihovu inkapsulaciju. U okviru ovog istraživanja pripremljeni su ekstrakti liofilizovanih plodova zove primenom mikrotalasne ekstrakcije, koji su zatim osušeni savremenim tehnologijama: liofilizacijom i sušenjem raspršivanjem. Primenom spektrofotometrijskih metoda određen je sadržaj ukupnih fenola, flavonoida i antocijana, a kroz niz *in vitro* testova analiziran je antioksidantni, hipolipidemijski i hipoglikemijski potencijal navedenih ekstrakata. Rezultati pokazuju da proces sušenja utiče kako na hemijski sastav tako i na biološku aktivnost ekstrakata. Takođe, objedinjeni rezultati svedoče o potencijalu inkapsulacije ekstrakata zove u formulaciji novih prehrambenih i farmaceutskih proizvoda.

The influence of modern drying technologies on the biological activity of elderberry extracts

Tatjana M. Majkić[1], Jelena D. Bajac[2], Vladimir S. Filipović[2], Ivana N. Beara[1], Marija M. Radojković[1], Ljiljana S. Milovanović[1], Milena D. Terzić[2].
[1] *University of Novi Sad - Faculty of Sciences, Trg Dositeja Obradovića 3, Novi Sad, Srbija*
[2] *University of Novi Sad - Faculty of Technology, Bulevar cara Lazara 1, Novi Sad, Srbija*

Elderberry (*Sambucus nigra* L.) is a wild-growing plant species that is extremely rich in polyphenolic compounds. Application of modern technologies has enabled more efficient isolation of bioactive compounds and their encapsulation. Extracts of lyophilized elderberry fruits were prepared using microwave extraction and afterwards were dried using modern drying technologies: lyophilization and spray drying. The content of total phenols, flavonoids and anthocyanins was determined using spectrophotometric methods, while the antioxidant, hypolipidemic and hypoglycemic potential of the extracts were analyzed through different *in vitro* assays. The results show that the drying process affects the chemical composition and biological activity of the extracts. Also, the obtained results testify about the potential of the encapsulation of the elderberry extracts in the formulation of new food and pharmaceutical products.

BH-4

Prečišćavanje i strukturna karakterizacija R-fikocijanina

Luka Veličković[1], Ana Simović[1], Nikola Gligorijević[2], Milica Obradović[1], Georgios Sotiroudis[3], Maria Zoumpanioti[3], Simeon Minić[1] i Milan Nikolić[1]

[1]Univerzitet u Beogradu – Hemijski fakultet, Katedra za biohemiju i Centar izuzetnih vrednosti za molekularne nauke o hrani, Beograd, Srbija

[2] Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju – Centar za hemiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Srbija

[3] Nacionalni helenski istraživački centar, Institut za biologiju, medicinsku hemiju i biotehnologiju, Atina, Grčka

Ljubičasti R-fikocijanin je protein crvenih algi sa mogućnostima primene u industriji hrane (kolorant) i za tretman otpadnih voda (vezuje teške metale). R-fikocijanin analitičke čistoće je izolovan iz puferisanog ekstrakta osušenih Nori algi (*Porphyra* spp.), kombinacijom taloženja amonijum-sulfatom, hidroksiapatitne i hromatografije na DEAE-Sepharose koloni. Multimerni protein imao je apsorpcione maksimume karakteristične za fikoeritrobilinsku (na 580 nm) i fikocijanobilinsku (na 640 nm) hromoforu, visok sadržaj α-zavojnica i temperaturu topljenja od 52°C. Sekundarna struktura proteina bila je stabilna u širokom rasponu pH vrednosti (3–9). R-fikocijanin imobilisan u kuglice kalcijum-alginata pokazao je povećanu toplotnu stabilnost i očuvana antioksidativna svojstva.

Purification and structural characterization of R-phycocyanin

Luka Veličković[1], Ana Simović[1], Nikola Gligorijević[2], Milica Obradović[1], Georgios Sotiroudis[3], Maria Zoumpanioti[3], Simeon Minić[1] and Milan Nikolić[1]

[1] University of Belgrade – Faculty of Chemistry, Department of Biochemistry and Center of Excellence for Molecular Food SciencesBelgrade, Serbia

[2] University of Belgrade, Institute of Chemistry, Technology, and Metallurgy – Center for Chemistry, National Institute of the Republic of Serbia, Belgrade, Serbia

[3] National Hellenic Research Foundation, Institute of Biology, Medicinal Chemistry and Biotechnology, Athens, Greece

Purple R-phycocyanin is a protein from red algae with the potential for application in the food industry (colorant) and wastewater treatment (binding of heavy metals). Analytical grade R-phycocyanin was purified from the buffered extract of dried Nori flakes (*Porphyra* spp.) by combining ammonium sulfate precipitation, hydroxyapatite, and DEAE-Sepharose column chromatography. The multimeric protein had absorption maxima characteristic for phycoerythrobilin (at 580 nm) and phycocyanobilin (at 640 nm) chromophores, high α-helical content, and melting temperature of 52°C. The secondary R-PC structure was stable under a wide range of pH values (3–9). R-phycocyanin immobilized in calcium alginate beads showed increased thermal stability and preserved antioxidant activity.

This work was supported by the PRESSION ANSO project (No: ANSO-CR-PP-2021-01).

BH-5

Korelacija između renalne eliminacije i izračunatih fizičko-hemijskih deskriptora više odabranih antihipertenziva

Jadranka V. Odović
[1]*Farmaceutski fakultet, Univerzitet u Beogradu, Srbija*

U lečenju hipertenzije, najčešće propisivane lekove danas predstavljaju inhibitori enzima koji konvertuje angiotenzin, blokatori kalcijumovih kanala i antagonisti receptora angiotenzina II. Cilj ovog rada bio je da se za dvadeset sedam lekova iz ove tri grupe, ispita zavisnost između renalne eliminacije i fizičko-hemijskih osobina molekula. Za odabrane lekove su primenom softverskih paketa izračunati: deskriptori lipofilnosti, rastvorljivosti u vodi, molekulska masa, volumen i polarna površina molekula. Između podataka o renalnoj eliminaciji i vrednosti molekulske mase, volumena i polarne površine molekula, primenom proste linearne regresione analize, dobijene su niske vrednosti koeficijenata korelacije ($R < 0{,}10$), nešto bolja korelacija je dobijena za vrednosti rastvorljivosti ($R = 0{,}64$), dok je najbolja zavisnost ($R = 0{,}80$) dobijena između vrednosti renalne eliminacije i lipofilnosti ispitivanih molekula. Dobijeni rezultati ukazuju na značaj lipofilnosti i rastvorljivosti za stepen renalne eliminacije ispitivanih antihipertenziva.

The correlation between renal elimination and computed molecular descriptors of selected antihypertensive drugs

Jadranka V. Odović
[1]*Faculty of Pharmacy, University of Belgrade, Serbia*

Today, angiotensin-converting enzyme inhibitors, calcium channel blockers and angiotensin II receptor antagonists represent commonly prescribed antihypertensive drugs. The aim of this work was to investigate relationship between renal elimination and calculated molecular properties for twenty-seven drugs from these three different groups. Several molecular descriptors of selected drugs, such as lipophilicity descriptors, solubility, polar surface area, molecular mass and volume were calculated by the application of software packages. Simple linear regression analysis provided low correlation ($R < 0.10$) between renal elimination of selected drugs and their calculated polar surface area, molecular mass and volume, better correlation was obtained for solubility of selected antihypertensive drugs ($R = 0.64$), while the best correlation was obtained for lipophilicity values ($R = 0.80$). The obtained results indicate the importance of lipophilicity as well as water solubility on renal elimination of antihypertensive drugs.

BH-6

Skrining pektinaznih proizvođača *Aspergillus* spp. za upotrebu u izbistravanju soka od jagode

Marija G. Pavlović[1], Miloš D. Momčilović[1], Sanja M. Živković[1], Marinela V. Šokarda Slavić[2], Marina B. Ristović[2], Zoran M. Vujčić[3]

[1] *Institut za nuklearne nauke „Vinča" - Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija*

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

[3]Katedra za Biohemiju, Hemijski fakultet, Univerzitet u Beogradu, Beograd, Srbija

U ovom radu urađen je skrining sojeva *Aspergillus* spp. koji proizvode pektinaze fermentacijom u tečnom medijumu, a koje su efikasne u izbistravanju soka od jagode. Endo-pektinaze su detektovane difuzionim testom, a ukupna pektinazna aktivnost određena je DNS metodom. Izbistravanje soka nakon tretmana pektinazama određeno je merenjem transmitancije na 660 nm, a povećanje prinosa soka izmereno je centrifugiranjem. Dobijeni rezultati su pokazali da su ove pektinaze visokoefikasne za tretman soka od jagode u poređenju sa komercijalnim pektinaznim preparatom Lafase Fruit.

Screening of pectinase-producing *Aspergillus* spp. for use in strawberry juice clarification

Marija G. Pavlović[1], Miloš D. Momčilović[1], Sanja M. Živković[1], Marinela V. Šokarda Slavić[2], Marina B. Ristović[2], Zoran M.Vujčić[3]

[1] *„VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[2] *Institute of chemistry, technology and metallurgy- National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

[3]*Department of Biochemistry, University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

In this work, the screening of *Aspergillus* spp which produce pectinases by fermentation in a liquid medium was performed, as pectinases are effective in clarifying strawberry juice. Endo-pectinases were detected by the diffusion assay, and total pectinase activity was determined by the DNS method. The clarification of juice after pectinase treatment was determined by measuring the transmission at 660 nm, and an increase in juice yield was measured by centrifugation. The results obtained showed that these pectinases are very effective for the treatment of strawberry juice in comparison with the commercial pectinase preparation Lafase Fruit.

Zahvalnica: Autori se zahvaljuju MNTRI Republike Srbije za finansijsku podršku istraživanju kroz institucionalno finansiranje (Broj ugovora 451-03-9/2023-14/200017, 451-03-47/2023-01/200026 i *451-03-68/2023-14/200168)*

BH-7

Fenolni profil dekokta latica novih genotipova baštenskih ruža gajenih u Vojvodini

Nemanja Đ. Živanović[1], Marija M. Lesjak[1], Biljana Z. Božanić Tanjga[2], Dejan Z. Orčić[1],
Mirjana Z. Ljubojević[2], Nataša Đ. Simin[1]
[1] Univerzitet u Novom Sadu, Prirodno-metematički fakultet, Novi Sad, Srbija
[2] Univerzitet u Novom Sadu, Poljoprivredni fakultet, Novi Sad, Srbija

Baštenske ruže se gaje širom sveta kao ukrasne biljke i koriste se za izolaciju etarskog ulja [1]. Nakon izolacije etarskog ulja hidrodestilacijom nastaje dekokt kao otpadni produkt. Cilj ovog rada bio je procena potencijala dekokta kao izvora farmakološki aktivnih jedinjenja u cilju smanjenja otpada prilikom proizvodnje etarskih ulja ruža. Odabrani su dekokti ostali nakon izolacije etarskog ulja iz latica 3 nova genotipa baštenskih ruža gajenih u Vojvodini. Hemijski sastav dekokta je određen LC-MS-MS [2]. Kvantifikovani su polifenoli u značajnim količinama, posebno galna kiselina, kvercitrin i glikozidi kemferola i kvercetina. Dekokt ružinih latica je bogat izvor polifenola i mogao bi biti izvor biološki aktivnih jedinjenja za kozmetičku idustriju i doprineti smanjenju industrijskog otpada.

Phenolic profile of petals decoct from new genotypes of garden rose grown in Vojvodina

Nemanja Đ. Živanović[1], Marija M. Lesjak[1], Biljana Z. Božanić Tanjga[2], Dejan Z. Orčić[1],
Mirjana Z. Ljubojević[2], Nataša Đ. Simin[1]
[1] University of Novi Sad Faculty of Sciences, Novi Sad, Serbia
[2] University of Novi Sad Faculty of Agriculture, Novi Sad, Serbia

Garden roses are cultivated across the world and are used for the isolation of essential oil [1]. After the isolation of essential oil by hydrodistillation, decoct remains as a byproduct. The aim of this study was to evaluate the potential of decoct as a source of pharmacologically active compounds and to reduce waste during rose essential oil production. Decocts obtained after the isolation of essential oils from petals of 3 new genotypes of garden roses grown in Vojvodina were selected and their chemical composition was determined by the LC-MS-MS [2]. Phenolic compounds were quantified in significant amounts, especially gallic acid, quercitrin, kaempferol and quercetin glucosides. Decoct of rose petals is a rich source of phenolics and could be a source of biologically active compounds for the cosmetic industry and contribute to the reduction of industrial waste.

1. B. Božanić Tanjga, et al., *Horticulturae*. **2022**, *8*, 895.
2. D. Orčić, et al., *Food Chem*. **2014**, *143*, 48-53.

Acknowledgment: This study was supported by the Secretary for Higher Education and Scientific Research, Autonomous Province of Vojvodina (Grant No.142-451-2658/2021-01/1).

Elektrohemija

Electrochemistry

EH-1

Elektroforetski taložene kompozitne prevlake sa gentamicinom

Marija S. Djošić[1], Ana Janković[2], Milena Stevanović[2], Maja Vukašinović-Sekulić[2], Vesna Mišković-Stanković[3]

[1] Institut za tehnologiju nuklearnih i drugih mineralnih sirovina, Beograd, Srbija
[2] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija
[3] Fakultet za ekologiju i zaštitu životne sredine, Univerzitet Union – Nikola Tesla, Beograd, Srbija

Uvođenje antibiotika u polimer/mineralnu kompozitnu prevlaku poboljšava antibakterijska svojstva prevlaka. Kompozitna prevlaka (hidroksiapatit - HAP, poli(vinilalkohol), hitozan, gentamicin) dobijena je elektroforetskim taloženjem iz četvorokomponentne vodene suspenzije. Primenom termogravimetrijske i rendgenske difrakcione analize pokazano je prisustvo karbonatno-supstituisanog HAP. Antibakterijska aktivnost kompozitne prevlake sa gentamicinom potvrđena je protiv soja *S. aureus* i *E. coli*, čineći ovu prevlaku pogodnom za potencijalnu primenu u biomedicini.

Electrophoretically deposited gentamicin-loaded composite coating

Marija S. Djošić[1], Ana Janković[2], Milena Stevanović[2], Maja Vukašinović-Sekulić[2], Vesna Mišković-Stanković[3]

[1] Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia
[2] University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
[3] Faculty of Ecology and Environmental Protection, University Union – Nikola Tesla, Belgrade, Serbia

Antibiotic introduction in polymer/mineral coating can improve the antibacterial properties of coatings. Composite coating (hydroxyapatite, poly(vinyl alcohol), chitosan, gentamicin) was fabricated from a four-component aqueous suspension using electrophoretic deposition. Structural and morphological characterization of the coating was investigated by X-ray diffraction and thermogravimetric analysis proving carbonate-substituted HAP. The presence of gentamicin contributed to the antibacterial activity of composite coating against *S. aureus* and *E. coli* strains, representing a suitable material for possible application in biomedicine.

Acknowledgment: This research is supported by the Ministry of Science, Technological Development and Innovation, Republic of Serbia, (Contract No. 451-03-47/2023–01/200287 and 451-03-47/2023–01/200023) and University Union – Nikola Tesla, Belgrade, Republic of Serbia. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 952033.

EH-2

Hidrogelni materijali za obloge rana sa elektrohemijski sintetisanim nanočesticama srebra

Ana D. Janković[1], Maja Vukašinović-Sekulić[1], Vesna Kojić[2], Vesna Mišković-Stanković[3]
[1] *Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2] *Univerzitet u Novom Sadu, Institut za onkologiju Vojvodine, Sremska Kamenica, Srbija*
[3] *Univerzitet Union – Nikola Tesla, Fakultet za ekologiju i zaštitu životne sredine Beograd, Srbija*

Široko rasprostranjena sistemska primena antibiotika dovela je do razvoja rezistencije kod mnogih bakterijskih sojeva. Komercijalni materijali za obloge rana sada se uglavnom oslanjaju na jonsko srebro, efikasno samo u većim dozama, kao antibakterijsko sredstvo. Zbog toga su proizvedeni novi materijali, kompoziti polielektrolitnog kompleksa sa antibakterijskim nanočesticama srebra za primenu kao obloge za rane, na bazi polisaharida prirodnog porekla-alginata sa sintetičkim biokompatibilnim polimerom-poli(vinil alkohol) kao elastičnom matricom. Kinetika antibakterijske aktivnosti hidrogelova praćena je prema sojevima bakterija *S. aureus* i *E. coli*, a citotoksičnost je ispitana MTT i DET testovima prema dve različite ćelijske linije fibroblasta.

Hydrogel wound dressing materials with electrochemically embedded silver nanoparticles

Ana D. Janković[1], Maja Vukašinović-Sekulić[1], Vesna Kojić[2], Vesna Mišković-Stanković[3]
[1] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Novi Sad, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia*
[3] *University Union – Nikola Tesla, Faculty of Ecology and Environmental Protection, Belgrade, Serbia*

The widespread systemic administration of antibiotics led to resistance developing in many bacterial strains. Commercial wound dressing materials now rely mostly on ionic silver, only effective in higher doses, as an antibacterial agent. Therefore, novel materials antibacterial silver nanoparticles-loaded polyelectrolyte complex composites for wound dressing applications were produced, based on natural-origin polysaccharide-alginate with synthetic biocompatible polymer-poly(vinyl alcohol) as an elastic matrix. The antibacterial activity kinetics of the hydrogels was determined against *S. aureus* and *E. coli* strains. Cytotoxicity was tested by MTT and DET tests on two different fibroblast cell lines.

This research is supported by the Ministry of Science, Technological Development and Innovation, Republic of Serbia, (Grant No. 451-03-47/2023–01/200287 and 451-03-47/2023–01/200023) and University Union – Nikola Tesla, Belgrade, RS. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952033.

EH-3

Peptidi i njihove sastavne komponente kao inhibitori korozije čelika: eksperimentalni i teorijski pristup

Anđela R. Simović[1], Sanja Stevanović[1], Branislav Milovanović[2], Mihajlo Etinski[2], Jelena B. Bajat[3]

[1]Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija
[2]Univerzitet u Beogradu, Fakultet za fizičku hemiju, Beograd, Srbija
[3]Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija

Ekološki prihvatljivi inhibitori privlače pažnju mnogih istraživača zbog povoljnih svojstava: biorazgradivost, netoksičnost, dostupnost i obnovljivost. U njih spadaju i amonokiseline (AK), kao sastojci od vitalnog značaja za sva živa bića. U radu je ispitan inhibitorski efekat nekoliko AK na čeliku u 1 M HCl: tri samostalne AK, glicin, glutaminska kiselina i cistein; smeša ove tri AK, kao i njihov dipeptid (glicin i glutaminska kiselina) i tripeptid glutation (glicin, glutaminska kiselina i cistein). Inhibitorska efikasnot AK je određena elektrohemijskim merenjima. Meren je ugao kvašenja površine čelika sa adsorbovanim inhibitorom, energija veza inhibitora i supstrata je određivana XPS metodom, a topografija AFM. Razlike u vezivanju inhibitora za supstrat su analizirane teorijskim proračunima.

Peptides and their constituents as steel corrosion inhibitors: an experimental and theoretical approach

Anđela R. Simović[1], Sanja Stevanović[1], Branislav Milovanović[2], Mihajlo Etinski[2], Jelena B. Bajat[3]

[1]University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Belgrade, Serbia
[2]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia
[3]University of Belgrade, Faculty for Technology and Metallurgy, Belgrade, Serbia

Green eco-friendly inhibitors have become very popular due to their remarkable properties such as biodegradability, environmental acceptability, safety, availability, and renewability. Amino acids (ACs) are one of them, as constituents of vital importance for all living beings. Several AC systems were examined in this study as steel inhibitors in 1 M HCl solution: three ACs separately, glycine, glutamic acid and cysteine; their mixture, as well as their dipeptide (glycine and glutamic acid) and tripeptide glutathione (glycine, glutamic acid and cysteine). Their inhibition efficiency was evaluated and compared by electrochemical methods. The steel surface with adsorbed inhibitor was analyzed by contact angle measurements, AFM and XPS. The intrinsic differences in adsorption between these green inhibitors were analyzed by theoretical calculations.

EH-4

Poboljšanje oksidacije etanola na Pd elektrohemijski nataloženom preko Sb_2O_3

Milica G. Košević[1], Jelena D. Lović[1,*]

[1]Centar za elektrohemiju, Institut za hemiju, tehnologiju i metalurgiju, Univerzitet u Beogradu, Njegoševa 12, 11000 Beograd, Srbija

Elektrohemijski nataloženi Pd i Sb-Pd katalizatori su ispitivani u reakciji oksidacije etanola cikličnom voltametrijom i hronoampeometrijskom metodom. Paladijum-antimon je sintetisan na nosaču od staklastog ugljenika u dvo-stepenom procesu, tako što je najpre nataložen Sb, a zatim Pd. Tako je dobijen Sb-Pd elektrokatalizator sa atomskim odnosom Sn:Pd (0.2:0.8). U odnosu na nemodifikovanu Pd elektrodu, dodatak Sb rezultuje u povećanoj aktivnosti i stabilnosti bimetalnog katalizaotora u elektrohemijskoj oksidaciji etanola. Posle hronoamperometrijskih ispitivanja, Sb-Pd katalizator je podvrgnut cikliziranju kako bi se povratila aktivnost, čime je utvrđena stabilnost sastava elektrode. Poboljšane karakteristike Sb-Pd su pripisane bifunkcionalnom mehanizmu delovanja i elektronskom efektu.

Enhancement of ethanol oxidation on Pd electrodeposited over Sb_2O_3

Milica G. Košević[1], Jelena D. Lović[1,*]

[1] Department of Electrochemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

Electrodeposited Pd and Sb-Pd catalysts were tested for the ethanol oxidation reaction by cyclic voltammetry and chronoamperometry. Palladium-antimony deposit was synthesized on a glassy carbon substrate by a two-step process, comprising deposition of Sb followed by deposition of Pd. The Sb-Pd electrocatalyst with the Sn:Pd atomic ratio 0.2:0.8 was obtained. Compared with pure Pd, the incorporation of Sb results in the increase of activity and stability of bimetallic catalyst for the electrocatalytic ethanol oxidation reaction. Besides upon the end of the current-time transient, the investigated Sb-Pd catalyst was subjected to the potential cycling showing the ability to recover activity loss implying the surface composition stability. The enhanced performance of Sb-Pd is mainly ascribed to the bifunctional mechanism and electronic effect.

Acknowledgments: This work was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (RS) (Grant No. 451-03-47/2023-01/200026).

EH-5

Elektroanalitičko određivanje prehrambene boje Sunset Yellow u sokovima i piću

Tamara G. Milosavljević[1], Kristina M. Jovanović[1], Jovana S. Acković[2], Ružica J. Micić[2],
Branka B. Petković[2]
[1] Univerzitet u Nišu – Tehnološki fakultet, Leskovac, Srbija
[2] Univerzitet u Prištini – Prirodno-matematički fakultet, Kosovska Mitrovica, Srbija

U današnje vreme razvoj ekonomičnih i dostupnih metoda za određivanje široko korišćenih sintetičkih prehrambenih azo boja je prioritet jer konzumiranje njihovih većih količina može dovesti do ozbiljnih zdravstvenih poremećaja. U ovom radu je ispitano elektrohemijsko ponašanje boje Sunset Yellow E110 (SY), na elektrodama od staklastog ugljenika (GC) i borom dopovanog dijamanta. Usled boljeg elektrohemijskog odziva na GC-u, razrađena je kvadratno-talasna voltametriska metoda pod optimizovanim eksperimentalnim uslovima i parametrima tehnike. U Britton-Robinson-ovom puferu, na pH 5, dobijen je radni opseg od 0,1-100 µM sa granicom detekcije (LOD) od 0,027 µM, što je za dva reda veličina niža granica detekcije od one dobijene spektrofotometrijskom metodom. Metoda je uspešno primenjena u uzorcima različitih sokova i pića pa može biti primenjena i za testiranje prisustva veštačke boje SY u sličnim uzorcima.

Electroanalytical determination of food dye Sunset Yellow in beverage products

Tamara G. Milosavljević[1], Kristina M. Jovanović[1], Jovana S. Acković[2], Ružica J. Micić[2],
Branka B. Petković[2]
[1] University of Niš – Faculty of Technology, Leskovac, Serbia
[2] University of Priština – Faculty of Sciences and Mathematics in Kosovska Mitrovica, Serbia

Nowadays, the development of economical and accessible methods for the determination of widely used synthetic azo dye is a priority because consuming their larger amounts in food can lead to serious health disorders. In this work, the electrochemical investigation of Sunset Yellow E110 (SY) on glassy carbon (GC) and boron-doped diamond electrodes was investigated. Due to the better electrochemical response on the GC, a square-wave voltammetric method was developed under optimized experimental conditions and parameters. In the Britton-Robinson buffer, at pH 5, a working range of 0.1-100 µM was obtained with a limit of detection (LOD) of 0.027 µM which is two orders of magnitude lower than the detection limit obtained by the spectrophotometric method. The method was successfully applied in samples of various juices and drinks, so it can be applied to test the presence of artificial color SY in similar samples.

Acknowledgment: Thanks to the Ministry of Science, Technological Development and Innovation of RS, grant no. 451-03-47/2023-01/ 200123.

EH-6

Cerijum laktat kao zeleni inhibitor korozije AA2024 aluminijumske legure

Anđela R. Simović[1], Bojana M. Radojković[1], Bore V. Jegdić[1], Milica Milojević[2], Jelena B. Bajat[3]
[1]Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Njegoševa 12, Beograd
[2]Univerzitet u Beogradu, Fizički fakultet, Studentski trg 12, Beograd
[3]Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Karnegijeva 4, Beograd

U ovom radu je ispitan inhibitorni efekat smeše Ce-hlorida i Na-laktata na leguru aluminijuma AA2024 u 0,1 M rastvoru NaCl. Za ispitivanje opšte otpornosti na koroziju primenjena je elektrohemijska impedansna spektroskopija (EIS), dok su polarizaciona merenja primenjena za određivanje otpornosti legure na pitting koroziju u rastvoru sa NaCl i rastvorima koji sadrže inhibitor. Prisustvo cerijuma na katodnim intermetalnim česticama potvrđeno je SEM/EDS analizom. Sinergija Ce-hlorida i Na-laktata je bila efikasniji inhibitor korozije od samog Ce-hlorida. Mešavina inhibitora je mešoviti inhibitor korozije sa većim uticajem na usporavanje katodne reakcije redukcije kiseonika. Adsorpcija inhibitora, odnosno prisustvo cerijuma u različitim oksidacionim stanjima (Ce^{3+}, i Ce^{4+}), i laktatnog anjona (C–C/C–H, C–OH, C = O, i O–C=O grupa) potvrđeno je XPS analizom. Predložen je mehanizam adsorpcije inhibitora na površini legure AA2024 u rastvoru NaCl.

Cerium lactate as green corrosion inhibitor of AA2024 alloy

Anđela R. Simović[1], Bojana M. Radojković[1], Bore V. Jegdić[1], Milica Milojević[2], Jelena B. Bajat[3]
[1]University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Njegoševa 12, Belgrade
[2]University of Belgrade, Faculty of Physics, Studentski trg 12, 11000 Belgrade
[3]University of Belgrade, Faculty for Technology and Metallurgy, Karnegijeva 4, Belgrade

This paper evaluated the inhibitory effect of Ce-chloride and Na-lactate mixture on the AA2024 aluminium alloy in 0.1 M NaCl solution. Electrochemical impedance spectroscopy (EIS) was applied for testing the general corrosion resistance, while potentiodynamic polarisation measurement was applied for determining the alloy pitting corrosion resistance in NaCl and inhibitive solutions. The presence of cerium on the cathodic intermetallic particles was confirmed by SEM/EDS analysis. The mixture of Ce-chloride and Na-lactate was a more effective corrosion inhibitor than Ce-chloride alone. The inhibitors mixture is a mixed-type corrosion inhibitor with a higher influence on slowing down the cathodic reaction of oxygen reduction. The adsorption of the inhibitor, the presence of cerium in different oxidation states (Ce^{3+}, and Ce^{4+}), and lactate anion (C–C/C–H, C–OH, C = O, and O–C=O group) were confirmed by XPS analysis. A mechanism of inhibitor adsorption on the surface of AA2024 alloy in NaCl solution was proposed.

EH-7

Bioaktivne kompozitne prevlake na bazi hidroksiapatita na titanu za primene u ortopediji

Milena Lj. Stevanović[1], Marija Djošić[2], Ana Janković[1], Vesna Kojić[3], Vesna Mišković-Stanković[4]

[1] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija
[2]Institut za tehnologiju nuklearnih i drugih mineralnih sirovina, Beograd, Srbija
[3]Univerzitet u Novom Sadu, Institut za onkologiju Vojvodine, Sremska Kamenica, Srbija
[4]Univerzitet Union – Nikola Tesla, Fakultet za ekologiju i zaštitu životne sredine Beograd, Srbija

Kompozitna prevlaka hidroksiapatita (HAP) sa prirodnim polimerima hitozanom (CS) i polivinil-alkoholom (PVA), kao i sa antibiotikom gentamicinom (Gent) je elektroforetski taložena na titanu, pri konstantnom naponu. Formiranje nove kompozitne HAP/PVA/CS/Gent prevlake je potvrđeno infracrvenom spektroskopijom sa Furijeovom transformacijom. Necitotoksični efekat istaložene HAP/PVA/CS/Gent prevlake je dokazan MTT testom prema dve ćelijske linije (MRC-5 i L929). Sposobnost HAP/PVA/CS/Gent prevlake da indukuje i promoviše osteointegraciju je pokazana ALP testom.

Bioactive hydroxyapatite-based composite coatings on titanium for orthopedic applications

Milena Lj. Stevanović[1], Marija Djošić[2], Ana Janković[1], Vesna Kojić[3], Vesna Mišković-Stanković[4]

[1] University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
[2]Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia
[3]University of Novi Sad, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia
[4]University Union – Nikola Tesla, Faculty of Ecology and Environmental Protection, Belgrade, Serbia

Composite coating of hydroxyapatite (HAP) with natural polymers chitosan (CS) and poly(vinyl alcohol) (PVA) with the antibiotic gentamicin (Gent) was electrophoretically deposited on titanium from an aqueous suspension, at a constant voltage. Formation of a new composite HAP/PVA/CS/Gent coating was confirmed by Fourier transform infrared spectroscopy. Non-cytotoxicity of deposited HAP/PVA/CS/Gent coating was demonstrated by MTT assay towards two types of cell lines (MRC-5 and L929). HAP/PVA/CS/Gent coating ability to induce and promote the osseointegration process was proved by the ALP assay.

Acknowledgment: This research is supported by the Ministry of Science, Technological Development and Innovation, Republic of Serbia, (Contract No. 451-03-47/2023–01/200287 and 451-03-47/2023–01/200023) and University Union – Nikola Tesla, Belgrade, Republic of Serbia. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952033.

Zelena hemija

Green Chemistry

GC-1

Odabir NaDES rastvarača za održive, ekološki prihvatljive kozmetičke sastojke pomoću COSMO-RS metode

Ilija N. Cvijetić[1], Đurđa Ivković[2], Petar Todorović[1], Filip Andrić[1], Petar Ristivojević[1]
[1] *Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu - Inovacioni centar Hemijskog fakulteta, Beograd, Srbija*

Prirodne eutektičke smeše (Natural Deep Eutectic Solvents, NaDES) sastoje se od donora i akceptora vodonične veze i imaju niže tačke topljenja od pojedinačnih komponenti. Svojstva ovih rastvarača mogu se podesiti odabirom sastojaka i njihovog molskog odnosa. U ovoj studiji koristili smo COSMO-RS metodu za predviđanje koeficijenata aktiviteta 12 fenolnih jedinjenja u 105 NaDES-a. Ovi rastvarači su se sastojali od ekvimolarne smeše betaina, karnitina, kreatina i ornitina kao donora vodonične veze i različitih šećera i aminokiselina kao akceptora vodonične veze. Nekoliko NaDES-a je pokazalo veći afinitet prema svim fenolima u poređenju sa metanolom, a betain-glicerol, betain-ksilitol i karnitin-urea su smeše koje su pokazale najveći afinitet prema svim svim polifenolima.

Screening natural deep eutectic solvents (NaDES) using COSMO-RS for sustainable and environmentally-friendly cosmetic ingredients

Ilija N. Cvijetić[1], Đurđa Ivković[2], Petar Todorović[1], Filip Andrić[1], Petar Ristivojević[1]
[1] *University of Belgrade - Faculty of chemistry, Belgrade, Serbia*
[2] *University of Belgrade -Iinovative centre of Faculty of Chemistry, Belgrade, Serbia*

DES are mixtures of a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA) that, when combined in a specific molar ratio, exhibit a significant decrease in melting point and become liquid at room temperature. DES can be tailored to meet different physicochemical requirements by altering the HBA:HBD ratio or the nature of the compounds. In this study, we utilized the COSMO-RS method to predict the activity coefficients of 12 phenolic compounds in 105 NaDES. These NaDES contained equimolar mixtures of betaine, carnitine, creatine, and ornithine as HBAs and various sugars and amino acids as HBDs. The NaDES were compared to methanol, and several mixtures exhibited higher affinities to all phenolics. The most promising NaDES were betaine-glycerol, betaine-xylitol, and carnitine-urea. We are currently conducting experimental validation of the extraction efficiency of these cosmetically acceptable solvents. In summary, we have identified promising NaDES mixtures that could replace conventional solvents and contribute to the development of sustainable, bio-based extracts.

