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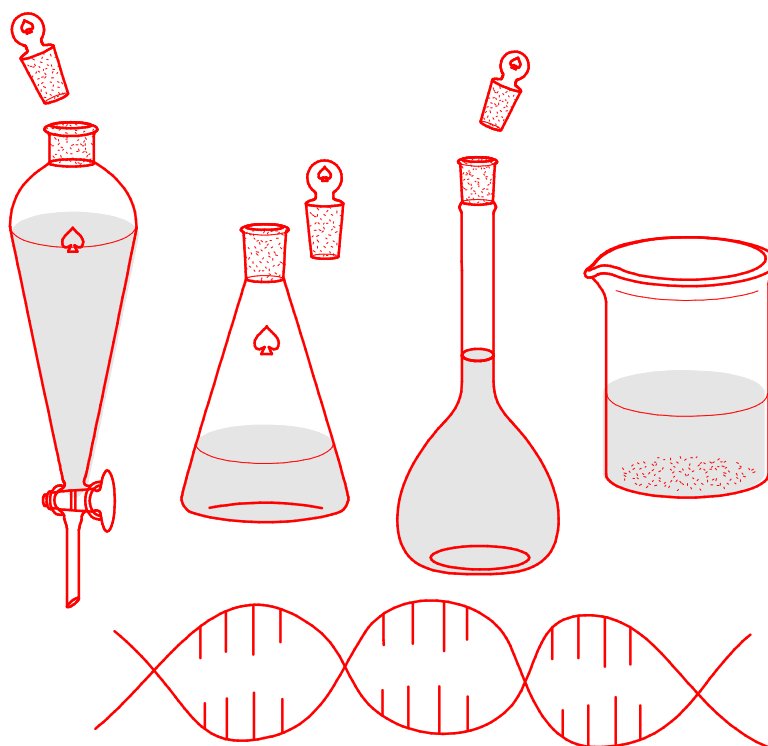
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**Chromium(VI) removal from aqueous solutions using powdered coconut shell
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Plenarna predavanja

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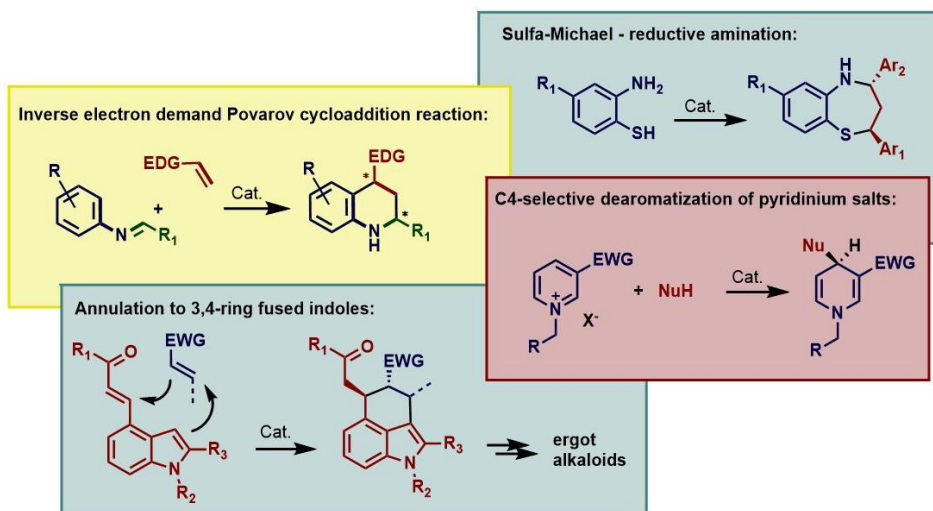
PP-1

Asymmetric organocatalysis: stereoselective approaches to nitrogen heterocycles

Luca Bernardi

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The curiosity of exploring new substrate reactivity, induced by organic catalysts, has led to the disclosure of stereoselective entries to a range of otherwise difficult to access heterocyclic structures. In this context, examples of transformations studied in our laboratory include dearomatizations of pyridinium salts, annulations to 3,4-ring fused indoles, inverse-electron demand Povarov cycloaddition reactions, and sulfa-Michael – reductive amination sequences towards tetrahydro-1,5-benzothiazepines. Some of these examples will be highlighted in the presentation, emphasizing mechanistic aspects and applications to targets such as ergot alkaloids and active pharmaceutical ingredients.



PP-2

Ligand Based (Machine Learning) and Structure-Based Approaches in Medicinal Chemistry: Application to Drug Discovery (and Essential Oils)

Rino Ragno

Rome Center for Molecular Design – Department of Drug Chemistry and Technology – Faculty of Pharmacy and Medicine -Sapienza University of Rome

In the past two decades we have been witnessing to a impressive technology update on the way how drug are designed. The role of classical medicinal chemists much involved in the design and hence in the preparation of new chemical entities (NCE) is now definitively transformed in a multidisciplinary approach. Increasingly, NCE are designed by teams of experts comprising medicinal chemists, pharmacologists, biochemists, structural (bio)chemists and computational chemists. During the years many classical medicinal chemists have turned to use the computer to design their NCE so that a new figure has born: the computational medicinal chemist (CMC). The role of a CMC is crucial as it has to be ready not only to use all possible computational techniques to predict which molecules deserve to be prioritized but he/she should be also able to give advice for synthetically accessible molecules as well as to drive the experiments' chronology to achieve as fast as possible the aims of the undergoing project. At Rome Center for Molecular Design (www.rcmd.it) in the last twenty years we have been developing procedures to aid drug design and NCE selection. In particular ligand-based (LB) and structure-based (SB) methods have been routinely applied gathering during the years a level of expertise leading to a list of high level of peer reviewed publications. During the summer of 2016 the very first free 3-D QSAR portal (www.3d-qsar.com) was opened to the public initially including only LB web applications overlapping the well known Comparative Molecular Field Analysis (CoMFA) software developed by Richard Cramer at the former TRIPOS. After two years and more than a thousands of active users, SB web application were also implemented including molecular docking and the full SB 3-D QSAR technique Comparative Molecular Binding Energy (COMBINE) analysis. At the moment 3d-qsar.com counts more than 2500 active users spread over 93 countries and include a list of specialized computational medicinal chemistry web application that allow any user to develop LB models just using the least amount of starting information as a list of molecules described by SMILES strings and the associated bioactivities. On the other side with the availability of a co-crystallized ligand into its target, 3d-qsar.com enable the user to undertake a full docking assessment protocol and the building of COMBINE models. In parallel to the drug design efforts, 15 years ago at RCMD we started to study essential oils (EOs) in particular their extraction and their chemical and biological characterization. During the years we collected a good amount of data that recently allowed us to undertaken investigations leading to converge the two fields (computational and EOs). In particular by the application of machine learning (ML) algorithms we were able to develop quantitative composition-activity relationships (QCAR) models as tools to investigate complex mixtures (EOs) and disclose the more important chemical components for a given biological activity. At the best of our knowledge such a conjugation of ML and EOs has not been yet reported by other investigators. We are still developing protocols in this new field and for this purpose one year ago we started the realization of a new EOs database (Py-EO) from data gathered either from experiments or from literature and focused on the EOs' chemical composition and associated biological activities. At the present in Py-EO have been already loaded more than 2000 essential oil compositions and more than 15000 activity data. In the near future such amount of growing data will be used to develop robust ML models to open a new frontier on the design of complex mixtures.

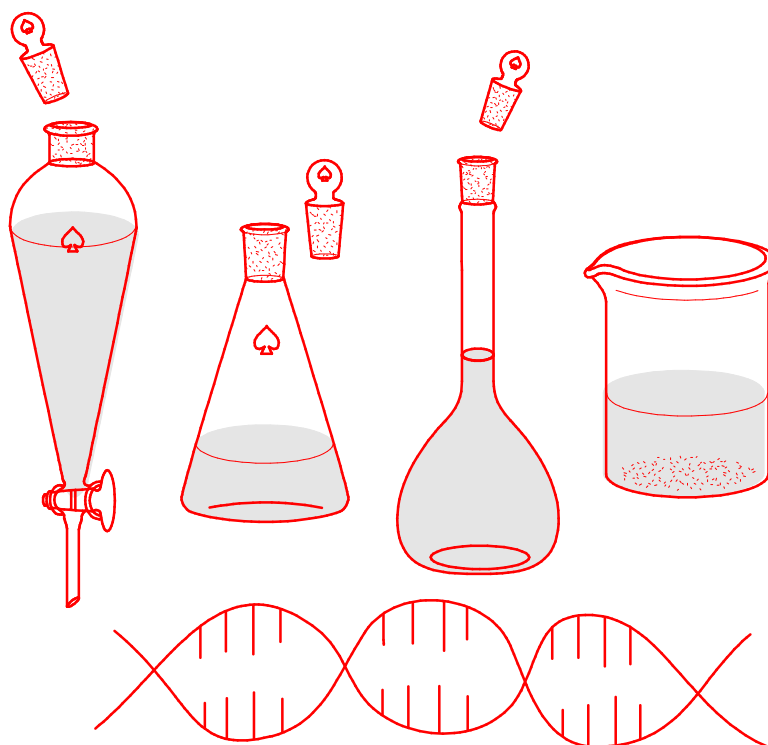
Pristupi u medicinskoj hemiji zasnovani na strukturi liganda (mašinskom učenju) i strukturi molekulske mete: Primena u otkrivanju lekova (i analizi esencijalnih ulja)

Rino Ragno

U poslednje dve decenije svedoci smo impresivnog napretka u tehnologiji dizajna lekova. Uloga klasičnih medicinskih hemičara, do sada uglavnom prepoznata u dizajnu i sintezi novih hemijskih entiteta (NHE) je definitivno transformisana u vidu multidisciplinarnog pristupa. Veliki broj NHE dizajnirani su u timovima sačinjenim od eksperata u oblasti medicinske hemije, farmakologije, biohemije, strukturne (bio)hemije i kompjutacione hemije. Tokom godina, mnogi medicinski hemičari počeli su koristiti računar da bi dizajnirali svoje NHE, a kao posledica toga nastalo je novo zanimanje: kompjutacioni medicinski hemičar (KMH). Uloga KMH-a je od presudne važnosti jer ekspert u toj oblasti mora da poznaje ne samo sve razvijene računarske tehnike da bi predvideo koji molekuli zaslužuju da se označe kao prioritetni, već on/ona mora da prepozna i predloži molekule koji se mogu relativno jednostavno sintetisati, kao i da vodi eksperimentalne protokole pomoću kojih se na najbrži mogući način mogu ostvariti ciljevi zadanog projekta. U Rimskom centru za molekularni dizajn (eng. Rome Center for Molecular Design, RCMD, www.rcmd.it) u poslednjih dvadeset godina razvijamo procedure za dizajn lekova i selekciju HNE. Naročito se rutinski primenjuju metode bazirane na strukturi liganada (eng. ligand-based, LB) i strukturi molekulske meta (eng. structure-based, SB), čime smo dostigli nivo kompetencije i ekspertize dovoljan za publikaciju velikog broja jako kvalitetnih naučnih radova. Tokom leta 2016. godine otvoren je za javnosti prvi besplatni veb portal za generisanje 3-D QSAR studija (www.3d-qsar.com), inicijalno pružajući mogućnost za razvijanje LB modela komparativnih sa poznatim Comparative Molecular Field Analysis (CoMFA) softverom razvijenim od strane Ričarda Kramera (Richard Cramer) u nekadašnjoj kompaniji TRIPOS. Nakon dve godine i više od hiljadu aktivnih korisnika, SB veb aplikacije su takođe implementirane, uključujući molekularno dokovanje i SB 3-D QSAR tehniku nazvanu Comparative Molecular Binding Energy (COMBINE). U ovom trenutku, 3d-qsar.com ima više od 2500 aktivnih korisnika u 93 zemlje i sadrži listu specijalizovanih veb aplikacija u okviru kompjutacione medicinske hemije koje omogućavaju bilo kom korisniku da razvije LB modele koristeći najmanju moguću količinu početnih informacija za set molekula opisanu pomoću SMILES stringova i povezanih vrednosti bioaktivnosti. Sa druge strane, usled dostupnosti liganada ko-kristalizovanih sa svojim molekularnim meta, portal 3d-qsar.com omogućava korisniku da sprovede potpuni protokol primenljivosti molekularnog dokovanja i generisanje COMBINE modela. Paralelno sa naporima vezanim za dizajn lekova, pre 15 godina smo u RCMD počeli sa proučavanjem esencijalnih ulja (eng. essential oils, EOs), naročito njihovu ekstrakciju i hemijsku i biološku karakterizaciju. Tokom godina, sakupljena je velika količina podataka koja nam je skorije omogućila da počnemo sa istraživanjima koja su rezultovala spajanjem dve oblasti (kompjutacione hemije i EOs). Konkretno, primenom algoritama mašinskog učenja (eng. machine learning, ML) bili smo u mogućnosti da razvijemo modele kvantitativne zavisnosti sastava EO u odnosu na aktivnost (eng. quantitative composition-activity relationships, QCAR) kao alat za istraživanje kompleksnih smeša EOs i otkrivanje najvažnijih hemijskih jedinjenja koja dovode do aktivnosti. Prema našim najboljim saznanjima, ovakva primena ML u analizi EOs do sada nije objavljena. Trenutno još uvek razvijamo protokole u ovoj novoj oblasti i s tim u vezi pre godinu dana počeli smo sa kreiranjem nove baze podataka za analizu EOs (Py-EO) iz podataka sakupljenih iz eksperimenata i iz literature, koja će se fokusirati na hemijski sastav EOs i povezane biološke aktivnosti. U ovom trenutku je u Py-EO ubačeno više od 2000 esencijalnih ulja sa definisanim hemijskim sastavom i podaci aktivnosti za preko 15000 jedinjenja. U skorijoj budućnosti, takva količina rastućih podataka biće korišćena za razvoj robustnih ML modela i otvoriće nove perspektive u dizajnu još kompleksnijih smeša.

Predavanja po pozivu

Invited Lectures



PPP-1

Steroidi u medicinskoj hemiji - hemijom i biologijom vođen razvoj lekova

Suzana Jovanović-Šanta

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Medicinska hemija obuhvata dizajn i sintezu biološki aktivnih jedinjenja, proučavanje njihovog metabolizma i načina delovanja i definisanje odnosa između strukture i aktivnosti. Prirodni steroidi pokazuju specifične fiziološke efekte, u zavisnosti od strukture i ciljnog tkiva. Modifikacija strukture steroida obično dovodi do promene njihove biološke/farmakološke aktivnosti. Neki modifikovani steroidi utiču na enzime uključene u steroidogenezu ili karcinogenezu, neki kompetituju sa receptorima, neki uzrokuju smrt ćelija kancera, najčešće indukovanjem apoptoze, dok neki deluju na druge načine. Otkrivanje lekova zasnovano na hemiji obuhvata dizajn modifikovanih steroida, zasnovan na biološkim efektima prirodnih ili sintetičkih jedinjenja na ciljne molekule, optimizaciju aktivnih molekula sintezom niza sličnih jedinjenja sa različitim farmakoforama, izosterama ili bioizosterama i upoređivanje struktura i aktivnosti. U razvoju lekova vođenom biologijom ciljni biomolekul se može identifikovati nakon uočenog i kvantifikovanog biološkog ili farmakološkog efekta ispitivanog jedinjenja u određenom model-sistemu.

Steroids in medicinal chemistry - chemistry and biology driven drug development

Suzana Jovanović-Šanta

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Medicinal chemistry encompasses the design and synthesis of biologically active compounds, studying of their metabolism and mode of action and defining the relationship between structure and activity. Natural steroids exhibit specific physiological effects, depending on the structure and target tissue. Modifying the structure of steroids usually leads to a change in their biological/pharmacological activity. Some modified steroids affect enzymes involved in steroidogenesis or carcinogenesis, some compete with receptors, some cause cancer cell death, mostly by inducing apoptosis, while some act in other ways. Chemistry-driven drug discovery includes modified steroids design, based on the biological effects of natural or synthetic compounds on target molecules, optimizing active molecules by synthesizing a series of similar compounds, with different pharmacophores, isosters or bioisosteres and comparing structures and activities. In the biology-driven drug discovery the target biomolecule can be identified after the observed and quantified biological or pharmacological effect of the test compound in a particular model system.

The research was conducted within the Program funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (451-03-9/2021-14/200125) and Belarus-Serbia bilateral projects (51-03-003036/2017-09/02 and 337-00-00612/2019-09/04).

PPP-2

Organokatalitičke enantioselektivne C-H funkcionalizacije u prisustvu organskih oksidanata

Bojan Bondžić

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U prisustvu hiralnih diaril prolinola kao organokatalizatora i organskog oksidacionog sredstva postignuta je reakcija formalne C-H oksidacije zasićenih aldehida, mehanizmom oksidacije elektron bogatog enamina do elektron deficitarnog iminijum jona. Ova reakciona vrsta zatim učestvuje u reakciji funkcionalizacije sa reakcionom vrstom prisutnom u reakcionoj smesi ili dodatoj nakon završetka oksidacionog procesa. Na ovaj način reakcija formalne C-H oksidacije je kombinovana sa Diels-Alderovom reakcijom (u prisustvu diena) i reakcijom ciklopropanovanja iniciranom Majklovom adicijom (u prisustvu odgovarajućeg nuleofila). Na ovaj način dobijeni su proizvodi Diels-Alderove reakcije i reakcije ciklopropanovanja u visokim prinosisima i sa visokim diastereo- i enantio-selektivnostima. Dodatno, razvijen je i proces funkcionalizacije tetrahidroizohinolina reakcijom ukrštenog dehidrogenativnog kuplovanja u prisustvu DDQ ili IBXa kao organskih oksidanasa.

Organocatalytic enantioselective C-H functionalizations promoted by organic oxidants

Bojan Bondžić

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Organic, single-electron oxidant in the presence of diarylprolinol silylether type catalyst serves as a tool for the transformation of electron-rich enamines to iminium ions. These iminium ions take part in a subsequent Diels-Alder or Michael-initiated ring-closure (MIRC) reaction with in situ present reaction partners giving rise to overall Diels-Alder or cyclopropanation reaction products. Stereodefined products are obtained in high yields and dia- and enantio-selectivities. In addition, Cross Dehydrogenative Coupling protocol for the functionalisation of tetrahydroisoquinolines promoted by organic oxidants was developed

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PPP-3

Zamena sumpora selenom; Supramolekulski pristup

Goran V. Janjić

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Supramolekulski pristup zasnovan je na statističkoj analizi podataka dobijenih iz kristalnih struktura, ekstrahovanih iz CSD-a (od eng. Cambridge Structural Database), kvantno-hemijskim proračunima za procenu jačine tipičnih interakcija, i na doking studiji za određivanje vezivanja S/Se jedinjenja za odabrane biomolekule. Statistička analiza je pokazala da atomi S i Se, u fragmentima koji odgovaraju bočnim lancima cisteina (Cis), metionina (Met), selenocisteina (Sec) i selenometionina (Mse), pokazuju sličnu tendenciju ka određenim vrstama interakcija. Najbrojnije su strukture sa C-H/Se i C-H/S interakcijama (~80%). Strukture sa Se/Se i S/S interakcijama su znatno manje zastupljene u kristalnim strukturama (~5%), iako su C-H/Se i C-H/S interakcije (~ -0,8 kcal/mol) slabije od najstabilnijih Se/Se i S/S interakcija sa paralelnih orijentacijom (~ -3,3 kcal/mol) i njihovih elektrostatičkih interakcija σ/π tipa (~ -2,6 kcal/mol). Značajna razlika u brojnosti može se objasniti obiljem C-H grupa u analiziranim kristalnim strukturama. Doking studija je pokazala da S i Se atomi retko uključeni u interakcijama sa amino-kiselinskim ostacima ciljanih enzima, ali su razlike u broju i položajima vezivnih mesta izraženije ako su supstituenti vezani za S/Se polarni, ali i ako ligand poseduje više od jednog Se ili S atoma.

Substitution of sulfur by selenium; The supramolecular insight

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The supramolecular approach is based on statistical analysis of data from crystal structures extracted from the Cambridge Structural Database (CSD), quantum-chemical calculations for assess the strength of typical interactions, and docking study for determination of the binding of S/Se compounds to selected biomolecules. The statistical analysis has shown that S and Se atoms, in fragments that corresponds to the side chains of cysteine (Cys), methionine (Met) selenocysteine (Sec) and selenomethionine (Mse), display a similar tendency towards specific types of interaction. The most numerous are structures with C-H/Se and C-H/S interactions (~80%). The structures with Se/Se and S/S interactions are notably less numerous (~5%), although the C-H/Se and C-H/S interactions (~-0.8 kcal/mol) are weaker than the most stable parallel Se/Se and S/S interactions (~-3.3 kcal/mol) and electrostatic interactions of σ/π type (~-2.6 kcal/mol). The significant difference in numerosity can be explained by the abundance of C-H groups in analyzed crystal structures. Docking studies revealed that S and Se rarely participate in interactions with the amino acid residues of target enzymes, but the differences in the number and positions of their binding sites between Se and S compounds are more pronounced if the substituents of S/Se atom are polar and if there are more Se/S atoms in the ligand.

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PPP-4

The art of structure-based drug design: Demystifying Molecular Docking

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Molecular docking is nowadays considered a mainstream structure-based drug discovery method in medicinal chemistry. Still, the critical analysis of scientific papers reporting the usage of molecular docking reveals that the method is often improperly used, mostly in terms of the experimental setup, and that the results are sometimes misinterpreted as a consequence of the *ad hoc* acknowledgment and presentation of the outcomes of the analysis, neglecting the basic or advanced biochemistry principles of ligand-molecular target interactions. The herein lecture aims to provide the guidelines for either novice or experienced users on how to consider molecular docking as an experimental procedure and not a tool whose usage is dependent on the program's graphical user interface as installed on the user's personal computer. Hence, some of the most important topics will be covered while performing molecular docking: (1) What is molecular docking and when to use it?; (2) How to validate molecular target for your ligand?; (3) Before we begin: What is an optimal platform for molecular docking, Windows, Linux, or MacOS?; (4) How to perform molecular docking: graphical user interface or command-line application?; (5) How to prepare a molecular target?; (6) How to prepare a ligand?; (7) How to work with multiple targets and ligands?; (8) How to define grid spacing and molecular coordinates, *i.e.* characterize the active site?; (9) How to approach when the information about the active site is missing?; (10) How to perform molecular docking: rigid docking, flexible docking, or other approaches?; (11) How to choose optimal scoring function/docking algorithm?; (12) How and when to perform covalent docking?; (13) How to interpret the results and define the ligand's bioactive conformation?; (14) How to surpass the limitations of molecular docking: predicted binding affinity (and other enzyme kinetics parameters) *vs.* the bioactive conformation?; (15) How to approach when the quality of structure-based alignment is uncertain? The lecture will address the theoretical considerations from the practical-like point of view (*viz.* by discussing the real case studies) upon which the users will be motivated to master molecular docking.

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PPP-5

Uticaj inertnog liganda na biološku aktivnost Rh(III) i Os(II) kompleksa u odsustvu i prisustvu jonskih tečnosti

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Zbog svoje inertnosti metalni kompleksi koji sadrže Rh i Os, od nedavno dobijaju sve veću pažnju. Inertnost kao specifična karakteristika ovih metalnih kompleksa, koja se u početku videla kao nedostatak, doprinela je dizajniranju kompleksa sa specifičnim ciljevima za vezivanje za proteine, inhibitore enzima, kao i DNK. Shodno tome sintetisali smo i okarakterisali dva nova Rh(III) kompleksa sa kamfor derivatima bis-pirazolpiridinskih liganada. Ispitivane su reakcije supstitucije sa biomolekulama i ispitivana je sposobnost interakcije sa CT-DNK i albumin serum proteinom. Citotoksičnost kompleksa metala je ispitana MTT testom na HCT-116 liniji. Takođe, uticaj biokompatibilnih jonskih tečnosti na reakcije sintetisanih kompleksa su ispitivane.

Navedeno istraživanje je finansijski pomoglo Ministarstvo prosvete, nauke i tehnološkog razvoja.

Influence of an inert ligand on the biological activity of Rh(III) and Os(II) complexes in the absence and in presence of ionic liquids

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Because of their inertness metal complexes containing Rh and Os, have just recently received increasing attention. Inertness as a specific characteristic of these metals complexes, that was in the beginning seen as a drawback has contributed to the design of complexes with a specific target for proteins, enzyme inhibitors, as well as DNA. Therefore we have designed and fully characterized a few new Rh(III) and Os(II) complexes with the bis-pyrazolylpyridine ligands. The substitutive reactions with biomolecules were studied and the interaction ability with CT-DNA and protein bovine serum albumin were examined. The impact of the metal complex on cytotoxicity was tested by MTT assay on HCT-116 line. As well as a influence of of biocompatible ionic liquids on reactions of synthesized complexes were examined.

PPP-6

**BISBIBENZILI, FLAVONOLIGNANI I FLAVONOIDNI DIMERI,
RASPROSTRANJENOST I BIOLOŠKE AKTIVNOSTI**

Miroslav Novaković

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Bisbibenzili su hemotaksonomski markeri jetrenjača, predaka viših biljaka. Maršancin A, kao najispitivaniji bisbibenzil, poseduje brojne biološke aktivnosti. Najbolje rezultate pokazao je u ispitivanjima antitumorske aktivnosti ka ćelijama raka dojke. Hemijskom i enzimskom derivatizacijom, tačnije acilovanjem, dobijeni su estri sa generalno sličnom aktivnošću polaznom maršancinu A ka ćelijama MDA-MB-231 raka dojke, ali boljom selektivnošću, posebno monoheksanoil estar. Bisbibenzili su po prvi put u višim biljkama nađeni u sibirskim jagorčevinama. Njihovo prisustvo je potvrđeno i u dvema vrstama istog roda iz Srbije, odnosno otkrivena su i dva potpuno nova bisbibenzila po prvi put.

Flavonolignani su jedinjenja nastala u prirodi kuplovanjem flavonoida i fenilpropanske grupe zahvaljujući prisustvu enzima oksidaza. Najpoznatiji su silimarini iz sikavice, *Silibum marianum*, sa hepatoprotektivnom aktivnošću. Dva nova auronolignana nastala na isti način izolovana su iz biljne vrste *Cotinus coggygria*. Sličnom je reakcijom iz 2'-hidroksihalkona buteina izolovanog iz *C. coggygria* dobijen prvo auron sulfuretin, a potom četiri nova auronska dimera. Proizvodi reakcije zavise od vrste lakaze (oksidaze) koja je korišćena, tj. njenog izvora.

**BISBIBENZYLs, FLAVONOLIGNANS AND FLAVONOID DIMERS,
ABUNDANCE AND BIOLOGICAL ACTIVITY**

Miroslav Novaković

University of Belgrade – Institut of Chemistry, Technology and Metallurgy – Department of Chemistry

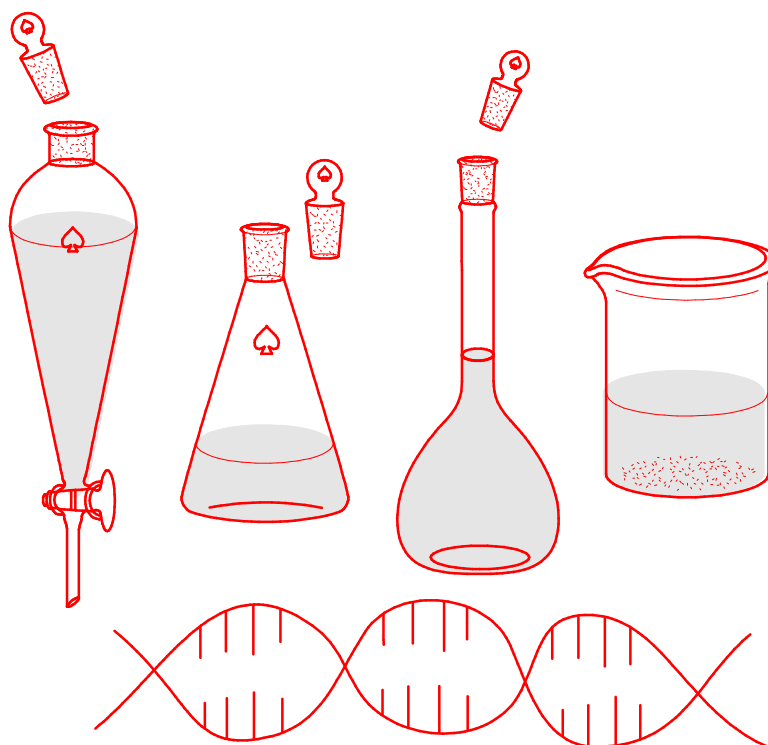
Bisbibenzyls are chemotaxonomic markers of liverworts, ancestors of higher plants. Marchantin A, as the most investigated bisbibenzyl, possess numerous biological activities. The best results marchantin A exhibited in investigations of antitumor activity against breast cancer. Chemical and enzymatic derivatization, acylation, provided esters with generally similar activity to starting marchantin A against MDA-MB-231 breast cancer cells, but with better selectivity, especially monohexanoil ester. For the first time bisbibenzyls were found in higher plants in Siberian *Primula* species. Their presence was confirmed in two Serbian *Primula* species as well, *ie.* two new bisbibenzyls were discovered for the first time. Flavonolignans are compounds formed in nature by coupling of molecules of flavonoid and phenyl-propane group using enzyme oxidase. The best known are silimarins from *Silibum marianum*, known for their hepatoprotective activity. Two new auronolignans formed in the same way were discovered in *Cotinus coggygria* plant species. In similar way from 2'-hydroxyhalcone butein isolated from *C. coggygria* were obtained firstly aurone sulfuretin, and later four new aurone dimers. Products of the reaction depends on the type of laccase (oxidase) used, *ie.* its source.