Acknowledgment: *This research was funded by The Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Program, N°. 389927, and the MNTR, contracts N°. 451-03-47/2023-01/200168 and 451-03-47/2023-01/200288.*

Medicinska hemija

Medicinal Chemistry

MH-1

Totalna sinteza 6-*epi*-(−)-kleistenolida

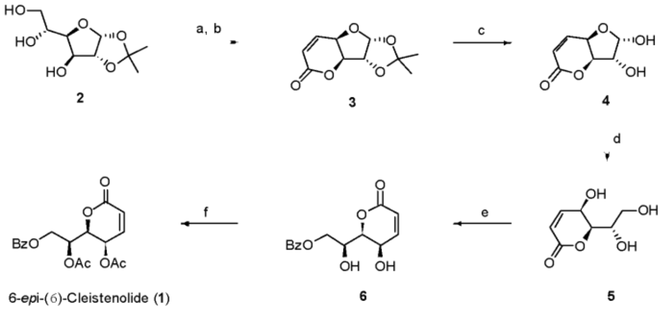
Goran Benedeković[1], Mirjana Popsavin[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] *Univerzitet u Novom Sadu – Prirodno-matematički fakultet, Novi Sad, Srbija*
[2] *Univerzitet u Novom Sadu – Medicinski fakultet, Institut za onkologiju Vojvodine, Sremska Kamenica, Srbija*
[3] *Srpska akademija nauka i umetnosti, Beograd, Srbija*

6-*epi*-(−)-Kleistenolid (**1**) je C-6 epimer prirodnog proizvoda (−)-kleistenolida koji pokazuje antibakterijsku, antigljivičnu i antiproliferativnu aktivnost. U ovom radu je prikazana nova totalna sinteza 6-*epi*-(−)-kleistenolida (**1**). Polazno jedinjenje je diol **4** koji je dobijen iz monoacetonida D-glukoze **2** u dve sintetičke faze. Molekul **4** sa prikazane sheme je preveden u intermedijerni monobenzoat **6** koji nakon acetilovanja daje finalni proizvod **1**.

Total synthesis of 6-*epi*-(−)-cleistenolide

Goran Benedeković[1], Mirjana Popsavin[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] *University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia*
[2] *University of Novi Sad – Faculty of Medicine, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia*
[3] *Serbian Academy of Sciences and Arts, Belgrade, Serbia*

6-*epi*-(−)-Cleistenolide (**1**) is a C-6 epimer of natural product (−)-cleistenolide that exhibits antibacterial, antifungal and antiproliferative activity. Herein, we report a new total synthesis of 6-*epi*-(−)-cleistenolide (**1**). Diol **4**, readily available from monoacetone D-glucose (**2**) over two steps, has served as a convenient starting material in this work. Molecule **4,** from the scheme, was converted to the intermediary monobenzoate **6,** which was finally acetylated to final product **1**.



Reagents and conditions: (a) $NaIO_4$, rt, aq 90% MeOH, MCMP, 0 °C, rt; (b) TsOH × H_2O, CH_2Cl_2, rt; (c) aq 90% TFA, CH_2Cl_2, 0 °C, rt; (d) $(Bu)_4N(BH_3CN)$, AcOH, rt; (e) BzCl, 1:1 Py/CH_2Cl_2, rt; (f) Ac_2O, TsOH × H_2O, rt.

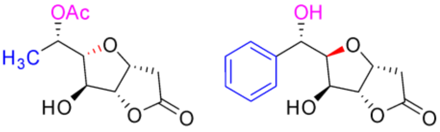
Acknowledgment to the financial support of a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-47/2023-01/200125), and (in part) by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

MH-2

Novi analozi (+)-protulaktona A i 7-*epi*-(+)-goniofufurona

Sanja Đokić[1], Jovana Francuz[1], Mirjana Popsavin[1], Marko V. Rodić[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] Univerzitet u Novom Sadu – Prirodno-matematički fakultet, Novi Sad, Srbija
[2] *Univerzitet u Novom Sadu – Medicinski fakultet, Institut za onkologiju Vojvodine, Sremska Kamenica, Srbija*
[3] *Srpska akademija nauka i umetnosti, Beograd, Srbija*

(+)-Protulakton A (**1**) je poliketid izolovan iz morske gljive *Aspergillus sp*. SF-5044, dok je 7-*epi*-(+)-goniofufuron (**2**) stiril-lakton izolovan iz etanolnog ekstrakta kore drveta *Goniothalamus giganteus* (Slika 1.).[1,2] Ova dva prirodna proizvoda pokazuju zadovoljavajuću antiproliferativnu aktivnost. Kombinacijom strukturnih elemenata ovih citotoksičnih laktona sintetizovani su novi analozi, kojima je ispitana antiproliferativna aktivnost. Uticaj strukturnih promena na ispoljenu citotoksičnu aktivnost novih analoga će biti diskutovan.



1 **2**

*Slika 1. Strukture (+)-protulaktona A (**1**) i 7-epi-(+)-goniofufurona (**2**).*

Novel analogues of (+)-protulactone A and 7-*epi*-(+)-goniofufurone

Sanja Đokić[1], Jovana Francuz[1], Mirjana Popsavin[1], Marko V. Rodić[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] *University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia*
[2] *University of Novi Sad – Faculty of Medicine, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia*
[3] *Serbian Academy of Sciences and Arts, Belgrade, Serbia*

(+)-Protulactone A (**1**) is a polyketide isolated from the marine fungus *Aspergillus sp.* SF-5044, while 7-*epi*-(+)-goniofufurone (**2**) is a styryl-lactone isolated from the ethanolic extract of the bark of *Goniothalamus giganteus*.[1,2] These two natural products show satisfactory antiproliferative activities. By combining the structural elements of these cytotoxic lactones, new analogues were synthesized, which were tested for their antiproliferative activity. The influence of structural changes on manifested cytotoxic activities of the new analogues will be discussed.

1. J. H. Sohn, H. Oh, *Bull. Korean Chem. Soc*. **2010**, *31(6)*, 1695.
2. X. P. Fang, J. E. Anderson, C. J. Chang, J. L. Mclaughlin, *J. Nat. Prod.* **1991**, *54*, 1034.

Acknowledgment to the financial support of a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-47/2023-01/200125), and (in part) by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

MH-3

Sinteza novih derivata artemizinina sa antitumorskom aktivnošću na rezistentne ćelije raka

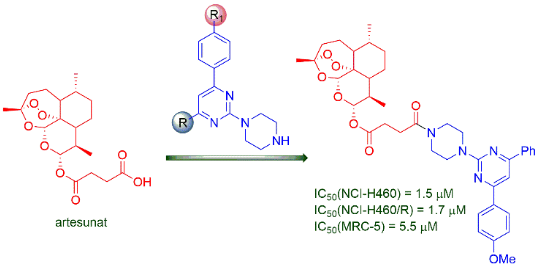
Ljiljana K. Koračak[1], Ema Lupšić[2], Mirna Jovanović[2], Miroslav Novakovic[3], Milica Pešić[2], Igor M. Opsenica[4]
[1]Inovacioni centar Hemijskog fakulteta u Beogradu, d.o.o., Beograd, Srbija
[2]Univerzitet u Beogradu – Institut za biološka istraživanja „Siniša Stanković“, Beograd, Srbija
[3]Univerzitet u Beogradu – Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija
[4]Univerzitet u Beogradu – Hemijski fakultet, Beograd, Srbija

Značaj artemizinina i njegovih derivata se ogleda u biološkoj aktivnosti jer osim što su našli primjenu kao efikasni lijekovi za liječenje malarije, pokazuju i antitumorsku aktivnost. Pirimidinsko jezgro je važno zbog prisustva ovog strukturnog motiva u prirodnim proizvodima, u odobrenim lijekovima, ali i u biološki aktivnim molekulima. U okviru ovog istraživanja prijavljena je sinteza novih hibridnih molekula dobijenih povezivanjem dvije farmakofore, kao i njihova antitumorska aktivnost na rezistentnim i osjetljivim ćelijama nesitnoćelijskog karcinoma pluća.

Synthesis of novel artemisinin derivatives with anticancer activity against multidrug-resistant cancer cells

Ljiljana K. Koračak[1], Ema Lupšić[2], Mirna Jovanović[2], Miroslav Novakovic[3], Milica Pešić[2], Igor M. Opsenica[4]
[1]Innovative Centre, Faculty of Chemistry, Belgrade, Ltd., Serbia
[2]University of Belgrade – Institute for Biological Research “Siniša Stanković” Belgrade, Serbia
[3]University of Belgrade – Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia [4]University of Belgrade – Faculty of Chemistry, Belgrade, Serbia

In addition to being used for the effective treatment of malaria, artemisinin and derivatives also exhibit anticancer activity. The importance of the pyrimidine scaffold is evidenced by its presence in natural products and approved drugs, as well as in biologically active compounds. In this study, we report the synthesis of novel hybrid molecules comprising two pharmacophores and their activity against sensitive and multidrug-resistant human non-small cell lung carcinoma cells.



Slika 1. Sinteza novih artemizinin-pirimidinskih hibrida

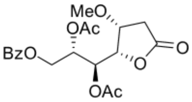
Zahvalnica: Ovo istraživanje je finansirano od strane Ministarstva nauke, tehnološkog razvoja i inovacija Republike Srbije (evidencioni broj: 451-03-47/2023-01/200168, 451-03-47/2023-01/200288).

MH-4

Citotoksičnost i SAR analiza novih analoga kleistanolata

Ivana Kovačević[1], Jelena Kesić[1], Mirjana Popsavin[1], Marko V. Rodić[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] *Univerzitet u Novom Sadu – Prirodno-matematički fakultet, Novi Sad, Srbija*
[2] *Univerzitet u Novom Sadu – Medicinski fakultet, Institut za onkologiju Vojvodine, Sremska Kamenica, Srbija*
[3] *Srpska akademija nauka i umetnosti, Beograd, Srbija*

Prirodni kleistanolat je izolovan iz metanolnog ekstrakta listova *Chleistochlamys kirkii*.[1] Nedavno smo publikovali njegovu prvu totalnu sintezu i preliminarna ispitivanja antitumorske aktivnosti. U cilju utvrđivanja strukturnih karakteristika važnih za aktivnost, sintetizovali smo veći broj analoga kleistanolata, i istražili odnos struktura-aktivnost. Ovde želimo da predstavimo i detaljno prodiskutujemo naše najnovije rezultate.



(–)-Kleistanolat

Cytotoxicity and SAR analysis of new cleistanolate analogues

Ivana Kovačević[1], Jelena Kesić[1], Mirjana Popsavin[1], Marko V. Rodić[1], Vesna Kojić[2], Velimir Popsavin[1,3]
[1] *University of Novi Sad – Faculty of Sciences, Novi Sad, Serbia*
[2] *University of Novi Sad – Faculty of Medicine, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia*
[3] *Serbian academy of sciences and arts, Belgrade, Serbia*

Natural cleistanolate is isolated from the methanol extract of leaves of *Cleistochlamys kirkii*.[1] We recently published its first synthesis along with preliminary investigation of antitumor activity.[2] In order to determine structural characteristics important for activity, we synthesized a number of cleistanolate analogs, and investigated the structure-activity relationship. Herein we want to present and discuss in detail our newest results.

1. S. S. Nyandoro, J. J. E. Munisii, A. Gruhonjic, S. Duffu, 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.
2. J. Kesić, I. Kovačević, M. Popsavin, G. Benedeković, M. V. Rodić, V. Kojić, V. Popsavin, *Bioorg. Chem.* **2022**, *128*, 106073.

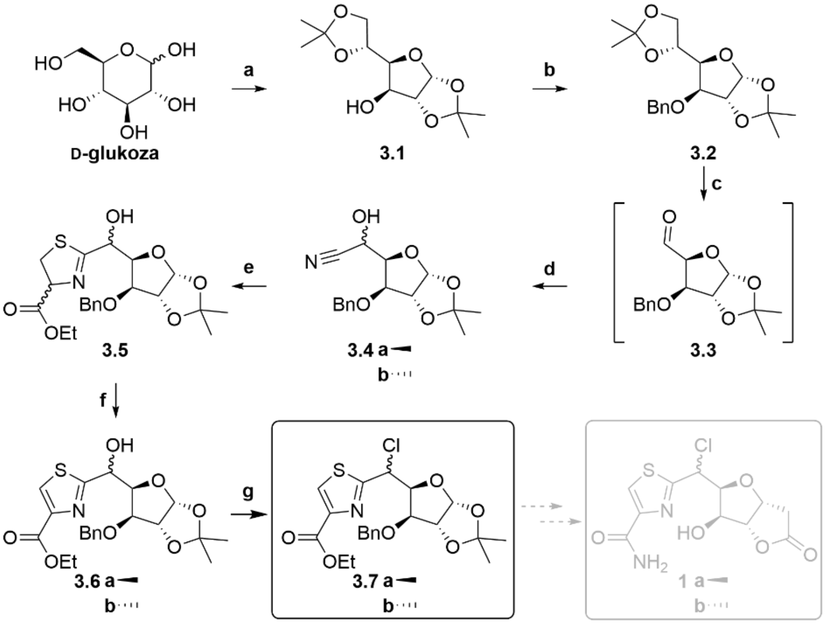
Acknowledgment to the financial support from Ministry of Education, Science and Technological Development (Grant No. 451-03-47/2023-01/200125), and (in part) by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

MH-5

Sinteza intermedijera na putu do hlorovanih hibrida tiazofurina i goniofufurona

Bojan D. Levovnik[1], Jelena D. Kesić[1], Sanja M. Đokić[1], Miloš M. Svirčev[1]
[1] *Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Novi Sad, Srbija*

Opisana je sinteza dva hlorovana derivata D-glukoze (**3.7a** i **3.7b**) u sedam faza. Sintetisani epimeri su intermedijeri na putu do ciljnih jedinjenja (**1a** i **1b**, Šema 1), hlorovanih hibrida sintetskog *C*-nukleozida tiazofurina i prirodnog stiril-laktona (+)-goniofufurona, i deo su planirane serije halogenovanih homologa čija će antiproliferativna aktivnost biti ispitana i 3D-QSAR model napravljen.



*Šema 1. Sintetski put do intermedijera **3.7a** i **3.7b** i planirana ciljna jedinjenja **1a** i **1b**.*

Synthesis of the intermediates on the pathway to chlorinated hybrids of tiazofurin and goniofufurone

Bojan D. Levovnik[1], Jelena D. Kesić[1], Sanja M. Đokić[1], Miloš M. Svirčev[1]
[1] *University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia*

The 7-step synthesis of 2 chlorinated derivatives of D-glucose (**3.7a** and **3.7b**) has been described. The synthesized epimers are the intermediates on the pathway to final compounds (**1a** and **1b**, Scheme 1), chlorinated hybrids of synthetic *C*-nucleoside tiazofurin and natural styryl-lactone (+)-goniofufurone. They are a part of the outlined library of halogenated homologs whose antiproliferative activity will be determined and the 3D-QSAR model built.

MH-6

Potencijal monoterpena karvakrola i geraniola u inhibiciji oralnih patogena

Milica Nemoda[1], Biljana Nikolić[2], Miloš Momčilović[1], Sanja Živković[1], Dejan Marković[3], Lada Živković[4], Jelena Marinković[1]

[1] *Univerzitet u Beogradu – Institut za nuklearne nauke „Vinča“- Institut od nacionalnog značaja za Repubiku Srbiju, Beograd, Srbija*
[2] *Univerzitet u Beogradu - Biološki fakultet, Beograd, Srbija*
[3] *Univerzitet u Beogradu - Stomatološki fakultet, Beograd, Srbija*
[4] *Univerzitet u Beogradu – Farmaceutski fakultet, Beograd, Srbija*

Cilj istraživanja bio je ispitivanje antimikrobnog potencijala monoterpena karvakrola i geraniola na bakterijskim izolatima *Streptococcus* spp. od značaja za etiologiju karijesa (*S. mutans, S. sanguinis, S. parasanguinis, S. gordonii*). Antimikrobni potencijal karvakrola i geraniola testiran je mikrodilucionim testom, kojim su određene minimalna inhibitorna koncentracija (MIC) i minimalna baktericidna koncentracija (MBC). Testirani monoterpeni ispoljili su značajan antimikrobni potencijal, MIC je bio u opsegu od 0.55 mg/mL do 4.39 mg/mL, a MBC od 2.20 mg/mL do 19.54 mg/mL.

Antibacterial potential of the monoterpenes carvacrol and geraniol against oral pathogens

Milica Nemoda[1], Biljana Nikolić[2], Miloš Momčilović[1], Sanja Živković[1], Dejan Marković[3], Lada Živković[4], Jelena Marinković[1]

[1] *University of Belgrade - Vinca Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Belgrade, Serbia*
[2] *University of Belgrade - Faculty of Biology, Belgrade, Serbia*
[3] *University of Belgrade - Faculty of Dentistry, Belgrade, Serbia*
[4] *University of Belgrade - Faculty of Pharmacy, Belgrade, Serbia*

The aim of our study was to investigate the antimicrobial potential of monoterpenes carvacrol and geraniol towards the *Streptococcus* spp. isolates relevant to tooth caries (*S.* mutans, *S. sanguinis, S. parasanguinis, S gordonii*). Microdilution test was used for the assessment of the antimicrobial potential of carvacrol and geraniol, and the minimal inhibitory concentrations (MICs) and minimal bactericidal concentrations (MBCs) were determined. Tested monoterpenes achieved notable antimicrobial activity, with MICs ranging from 0.55 mg/mL to 4.39 mg/mL, and MBCs from 2.20 mg/mL to 19.54 mg/mL.

Acknowledgment: Authors thank the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia for the financial support to the research through institutional funding (Contract numbers 451-03-47/2023-01/200017)

MH-7

Ru(II) arenski kompleksi sa piridinskim ligandima: sinteza i antimikrobna aktivnost

Marija V. Dimitrijević[1], Ljiljana E. Mihajlović-Lalić[2], Sanja Grgurić-Šipka[3], Stefan R. Nikolić[2], Tamara A. Petrović[3], Jelena M. Poljarević[3]
[1]*Univerzitet u Nišu – Medicinski fakultet, Niš, Srbija*
[2]*Inovacioni centar Hemijskog fakulteta u Beogradu, d.o.o, Beograd, Srbija*
[3]*Univerzitet u Beogradu – Hemijski fakultet, Beograd, Srbija*

Kompleksi metala retko se koriste kao potencijalni antimikrobni agensi. U ovom radu smo prikazali sintezu, hemijsku karakterizaciju i antimikrobnu aktivnost 14 arenskih Ru(II) kompleksa sa piridinskim ligandima. Strukturu i čistoću dobijenih jedinjenja potvrdili smo koristeći ^{1}H, ^{13}C NMR i IC spektroskopiju, MS i EA. Mikrodilucioni esej je korišćen za određivanje minimalne inhibitorne koncentracije (MIC) i minimalne baktericidne koncentracije sintetisanih jedinjenja. Streptomicin i hloramfenikol su korišćeni kao standard. Najbolja aktivnost prema ispitivanim sojevima bakterija zapažena je na soju *E. coli*, sa MIC vrednošću 1,25 mg/mL, kompleksa sa 2,4- i 2,5-piridindikarboksilnim ligandima. Svi sintetisani kompleksi pokazali su podjednako dobru aktivnost prema *C. Albicans.*

Ru(II) arene based pyridil complexes: synthesis and antimicrobial potency

Marija V. Dimitrijević[1], Ljiljana E. Mihajlović-Lalić[2], Sanja Grgurić-Šipka[3], Stefan R. Nikolić[2], Tamara A. Petrović[3], Jelena M. Poljarević[3]
[1]*University of Niš – Faculty of Medicine, Department of Pharmacy, Niš, Serbia*
[2]*Innovation Center of the Faculty of Chemistry d.o.o, Serbia*
[3]*University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*

Metal-based compounds are rarely good antimicrobial compounds. Here we report synthesis, chemical characterization and antimicrobial potency of fourteen Ru(II) arene complexes with pyridine-based ligands. The structures and purity of synthesized compounds were confirmed using ^{1}H and ^{13}C NMR spectroscopy, IR spectroscopy, MS, and EA. A micro-well dilution assay was used to determine the minimum inhibitory concentration (MIC), and minimum bactericidal concentration. of evaluated compounds. Streptomycin and chloramphenicol were used as a positive control. The best activity of all tested bacteria was observed against *E. coli*, with a MIC value of 1.25 mg/mL, for complexes with 2,4- i 2,5-pyridinedicarboxylic ligands. Also, all synthesized complexes showed the same activity against *C. Albicans.*

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia Contract numbers 451-03-47/2023-01/200168, 451-03-47/2023-01/200288 and 451-03-68/2023-14/200113.

MH-8

Novi derivati 4-azasteroidnog 17-hidrazona: Sinteza, *in silico* ADMET i *in vitro* biološka ispitivanja

Tijana Lj. Šestić[1], Julia Scholda[2], Ivana Z. Kuzminac[1], Jovana Ajduković[1], Florian Kopp[2], Marina P. Savić[1]

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

[2] *University of Vienna, Faculty of Life Sciences, Department of Pharmaceutical Sciences, Clinical Pharmacy Group, Vienna, Austria*

U ovom radu je prikazana sinteza novih derivata 4-azasteroidnog 17-hidrazona, kao i *in silico* ispitivanje fizičko-hemijskih svojstava i procena njihove farmakokinetike i toksičnosti (ADMET). Jedinjenja su testirana i *in vitro* na četiri humane ćelijske linije kancera: HCT116 (kancer debelog creva), MCF7 (estrogen receptor pozitivni kancer dojke), MDA-MB-231 (trostruko negativni kancer dojke) i Huh7 (humani hepatom). Rezultati su pokazali da pojedina ispitivana jedinjenja pokazuju jaku citotoksičnost, kao i odgovarajuću bioraspoloživost i ADMET svojstva, koja su neophodna za potencijalne kandidate za lek.

New 4-azasteroid 17-hydrazone derivatives: Synthesis, *in silico* ADMET and *in vitro* biological testing

Tijana Lj. Šestić[1], Julia Scholda[2], Ivana Z. Kuzminac[1], Jovana Ajduković[1], Florian Kopp[2], Marina P. Savić[1]

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

[2] *University of Vienna, Faculty of Life Sciences, Department of Pharmaceutical Sciences, Clinical Pharmacy Group, Vienna, Austria*

This paper presents the synthesis of new derivatives of 4-azasteroid 17-hydrazone, as well as *in silico* testing of their physicochemical properties and evaluation of their pharmacokinetics and toxicity (ADMET). The compounds were also tested in *vitro* against four human cancer cell lines HCT116 (colon cancer), MCF7 (estrogen receptor-positive breast cancer), MDA-MB-231 (triple negative breast cancer) and Huh7 (human hepatoma). Results showed that some tested compounds exhibit strong cytotoxicity in addition to good bioavailability and ADMET properties, which are essential for potential drug candidates.

Presented results were obtained within the framework of the bilateral cooperation between the Republic of Austria and the Republic of Serbia [Project No. 337-00-577/2021-09/27 and OeAD RS15/2022]. The authors also acknowledge the financial support of the Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina [Project No. 142-451-3133/2022-01], the Ministry of Science, Technological Development and Innovation of the Republic of Serbia and Austria's Agency for Education and Internalisation (OeAD).

MH-9

Defenilovani analozi (–)-goniofufurona: SAR i 3D-QSAR model

Bojana M. Srećo Zelenović[1], Slađana M. Stanisavljević[1], Mirjana Popsavin[1], Vesna Kojić[2], Vladimir Vukić[3], Dajana Vukić[3], Velimir Popsavin[1,4]

[1] *Prirodno-matematički fakultet, Trg Dositeja Obradovića 3, Novi Sad, Srbija*
[2] *Institut za onkologiju Vojvodine, Put dr Goldmana 4, Sremska Kamenica, Srbija*
[3] *Tehnološki fakultet Novi Sad, Bulevar cara Lazara 1, Novi Sad, Srbija*
[4] *Srpska akademija nauka i umetnosti, Kneza Mihaila 35, Beograd, Srbija*

(–)-Goniofufuron je neprirodni stiril lakton, koji je poslužio kao 'vodeće jedinjenje' za sintezu velikog broja defenilovanih analoga. Pored rezultata antiproliferativne aktivnosti prema većem broju malignih ćelijskih linija, u ovom radu biće detaljno prikazan odnos strukture i aktivnosti (SAR) analoga i (–)-goniofufurona. U cilju ispitivanja uticaja 3D konformacije analiziranih jedinjenja na biološku aktivnost prema ćelijskoj liniji K562, korišćen je statistički pogodan 3D-QSAR model sa dobrim koeficijentom korelacije (r 2=0,700), koeficijentom unakrsne validacije (q2=0,560) i visokim Fišerovim odnosom (F=14,6). Konačno, CoMFA model je korelisan sa biološkim aktivnostima upotrebom statističke metode PLS (eng. Partial Least Squares).

Dephenylated (–)-goniofufurone analogues: SAR and 3D-QSAR model

Bojana M. Srećo Zelenović[1], Slađana M. Stanisavljević[1], Mirjana Popsavin[1], Vesna Kojić[2], Vladimir Vukić[3], Dajana Vukić[3], Velimir Popsavin[1,4]

[1] *Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, Novi Sad, Serbia*
[2] *Oncology Institute of Vojvodina, Put Dr. Goldmana 4, Sremska Kamenica, Serbia*
[3] *Faculty of Technology Novi Sad, University of Novi Sad, Bulevar cara Lazara 1, Novi Sad, Serbia*
[4] *Serbian Academy of Sciences and Arts, Kneza Mihaila 35, Belgrade, Serbia*

(–)-Goniofufurone is an unnatural styryl lactone, which served as a *lead compound* for the synthesis of many dephenylated analogues. In addition to the results of antiproliferative activity against a number of malignant cell lines, the structure-activity relationship (SAR) of analogs and (–)-goniofufurone will be presented in details. In order to examine the influence of the 3D conformation of the analyzed compounds on the biological activity against the K562 cell line, a statistically adequate 3D-QSAR model was used with a good correlation coefficient (r 2=0.700), cross-validation coefficient (q2=0.560) and a high Fisher's ratio (F= 14,6). Finally, the CoMFA model was correlated with biological activities using the PLS (Partial Least Squares) statistical method.

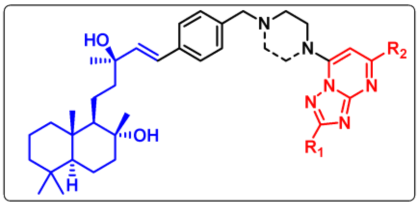
Acknowledgment: The work was supported by a grant from Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125 and 451-03-47/2023-01/200134).

MH-10

Sinteza i citotoksičnost novih derivata sklareola

Pavle A. Stojković[1], Ana Kostić[2], Ema Lupšić[2], Nataša Terzić Jovanović[3], Miroslav Novaković[3], Milica Pešić[2], Igor M. Opsenica[1]
[1]*Univerzitet u Beogradu – Hemijski fakultet, Beograd, Srbija*
[2]*Institut za biološka istraživanja "Siniša Stanković" – Univerzitet u Beogradu, Beograd, Srbija*
[3] *Univerzitet u Beogradu – Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija*

Sklareol, biološki aktivan diterpen, je iskorišćen kao polazna supstanca za sintezu novih hibridnih molekula sa 1,2,4-triazolo[1,5-*a*]-pirimidinskim jezgrom (Slika 1). Svi derivati sklareola su testirani na ćelijsku liniju ljudskog glioblastoma U87 i ćelijsku liniju U87-TxR koja ispoljava višestruku rezistenciju na lekove. Jedinjenja su modifikovala aktivnost P-glikoproteina u sličnoj meri kao P-gp inhibitor treće generacije – tarikvidar. Ispitan je uticaj novih jedinjenja na različite ćelijske procese među kojima su ćelijski ciklus i ćelijska smrt, kao i na koncentraciju reaktivnih kiseoničnih i azotnih vrsta (ROS/RNS) u ćelijama glioblastoma i na potencijal membrane mitohondrija.



Slika 1. Hibridi sklareola i1,2,4-triazolo[1,5-a]-pirimidina.

Synthesis and cytotoxic activity of novel sclareol derivatives

Pavle A. Stojković[1], Ana Kostić[2], Ema Lupšić[2], Nataša Terzić Jovanović[3], Miroslav Novaković[3], Milica Pešić[2], Igor M. Opsenica[1]
[1]*University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*
[2]*Institute for Biological Research "Siniša Stanković" – University of Belgrade, Belgrade, Serbia*
[3]*University of Belgrade - Institute of Chemistry, Technology, and Metallurgy, Belgrade, Serbia*

Sclareol, a biologically active diterpenoid, was used as the starting material for the synthesis of novel hybrid molecules containing the 1,2,4-triazolo[1,5-*a*]-pyrimidine moiety. All sclareol derivatives were tested on human glioblastoma U87 and multi-drug resistant U87-TxR cells. Hybrid compounds decreased P-gp activity to the same extent as a third generation P-gp inhibitor - tariquidar. We examined the effect of novel compounds on various cellular processes including the cell cycle and cell death, as well as their influence on the levels of reactive oxygen and nitrogen species (ROS/RNS) and mitochondrial membrane potential in glioblastoma cells.

Zahvalnica: Ovo istraživanje je finansirano od strane Ministarstva nauke, tehnološkog razvoja i inovacija Republike Srbije (evidencioni broj: 451-03-47/2023-01/200168).

Nastava i istorija hemije

Education in and History of Chemistry

NIH-1

Kako učenici gimnazije tumače i integrišu različite nivoe predstavljanja strukture, svojstava i promena supstanci?

Vesna D. Milanović Maštrapović, Lidija R. Ralević, Dragica D. Trivić, Biljana I. Tomašević
Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija

Nastava/učenje hemije podrazumeva razmatranje sadržaja hemije na tri nivoa: makroskopskom (čulno uočljiva svojstva i promene supstanci), submikroskopskom (struktura supstance na nivou čestica) i simboličkom (hemijski simboli, formule i jednačine). Cilj istraživanja je bio da se ispita kako učenici gimnazije razumeju strukturu, svojstva i promene supstanci na osnovu tumačenja i integracije reprezentacija na makroskopskom, submikroskopskom i simboličkom nivou. Za potrebe istraživanja pripremljen je test sa 10 zadataka. Istraživanje je realizovano onlajn na kraju školske 2021/22. godine, a u njemu je učestvovalo ukupno 290 učenika prvog, drugog i trećeg razreda iz sedam gimnazija. Gimnazijalci su bili uspešniji u rešavanju zadataka u kojima se zahtevalo tumačenje reprezentacija na makroskopskom ili simboličkom nivou i njihovo povezivanje sa submikroskopskim nivoom nego u obrnutom slučaju.

Zahvalnica: Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije Evidencioni broj:451-03-47/2023-01/200168

How do grammar school students interpret and integrate different levels of representation of the structure, properties and changes of substances?

Vesna D. Milanović Maštrapović, Lidija R. Ralević, Dragica D. Trivić, Biljana I. Tomašević
University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

Teaching/learning chemistry involves considering the chemistry contents at three levels: macroscopic (properties and changes of substances noticeable by the senses), submicroscopic (structure of substances at the particle level) and symbolic (chemical symbols, formulas and equations). The aim of the research was to examine how grammar school students understand the structure, properties and changes of substances based on the interpretation and integration of representations at the macroscopic, submicroscopic and symbolic levels. For the purposes of the research, a test with 10 tasks was prepared. The research was conducted online at the end of the 2021/22 school year, and a total of 290 students of the first, second and third grade from seven grammar schools took participation. Grammar school students were more successful in solving tasks that required the interpretation of representations at the macroscopic or symbolic level and making connection with the submicroscopic level than in the reverse case.

NIH-2

Ко публикује у часопису Journal of the Serbian Chemical Society?

Олгица Недић[1], Maciej Mrowinski[2], Agata Fronczak[2], Piotr Fronczak[2] и Александар Декански[3]

[1] *Универзитет у Београду - Институт за примену нуклеарне енергије (ИНЕП), Београд, Србија*
[2] *University of Warsaw Technology - Faculty of Physics, Warsaw, Poland*
[3] *Универзитет у Београду - Институт за хемију, технологију и металургију, Београд, Србија*

Анализирани су подаци из базе података часописа Journal of the Serbian Chemical Society који се односе на поднете радове у периоду 2015-2016.[1] Већина приспелих радова је била из Индије, Ирана и Кине (укупно 49 %), док су радови из Србије били у мањини (12 %). Велики број радова је одбијен из техничких разлога. Укупно 1010 поднетих радова је послато 2089 пута. Само 279 радова (28 %) је прослеђено уредницима. 78 % аутора је поднело само један рад, 18 % два и 3 % три рада. Процес рецензирања за ауторе из Србије траје краће него за иностране ауторе и већа је вероватноћа прихватања рада. Међу иностраним ауторима је више мушкараца, а међу домаћим жена. Вероватноћа прихватања рада је већа за женске него за мушке ауторе. Просечан број аутора из Србије на једном раду је 5, док је просечан број иностраних аутора по раду 2.

Who is publishing in the Journal of the Serbian Chemical Society?

Olgica Nedić[1], Maciej Mrowinski[2], Agata Fronczak[2], Piotr Fronczak[2] and Aleksandar Dekanski[3]

[1] *University of Belgrade - Institute for the Application of Nuclear Energy (INEP), Belgrade, Serbia*
[2] *Warsaw University of Technology - Faculty of Physics, Warsaw, Poland*
[3] *University of Belgrade - Institute for Chemistry, Technology and Metallurgy, Belgrade, Serbia*

A dataset which contains information on the submitted manuscripts in the Journal of the Serbian Chemical Society in the period 2015-2016 was evaluated.[1] Majority of submissions were from India, Iran and China (49 % altogether), while Serbian submissions were in the minority (12 %). Many submissions were rejected due to technical reasons. A total of 1010 submitted papers were submitted 2089 times. Only 279 papers (28 %) were sent to editors. 78 % of authors submitted just one manuscript, 18 % two and 3 % three. The peer review process for Serbian submissions takes less time than for external authors and submissions are more likely to be accepted. There are more men than women among external authors, whereas there are more females among Serbian authors. Articles submitted by women are more likely to be published than those submitted by men. An average number of authors for submissions from Serbia is 5, while for external submissions it is 2.