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Saopštenja / Contributions

Analitička hemija

Analytical Chemistry



AH-P-1

Elektroda od ugljenične paste modifikovana jonskom tečnošću 1-butil-3-metilpiridinium hloridom za voltometrijsko određivanje UV filtera avobenzona

Sanja Mutić, Jasmina Anojić, Milan Vraneš, Snežana Papović, Jovana Panić, Aleksandar Tot, Nikolet Baganj, Teona Teodora Borović

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Ispitana je primenljivost elektrode od ugljenične paste (CPE) zapreminski modifikovane piridiniumovom jonskom tečnošću (IL), kao što je 1-butil-3-metilpiridinium hlorid (N-C₄-3MPyCl), za voltometrijsko određivanje UV filtera avobenzona (AVO). Primenjena je direktna anodna voltimetrija sa pravougaonim talasima. Optimizovani su različiti eksperimentalni parametri, uključujući pH pomoćnog elektrolita i količinu IL modifikatora u CPE. Za analitičke svrhe, optimalna vrednost Britton-Robinson pufera je pH 11,98 i 3,3 mas.% IL modifikatora. Modifikacija CPE sa N-C₄-3MPyCl obezbeđuje 2 puta intenzivniji oksidacioni pik AVO u poređenju sa istim na nemodifikovanoj CPE. Linearost kalibracione krive postignuta je u opsegu od 0,10 do 3,85 µg mL⁻¹ AVO sa N-C₄-3MPyCl-CPE. Procenjena granica detekcije je 0,03 µg mL⁻¹ AVO, a relativna standardna devijacija nije prelazila 3,6%.

Zahvalnica: *Autori se zahvaljuju za finansijsku podršku Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (br. ugovora 451-03-9/2021-14/200125) i projektu Sekretarijata za nauku i tehnološki razvoj Autonomne pokrajine Vojvodine, Srbija (broj 142-451-3167/2020).*

Carbon paste electrode modified with ionic liquid 1-butyl-3-methylpyridinium chloride for voltammetric determination of UV filter avobenzone

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The applicability of carbon paste electrode (CPE) bulk modified by pyridinium ionic liquid (IL) such as 1-butyl-3-methylpyridinium chloride (N-C₄-3MPyCl) for voltammetric determination of avobenzone UV filter (AVO) was investigated. Direct anodic square wave voltammetry was applied and various experimental parameters were optimized including the pH of the supporting electrolyte and the amount of IL modifier in the CPE. For analytical purposes, Britton-Robinson buffer pH 11.98 and 3.3 wt% of IL modifier was optimal. The modification of CPE by N-C₄-3MPyCl provides 2 times more intensive AVO oxidation signal compared to an unmodified CPE. The linearity of calibration curve was obtained in the range from 0.10 to 3.85 µg mL⁻¹ of AVO at N-C₄-3MPyCl-CPE. The evaluated limit of detection was 0.03 µg mL⁻¹ AVO and relative standard deviation did not exceed 3.6%.

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AH-P-2

Sadržaj ukupnih polifenola, flavonoida i derivata dihidroksicimetne kiseline u rizomu i vegetativnom delu biljke *Corydalis ochroleuca*

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Ispitivanje fitohemijskog sastava biljaka i određivanje sadržaja odabranih sekundarnih metabolita u njima predstavlja i dalje veoma aktuelnu oblast istraživanja. U okviru ovog rada izvršeno je ispitivanje sadržaja odabranih sekundarnih metabolita u rizomu i nadzemnom vegetativnom delu biljke *Corydalis ochroleuca*. Biljni materijal je sakupljen u kanjonu reke Dervente (Srbija). Ekstrakcija (1,5 g) je izvršena pomoću 80% metanola (15 mL) u trajanju od 3h, a dobijeni ekstrakti su čuvani na hladnom i tamnom mestu. Sadržaj ukupnih polifenola (TPC), flavonoida (TFC) i derivata dihidroksicimetne kiseline (THD) je utvrđen standardnim spektrofotometrijskim metodama i izražen kao mg/g ekvivalenata galne kiseline (GAE), kvercetina (QE) i hlorogenske kiseline (CGAE) na suhu masu uzorka. Utvrđeno je da nadzemni deo biljke sadrži više bioaktivnih jedinjenja (3,45 mg/g GAE; 1,18 mg/g QE; 1,50 mg/g CGAE) u odnosu na rizom biljke (2,54 mg/g GAE; 0,28 mg/g QE; 1,28 mg/g CGAE). Na osnovu dobijenih rezultata može se reći da je nadzemni vegetativni deo biljke *C. ochroleuca* bolji izvor odabranih sekundarnih metabolita u odnosu na rizom.

The content of total phenolics, flavonoids and dihydroxycinnamic acid derivatives in rhizome and vegetative parts of *Corydalis ochroleuca*

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Phytochemical analysis with determination of the content of secondary plant metabolites is still very popular research topic. The aim of present study was to determine the content of selected bioactive compounds in rhizome and aerial vegetative parts of the plant *Corydalis ochroleuca*. Plant material was collected in Derventa river canyon (Serbia). Extraction (1.5 g) was performed with 80% methanol (15 mL) as solvent for 3 h. Extracts were stored at cold and dark place until further analysis. The content of total phenolics (TPC), flavonoids (TFC), and hydroxycinnamic acid derivatives (THD) was determined via standard spectrophotometric methods and expressed as mg/g per dry weights of galic acid (GAE), quercetin (QE) and chlorogenic acid (CGAE) equivalents, respectively. It was observed that TPC, TFC and THD values were higher in vegetative part (3.45 mg/g GAE; 1.18 mg/g QE; 1.50 mg/g CGAE) compared to rhizome (2.54 mg/g GAE; 0.28 mg/g QE; 1.28 mg/g CGAE). It can be concluded that aerial vegetative parts of *C. ochroleuca* are better source of secondary metabolites compared to rhizome.

AH-P-3

pH-Zavisna rastvorljivost nortriptilin-hidrohlorida

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Rastvorljivost je značajno fizičko-hemijsko svojstvo biološki aktivnih i potencijalno biološki aktivnih supstancija, koje određuje stabilnost, biodostupnost i terapeutsko dejstvo leka. Cilj ovog rada je ispitivanje rastvorljivosti nortriptilin-hidrohlorida, pomoću pH-Ramp *Shake-Flask* metode, prethodno primenjene na desipramin-hidrohlorid [1]. Eksperimenti su izvedeni prema novim preporukama iz literature [2]. Rastvorljivost je određena u fosfatnom puferu, u sistemu bez hlorida i sistemu bez fosfata, koristeći nortriptilin bazu i nortriptilin-hidrohlorid. Urađena je i katakterizacija čvrste faze pomoću elementalne analize, termogravimetrije, diferencijalne skenirajuće kalorimetrije i difrakcije X-zraka.

pH-Dependent solubility profile of nortriptyline hydrochloride

Olivera S. Marković, Nemanja Ž. Marjanović*, Nirali Patel**, Abu T. M. Serajuddin**, Alex Avdeef***, Tatjana Ž. Verbić*

Solubility is important physicochemical parameter and determines drug stability, bioavailability and therapeutic action. The aim of this study was to examine solubility of nortriptyline hydrochloride in a wide pH range, using pH-Ramp *Shake-Flask* method, already applied to desipramine hydrochloride [1] and based of recently published recommendations [2]. Solubility was measured in phosphate buffer, in chloride-free media and phoshate-free media, using both nortriptyline base and nortriptyline hydrochloride as starting material. Elemental analysis, termogravimetric analysis, differential scanning calorimetric analysis and powder X-ray diffraction analysis were used for solid precipitate analysis.

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AH-P-4

Imobilizacija govedeg serum albumina na silika gelu i primena u ekstrakciji čvrstom fazom

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Goveđi serum albumin (BSA), jeftin, dostupan i stabilan protein, imobilizovan na različitim nosačima se koristi i kao stacionarna faza u hromatografiji za hiralno razdvajanje i u ekstrakciji čvrstom fazom.¹ U ovom radu sintetisano je nekoliko modifikacija silika gela različite poroznosti sa imobilizovanim BSA i ispitano je vezivanje model molekula – progesterona i desipramin-hidrohlorida za dobijene sorbente pri različitim pH vrednostima (4,5; 6,0 i 7,4). Sorbenti su okarakterisani elementalnom analizom i infracrvenom spektroskopijom. Rezultati pokazuju da se desipramin-hidrohlid najbolje vezuje na pH 4,5, dok je vezivanje progesterona najbolje na pH 7,4. Dobijeni sorbenti primenjeni su u ekstrakciji progesterona čvrstom fazom, pri čemu je rastvor progesterona koncentracije 0,2 μM uspešno koncentrovan 25 puta sa prinosom metode od 100%.

Zahvalnica: Ovaj rad je finansiran sredstvima koje je obezbedilo Ministarstvo prosvete, nauke i tehnološkog razvoja – evidencioni broj 451-03-9/2021-14/200168.

Bovine serum albumin immobilization on silica gel and application in solid phase extraction

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BSA is a cheap, easily available and stable protein. When immobilized on different carriers, it can be used as a stationary phase in chiral chromatography and solid-phase extraction.¹ Several BSA-silica gel modifications of different porosity were prepared within this study and binding of two model molecules – progesterone and desipramine hydrochloride was examined at different pH values (4.5; 6.0 and 7.4). Sorbents were characterized using elemental microanalysis and infrared spectroscopy. Results show that desipramine hydrochloride binds best at pH 4.5, while progesterone binds best at pH 7.4. Prepared sorbents were applied as progesterone solid-phase extraction sorbents. The results show that progesterone solution can be concentrated up to 25 times with 100% recovery.

Literatura: 1. S. Andresson, S. Allenmark, *Journal of Chromatography A*, **498** (1990) 81-91

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AH-P-5

Optimizacija uslova za degradaciju ibuprofena pomoću hlor – dioksida

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Ibuprofen (IBP) zbog svoje široke primene, velike konzumacije, relativno brzog metabolizma i eliminacije iz organizma, predstavlja potencionalni rizik po životnu sredinu.. Hlor - dioksid, kao jako oksidaciono sredstvo, pokazao se kao dobar reagens za uklanjanje određenih grupa pesticida iz hrane i vode, kao i za degradaciju određenih lekova. Cilj ovog rada bio je da se ispita pod kojim uslovima i u kojoj meri hlor - dioksid može da ukloni IBP u vodi. Ispitivana je degradacija IBP različitih koncentracija (10, 20, 35 i 60 mg/L) sa različitim koncentracijama hlor - dioksida (5, 10 i 15 mg/L) na pH vrednostima 3,00, 7,00 i 10,00 i pri različitim reakcionim vremenima (0,5 h, 1 h, 2 h, 3 h, 6 h, 24 h). Rezultati HPLC - DAD analize su pokazali da je IBP moguće efikasno ukloniti iz vode. Najveća efikasnost degradacije od 99% postignuta je kada je koncentracija IBP u vodi bila 10 mg/L, a rastvor je bio tretiran sa 15 mg/L hlor - dioksida na pH 10,00 posle 24 h tretiranja hlor - dioksidom.

Optimization of conditions for degradation of ibuprofen using chlorine dioxide

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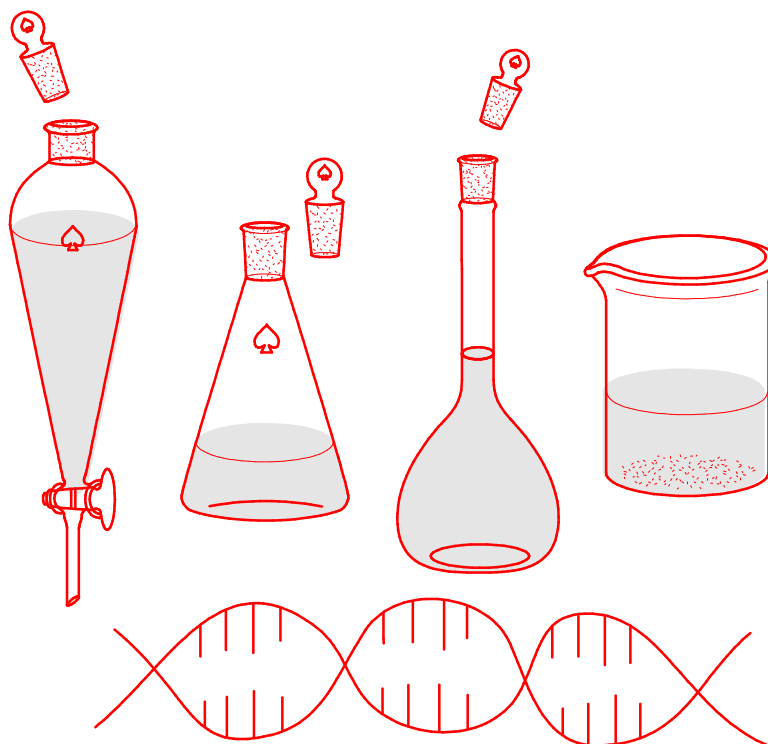
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Due to ibuprofen (IBP) wide application, high consumption, relatively fast metabolism and elimination from the organism, it represents a potential risk to the environment. Chlorine dioxide, as a strong oxidizing agent, has been shown to be a good reagent for removing certain groups of pesticides from food and water, as well as for degrading certain drugs. The aim of this study was to find optimal conditions for IBP removal from water using chlorine dioxide. Degradation of IBP of different concentrations (10, 20, 35 and 60 mg / L) with different concentrations of chlorine dioxide (5, 10 and 15 mg / L) at pH values of 3.00, 7.00 and 10.00 and at different reaction times (0.5 h, 1 h, 2 h, 3 h, 6 h, 24 h), was investigated. The results of HPLC - DAD analysis showed that IBP can be effectively removed from water. The highest degradation efficiency of 99% was achieved when the concentration of IBP in water was 10 mg / L, and the solution was treated with 15 mg / L of chlorine dioxide at pH 10.00 after 24 h of chlorine dioxide treatment.

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Fizička hemija

Physical Chemistry



FH-P-1

LIBS kao obećavajući alat za brzu elementnu analizu humanih zuba

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U ovom radu je ispitivana mogućnost upotrebe originalne LIBS (spektroskopija laserski indukovane plazma) laboratorijske postavke za elementnu analizu tkiva humanih zuba. U ovoj studiji su korišćeni različiti uzorci zuba, zdravi i stomatoloski tretirani. Plazma je indukovana na vazduhu na atmosferskom pritisku. Dobijeni su optički emisijski spektri sa veoma oštrim linijama i zanemarljivom pozadinom. Identifikacija linija pokazala je prisustvo različitih elemenata u zubnim tkivima. Takođe, proučavan je elementni sastav materijala za ispune zuba i posmatrana je mogućnost difuzije teških metala iz ispuna u zdrava tkiva zuba. Pored toga, optička mikroskopija i profilometrijska analiza su pokazale da je primenjena LIBS metoda skoro nedestruktivna za zube. Ovi preliminarni rezultati vode do zaključka da ovaj alternativni i ekonomični LIBS sistem može naći svoju primenu kao korisni alat u daljnjim istraživanjima vezanim za primenu laserski indukovane plazme u stomatologiji.

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LIBS as a promising tool for fast elemental analysis of human teeth

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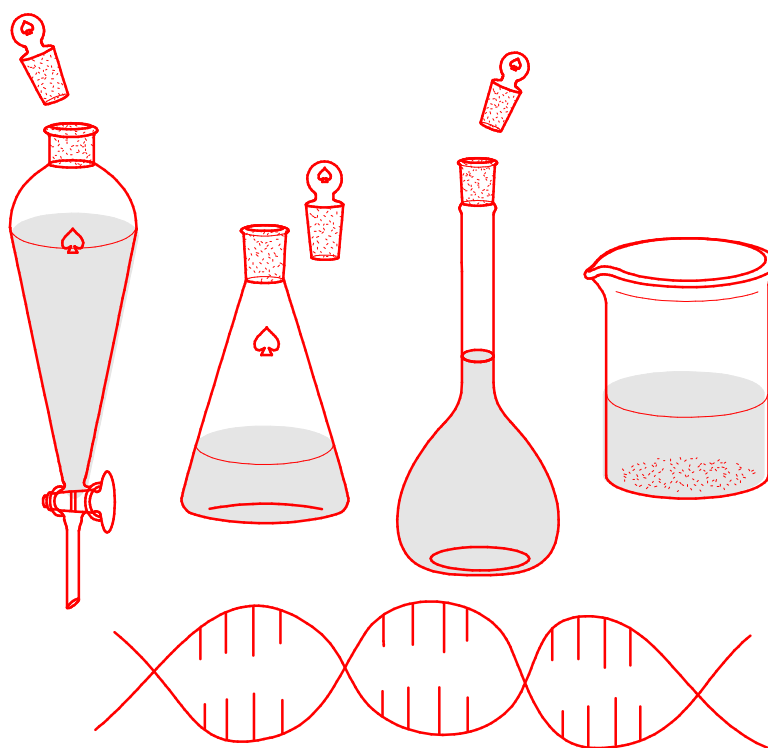
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This work assesses the capabilities of the original LIBS (Laser Induced Breakdown Spectroscopy) laboratory setup for elemental analysis of human teeth tissues. Different tooth samples, healthy and restored, were used in this study. The plasma was induced in air at atmospheric pressure. The optical emission spectra with sharp and well resolved spectral lines and negligibly low background were obtained. The results of the elemental analysis show the presence of different trace elements in teeth tissues. Also, the elemental analysis of teeth filling materials and the possibility of heavy metals diffusion into the healthy tissues of the tooth has been studied. Additionally, optical microscopy and profilometer measurements showed that the applied LIBS method is almost nondestructive for teeth. These preliminary results led to the conclusion that this alternative and cost-effective LIBS system can find applications as a useful tool for further explorations of laser-induced plasma in dentistry.

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Elektrohemija

Electrochemistry



EH-P-1

Brzina korozije cevi od nerđajućih čelika izračunata pomoću elektrohemijske frekvencione modulacije

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Nerđajući čelici su omiljeni materijali u nuklearnoj medicini zbog jednostavnog održavanja (brisanje, dekontaminacija, itd.). Otpornost na rđanje ovih materijala je smanjena usled istovremenog delovanja hloridnih jona i jonizujućeg zračenja. Brza i nedestruktivna tehnika merenja korozije, kao što je elektrohemijska frekvenciona modulacija (EFM), korisna je za brzu procenu materijala koji moraju biti otporni na rđanje. Tri različite cevi od nerđajućeg čelika su analizirane pomoću EFM metode i izračunate su njihove brzine korozije. Uzorak označen kao S II, koji ne sadrži Mo u svom sastavu pokazuje veću brzinu korozije u odnosu na uzorke koji sadrže Mo ako je istovremeno izložen hloridnim jonima i gama zračenju. Ovaj rezultat je u sagalsnosti sa sastavom nerđajućeg čelika dobijenim rentgenskim fluorescentnim spektrometrom koji pokazuje nedostatak bakra i vanadjuma u tragovima, uključujući molibden.

Corrosion Rate of Stainless Steel Tubes Calculated by Electrochemical Frequency Modulation

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Stainless steels (SS) are favored materials in nuclear medicine due to their easy maintenance (wiping, decontamination, etc). Rust resistance of these materials is reduced due to the simultaneous action of chloride ions and ionizing radiation. A fast and nondestructive corrosion-measurement technique such as Electrochemical Frequency Modulation (EFM) is useful for quick assessment of materials that need to be resistant to rust. Three different tubes of SS were analyzed using EFM technique and their corrosion rates were calculated. The sample labelled as S II, which does not contain Mo in its composition, shows an increase in corrosion rate than others if it is simultaneously exposed to chloride ions and gamma radiation. This result coincides with the SS composition obtained by X-ray fluorescence spectrometer which shows the lack of copper and vanadium besides molybdenum.

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EH-P-2

Uticaj prisustva vode na koroziju Mg u etalinu

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Etalin je komercijalni naziv za eutektičku smešu etilen glikola i holin hlorida koja nalazi različite primene. Neminovno je da će u industrijskoj primeni, različiti materijali biti u kontaktu sa etalinom i stoga je važno poznavati njegovu korozivnost. Međutim, po našem mišljenju, još je važnije poznavati korozivnost smeša vode i etalina. Naime, etalin je izuzetno higroskopna smeša: prema našim merenjima, kada je izložen vlažnom vazduhu, tokom 24 h može apsorbovati više od 50 mas.% vlage.

U ovom radu merena je brzina korozije magnezijuma visoke čistoće, u osušenom etalinu i smešama sa različitim odnosima etalin:voda. Kao tehnika za merenje primenjena je spektroskopija elektrohemijske impedancije. Rezultati su pokazali da u celom opsegu odnosa sadržaja etalina i vode u smeši (od 0 do 100% vode), važi jedno pravilo: korozija je brža sa većim sadržajem vode.

Water influence on Mg corrosion in ethaline

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Ethaline is the commercial name for an eutectic mixture of ethylene glycol and choline chloride with the applications in various fields. It is inevitable that various materials will be in contact with ethaline in industrial applications, and therefore, it is important to know its corrosivity. However, in our opinion, it may be even more important to know the corrosivity of a mixture of water and ethaline. Namely, ethaline is an extremely hygroscopic mixture: it can absorb more than 50 mass. % of water during 24h.

In this paper, the corrosion rate of high purity magnesium was measured in dried ethaline as well as in mixtures with different etalin: water ratios. Electrochemical impedance spectroscopy was used as the measurement technique. The results showed that for the whole range of the ratio of ethaline and water (from 0 to 100% water), one rule applies: the corrosion rate is higher with higher water content in the mixture.

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EH-P-3

Aminokiseline kao zeleni inhibitori korozije AA2024-T42 legure

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Aluminijum ima ogromni ekonomski, tehnološki i industrijski značaj. Njegova velika reaktivnost dovodi do formiranja prirodne zaštite od korozije, odnosno do obrazovanja tankog, zaštitnog, oksidnog filma (Al_2O_3) koji delimično štiti metal od agresivne okolne sredine. Joni hlorida dovode do razaranja oksidnog filma i izazivaju lokalnu koroziju. Prisustvo aminokiselina u panorami zelenih inhibitora korozije opravdava njihova struktura u kojoj se nalaze karboksilna i amino grupa koje su vezane za isti ugljenikov atom. Pored ove dvije funkcionalne grupe za ugljenikov atom mogu biti vezane i mnoge druge koje se razlikuju po hemijskim svojstvima, obliku i veličini.

U radu će spektroskopijom elektrohemijske impedancije biti ispitivano zaštitno dejstvo različitih aminokiselina na leguri aluminijuma AA2024-T42 u rastvoru NaCl različitih koncentracija. Aminokiseline čije će se inhibitorsko dejstvo ispitivati su glicin, glutamin, triptofan, asparaginska kiselina i arginin. Takođe, ispitaće se dejstvo dipeptida aminokiseline glicin.

Amino acids as green corrosion inhibitors for AA2024-T42 alloy

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Aluminum has enormous economic, technological and industrial value. Its high reactivity leads to the formation of natural corrosion protection, ie to the formation of a thin, protective, oxide film (Al_2O_3) which provides temporary protection to the metal from the aggressive environment. Chloride ions lead to the destruction of the oxide film and cause local corrosion. The presence of amino acids in the panorama of green corrosion inhibitors is justified by their structure, composed of carboxyl and amino groups that are attached to the same carbon atom. The other carbon ligands are -H and R-group of different chemical properties, shape, and size.

The protective effect of different amino acids on aluminum alloy AA2024-T42 in NaCl solution of different concentrations will be examined by electrochemical impedance spectroscopy. Amino acids whose inhibitory effect will be tested are glycine, glutamine, tryptophan, aspartic acid and arginine. In addition, the effect of the amino acid dipeptide glycine will be examined.

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EH-P-4

Primena senzora na bazi modifikovane ugljenične paste za određivanje riboflavina

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Riboflavin (vitamin B₂) pripada grupi vitamina B, i predstavlja prekursor flavinskih koenzima: flavin adenin mononukleotida i dinukleotida, koji katalizuju brojne hemijske reakcije, i ključni su za stvaranje energije. Klinička slika nedostatka riboflavina uključuje dermatitis, anemiju i disfunkciju mozga. Analiza ovog vitamina često je ograničena na metode koje podrazumevaju dugotrajnu pripremu uzoraka i skupu instrumentaciju. Uzimajući u obzir elektroaktivnost molekula riboflavina, elektroanaliza može služiti kao alternativna metodologija uz brojne prednosti.

U ovom radu opisani su preliminarni rezultati uz upotrebu modifikovane elektrode od ugljenične paste u cilju određivanja riboflavina primenom voltametrijе sa pravougaonim talasom. Kao modifikator korišćene su funkcionalizovane višeslojne ugljenične nanocevi uz primenu gvožđa, pripremljene u laboratoriji. Voltamogrami su snimani u pozitivnom i negativnom rasponu potencijala u acetatnom puferu pH 4, pri čemu su dobijeni oksidacioni i redukcionni pikovi. Za određivanje riboflavina odabran je oksidacioni pik koji je bio nešto većeg intenziteta. U poređenju sa elektrodom od ugljenične paste, modifikovana elektroda pokazala je znatno bolje performanse u smislu osetljivosti određivanja, te poseduje značajan potencijal za voltametrijsko određivanje riboflavina.

Application of the sensor based on modified carbon paste electrode as an electroanalytical approach for riboflavin determination

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Riboflavin (vitamin B₂) belongs to the group of vitamin B and is the precursor of the flavin coenzymes: flavin adenine mononucleotide and dinucleotide, which catalyze numerous redox reactions, and are crucial for energy production. The clinical features of riboflavin deficiency include dermatitis, anemia and brain dysfunction. Analysis of this vitamin is often limited to methods that involve tedious sample preparation and expensive instrumentation. Considering the electro-activity of riboflavin molecule, electroanalysis serves as an attractive alternative methodology with numerous benefits.

This paper describes the preliminary results of the use of modified carbon paste electrode for determination of riboflavin using square-wave voltammetry. As the modifier laboratory made functionalized multi-walled carbon nanotubes supported with iron were used. Voltammograms were recorded in the positive and negative potential range in the acetate buffer pH 4, whereby oxidation and reduction peaks were obtained. An oxidation peak of slightly higher intensity was selected for the analysis of riboflavin. Compared to the carbon paste electrode, the modified electrode showed significantly better performance in terms of sensitivity, and thus possesses significant potential for voltammetric determination of riboflavin.

EH-P-5

Poređenje elektrohemijskog ponašanja folne kiseline na različitim elektrohemijskim senzorima

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Dnevna suplementacija folnom kiselinom izuzetno je važna tokom rane trudnoće jer znatno smanjuje rizik oštećenja nerne cevi kod novorođenčadi, dok je nedostatak ovog vitamina povezan sa pojedinim bolestima. U ovom radu predstavljena je voltametrijska studija za određivanje folne kiseline, a poređene su performanse različitih radnih elektroda. Studija uključuje primenu elektrode od staklastog ugljenika (GCE) i borom dopovane dijamantska elektrode (BDDE). Kao voltametrijske tehnike korišćene su ciklična voltametrija i voltametrija sa pravougaonim talasom. Potencijal je skeniran u anodnom opsegu od +0,4 V do +1,2 V u Briton-Robinsonovom puferu pH 6,0 kao pomoćnom elektrolitu. Folna kiselina pokazala je slično elektrohemijsko ponašanje primenom obe elektrode, uz dobro definisan oksidacioni pik na +0,87 V i +0,89 V na GCE i BDDE redom. Skeniranjem potencijala u obrnutom smeru ne javlja se katodni pik, što ukazuje na ireverzibilnu oksidaciju vitamina. Poređenjem radnih elektroda korišćenih u ovoj studiji u smislu osetljivosti i opsega linearanosti (1–50 μM), bolje performanse uočene su u slučaju BDDE. Dalji eksperimenti su usmereni ka razvoju analitičke metodologije u cilju određivanje sadržaja folne kiseline u farmaceutskim preparatima.

Comparison of electrochemical behavior of folic acid on different electrochemical sensors

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Daily supplementation of folic acid during early pregnancy is extremely important because it significantly reduces the risk of neural tube defects in newborns, while deficiency of this vitamin is associated to some diseases. In this paper a voltammetric study for the determination of folic acid is presented, and the performances of different working electrodes are compared. The study included the use of glassy carbon electrode (GCE), and boron-doped diamond electrode (BDDE). Cyclic voltammetry and square-wave voltammetry are used as voltammetric techniques. The potential is scanned in the anodic range from +0.4 V to +1.2 V in Britton-Robinson buffer pH 6.0 as the supporting electrolyte. Folic acid demonstrated similar behavior on both studied working electrodes, with one well defined oxidation peak at +0.87 V and +0.89 V using GCE and BDDE as a working electrode, respectively. No cathodic peak is seen in the reverse scan, indicating on the irreversible oxidation of the vitamin. By comparing the working electrodes used in this study in terms of sensitivity and linearity range (1–50 μM), better performance is observed in the case of BDDE. Further studies are directed on development of analytical methodology toward determination of folic acid content in pharmaceuticals.