1. M. J. Mrowinski, A. Fronczak, P. Fronczak, O. Nedic, A. Dekanski, *Scientometrics*, **2020**, *125*, 115.

NIH-3

Radionica za unapređivanje razumevanja karakteristika asinhronog i sinhronog onlajn učenja kod nastavnika hemije

Biljana I. Tomašević, Lidija R. Ralević, Dragica D. Trivić,
Vesna D. Milanović Maštrapović
Univerzitet u Beogradu - Hemijski fakultet, Beograd, Srbija

Cilj istraživanja je bio da se ispita koliko nastavnici hemije poznaju vidove i karakteristike onlajn nastave i učenja. Takođe, cilj je bio i da se ispita koliko se mogu unaprediti viđenja nastavnika kroz aktivnosti u okviru radionice usmerene na karakteristike asinhronog i sinhronog onlajn učenja hemije. Prema ciljevima istraživanja i istraživačkim pitanjima pripremljen je onlajn upitnik. Uzorak je obuhvatio 36 nastavnika hemije koji su odgovorili na pitanja u upitniku pre i posle radionice. Rezultati su pokazali da su posle radionice nastavnici statistički značajno unapredili razumevanje šta je asinhrono onlajn učenje, kao i da bolje sagledavaju karakteristike asinhronog i sinhronog onlajn učenja/nastave.

Zahvalnica: Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije Evidencioni broj: 451-03-47/2023-01/200168

Workshop for the improvement of chemistry teachers' understanding of the characteristics of asynchronous and synchronous online learning

Biljana I. Tomašević, Lidija R. Ralević, Dragica D. Trivić,
Vesna D. Milanović Maštrapović
University of Belgrade - Faculty of Chemistry

The research examined how well chemistry teachers know the types and characteristics of online teaching and learning. Also, the goal was to examine whether teachers' perceptions can be improved through activities within the workshop focused on the characteristics of asynchronous and synchronous online chemistry learning. An online questionnaire was prepared according to the research objectives and research questions. The sample included 36 chemistry teachers who filled out the questionnaire before and after the workshop. The results showed that after the workshop, the teachers statistically significantly improved their understanding of asynchronous online learning and the characteristics of asynchronous and synchronous online learning/teaching.

Neorganska hemija

Inorganic Chemistry

NH-1

Strukturna karakterizacija i DNA/BSA interakcije zlato(III) kompleksa sa dimetil-piridin-4,5-dikarboksilatnim estrima

Tina P. Andrejević[1], Darko P. Ašanin[2], Jakob Kljun[3], Iztok Turel[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]
[1] Univerzitet u Kragujevcu - Prirodno-matematički fakultet, Institut za hemiju, Radoja Domanovića 12, 34000 Kragujevac, Srbija
[2] Univerzitet u Kragujevcu - Institut za informacione tehnologije Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Srbija
[3] Univerzitet u Ljubljani - Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, SI-1000 Ljubljana, Slovenija
[4] Srpska akademija nauka i umetnosti - Knez Mihailova 35, 11000 Beograd, Srbija

Dimetil 2,2’-bipiridin-4,5-dikarboksilat (py-2py) i dimetil 2-(tiazol-2-il) piridin-4,5-dikarboksilat (py-2tz) korišćeni su kao ligandi za sintezu novih kompleksa zlata(III). Sintetisani kompleksi $[AuCl_2(py\text{-}2py)][AuCl_4]$ (**1**) i $[AuCl_2(py\text{-}2tz)][AuCl_4]$ (**2**) su okarakterisani primenom spektroskopskih metoda, kao i rendgenske strukturne analize. U cilju ispitivanja reaktivnosti sintetisanih kompleksa prema biološki značajnim molekulima, ispitivane su njihove reakcije sa DNK i BSA.

Structural characterization and DNA/BSA interactions of gold(III) complexes with dimethyl pyridine-4,5-dicarboxylate esters

Tina P. Andrejević[1], Darko P. Ašanin[2], Jakob Kljun[3], Iztok Turel[3], Miloš I. Djuran[4], Biljana Đ. Glišić[1]
[1] University of Kragujevac - Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia
[2] University of Kragujevac - Institute for Information Technologies Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Serbia
[3] University of Ljubljana - Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia
[4] Serbian Academy of Sciences and Arts - Knez Mihailova 35, 11000 Belgrade, Serbia

Dimethyl 2,2’-bipyridine-4,5-dicarboxylate (py-2py) and dimethyl 2-(thiazol-2-yl) pyridine-4,5-dicarboxylate (py-2tz) were used as ligands for the synthesis of new gold(III) complexes. The synthesized complexes, $[AuCl_2(py\text{-}2py)][AuCl_4]$ (**1**) and $[AuCl_2(py\text{-}2tz)][AuCl_4]$ (**2**) were characterized by spectroscopic methods, while their structures were determined by single-crystal X-ray diffraction analysis. To examine the affinity of the synthesized complexes towards biologically important molecules, their interactions with DNA and BSA were performed.

NH-2

Sinteza i kristalna struktura monomernog kompleksa Cu(II) sa Šifovom bazom bifenildikarboksilne kiseline

Milica G. Bogdanović, Nikola D. Radnović, Marko V. Rodić
Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Novi Sad, Srbija

Kompleks formule $[Et_3NH]_2[CuL]\cdot xH_2O$ je dobijen reakcijom metanolnog rastvora anhidrovanog $CuCl_2$ sa ligandom 2,2′-bis(((*E*)-2-hidroksibenziliden) amino)-[1,1′-bifenil]-4,4′-dikarboksilnom kiselinom (H_4L), u prisustvu NEt_3 i kasnijom prekristalizacijom iz MeCN. Kristalna struktura se sastoji od organskih katjona $[Et_3NH]^+$ i kompleksnih anjona $[CuL]^{2-}$ koji pakovanjem stvaraju šupljine u koje se smeštaju molekuli H_2O. Ligand se u kompleksu nalazi u tetraanjonskoj formi L^{4-} i koordinuje se kao *OONN* tetradentat (slika 1), dok je Cu(II) smešten u deformisanom tetraedarskom okruženju (τ_4 = 0,46) dva fenoksidna atoma kiseonika i oba azometinska atoma azota liganda. Ovakvom koordinacijom nastaju dva šestočlana i jedan sedmočlani fuzionisani metalocikl, a nastali kompleksni anjon poseduje kristalografsku osu rotacije drugog reda. Poređenje deformacija koordinacionog poliedra ispitivanog kompleksa i njemu sličnih struktura deponovanih u Kembričku banku podataka je izvršeno računanjem kontinualne mere oblika.

Slika 1. Molekulska struktura kompleksa $[Et_3NH]_2[CuL]\cdot xH_2O$.

Synthesis and crystal structure of monomeric Cu(II) complex with a biphenyldicarboxylic acid Schiff base ligand

Milica G. Bogdanović, Nikola D. Radnović, Marko V. Rodić
University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia

The complex of the formula $[Et_3NH]_2[CuL]\cdot xH_2O$ was obtained by the reaction of a methanolic solutions of anhydrous $CuCl_2$, and the ligand 2,2′-bis(((*E*)-2-hydroxybenzylidene)amino)-[1,1′-biphenyl]-4,4′-dicarboxylic acid (H_4L), in the presence of NEt_3, followed by recrystallization from MeCN. The crystal structure consists of organic cations $[Et_3NH]^+$ and complex anions $[CuL]^{2-}$, which by packing create voids in which H_2O molecules are placed. In this complex, the ligand is in its tetraanionic form (L^{4-}) and it is coordinated as *OONN* tetradentate, while Cu(II) is located in a deformed tetrahedral environment (τ_4 = 0.46) of two phenoxide oxygen atoms and both azomethine nitrogen atoms of the ligand. The comparison of the deformations of the coordination polyhedron of this complex and similar structures deposited in the Cambridge Structural Database was performed by calculating the continuous shape measures.

NH-3

Citotoksična aktivnost i ispitivanje interakcija dinuklearnih paladijum(II) kompleksa sa DNK i BSA

Anđela A. Franich[1], Marija D. Živković[2], Sanja Zornić[3,4], Bojana Simović Marković[3],
Nebojša N. Arsenijević[3], Gordana D. Radosavljević[3], Jelena Pantić[3]
Snežana Rajković[1]
[1] Univerzitet u Kragujevcu - Institut za hemiju, Kragujevac, Srbija
[2] Univerzitet u Kragujevcu - Fakultet medicinskih nauka, Institut za farmaciju, S. Markovića 69, Kragujevac, Srbija
[3] Univerzitet u Kragujevcu - Fakultet medicinskih nauka, Centar za molekulsku medicinu i istraživanje matičnih ćelija, S. Markovića 69, Kragujevac, Srbija
[4] Univerzitetski klinički centar Kragujevac - Odeljenje za Mikrobiologiju, Z. Jovina 30, Kragujevac, Srbija

Ispitivanje interakcija kompleksa prelaznih metala sa dezoksiribonukleinskom kiselinom (DNK) i serum albuminima poslednjih godina predmet su istraživanja. U ovom radu ispitivane su interakcije dinuklearnih paladijum(II) kompleksa $[\{Pd(en)Cl\}_2(\mu\text{-pz})](NO_3)_2$ i $[\{Pd(en)Cl\}_2(\mu\text{-pydz})](NO_3)_2$ (en je bidentatno koordinovani etilendiamin, dok su pirazin (pz) i piridazin (pydz) mostni ligandi) sa CT-DNK i serum albuminom (BSA), primenom UV-Vis i fluorescentne spektroskopije. Analiza citotoksičnog efekta pokazuje da kompleksi nisu selektivni prema tumorskim linijama ali su manje toksični u odnosu na cisplatinu.

Cytotoxic effects and interaction of dinuclear palladium(II) complexes with DNA and BSA

Anđela A. Franich[1], Marija D. Živković[2], Sanja Zornić[3,4], Bojana Simović Marković[3],
Nebojša N. Arsenijević[3], Gordana D. Radosavljević[3], Jelena Pantić[3]
Snežana Rajković[1]
[1] University of Kragujevac - Faculty of Science, Department of Chemistry, Kragujevac, Serbia
[2] University of Kragujevac - Faculty of Medical Sciences, Department of Pharmacy, S. Markovića 69, Kragujevac, Serbia
[3] University of Kragujevac - Faculty of Medical Sciences, Center for Molecular Medicine and Stem Cell Research, S. Markovića 69, 34000 Kragujevac, Serbia
[4] University Clinical Center Kragujevac - Department of Microbiology, Z. Jovina 30, 34000 Kragujevac, Serbia

The interactions of transition metal complexes with deoxyribonucleic acid (DNA) and serum albumins have been investigated in recent years. In the present study, the interactions of dinuclear palladium(II) complexes, $[\{Pd(en)Cl\}_2(\mu\text{-pz})](NO_3)_2$ and $[\{Pd(en)Cl\}_2(\mu\text{-pydz})](NO_3)_2$ (en is bidentate coordinated ethylenediamine, pirazine (pz) and pyridazine (pydz) are bridging ligands) with CT-DNA and bovine serum albumin (BSA) were investigated by UV-Vis and fluorescence spectroscopy. Analysis of the cytotoxic effect shows that the complexes were not selective towards tumor cell lines but showed less toxicity compared to cisplatin.

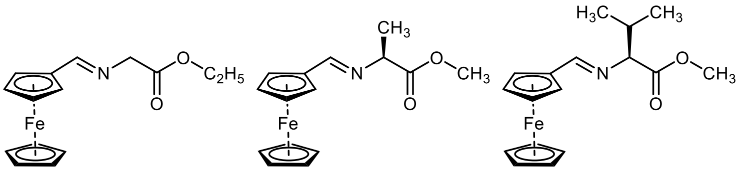
Acknowledgment: Financially supported by Ministry of Science, Technological Development and Innovation of Republic of Serbia (No. 451-03-47/2023-01/ 200122, 451-03-47/2023-01/ 200111)

NH-4

Sinteza i karakterizacija srebro(I) kompleksa sa ligandima na bazi ferocena

Andrija D. Gigić[1], Angelina Z. Caković[1], Dragana D. Stevanović[1], Jovana V. Bogojeski[1],
Ana S. Kesić[2]
[1] Univerzitet u Kragujevcu - Prirodno-matematički fakultet, R. Domanovića 12, Kragujevac, Srbija
[2] Univerzitet u Kragujevcu - Institut za informacione tehnologije, J. Cvijića bb, Kragujevac, Srbija

Kompleksi srebra su poznati po svojim antibakterijskim i antimikrobnim svojstvima, a ligandi na bazi ferocena grade stabilne komplekse sa jonima prelaznih metala. Ovaj rad obuhvata sintezu i strukturnu karakterizaciju novih kompleksa srebra(I) sa iminima koji sadrže ferocensko jezgro prikazanim na Slici 1. U reakcijama između srebro-tetrafluoroborata ($AgBF_4$) i ferocenskih imina, etil 2-((ferocenilmetilen)amino)acetat (**1**), metil 2-((ferocenilmetilen)amino)propanoat (**2**) i metil 2-((ferocenilmetilen)amino)-3-metilbutanoat (**3**) nastaju kompleksna jedinjenja srebra(I) tipa 1:1. Sintetizovani kompleksi srebra(I) su okarakterisani spektroskopskim tehnikama (^{1}H NMR, ^{13}C NMR, IR, UV-Vis). Sinteza novih kompleksa Ag(I) sa ferocenskim ligandima može značajno pomoći razvoju novih antibakterijskih i antimikrobnih agenasa sa poboljšanim karakteristikama.



1 **2** **3**

Slika 1. Strukturne formule ispitivanih liganada.

Synthesis and characterization of silver(I) complexes with ferrocene-based ligands

Andrija D. Gigić[1], Angelina Z. Caković[1], Dragana D. Stevanović[1], Jovana V. Bogojeski[1],
Ana S. Kesić[2]
[1] University of Kragujevac - Faculty of Science, R. Domanovića 12, Kragujevac, Serbia
[2] University of Kragujevac - Institute for Information Technologies, J. Cvijića bb, Kragujevac, Serbia

Silver complexes are known for their antibacterial and antimicrobial properties, and ferrocene-based ligands form stable complexes with transition metal ions. This work involves the synthesis and structural characterization of new silver(I) complexes with ferrocene-containing imines, shown in Figure 1. In the reactions between silver tetrafluoroborate ($AgBF_4$) and ferrocene-containing imines, ethyl 2-((ferrocenylmethylene)amino)acetate (**1**), methyl 2-((ferrocenylmethylene)amino propanoate (**2**), and methyl 2-((ferrocenylmethylene)amino)-3-methylbutanoate (**3**) form silver(I)-type complex compounds 1:1. Synthesized silver(I) complexes were characterized by spectroscopic techniques (^{1}H NMR, ^{13}C NMR, IR, UV-Vis).

NH-5

Sinteza i karakterizacija kompleksa tributilkalaja(IV) sa 2-(4-hidroksi-2-oksohinolinil)propanskom kiselinom

Marijana P. Kasalović[1,2], Jelena Lađarević[3], Bojan Božić[4], Verica V. Jevtić[2], Goran N. Kaluđerović[1], Nebojša Đ. Pantelić[5]

[1] University of Applied Sciences - Department of Engineering and Natural Sciences, Merseburg, Nemačka
[2] Univerzitet u Kragujevcu - Prirodno-matematički fakultet, Institut za hemiju, Kragujevac, Srbija
[3] Univerzitet u Beogradu - Tehnološko-metalurški fakultet, Katedra za organsku hemiju, Beograd, Srbija
[4] Univerzitet u Beogradu - Biološki fakultet, Institut za fiziologiju i biohemiju „Ivan Đaja“, Beograd, Srbija
[5] Univerzitet u Beogradu - Poljoprivredni fakultet, Katedra za hemiju i biohemiju, Beograd, Srbija

U datom radu opisana je sinteza 2-(4-hidroksi-2-oksohinolinil)propanske kiseline i njenog kompleksa tributilkalaja(IV). Ligand prekursor je dobijen hidrolizom metil-estra sintetisanog u reakciji između 4-hidroksi-2-hinolona i metil-2-bromopropanoata. U reakciji deprotonovanog liganda i ekvimolarne količine Bu_3SnCl dobijen je kompleks u obliku belog taloga. Sintetisana jedinjenja su okarakterisana standardnim analitičkim metodama. Ligand prekursor i odgovarajući kompleks tributilkalaja(IV) biće testirani na antitumorsku aktivnost prema raznim tumorskim ćelijskim linijama.

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

Marijana P. Kasalović[1,2], Jelena Lađarević[3], Bojan Božić[4], Verica V. Jevtić[2], Goran N. Kaluđerović[1], Nebojša Đ. Pantelić[5]

[1] University of Applied Sciences - Department of Engineering and Natural Sciences, Merseburg, Germany
[2] University of Kragujevac - Faculty of Science, Department of Chemistry, Kragujevac, Serbia
[3] University of Belgrade - Faculty of Technology and Metallurgy, Department of Organic Chemistry, Belgrade, Serbia
[4] University of Belgrade - Faculty of Biology, Institute of Physiology and Biochemisty „Ivan Đaja“, Belgrade, Serbia
[5] University of Belgrade - Faculty of Agriculture, Department of Chemistry and Biochemistry, Belgrade, Serbia

Synthesis of 2-(4-methyl-2-oxoquinolinyl)propanoic acid and its tributyltin(IV) complex has been performed. The ligand precursor has been obtained by the hydrolysis of methyl ester synthesized in the reaction between 4-hydroxy-2-quinolone and methyl 2-bromopropanoate. In the reaction of deprotonated ligand with equimolar amount of Bu_3SnCl, the desired complex was precipitated as a white solid. The synthesized compounds have been characterized using standard analytical methods. The following research of ligand precursor and corresponding tributyltin(IV) complex will be focused on examining their antitumor activity against various cancer cell lines.

NH-6

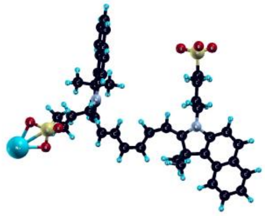
Mikroskopska i teorijska studija adsorpcije boje Indocijanin zeleno na površini nanočestica srebra

Bojana B. Laban[1], Ana V. Vujačić Nikezić[2], Mirjana Novaković[2], Marija Kovačević[2], Dragana Vasić Anićijević[2]

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

[2] Univerzitet u Beogradu - Institut za nuklearne nauke Vinča, Institut od nacionalnog značaja za Republiku Srbiju, 11351 Beograd, Srbija

U ovom radu, transmisionom elektronskom mikroskopijom (TEM) i teorijskim proračunom (DFT), izučavana je adsorpcija boje Indocijanin zeleno (ICG) na površini nanočestica srebra (AgNPs). Studija je pokazala da su dobijene hibridne nanočestice sastava Ag-jezgro-ICG-omotač. TEM merenjima potvrđeno je formiranje omotača boje oko AgNPs debljine ~ 3 do 4 nm, dok su HRTEM merenja pokazala mikrostrukturne promene AgNPs usled adsorpcije boje ICG. Teorijskim proračunom utvrđeno je da se molekul ICG boje vezuje kovalentno za atom Ag, na površini AgNPs, preko svoje SO_3^- grupe.



Slika 1. Strukutra ICG molekula. Figure 1. DFT optimized structure of ICG.

TEM and DFT study of Indocyanine green adsorption on a silver nanoparticle surface

Bojana B. Laban[1], Ana V. Vujačić Nikezić[2], Mirjana Novaković[2], Marija Kovačević[2], Dragana Vasić Anićijević[2]

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

[2] University of Belgrade - Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, 11351 Belgrade, Serbia

Here we present the TEM and DFT study of hybrid nanoparticles consisting of an Ag core and Indocyanine green (ICG) shell. TEM measurements revealed the formation of a distinctive ~ 3 to 4 nm thick halo around the particles, while HRTEM measurements show microstructural changes in NPs. The DFT calculations were used to investigate the energetics of interaction between ICG molecule and Ag-surface. The obtained data indicate a strong interaction between Ag-atom from NPs surface and SO_3^- group of ICG molecule.

Acknowledgment This work was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia Grant No. 451-03-47/2023-01/ 200123.

NH-7

Ispitivanje mehanohemijske reakcije Fe(II)-soli sa iminodiacetatoditiokarbamato-ligandom (idadtc^{3-})

Zorica B. Leka[1], Danijela M. Čukić[1], Aleksandra R.Gezović[1]
[1] *Univerzitet Crne Gore - Metalurško tehnološki fakultet, Dž. Vašingtona, Podgorica, Crna Gora*

Mehanohemijskom sintezom se može eliminisati potreba za inertnom atmosferom i potrebnom aparaturom. Pored toga, reakcija može da se isproba, prije optimizacije, sa malim količinama reaktanata, ručnim mljevenjem. U ovom radu je praćena mehanohemijska reakcija između $FeSO_4$ i $(NH_4)_3$idadtc pomoću infracrvene (IC) spektroskopije. Praćen je položaj i oblik traka u IC spektru proizvoda reakcije tokom vremena i zaključeno da se ditiokarbamato-ligand koordinovao preko atoma sumpora u bidentatnoj formi unutar 30 min. Oksidaciono stanje nastalog proizvoda je ispitano cikličnom voltametrijom (CV) . Mjerenja CV su potvrdila da mehanohemijskom reakcijom ne dolazi do oksidacije Fe(II)-jona što se dešava reakcijom iz rastvora. Na osnovu spektralne i elektrohemijske analize zaključeno je da se navedenom mehanohemijskom reakcijom dobija Fe(II)-ditiokarbamato kompleks sa pretpostavljenom strukturom $(NH_4)_4[Fe^{II}(idadtc)_2]$, dok reakcijom iz vodenog rastvora nastaje Fe(III)-ditiokarbamato proizvod složenijeg i nedefinisanog sastava.

Examination of the mechanochemical reaction of Fe(II)- salt with iminodiacetatodithiocarbamato-ligand (idadtc^{3-})

Zorica B. Leka[1], Danijela Čukić[1], Aleksandra Gezović[1]
[1] *University of Montenegro - Faculty of Metallurgy and Technology, Dž.Vašingtona, Podgorica, Montenegro*

Mechanochemical synthesis can eliminate the need for an inert atmosphere and the necessary apparatus. In addition, the reaction can be tried, before optimization, with small amounts of reactants, by manual grinding. In this work, the mechanochemical reaction between $FeSO_4$ and $(NH_4)_3$idadtc was monitored using infrared (IR) spectroscopy. The position and shape of the bands in the IR spectrum of the reaction product were monitored over time and it was concluded that the dithiocarbamate ligand was coordinated via the sulfur atoms in the bidentate form within 30 min. The oxidation state of the resulting product was examined by cyclic voltammetry (CV). The measurements confirmed that during the mechanochemical reaction, the oxidation of Fe(II)-ion, which occurs during the reaction from the solution, does not occur. Based on the spectral and electrochemical analysis, it was concluded that the mentioned mechanochemical reaction produces Fe(II)-dithiocarbamate complex with the assumed structure $(NH_4)_4[Fe^{II}(idadtc)_2]$, while the reaction from aqueous solution produces Fe(III) - dithiocarbamate product with a more complex and undefined composition.

NH-8

Ispitivanje interakcija novih rutenijum(II)-polipiridil kompleksa sa DNK i HSA

Milica G. Međedović[1], Ana M. Rilak Simović[2], Biljana V. Petrović[1]
[1] Univerzitet u Kragujevcu - Prirodno-matematički fakultet, Kragujevac, Srbija
[2] Univerzitet u Kragujevcu - Institut za informacione tehnologije, Kragujevac, Srbija

U cilju pronalaska kompleksnih jedinjenja različitih jona prelaznih metala koji bi zamenili komplekse platine, naročito su se izdvojili rutenijum-polipiridil kompleksi kao potencijalni antitumorski agensi.[1] U okviru ovih istraživanja sintetisana su dva nova rutenijum(II)-polipiridil kompleksa opšte formule [Ru(L)(*N*-*N*)Cl]Cl, u kojoj je L = 2,2':6',2''-terpiridin sa dodatnom funkcionalnom grupom 2-tienil u 4'-položaju, a *N*-*N* = bpy (2,2'-bipiridin, za kompleks **1**) ili phen (fenantrolin, za kompleks **2**). Ispitivani kompleksi okarakterisani su elementalnom analizom i nizom spektroskopskih metoda, kao što su: UV-Vis, IR, ESI MS, ^{1}H and ^{13}C NMR. Ispitivane su interakcije kompleksa sa biološki važnim molekulima, DNK i humanim serum albuminom (HSA). Dobijeni rezultati upoređeni su sa rezultatima za slične sisteme, u cilju definisanja uticaja prirode helatnih liganada na aktivnost rutenijum(II)-polipiridil kompleksa.

Study of the interactions of new ruthenium(II)-polypyridyl complexes with DNA and HSA

Milica G. Medjedovic[1], Ana M. Rilak Simovic[2], Biljana V. Petrovic[1]
[1] University of Kragujevac - Faculty of Science, 34000 Kragujevac, Serbia
[2] University of Kragujevac - Institute for Information Technologies, Kragujevac, Serbia

To find transition metal ion complexes that would replace well-known antitumor active platinum-based complexes, ruthenium-polypyridyl complexes have shown great potential.[1] In this study we have synthesized two new ruthenium(II) complexes with general formula [Ru(L)(*N*-*N*)Cl]Cl, where L = 2,2':6',2''-terpyridine with the additional functional group 2-thienyl at 4'-position, and *N*-*N*= bpy (2,2'-bypyridine, for complex **1**) and phen (phenanthroline, for complex **2**). These complexes were characterized by elemental analysis and by various spectroscopic techniques, such as IR, UV-Vis, ESI MS, ^{1}H and ^{13}C NMR. We have also studied the interactions of these complexes with some important biomolecules, DNA and human serum albumin (HSA). Obtained results were compared with the results for similar systems, in order to provide the influence of the nature of chelating ligands on the activity of ruthenium(II)-polypyridyl complexes toward biomolecules.

1. M. Medjedovic, A. Rilak Simovic, D. Cocic, L. Senft, S. Matic, D. Todorovic, S. Popovic, D. Baskic, B. Petrovic, Dalton Trans., **2023**, 52, 1323-1344.

Zahvalnica: *Istraživanje je finansijski pomoglo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (broj ugovora 451-03-47/2023-01/200122; 451-03-47/2023-01/200378).*

NH-9

Sinteza, strukturna karakterizacija i DNK/BSA interakcije kompleksa galijuma(III) sa 1,3-propandiamin-*N,N,N',N'*-tetraacetatom

Bojana V. Pantović[1], Darko P. Ašanin[2], Franc Perdih[3], Iztok Turel[3], Miloš I. Djuran[4]
Biljana Đ. Glišić[1]
[1] Univerzitet u Kragujevcu - Prirodno-matematički fakultet, R. Domanovića 12, 34000 Kragujevac, Srbija
[2] Univerzitet u Kragujevcu - Institut za informacione tehnologije, Jovana Cvijića bb, 34000 Kragujevac, Srbija
[3] Univerzitet u Ljubljani - Fakultet za hemiju i hemijsku tehnologiju, Večna pot 113, SI-1000 Ljubljana, Slovenija
[4] Srpska akademija nauka i umetnosti - Knez Mihailova 35, 11000 Beograd, Srbija

U ovom radu, 1,3-propandiamin-*N,N,N',N'*-tetraacetato (1,3-pdta) ligand je upotrebljen za sintezu galijum(III) kompleksa, $Na[Ga(1,3\text{-pdta})]\cdot 3H_2O$. Kompleks je okarakterisan spektroskopskim (IR, ^{1}H i ^{13}C NMR) i elektrohemijskim (CV) metodama, dok je njegova kristalna struktura određena difrakcijom rendgenskih X zraka sa kristala. Primenom fluorescentne emisione spektroskopije ispitivane su interakcije $Na[Ga(1,3\text{-pdta})]\cdot 3H_2O$ kompleksa sa DNK izolovanom iz timusa teleta (ct-DNA) i goveđeg serum albumina (BSA).

Synthesis, structural characterization and DNA/BSA interactions of gallium(III) complex with 1,3-propanediamine-*N,N,N',N'*-tetraacetate

Bojana V. Pantović[1], Darko P. Ašanin[2], Franc Perdih[3], Iztok Turel[3], Miloš I. Djuran[4]
Biljana Đ. Glišić[1]
[1] University of Kragujevac - Faculty of Science, R. Domanovića 12, 34000 Kragujevac, Serbia
[2] University of Kragujevac - Institute for Information Technologies Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Serbia
[3] University of Ljubljana - Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia
[4] Serbian Academy of Sciences and Arts - Knez Mihailova 35, 11000 Belgrade, Serbia

In this study, 1,3-propanediamine-*N,N,N',N'*-tetraacetate (1,3-pdta) was used as a ligand for the synthesis of a new gallium(III) complex, $Na[Ga(1,3\text{-pdta})]\cdot 3H_2O$. This complex was characterized by spectroscopic (IR, ^{1}H and ^{13}C NMR) and electrochemical (CV) methods, while its crystal structure was determined by single-crystal X-ray diffraction analysis. The interactions of $Na[Ga(1,3\text{-pdta})]\cdot 3H_2O$ complex with calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) were investigated by fluorescence emission spectroscopy.

NH-10

Reakcija Co(II) sa 4-bromo-3-nitro-1Hpirazol-5-karboksilnom kiselinom

Ana Radović[1], Željko Jaćimović[2]*, Ljiljana S. Vojinović Ješić[3], Vukadin M. Leovac[3],
Mirjana M. Radanović[3], Berta Barta Holló[3]
[1] Akreditaciono tijelo Crne Gore - Podgorica, Crna Gora
[2] Univerzitet Crne Gore - Metalurško-tehnološki fakultet, Podgorica, Crna Gora
[3] Univerzitet u Novom Sadu - Departman za hemiju, biohemiju i zaštitu životne sredine Prirodno-matematički fakultet, Novi Sad, Serbia

Veliki broj derivata pirazola pokazuje raznolika biološka dejstva, kao npr. antipiretičko, analgetičko, antimikrobno. Jedno od tih jedinjenja je i 4-bromo-3-nitro-1Hpirazol-5-karboksilna kiselina (L), antagonista Bradykinin B1 receptora. Kako prisustvo jona metala može povoljno uticati na biološku aktivnost liganda, cilj ovog rada je ispitivanje sposobnosti koordinacije L sa kobalt(II)-acetatom. Dobijeni kompleks okarakterisan je podacima elementalne analize, IR spektrima, TG i XRD analizom.

Reaction of Co(II) with 4-bromo-3-nitro-1Hpyrazole-5-carboxylic acid

Ana Radović[1], Željko Jaćimović[2]*, Ljiljana S. Vojinović Ješić[3], Vukadin M. Leovac[3],
Mirjana M. Radanović[3], Berta Barta Holló[3]
[1]Accreditation body of Montenegro - Podgorica, Montenegro
[2] University of Montenegro - Faculty of Metallurgy and Technology, Podgorica, Montenegro
[3] University of Novi Sad - Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, Novi Sad, Serbia

Numerous pyrazole derivatives show some kind of biological activity, such as antipyretic, analgetic, antimicrobic, etc. 4-Bromo-3-nitro-1Hpyrazole-5-carboxylic acid, one of those biologically active compounds, is an antagonist of the Bradykinin B1 receptor. Since the presence of metal ions could enhance the activity of the ligand, the aim of this work is to investigate the coordination abilities of L with cobalt(II) acetate, thus obtaining knowledge on the structure and properties of the complex. The formed complex is characterized by elemental analysis, FTIR and thermogravimetric data, as well as by powder X-ray diffraction pattern.

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125).

NH-11

Ispitivanje interakcija dinuklearnog zlato(III) kompleksa sa BSA pomoću markera eozina Y i ibuprofena

Snežana R. Radisavljević, Biljana V. Petrović
Univerzitet u Kragujevcu - Prirodno-matematički fakultet, R. Domanovića 12, Kragujevac, Srbija

Serum albumini (SA) su najzastupljeniji plazma proteini, koji su, pre svega, odgovorni za transport jona i lekova kroz krvnu plazmu. S tim u vezi, proučavanje interakcija između kompleksnih jedinjenja različitih jona prelaznih metala i serum albumina ima značajnu ulogu prilikom određivanja biološkog potencijala kompleksa. U okviru ovog istraživanja ispitivane su interakcije dinuklearnog zlato(III) kompleksa, koji kao mostni ligand sadrži 1,5-naftiridin, sa goveđim serum albuminom (BSA) u prisustvu markera eozina Y i ibuprofena. Naime, humani serum albumin (HSA) i goveđi serum albumin (BSA) se sastoje od tri strukturno slična domena (I, II i III), koji su podeljeni na poddomene A i B.[1] Eozin predstavlja marker za domen I i poddomen IIA, dok je ibuprofen marker za domen II i poddomen IIIA. Eksperimentalno dobijeni rezultati naših ispitivanja pokazali su prisustvo konkurentnih reakcija između kompleksa i eozina Y prema proteinu, što je dovelo do zaključka da se ispitivani kompleks vezuje za domen I, poddomen IIA u strukturi BSA.

Investigation of the interactions between dinuclear gold(III) complex and BSA with markers eosin Y and ibuprofen

Snežana R. Radisavljević, Biljana V. Petrović
University of Kragujevac - Faculty of Science, R. Domanovića 12, Kragujevac, Serbia

Serum albumins (SA) are the most abundant plasma proteins, which are responsible for the transportation of ions or drugs through the bloodstream. Considering this, the study of the interactions between different transition metal ion complexes and serum albumins plays a crucial role in the determination of the biological potential of complexes. In this work, we have investigated the interactions between dinuclear gold(III) complex, with 1,5-naphtiridine as bringing ligand, and bovine serum albumin (BSA) in the presence of site markers, eosin Y and ibuprofen. Namely, human serum albumin (HSA) and bovine serum albumin (BSA) consist of three structurally different domains (I, II and III), which are divided into subdomains A and B.[1] Eosin Y represents marker for site I and subdomain IIA, while ibuprofen represents marker for site II and subdomain IIIA. Experimentally obtained results have confirmed competitive reactions between studied Au(III) complex and eosin Y in binding toward protein, indicating that interaction probably occurs to site I subdomain IIA of BSA.