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EH-P-6

Određivanje elektrohemijski aktivne površine nikal-oksi-hidroksida

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Filmovi Ni-oksi-hidroksida (NiO_xH_y) na niklenoj mrežici su elektrohemijski formirani u rastvoru 0,1 M KOH koristeći voltametrijski protokol sa različitim brojem ciklusa i različitim granicama potencijala. Dobijeni filmovi NiO_xH_y su se razlikovali po stepenu hidratacije i debljini. Karakteristike početnog oksidnog filma i taloženih NiO_xH_y filmova, kao što su količina elektrohemijski aktivnih mesta unutar Ni-oksida, kapacitivnost dvojnog sloja i adsorpciona pseudokapacitivnost intermedijara reakcije izdvajanja kiseonika ispitivani su cikličnom voltametrijom i spektroskopijom elektrohemijske impedancije. Iz linearne zavisnosti kapacitivnosti dvojnog sloja od debljine filma izračunate su vrednosti specifičnih kapacitivnosti i dobijene su veće vrednosti za hidratizane u odnosu na anhidrovane NiO_xH_y filmove. Dobijena je jedinstvena linearna zavisnost adsorpcione pseudokapacitivnosti intermedijara u reakciji izdvajanja kiseonika od količine naelektrisanja koja utrošena za oksidaciju $\text{Ni}(\text{OH})_2$. Na osnovu dobijenih specifičnih kapacitivnosti i adsorpcione pseudokapacitivnosti moguće je određivanje elektrohemijski aktivne površine NiO_xH_y filmova sa različitim stepenom hidratacije, koja je neophodna za procenu stvarne katalitičke aktivnosti za reakciju izdvajanja kiseonika.

Estimation of the electrochemically active surface area of nickel-oxy-hydroxides

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Ni-oxy-hydroxides films (NiO_xH_y) were electrochemically deposited on nickel gauze electrode in 0.1 M KOH solution using a potential cycling protocol with variation of cycle number and potential limits. The prepared NiO_xH_y films varied in hydration degree and the thickness. Characteristics of incipient and deposited NiO_xH_y films, such as an amount of Ni-active oxide species, a double-layer capacitance and the pseudo-adsorption capacitance of the oxygen evolution reaction (OER) intermediates were examined by cycling voltammetry and electrochemical impedance spectroscopy. From a linear correlation of the double-layer capacitances and the film thickness, the specific capacitances were calculated and it was found to be higher for hydrous than for anhydrous NiO_xH_y films. A unique linear correlation between the adsorption pseudocapacitance of OER intermediates and the charge for the oxidation of $\text{Ni}(\text{OH})_2$. Based on the determined specific capacitances and adsorption pseudocapacitance it is possible to estimate the electrochemically active surface area of NiO_xH_y films with initially different degrees of hydration, which is necessary for the insight in their intrinsic activity for OER.

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EH-P-7

Elektrohemijska sinteza nanočestica srebra u hidrogelovima polivinil-alkohola i alginata

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Hidrogelovi su se pokazali kao odlični materijali za obloge za rane. Inkorporisanjem nanočestica srebra unutar hidrogelova dobijaju se materijali sa antibakterijskim svojstvima i sa mogućnošću kontrolisanog otpuštanja srebra, a izbegava se dugotrajno korišćenje antibiotika koje dovodi do bakterijske rezistencije. U ovom radu sintetisani su hidrogelovi polivinil-alkohola i alginata sa nanočesticama srebra sintetisanim elektrohemijskom redukcijom. UV-vidljivom sprektroskopijom je potvrđeno prisustvo nanočestica srebra. Antibakterijska aktivnost hidrogelova određena je agar-difuzionim testom prema sojevima bakterija *S. aureus* TL i *E. coli* ATCC25922, a citotoksičnost je ispitana MTT i DET testovima prema dve ćelijske linije fibroblasta – MRC-5 (humani) i L929 (mišji). Otpuštanje srebra praćeno je 28 dana u fosfatnom puferu na 37°C (uslovi koji simuliraju fiziološku sredinu), a koncentracija otpuštenog srebra je određena atomskom apsorpcionom spektroskopijom. Dobijeni rezultati su ukazali na dobra antibakterijska svojstva sintetisanih hidrogelova, koji se mogu smatrati pogodnim materijalima za obloge za rane.

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Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol) and alginate hydrogels

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Hydrogels have been proven to be excellent wound dressing materials. By incorporating silver nanoparticles (AgNPs) within their matrix, materials with antibacterial properties and the possibility of controlled silver release are obtained, and long-term use of antibiotics that leads to bacterial resistance is avoided. In this work, poly(vinyl alcohol) and alginate hydrogels were synthesized with electrochemically embedded AgNPs. The presence of AgNPs was confirmed using UV-visible spectroscopy. The antibacterial activity of the hydrogels was determined by agar-diffusion test against *S. aureus* TL and *E. coli* ATCC25922 strains. Cytotoxicity was tested by MTT and DET tests using mouse L929 fibroblasts and human MRC-5 fibroblast cell lines. Silver release was monitored during 28 days in phosphate buffer at 37 °C (mimicking physiological environment), while the released silver concentration was determined by atomic absorption spectroscopy. The obtained results indicated good antibacterial properties of the synthesized hydrogels, so they can be considered suitable materials for wound dressing application.

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EH-P-8

Optimizacija elektrohemijske sinteze nanočestica srebra u polivinil-alkohol/hitozan hidrogelovima pomoću eksperimentalnih i simuliranih UV-vidljivih spektara

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Hidrogelovi su biokompatibilni netoksični materijali koji imaju sposobnost apsorpcije tečnosti i kontrolisanog otpuštanja imobilisanih aktivnih agenasa, te nalaze široku primenu u medicini, uključujući i obloge za saniranje rana. U cilju poboljšanja antibakterijskog dejstva, vrši se inkorporacija različitih lekova i antibakterijskih agenasa unutar hidrogelnih materijala, a jedan od najčešćih agenasa su nanočestice srebra. U ovom radu, izvršena je sinteza hidrogelova polivinil-alkohola i hitozana sa i bez grafena. Inkorporacija nanočestica srebra odgovarajućih dimenzija i sa jakim antibakterijskim efektom, ostvarena je metodom elektrohemijske sinteze pri konstantnom naponu, koja ujedno ne zahteva korišćenje toksičnih hemijskih agenasa. Optimizacija uslova elektrohemijske sinteze nanočestica srebra unutar dobijenih hidrogelova izvršena je variranjem primenjenog napona, dok je prisustvo nanočestica srebra potvrđeno UV-vidljivom spektroskopijom. Izvršena je i simulacija teorijskih UV-vidljivih spektara nanočestica srebra pomoću programa MiePlot, kako bi se, na osnovu poređenja eksperimentalnih i teorijskih spektara, procenile dimenzije nanočestica srebra u zavisnosti od primenjivanog napona.

Optimization of electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)/chitosan hydrogels using experimental and simulated UV-visible spectra

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Hydrogels are biocompatible non-toxic materials with the capability for absorption of liquids and controlled release of immobilized active agents, which is why they have broad application in medicine, including wound dressing. To improve antibacterial activity, different drugs and antibacterial agents are incorporated in hydrogel materials, and one of the frequently used agents are silver nanoparticles (AgNPs). In this work, poly(vinyl alcohol) and chitosan hydrogels have been synthesized with or without graphene. To achieve the incorporation of AgNPs with defined particle size and strong antibacterial effect, a constant-voltage electrochemical synthesis method was applied, without using toxic chemical agents. Optimization of parameters for the electrochemical synthesis of AgNPs within the obtained hydrogels was performed by variation of applied voltage, while the presence of AgNPs was confirmed by UV-visible spectroscopy. Simulation of theoretical UV-visible spectra of silver nanoparticles was done using MiePlot software, to estimate the dependence of silver nanoparticles dimensions on the applied voltage.

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EH-P-9

Bioaktivne kompozitne prevlake na titanu koje otpuštaju gentamicin

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Trenutni trendovi u nauci o biomaterijalima favorizuju dizajniranje multifunkcionalnih prevlaka za implantate koji služe kao nosači antibakterijskih sredstava sa primarnom namerom da inhibiraju rast bakterija na površini kontakta implantata i tkiva, a da istovremeno promovišu osteointegraciju. Elektroforetskim taloženjem (EPD) u jednom koraku pri konstantnom naponu, uspešno je dobijena kompozitna prevlaka na bazi hidroksiapatita (HAP), hitozana (CS) i gentamicina (Gent) iz vodene suspenzije na titanu. Kinetika otpuštanja leka ispitivana je u dejonizovanoj vodi na 37 °C tečnom hromatografijom visokih performansi u kombinaciji sa masenom spektrometrijom. Sposobnost osteointegracije dalje je potvrđena merenjem aktivnosti alkalne fosfataze (ALP), što ukazuje na povoljne osteopromotivne osobine taloženih prevlaka. Kada su testirane na humane i mišje fibroblastne ćelijske linije (MRC-5 i L929), kompozitna prevlaka pokazala je necitotoksični efekat. HAP/CS/Gent prevlaka je pokazala dobru antibakterijsku aktivnost prema *Staphylococcus aureus* i *Escherichia coli*, što ukazuje na visok potencijal za biomedicinske primene.

Bioactive Gentamicin-Eluting Composite Coatings on Titanium

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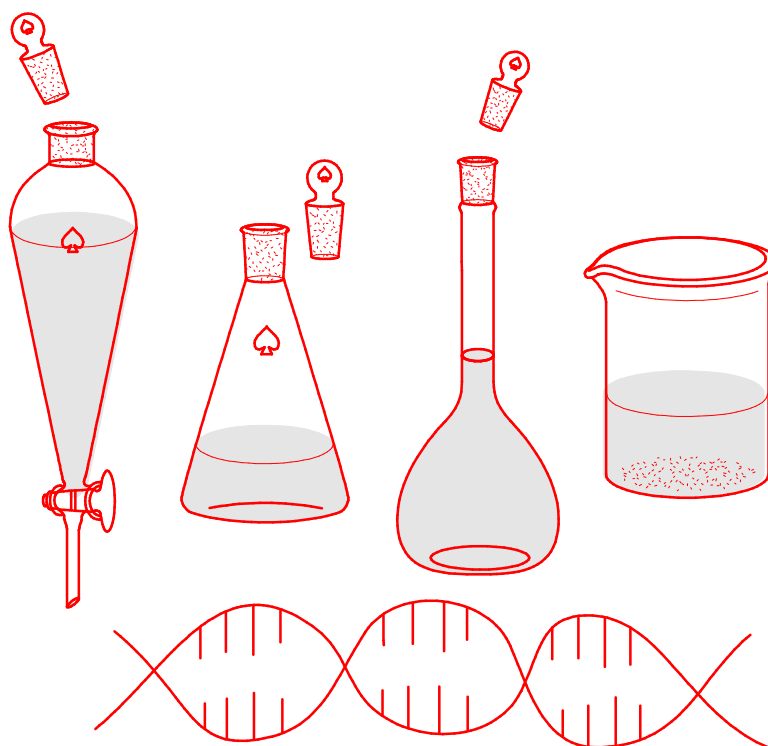
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Current trends in biomaterials science favor designing multifunctional implant coatings that serve as carriers of antibacterial agents with the primary intention of inhibiting bacterial growth on the implant-tissue interface, while still promoting osseointegration. Electrophoretic deposition (EPD) in a single step at the constant voltage was successfully used to obtain composite coating based on hydroxyapatite (HAP), chitosan (CS) and gentamicin (Gent) from an aqueous suspension on titanium. Drug-release kinetics was investigated in deionized water at 37 °C by liquid chromatography coupled with mass spectrometry. The osseointegration ability was further validated by measuring the alkaline phosphatase activity (ALP) indicating the favorable osseopromotive properties of deposited coatings. When tested against human and mice fibroblast cells lines (MRC-5 and L929), composite coatings showed a noncytotoxic effect. HAP/CS/Gent coating exhibited good antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*, indicating the high potential for biomedical applications.

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Hemijsko inženjerstvo

Chemical Engineering



HI-P-1

Termodinamička svojstva i modelovanje međumolekulske interakcije dvokomponentne smeše limonena i hloroforma

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U cilju proučavanja termodinamičkih svojstava binarne smeše limonen + hloroform eksperimentalno su određene gustine (ρ), viskoznosti (η) i indeksi refrakcije (n_D) za ovu smešu. Eksperimentalna merenja su rađena u opsegu temperatura od 288,15 do 323,15 K na atmosferskom pritisku, za ceo opseg udela. Na osnovu eksperimentalno dobijenih rezultata izračunate su vrednosti dopunske molarne zapremine V^E , vrednosti promene viskoznosti $\Delta\eta$ i vrednosti promene indeksa refrakcije Δn_D . Za izvedene vrednosti rezultati su dobijeni fitovanjem Redlich-Kister polinomskom jednačinom. Na osnovu ovih rezultata izvedeni su zaključci o međumolekulskim interakcijama u limonen + hloroform binarnom sistemu. Vrednosti dopunske molarne zapremine, kao i vrednosti promene viskoznosti i indeksa refrakcije pokazuju pozitivno odstupanje u celom opsegu molskih udela. Povećanje dopunske molarne zapremine pokazuje da je pakovanje molekula u smeši manje efikasno nego u čistim komponentama.

Thermodynamic properties and modeling intermolecular interaction of binary mixture of limonene and chloroform

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In order to study the thermodynamic properties of the binary mixture limonene + chloroform, the densities (ρ), viscosities (η) and refractive indices (n_D) for this mixture were experimentally determined. Experimental measurements were performed in the temperature range from 288.15 K to 323.15 K at atmospheric pressure, for the entire range of composition. Based on the experimental results, the values of excess molar volume V^E , the viscosity deviation $\Delta\eta$ and the refractive index deviation Δn_D were calculated. Additionally, the excess molar volume and viscosity and refractive index deviations were fitted with the Redlich-Kister polynomial equation. Based on these results, conclusions can be made on intermolecular interactions in the limonene + chloroform binary system. Values of excess molar volume, viscosity and refractive index deviations have shown a positive non-ideal behavior in the entire composition range. An increase in the values of excess molar volume indicates that the packaging of the molecules in the mixture is less efficient than in the pure components.

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HI-U-2

Eksperimentalno određivanje gustina linalola, alfa-pinena i beta-pinena na visokom pritisku

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U cilju smanjenja zagađenja na globalnom nivou poslednjih godina aktuelna je tema zamene fosilnih goriva nekim novim biogorivima. Terpeni, koji su sastavni delovi biljaka, mogu se koristiti u ove svrhe kao dodatak standardnim gorivima. Neke od termodinamičkih svojstva pod uslovima visokog pritiska i određenih temperatura su od velike važnosti za efikasnost motora. U ovom radu su dobijene gustine linalola, alfa-pinena i beta-pinena u temperaturnom intervalu 293,15-413,15 K i na pritiscima do 60 MPa. Na osnovu ovih rezultata utvrđeno je da s porastom temperature pri konstantnom pritisku gustina navedenih terpena opada, dok sa povećanjem pritiska pri konstantnoj temperaturi gustina raste.

Experimental determination of linalool, α -pinene and β -pinene densities at high pressure

Zoran Simić, Nikola Grozdanic, Ksenija Miletić, Mirjana Kijevčanin, Ivona Radović

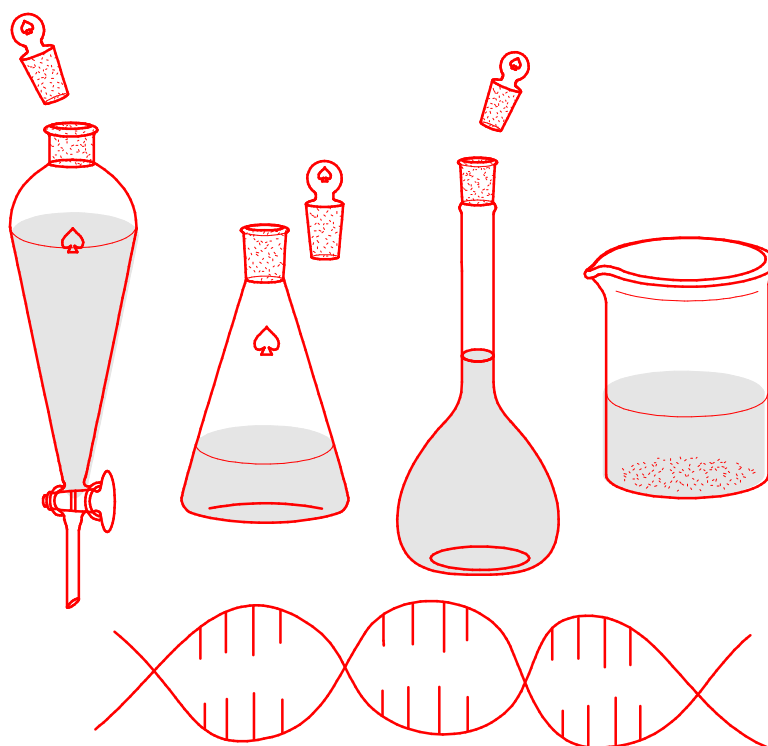
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In order to reduce pollution at the global level in recent years, the main topic is replacing fossil fuels with some new biofuels. Terpenes, which are integral parts of plants, can be used for these purposes as an addition to standard petroelum fuels. Some of thermodynamic properties under high pressure conditions and moderate temperatures are of significant importance for engine efficiency. In this work, the densities of linalool, α -pinene and β -pinene were obtained in the temperature range 293.15-413.15 K and at pressures up to 60 MPa. Based on these results, it was found that with increasing temperature at constant pressure the density of these terpenes decreases, while with increasing pressure at constant temperature the density increases.

The authors are grateful for the financial support they received from the research fund of the Ministry of Education, Science and Technological Development, the Republic of Serbia and the Faculty of Technology and Metallurgy, University of Belgrade (contract no. 451-03-9 / 2021-14 / 200135).

Tekstilno inženjerstvo

Textile Engineering



TI-P-1

Antimikrobna aktivnost nanolistića CuO *in situ* sintetisanih na pamučnoj tkanini prethodno oksidisanom sa NaIO₄/NaClO₂

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U ovom radu diskutovana je mogućnost sinteze nanolistića na bazi Cu na pamučnoj tkanini koji bi pružili željeni nivo antimikrobne aktivnosti. Da bi se obezbedio dovoljan broj karboksilnih grupa za vezivanje Cu²⁺-jona iz rastvora soli prekursora pamučna tkanina je selektivno oksidisana u dvostepenom procesu sa NaIO₄ i NaClO₂. Sorbovani Cu²⁺-joni su redukovani galnom kiselinom. FESEM i XRD analize su pokazale da nanolistići CuO organizovani u fine slojeve ravnomerno pokrivaju površinu vlakana. Što je veća početna koncentracija NaIO₄, veći je broj karboksilnih grupa i posledično količina sintetisanih nanolistića CuO. Razvijeni tekstilni nanokompoziti su pokazali odličnu antibakterijsku aktivnost prema Gram-negativnoj bakteriji *Escherichia Coli* i Gram-pozitivnoj bakteriji *Staphylococcus aureus*, kao i zadovoljavajuću antifungalnu aktivnost prema kvascu *Candida albicans*.

Zahvalnica: Ovo istraživanje je podržalo Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije (Ugovori br. 451-03-9/2021-14/200135 and 451-03-68/2021-14/200287).

Antimicrobial activity of CuO nanosheets *in situ* synthesized on cotton fabric previously oxidized with NaIO₄/NaClO₂

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This study discussed the possibility of synthesizing Cu-based nanosheets on cotton fabric which could provide desired level of antimicrobial activity. In order to ensure a sufficient number of carboxyl groups that could efficiently bind Cu²⁺-ions from precursor salt solution, cotton fabric was selectively oxidized in two-step process with NaIO₄ and NaClO₂. Sorbed Cu²⁺-ions were reduced with gallic acid. FESEM and XRD analyses revealed that CuO nanosheets organized in fine layers evenly covered the surface of cotton fibers. The larger the initial concentration of NaIO₄, the larger the number of carboxyl groups and consequently the amounts of synthesized CuO nanosheets. Fabricated textile nanocomposites exhibited excellent antibacterial activity against Gram-negative bacterium *Escherichia Coli* and Gram-positive bacterium *Staphylococcus aureus* as well as satisfactory antifungal activity against yeast *Candida albicans*.

TI-P-2

Sposobnost jednosmernog upravljanja tečnošću glatkih DL pletenina

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U ovom istraživanju izvršena je analiza sposobnosti jednosmernog upravljanja tečnošću glatkih DL pletenina upotrebom testa kapilarnog kvašenja u okviru koga su određena dva parametra – standardni indeks kapilarnosti i maksimalna visina kvašenja. Pletenine sa većim vrednostima ovih parametara imaju prednost u pogledu toplotnog komfora. Eksperimentalni materijal je obuhvatio glatke DL pletenine izrađene od hidrofilnih (konoplja), hidrofobnih (poliakrilonitril), i mešavine hidrofilnih/hidrofobnih (konoplja/poliakrilonitril) vlakana. Dobijeni rezultati ukazali su na različite vrednosti indeksa kapilarnosti u zavisnosti od sirovinskog sastava ispitivanih pletenina, i pravca kapilarnog kvašenja (izuzev kod poliakrilonitrilne pletenine). Najvećim indeksom kapilarnosti okarakterisana je poliakrilonitrilna pletenina, pračena konoplja/poliakrilonitril i konopljinom pleteninom, ili obrnuto (konoplja i konoplja/poliakrilonitril) zavisno od smera kapilarnog kvašenja. Vrednosti maksimalne visine kvašenja bile su uslovljene sirovinskim sastavom pletenina. Poliakrilonitrilna pletenina je okarakterisana najvećom vrednošću maksimalne visine kvašenja, dok se pletenina od konoplje odlikovala najnižom vrednošću ovog parametra. Međutim, efekat pravca kapilarnog kvašenja pletenina (nizovi ili redovi) na maksimalnu visinu kapilarnog kvašenja uočen je samo kod pletenine od hidrofilnih (konopljinih) vlakana.

Zahvalnica: Rad u okviru MPNT (451-03-68/2020-14/200135)

Unidirectional liquid management properties of plain weft knitted fabrics

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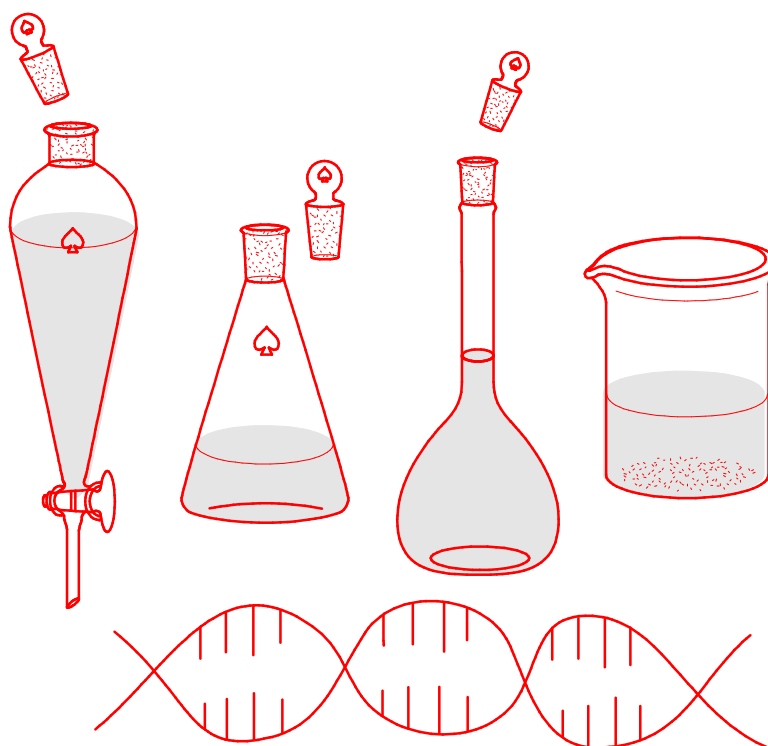
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In this investigation, an attempt was made to assess the unidirectional liquid management properties of plain knitted fabrics using the wicking test. Two parameters were determined in the wicking tests conducted: capillary index and maximum wicking height. In terms of thermal comfort, higher values of these parameters are desirable. The experimental material included the plain weft knitted fabrics made from pure hydrophilic (hemp), pure hydrophobic (acrylic) and hydrophilic/hydrophobic (hemp/acrylic) fibre blend. The obtained results indicated the differences in the capillary index in respect to the composition of the knitted fabrics and wicking direction (except acrylic knit). The highest capillary index was observed in the acrylic knitted fabric, followed by the hemp/acrylic and hemp knits, or vice versa depending on wicking direction. Maximum wicking height depended on the knit composition. The highest value of the maximum wicking height appeared in the acrylic knit, while the hemp knit exhibited the lowest max wicking height. However, the influence of the wicking direction (wale or course) on the maximum wicking height was confirmed only for the pure hydrophilic (hemp) knitted fabric.

Acknowledgement: Within the Contract No. 451-03-68/2020-14/200135

Hemija materijala

Material Science



HM-P-1

Sinteza i karakterizacija hidrougljeva dobijenih iz drvene biomase

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Hidrougljevi (HC) se dobijaju postupkom hidrotermalne karbonizacije različitih vrsta biomase i predstavljaju multifunkcionalne proizvode, koji između ostalog mogu da se primenjuju i kao alternativni obnovljiv izvor energije. U ovom radu su prikazane karakteristike HC, koji su sintetisani u komercijalnom reaktoru pri različitim radnim uslovima temperature (200-300 °C), pritiska (15-100 bar), vremena trajanja reakcije (30-165 min) i odnosa čvrste i tečne faze (1:5 - 1:15), kao i uticaj ovih parametara na prinos i elementarni sastav HC. U zavisnosti od reakcionih uslova, prinos HC se kreće u opsegu 38-64%. Prinos HC značajno opada sa povišenjem temperature, dok je uticaj drugih faktora znatno niži. Na osnovu SEM analize svi uzorci HC karakterišu se heterogenom površinom i razvijenom poroznom strukturom (2-16 nm). Sastav HC, određen EDS analizom najvećim delom čine C (67-82%) i O (17-33%), dok se Al, Ca i K nalaze u tragovima.

Synthesis and characterization of wood-derived hydrochars

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Hydrochars (HC) are obtained by hydrothermal carbonization of different types of biomass and represent multifunctional products, which can be used also as an alternative source of renewable energy. This paper presents the characteristics of HC synthesized in a commercial reactor at different working conditions of temperature (200-300 °C), pressure (15-100 bar), reaction time (30-165 min) and the ratio of solid and liquid phases (1:5 - 1:15), as well as the influence of these parameters on the yield and elemental composition of HC. Depending on the reaction conditions, the yield of HC ranges from 38-64%. The yield of HC decreases significantly with increasing temperature, while the influence of other factors is significantly lower. Based on SEM analysis, all HC samples are characterized by a heterogeneous surface and a developed porous structure (size of pore 2-16 nm). The composition of HC, determined by EDS analysis, consists mostly of C (67-82%) and O (17-33%), while Al, Ca and K were found in traces.

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HM-P-2

Morfološka i elektrohemijska karakterizacija nanočestica srebra i gvožđe-oksida namenjenih za elektroanalizu

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Nanočestice metala i oksida metala (NPs) privlače pažnju mnogih istraživača zbog svojih jedinstvenih optičkih i električnih svojstva. Ove nanočestice nalaze primenu u biologiji, medicini, kao i u elektronici, za izradu senzora. U ovom radu sintetisane su nanočestice srebra (Ag NPs) i gvožđe(III)-oksida (Fe_2O_3 NPs), jednostavnom „*solid-state*“ metodom iz čvrstog stanja uz prisustvo različitih soli kao stabilizatora. Sintetisane su Ag i Fe_2O_3 NPs uz trinatrijum citrat kao stabilizator, kao i Fe_2O_3 NPs u prisustvu kalijum-hlorida. TEM merenjima nađeno je da su Ag NPs sferne, prosečne veličine od 25 nm, dok su Fe_2O_3 NPs takođe sferne i veličine 3 nm, u oba slučaja. Elektrohemijska karakterizacija sintetisanih Fe_2O_3 NPs i Ag NPs ugrađenih u elektrodu od ugljenične paste (CPE) izvedena je cikličnom voltametrijom (CV) u $[\text{Fe}(\text{CN})_6]^{3-/4-}$ redoks sistemu. Izračunate su efektivne površine svih modifikovanih CPE, a električna provodljivost je poređena elektrohemijskom impedansnom spektroskopijom (EIS). Međusobnim upoređivanjem, utvrđeno je da CPE modifikovane sa Fe_2O_3 NPs pripremljene uz KCl, kao i AgNPs stabilizovane citratnim jonima pokazuju najbolji elektrohemijski odgovor. Ove NPs su i izabrane kao potencijalno aktivni materijali za elektrohemijske senzore.