1. S. Radisavljević, A. Kesić, D. Ćoćić, V. Marković, J. Milovanović, B. Petrović, A. Rilak Simović, *Appl. Organomet. Chem.*, **2022,** e6922.

Zahvalnica: Istraživanje je finansijski pomoglo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (broj ugovora 451-03-47/2023-01/200122).

NH-12

Sinteza i karakterizacija nanostrukturnog $Ca_{0.9}Er_{0.1}MnO_3$

Tijana B. Vlašković[1], Bojana Laban[1], Maja Milošević[2], Maria Čebela[3], Vladimir Dodevski[3], Milena Rosić[3]

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

[2] Univerzitet u Beogradu - Katedra za mineralogiju, kristalografiju, petrologiju i geohemiju, Rudarsko-geološki fakultet Đušina 7, 11000 Beograd, Srbija

[3] Univerzitet u Beogradu - Laboratorija za nauku o materijalima, Institut za nuklearne nauke „Vinča“, Nacionalni institut Republike Srbije, P.O. Bok 522, 11001 Beograd, Srbija

Nanostrukturni $Ca_{0.9}Er_{0.1}MnO_3$ je sintetisan saharoza-nitratnon procedurom (SNP). Tokom ove metode sagorevanja su korišćene sledeće hemikalije: saharoza $C_{12}H_{22}O_{11}$ koja ima dvostruku ulogu i goriva i kompleksanta, kalcijum-nitrat tetrahidrat, mangan(II)-nitrat hidrat i erbijum(III)-nitrat pentahidrat. Nitrati metala i saharoza su kombinovani u njihovim odgovarajućim stehiometrijskim odnosima da bi se pripremio složeni oksid perovskitske nanostrukture. Dobijeni prah $Ca_{0.9}Er_{0.1}MnO_3$ je kalcinisan u temperaturnom opsegu od 800-1000°C tokom 15 min. Ispitani su veličina čestica, parametri rešetke, strukturne promene i površina. Za karakterizaciju sintetisanih uzoraka korišćena je diferencijalno termijska analiza (DTA), rendgenska difrakciona analiza (XRD), Furijeova transformaciona infracrvena spektroskopija (FTIR) i skenirajuća elektronska mikroskopija (SEM).

Synthesis and characterization of nanostructured $Ca_{0.9}Er_{0.1}MnO_3$

Tijana B. Vlašković[1], Bojana Laban[1], Maja Milošević[2], Maria Čebela[3], Vladimir Dodevski[3], Milena Rosić[3]

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

[2] University of Belgrade - Department of Mineralogy, Crystallography, Petrology and Geochemistry, Faculty of Mining and Geology, Đušina 7, 11000 Belgrade, Serbia

[3] University of Belgrade - Laboratory for Material Science, Institute of Nuclear Science „Vinča“, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, Serbia

Nanostructured $Ca_{0.9}Er_{0.1}MnO_3$ was synthesized by the sucrose-nitrate procedure (SNP). During this combustion method, sucrose $C_{12}H_{22}O_{11}$ which is both fuel and complexant and metal ions in the form of calcium nitrate tetrahydrate, manganese(II) nitrate hydrate, erbium(III) nitrate pentahydrate were used. Metal nitrates and sucrose were combined to prepare this nanostructured in their appropriate stoichiometric ratios. Obtained $Ca_{0,9}Er_{0,1}MnO_3$ powder was calcined in a temperature range of 800-1000 °C for 15min. Particle size, lattice parameters, structural changes, and specific surface area were investigated. DTA, X-ray diffraction (XRD), FTIR, and Field emission scanning electron microscopy (SEM) were used to characterize the synthesized samples at room temperature.

This work was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia Grant No. 451-03-47/2023-01/ 200123.

Organska hemija

Organic Chemistry

OH-1

Sinteza novih *N*-aril-azola kao potencijalnih antiandrogena

Ljubica M. Brenjo[1], Vukašin S. Mitrović[1], Ksenija J. Pavlović[1], Aleksandar M. Oklješa[1]
[1] Univerzitet u Novom Sadu - Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Srbija

Kancer prostate (KP) je drugi najčešći kancer i peti kancer po smrtnom ishodu kod muškaraca. Rast tumorskih ćelija kod KP je uglavnom androgen-zavisan, tako da terapija deprivacije androgena (TDA), koja podrazumijeva inhibiciju biosinteze androgena ili blokiranje funkcije androgenih receptora (AR) sa lijekovima, može da uspori ili zaustavi ovaj rast. Nesteroidni antiandrogeni kao flutamid i nilutamid smanjuju androgeni efekat kompetitivnim vezivanjem za AR. Hidroksilni derivat flutamida je njegov aktivni metabolit. Odnos strukture i aktivnosti ukazuje na to da najaktivniji antiandrogeni sadrže aromatični prsten sa dvije elektron-akceptorske grupe (nitro, cijano, trifluormetil).[1] S druge strane, triazoli i tetrazoli su poznati po svojoj biološkoj aktivnosti. Prijavljujemo sinteze dva jedinjenja, *N*-aril-triazola i *N*-aril-tetrazola koji sadrže hidroksimetilnu funkciju na heteroaromatičnom dijelu i elektron-akceptorske grupe na aromatičnom prstenu.

Synthesis of new *N*-aryl azoles as potential antiandrogens

Ljubica M. Brenjo[1], Vukašin S. Mitrović[1], Ksenija J. Pavlović[1], Aleksandar M. Oklješa[1]
[1]University of Novi Sad - Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia

Prostate cancer (PC) is the second most frequent cancer and the fifth leading cause of cancer death among males. PC tumor growth is mainly androgen-dependent, so androgen deprivation therapy (ADT), which implies inhibition of the biosynthesis of androgens and blocking the function of androgen receptors (AR) with drugs, may slow or stop this growth. Nonsteroidal antiandrogens such as flutamide and nilutamide diminish androgenic effects by competitively binding to the AR. The hydroxylated derivative of flutamide is the active metabolite. Structure-activity relationships infer that the most active antiandrogens contain an aromatic ring with two electron-withdrawing groups (nitro, cyano, trifluoromethyl).[1] On the other hand, triazoles and tetrazoles are known for their biological activity. We report the syntheses of two compounds, an *N*-aryl triazole and an *N*-aryl tetrazole which contain a hydroxymethyl group in the heteroaromatic moiety, and electron-withdrawing groups in the aromatic ring.

1. S. Singh, S. Gauthier, F. Labrie, *Curr. Med. Chem.* **2000**, *7*, 211.

Zahvalnica: Istraživanja je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Ev.br. 451-03-47/2023-01/200125).

OH-2

Razvoj održivih metoda za sintezu pirazolopirazolona

Jovana Bugarinović[1], Ivan Damljanović[1], Dragana Stevanović[1], Marko Pešić[1], Anka Todosijević[2]
[1] Univerzitet u Kragujevcu, Prirodno-matematički fakultet, R. Domanovića 12, Kragujevac
[2] Univerzitet u Nišu, Poljoprivredni fakultet, Kosančićeva 4, Kruševac

Heterociklični prstenovi, poput pirazolopirazolona predstavljaju farmakofore brojnih biološki aktivnih jedinjenja. Najefikasnija metoda za sintezu ovih *N,N* bicikličnih heterocikala je zasnovana na dipolarnoj cikloadiciji azometinimina[1]. Nedostatak metoda zasnovanih na cikloadicijama je što najčešće podrazumevaju drastične reakcione uslove i korišćenje toksičnih reagenasa. Iz tog razloga, rešili smo da razvijemo „zeleniju" metodu za sintezu pirazolopirazolona u prisustvu sirćetne kiseline. Željeni pirazolopirazoloni su uspešno sintetisani mešanjem odgovarajućih vinil-enona i azometinimina u sirćetnoj kiselini tokom 12 h. Nakon toga, ispitivana je i primena različitih metoda prenosa energije poput ultrazvučnog kupatila i mikrotalasnog reaktora. Najbolji rezultati su postignuti ozračivanjem reakcione smeše mikrotalasima jačine 100 W tokom 15 min. Ovi novi protokoli za sintezu pirazolopirazolona predstavljaju značajan pomak u istraživanju ekološki održivih metoda za dobijanje heterocikličnih jedinjenja.

Sustainable methods for the synthesis of pyrazolopyrazolones

Jovana Bugarinović[1], Ivan Damljanović[1], Dragana Stevanović[1], Marko Pešić[1], Anka Todosijević[2]
[1] University of Kragujevac, Faculty of Science, R. Domanovića 12, Kragujevac
[2] University of Niš, Faculty of Agriculture, Kosančićeva 4, Kruševac

Heterocyclic rings such as pyrazolopyrazolones are pharmacophores of numerous biologically active compounds. The most efficient method for the synthesis of these *N,N* bicyclic heterocycles is based on dipolar cycloaddition of azomethine imines[1]. Lack of methods based on the cycloadditions is that they often require drastic reaction conditions and usage of toxic reagents. For that reason, we decided to develop a more sustainable method for the synthesis of the pyrazolopyrazolones in the presence of acetic acid. Wanted pyrazolopyrazolones were successfully synthesized by stirring the corresponding vinyl enones and azomethine imines in acetic acid for 12 h. After that, we examined different methods of energy transfer such as ultrasonic bath and a microwave reactor. The best results were achieved by the irradiation of the reaction mixture with 100 W power waves for 15 minutes. These novel protocols for the synthesis of pyrazolopyrazolones represent significant improvement in research of sustainable methods for obtaining heterocycles.

Acknowledgements: Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant no. 451-03-47/2023-01/ 200122).

J. P. Jovanovic, G. A. Bogdanovic, I. Damljanovic, *Synlett* **2017**, *28*, 664.

ОН-3

Синтеза пироло[3,4-*c*]хинолин-1,3-диона као ефикасних инхибитора хумане дихидрооротат-дехидрогеназе

Марина Г. Димитријевић [1], Милан Д. Јоксовић [1], Cornelia Roschger [2], Kevin Lang [2], Andreas Zierer [2]

[1] Универзитет у Крагујевцу, Природно-математички факултет, Институт за хемију, Р. Домановића 12, 34000 Крагујевац, Србија

[2] Јоханес Кеплер Универзитет Линц, Медицински факултет, Krankenhausstraße 7a, 4020 Линц, Аустрија

Хумана дихидрооротат-дехидрогеназа (*h*DHODH) је ензим који се налази у унутрашњој мембрани митохондрија и катализује четврту фазу *de novo* биосинтезе пиримидинских нуклеотида. Овај редокс ензим игра кључну улогу у каталитичкој конверзији дихидрооротата у оротат, кораку који одређује брзину у *de novo* биосинтези пиримидина и стога представља потенцијалну мету за лечење канцера и аутоимуних болести. Самим тим, синтетизовали смо нову класу инхибитора *h*DHODH који садрже пироло[3,4-*c*]хинолински фрагмент каскадном реакцијом Pfitzinger-овог естра са примарним алифатичним и ароматичним аминима. Добијена једињења са ниском цитотоксичношћу према здравој HaCaT ћелији (IC_{50} > 200 μM) показала су бољу инхибиторну активност (IC_{50}=0,12-0,43 μM) у поређењу са референтним леком лефлуномидом (IC_{50}= 0.79 μM).

Synthesis of pyrrolo[3,4-*c*]quinoline-1,3-diones as potent human dihydroorotate dehydrogenase inhibitors

Marina G. Dimitrijević [1], Milan D. Joksović [1], Cornelia Roschger [2], Kevin Lang [2], Andreas Zierer [2]

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

[2] Johannes Kepler University Linz, Medical Faculty, Krankenhausstraße 7a, 4020 Linz, Austria

Human dihydroorotate dehydrogenase (*h*DHODH) is an inner mitochondrial membrane enzyme that catalyzes the fourth step of the *de novo* biosynthesis of pyrimidine nucleotides. This redox enzyme plays a crucial role in the catalytic conversion of dihydroorotate to orotate, a rate-determining step in the *de novo* biosynthesis, and therefore represents a potential target for cancer treatment and autoimmune diseases. Hence, we synthesized a new class of potent *h*DHODH inhibitors with a pyrrolo[3,4-c]quinoline scaffold by cascade reaction of Pfitzinger's ester precursor and primary aliphatic and aromatic amines. The obtained compounds with low cytotoxicity toward healthy HaCaT cells (IC_{50} > 200 μM) showed better inhibitory activity (IC_{50}=0.12-0.43 μM) than the reference drug Leflunomide (0.79 μM).

Acknowledgment – This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreement No. 451-03-47/2023-01/200122).

OH-4

Sinteza novih hidrazidnih derivata androstanske serije, *in silico* ADME/T svojstva i *in vitro* biološka aktivnost

Đorđe D. Janković[1], Marina P. Savić[1], Sofija S. Bekić[1], Anđelka S. Ćelić[2], Edward T. Petri[2], Andrea R. Nikolić[1], Jovana J. Ajduković[1]
[1] Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija
[2] Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za biologiju i ekologiju, Trg Dositeja Obradovića 2, 21000 Novi Sad, Srbija

U ovom radu sintetizovani su hidrazidni derivati 17α-(piridin-2-ilmetil)androstanske serije u cilju dobijanja biološki aktivnih molekula. S obzirom na to da hidrazidi pokazuju zapaženu biološku aktivnost, urađena je *in silico* ADME/T analiza i farmakokinetika, a ispitana je i *in vitro* biološka aktivnost. Određeni su relativni afinitet vezivanja novih hidrazidnih derivata za ligand-vezujuće domene odabranih steroidnih receptora i inhibicija rekombinantnih enzima iz potfamilije aldo-keto reduktaza 1C, značajne mete za lečenje kancera.

Synthesis of new androstane hydrazide derivatives, *in silico* ADME/T properties and *in vitro* biological activity

Đorđe D. Janković[1], Marina P. Savić[1], Sofija S. Bekić[1], Anđelka S. Ćelić[2], Edward T. Petri[2], Andrea R. Nikolić[1], Jovana J. Ajduković[1]
[1] University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Enviromental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[2] University of Novi Sad, Faculty of Sciences, Department of Biology and Ecology, Trg Dositeja Obradovića 2, 21000 Novi Sad, Serbia

In the present study, new steroid hydrazide derivatives in 17α-(pyridine-2-ylmethyl)androstane series were synthesized in order to investigate their biological activity. Because hydrazides show specific biological activity, we performed *in silico* ADME/T and pharmacokinetic analysis and examined *in vitro* biological activity. New hydrazide derivatives were evaluated for relative binding affinities to the ligand-binding domains of selected steroid receptors and inhibition potential against recombinant enzymes from aldo-keto reductase 1C subfamily, promising drug targets for cancer treatment.

The authors acknowledge the financial support of the Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina (Project No. 142-451-3133/2022-01) and the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125).

OH-5

Fluorescentno i UV-Vis ispitivanje interakcije A/B-modifikovanih androstanskih derivata sa DNK

Nezrina Kurtanović[1], Jovana J. Ajduković[2], Anđela A. Franich[1], Snežana Rajković[1]
[1] *Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, R. Domanovića 12, 34000 Kragujevac, Srbija, nezrina.mihovic@pmf.kg.ac.rs*
[2] *Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija*

Steroidna jedinjenja čine važnu klasu policikličnih molekula koja ispoljavaju raznovrsnu biološku aktivnost. Uvođenje heteroatoma ili heterocikla u steroidno jezgro, ili zamena jednog ili više atoma ugljenika heteroatomom, može dovesti do promene biološke aktivnosti steroida, pri čemu je od naročitog značaja citotoksična aktivnost prema tumorskim ćelijskim linijama. Interakcije 17-supstituisanih A i B-modifikovanih androstanskih derivata sa DNK ispitivane su primenom UV-Vis i fluorescentne spektroskopije. Na osnovu dobijenih rezultata utvrđeno je da androstanski derivati stabilizuju DNK lanac, međutim ne mogu istisnuti etidijum-bromid (EtBr) iz DNK-EtBr te stoga nisu interkalatori.

Fluorescent and UV-Vis investigation of the interaction of A/B-modified androstane derivatives with DNA

Nezrina Kurtanović[1], Jovana J. Ajduković[2], Anđela A. Franich[1], Snežana Rajković[1]
[1] *University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia, nezrina.mihovic@pmf.kg.ac.rs*
[2] *University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia*

Steroid compounds constitute an important class of polycyclic molecules that exhibit diverse biological activity. The introduction of a heteroatom or heterocycle into the steroid core, or the replacement of one or more carbon atoms by a heteroatom, can lead to a change in the biological activities of steroids, where cytotoxic activity against tumor cell lines could be of grate importance. Interactions of 17-substituted A and B-modified androstane derivatives with DNA were investigated using UV-Vis and fluorescence spectroscopy. Based on the obtained results, it was determined that androstane derivatives stabilize the DNA chain, however, they cannot displace ethidium bromide (EtBr) from DNA-EtBr and are therefore not intercalators.

Acknowledgement: The authors acknowledge financial support of the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200122 and 451-03-47/2023-01/200125).

OH-6

Solvatohromna svojstva novih boja na bazi stilbazolijum-soli

Luka R. Matović[1], Aleksandra D. Mašulović[1], Anita M. Lazić[1], Kristina G. Gak Simić[1],
Jelena M. Lađarević[2], Nemanja P. Trišović[2], Dušan Ž. Mijin[2]
[1]Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija
[2] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija

Pet novih jedinjenja na bazi stilbazolijum-soli, D-π-A strukture, sintetizovano je i detaljno okarakterisano. Solvatohromizam sintetizovanih jedinjenja ispitan je korišćenjem četiri rastvarača različite prirode pomoću UV-Vis spektroskopije. Takođe, ispitan je uticaj različitih elektron-donorskih grupa na solvatohromna svojstva molekula. Zahvaljujući prirodi kvaternarnog atoma azota, piridinijumov prsten u ovim jedinjenjima ispoljava jak elektron-akceptorski karakter, promovišući intramolekulski transfer naelektrisanja. Zahvaljujući ovom svojstvu, jedinjenja na bazi stilbazolijum-soli su primenu našla u brojnim granama industrije i nauke.

Solvatochromic properties of novel dyes derived from stilbazolium salts

Luka R. Matović[1], Aleksandra D. Mašulović[1], Anita M. Lazić[1], Kristina G. Gak Simić[1],
Jelena M. Lađarević[2], Nemanja P. Trišović[2], Dušan Ž. Mijin[2]
[1] Innovation Center, Faculty of Technology and Metallurgy, Belgrade, Serbia
[2] University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Five novel dyes derived from stilbazolium salts, bearing D-π-A structure, were synthesized and completely characterized. The solvatochromism of the synthesized dyes was investigated using four different solvents by means of UV-Vis spectroscopy. Also, the influence of different electron-donor groups on the solvatochromic properties of dyes was examined. Due to the nature of the quaternary nitrogen atom, the pyridinium ring in these compounds exhibits a strong electron-accepting character, promoting intramolecular charge transfer. This property has enabled compounds derived from stilbazolium salts to find applications in numerous branches of industry and science.

Acknowledgements: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-47/2023-01/200135 and 451-03-47/2023-01/200287).

OH-7

Modifikovani steroidi kao inhibitori SARS-CoV-2 Mpro

Andrea R. Nikolić[1], Ivana Z. Kuzminac[1], Edward T. Petri[2], Andjelka S. Ćelić[2], Sofija S. Bekić[2], Maja A. Marinović[2], Marija N. Sakač[1]
[1]Departman za hemiju, biohemiju i zaštitu životne sredine, Prirodno-matematički fakultet, Univerzitet u Novom Sadu, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija
[2] Departman za biologiju i ekologiju, Prirodno-matematički fakultet, Univerzitet u Novom Sadu, Trg Dositeja Obradovića 2, 21000 Novi Sad, Srbija

U cilju ispitivanja anti-COVID potencijala steroidnih jedinjenja sintetizovani su novi B,D-diseko 16,17a-dinitrili. *In silico* ADMET analiza je pokazala da sintetizovana jedinjenja imaju poželjne osobine leka i dobar bezbednosni profil, a virtuelni skrining predviđa njihovu potencijalnu inhibitorsku aktivnost prema proteazama. Molekulski doking pokazuje specifično vezivanje steroidnih dinitrila za glavnu proteazu COVID-a, Mpro. Proteaza Mpro je atraktivna meta za razvoj inhibitora protiv SARS-CoV-2, zbog svog značaja u životnom ciklusu virusa i visoke očuvanosti među različitim koronavirusima.

Modified steroids in the search for SARS-CoV-2 main protease inhibitors

Andrea R. Nikolić[1], Ivana Z. Kuzminac[1], Edward T. Petri[2], Andjelka S. Ćelić[2], Sofija S. Bekić[2], Maja A. Marinović[2], Marija N. Sakač[1]
[1]Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[2]Department of Biology and Ecology, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 2, 21000 Novi Sad, Serbia

Aiming to investigate the anti-COVID potential of dinitrile-modified steroidal compounds, we synthesized new B,D-diseco 16,17a-dinitriles. *In silico* ADMET analysis showed that synthesized compounds possess drug-like properties and no predicted toxicities, while structural similarity analysis predicts potential as protease inhibitors. Molecular docking simulations show that steroidal dinitriles can specifically bind the peptide binding site of the COVID main protease, Mpro. Mpro is an attractive drug target for the development of inhibitors against SARS-CoV-2, because of its importance in the viral life cycle and high conservation among different coronaviruses.

Acknowledgment: The authors acknowledge the financial support the Ministry of Science, Technological Development and Innovation of the Republic of Serbia grant number 451-03-47/2023-01/200125 and the Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina Project grant number 142-451-3133/2022-01.

OH-8

Optimizacija sinteze C-homo laktonskog derivata deoksiholne kiseline

Ksenija J. Pavlović, Aleksandar M. Oklješa, Srđan Bjedov
Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Srbija

Žučne kiseline (BAs) su hidroksilovani steroidi koji imaju značajnu ulogu u digestiji i apsorpciji holesterola, triglicerida i liposolubilnih vitamina, regulišu homeostazu lipida i glukoze, kao i inflamatorne procese. Uvođenje heteroatoma ili zamena atoma ugljenika heteroatomom u steroidnom skeletu utiče na hemijska svojstva žučnih kiselina i često dovodi do promene njihove biološke aktivnosti.

Pokazano je da proširenje prstena, odnosno umetanje laktonske funkcije u prsten C steroidnog skeleta žučnih kiselina znatno utiče na inhibiciju sijalil-transferaza,[1] stoga je razvoj efikasnog sintetskog puta važan za dobijanje niza novih derivata i dalji razvoj ovog područja. Ovde želimo da saopštimo optimizaciju sinteze 3α-hidroksi-13-oksa-12-okso-C-homo-5β-holanske kiseline menjanjem oksidacionog sredstva ali i reakcionih uslova. Najbolji rezultati su postignuti mikrotalasnom sintezom. Detalji ove sinteze i optimizacije će biti prezentovani.

Optimization of the synthesis of C-homo lactone derivative of deoxycholic acid

Ksenija J. Pavlović, Aleksandar M. Oklješa, Srđan Bjedov
University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia

Bile acids (BAs) are hydroxylated steroids that play a significant role in the digestion and absorption of cholesterol, triglycerides, and liposoluble vitamins, regulate lipid, glucose, and energy homeostasis, as well as inflammatory processes. The introduction of a heteroatom or replacement of carbon atoms in a steroidal skeleton by a heteroatom affects the chemical properties of bile acids and often results in alterations of their biological activities.

It has been shown that the expansion of the ring, i.e. the insertion of a lactone function into ring C of the steroid skeleton of bile acids significantly affects the inhibition of sialyltransferases,[1] therefore the development of an efficient synthetic route is important for obtaining several new derivatives and further development of this area. Here we would like to report the optimization of the synthesis of 3α-hydroxy-13-oxa-12-oxo-C-homo-5β-cholanoic acid by changing the oxidizing agent and the reaction conditions. The best results are obtained by microwave synthesis. Details of this synthesis and optimization will be presented.

[1] H. H. M. Abdu-Allah, T. T. Chang, W. Li, *Steroids* **2016**, *112*, 54.

Zahvalnica: Istraživanja je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Ev.br. 451-03-47/2023-01/200125)

OH-9

Dizajn, sinteza i biološki potencijal novih indol-pirazolskih hibrida

Milena M. Petrović[1], Nikola Srećković[1]
[1] *Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Instiitut za hemiju, R. Domanovića 12, 34000 Kragujevac, Srbija*

Indolski i pirazolski fragmenti se veoma često sreću u sintezi potencijalnih medicinskih agenasa zahvaljujući brojnim biološkim aktivnostima koje ispoljavaju. Derivati koji u svojoj strukturi sadrže indol pokazali su veoma značajne aktivnosti u mnogobrojnim biološkim ispitivanjima. Sa druge strane, mnogi agensi koji imaju široku primenu u lečenju različitih bolesti sadrže pirazolski fragment. Imajući ovo u vidu, može se pretpostaviti da će kombinacija ovih biološki značajnih fragmenata doprineti boljoj biološkoj aktivnosti željenog molekula usled sinergističkih efekata. Samim tim, osmišljena je i sintetisana serija novih indol-pirazolskih hibrida. Sinteza finalnih jedinjenja se sastojala iz dva koraka: prvo su sintetisani polazni halkoni Claisen-Schmidt-ovom kondenzacijom, a zatim u daljoj reakciji sa tiosemikarbazidom dolazi do formiranja pirazolskih derivata. Sintetisana jedinjenja će dalje biti podvrgnuta biološkim ispitivanjima, uključujući antimikrobni potencijal kao i citotoksičnu aktivnost prema kancerogenim ćelijskim linijama u *in vitro* uslovima.

Design, synthesis and biological potential of novel indole-pyrazole hybrids

Milena M. Petrović[1], Nikola Srećković[1]
[1] *University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34000 Kragujevac, Serbia*

Indole and pyrazole moieties are widely used in the synthesis of prospective medicinal agents due to the diversity of their biological activities. Derivatives containing indole fragment demonstrated very potent activities in various biological assays. On the other hand, pyrazole represents a core ring in most drugs broadly used in the treatment of various diseases. Considering this, it can be expected that combining these physiologically significant fragments will enhance the biological activity of the designed molecules due to synergistic effects. Hence, a series of novel indole-pyrazole hybrids was designed and prepared. The synthetic route of the final compounds consisted of two steps: the synthesis of starting chalcones by Claisen–Schmidt condensation, and further reaction with thiosemicarbazide to afford pyrazole derivatives. The synthesized compounds will be subjected to biological assays, including examination of antimicrobial potential and cytotoxic activity against human cancer cell lines *in vitro*.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreement No. 451-03-47/2023-01/200122).

OH-10

Sinteza i spektralna karakterizacija novih alizarinskih diacilhidrazina izvedenih iz vanilina

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

[1] Univerzitet u Kragujevcu, Institut za informacione tehnologije, Departman za prirodno-matematičke nauke, Jovana Cvijića bb, 34 000 Kragujevac, Srbija [2] Univerzitet u Kragujevcu, Prirodno-matematički fakultet, Institut za hemiju, R. Domanovića 12, 34 000 Kragujevac, Srbija

Alizarin i vanillin, kao i njihovi sintetički derivati pokazuju širok spektar bioloških aktivnosti.[1] Pretpostavka je da bi molekuli koji sadrže obe farmakofore mogli pokazati unapređen biološki potencijal. Iz tog razloga, izvršena je sinteza i spektralna karakterizacija serije novih diacilhidrazina. Prvi korak u dobijanju finalnih derivata predstavlja alkilovanje OH grupe u položaju 2 alizarina pomoću etil bromacetata i sukcesivna hidroliza dobijenog estra do odgovarajuće kiseline. Dobijena kiselina prevedena je u hlorid, koji je dalje derivatizovan reakcijom sa acilhidrazinima izvedenim iz odgovarajućih *O*-alkilovanih derivata vanilinske kiseline. Sva finalna jedinjenja su strukturno okarakterisana primenom IR i NMR spektroskopije.

Synthesis and spectral characterization of novel alizarin diacylhydrazines derived from vanillin

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

[1] University of Kragujevac, Institute for Information Technologies, Department of Science, Jovana Cvijića bb, 34 000 Kragujevac, Serbia, [2] University of Kragujevac, Faculty of Science, Department of Chemistry, R. Domanovića 12, 34 000 Kragujevac, Serbia

Alizarin and vanillin, as well as their synthetic analogues possess a broad spectrum of biological activities.[1] It can be hypothesized that molecules containing both pharmacophores could show an enhanced biological potential. For that reason, synthesis, and spectral characterization of a series of novel diacylhydrazines is performed. The first step in preparation of the final derivatives was an alkylation of OH group at position 2 of alizarin, using ethyl bromoacetate and subsequent hydrolysis of obtained ester to corresponding acid. The formed acid was converted to chloride and then treated with acylhydrazines prepared from corresponding *O*-alkylated derivatives of vanillic acid. All compounds are structurally characterized using IR and NMR spectroscopy.

1. a) A. Khan, P. Ezati, J.-W. Rhim, *Colloid Surface B.* **2023**, *223*, 113169; b) A. Olatunde *et al*, *Eur. J. Med. Chem.* **2022**, *5*, 100055.

Acknowledgment: This research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Agreements No. 451-03-47/2023-01/200122 and 451-03-47/2023-01/200378).

OH-11

Dizajn novog fotoreaktora za fotokatalizu pomoću vidljive svetlosti

Bojan Z. Vulović, Marko P. Slijepčević, Milica B. Plazinić, Filip J. Bihelović
Univerzitet u Beogradu – Hemijski fakultet, Beograd, Srbija

Fotokataliza pomoću vidljive svetlosti je od nedavno u prvom planu sintetičke organske hemije kao neophodan alat za selektivnu aktivaciju malih molekula i stvaranje novih veza. Međutim, nedostatak standardizacije eksperimentalnog izvođenja fotokatalizovanih reakcija i dalje postoji. Šira upotreba komercijalno dostupnih fotoreaktora kao standardnih je ograničena zbog njihove visoke cene. Ovde predstavljamo novi dizajn fotoreaktora koji omogućuje efikasnije izvođenje fotohemijskih reakcija. Performanse novog fotoreaktora testirane su na literaturnim transformacijama potpomognutim vidljivom svetlošću. U poređenju sa tradicionalnim načinom izvođenja reakcija, fotoreaktor obezbeđuje povećanu optičku snagu i značajno ubrzanje svih testiranih i fotokatalitičkih reakcija. Ekonomičan, modularan i prilagodljiv, fotoreaktor uvećava osvetljenost reakcione smese čak i kada se koriste jaki i fokusirani izvori svetla (serija Kessil PR160L). Dodatno, novi pristup značajno smanjuje svetlosno zagađenje u laboratoriji prilikom eksperimentalnog rada.

A novel photoreactor design for visible-light photocataysis

Bojan Z. Vulović, Marko P. Slijepčević, Milica B. Plazinić, Filip J. Bihelović
University of Belgrade – Faculty of Chemistry, Belgrade, Serbia

Visible-light photocatalysis has emerged to the forefront of synthetic organic chemistry as an indispensable tool for selective activation of small molecules and formation of new chemical bonds. However, the lack of standardization for experimental setup still persists in the field. Moreover, widespread use of commercial photoreactors as standards for photocatalysis research could be limited by high cost. Herein we report a novel photoreactor design for enhanced reaction efficiency. New photoreactor performance is evaluated using literature light-driven transformations. In comparison to standard reaction setup, the photoreactor enables increase in optical power thus providing significant rate acceleration of photocatalytic reactions in all cases. Inexpensive, modular and adaptable, the reactor offers enhanced light exposure even when strong and focused light sources (Kessil PR160L series) are employed. In addition, this novel approach to experimental setup significantly reduces light pollution in the lab.

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

Teorijska hemija

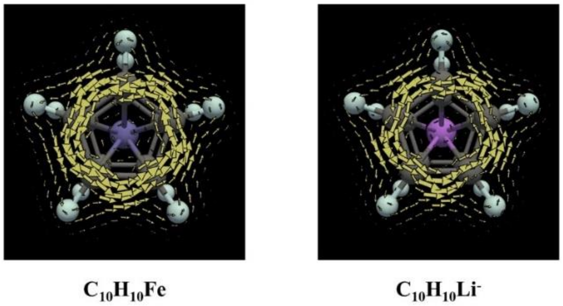
Theoretical Chemistry

TH-1

Cilindrična aromatičnost u ferocenu i njegovim analozima

Slađana Đorđević[1], Slavko Radenković[1]
[1]Univerzitet u Kragujevcu Prirodno-matematički fakultet, Kragujevac, Republika Srbija

Još od otkrića ferocena, aromatični karakter ovog molekula bio je predmet mnogih istraživanja. U ovom radu, aromatičnost ferocena i njegovih analoga analizirana je primenom modela čestice u cilindru. Naime, rešenja Šredingerove jednačine za česticu koja se kreće u cilindru su funkcije koje se razlikuju po broju i prirodi nodalnih površina. Nađeno je da se molekulske orbitale ispitivanih molekula mogu povezati sa sopstvenim funkcijama modela čestice u cilindru. Gustine magnetno indukovanih struja su izračunate primenom CTOCD-DZ metode na B3LYP/LANL2DZ nivou teorije za svaku od podgrupa molekulskih orbitala. Pokazano je da popunjenost dobijenih podgrupa molekulskih orbitala u ferocenu prati Hikelovo 4n+2 pravilo.


$C_{10}H_{10}Fe$ $C_{10}H_{10}Li^-$

Slika 1. Mape gustine struja za $C_{10}H_{10}Fe$ i $C_{10}H_{10}Li^-$.

Cylindrical aromaticity in ferrocene and its analogues

Slađana Đorđević[1], Slavko Radenković[1]
[1]University of Kragujevac Faculty of Science, Kragujevac, Republic of Serbia

The aromatic character of ferrocene has been extensively investigated since its discovery. In this work the aromaticity of ferrocene and its analogues was rationalized by the hollow cylinder model. Solving the Schrödinger equation for a particle in the hollow cylinder model gives eigenfunctions which can be classified based on their nodal characteristics. It was found that the molecular orbitals of the studied molecules follow the nodal properties of the eigenvectors of the simple cylinder model. Magnetically induced current densities were calculated using the CTOCD-DZ method at the B3LYP/LANL2DZ level of theory for each molecular orbital subgroup. It was found that populations of the orbital subgroups follow the Hückel 4n+2 rule.

Acknowledgment: Authors thanks the Ministry of Education, Science and Technological Development of the Republic of Serbia (Agreement No. 451-03-47/2023-01/200122).

TH-2

Интеракције јона са ароматичним лигандима у (полу)сендвич-једињењима: нове врсте π-система за препознавање јона

Душан П. Маленов[1], Катарина А. Ћеранић[2], Снежана Д. Зарић[1]
[1] *Универзитет у Београду - Хемијски факултет, Београд, Србија*
[2] *Иновациони центар Хемијског факултета, Београд, Србија*

Катјон-π и анјон-π интеракције сендвич- и полусендвич-једињења проучаване су квантнохемијским методама. DFT прорачуни показују да фероцен формира веома јаке катјон-π интеракције са катјонима алкалних метала, што је у сагласности са негативним електростатичким потенцијалом изнад ароматичних лиганада у сендвич-једињењима. С друге стране, DFT прорачуни показују да лиганди Cp типа у полусендвич-једињењима формирају јаке анјон-π интеракције са халогенидима,[1] услед позитивних електростатичких потенцијала изнад ових ароматичних лиганада. Интеракције катјона и анјона са ароматичним лигандима у сендвич, односно полусендвич-једињењима могу бити јаче него интеракције јона са органским ароматичним молекулима,[1] што може да пружи смернице за дизајн нових рецептора за јоне.

Interactions of ions with aromatic ligands in (half-)sandwich compounds: new types of π-systems for ion recognition

Dušan P. Malenov[1], Katarina A. Ćeranić[2], Snežana D. Zarić[1]
[1] *University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*
[2] *Innovative Centre of the Faculty of Chemistry, Belgrade, Serbia*

Cation-π and anion-π interactions of sandwich and half-sandwich compounds were studied using quantum chemical methods. DFT calculations show that ferrocene forms very strong cation-π interactions with alkali metal cations, which is in agreement with negative electrostatic potentials above aromatic ligands in sandwich compounds. On the other hand, DFT calculations show that Cp-based ligands in half-sandwich compounds form strong anion-π interactions with halide anions,[1] due to positive electrostatic potentials above these aromatic ligands. Interactions of cations and anions with aromatic ligands in sandwich and half-sandwich compounds, respectively, can be stronger than interactions of ions with organic aromatic molecules,[1] which can provide guidelines for the design of novel ion receptors.

2. D. P. Malenov, S. D. Zarić, *Chem Eur J.* **2021**, *27*, 17862.

This research was funded by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contracts 451-03-47/2023-01/200168 and 451-03-47/2023-01/200288).

TH-3

Neočekivani Ni(III) komleks sa hidrazonskim ligandom – analiza spinskih stanja

Miloš K. Milčić[1], Maja A. Gruden[1], Matija S. Zlatar[2]
[1] Univerzitet u Beogradu – Hemijski fakultet, Studentski trg 12 – 16, Beograd, Srbija
[2] Univerzitet u Beogradu – Institut za hemiju, tehnologiju I metalurgiju, Njegoševa 12, 11000 Beograd, Srbija

Tokom sinteze kompleksa nikla(II) sa tridentatnim I−1-(2-okso-2-(2-(1-(piridin-2-il)etiliden)hydrazinil)etil)piridin-1-ijum ligandom (**L**) došlo je do neočekivane oksidacije Ni(II) u Ni(III), vazdušnim kiseonikom, pri veoma blagim uslovima. Nastali oktaedarski [Ni**L**(N_3)$_3$] kompleks pokazuje veoma zanimljive spinske I magnetne osobine, koje su proučavane metodama teorije funkcionala gustine (DFT). Proračuni su pokazali da će u vodenom rastvoru, dubletno spinsko stanje biti osnovno stanje ovog kompleksa, dok je energija kvartetnog spinskog stanja za 16,55 kcal/mol visa. U osnovnom stanju, spinska gustina nesparenog elektrona je locirana najvećim delom na jonu Ni(III) (76,5%), I atomima azota (10,7%) I kiseonika (7,5%) iz prve kooridnacione sfere kompleksa.

Unexpected Ni(III) complex with hydrazone lignad – spin state analysis

Miloš K. Milčić[1], Maja A. Gruden[1], Matija S. Zlatar[2]
[1] University of Belgrade – Faculty of Chemistry, Studenstki trg 12-16, 11000 Belgrade, Serbia
[2] University of Belgrade – Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia

During synthesis of Ni(II) complex with (E)−1-(2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethyl)pyridin-1-ium ligand (**L**) unexpected oxidation of Ni(II) to Ni(III) with atmospheric oxygen occurred at mild conditions. Unusual spin and magnetic properties of the synthesized octahedral [Ni**L**(N_3)$_3$] complex, were further investigated with Density Functional Theory (DFT) methods. These DFT calculations have shown that, in water solution, doublet state is the ground state for Ni(III) complex, with the quartet state higher in energy for 16.55 kcal/mol. Spin density calculations have revealed that most of the spin density is located on Ni(III) ion (76.5%), and N (10.7%) and O (7.5%) atoms from the first coordination sphere of the complex.

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.

TH-4

Теоријско проучавање утицаја халогених супституената на осетљивост полицикличних нитроароматичних експлозива

Ивана С. Вељковић[1], Александра Б. Ђуновић[2], Душан Ж. Вељковић[3]
[1] Универзитет у Београду – Институт за хемију, технологију и металургију – Институт од националног значаја за Републику Србију, Његошева 12, Београд
[2] Иновациони центар Хемијског факултета у Београду, Студентски трг 12-16, Београд
[3] Универзитет у Београду – Хемијски факултет, Студентски трг 12-16, Београд

Позитивне вредности електростатичких потенцијала на површини високоенергетских молекула представљају добар индикатор њихове детонабилности. У овом раду смо на основу прорачуна енергија дисоцијације веза и електростатичких потенцијала анализирали утицај присуства халогених супституената на детонационе особине одабраних динитронафталена са халогеним супституентима. Резултати *ab initio* прорачуна указују да халогени супституенти могу да утичу на геометрију нитро-група и да доведу до смањења стабилности најслабијих C-N веза. Халогени супституенти такође утичу на вредности електростатичких потенцијала у централним деловима површине испитиваних молекула.

Theoretical study of the influence of halogen substituents on sensitivity of polycyclic nitroaromatic explosives

Ivana S. Veljković[1], Aleksandra B. Đunović[2], Dušan Ž. Veljković[3]
[1] University of Belgrade – Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia, Njegoševa 12, Belgrade
[2] Innovative Centre of the Faculty of Chemistry, Studentski trg 12-16, Belgrade
[3] University of Belgrade–Faculty of Chemistry, Studentski trg 12-16, Belgrade

Positive values of electrostatic potential on the surface of high-energy molecules are a good indicator of the high sensitivity towards detonation. Here we used Bond Dissociation Energy and Molecular Electrostatic Potential calculations to predict the influence of the halogen substituents on the detonation properties of selected halogen-containing dinitronaphthalenes. Results of *ab initio* calculations indicated that halogen substituents may affect the geometry of the nitro- groups and lead to decreased stability of the weakest C-N bonds. Presence of halogen substituents also affects the values of the electrostatic potentials in the central regions of the molecular surfaces.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, PROMIS, #6066886, CD-HEM. This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No: 451-03-47/2023-01/200026, 451-03-47/2023-01/200288 and 451-03-47/2023-01/200168).

Fizička hemija

Physical Chemistry

FH-1

Nanokompozitni prah ZrO_2/magnetit kao fotokatalizator u reakciji degradacije odabranih hlorofenola

Tatjana D. Vulić[1], Milica V. Carević[1], Nadica D. Abazović[1], Mirjana I. Čomor[1]

[1]Institut za nuklearne nauke Vinča, Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Republika Srbija

Nanokompozitni prah ZrO_2/Fe_3O_4 sintetisan je uspešno u nekoliko koraka. Prvo su sintetisane nanočestice magnetita sa zaštitnim slojem od SiO_2 koji sprečava prenos elektrona iz provodne zone ZrO_2 na magnetit prilikom ozračivanja. Potom je na nanočestice nanet sloj ZrO_2 solvotermalnom metodom. Dobijeni prah je prečišćen uz pomoć permanentnog magneta koji obezbeđuje potpuno ukalanjanje magnetnog materijala iz rastvora. Ovako sintetisan magnetni materijal je upotrebljen kao fotokatalizator u reakcijama razgradnje 2,4 dihlorofenolai 2,4,6 trihlorofenola u vodenim rastvorima. Rezultati su pokazali da je nanokompozit efikasan adsorber i fotokatalizator za odabrana jedinjenja. Hlorofenoli su izabrani kao model jedinjenja u ovoj studiji zbog toga što se često nalaze u prirodnim vodama, u koje stižu iz pesticida koji se upotrebljavaju u poljoprivredi. Njihova toksičnost se najviše ogleda u uticaju na nervini sistem životinja i ljudi.

ZrO_2/magnetite nanocomposite as photocatalyst in degradation of selected chlorophenols

Tatjana D. Vulić[1], Milica V. Carević[1], Nadica D. Abazović[1], Mirjana I. Čomor[1]

[1]Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Republic of Serbia

Nanocomposite powder ZrO_2/Fe_3O_4 was synthesized in several steps. Firstly, magnetite nanoparticles with a protective layer of SiO_2 were synthesized. Silica layer protects magnetite core and prevents the transfer of electrons from the conduction band of ZrO_2 to magnetite during illumination. Secondly, a layer of ZrO_2 was added to the nanoparticles by the solvothermal method. The resulting powder was purified with the help of a strong magnet that ensures complete separation of the magnetic material from the solution. The magnetic material thus synthesized was used as a photocatalyst in the decomposition reactions of 2,4 dichloro- and 2,4,6 trichloro- phenols in aqueous solutions with Simulated Solar light as an irradiation source. The results showed that nanocomposite is an effective adsorber and photocatalyst for selected compounds. Chlorophenols were chosen as a model of compounds in this study because they are often found in natural waters, which come from pesticides used in agriculture. Their toxicity is mostly reflected in the impact on the nervous system of animals and humans.

FH-2

Karakterizacija post-modifikovanih metalo-organskih umreženih struktura sa Šifovom bazom sorpcijom gasova i ispitivanje njihove stabilnosti u vodi

Branko B. Kordić[1], Nikola D. Radnović[1], Milica G. Bogdanović[1], Mirjana M. Radanović[1],
Berta Barta Holló[1], Marko V. Rodić[1]
[1]*Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija*

Novi, post-modifikovani derivati metalo-organske umrežene strukture (MOFs) UiO-67 su ispitani kao hvatači ugljen dioksida. Ispitana je i njihova stabilnost u vodi. Ispitivanja su vršina na mono i diamino derivatima UiO-67 koji su post-modifikovani uvođenjem 4-formilbenzonitrila uz građenje Šifove baze. Poroznost MOFs-ova je ispitana sorpcijom N_2, dok je adsorbovana količina CO_2 određena na 283, 288 i 293 K. Izosterična entalpija za adsorpciju CO_2 je određena virijalnom jednačinom. Hidroliza MOFs-ova u vodenoj suspenziji je praćena UV-Vid spektroskopijom. Detektovana je traka na 252 nm koja potiče od 4-formilbenzonitrila.

Gas sorption characterization and water stability investigation of post modified Schiff-base containing Metal-organic frameworks

Branko B. Kordić[1], Nikola D. Radnović[1], Milica G. Bogdanović[1], Mirjana M. Radanović[1],
Berta Barta Holló[1], Marko V. Rodić[1]
[1]*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*

Novel post-modified derivatives of UiO-67 Metal-organic framework (MOFs) have been investigated for their carbon-capture capabilities and water stability. Mono and diamino derivatives of UiO-67 MOFs have been post-synthetically modified with 4-formylbenzonytrile that can be incorporated as animine, forming Schiff base. The porosity of MOFs has been investigated with the sorption of N_2 gas, while CO_2 uptake has been determined at 283, 288 and 293 K. Isosteric enthalpy of CO_2 adsorption has been obtained from the virial fit of the experimental data. UV-VIS spectroscopy has been used for hydrolysis investigation. A band of 4-formylbenzonitrile (252 nm) has been detected in the samples taken from MOFs water suspension.

1. N. Ko, J. Hong, S. Sung, K.E. Cordova, H.J. Park, J.K. Yang, J. Kim, *Dalton Trans.* **2015**, *44*, 2047.

Zahvalnica: ovo istraživanje je finansirano sa projekta Fonda za nauku Republike Srbije PROMIS, pod brojem 6066708 (CASCH-MOF).

FH-3

Елементна анализа и дијагностика плазме хуманих зуба применом LIBS-a

Јелена Д. Петровић[1], Јелена М. Маринковић[1], Марина Б. Раденковић[1], Сања М. Живковић[1], Јован В. Цигановић[1], Милош Д. Момчиловић[1]
[1] *Универзитет у Београду, Институт за нуклеарне науке „Винча“, Институт од националног значаја за Републику Србију, Београд, Србија*

У овом раду се испитује примена спектроскопије ласерски индуковане плазме (LIBS) за анализу елементног састава зуба и пломбе. Коришћењем CO_2 ласера као извора побуђивања, добијени су емисиони спектри са оштрим спектралним линијама и ниском позадином који су омогућили идентификацију елементног састава ткива зуба и пломбе. Испитивани су и параметри плазме, температура и густина електрона, што је важно за разумевање процеса током LIBS анализе. Добијени резултати показују да LIBS техника са CO_2 ласером може пружити корисне информације о елементном саставу зуба и пломбе, што је значајно за стоматологију, археологију и форензику [1].

Elemental analysis and plasma diagnostics of human teeth using LIBS

Jelena D. Petrović[1], Jelena M. Marinković[1], Marina B. Radenković[1], Sanja M. Živković[1], Jovan V. Ciganović[1], Miloš D. Momčilović[1]
[1] *University of Belgrade, „Vinča“, Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade, Serbia*

This study investigates the application of laser-induced breakdown spectroscopy (LIBS) for analyzing the elemental composition of teeth and dental fillings. Using a CO_2 laser as the excitation source, emission spectra with sharp spectral lines and low background were obtained, allowing for the identification of the elemental composition of tooth and filling tissue. Plasma parameters, including electron temperature and density, were also examined, which is important for understanding the process during LIBS analysis. The results show that the LIBS technique with a CO_2 laser can provide useful information on the elemental composition of teeth and fillings, which is significant for dentistry, archaeology, and forensics [1].

1. E. Castellon, P. Pacheco Martinez, J. Alvarez, F. Bredice, F. Borges, M. V. Muniz, C. Sanchez-Ake, V. Palleschi, R. Sarmiento, *Spectroc. Acta B.* **2018**, *149*, 229–35.

Acknowledgment: The authors thank the financial support from the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (No. 451-03-47/2023-01/ 200017).

FH-4

Multivarijantna analiza parametara lipofilnosti novih derivata spirohidantoina

Kristina A. Tot[1], Tatjana Lj. Đaković Sekulić[1]
[1]*Univerzitet u Novom Sadu, Departman za hemiju, biohemiju i zaštitu životne sredine, Prirodno-matematički fakultet, Novi Sad, Republika Srbija*

Lipofilnost predstavlja fizičko-hemijsko svojstvo molekula koje otkriva mnoštvo informacija o međumolekulskim silama, intramolekulskim interakcijama i molekulskoj strukturi u najširem smislu. Parametri lipofilnosti (R_M^0) novosintetisanih derivata cikloalkilspiro-5-hidantoina određeni su primenom hromatografije na tankom sloju na obrnutim fazama. Kao nepokretna faza korišćen je C-18 modifikovani silika gel, a kao pokretne faze korišćene su dvokomponentne smeše vode i organskih rastvarača. Uticaj supstituenata, organskog rastvarača, kao i sličnosti među proučavanim parametrima lipofilnosti i derivatima spirohidantoina ispitane su multivarijantnom analizom, odnosno analizom glavnih komponenti (PCA) i hijerahijskom klaster analizom (HCA).

Zahvalnica: Istraživanje je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Ev.br. 451-03-47/2023-01/200125)

Multivariate analysis of lipophilicity parameters of new spirohydantoin derivatives

Kristina A. Tot[1], Tatjana Lj. Đaković Sekulić[1]
[1] *University of Novi Sad, Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Science, Novi Sad, Republic of Serbia*

Lipophilicity reperesent physico-chemical property that reveals a wealth of information on intermolecular forces, intramolecular interactions, and molecular structure in the broadest senses. Parameters of lipophilicity (R_M^0) of newly synthesized derivatives of cycloalkylspiro-5-hydantoins were determined by reverse phase thin layer chromatography on C-18 modified silica gel. Mobile phases were two-component mixtures of water and organic solvents. The effect of the substituents, organic solvents, as well as similarities among the studied lipophilicity measures and spirohydantoin derivatives were examined by the multivariate exploratory analysis such as principal component analysis (PCA) and hierarchical cluster analysis (HCA).

Hemija životne sredine

Environmental Chemistry

HŽS-1

Sorpcija lindana iz vode pomoću makroporoznog kopolimera na bazi glicidil metakrilata

Sandra S. Bulatović[1], Tamara T. Tadić[1], Bojana M. Marković[1],
Aleksandra B. Nastasović[1], Mila V. Ilić[1], Natalija Ž. Nedić[2]
[1]Univerzitet u Beogradu, Institut za Hemiju, Tehnologiju i Metalurgiju, Beograd, Srbija
[2]Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija

Organohlorni pesticid - lindan, smatra se potencijalno kancerogenim jedinjenjem. Lindan i njegovi ostaci mogu da opstanu u životnoj sredini veoma dugo, migrirajući i potencijalno izazivajući zagađenje životne sredine. Ostaci lindana mogu dospeti i u ljudski organizam kroz lanac ishrane, jer je ovo potencijalno toksično jedinjenje sklono bioakumulaciji. Kontaminacija lindanom je globalni problem, a njegovo uklanjanje iz životne sredine je neophodno. U ovom istraživanju sorpcija lindana iz vodenog rastvora urađena je sa makroporoznim kopolimerom na bazi glicidil metakrilata, koji se pokazao kao veoma efikasan sorbent, sa sorpcijom lindana od oko 80%. Za određivanje koncentracije lindana korišćena je analitička tehnika, gasna hromatografija sa detektorom za hvatanje elektrona GC-ECD. Osim sorpcije, uspešno je urađena i desorpcija lindana.

Sorption of lindane from water using a macroporous copolymer based on glycidyl methacrylate

Sandra S. Bulatović[1], Tamara T. Tadić[1], Bojana M. Marković[1],
Aleksandra B. Nastasović[1], Mila V. Ilić[1], Natalija Ž. Nedić[2]
[1]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia
[2]University of Belgrade, Faculty of Chemistry, Belgrade, Serbia

Organochlorine pesticide - lindane, is considered as potentially carcinogenic compound. Lindane and its residues can persist in the environment for a very long period, migrating and potentially causing environmental pollution. Residues of lindane can also enter the human body through the food chain, because this potentially toxic compound is prone to bioaccumulation. Lindane contamination is a global problem, and its removal from the environment is essential. In this research, the sorption of lindane from an aqueous solution was performed with a macroporous copolymer based on glycidyl methacrylate, which proved to be a very effective sorbent, with lindane sorption of about 80%. An analytical technique, gas chromatography with an electron capture detector GC-ECD, was used to determine the concentration of lindane. In addition to sorption, desorption of lindane was also successfully performed.

Zahvalnica: Izradu ovog rada je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Broj ugovora: 451-03-47/2023-01/200026 i 451-03-47/2023-01/200168).

HŽS-2

Efikasnost fotokatalitičke razgradnje odabranih herbicida u prisustvu zelenih ZnO nanočestica

Vesna N. Despotović[1], Nataša Zec[2], Nina L. Finčur[1], Tamara B. Ivetić[3], Szabolcs I. Bognár[1], Dušica K. Jovanović[1], Daniela V. Šojić Merkulov[1]
[1]Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija
[2]Visoka tehnička škola strukovnih studija u Zrenjaninu, Đorđa Stanimirovića 23, 23000 Zrenjanin, Srbija
[3]Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za fiziku,Trg Dositeja Obradovića 4, 21000 Novi Sad, Srbija

Cilj ovoga rada je bio ispitivanje fotokatalitičke aktivnosti novosintetisanih zelenih ZnO nanočestica na bazi ekstrakta kore banane i vinske kiseline za uklanjanje herbicida klomazona i kvinmeraka iz vodene sredine. Za uklanjanje odabranih herbicida korišćen je fotokatalitički reaktor sa ksenonskom lampom. Rezultati su pokazali da se bolja efikasnost uklanjanja klomazona i kvinmeraka postiže primenom ZnO nanoprahova na bazi vinske kiseline kao fotokatalizatora u poređenju sa zelenim nanoprahovima na bazi ekstrakta kore banane, nakon 60 min ozračivanja.

Efficiency of photocatalytic degradation of selected herbicides in the presence of green ZnO nanoparticles

Vesna N. Despotović[1], Nataša Zec[2], Nina L. Finčur[1], Tamara B. Ivetić[3], Szabolcs I. Bognár[1], Dušica K. Jovanović[1], Daniela V. Šojić Merkulov[1]
[1]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[2]Technical College of Applied Sciences in Zrenjanin, Đorđa Stratimirovića 23, 23000 Zrenjanin, Serbia
[3]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia

The aim of this work was to investigate the photocatalytic activity of newly synthesized green ZnO nanoparticles based on banana peel extract and tartaric acid for the removal of clomazone and quinmerac herbicides from aquatic environment. The photocatalytic reactor with xenon lamp was used for the removal of selected herbicides. The results showed that after 60 min of irradiation higher efficiency of clomazone and quinmerac removal was achieved by using ZnO nanopowders based on tartaric acid as a photocatalyst compared to green nanopowders based on banana peel extract.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia (Grant No 7747845, In situ pollutants removal from waters by sustainable green nanotechnologies-CleanNanoCatalyze).

HŽS-3

Spektroskopska karakterizacija glomalinskih ekstrakata zemljišta Novog Sada

Branislav D. Jović[1], Nataša Negru, Slavica Mitrović, Stefan Vidović
Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Trg Dossiteja Oradovića3 Novi Sad, Srbija

Gloamalinski proteini zemljišta veoma su bitna komponenta zemljišta odgovorna za stabilnost organske materije i agregaciju čestica. Do sada ekstrakti glomalinskih proteina nisu sistematski izučavani na zemljištima sa područja Srbije. U ovom istraživanju prvi put su ispitivani ekstrakti glomalinskih proteina zemljišta spektroskopskim metodama. Korišćenjem UV VIS, FTIR i SEM instrumentalnih tehnika određene su osnovne spektralne karakteristike ove nove grupe jedinjenja a takođe je izvršena i kvantifikacija glomalinskih proteina. Za lokalno zemljište sa područja Novog Sada utvrđeno je da glomalinski proteini čine oko 20 % ukupne organske materije. Spektroskopskim metodama utvrđene su glavne trake za identifikaciju. Takođe su i procenjeni problemi koekstrakcije huminske organske materije manje molarne mase i visoke aromatičnosti.

Spectroscopic characterization of glomalin extracts from the soil of Novi Sad

Branislav D. Jović[1], Nataša Negru, Slavica Mitrović, Stefan Vidović
University of Novi Sad, Faculty of Sciences, Trg Dositeja Obradovića 3, Novi Sad. Serbia

Soil gloamalin proteins are very important component of the soil responsible for the stability of organic matter and the aggregation of particles. Until now, glomaline protein extracts have not been systematically studied on soils from Serbia. In this research, for the first time, extracts of soil glomalin proteins were examined by spectroscopic methods. Using UV VIS, FTIR and SEM instrumental techniques, the basic spectral characteristics of this new group of compounds were determined, and the quantification of glomalin proteins was also performed. For the local soil from the area of Novi Sad, it was determined that glomaline proteins represent about 20% of the total organic matter. Spectroscopic methods were used to determine the main bands for identification. The problems of co-extraction of humic organic matter with lower molar mass and high aromaticity were also assessed.

B. Jović, S. Maletić, B. Kordić, J. Beljin, *Environ Monit Assess* **2023**. *195*,473

This work was supported by the Provincial Secretariat for Science and Technological Development, Autonomous Province of Vojvodina, project no. 142–451-2198/2022–01.

HŽS-4

Ekstrakcija retkih elemenata zemljine kore iz letećeg pepela TCLP metodom

Jelena D. Lukić[1], Latinka J. Slavković-Beškoski[2], Katarina V. Trivunac[3], Antonije E. Onjia[3]
[1] Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija
[2] Laboratorija Anahem, Beograd, Srbija
[3] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija

Retki elementi zemljine kore (engl. Rare Earth Elements, REE) koriste se u proizvodnji uređaja visoke tehnologije, optičkih vlakana, superprovodnika, itd. Osim ruda koje su glavni izvor REE, u novije vreme oni se dobijaju iz nusproizvoda ili otpadnih materijala. Sve češće se ispituje mogućnost primene letećeg pepela kao sirovine za dobijanje REE. Uzorci letećeg pepela korišćeni u ovom radu potiču iz četiri termoelektrane sa teritorije Republike Srbije (Tent B, Morava, Kostolac i Kolubara). Ekstrakcija REE je vršena pomoću TCLP ekstrakcionog fluida. Metodom masene spektrometrije sa indukovano spregnutom plazmom analizirano je 17 elemenata (Sc, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Th). Najviše koncentracije REE izmerene su u uzorku pepela iz termoelektrane Tent B.

Extraction of the Rare Earth elements from coal fly ash by the TCLP method

Jelena D. Lukić[1], Latinka J. Slavković-Beškoski[2], Katarina V. Trivunac[3], Antonije E. Onjia[3]
[1] Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia
[2] Anahem Laboratory, Belgrade, Serbia
[3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Rare earth elements (REEs) are used as components in high-technology devices, fiber optics, superconductors, etc. In addition to ores, by-products or waste materials are being considered as alternative sources for obtaining REEs. The potential for extracting REE from fly ash is being intensively studied. The fly ash samples used in this work were obtained from four thermal power plants from the Republic of Serbia (Tent B, Morava, Kostolac and Kolubara). The REE were extracted by TCLP extraction fluid. The ICP MS method was used for the analysis of 17 elements (Sc, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Th). The highest concentrations of REE were measured in the sample of fly ash from the Tent B power plant.

Zahvalnica: Ovo istraživanje je podržano od stane Fonda za nauku Republike Srbije, GRANT No 7743343, Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants - SIW4SE, Program IDEJE.

HŽS-5

Alkalno aktivirani leteći pepeo modifikovan polietileniminom kao adsorbent za uklanjanje metilensko plavog iz vode

Marina M. Maletić[1], Sara D. Žižović[2], Marija M. Vukčević[2], Milena D. Milošević[3], Nataša V. Karić[1], Katarina V. Trivunac[2], Aleksandra A. Perić Grujić[2]

[1] Inovacioni Centar Tehnološko-metalurškog fakulteta, Beograd, Srbija

[2] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija

[3] Univerzitet u Beogradu, Institut za Hemiju, Tehnologiju i Metalurgiju, Institut od nacionalnog značaja za Republiku Srbiju, Beograd, Srbija

U cilju iskorišćenja industrijskog otpada, leteći pepeo je modifikovan radi dobijanja efikasnih adsorbenata za uklanjanje metilensko plavog iz vode. Leteći pepeo je aktiviran u prisustvu NaOH na 550°C, i modifikovan različitim količinama polietilenimina. Karakterizacija polaznog i modifikovanih uzoraka izvršena je skenirajućom elektronskom mikroskopijom i infracrvenom spektroskopijom sa Furijeovom transformacijom. Ispitan je uticaj vremena kontakta i početne koncentracije adsorbata na adsorpcione kapacitete nemodifikovanog i modifikovanog letećeg pepela. Pokazano je da adsorpcione karakteristike zavise od količine dodatog polietilenimina, kao i da adsorpcija prati brzinu pseudo-drugog reda, a ravnotežni adsorpcioni podaci pokazuju bolje slaganje sa Frojndlihovom izotermom.

Alkali-activated fly ash modified with polyethyleneimine as adsorbent for methylene blue removal from water

Marina M. Maletić[1], Sara D. Žižović[2], Marija M. Vukčević[2], Milena D. Milošević[3], Nataša V. Karić[1], Katarina V. Trivunac[2], Aleksandra A. Perić Grujić[2]

[1] Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia

[2] University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

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

In attempt to reuse industrial waste, fly ash was modified and converted into efficient adsorbent for the removal of methylene blue from water. Fly ash was activated in the presence of NaOH at 550°C, and modified with different amounts of polyethyleneimine. The raw and modified samples were characterized by scanning electron microscopy and Fourier transform infrared spectroscopy. The influence of contact time and initial adsorbate concentration on the adsorption capacity of unmodified and modified fly ash was also examined. It has been shown that the adsorption characteristics depend on the amount of polyethyleneimine added, that the adsorption follows a pseudo-second-order rate, and the equilibrium adsorption data show better agreement with the Freundlich isotherm.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, GRANT No 7743343, Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants - SIW4SE, Program IDEAS.

HŽS-6

Sinteza nanobiokatalizatora na bazi ugljeničnih nanocevi za tretman fenolnih otpadnih voda

Mirjana Ž. Petronijević, Sanja N. Panić
Univerzitet u Novom Sadu – Tehnološki fakultet Novi Sad, Novi Sad, Srbija

Fenolne komponente su polutanti koji se često mogu naći u industrijskim otpadnim vodama i poznato je da imaju toksičan uticaj na ljude i vodene organizme. Tretman fenolnih otpadnih voda zasnovan na primeni enzima pokazao je veliki potencijal zbog svoje visoke efikasnosti, selektivnosti i blagih uslova rada. Cilj ovog istraživanja bila je sinteza površinski modifikovanih ugljeničnih nanocevi (UNC) pogodnih za kovalentnu imobilizaciju peroksidaze dobijene iz rena (HRP), kao i njihova dalja primena kao biokatalizatora za tretman fenolnih otpadnih voda. Sintetisane UNC su funkcionalizovane sa ccHNO_3 i modifikovane sa tionil-hloridom, a potom primenjene kao nosač za imobilizaciju HRP. Dobijeni rezultati ukazuju da primena HRP imobilisane na UNC predstavlja dobro rešenje za tretman fenolnih otpadnih voda. Naime, primenom imobilisane HRP postignuto je uklanjanje 80% fenola iz vode nakon 10 min, pri čemu povećanje dužine trajanja reakcije nije značajno povećalo efikasnosti procesa (88% nakon 90 min).

Synthesis of nanobiocatalyst based on carbon nanotubes for phenolic wastewater treatment

Mirjana Ž. Petronijević, Sanja N. Panić
University of Novi Sad – Faculty of Technology Novi Sad, Novi Sad, Serbia

Phenols are common pollutants found in industrial wastewaters and are known to have toxic effects on both humans and aquatic organisms. Enzyme-based phenol-containing wastewater treatment has shown a great potential due to its high efficiency, selectivity, and mild operating conditions. The objective of this study was to synthesize surface modified carbon nanotubes (CNTs) suitable for covalent horseradish peroxidase (HRP) immobilization and their further utilization as biocatalyst for phenolic wastewater treatment. CNTs were initially functionalized with ccHNO_3, modified with thionyl chloride and then applied as a support for HRP immobilization. The obtained results suggest that the application of HRP immobilized onto CNTs offers a promising solution for the treatment of phenolic wastewater. Namely, 80% of phenol was removed from water after 10 min by immobilized HRP, whereas the increase of the duration of the reaction did not significantly contribute to the efficiency of the process (88% after 90 min).

Acknowledgment: The research was financed by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia under Grant 451-03-47/2023-01/200134.

HŽS-7

Adsorpcione karakteristike hidrogelova hitozana za uklanjanje boje kongo crveno iz vodenih rastvora

Đorđe Ž. Petrović, Katarina V. Stanković, Ksenija R. Kumrić
University of Belgrade, "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade, Serbia

Istraživanja u okviru ove studije okrenuta su ka ispitivanju mogućnosti primene hidrogelova hitozana, u obliku sfera, za uklanjanje boje kongo crveno (CR) iz vodenih rastvora. Sfere hidrogela hitozana (CHBs) pripremljene su spregnutim jonskim i kovalentnim umrežavanjem, pri čemu su limunska kiselina (CA) i glutaraldehid (Glu) korišćeni kao jonski i kovalentni umreživač, respektivno. Eksperimenti su rađeni u šaržnom sistemu kako bi se optimizovali uslovi za efikasno uklanjanje CR iz vode i odredili adsorpcioni kapaciteti sintetisanih CHBs. Eksperimentalni rezultati su pokazali da je efikasnost uklanjanja CR najveća u pH intervalu od 6 do 10, a da se ravnoteža uspostavlja nakon 180 minuta. Langmirova izoterma pokazala je najbolju korelaciju za adsorpciju CR boje na CA/Glu umreženim sferama hidrogelova hitozana, pri čemu maksimalni adsorpcioni kapacitet (q_m) iznosi 544.2 mg g^{-1}.