Morphological and electrochemical characterization of silver and iron-oxide nanoparticles intended for electroanalysis

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Metal and metal oxide nanoparticles (NPs) attract the great attention of researchers due to their unique optical and electrical properties. These NPs are used in various biological and medical applications, as in electronics as sensors. In this work, silver and iron(III)-oxide NPs (Ag, Fe_2O_3 NPs) were synthesized by a simple solid-state chemical method in the presence of different stabilizers. Ag and Fe_2O_3 NPs were obtained with trisodium citrate as stabilizing agents. The second sample of Fe_2O_3 NPs was synthesized in the presence of potassium chloride. TEM measurements showed that the Ag NPs are spherical with a diameter of 25 nm, while Fe_2O_3 NPs were spherical with 3 nm in both cases. Electrochemical characterization of synthesized Fe_2O_3 NPs and Ag NPs incorporated in carbon paste electrode (CPE) was performed by cyclic voltammetry (CV) in $[\text{Fe}(\text{CN})_6]^{3-/4-}$ redox system. Effective surface areas of all modified CPEs were calculated, and electrical conductivity was compared by electrochemical impedance spectroscopy (EIS). By mutual comparison, it was found that Fe_2O_3 NPs synthesized in the presence of KCl incorporated into CPE, and AgNPs surrounded by citrates, show the best electrochemical response. These NPs were selected as potentially active materials for electrochemical sensors.

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HM-P-3

Bio-sinteza nanočestica magnetita primenom vodenih ekstrakata cveta biljke *Sambucus ebulus* L.

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U poslednje vreme velika pažnja posvećena je razvoju nanomaterijala zasnovanih na primeni biljnih ekstrakata, kako bi se poboljšale njihove karakteristike i biološka svojstva. Tokom procesa sinteze bioaktivna jedinjenja prisutna u biljkama (polifenoli, flavonoidi, itd.) imaju značajan uticaj na veličinu sintetisanih čestica, kao i na njihovu biološku aktivnost. U ovom radu su predstavljene karakteristike Fe₃O₄-MNp koji je sintetisan primenom vodenih ekstrakata cveta biljke *Sambucus ebulus*. Ekstrakt biljke pokazuje visok antiradikalni potencijal (određen DPPH testom), što je posledica visokog sadržaja polifenola. Magnetit je sintetisan iz Fe²⁺ i Fe³⁺ sulfatnih soli u prisustvu biljnog ekstrakta na 80°C. Na osnovu XRD analize srednja vrednost veličine kristalita sintetisanog magnetita je iznosila 10,3 nm.

Bio-synthesis of magnetite nanoparticles using *Sambucus ebulus* flower water extract

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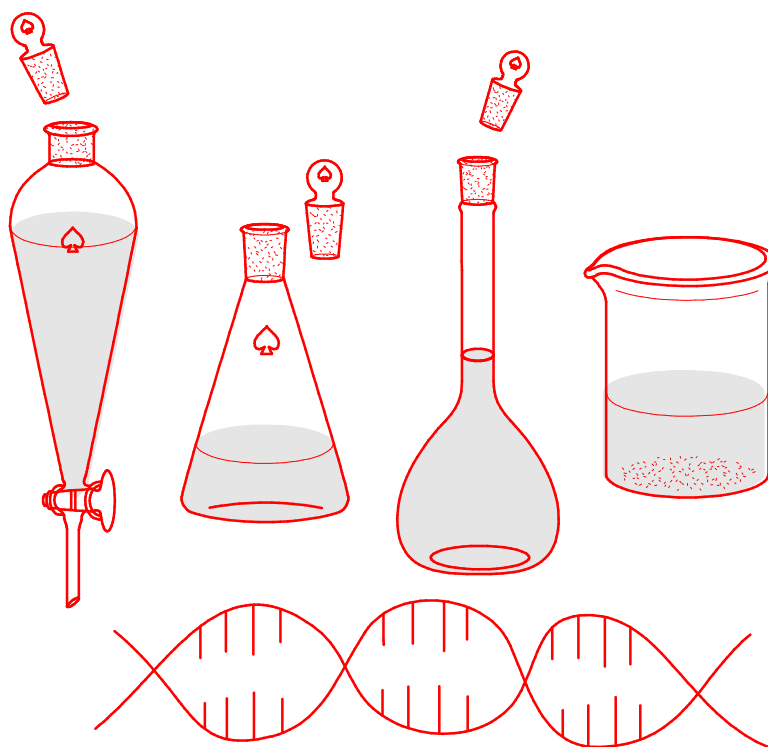
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Recently, great attention has been paid to development of various nanomaterials based on plant extracts, in order to improve their characteristics and biological properties. During the synthesis process, bioactive compounds present in plants (such as polyphenols, flavonoids, proteins, etc.) have a significant impact on the size of the synthesized particles, as well as on their biological activity. This paper presents the characteristics of biogenic Fe₃O₄-MNp synthesized by using *Sambucus ebulus* flower water extract. The plant extract showed a high antiradical potential (according to DPPH assay), which is connected with the high polyphenolic content. Magnetite was synthesized from Fe²⁺ and Fe³⁺ sulfate salts in the presence of plant extract at 80°C. Based on XRD analysis the mean crystallite size value of magnetite was 10.3 nm.

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Neorganska hemija

Inorganic Chemistry



NH-P-1

Ispitivanje supstitucionih reakcija kompleksa Pd(II) sa biološki značajnim ligandima

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S obzirom da su kompleksi Pd(II) poslednjih godina pokazali značajnu antitumorsku aktivnost prema mnogobrojnim kancerogenim ćelijama, ispitivanje reakcija supstitucije kompleksa Pd(II) sa biomolekulama koje sadrže azot i sumpor može značajno pomoći razvoju novih antitumorskih lekova sa poboljšanim karakteristikama. Kinetika supstitucionih reakcija kompleksa Pd(II), 3-(1-(2-hidroksipropilamino)-etilidene)-hroman-2,4-dione-paladijum(II) (C1) i 3-(1-(2-merkaptometilamino)-etilidene)-hroman-2,4-dione-paladijum(II) (C2), sa biološki značajnim ligandima kao što su L-cistein (L-cys), L-metionin (L-met) i guanozin-5'-monofosfat (5'-GMP) ispitivana je pod uslovima reakcija pseudo-prvog reda, primenom stopped-flow metode. Sve reakcije su proučavane na pH = 7.2 (u 25 mM Hepes puferu uz dodatak 50 mM NaCl) na 37 °C. Dobijeni kinetički podaci su pokazali da je kompleks C2 reaktivniji u odnosu na C1, što potvrđuje da strukturne i elektronske karakteristike ispitivanih kompleksa značajno utiču na njihovu reaktivnost prema odabranim ligandima. Reaktivnost ispitivanih nukleofila opada u nizu: L-cys > L-met > 5'-GMP.

Study of the substitution reactions between Pd(II) complexes and biologically significant ligands

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Considering that Pd(II) complexes in recent years have shown the significant antitumor activity against numerous cancer cells, study of the substitution reactions of Pd(II) complexes with nitrogen and sulfur containing biomolecules can help to develop new antitumor drugs with improved characteristics. Kinetics of the substitution reactions of Pd(II) complexes, 3-(1-(2-hydroxypropylamino)-ethylidene)-chroman-2,4-dione-palladium(II) (C1) and 3-(1-(2-mercaptoethylamino)ethylidene)-chroman-2,4-dione-palladium(II) (C2), with biologically relevant ligands, such as L-cysteine (L-cys), L-methionine (L-met) and guanosine-5'-monophosphate (5'-GMP) were studied under the pseudo-first order conditions, using stopped-flow method. All reactions were performed at pH = 7.2 (25 mM Hepes buffer in the presence of 50 mM NaCl) at 37 °C. The obtained kinetic data showed that C2 complex is more reactive than C1, confirming that structural and electronic characteristics of the investigated complexes strongly affect on their reactivity toward selected ligands. The reactivity of the studied nucleophiles decreases in order: L-cys > L-met > 5'-GMP.

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NH-P-2

Kompleksi platine(II) sa malonskom kiselinom: Sinteza, karakterizacija i interakcije sa DNK

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Kompleks karboplatina, koji je poznat kao hemoterapijski lek druge generacije, je pokazao značajnu antitumorsku aktivnost i manju nefrotoksičnost, kao i manje druge neželjene efekte u odnosu na cisplatinu, što je posledica prisustva bidentatno koordinovanog cbdca (ciklobutan-1,1-dikarboksilat) liganda.¹ S obzirom na to da je cbdca derivat malonske kiseline, u ovom radu sintetizovana su tri Pt(II) kompleksa opšte formule [Pt(L)(5,6-epoxy-1,10-phen)], gde je L anjon malonske (mal, Pt1), 2-metilmalonske (Me-mal, Pt2) ili 2,2-dimetilmalonske kiseline (Me₂-mal, Pt3), dok je 5,6-epoxy-1,10-phen bidentatno koordinovani 5,6-epoksi-5,6-dihidro-1,10-fenantrolin. Kompleksi su okarakterisani na osnovu rezultata elementalne mikroanalize, IR, UV-Vis i NMR (¹H i ¹³C) spektroskopije. Interakcije kompleksa sa DNK ispitivane su primenom UV-Vis i fluorescentne spektroskopije. Rezultati ispitivanja su pokazali da ovi kompleksi interaguju sa DNK i da mogu istisnuti etidijum-bromid (EtBr) iz DNK-EtBr.

Platinum(II) complexes with malonic acid: Synthesis, characterization and interactions with DNA

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Carboplatin, as a second-generation chemotherapeutic drug, showed antitumor activity without nephrotoxic effects of cisplatin, as well as less side effects, due to the presence of bidentate-coordinated cbdca (cyclobutane-1,1-dicarboxylate) ligand.¹ Since cbdca is a derivative of malonic acid, three Pt(II) complexes of the general formula [Pt(L)(5,6-epoxy-1,10-phen)], where L is anion of malonic (mal, Pt1), 2-methylmalonic (Me-mal, Pt2) or 2,2-dimethylmalonic (Me₂-mal, Pt3) acid, while 5,6-epoxy-1,10-phen is bidentately coordinated 5,6-epoxy-5,6-dihydro-1,10-phenanthroline. These complexes were characterized by elemental microanalysis, IR, UV-Vis and NMR (¹H i ¹³C) spectroscopic techniques. The binding of these complexes to DNA was investigated by UV-Vis and fluorescence spectroscopy. The obtained results showed that the complexes interact with DNA and can displace ethidium bromide (EtBr) from DNA-EtBr adduct.

1. H. Gao, X. Wei, X. Liu, T. Yan, *J. Phys. Chem. B*, **114** (2010) 4056–4062

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NH-P-3

***In-vitro* ispitivanje interakcija dva strukturno slična kompleksa Šifovih baza Rh(III) sa HSA/DNK i molekularni doking**

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Kompleksi metala sa tetradentatnim Šifovim bazama ispoljavaju različitu biološku aktivnost, što omogućava ciljne sinteze novih biološki aktivnih jedinjenja¹. Proučavane su interakcije H[Rh(acac₂en)Cl₂] (1) i H[Rh(phacac₂en)Cl₂] (2) sa humanim serum albuminom (HSA) i sa DNK, primenom fluorescentne i UV-Vis spektroskopije (298 K, pH 7,4). Dobijene su relativno visoke vrednosti dinamičke konstante vezivanja (K_{sv}) i to $3,88 \times 10^4 M^{-1}$ za (1), $7,02 \times 10^4 M^{-1}$ za (2), što ukazuje na značajno vezivanje za HSA. Izračunate konstante unutrašnjeg vezivanja (K_b) su: $2,87 \times 10^5 M^{-1}$ za (1), $4,22 \times 10^5 M^{-1}$ za (2). Vrednosti navednih konstanti ukazuju na dobru interakciju između kompleksa Rh(III) i DNK. Ponašanje ispitivanih kompleksa je u saglasnosti sa razlikama u njihovim strukturama. Molekulski doking potvrđuje dobijene eksperimentalne podatke različitih interakcija u kojima se kompleks vezuje za molekul proteina.

***In-vitro* investigation of interaction of two structurally similar Schiff base Rh(III) complexes with HSA/DNA and molecular docking**

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Tetradentate Schiff base metal complexes exhibit different biological activity, which enables targeted syntheses of new biologically active compounds¹. The interaction of H[Rh(acac₂en)Cl₂] (1) and H[Rh(phacac₂en)Cl₂] (2) with human serum albumine (HSA) and with DNA by fluorescence and UV-Vis spectroscopy (at 298 K, pH 7.4) were investigated. Relatively high values of the dynamic quenching constant (K_{sv}) are obtained: $3.88 \times 10^4 M^{-1}$ for (1), $7.02 \times 10^4 M^{-1}$ for (2), which indicates binding to HSA. Calculated intrinsic binding constants (K_b) which are $2.87 \times 10^5 M^{-1}$ for (1), $4.22 \times 10^5 M^{-1}$ for (2) suggest a good interaction between the Rh(III) complexes and DNA. The behavior is in accordance with differences in structures of investigated compounds. Molecular docking studies confirm experimental findings of different interactions through which complexes are bound to the protein molecule.

[1] S.Mistria, H.Puschmannb, S. ChandraManna, Polyhedron 115 (2016) 155-163.

Ministry of Education, Science and Technological Development of Republic of Serbia, Contract numbers: 451-03-9/2021-14/200126, 451-03-9/2021-14/200168, 451-03-68/2021-14/200122.

NH-P-4

Antimikrobna aktivnost platine(IV) kompleksa sa *O,O'*-dialkil estrima (*S,S*)-etilendiamin-*N,N'*-di-2-(4-metil)-pentanske kiseline

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Od otkrića cisplatine od strane Rosenberga, kompleksi platine su u fokusu istraživanja. Kompleksi platine(IV) privukli su značajnu pažnju zbog mogućnosti oralne upotrebe i njihove kinetičke inertnosti. Brojni kompleksi platine(IV) su sintetisani i zabeležene su njihove različite biološke aktivnosti. Proučavan je uticaj različitih kompleksa platine na rast i metabolizam različitih grupa mikroorganizama. Sintetisani su kompleksi platine(IV) (1–4) sa *O,O'*-dialkil esterima (alkil = etil, *n*-propil, *n*-butil i *n*-pentil), (*S,S*) -etilendiamin-*N,N'*- di-2-(4-metil) pentanske kiseline (L1·2HCl–L4·2HCl). Antimikrobna aktivnost je urađena za sva sintetisana jedinjenja. *In vitro* antimikrobna aktivnost sintetisanih jedinjenja izvršena je na šest bakterija: *Staphylococcus aureus* ATCC 25923, *Klebsiella pneumoniae* ATCC 13883, *Escherichia coli* ATCC 25922, *Proteus vulgaris* ATCC 13315, *Proteus mirabilis* ATCC 14153, *Bacillus subtilis* ATCC 6633 i dve gljive: *Candida albicans* ATCC 10231 i *Aspergillus niger* ATCC 16404 minimalnom inhibitornom koncentracijom (MIC). Rezultati antimikrobne aktivnosti platine(IV) kompleksa i liganada pokazuju MIC vrednosti od 19,5 mg/mL do 625 mg/mL za bakterije i 39,1 mg/mL do 312,5 mg/mL za gljive. Najvišu antimikrobnu aktivnost pokazao je kompleks 4 od svih testiranih jedinjenja.