Adsorption characteristics of chitosan hydrogel beads toward removal of Congo red dye from aqueous solutions

Đorđe Ž. Petrović, Katarina V. Stanković, Ksenija R. Kumrić
University of Belgrade, "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade, Serbia

The present study investigated potential application of biopolymer chitosan, in the form of gel beads, for the removal of Congo red (CR) dye from aqueous solution. Chitosan hydrogel beads (CHBs) were prepared by a coupled ionic and covalent co-cross-linking, employing citric acid (CA) and glutaraldehyde (Glu) as an ionic and a chemical cross-linker, respectively. Batch experiments were carried out to optimize the process conditions for efficient removal of CR dye and to determine the adsorption capacity of prepared CHBs. The results showed that the highest removal efficiency of CR was obtained in the pH range from 6 to 10, and that the equilibrium was attained after 180 min. The Langmuir isotherm model provided the best correlation for the adsorption of CR onto CA/Glu co-cross-linked CHBs, with the maximum adsorption capacity (q_m) of 544.2 mg g^{-1}.

HŽS-8

Statistička optimizacija adsorpcije bakra iz vodenih rastvora korišćenjem aktiviranog ugljeničnog materijala agroindustrijskog otpada suncokreta

Marina B.Radenković[1], Jelena D. Petrović[1], Sabolč I. Pap[2], Ana M. Kalijadis[1], Miloš D. Momčilović[1], Sanja M. Živković[1]

[1] Institut za nuklearne nauke „Vinča" - Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija .

[2] Departman za inženjerstvo zaštite životne sredine i zaštite na radu, Fakultet tehničkih nauka, Univerzitet u Novom Sadu, Novi Sad, Srbija , Environmental Research Institute, UHI North Highland, University of the Highlands and Islands, Thurso, Scotland KW14 7JD, UK.

U ovom radu za procenu efikasnosti uklanjanja bakra iz vodenih rastvora korišćen je aktivni ugalj dobijen od agroindustrijskog otpada suncokreta. Boks-Benkenov dizajn i metoda odzivne površine korišćeni su za optimizaciju procesnih parametara adsorpcije kao i međusobni uticaj varijabli na efikasnost uklanjanja. Sintetizovani aktivni ugalj primenjen je za uklanjanje bakra iz realnog uzorka otpadne vode, a dobijeni rezultati ukazuju na veliki afinitet za separaciju bakra (98,6% ± 2,0%).

Statistical optimization of copper adsorption from aqueous solutions by sunflower waste derived activated carbon

Marina B.Radenković[1], Jelena D. Petrović[1], Sabolc I. Pap[2], Ana M. Kalijadis[1], Miloš D. Momčilović[1], Sanja M. Živković[1]

[1] „VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia.

[2] Department of Environmental Engineering and Occupational Safety and Health, Faculty of Technical Sciences, University of Novi Sad, Novi Sad, Serbia, Environmental Research Institute, UHI North Highland, University of the Highlands and Islands, Thurso, Scotland KW14 7JD, UK.

In this work, activated carbon obtained from sunflower agro-industrial waste was used to evaluate the removal efficiency of copper from aqueous solutions. The Box-Behnken design combined with the response surface method was employed to optimize the adsorption process parameters as well as the mutual influence of the variables on removal efficiency. The synthesized activated carbon was applied to remove copper from a real wastewater sample, and the obtained results indicate a high affinity for copper separation (98,6% ± 2,0%).

Zahvalnica: Autori se zahvaljuju MNTRI razvoja Republike Srbije za finansijsku podršku istraživanju kroz institucionalno finansiranje (Broj ugovora 451-03-9/2023-14/200017).

HŽS-9

Primena unapređenih oksidacionih procesa za degradaciju 2-etilheksil-4-metoksicinamata iz vode

Tajana M. Simetić[1], Jelena J. Molnar Jazić[1], Sanja V.Vasiljević[1], Aleksandra M. Tubić[1], Jelena M. Beljin[1], Marijana M. Kragulj Isakovski[1], Jasmina R. Agbaba[1]
[1] Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za hemiju, biohemiju i zaštitu životne sredine, Trg Dositeja Obradovića 3, Novi Sad, Republika Srbija

U radu su prikazani rezultati ispitivanja efikasnosti fotohemijskih unapređenih oksidacionih procesa (eng. *advanced oxidation processes*, AOPs) zasnovanih na generisanju hidroksil radikala (UV/H_2O_2 proces) i sulfatnih radikala (UV/$S_2O_8^{2-}$ i UV/HSO_5^- procesi) na stepen oksidativne degradacije 2-etilheksil-4-metoksicinamata (EHMC) u vodi. EHMC pripada grupi organskih UV filtera svrstanih na listu emergentnih supstanci i predstavlja važnu aktivnu komponentu sredstava za ličnu higijenu. Dobijeni rezultati ukazuju da je značajno efikasnija degradacija EHMC dobijena primenom fotohemijskih AOPs u odnosu na direktnu UV fotolizu. Stepen oksidativne degradacije EHMC opada prema sledećem nizu u odnos na proces: UV/H_2O_2 (40-93%) > UV/HSO_5^- (32-88%) > UV/$S_2O_8^{2-}$ (14-79%).

Zahvalnica: Istraživanje je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Ev.br. 451-03-47/2023-01/200125) i SAFEWAT 17243/EUREKA Projekat (Ev. br. 337-00-00294/2021/09/05).

Application of advanced oxidation processes for degradation of 2-ethylhexyl-4-methoxycinnamate from water

Tajana M. Simetić[1], Jelena J. Molnar Jazić[1], Sanja V.Vasiljević[1], Aleksandra M. Tubić[1], Jelena M. Beljin[1], Marijana M. Kragulj Isakovski[1], Jasmina R. Agbaba[1]
[1] University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Republic of Serbia

In study presents the results of a comparison of the efficiency of photochemical advanced oxidation processes (AOPs) based on the generation of hydroxyl radicals (UV/H_2O_2 process) and sulfate radicals (UV/$S_2O_8^{2-}$ and UV/HSO_5^- processes) on the degree of oxidative degradation of 2-ethylhexyl-4-methoxycinnamate (EHMC) in water. EHMC belongs to the group of organic UV filters included in the list of emerging substances and is an important active component of personal care products. The obtained results indicate that the degradation of EHMC is a significantly more effective using the photochemical AOPs compared to direct UV photolysis. The degree of oxidative degradation of EHMC decreases in the following order in relation to the process: UV/H_2O_2 (40-93%) > UV/HSO_5^- (32-88%) > UV/$S_2O_8^{2-}$ (14-79%).

HŽS-10

Uklanjanje teških metala iz vodenih rastvora primenom cijanobakterija

Irena Z. Rakić[1], Žarko S. Kevrešan[2], Renata Kovač[2], Snežana Ž. Kravić[1], Zorica B. Svirčev[3], Ana D. Đurović[1], Zorica S. Stojanović[1]

[1] Univerzitet u Novom Sadu, Tehnološki fakultet Novi Sad, Novi Sad, Srbija

[2] Naučni institut za prehrambene tehnologije, Univerzitet u Novom Sadu, Novi Sad, Srbija

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

Poslednjih godina biološke metode privlače pažnju za uklanjanje teških metala iz industrijskih otpadnih voda. U ovom radu, ispitana je sposobnost cijanobakterija *Nostoc* sp. da apsorbuju jone teških metala (Cd^{2+}, Cu^{2+}, Pb^{2+}, Ni^{2+}, Zn^{2+}) iz vodenih rastvora upotrebom živih ćelija. Rezultati su pokazali da su koncentracije metala imale značajan uticaj na apsorpciju metala putem biosorpcije. Do najveće akumulacije Cd^{2+}, Cu^{2+}, Zn^{2+}, i Ni^{2+} je došlo pri početnoj koncentraciji od 20 mg/l, osim za Pb^{2+}, gde je zabeležena najveća bioakumulaciju pri 80 mg/l. Najmanja sposobnost bioakumulacije od 38% ostvarena je za Ni^{2+}, dok je najveća bioakumulacija od 98,15% postignuta za Pb^{2+}. Dobijeni rezultati ukazuju na potencijal cijanobakterija kao biosorbenta za efikasno uklanjanje teških metala iz vodenih rastvora.

Removal of heavy metals from aqueous solutions using cyanobacteria

Irena Z. Rakić[1], Žarko S. Kevrešan[2], Renata Kovač[2], Snežana Ž. Kravić[1], Zorica B. Svirčev[3], Ana D. Đurović[1], Zorica S. Stojanović[1]

[1] University in Novi Sad, Faculty of Technology Novi Sad, Novi Sad, Serbia

[2] Institute of Food Technology in Novi Sad, University of Novi Sad, Novi Sad, Republic of Serbia

[3] Faculty of Sciences, Department of Biology and Ecology, University of Novi Sad, Novi Sad, Serbia

In recent years, researchers have resorted to biological methods to remove toxic heavy metals from industrial wastewater. In the present study, the ability of cyanobacteria *Nostoc* sp. to absorb heavy metal ions (Cd^{2+}, Cu^{2+}, Pb^{2+}, Ni^{2+}, Zn^{2+}) from aqueous solutions was investigated by optimizing the absorption conditions for cyanobacteria live cells. The results revealed that the metal concentrations had a significant impact on the uptake of metals through biosorption. The greatest accumulation of Cd^{2+}, Cu^{2+}, Zn^{2+}, and Ni^{2+} occurred at an initial concentration of 20 mg/l, except for Pb^{2+}, which showed the highest bioaccumulation at a concentration of 80 mg/l. The lowest bioaccumulation power of 38% was achieved for Ni^{2+}, while the highest bioaccumulation of 98.15% was achieved for Pb^{2+}. The obtained results highlight the significance of cyanobacteria as a favorable and promising biosorbent for effectively removing heavy metals from aqueous solutions.

Hemijsko inženjerstvo

Chemical Engineering

HI-1

Dobijanje eteričnog ulja ploda kleke (*Juniperis communis* L.) mikrotalasnom hidrodestilacijom

Jelena D. Bajac[1], Milena D. Terzić[1], Branislava G. Nikolovski[1], Igor S. Antić[1], Marija M. Radojković[1]
[1] *Univerzitet u Novom Sadu - Tehnološki fakultet Novi Sad, Novi Sad, Srbija*

Primena mikrotalasne hidrodestilacije za izolovanje eteričnog ulja kleke, kao savremene tehnologije izolovanja eteričnih ulja, razvijena je u cilju smanjenja utroška energije u odnosu na konvencionalne tehnike dobijanja. U radu je opisan uticaj vremena mikrotalasne hidrodestilacije, koji je variran od 5 do 120 minuta pri snazi od 200 W, na prinos eteričnog ulja, njegov kvalitativni i kvantitativni hemijski sastav. Rezultati istraživanja su pokazali da se najveći procenat monoterpena izoluje već u prvim minutama procesa (ulje dobijeno nakon 5 min. sadrži 84,15% monoterpena, 0,32% oksidovanih monoterpena i 15,40% seskviterpena), dok duže delovanje mikrotalasnog zračenja doprinosi povećanju procenta oksidovanih monoterpena i seskviterpena (nakon 120 min. sadržaj monoterpena je 67,23%, oksidovanih monoterpena 0,97% i seskviterpena 31,64%).

Juniper berry (*Juniperis communis* L.) essential oil isolation by microwave hydrodistillation

Jelena D. Bajac[1], Milena D. Terzić[1], Branislava G. Nikolovski[1], Igor S. Antić[1], Marija M. Radojković[1]
[1] *University of Novi Sad - Faculty of Technology Novi Sad, Novi Sad, Serbia*

The application of microwave hydrodistillation for the isolation of juniper berry essential oil, as a modern technology for obtaining essential oils, was developed in order to reduce energy consumption compared to conventional techniques of extraction. The paper describes the influence of microwave hydrodistillation time (varied from 5 to 120 minutes at a power of 200 W) on the essential oil yield, qualitative and quantitative chemical composition. The results of investigation showed that the highest percentage of monoterpenes was isolated during the first minutes of the process (the oil obtained after 5 min. had 84.15% of monoterpenes, 0.32% of oxidized monoterpenes and 15.40% of sesquiterpenes), while longer exposure to microwave radiation was contributed to a higher percent of oxidized monoterpenes and sesquiterpenes fractions (after 120 min. monoterpenes, oxidized monoterpenes and sesquiterpenes fractions were 67.23%, 0.97% and 31.64%, respectively).

Acknowledgment: This work was supported by Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Project No. 451-03-47/2023-01/200134)

HI-2

Analiza molekulskih interakcija prema dopunskim veličinama za binarnu smešu etil oktanoat + 1-butanol

Divna M. Majstorović[1], Emila M. Živković[1], Mirjana Lj. Kijevčanin[1]

[1]Univerzitet u Beogradu Tehnološko-metalurški fakultet, Karnegijeva 4, Beograd, Srbija

Gustina i viskoznost za binarni sistem koji sadrži estar etil oktanoat i alkohol 1-butanol mereni su na osam temperatura u opsegu (288,15-323,15) K i na atmosferskom pritisku. Ovi podaci omogućili su izračunavanje dopunskih veličina kao što su dopunska molarna zapremina, promena viskoznosti i dopunska molarna Gibsova energija aktivacije viskoznog toka. Izračunati podaci su korelisani Redlich-Kister jednačinom i korišćeni za diskusiju o strukturnim efektima i efektima pakovanja koji se dešavaju u ispitivanoj smeši. Rezultati su pokazali da je efekat raskidanja vodoničnih veza molekula alkohola i dipol-dipol interakcija molekula estara, koji uslovljava ekspanziju zapremine, kvantitativno nadmašio slabe intermolekulske vodonične veze između ovih molekula i intersticijalno smeštanje molekula estara u multimere alkohola.

Molecular interaction analysis according to the excess and deviation properties for the binary mixture ethyl octanoate + 1-butanol

Divna M. Majstorović[1], Emila M. Živković[1], Mirjana Lj. Kijevčanin[1]

[1]University of Belgrade Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

Density and viscosity data for the binary system containing ester ethyl octanoate and alcohol 1-butanol are obtained at eight temperatures in the range (288.15-323.15) K and at atmospheric pressure. These property data allowed the calculation of the excess and deviation properties such as excess molar volume, viscosity deviations and excess molar Gibbs energy of activation of viscous flow. Calculated property data are correlated with the Redlich-Kister equation and used for discussion of structural and packing effects taking place in the investigated mixture. The results showed that the effect of breaking hydrogen bonds of alcohol molecules and dipole-dipole interactions of ester molecules, which attributes the volume expansion, quantitatively exceeded the weak intermolecular hydrogen bonds between these molecules and the interstitial placement of ester molecules in alcohol multimers.

Acknowledgment: The authors gratefully acknowledge the financial support received from the Research Fund of Ministry of Science, Technological Development and Innovation Republic of Serbia and the Faculty of Technology and Metallurgy University of Belgrade (Contract No. 451-03-47/2023-01/200135).

HI-3

Superupijajući hidrogelovi natrijum-karboksimetilceluloze za zeleno uklanjanje organskih zagađujućih materija

Ksenija D. Milošević[1], Melina T. Kalagasidis Krušić[2]
[1] *Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija*
[2] *Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*

U prirodi su prisutne različite zagađujuće materije, poput organskih nerazgradivih materija. Upotreba ekoloških, „zelenih“ materijala na bazi prirodnih polimera, za njihovo uklanjanje predstavlja korak napred u odstranjivanju zagađenja. Prirodni polimeri imaju odličnu perspektivu zbog svoje netoksičnosti, različitih izvora dobijanja, niske cene i biodegradabilnosti. Natrijum-karboksimetilceluloza (CMC) je široko dostupan i jeftin polimer koji može da se koristi za sintezu ekološki prihvatljivih superupijajućih hidrogelova. Tema ovog istraživanja je upotreba materijala na bazi CMC umrežene limunskom kiselinom za sorpciju zagađujućih materija iz vode. Kao model supstanca korišćena je boja Basic Yellow 9. Parametri kao što su koncentracija boje, temperatura, vreme kontakta, odnos polimera i umreživača praćeni su tokom procesa sorpcije. Rezultati istraživanja su pokazali da se hidorgelovi na bazi CMC dobijaju jednostavnom sintezom i da imaju odličnu moć sorpcije zagađujućih materija.

Superabsorbent sodium carboxymethylcellulose hydrogels for green removal of organic pollutants

Ksenija D. Milošević[1], Melina T. Kalagasidis Krušić[2]
[1] *University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*

Various pollutants are present in nature, such as organic non-degradable substances. The use of ecological, "green" materials such as natural polymers, for their removal represents a step forward in removing pollution. Natural polymers have an excellent perspective due to their non-toxicity, various sources of production, low cost, and biodegradability. Sodium carboxymethylcellulose (CMC) is a widely available and inexpensive polymer that can be used to synthesize environmentally-friendly superabsorbent hydrogels. The topic of this research is the use of materials based on CMC crosslinked with citric acid for the sorption of pollutants from water. Basic Yellow 9 dye was used as a model pollutant. Parameters such as dye concentration, temperature, contact time, and polymer/crosslinker ratio were monitored during the sorption process. The results of the research showed that hydrogels based on CMC are obtained by a simple synthesis and that they have excellent sorption properties of pollutants.

Zahvalnica: Sredstva za realizaciju istraživanja obezbedilo je Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (ugovor br. 451-03-47/2023-01/200135 i 451-03-47/2023-01/200026).

HI-4

Ispitivanje međumolekulskih interakcija računarskim simulacijama

Milana M. Zaric[1,2], Mirjana Lj. Kijevcanin[3], Ivona R. Radovic[3]
[1] Univerzitet u Beogradu, Institut za hemiju, tehnologiju i metalurgiju, Beograd, Srbija
[2]Univerzitet u Beogradu, Centar za hemiju i inženjering životne sredine, Centar izuzetnih vrednosti IHTM, Beograd, Srbija
[3] Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija

Експериментална мерења и подаци су од суштинског значаја за пружање информација о својствима и понашању смеша. Међутим, компјутерски прорачуни у комбинацији са експерименталним мерењем могу пружити дубљи увид у понашање и интеракције на молекулском нивоу.[1] За течне бинарне смеше нековалентне интеракције су проучаване квантним хемијским прорачунима и молекулско-динамичким симулацијама. Истражен је утицај различитих функционалних група, попут двоструке везе са могућношћу π-π интеракције и -OH групе са могућношћу водоничне везе. Поред тога, проучавали смо утицај геометрије молекула на својства бинарних смеша.

Investigation of intermolecular interactions using computer simulations

Milana M. Zaric[1,2], Mirjana Lj. Kijevcanin[3], Ivona R. Radovic[3]
[1] University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia
[2] University of Belgrade, Centre of Excellence in Environmental Chemistry and Engineering – ICTM, Belgrade, Serbia
[3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Experimental measurement and data are essential for providing the information of properties and behavior of mixtures. However, the computer calculations combined with experimental measurement can provide a deeper insight of behavior and interactions at the molecular level[1]. For liquid binary mixtures the non-covalent interactions were studied with quantum chemical calculations and molecular dynamic simulations. The influence of different functional groups, like the double bond with possibility for the π-π interactions and the -OH group with possibility for the hydrogen bonding was investigated. In addition, we studied the influence of the geometry of the molecule on the properties of binary mixtures.

1. M. M. Zarić, I. R. Radović, M. Lj. Kijevčanin, *J. Mol. Liq.* **2020**, *303*,112486

Acknowledgment This work was supported by the Science Fund of the Republic of Serbia, Program DIJASPORA #6388652, PAMD, and the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-47/2023-01/200026)

Hemija i tehnologija materijala

Chemistry and Technology of Materials

HTM-1

Sinteza i karakterizacija hibridnih nanomaterijala na bazi ZnO

Miljana M. Dukić[1], Valentina Z. Nikšić[1], Dušan N. Sredojević[2], Vesna M. Lazić[2], Jovan M. Nedeljković[2]

[1] *Institut za nuklearne nauke Vinča, Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija*

[2] *Centar za konverziju svetlosne energije, Institut za nuklearne nauke Vinča, Univerzitet u Beogradu, Beograd, Srbija*

Cink oksid (ZnO) je poluprovodni material sa velikim energetskim procepom, sa najčešćom primenom u fotokatalizi. Površinska modifikacija nanočestica ZnO ligandima salicilatnog tipa (salicilna kiselina i 5-aminosalicilna kiselina) kao i ligandima kateholatnog tipa (katehol, 3,4-dihidroksibenzoeva kiselina i kafeinska kiselina) dovodi do pomeranja apsorpcije ka vidljivom delu spectra usled formiranja kompleksa sa prenosom naelektrisanja (ICT). Pripremljeni uzorci su okarakterisani infracrvenom spektroskopijom (FTIR) koja je korišćena za identifikaciju načina vezivanja između liganada i ZnO. Proračuni teorije funkcionalne gustine (DFT) sa pravilno dizajniranim klasterima, izvedeni su za procenu usklađenosti energetskih nivoa različitih neorganskih/organskih hibrida. Utvrđena je značajna usaglašenost između izračunatih i eksperimentalnih vrednosti za FTIR i refleksione spektre.

Synthesis and characterization of hybrid nanomaterials based on ZnO

Miljana M. Dukić[1], Valentina Z. Nikšić[1], Dušan N. Sredojević[2], Vesna M. Lazić[2], Jovan M. Nedeljković[2]

[1] *Vinča institute for nuclear sciences − National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia.*

[2] *Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia.*

Zinc oxide (ZnO) is a wide bandgap ceramic material with various potential applications like photocatalysis. Surface modification of ZnO nano-powder with salicylate-type ligands (salicylic acid and 5-aminosalicylic acid) as well as catecholate-type ligands (catechol, 3,4-dihydroxybenzoic acid, and caffeic acid), induces the appearance of absorption in the visible spectral region due to the interfacial charge transfer (ICT) complex formation. The prepared samples were characterized by Fourier-transform infrared spectroscopy (FTIR), used to identify the binding mode between ligands and the surface of ZnO. The density functional theory (DFT) calculations with properly designed model systems, were performed to estimate the alignment of energy levels of various inorganic/organic hybrids. A reasonably good agreement between calculated values and experimental data for FTIR and reflectance spectra was found.

HTM-2

Fluorescencija heterospojenih TiO_2/MoO_3 poluprovodnika za remedijaciju i monitoring životne sredine

Tamara B. Ivetić[1], Kristina O. Čajko[1], Dalibor L. Sekulić[2]

[1] *Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Departman za fiziku, Trg Dositeja Obradovića 3, 21000 Novi Sad, Srbija*

[2] *Univerzitet u Novom Sadu, Fakultet tehničkih nauka, Departman za energetiku, elektroniku i telekomunikacije, Trg Dositeja Obradovića 6, 21000 Novi Sad, Srbija*

Fluorescencija heterospojnih TiO_2/MoO_3 poluprovodnika pod 324 nm ekscitacijom pokazala je široku i intenzivnu traku u vidljivom opsegu koja sadrži najmanje dva pika koja prikazuju karakteristike fluorescencije pojedinačnih oksida ali sa smanjenim intenzitetom. Ovo potvrđuje formiranje heterospojne TiO_2/MoO_3 strukture bliskog kontakta koja razdvaja fotogenerisane parove elektron-šupljina više nego u pojedinačnim metal oksidima i doprinosi poboljšanju efikasnosti ovog materijala u remedijaciji životne sredine [1].

Fluorescence of heterojunction TiO_2/MoO_3 semiconductors for environmental remediation and monitoring

Tamara B. Ivetić[1], Kristina O. Čajko[1], Dalibor L. Sekulić[2]

[1] *University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia*

[2] *University of Novi Sad, Faculty of Technical Sciences, Department of Power, Electronic and Telecommunication Engineering, Trg Dositeja Obradovića 6, 21000 Novi Sad, Serbia*

Fluorescence of heterojunction TiO_2/MoO_3 semiconductors under the 325 nm excitation showed a broad and intense band in the visible range containing at least two peaks depicting the fluorescence characteristics of a single oxide but with reduced peak intensity. This confirms the formation of a TiO_2/MoO_3 close-contact heterojunction structure that separates the photogenerated electron-hole pairs more than in individual metal oxides and contributes to the improvement of efficiency in environmental remediation [1].

1. T. Ivetić et al., *Catalysts*. **2021**, *11*, 1054.

Acknowledgment: This research is financed by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (grant no. 451-03-47/2023-01/200125) and partially by the APV Provincial Secretariat for Higher Education and Scientific Research (project title: Development of new highly-sensitive sensors for monitoring of gas pollution and humidity in Vojvodina, project no. 142-451-3154/2022-01/2).

HTM-3

Mikrotalasna sinteza biorazgradivih hidrogelova

Teodora J. Pušac[1], Marija G. Kostić[1], Jelena M. Tanasić[1], Suzana M. Cakić[2], Ivan S. Ristić[1]
[1] *Univerzitet u Novom Sadu – Tehnološki fakultet Novi Sad, Novi Sad, Srbija*
[2] *Univerzitet u Nišu – Tehnološki fakultet Leskovac, Leskovac, Srbija*

U ovom radu sintetisani su biorazgradivi hidrogelovi na bazi natrijum alginata i hitozana. Varirani su odnosi Na-alginat/hitozan (od 4:1 do 1:4) kako bi se ispitao njihov uticaj na svojstva gelova. Pored klasične sinteze, isproban je novi pristup za sintezu pomoću mikrotalasa. Karakterizacija je vršena pomoću infracrvene spektroskopije sa Furijeovom transformacijom (FTIR), diferencijalne skenirajuće kalorimetrije (DSC) i određivanjem stepena bubrenja pri različitim pH vrednostima. Mikrotalasna sinteza doprinela je skraćivanju vremena formiranja hidrogelova (sa 3 h na 3 min) i njihovoj većoj poroznosti omogućavajući veći stepen bubrenja (do 8000%). Na bubrenje takođe utiče i promena pH vrednosti medijuma. Rezultati su pokazali da ovi hidrogelovi imaju veliki potencijal kao biomaterijali za medicinske primene, prečišćavanje voda i u sistemima gde se zahteva velika sposobnost upijanja vode.

Microwave-assisted synthesis of biodegradable hydrogels

Teodora J. Pušac[1], Marija G. Kostić[1], Jelena M. Tanasić[1], Suzana M. Cakić[2], Ivan S. Ristić[1].
[1] *University of Novi Sad – Faculty of Technology Novi Sad, Novi Sad, Serbia*
[2] *University of Niš – Faculty of Technology Leskovac, Leskovac, Serbia*

Biodegradable hydrogels based on sodium alginate and chitosan were synthesized in this work. The ratios of Na-alginate/chitosan (from 4:1 to 1:4) were varied to investigate the influence on the properties of the gels. In addition to the classical synthesis, a new approach for the synthesis using microwaves was tried. Characterization of the gels was performed using Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), and determination of the degree of swelling at different pH values. Microwave synthesis contributed to shortening the formation time of hydrogels (from 3 h to 3 min) and their greater porosity, enabling a higher degree of swelling (up to 8000%). Swelling is also affected by a change in the pH value of the solution. The results showed that these hydrogels have great potential as biomaterials for medical applications, in water purification, and in systems where high-water absorption capacity is required.

Acknowledgment: to the Ministry of Education, Science and Technological Development, Republic of Serbia, project numbers 451-03-68/2023-14/200134, 451-03-9/2023-14/200125 for financial support.

HTM-4

Čišćenje naftnih mrlja pomoću netkanog sorbenta proizvedenog od post-industrijskog tekstilnog otpada

Aleksandar G. Kovačević[1], Darka D. Marković[2], Marija B. Radoičić[3],
Maja M. Radetić[1]
[1]Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija,
[2]Univerzitet u Beogradu, Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija
[3]Univerzitet u Beogradu, Institut za nuklearne nauke "Vinča", Beograd, Srbija

Efikasno i jeftino čišćenje naftnih mrlja sa vode i tla kao i generisanje ogromnih količina tekstilnog otpada su goreći ekološki problemi koji zahtevaju hitno rešavanje. U pokušaju da se odgovori na oba izazova, proizveden je iglovani netkani sorbent od recikliranih vlakana jute iz industrije tepiha. Ispitan je uticaj površinske mase i debljine sorbenata na sorpcioni kapacitet za naftu u vodi i u nafti bez vode, sposobnost plutanja, sposobnost zadržavanja nafte i mogućnost ponovne upotrebe. Svi sorbenti su položili test plutanja. Površinska masa sorbenata i viskozitet testirane nafte i naftnih derivata (sirova nafta, dizel gorivo i dva motorna ulja) imaju snažan uticaj na sorpcioni kapacitet i sposobnost zadržavanja nafte. Sorbenti uglavnom zadržavaju do 50% svojih početnih sorpcionih kapaciteta nakon 5 ponovljenih ciklusa sorpcije što ukazuje da se mogu višekratno koristiti.

Oil spills cleanup with non-woven sorbent produced from post-industrial textile waste

Aleksandar G. Kovačević[1], Darka D. Marković[2], Marija B. Radoičić[3],
Maja M. Radetić[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
[2]University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia
[3]University of Belgrade, "Vinča" Institute of Nuclear Sciences, Belgrade, Serbia

Efficient and inexpensive cleanup of oil spills on water or land and huge generation of textile waste are burning environmental issues that are seeking urgent solutions. In an attempt to address both challenges, needle-punched non-woven sorbents (NWSs) based on recycled jute fibers from the carpet industry were manufactured. The influence of NWS area density and thickness on oil sorption capacity in water and oil without water, buoyancy, oil retention and reusability were studied. All NWSs passed the buoyancy test. The area density of NWSs and viscosity of tested oils (crude oil, diesel oil and two motor oils) strongly affect the oil sorption capacity and oil retention. NWSs mainly retain 50% of their initial oil sorption capacities after 5 repeated sorption cycles indicating that NWSs could be used several times.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, GRANT No.7673808, SORBTEX

HTM-5

Nanokompoziti TiO_2/PPy za primenu u fotokatalizi

Natalija D. Milojković[1], Bojana M. Simović[2], Milan M. Žunić[2], Lidija D. Radovanović[3],
Aleksandra H. Dapčević[1]
[1] *Univerzitet u Beogradu - Tehnološko-metalurški fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu - Institut za multidisciplinarna istraživanja, Beograd, Srbija*
[3] *Univerzitet u Beogradu - Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*

Titan(IV)-oksid je jedan od najčešće korišćenih fotokatalizatora, dok za polipirol (PPy) postoje potvrde da je pogodan za ovu primenu. Cilj ovog rada bio je dobijanje kompozita TiO_2/PPy sa boljom fotokatalitičkom aktivnosti u odnosu na TiO_2. Kako bi se optimizovao sadržaj PPy u kompozitu, sintetisani su uzorci TiO_2/x%PPy (x = 0, 0,5, 1, 1,5, 3, 5 mas.%), koji su okarakterisani TG/DTA, XRD, FTIR, FESEM i UV-Vis metodama, dok su njihova fotokatalitička svojstva ispitana kroz razgradnju tekstilne boje RO16. Nanokristalni TiO_2 je dobijen u obliku anatasa veličine kristalita oko 26 nm, dok su izračunati parametri jedinične ćelije potvrdili da je kristalna struktura anatasa ostala nepromenjena nakon dodatka PPy. Gotovo svi uzorci (izuzev TiO_2/3%PPy) su fotokatalitički aktivniji od TiO_2, dok je TiO_2/1%PPy pokazao najizraženiju fotokatalitičku aktivnost razgradivši 98 % boje nakon 75 min.

TiO_2/PPy nanocomposites for photocatalytic application

Natalija D. Milojković[1], Bojana M. Simović[2], Milan M. Žunić[2], Lidija D. Radovanović[3],
Aleksandra H. Dapčević[1]
[1] *University of Belgrade - Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade - Institute for Multidisciplinary Research, Belgrade, Serbia*
[3] *University of Belgrade - Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*

Titanium(IV) oxide is one of the most used photocatalysts while polypyrrole (PPy) is a promising material for photocatalytic application. The aim of this work was to obtain TiO_2/PPy composites exhibiting higher photocatalytic activity than TiO_2. In order to determine the optimal PPy content in a composite, TiO_2/x%PPy (x = 0, 0.5, 1, 1.5, 3, 5 wt.%) samples were synthesized and characterized by TG/DTA, XRD, FTIR, FESEM and UV-Vis methods, while the photocatalytic behavior was examined towards the degradation of the textile dye RO16. Nanocrystalline TiO_2 was obtained in anatase form with crystallite size around 26 nm and preserved anatase crystal structure despite the addition of PPy according to the calculated unit cell parameters. Almost all samples (except TiO_2/3%PPy) showed better photocatalytic activity than TiO_2 while the best photocatalytic activity was demonstrated by TiO_2/1%PPy which degraded 98 % of the dye after 75 min.

HTM-6

Tretman natrijum-alginatom kao način da se poboljšaju sorpciona svojstva sirove tkanine jute

Marija D. Milošević[1], Aleksandra M. Ivanovska[2], Mirjana M. Kostić[1], Zorica B. Svirčev[3,4]
[1] *Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu, Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[3] *Univerzitet u NovomSadu, Prirodno-matematički fakultet, Novi Sad, Srbija*
[4] *Abo Akademi Univerzitet, Prirodno-tehnički fakultet, Turku, Finska*

Rastvori natrijum-alginata različitih koncentracija (0, 5, 1,0 ili 2,0%) korišćeni su za poboljšanje sorpcionih svojstava (sposobnost zadržavanja vode (WRP) i vreme kvašenja (WT)) sirove tkanine jute. Proučavan je uticaj uslova sušenja (neosušeni uzorci, uzorci sušeni na 60 °C ili na sobnoj temperaturi) na sorpciona svojstva tkanina jute tretiranih alginatom. Tkanine tretirane alginatom imale su do 4,8 puta veću posobnost zadržavanja vode i više od 120 puta kraće vreme kvašenja. Poboljšana sorpciona svojstva tkanina jute tretiranih alginatom pripisuju se sloju alginate na njihovoj površini sa većim brojem dostupnih funkcionalnih grupa sposobnih da formiraju nove vodonične veze sa molekulima vode.

A way to improve the sorption properties of raw jute fabric by sodium alginate treatment

Marija D. Milošević[1], Aleksandra M. Ivanovska[2], Mirjana M. Kostić[1], Zorica B. Svirčev[3,4]
[1] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[3] *University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*
[4] *Åbo Akademi University, Faculty of Science and Engineering, Turku, Finland*

Sodium alginate solutions of different concentrations (0.5, 1.0, or 2.0%) were used for improving the sorption properties (the water retention power (WRP) and wetting time (WT)) of raw jute fabric. The influence of drying conditions (never-dried samples, samples dried at 60 °C or at room temperature) on the sorption properties of alginate-treated jute fabrics was studied. The WRP of alginate-treated fabric increased up to 4.8 times compared to raw jute fabric, while the WT of jute fabrics decreased more than 120 times after the alginate treatment. The improved sorption properties of alginate-treated jute fabrics are attributed to the alginate layer on the fabric surface having a higher number of accessible functional groups capable of forming new hydrogen bonds with water molecules.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #7726976, Integrated Strategy for Rehabilitation of Disturbed Land Surfaces and Control of Air Pollution– RECAP.

HTM-7

Toksičnost nanočestica TiO_2 modifikovanih dihidrokvarcetinom

Valentina Z. Nikšić[1], Miljana M. Dukić[1], Andrea M. Pirković[2], Vesna M. Lazić[3]
[1] Institut za nuklearne nauke Vinča, Institut od nacionalnog značaja za Republiku Srbiju, Univerzitet u Beogradu, Beograd, Srbija
[2] INEP Institut za primenu nuklearne energije, Univerzitet u Beogradu, Beograd, Srbija
[3] Centar za konverziju svetlosne energije, Institut za nuklearne nauke Vinča, Univerzitet u Beogradu, Beograd, Srbija

Cilj ovog rada je modifikacija površine nanočestica TiO_2 bioaktivnim ligandima, kao što je dihidrokvercetin (DHQ), formiranjem interfacijalnog kompleksa sa prenosom naelektrisanja, kako bi se postigla njegova aktivacija pod vidljivom svetlošću. Neorgansko-organski hibridni nanokompozit TiO_2/DHQ okarakterisan je infracrvenom (FTIR) i refleksionom spektroskopijom. FTIR spektri su identifikovali C=O grupe flavonoida, O-H, C-O i C-O-C grupe fenola, potvrđujući prisustvo liganada na površini nanočestica TiO_2. Kubelka-Munk transformacijom spektara difuzione refleksije vidi se pomeraj ekscitacije TiO_2/DHQ prema vidljivom delu spektra. Ispitivanje citotoksičnosti MTT testom urađeno je na zdravim ljudskim MRC-5 ćelijama, kao i na ljudskim HeLa ćelijama raka grlića materice. Takođe, H2DCFDA testom ispitan je efekat TiO_2/DHQ na proizvodnju reaktivnih vrsta kiseonika u MRC-5 ćelijama.

Toxicity of TiO_2 nanoparticles modified with dihydroquercetin

Valentina Z. Nikšić[1], Miljana M. Dukić[1], Andrea M. Pirković[2], Vesna M. Lazić[3]
[1] Vinča institute for nuclear sciences , National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia
[2] INEP Institute for Application of Nuclear Energy, University of Belgrade, Belgrade, Serbia
[3] Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

This study aims to modify the surface of TiO_2 nanoparticles with bioactive ligands, forming an interfacial charge transfer complex to achieve its activation under visible light. Dihydroquercetin (DHQ) is a catechol-type ligand with pronounced antioxidant and valuable biological performance. The inorganic-organic hybrid nanocomposite TiO_2/DHQ was characterized by Fourier transform infrared (FTIR) and Reflectance spectroscopy. FTIR spectra identified C=O stretching in flavones, O-H, C-O and C-O-C starching in phenolic compounds, demonstrating the presence of ligands on the surface of TiO_2 nanoparticles. The Kubelka-Munk transformation of the diffuse reflection spectra shows a shift in the excitation of the TiO_2/DHQ towards the visible part of the spectrum. Cytotoxicity testing was performed on healthy human MRC-5 cells and human cervical cancer HeLa cells determined by MTT assay. Also, the effect of TiO_2/DHQ on the production of reactive oxygen species in MRC-5 cells was determined by the H2DCFDA assay.

HTM-8

Ispitivanje uticaja vlažnosti pletenina na njihovu propustljivost vazduha

Milada Novaković[1], Gordana Popović[2], Snežana Stanković[3]
[1] *Visoka tehnička škola strukovnih studija, Zrenjanin, Srbija*
[2] *Profi Lab, Beograd, Srbija*
[3] *Univerzitet u Beogradu - Tehnološko-metalurški fakultet, Beograd, Srbija*

Sposobnost propuštanja vazduha predstavlja jedno od osnovnih higijenskih svojstava odevnih tekstilnih materijala zahvaljujući kome omogućavaju stalnu izmenu vazduha između tela i okruženja. Ispitivanje propustljivosti vazduha sprovedeno je na DL pleteninama u dinamičkim uslovima, odnosno pri različitom sadržaju vlage u pletenini (do 30%). Ispitivane su pletenine različitog sirovinskog sastava (100% konoplja, 100% poliakrilonitril - PAN i mešavina50% konoplja/50% PAN). Iako je sposobnost propuštanja vazduha ispitivanih DL pletenina u uslovima neravnotežnog sadržaja vlage bila uslovljena geometrijskim faktorima pletenine, pokazalo se da vlakna svojim afinitetom prema apsorpciji vode imaju dominantan efekat na propustljivost vazduha u dinamičkim uslovima.

Investigation of the influence of moisture content of knitted fabrics on their air permeability

Milada Novaković[1], Gordana Popović[2], Snežana Stanković[3]
[1] *High Technical College of Professional Studies, Zrenjanin, Serbia*
[2] *Profi Lab, Belgrade, Serbia*
[3] *University of Belgrade - Faculty of Technology and Metallurgy, Belgrade, Serbia*

The air permeability is one of the basic hygienic properties of clothing textiles thanks to which they enable a constant exchange of air between the human body and the environment. The air permeability of single jersey knitted fabrics under different moisture contents (up to 30%) was investigated. Knitted fabrics of different raw material compositions (100% hemp, 100% polyacrylonitrile- PAN, and 50% hemp/50% PAN) were tested in this study. Although the air permeability of the tested knitted fabrics under the unbalanced moisture content range was influenced by their geometric factors, it was shown that the water absorption ability of constituent fibers has a predominant effect on the air permeability of the knits under various moisture contents.

HTM-9

Kompozitni materijali na bazi otpadne ljuske jajeta i nezasićenih poliestarskih smola dobijenih iz bioobnovljivih izvora

Olga J. Pantić[1], Vesna V. Panić[2], Maja D. Marković[2], Pavle M. Spasojević[2], Sanja I. Savić[1], Melina T. Kalagasidis Krušić[3]

[1] Institut za hemiju, tehnologiju i metalurgijiu, Univerzitet u Beogradu, Srbija
[2] Inovacioni centar Tehnološko-metalurškog fakulteta, Univerzitet u Beogradu, Srbija
[3] Tehnološko-metalurški fakultet, Univerzitet u Beogradu, Srbija

Novi trendovi u polimernoj industriji podstiču upotrebu sirovina dobijenih iz bioobnovljivih izvora kao i prelazak na zelenu tehnologiju. Nezasićene poliestarske smole su najzastupljenije termoreaktivne smole u proizvodnji polimernih kompozitnih materijala. Otpadni materijali, kao što su ljuske preostale od upotrebe kokošijih jaja, nastaju u velikim količinama, pri čemu ne predstavljaju opasan otpad zbog čega su korišćena kao punila za proizvodnju polimernih kompozitnih materijala. Za sintezu matrice korišćene su itakonska kiselina, ćilibarna kiselina, neopentil glikol, pri čemu je kao reaktivni rastvarač korišćen dimetil itakonat. Karakterizacija dobijenih kompozitnih materijala se sastojala od mehaničkog ispitivanja jednoosnim istezanjem kao i savijanjem u tri tačke, dok su promene u hemijskoj strukturi ispitivane FTIR spektroskopijom, a stepen umreženja je određivan analizom sadržaja gel faze.

Composite materials prepared from waste eggshells and biobased unsaturated polyester resin

Olga J. Pantić[1], Vesna V. Panić[2], Maja D. Marković[2], Pavle M. Spasojević[2], Sanja I. Savić[1], Melina T. Kalagasidis Krušić[3]

[1] Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia
[2] Innovation Center of Faculty of Technology and Metallurgy, University of Belgrade, Serbia
[3] Faculty of Technology and Metallurgy, University of Belgrade, Serbia

Development of biobased thermoset polymers encourages the strategic use of biobased resources and migrating to greener technologies. Unsaturated polyester resins have an extensive array of properties which makes them the most used thermoset resins in the production of polymer composite materials. Waste materials, such as eggshells left over from the usage of chicken eggs, are abundant and non-hazardous materials which offer many benefits in potential use as a filler in developing a biobased composite material. Itaconic acid, succinic acid, and neopentyl glycol were employed in unsaturated polyester synthesis, while dimethyl itaconate was used as a reactive diluent. Characterization of the resulting composite materials included assessing mechanical properties (uniaxial tensile test, three-point bending test), FTIR spectroscopy, and gel content analysis.

This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No: 451-03-47/2023-01/200026,451-03-47/2023-01/200287,451-03-47/2023-01/200135).

HTM-10

Effect of the filler concentration on the toxic gas adsorption capability of rGO/CNT/polymer composites

Marija Prosheva, Jadranka Blazevska Gilev
Ss. Cyril and Methodius University in Skopje, Faculty of Technology and Metallurgy, Skopje, R. N. Macedonia

The effect of the concentration of the reduced graphene oxide/carbon nanotubes (rGO/CNT) hybrid filler on the adsorption ability of polymer composites based on rGO/CNT was investigated using Quartz crystal microbalance (QCM). The polymer composites were synthesized using the emulsion mixing technique. First, the polymer matrix consisting of methyl methacrylate/butyl acrylate/glycidyl methacrylate in a weight ratio of 49.5/49.5/1 was synthesized by emulsion polymerization. Afterwards, aqueous dispersion of rGO/CNT hybrid (the weight ratio of the rGO/CNT was 10:1) was added into the polymer matrix. The rGO/CNT hybrid was added in three different concentrations, i.e., 0.25 wt%, 0.5 wt% and 1 wt% based on the monomer content. The morphology of the composites was investigated by scanning electron microscopy and atomic force microscopy, while, the adsorption capability of the composites was investigated using QCM towards different toxic gases (CO, NH_3, NO and NO_2). The results suggested that the concentration of the filler has an important role when comes to the properties of the composites. Namely, the best distribution of the filler was achieved when its concentration was lowest, 0.25 wt%, also, this sample presented the highest adsorption of toxic gas molecules. The incorporation of rGO/CNT had a positive effect on the hydrophobicity and the conductivity, these two properties increased with the incorporation of the rGO/CNT hybrid filler.

HTM-11

Antimikrobna aktivnost i citotoksičnost nanočestica na bazi srebra *in situ* sintetisanih na pamučnoj tkanini primenom ekstrakta lista oraha

Ana G. Krkobabić[1], Darka D. Marković[2], Aleksandar G. Kovačević[1], Tatjana R. Ilić-Tomić[3], Vanja M. Tadić[4], Maja M. Radetić[1]
[1] *Univerzitet u Beogradu – Tehnološko-metalurški fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu – Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[3] *Univerzitet u Beogradu – Institut za molekularnu genetiku i genetsko inženjerstvo, Beograd, Srbija*
[4] *Institut za proučavanje lekovitog bilja „Dr Josif Pančić“, Beograd, Srbija*

U ovom radu je ispitana mogućnost *in situ* sinteze nanočestica na bazi srebra primenom ekstrakta lista oraha, na pamučnoj tkanini prethodno modifikovanoj limunskom kiselinom. Tokom sinteze su formirane sferne nanočestice prečnika oko 60 nm, koje su ravnomerno raspoređene po površini pamučnih vlakana. Prisustvo nanočestica na bazi srebra je obezbedilo odličnu antimikrobnu aktivnost prema bakterijama *Staphylococcus aureus* i *Escherichia coli,* kao i kvascu *Candida albicans.* Tekstilni nanokompozitni materijal nije citotoksičan prema ćelijama zdravih keratinocita kože (HaCaT linija) i zdravih fibroblasta (MRC-5 linija), što omogućava njegovu bezbednu primenu za medicinske potrebe.

Antimicrobial activity and cytotoxicity of silver-based nanoparticles *in situ* synthesized on cotton fabric using walnut leaf extract

Ana G. Krkobabić[1], Darka D. Marković[2], Aleksandar G. Kovačević[1], Tatjana R. Ilić-Tomić[3], Vanja M. Tadić[4], Maja M. Radetić[1]
[1] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[3] *University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia*
[4] *Institute for Medical Plant Research „Dr Josif Pančić“, Belgrade, Serbia*

This study discusses the possibility to utilize walnut leaf extract for *in situ* synthesis of silver-based nanoparticles on cotton fabric previously modified with citric acid. Synthetized spherical nanoparticles with an average diameter of 60 nm were evenly distributed over the surface of cotton fibers. The presence of silver-based nanoparticles provided excellent antimicrobial activity against bacteria *Staphylococcus aureus* and *Escherichia coli,* and yeast *Candida albicans*. The textile nanocomposite did not show any cytotoxicity towards healthy skin keratinocytes cells (HaCaT line) and healthy fibroblast cells (MRC-5 line). Thus, it could be considered as a safe for potential medical applications.

Hemija i tehnologija hrane

Chemistry and Technology of Food

HTH-1

Fenilamidni profil polena uljane repice kao potencijalno funkcionalnog dodatka hrani

Aleksandar Ž. Kostić[1], Danijel D. Milinčić[1], Nebojša Nedić[1], Živoslav Lj. Tešić[2], Slađana P. Stanojević[1], Mirjana B. Pešić[1]
[1] *Univerzitet u Beogradu, Poljoprivredni fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu, Hemijski fakultet, Beograd, Srbija*

Cilj ovog rada je bio ekstrakcija (80% metanol za ekstraktibilnu i alkalna digestija za vezanu frakciju) i identifikacija fenilamidnog profila pčelinjeg polena uljane repice (*Brassica napus* L.) primenom tečne hromatografije visokih performansi (UHPLC) spregnute sa masenom spektrometrijom (MS-QToF) (Agilent, 1290, USA). Za analizu dobijenih rezultata korišćen je Agilent MassHunter softver. Identifikovano je ukupno dvedeset pet fenilamidnih jedinjenja u ekstraktibilnoj frakciji kao i dva derivata prisutna u vezanoj frakciji. Izrazito dominantni su bili različiti kumaroil derivati (dvadeset jedinjenja). Vezana frakcija je sadržavala samo dva fenilamida: kumaroil i dikumaroil spermidine.

Phenylamides profile of rapeseed bee-collected pollen as potential functional food ingredient

Aleksandar Ž. Kostić[1], Danijel D. Milinčić[1], Nebojša Nedić[1], Živoslav Lj. Tešić[2], Slađana P. Stanojević[1], Mirjana B. Pešić[1]
[1] *University of Belgrade, Faculty of Agriculture, Belgrade, Serbia*
[2] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

The aim of current research was to obtain extracts (80% methanol for extractable and alkaline digestion for bound fraction) from bee-collected rapeseed (*Brassica napus* L.) pollen and to identify presented phenylamides. For that purpose, ultra-high-performance liquid chromatography (UHPLC) system (Agilent 1290, USA) coupled with a quadrupole time-of-flight mass spectrometry (MS-QToF) was applied. Agilent MassHunter softwer was used for the instrument control, data acquisition and data analysis. A total of twenty-five phenylamine phenylamide compounds were identified in the extractable fraction as well as two derivatives present in the bound fraction. In most of the compounds, the coumaroyl moiety was dominant, so we can say that various coumaroyl phenylamide (twenty compounds) were distinctly prevalent. The bound fraction contained only two phenylamines: coumaroyl and dicoumaroyl spermidine.

Acknowledgment: This work was supported by Ministry of Science, Technological Development and Innovation of the Republic of Serbia and the Faculty of Agriculture of the University of Belgrade contract no. 451-03-47/2023-01/200116.

KNJIGA RADOVA

Proceedings

Analitička hemija

Analytical Chemistry

R-AH-1

Mehlich-3 solution as an extractant for multi-element analysis of soil samples

Vibor Roje, Robert Potočnjak, Mario Sladin, Ivan Perković, Darko Bakšić
University of Zagreb - Faculty of Forestry and Wood Technology, Svetošimunska 23,
HR-10002 Zagreb, Croatia

This paper focuses on the Mehlich-3 solution for extracting the selected chemical elements from soil samples. The research used the certified reference material (CRM) for soil Metranal™ 33 (Analytika, Czech Republic) as a model sample. The quantification of the analytes in the extracts was done by means of ICP-AES. The results were compared to the values of the extracts prepared with deionized water and *aqua regia* as one-step extraction reagents.

Introduction

Amongst numerous and mutually different reagents and methods for extraction of metals, metalloids and non-metals from soil samples that have been described in the scientific literature and/or applied in practice, there is also the Mehlich-3 solution that becomes present in a wider application for analyses of soils in terms of macro- and micronutrients.

The solution mixture known under the above-cited name is a successor of the reagents nowadays referred to as Mehlich-2 and Mehlich-1. More precisely, distinguished American soil scientist of German origins Dr. Adolf Mehlich, devoted to research and optimization of methodologies for various chemical analyses of soil samples with a special interest in their multi-elemental characterisation, 1953 he has invented a dilute double-acid extractant which is nowadays referred to as Mehlich-1. It consists of two diluted acids: HCl (0.05 mol·dm^{-3}) and H_2SO_4 (0.0125 mol·dm^{-3}) [1]. The main shortcoming of the Mehlich-1 extraction reagent is its applicability to acid soils. In the cases of neutral or, especially, basic soils, a consummation of the reagent for neutralization reactions occurs before the extraction of cations begins [2].

To overcome the lack of the previously described reagent, Mehlich proposed a buffered acid-fluoride extractant that consists of: NH_4Cl (0.2 mol·dm^{-3}), HOAc (0.2 mol·dm^{-3}), NH_4F (0.015 mol·dm^{-3}), and HCl (0.012 mol·dm^{-3}) – it is known as Mehlich-2 [3]. Shortly after, the author considered this reagent too corrosive and decided to change chlorides with nitrates.

In 1983 the improved reagent was presented and it has remained in use up to now, becoming even more present among soil scientists – Mehlich-3 solution that is consisted of: HOAc (0.2 mol·dm^{-3}), NH_4NO_3 (0.25 mol·dm^{-3}), NH_4F (0.015 mol·dm^{-3}), HNO_3 (0.013 mol·dm^{-3}), and EDTA (0.001 mol·dm^{-3}). Initially, Mehlich-3 solution was mentioned as an extractant suitable for analysing macronutrients P, K, Na, Ca, Mg, and micronutrients Mn, Zn, and Cu in a broad range of soils [4] in the context of assessing their uptake by plants and crops. Finally, modern analytical techniques (especially ICP-MS and ICP-OES) allow simple and reliable quantification of these analytes in extracts prepared using the Mehlich-3 extraction solution.

This research was conducted in the context of our interests in the multi-element analysis of soils and tests of various extraction media [5,6]. Its main aim was to test the extraction ability of the Mehlich-3 solution in comparison to two extraction reagents (namely, *aqua regia* and deionized water) that are more commonly used and cited in the literature.

Results and Discussion

The results of the analyses of the soil CRM Metranal™ 31 are presented in Table 1. At the same time, Figure 1 gives an insight into the differences between the extraction abilities of the Mehlich-3 solution, deionized water and *aqua regia*. The recovery values obtained with the two latter reagents originate from our Laboratory for Ecology and Pedology research at the Faculty of Forestry and Wood Technology of the University of Zagreb [5,7].

Table 1. Mass fraction values (mg/kg) of the analytes in the soil certified reference material Metranal™ 31 obtained after the extraction with Mehlich-3 solution (N=4)

	Cert. tot. content	**Found after extraction with Mehlich-3 sol'n**	
	mg/kg	Av. ± Std.dev. (mg/kg)	RSD* (%)
Ca	10720	2144 ± 58	3
Cu	30.8 ± 0.9	1.72 ± 0.08	4
Fe	33083	2241 ± 59	3
K	26233	326 ± 7	2
Mg	7659	213 ± 5	3
Mn	540 ± 20	147 ± 5	3
Na	17434	25.2 ± 5.3	21
P	1484	39.5 ± 4.4	11
S	–	25.1 ± 0.3	1
Zn	120 ± 7	11.1 ± 0.2	2

* RSD – relative standard deviation

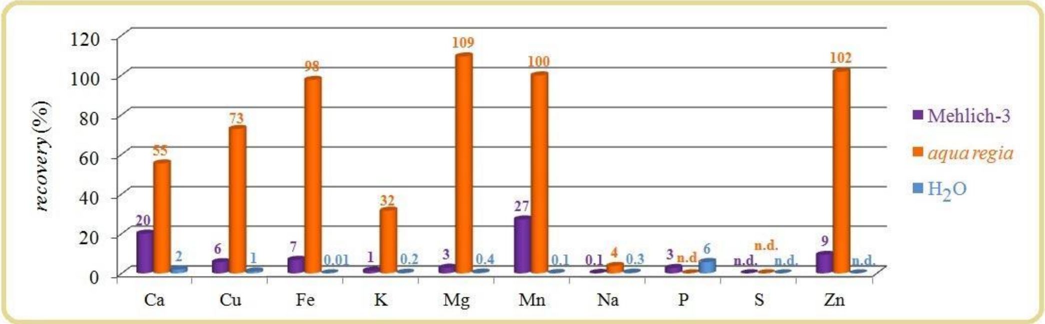


Figure 1. Comparison of the recoveries of the analysed elements in Metranal™ 31 obtained with three different extraction reagents

The data in Table 1 reveal that measurements of the analytes were generally performed with low uncertainty. Na and P are two elements whose determination was done with RSD values higher than 10 %. The uncertainty of the Na measurement probably arose from the contamination of the extracts with this element. Still, its relatively low concentration in the extracts should not be neglected as a possible cause of the noticed uncertainty.

Figure 1 illustrates the relationship between the recoveries (wfound/wtotal, certified) of the analytes obtained with Mehlich-3 extraction solution and, on the other hand, with two more often used extractants, *i.e. aqua regia* and water. These results also suggest that *aqua regia* is a too strong reagent for assessing the bioavailability of metals from soil.

Since very few soil CRMs are certified on the Mehlich-3 extraction procedure, the values given in this paper can be useful as information values in possible future uses of Metranal™ 31 for quality control purposes in the context of the same type of analysis.

Experimental

Chemicals

Certified reference material (CRM) for soil Metranal™ 31 (produced by Analytika Ltd, Prague, Czech Republic) was used as a model soil sample. It is a light sandy soil, with normal levels of the analytes.

Preparation of the Mehlich-3 solution was carried out according to the previously published instructions [8].

Multi-element Standard Solutions (100 ± 0.2 mg L^{-1}, 5% *v*/*v* HNO_3), CPAChem Ltd., Bulgaria as well as *Multielement standard solution III for ICP* TraceCERT® (Ca, K, Mg, Na), Fluka, Switzerland were used for the preparation of the series of standard solutions for performing an external calibration of the ICP-spectrometer.

Ultrapure water (Siemens Ultra clear, 0.055 μS/cm) was used to prepare all solutions.

Soil samples preparation and spectrometric quantification of the analytes

The aliquots of the CRM were weighted (~2.0000 g each) in 50-mL polypropylene cuvettes, mixed with 20 mL of the Mehlich-3 solution, and then shaken on the orbital shaker for 1 h at 200 rpm. Afterwards, the mixtures were filtered (Whatman® quantitative filter paper, ashless, Grade 42) and stored in 20-mL polypropylene scintillation vessels. The elements Cu, Fe, K, Mg, Mn, Na, P, S, and Zn were determined by direct measuring (*i.e.* without further dilution) in the prepared extracts, while Ca was quantified after 100-fold dilution of the extracts.

Quantifying the selected elements in the prepared extracts was made using an atomic emission spectrometer with inductively coupled plasma, ICP-AES (*Thermo Fischer iCAP6300 Duo*) [5]. The analytes were measured after the matrix-matched external calibration of the spectrometer had been performed.

Rastvor Melih-3 (*Mehlich-3)* kao ekstraktant za multielementarnu analizu uzoraka zemljišta

Vibor Roje, Robert Potočnjak, Mario Sladin, Ivan Perković, Darko Bakšić
Sveučilište u Zagrebu - Fakultet šumarstva i drvne tehnologije, Svetošimunska 23,
HR-10002 Zagreb, Croatia

U fokusu ovog rada jeste otopina Melih-3 (*Mehlich-3*) koja se koristi za ekstrakciju nekih hemijskih elemenata iz uzoraka zemljišta. Istraživanje je provedeno korišćenjem sertifikovanog referentnog materijala za zemljište Metranal^{TM} 33 (Analytika, Rapublika Češka) kao modelnog uzorka. Kvantifikacija određivanih elemenata u ekstraktima urađena je tehnikom atomske emisione spektrometrije uz induktivno spregnutu plazmu (ICP-AES). Dobiveni rezultati upoređeni su sa rezultatima određivanja istih analita u ekstraktima priređenima ekstrakcijom pomoću deionizovane vode odnosno carske vode, u jednom koraku.

References

[1] A. Mehlich, Determination of P, Ca, Mg, K, Na and NH_4, North Carolina Soil Test Division (mimeo), 1953.

[2] R. Mylavarapu, T. Obreza, K. Morgan, G. Hochmuth, V. Nair, A. Wright, *Department for Soil and Water Sciences – UF/IFAS Extension* **2014 (reviewed: 2020)**, SL 407 (https://edis.ifas.ufl.edu/publication/SS620)

[3] A. Mehlich, *Commun. Soil Sci. Plan. Anal.* **1978**, *9*, 477.

[4] A. Mehlich, *Commun. Soil Sci. Plan. Anal.* **1984**, *15*, 1409.

[5] V. Roje, F. Galinec, *Environ. Monit. Assess.* **2019**, *191*, 534.

[6] V. Roje, D. Buršić, I. Košutić, Comparison of nitric acid and *aqua regia* as extractants for heavy metals in soil samples in B. Šolaja (ed.), 58th Meeting of the Serbian chemical society, Belgrade, Serbia, 9-10 June 2022, Book of Abstracts/Proceedings, R-AH-2, pp. 190-194.

[7] D. Buršić, Recovery of the Trace Elements from Soil Samples in Dependence on the Digestion Temperature Applying Aqua Regia in Microwave Digestion System (in Croatian, Abstract in English), B.Sc. Thesis, University of Zagreb – Faculty of Forestry, Zagreb, Croatia, 2014.

[8] H. Zhang, D. Hardy, R. Mylavarapu, J. Wang, Mehlich-3 in F.J. Sikora and K.P. Moore, Soil Test Methods From the Southeastern United States, *Southern Cooperative Series Bulletin,* **2014**, *419*, 101.

Hemija životne sredine

Environmental Chemistry

R-HŽS-1

Sorption of lindane from water using a macroporous copolymer based on glycidyl methacrylate

Sandra S. Bulatović[1], Tamara T. Tadić[1], Bojana M. Marković[1], Aleksandra B. Nastasović[1], Mila V. Ilić[1], Natalija Ž. Nedić[2]

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

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

Organochlorine pesticide - lindane, according to the US EPA classification, is considered as potentially carcinogenic compound. Although the usage of this pesticide is banned in many countries, it is still used in some. As persistent organic compound, lindane and its residues can persist in the environment for a very long time, migrating over long distances, potentially causing environmental pollution. Lindane residues can reach the human body through the food chain, because this potentially toxic compound is prone to bioaccumulation, and this is serious toxicological problem especially at industrial and agricultural sites where lindane has been used directly, or has reached due to improper wastewater disposal. Despite bans on its use, lindane contamination remains a global problem, and its removal from the environment is of crucial importance. In this research, for the sorption of lindane from an aqueous solution, a macroporous copolymer based on glycidyl methacrylate was utilized, which proved to be a very effective sorbent, with lindane sorption of about 80 %. Analytical technique, Gas Chromatography with an Electron Capture Detector (GC-ECD), was used for determination of lindane concentration. In addition to sorption, desorption of lindane was also successfully performed using different solvents, which confirmed the possibility of recycling and reuse of the investigated polymer.

Introduction

Lindane is an organochlorine pesticide, which is prohibited in many countries because it is linked to numerous diseases, and it is also considered as a potential carcinogenic compound, which was established by the US EPA [1]. However, in some countries this pesticide is still in use and is therefore the subject of numerous researches related to environmental protection. Due to the growing awareness of the toxic effects of pesticides, a large number of methods have been developed that enable their removal from the environment. The sorption method can be observed to eliminate different substances, and different specific sorbents can be developed as needed. In this sense, polymer materials are the most popular sorbents due to their easy modification and versatility [2]. The subject and goal of this research was the investigation of the sorption and desorption of lindane from aqueous solutions by macroporous copolymer based on glycidyl methacrylate.

Results and Discussion

The results of the lindane removal from an aqueous solution using a macroporous copolymer are shown in Figure 1a. The efficiency of lindane removal in the first 5 minutes reaches a value of 85 %. After this fast phase, in the next 30 minutes, a second, slower phase is observed which leads to reaching the equilibrium state, and this phase can be seen as a plateau (Figure 1a). In addition to sorption, desorption of lindane from the macroporous copolymer was also performed, and the results are shown in Figure 1b. Various desorption solvents were used for this purpose. The solvent with highest desorption efficiency was acetone (65.4 %), then 2-propanol (63.1 %), then acetonitrile (54.4 %), followed by a mixture of hexane/ethyl acetate (37, 8 %), then ethyl acetate (31.8 %) and methanol as the weakest desorption solvent (10.9 %). These results confirmed the multiple application of the synthesized polymer, with the sorption and desorption abilities, confirming that the same polymer can be used multiple times.

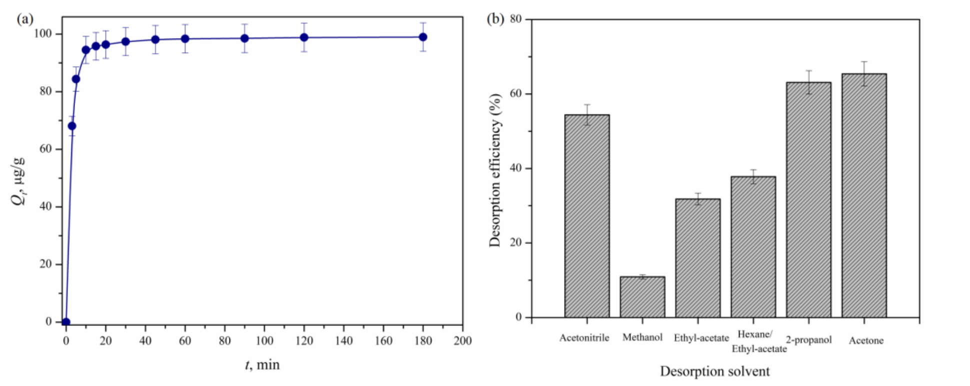


Figure 1. (a) Dependence of the removal efficiency of lindane by the macroporous copolymer on the contact time; (b) Lindane desorption with different desorption solvents.

Experimental Part

In this research, the cross-linked macroporous polymer poly(glycidyl methacrylate-*co*-ethylene glycol dimethacrylate) (poly(GMA-*co*-EGDMA)) was used as a sorbent of lindane, with a particle size fraction of 0.15 to 0.30 mm, which were obtained by suspension copolymerization in the presence of an inert component [3]. An analytical standard of lindane with a purity of 98.2 % ± 0.1 % (CPAchem Ltd, Bulgaria) was used for testing lindane sorption. For lindane desorption, the following desorption agents/solvents were used: acetonitrile, methanol, ethyl acetate, a mixture of hexane and ethyl acetate in a ratio of 3:2 v/v, 2-propanol and acetone. Lindane was extracted according to US EPA method 505 [4] and analyzed using an Agilent 7890A gas chromatograph connected to electron capture detector (GC-ECD), and a capillary column Thermo Scientific™ TraceGOLD™ TG-5MT (30 m x 0.25 mm ID x 0.25 µm). The initial heating temperature was 50 °C for 3 min, and then heating was reached at a rate of 30 °C/min up to 210 °C and held at this temperature for 20 min. The mode of injection was splitless. Hydrogen was used as a carrier gas with a flow rate of 60 mL/min.

Experiments of lindane sorption using a macroporous copolymer were performed in a batch process at room temperature (25 ± 0.2 °C). In an erlenmeyer flask with a volume of 100 mL, 400 mg of sorbent was measured and poured with 50 mL of an aqueous solution of lindane with a concentration of 500 µg/L (initial pH of the solution 8; ionic strength 3 % w/v). The lindane solution that was brought into contact with the sorbent was shaken for 180 min on an orbital shaker at a speed of 300 rpm/min. At appropriate time intervals (3, 5, 10, 15, 20, 30, 45, 60, 90, 120 and 180 min), 1 mL of the solution was sampled with a micropipette, which was diluted with 4 mL of deionized water and prepared for measurement by GC-ECD. All measurements were performed in duplicate and the results were expressed as the mean value. The efficiency of sorption (*E*, %) was calculated according to the following equation [5]:

$$E(\%) = \frac{(C_0 - C_e)}{C_0} \times 100\% \qquad (1)$$

where C_0 (µg/L) and C_e(µg/L) are the initial and equilibrium concentration of lindane in the solution. After the sorption process (60 min), the dried samples of macroporous copolymer with bound lindane were dried and used in desorption experiments. Desorption was performed by mixing 50 mg of sorbent (with bound lindane) with 5 mL of desorption agent (acetonitrile, methanol, ethyl acetate, mixture of hexane and ethyl acetate in the ratio 3:2 v/v, 2-propanol and acetone) for 60 min, on an orbital shaker (300 rpm) at room temperature (25 ± 0.2 °C). The samples after the sorption process were filtered and analyzed by GC-ECD. All measurements were performed in duplicate and the results were expressed as the mean value. Desorption efficiency (*D*, %) was calculated according to the following equation [6]:

$$D(\%) = \frac{C_d V_d}{(C_0 - C_e) V_i} \times 100\% \qquad (2)$$

where C_e (µg/L) is the equilibrium concentration of lindane in the solution after sorption, C_d (µg/L) is the concentration of lindane in the desorption solvent after desorption, V_i (L) and V_d (L) are the volume of the aqueous solution of lindane and the desorption solvent.

Sorpcija lindana iz vode pomoću makroporoznog kopolimera na bazi glicidil metakrilata

Sandra S. Bulatović[1], Tamara T. Tadić[1], Bojana M. Marković[1], Aleksandra B. Nastasović[1], Mila V. Ilić[1], Natalija Ž. Nedić[2]

[1]*Univerzitet u Beogradu, Institut za Hemiju, Tehnologiju i Metalurgiju, Beograd, Srbija*

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

Organohlorni pesticid - lindan, prema US EPA klasifikaciji, smatra se potencijalno kancerogenim jedinjenjem. Iako je upotreba ovog pesticida zabranjena u mnogim zemljama, u nekim se i dalje koristi. Kao perzistentno organsko jedinjenje, lindan i njegovi ostaci mogu da opstanu u životnoj sredini veoma dugo, migrirajući na velike udaljenosti, potencijalno izazivajući zagađenje životne sredine. Ostaci lindana mogu da dospeju u ljudski organizam kroz lanac ishrane, jer je ovo potencijalno toksično jedinjenje sklono bioakumulaciji, a to je ozbiljan toksikološki problem posebno u industrijskim i poljoprivrednim lokacijama gde se lindan direktno koristio ili je dospeo usled nepravilnog odlaganja otpadnih voda. Uprkos zabranama njegove upotrebe, kontaminacija lindanom ostaje globalni problem, a njegovo uklanjanje iz životne sredine je od ključnog značaja. U ovom istraživanju sorpcija lindana iz vodenog rastvora urađena je sa makroporoznim kopolimerom na bazi glicidil metakrilata, koji se pokazao kao veoma efikasan sorbent, sa sorpcijom lindana od oko 80 %. Za određivanje koncentracije lindana korišćena je analitička tehnika, gasna hromatografija sa detektorom za hvatanje elektrona GC-ECD (Gas Chromatography with an Electron Capture Detector). Osim sorpcije, uspešno je urađena i desorpcija lindana korišćenjem različitih rastvarača, što je potvrdilo mogućnost reciklaže i ponovne upotrebe ispitivanog polimera.

References

1. United States Environmental Protection Agency (US EPA, 2016). Lindane (Gamma-Hexachlorocyclohexane), 58-89-9.
2. I. A. Saleh, et al., *Environ. Technol. Innov*. **2020**, 19,101026.
3. Lj. T. Suručić, et al., *Serb. Chem. Soc*. **2019**, 84, 1391-1404.
4. J. W. Munch, US EPA Method 505 (1995).
5. K. Moradnejadi, et al., *J. Bas. Res. Med. Sci.* **2019**, 6, 57-66.
6. B. Liu, et al., *J. Chromatogr. B*, **2013**, 937, 84-90.

Zahvalnica: Izradu ovog rada je finansiralo Ministarstvo nauke, tehnološkog razvoja i inovacija Republike Srbije (Broj ugovora: 451-03-47/2023-01/200026 i 451-03-47/2023-01/200168).

R-HŽS-2

Adsorption characteristics of chitosan hydrogel beads toward removal of Congo red dye from aqueous solutions

Đorđe Ž. Petrović, Katarina V. Stanković, Ksenija R. Kumrić
University of Belgrade, "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade, Serbia

The present study investigated potential application of biopolymer chitosan, in the form of gel beads, for the removal of Congo red (CR) dye from aqueous solution. Chitosan hydrogel beads (CHBs) were prepared by a coupled ionic and covalent co-cross-linking, employing citric acid (CA) and glutaraldehyde (Glu) as an ionic and a chemical cross-linker, respectively. Batch experiments were carried out to optimize the process conditions for efficient removal of CR dye and to determine the adsorption capacity of prepared CHBs. The results showed that the highest removal efficiency of CR was obtained in the pH range from 6 to 10, and that the equilibrium was attained after 180 min. The Langmuir isotherm model provided the best correlation for the adsorption of CR onto CA/Glu co-cross-linked CHBs, with the maximum adsorption capacity (q_m) of 544.2 mg g^{-1}.

Introduction

In recent years, many investigations focus on the use of biopolymeric materials for the treatment of wastewaters containing dyes since these materials are non-toxic, biodegradable and can be obtained from renewable sources [1]. Among them, the biopolymer chitosan has caught particular attention because of its high affinity and adsorption capacity toward dyes. According to the literature data [2-4], the use of chitosan in the form of spherical gel beads, instead of flakes or powders, have shown better adsorption characteristics for the removal of dyes from aqueous solutions, primarily due to decreased crystallinity of hydrogels, improved porosity and large pore sizes. Because of that, the diffusion of dye molecules toward a large number of internal $-NH_2$ and –OH functional groups of chitosan may be facilitated, and consequently, its adsorption capacity could be enhanced.

The aim of the present study was to prepare CHBs via ionic/covalent co-cross-linking and to investigate their adsorption characteristics toward the removal of the anionic CR dye from aqueous solutions in a batch mode. The effects of the initial solution pH, contact time and initial CR concentration were evaluated with respect to the removal efficiency of CR dye from aqueous solution. Pseudo-first-order (PFO) and pseudo-second-order (PSO) adsorption kinetic models were employed to analyze the kinetics of CR adsorption on CHBs. The equilibrium adsorption data were analyzed using Langmuir and Freundlich isotherms.

Experimental part

Chitosan flakes (medium molecular weight), glacial acetic acid (AA), Glu solution and CA were purchased from Sigma-Aldrich (USA), while the CR dye was purchased from Acros

Organics (Belgium). All the chemicals were analytical reagent grade and used without further purification.

Preparation of chitosan adsorbent in the form of hydrogel beads was done by dissolving 1 g of chitosan flakes in 40 cm^3 of (1) 2 wt% of AA, (2) 1 wt% AA and 1 wt% CA and (3) 2 wt% of CA. Afterward, 5% (v/v) Glu solution was added in each of the 2.5% (w/v) chitosan solutions and the mixtures were magnetically stirred for 2 h at room temperature. Then, the obtained solutions, separately, were dropped into 1 mol dm^{-3} NaOH solution to form uniform CHBs. The samples of CHBs (denoted as CHB – 2% AA, CHB – 1% AA, 1% CA and CHB – 2% CA) were kept in the NaOH solution for 24 h. Finally, CHBs were rinsed with deionized water until neutral pH was reached and stored in deionized water until further use.

The study of CR adsorption onto CHBs was carried out in a batch mode. Typically, the experiments were conducted at room temperature by mixing approximately 0.5 g wet CHBs and 10 cm^3 of the CR solution of the desired concentration at pH 6. The mixtures were shaken at a speed of 150 rpm for 24 h. After that, the liquid phases were separated and the residual CR concentrations were determined by UV-Vis spectrophotometer (UV-2600, Shimadzu, Japan) at λ_{max} of 497 nm. CHBs were dried in an oven at 60°C and then, the mass of the dried CHBs were weighed.

The effect of pH was studied by changing pH of the CR solution (25 mg dm^{-3}) from 4 to 12. Kinetic adsorption experiments were performed by mixing 2.5 g wet CHBs and 50 cm^3 of the CR solution (25 mg dm^{-3}) at pH 6. The adsorption continued for 24 h and the CR concentration in the solution was measured at predetermined time intervals. The effect of the initial dye concentration was investigated in the range from 1 to 1000 mg dm^{-3} at pH 6. The obtained results were discussed in terms of removal efficiency, *E* (%), and adsorption capacity, q_e (mg g^{-1}), at equilibrium defined by the equations:

$$E = \left(\frac{C_i - C_e}{C_i}\right) 100$$

$$q_e = \left(\frac{C_i - C_t}{m}\right) V$$

where C_i and C_e (mg dm^{-3}) are the initial and equilibrium concentrations of CR in the solution, respectively, *V* (dm^3) is the volume of the solution, and *m* (g) is the mass of the dried adsorbent.

Results and discussion

The shape of the CA/Glu co-cross-linked CHBs was nearly spherical with the mean diameter of the gel beads about 3.0 mm. The water content of the three tested CHBs samples was in the range of 97.0-97.5%.

Variations in the initial solution pH affect the surface charge of the adsorbent and the degree of ionization of the adsorbate and, hence, influence the removal efficiency of the adsorbent. The effect of the initial solution pH on the CR dye removal by CHB – 2% AA, CHB – 1% AA, 1% CA and CHB – 2% CA was studied in the pH range of 4-12, while other experimental conditions were constant. The obtained results revealed that the highest removal efficiency (98-99%) of CR for the three tested adsorbents occurred in the pH range of 6-10. According to the literature data [5], it can be assumed that the removal of CR dye is driven by both electrostatic interaction between the positively charged surface of tested CHBs and the anionic CR dye and some physical forces (like hydrogen bonds or Van der Waals forces). pH 6 was selected as optimal for further experiments.

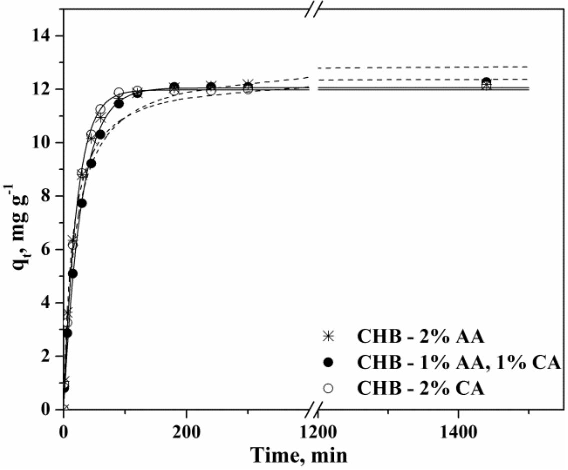


Figure 1. Effect of contact time on the removal of CR dye by CA/Glu co-cross-linked CHBs (solid and dashed lines represent PFO and PSO kinetic models, respectively)

As can be seen from Fig. 1, the adsorption of CR dye on CHB – 2% AA, CHB – 1% AA, 1% CA and CHB – 2% CA took place at relatively fast rate in the first 45 min, then slowed down and finally attained the equilibrium after 180 min of contact. The obtained experimental data were fitted by the non-linear forms of the PFO and PSO kinetic models. The resulting kinetic parameters and the determination coefficients (R^2) suggested that PSO model is more suitable for describing the adsorption of CR dye onto the CA/Glu co-cross-linked CHBs.

The equilibrium adsorption data on the effect of the initial CR concentration were fitted using the non-linear Langmuir and Freundlich isotherm models in order to determine the surface properties and the affinity of the adsorbent. The corresponding isotherm parameters and the determination coefficients of these two models are reported in Table 1. Based on the values of the R^2, it is evident that CR adsorption by CA/Glu co-cross-linked CHBs can be better described by the Langmuir isotherm. CA/Glu co-cross-linked CHBs with the higher content of CA showed better q_m value compared to other samples, probably due to incorporation of additional carboxylic groups that have positive impact on the features of CHBs.

Table 1 Langmuir and Freundlich parameters for the adsorption of CR onto CA/Glu co-cross-linked CHBs

Adsorbent	**Langmuir isotherm**			**Freundlich isotherm**		
	q_m, mg g^{-1}	***K_L**	**R^2**	**n_F**	****K_F**	**R^2**
CHB - 2% AA	445.8	0.039	0.992	3.52	64.43	0.955
CHB - 1% AA, 1% CA	490.4	0.040	0.999	3.07	65.06	0.963
CHB - 2% CA	544.2	0.046	0.999	2.98	69.49	0.952

13. *K_L, dm^3/mg; **K_F, (mg/g)(dm^3/mg)$^{1/n}$

In conclusion, the results presented in this study indicate that CA/Glu co-cross-linked chitosan in the form of hydrogel beads can be regarded as an efficient and low-cost adsorbent, which could be potentially applied in the treatment of wastewaters containing toxic anionic dyes such as CR. Further experiments will be oriented toward its application in dynamic systems.

Adsorpcione karakteristike hidrogelova hitozana za uklanjanje boje kongo crveno iz vodenih rastvora

Đorđe Ž. Petrović, Katarina V. Stanković, Ksenija R. Kumrić
University of Belgrade, "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade, Serbia

Istraživanja u okviru ove studije okrenuta su ka ispitivanju mogućnosti primene hidrogelova hitozana, u obliku sfera, za uklanjanje boje kongo crveno (CR) iz vodenih rastvora. Sfere hidrogela hitozana (CHBs) pripremljene su spregnutim jonskim i kovalentnim umrežavanjem, pri čemu su limunska kiselina (CA) i glutaraldehid (Glu) korišćeni kao jonski i kovalentni umreživač, respektivno. Eksperimenti su rađeni u šaržnom sistemu kako bi se optimizovali uslovi za efikasno uklanjanje CR iz vode i odredili adsorpcioni kapaciteti sintetisanih CHBs. Eksperimentalni rezultati su pokazali da je efikasnost uklanjanja CR najveća u pH intervalu od 6 do 10, a da se ravnoteža uspostavlja nakon 180 minuta. Langmirova izoterma pokazala je najbolju korelaciju za adsorpciju CR boje na CA/Glu umreženim sferama hidrogelova hitozana, pri čemu maksimalni adsorpcioni kapacitet (q_m) iznosi 544.2 mg g^{-1}.

References

1. A.M. Abu El-Soad, G. Lazzara, M.O. Abd El-Magied, G. Cavallaro, J.S. Al-Otaibi, M.I. Sayyed, E.G. Kovaleva, *Int. J. Mol. Sci.* **2022**, *23*, 2396.
2. F.C. Wu, R.L. Tseng, R.S. Juang, *J. Hazard. Mater.* **2000**, *73*, 63.
3. M.Y. Chang, R.S. Juang, *Colloids Surf., A.* **2005**, *269*, 35.
4. G. Crini, P.M. Badot, *Prog. Polym. Sci.* **2008**, *33*, 399.
5. S. Chatterjee, S. Chatterjee, B.P. Chatterjee, A.K. Guha, *Coll. Surf. Physicochem. Eng. Asp.* **2007**, *299*, 146.

Acknowledgement: This research was funded by the Ministry of Science and Technological Development of the R. Serbia (contract number: 451-03-47/2023-01/ 200017).

Hemijsko inženjerstvo

Chemical Engineering

R-HI-1

Molecular interaction analysis according to the excess and deviation properties for the binary mixture ethyl octanoate + 1-butanol

Divna M. Majstorović[1], Emila M. Živković[1], Mirjana Lj. Kijevčanin[1]
[1]*University of Belgrade Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia*

Density and viscosity data for the binary system containing ester ethyl octanoate and alcohol 1-butanol are obtained at eight temperatures in the range (288.15-323.15) K and at atmospheric pressure. These property data allowed the calculation of the excess and deviation properties such as excess molar volume, viscosity deviations and excess molar Gibbs energy of activation of viscous flow. Calculated property data are correlated with the Redlich-Kister equation and used for discussion of structural and packing effects taking place in the investigated mixture. The results showed that the effect of breaking hydrogen bonds of alcohol molecules and dipole-dipole interactions of ester molecules, which attributes the volume expansion, quantitatively exceeded the weak intermolecular hydrogen bonds between these molecules and the interstitial placement of ester molecules in alcohol multimers.

Introduction

The theoretical significance of the study of thermodynamic properties of liquid mixtures is reflected in the expansion of the database due to new experimental values and deepening of knowledge in the theory of solution. These property data are very important for process and equipment calculations in the chemical, process, food industry, medicine, as well as in product quality control. System included in this study is containing industrially important components: ester and alcohol.

Thermodynamic and thermophysical studies of esters are of increasing interest due to their wide usage in flavoring, perfumery, artificial essences, and generally in food and cosmetic industry, while alcohols are the most commonly used industrial solvents, mainly for resins and cellulose esters. Caprylic acid is a saturated fatty acid with eight carbon atoms, also known as octanoic acid, which is why its esters are called octanoates. Ethyl octanoate is approved by the FDA ("U.S. Food and Drug Administration") agency as an "additive permitted for direct addition to food for human consumption."

Density and viscosity are quantities significant for the understanding of matter at the microscopic level, but also for the behavior of the system because of the complex structure of molecules and intermolecular interactions that are present in every real mixture. Knowing these properties at multiple temperatures gives us a better insight into the structure of the mixture itself, the interactions that prevail in them, but also the changes of interactions in the entire temperature range. Density and excess molar volume, but also excess molar Gibbs energy of activation of viscous flow, are the best indicators of structural changes and packing effects in mixtures.

Experimental part

The experimental measurements of density and viscosity were performed at atmospheric pressure and in the temperature range 288.15 - 323.15 K. The viscosity of the pure components and their mixture was measured on an Anton Paar SVM 3000 viscometer, while density data are obtained from the Anton Paar DMA 5000 densimeter.

Results and Discussion

The results of the experimental measurements were used to further determine the viscosity deviations $\Delta\eta$ and the excess molar volume V^E for the tested mixture.

Based on experimentally measured density values of pure components ρ_1 and ρ_2, and their binary mixture ρ, equation for excess molar volume calculations will have the following form:

VE=x1M1+x2M2-x1M11+x2M22   (1)

where x_1 and x_2 are molar fractions of components and M_1 and M_2 are molar masses of pure components.

Viscosity deviations for binary systems are determined from experimentally measured viscosities according to the equation:

Δη=η-x11+x22   (2)

where η_1 and η_2 are the viscosities of the pure components, and η is the viscosity of the binary mixture.

Another supplementary property used in the analysis of molecular interactions present in mixtures is the excess molar Gibbs energy of activation of viscous flow ΔG^{*E} [1]. Since both density (molar volume) and viscosity enter the calculation of this property, it is considered more suitable for interpreting interactions than viscosity deviations.

The excess molar Gibbs energy of activation of viscous flow ΔG^{*E} for binary mixtures is calculated using the following equation:

ΔG*E=RTln ηV2V2 -x1ln⁡(1V1/2V2)   (3)

where η, V, η_1, η_2, V_1 and V_2 represent the viscosity and molar volume of the mixture, the viscosity of pure component 1, the viscosity of pure component 2, the molar volume of pure component 1 and the molar volume of pure component 2, respectively.

These calculated data were correlated using the empirical Redlich-Kister equation [2]:

Yij=xixjk=1mAkxi-xjk-1=xixjk=1mAk2xi-1k-1

where A_k are polynomial parameters, i, j are binary system components and Y_{ij} is either excess molar volume V^E, viscosity deviation $\Delta\eta$ or excess molar Gibbs energy of activation of viscous flow ΔG^{*E}.

Figure 1 graphically shows the values of excess molar volumes of investigated ethyl octanoate + 1-butanol system, covering the entire range of molar fractions at the investigated temperature range. The values of this property are positive.

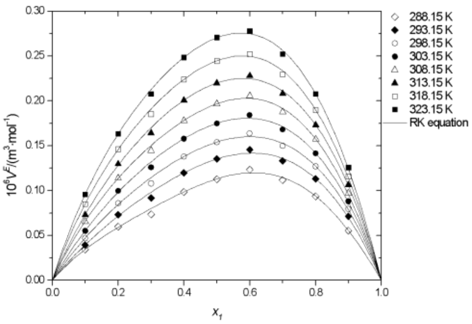
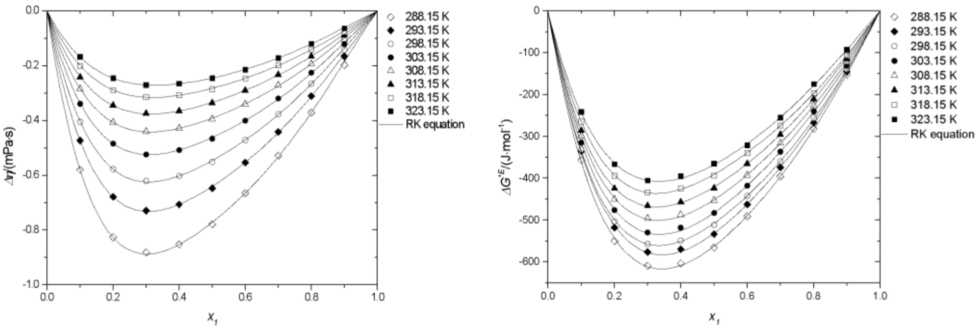


Figure 1. Experimental values of excess molar volume V^E as a function of the molar fraction of ethyl octanoate x_1 for the system ethyl octanoate (1) + 1-butanol (2).

Mixing esters with alcohols is expected to cause changes in the balance of hydrogen bonds and electrostatic interactions, resulting in different contributions to the volume of the mixtures. The analyzed compounds have good predispositions for the formation of H-bonds, as well as polar nature. Alcohols act as both hydrogen donors and acceptors, while ester molecules are H-bond acceptors. But it can be concluded that positive V^E values are a consequence of breaking of hydrogen bonds between strongly connected alcohol molecules and the weakening of dipole-dipole interactions between polar ester molecules in the mixture, as well as steric hindrances.

The values of viscosity deviations and excess molar Gibbs energies of activation of viscous flow are graphically given in Figure 2. These values are negative at all temperatures and for all molar fractions of ethyl octanoate. The values become less negative as temperature increases.



(a) (b)

Figure 2. Experimental values of (a) viscosity deviation $\Delta\eta$, (b) excess molar Gibbs energy of activation of viscous flow ΔG^{*E}, as a function of the molar fraction of ethyl octanoate x_1 for the system ethyl octanoate (1) + 1-butanol (2).

Physical interactions involving mainly dispersion forces or weak dipole-dipole interactions between mixture components lead to negative values of ΔG^{*E} and $\Delta\eta$. Negative deviations in viscosity indicate weaker interactions between different molecules, as a result of the dominance of strong attractive interactions between the same molecules.

Analiza molekulskih interakcija prema dopunskim veličinama za binarnu smešu etil oktanoat + 1-butanol

Divna M. Majstorović[1], Emila M. Živković[1], Mirjana Lj. Kijevčanin[1]
[1] *Univerzitet u Beogradu Tehnološko-metalurški fakultet, Karnegijeva 4, Beograd, Srbija*

Gustina i viskoznost za binarni sistem koji sadrži estar etil oktanoat i alkohol 1-butanol mereni su na osam temperatura u opsegu (288,15-323,15) K i na atmosferskom pritisku. Ovi podaci omogućili su izračunavanje dopunskih veličina kao što su dopunska molarna zapremina, promena viskoznosti i dopunska molarna Gibsova energija aktivacije viskoznog toka. Izračunati podaci su korelisani Redlich-Kister jednačinom i korišćeni za diskusiju o strukturnim efektima i efektima pakovanja koji se dešavaju u ispitivanoj smeši. Rezultati su pokazali da je efekat raskidanja vodoničnih veza molekula alkohola i dipol-dipol interakcija molekula estara, koji uslovljava ekspanziju zapremine, kvantitativno nadmašio slabe intermolekulske vodonične veze između ovih molekula i intersticijalno smeštanje molekula estara u multimere alkohola.

References

1. V.K. Misra, I. Vibhu, R. Singh, M. Gupta, J.P. Shukla, *J. Mol. Liq.* **2007**, *135*, 166–169.
2. O. Redlich, A.T. Kister, *Ind. Eng. Chem.* **1948**, *40*, 345–348.

Acknowledgment: The authors gratefully acknowledge the financial support received from the Research Fund of Ministry of Science, Technological Development and Innovation Republic of Serbia and the Faculty of Technology and Metallurgy University of Belgrade (Contract No. 451-03-47/2023-01/200135).

Hemija i tehnologija materijala

Chemistry and Technology of Materials

R-HTM-1

A way to improve the sorption properties of raw jute fabric by sodium alginate treatment

Marija D. Milošević[1], Aleksandra M. Ivanovska[2], Mirjana M. Kostić[1], Zorica B. Svirčev[3,4]
[1] *University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia*
[3] *University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*
[4] *Åbo Akademi University, Faculty of Science and Engineering, Turku, Finland*

Sodium alginate aqueous solutions of different concentrations (0.5, 1.0, or 2.0%) were used for improving the sorption properties (evaluated through the determination of water retention power (WRP) and wetting time (WT)) of raw jute fabric. The influence of drying conditions (never-dried samples, samples dried at 60 °C or at room temperature) on the sorption properties of alginate-treated jute fabrics was also studied. Independently on the examined method (centrifuge or water absorption method), the same trend of improvement in WRP of alginate-treated fabrics was observed. The WRP of never-dried fabric treated with 2.0% sodium alginate solution determined using the water absorption or centrifuge method increased by 4.8 or 3.3 times compared to raw jute fabric, respectively. Moreover, the WT of jute fabrics decreased from 206.9±6.6 s down to 1.7±0.1 s after the treatment with 0.5% sodium alginate solution. The improved sorption properties of alginate-treated jute fabrics are attributed to the alginate layer on the fabric surface having a higher number of accessible carboxyl groups as well as hydroxyl groups capable of forming new hydrogen bonds with water molecules.

Introduction

As the most important ligno cellulosic fiber, jute represents an economical, sustainable, readily available, and renewable resource. Thanks to its excellent physico-mechanical and chemical properties, this natural fiber can be used for various conventional and non-conventional applications. The well-known conventional application of jute fibers is for the production of packaging materials such as sacking cloth, hessian, as well as carpet backing. Non-conventional applications of jute fibers are usually connected with the production of various jute based-composites with defined properties and targeted end-uses. In light of that, jute fabric with enhanced sorption properties could find novel application as geo-prebiotic supports for cyanobacteria growth in biocarpet engineering, *i.e.*, to promote a sustainable relationship between the microbiota and abiotic constituents on the degraded land surface. In our previous work [1], we reported that the treatment with chitosan enhanced the sorption properties of raw jute fabric. As a continuation of the research within the topic, in this work, the influence of the treatment with another polysaccharide, *i.e.*, sodium alginate on the jute fabric sorption properties was studied. Sodium alginate is a non-toxic, biocompatible, anionic polysaccharide with good sorption properties originating from the presence of carboxyl and hydroxyl groups in its structure [2]. In order to obtain jute fabrics with enhanced sorption properties, raw jute fabric was treated with 0.5, 1.0, or 2.0% sodium alginate aqueous solutions. After the treatment, different methods were employed for fabric drying and their effect on water retention power and wetting time was studied.

Results and Discussion

Water retention power (WRP)

As an important indicator of fabric sorption properties, WRP, representing the total amount of retained water in its structure [3], was studied according to two different methods (*i.e.* centrifuge and water absorption methods), Figure 1.

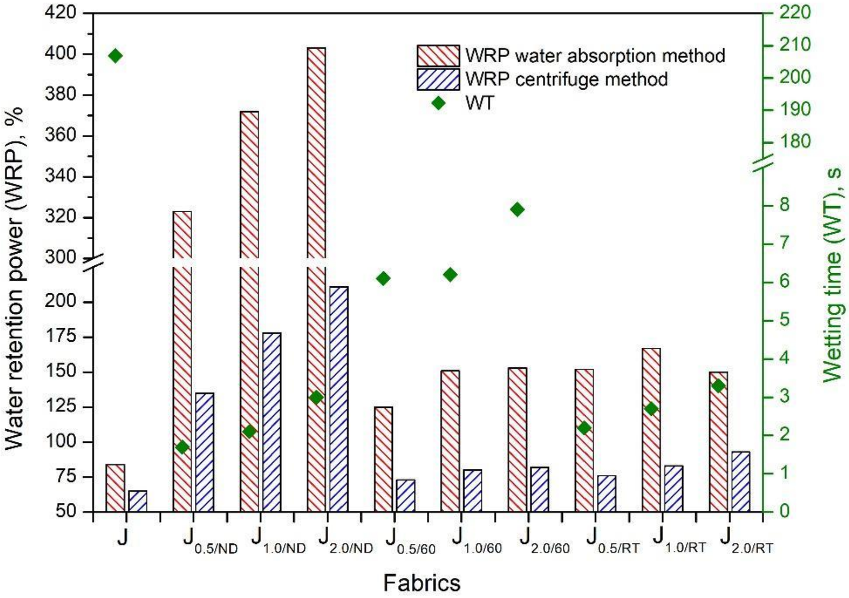


Figure 1. WRP and WT of raw and alginate-treated jute fabrics

The WRP of raw jute (J) determined by water absorption and centrifuge methods accounted for 84% and 65%, respectively. Among three sets of samples, never-dried ones ($J_{0.5/ND}$, $J_{1.0/ND}$, $J_{2.0/ND}$) possessed the highest increment in WRP, whereby $J_{2.0/ND}$ is characterized by 4.8 (water absorption method) or 3.3 times (centrifuge method) higher WRP compared to raw jute fabric. It is interesting to note that the results obtained for WRP using the different testing methods followed the same trend. Sodium alginate treatment enriched the jute fabrics’ surface with functional groups available for forming the new hydrogen bonds with water molecules contributing to higher WRP values. Considering in parallel the different drying methods (at 60 °C and at room temperature), it is evident that they significantly decreased the WRP in comparison to never-dried samples. A small difference between WRP of differently dried fabrics can be explained by the different rates of water evaporation from the samples’ surface affecting the structure of the formed alginate layer. Furthermore, its hornification makes dried fibers more resistant to reswelling and behaves as a kind of barrier to water penetration.

Wetting time (WT)

Besides WRP, WT is another important indicator of fabrics’ sorption properties. Before measuring the WT, the never-dried samples were left to dry under the same conditions as the samples dried at room temperature. As can be seen from Figure 1, the treatment with sodium alginate positively affect the WT. For example, the WT of raw jute (J) decreased from 206.9±6.6 s down to 1.7±0.1 s after the treatment with 0.5% sodium alginate solution (sample $J_{0.5/ND}$). There are no differences between the WT of never-dried samples subsequently dried at room temperature and those dried at room temperature. On the other hand, the drying samples at 60 °C resulted in higher WT compared to the samples dried at room temperature. Moreover, the effect of the concentration of sodium alginate aqueous solution on WT should not be neglected. Namely, the utilization of a higher concentration of sodium alginate aqueous solution implies the formation of a denser alginate layer which is more prone to hornification during the drying at 60 °C, Figure 1.

Experimental Part

Treatment of jute fabric with sodium alginate aqueous solution

Before the treatment with sodium alginate aqueous solution, raw jute fabric was washed in distilled water at boiling temperature for 30 min to remove water-soluble substances. Immediately after squeezing, jute fabric was dipped into 0.5, 1.0, or 2.0% sodium alginate (low viscosity, Alfa Aesar) aqueous solution (material to liquid ratio of 1:20) at an ambient temperature for 24 h. Thereafter, the fabrics were immersed in 2.0% aqueous solution of $CaCl_2$ (material to liquid ratio of 1:20) at an ambient temperature for 24 h, and rinsed with distilled water. Three sets of samples were prepared regarding the drying procedure. One set of samples was never-dried, the other was dried at 60 °C for 24 h, while the last set of samples was dried at room temperature.

Sorption properties

The WRP was determined following the standard centrifuge method ASTM D2402-07(2018), and the water absorption method based on ASTM D570-98(2018) standard, while the WT measurements were performed according to standard AATCC 79 (2018). The WRP and WT are presented as the mean values of six and three measurements per sample, respectively.

Tretman natrijum-alginatom kao način da se poboljšaju sorpciona svojstva sirove tkanine jute

Marija D. Milošević[1], Aleksandra M. Ivanovska[2], Mirjana M. Kostić[1], Zorica B. Svirčev[3,4]
[1] *Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Beograd, Srbija*
[2] *Univerzitet u Beogradu, Inovacioni centar Tehnološko-metalurškog fakulteta, Beograd, Srbija*
[3] *Univerzitet u Novom Sadu, Prirodno-matematički fakultet, Novi Sad, Srbija*
[4] *Abo Akademi Univerzitet, Prirodno-tehnički fakultet, Turku, Finska*

Vodeni rastvori natrijum-alginata različitih koncentracija (0,5, 1,0 ili 2,0%) korišćeni su za poboljšanje sorpcionih svojstava (procenjenih određivanjem sposobnosti zadržavanja vode (WRP) i vremena kvašenja (WT)) sirove tkanine jute. Takođe je proučavan uticaj uslova sušenja (neosušeni uzorci, uzorci sušeni na 60 °C ili na sobnoj temperaturi) na sorpciona svojstva tkanina jute tretiranih alginatom. Nezavisno od metode ispitivanja (centrifugiranjem ili apsorpcijom vode posle potapanja), dobijen je isti trend poboljšanja sposobnosti zadržavanja vode tkanina tretiranih alginatom. Sposobnost zadržavanja vode nesušene tkanine tretirane 2,0% rastvorom natrijum-alginata, određene metodom apsorpcije vode posle potapanja ili centrifugiranjem, povećana je 4,8 ili 3,3 puta u

poređenju sa sirovom tkaninom jute, respektivno. Štaviše, tretman tkanina jute 0,5% rastvorom natrijum-alginata dovodi do smanjenja vremena kvašenja sa 206,9±6,6 s na 1,7±0,1 s. Poboljšana sorpciona svojstva tkanina jute tretiranih alginatom pripisuju se sloju alginata na njihovoj površini sa većim brojem dostupnih karboksilnihi hidroksilnih grupa sposobnih da formiraju nove vodonične veze sa molekulima vode.

References

1. A. Ivanovska, M. Milošević, J. Lađarević, L. Pavun, Z. Svirčev, M. Kostić, J. Meriluoto, *Appl. Sci*. **2023**, *13*, 2512.
2. B. Wang, Y. Wan, Y. Zheng, X. Lee, T. Liu, Z. Yu, J. Huang, Y. S. Ok, J. Chen, B. Gao, *Crit. Rev. Env. Sci. Tec*. **2019**, *49*, 318.
3. A. Kramar, A. Ivanovska, M. Kostić, *Fiber Polym*. **2021**, *22*, 2177.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #7726976, Integrated Strategy for Rehabilitation of Disturbed Land Surfaces and Control of Air Pollution– RECAP.