Antimicrobial activity of platinum(IV) complexes with *O,O'*-dialkyl esters of (*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)-pentanoic acid

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Since discovery of cisplatin by Rosenberg, platinum complexes are in the focus of research. Platinum(IV) complexes have attracted considerable attention due to the resulting possibility of oral use and their kinetic inertness. Numerous platinum(IV) complexes have been synthesized and their various biological activities recorded. The influence of different platinum complexes on the growth and metabolism of different groups of microorganisms has been studied. Platinum(IV) complexes (1–4) with *O,O'*-dialkyl esters (alkyl = ethyl, *n*-propyl, *n*-butyl and *n*-pentyl), of (*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)pentanoic acid (L1·2HCl–L4·2HCl) were synthesized. Antimicrobial activity was performed for all synthesized compounds. *In vitro* antimicrobial activity of the synthesized compounds was done on six bacteria: *Staphylococcus aureus* ATCC 25923, *Klebsiella pneumoniae* ATCC 13883, *Escherichia coli* ATCC 25922, *Proteus vulgaris* ATCC 13315, *Proteus mirabilis* ATCC 14153, *Bacillus subtilis* ATCC 6633 and two fungi: *Candida albicans* ATCC 10231 and *Aspergillus niger* ATCC 16404 by minimum inhibitory concentration (MIC). The results of antimicrobial activity for platinum(IV) complexes and ligands show in the MIC concentration range from 19.5 mg/mL to 625 mg/mL for bacteria and 39.1 mg/mL to 312.5 mg/mL for fungi. The strongest antimicrobial activity was demonstrated by complex 4 of all compounds tested.

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NH-P-5

Sinteza i karakterizacija jedinjenja trifenilkalaja(IV) sa 3-(4-metil-2-oksohinolinil)propanskom kiselinom

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U poslednjoj deceniji jedinjenja organokalaja(IV) privukla su veliku pažnju istraživača zbog svoje izvanredne citotoksične aktivnosti protiv raznih oblika tumora. Ovde je prikazana sinteza 3-(4-metil-2-oksohinolinil)propanske kiseline i njenog kompleksa trifenilkalaja(IV). Ligand je dobijen u dva koraka. U prvom koraku, u reakciji između 4-metil-hinolin-2-ona i metil-3-bromopropionata sintetisan je odgovarajući metil-estar, čijom hidrolizom, u drugom koraku, je dobijen ligand. U reakciji liganda, koji je deprotonovan LiOH, i ekvimolarne količine Ph_3SnCl dobijen je kompleks u obliku belog taloga. Sintetisana jedinjenja su okarakterisana standardnim analitičkim metodama. Naredna istraživanja sintetisanih jedinjenja biće usmerena ka *in vitro* ispitivanju citotoksične aktivnosti prema raznim ćelijskim linijama karcinoma, kao i na ispitivanje mehanizma njihovog delovanja.

Synthesis and characterization of novel triphenyltin(IV) compound with 3-(4-methyl-2-oxoquinolinyl)propanoic acid

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Biochemistry

Organotin(IV) compounds have greatly attracted researchers' attention in the last decade for their outstanding cytotoxic activity against different tumor cells. Herein, the synthesis of 3-(4-methyl-2-oxoquinolinyl)propanoic acid and its triphenyltin(IV) complex has been performed. The ligand precursor has been synthesized in two steps. In the first step, reaction between 4-methylquinoline-2-on and methyl 3-bromopropionate afforded corresponding methyl ester, whose hydrolysis, in the second step, produced targeted ligand. In the reaction of ligand precursor, which was deprotonated with LiOH, with equimolar amount of Ph_3SnCl , the expected complex was obtained as white solid. The synthesized compounds have been characterized using standard analytical methods. The following research of synthesized compounds will be focused on *in vitro* cytotoxic activity against various cancer cell lines, as well as investigation of mechanism of their action.

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NH-P-6

Sinteze i kristalne strukture semikarbazona pirogroždane kiseline i njegovog kompleksa sa bakar(II) bromidom

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Monokristali liganda semikarbazona pirogroždane kiseline (L) dobijeni su reakcijom vodenih rastvora natrijum-piruvata i semikarbazid hidrohlorida. Asimetrična jedinica kristalne strukture liganda sadrži tri kristalografski nezavisna molekula, od kojih dva imaju konformaciju u kojoj su iminski i terminalni semikarbazidni atomi azota u *cis* položaju, dok treći molekul zauzima konformaciju u kojoj su ovi atomi u *trans* položaju. Osim atoma ugljenika metil grupe, svi ostali nevodonični atomi su sp^2 hibridizovani, što se reflektuje na dužine veza koje grade. Strukture sva tri molekula blago odstupaju od planarnosti.

Zeleni monokristali kompleksa $[Cu(L-H)Br(H_2O)] \cdot H_2O$, dobijeni su reakcijom toplih etanolnih rastvora $CuBr_2$ i L. Koordinaciono okruženje Cu(II) je deformisano kvadratno-piramidalno, koje se realizuje tridentatnom *ONO* koordinacijom Šifove baze u monoanjonskoj formi, i bromidnog jona u bazalnoj ravni, kao i molekula vode u apikalnom položaju.

Synthesis and crystal structures of pyruvate semicarbazone and its copper(II) bromide complex

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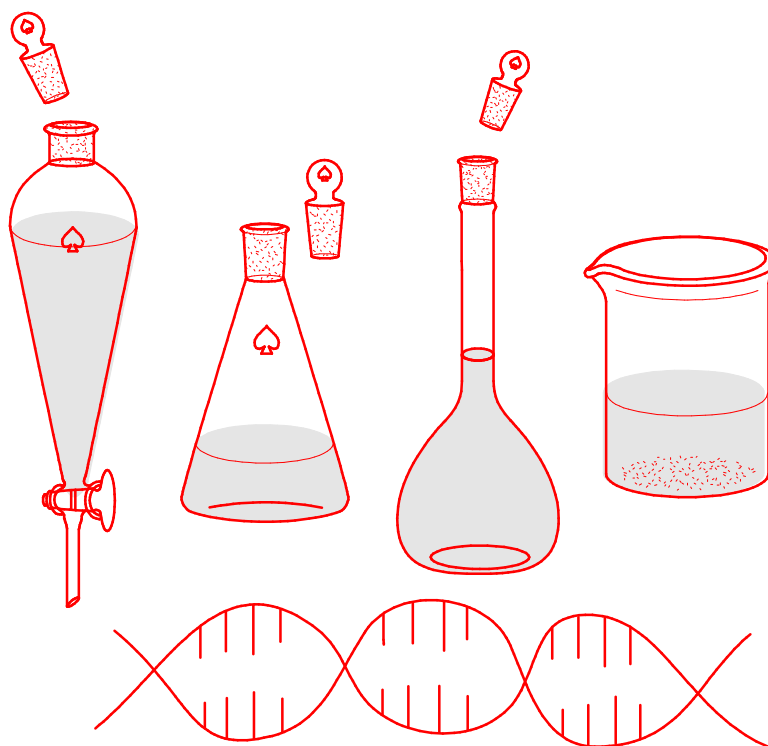
Single crystals of pyruvate semicarbazone (L) have been obtained in reaction of aqueous solutions of sodium pyruvate and semicarbazide hydrochloride. Asymmetric unit of the crystal structure consists of three crystallographically independent molecules. Two of these have same conformation, in which imine and terminal semicarbazide nitrogen atoms are mutually in *cis* position, while the third molecule adopts conformation in which these atoms are in *trans* position. Except methyl group carbon atom, all other non-hydrogen atoms are sp^2 hybridized, which is reflected in their bond lengths. All three molecular structures are slightly non-planar.

Green single crystals of $[Cu(L-H)Br(H_2O)] \cdot H_2O$ complex are obtained in reaction of warm ethanolic solutions of $CuBr_2$ and L. Cu(II) is situated in slightly deformed square pyramidal environment, composed of *ONO* tridentately coordinated Schiff base in its monoanionic form, and bromide anion in the basal plane, while apical position is occupied by water molecule.

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Hemija životne sredine

Environmental Chemistry



HŽS-U-1

Uklanjanje hroma(VI) iz vode primenom praškastog ugljeničnog materijala dobijenog iz kokosove ljuske kao jeftinog adsorbenta

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Praškast ugljenični materijal proizveden iz kokosove ljuske korišćen je kao adsorbent za uklanjanje Cr(VI) jona iz vodenih rastvora. Karakterizacija adsorbenta rađena je primenom dve analitičke tehnike, skenirajućom elektronskom mikroskopijom (SEM) i BET metodom. Eksperimenti adsorpcije rađeni su u šaržnom režimu, kako bi se istražili uticaji pH rastvora, vremena kontakta i početne koncentracije Cr(VI) jona. Eksperimentalni rezultati su pokazali da je efikasnost uklanjanja Cr(VI) najveća u pH intervalu od 2,0 do 3,5, a da se ravnoteža uspostavlja nakon 60 minuta. Dva ravnotežna adsorpciona modela, Langmirov i Frojndlihov, korišćena su za fitovanje dobijenih podataka. Frojndlihova izoterma je obezbedila najbolju korelaciju za adsorpciju Cr(VI) jona na ugljeničnom materijalu proizvedenom iz kokosove ljuske. Na osnovu dobijenih rezultata može se zaključiti da ugljenični materijal proizveden iz kokosove ljuske predstavlja jeftin i efikasan adsorbent koji bi potencijalno mogao biti korišćen za tretman otpadnih voda koje sadrže toksični Cr(VI).

Chromium(VI) removal from aqueous solutions using powdered coconut shell activated carbon as a low-cost adsorbent

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Powdered activated carbon produced from coconut shell was used as an adsorbent for the removal of Cr(VI) ions from aqueous solutions. The characterization of the investigated adsorbent was performed using the two analytical techniques, scanning electron microscopy (SEM) and BET method. Batch adsorption experiments were performed to investigate the effects of solution pH, contact time and initial concentration of Cr(VI) ions. Experimental results showed that the highest removal efficiency of Cr(VI) was obtained in the pH interval from 2.0 to 3.5, and that the equilibrium was restored after 60 minutes. Two equilibrium adsorption models, the Langmuir and the Freundlich, were used to fit the obtained data. The Freundlich isotherm provided the best correlation for the adsorption of Cr(VI) ions onto coconut shell activated carbon. Based on the obtained results, it can be concluded that the carbon material produced from coconut shell can be regarded as an inexpensive and effective adsorbent which could be potentially used in the treatment of wastewaters containing toxic Cr(VI).

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HŽS-P-2

Efikasnost fotokatalitičke razgradnje odabranih herbicida primenom simuliranog sunčevog zračenja

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Kao zagađujuće materije u vodi najčešće su prisutni lekovi, rastvarači, boje, pesticidi, teški metali i dr. Za fotorazgradnju pomenutih polutanata koriste se različiti komercijalni tipovi TiO₂ katalizatora koji se razlikuju po kristalnom sastavu, specifičnoj površini i veličini čestica. Cilj ovoga rada je bio ispitivanje efikasnosti uklanjanja herbicida kvinmeraka primenom tri komercijalna TiO₂ nanopraha (Wackherr, Aeroxide P25 i Kronos) u prisustvu simuliranog sunčevog zračenja. Takođe, proučavan je i uticaj pH rastvora na efikasnost procesa fotokatalitičke razgradnje herbicida upotrebom TiO₂ Wackherr kao najefikasnijeg fotokatalizatora. U cilju utvrđivanja uticaja strukture supstrata na efikasnost razgradnje, ispitana je pored kvinmeraka i kinetika fotorazgradnje herbicida fluoksipira i triklopira pri istim eksperimentalnim uslovima u prisustvu pomenutog katalizatora.

Efficiency of photocatalytic degradation of selected herbicides using simulated solar light

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Drugs, solvents, paints, pesticides, heavy metals etc. as pollutants are usually present in water. For the photodegradation of the mentioned pollutants, different commercial types of TiO₂ catalysts are used, which differ of crystal composition, specific surface area and particle size. The aim of this study was to investigate the removal efficiency of herbicide quinmerac herbicide using three commercial TiO₂ nanopowders (Wackherr, Aeroxide P25 and Kronos) in the presence of simulated solar radiation. Also, the influence of pH solution on the efficiency of the process of photocatalytic decomposition of herbicides was studied using TiO₂ Wackherr as the most efficient photocatalyst. In order to determine the influence of the substrate structure on the degradation efficiency, the photodegradation kinetics of the herbicide fluoxypyr and triclopyr were investigated under the same experimental conditions in the presence of the mentioned catalyst.

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HŽS-P-3

Sadržaj i distribucija teških metala u reci Ibar tokom poplava i izlivanja jalovišta

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У овом раду испитиван је утицај велике магнитуде поплава на загађење тешким металима у реци Ибар, северно Косово и Метохија. Подручје анализе је један од најважнијих индустријских региона Pb/Zn у Европи. Узорци речне воде су захваћени пре и након поплаве у јануару месецу 2021. Рад пружа информације о садржају тешких метала у речној води која се користи за прераду воде за пиће, као и корелацији близине извора загађења и природних акцидната-поплава. На основу резултата добијених у истраживању, примећено је значајно повећање концентрације тешких метала у речној води на месту изливања јаловишта, што говори о ризику загађења. Измерене концентрације током и након поплава су следеће: олово (Pb) 1502.3 ng/ml (RSD=1.95 %) и 42.95 ng/ml (RSD=0.77%), арсен (As) 1668.9 ng/ml (RSD=1.50%) и 8.56 ng/ml (RSD=0.29%), кадмијум (Cd) 18.87 (RSD=3.52%) ng/ml и 0.062 ng/ml (RSD=2.87%), хром (Cr) 9.59 ng/ml (RSD=1.49%) и 8.66 ng/ml (RSD=1.54%), жива (Hg) 37.85 ng/ml (RSD=0.012%) и 13.5 ng/ml (RSD=0.03%), талијум (Tl) 0.32 ng/ml (RSD=2.65%) и 0.05 ng/ml (RSD=2.43 %). Узорци су анализирани применом ICP – OES (ICP – OES, iCAP 6500 Duo, Thermo Scientific, UK) и ICP - MS (ICP-MS, iCAP Qc, Thermo Scientific, UK) технике.

Content and distribution of heavy metals in the river Ibar during floods and spills of mine tailings

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This paper examines the impact of high flood magnitude on heavy metal pollution in the Ibar River, northern Kosovo and Metohija. The area of analysis is one of the most important industrial regions of Pb / Zn in Europe. River water samples were taken during and after the flood in January, 2021. Almost all heavy metals cause various cancers and diseases, cumulative effect after prolonged intake through drinking water. The paper provides information on the content of heavy metals in river water used for the treatment of drinking water, as well as the correlation of the proximity of pollution sources and natural floods. Concentrations of toxic elements during and after floods are: lead (Pb) 1502.3 ng/ml (RSD=1.95 %) and 42.95 ng/ml (RSD=0.77%), arsenic (As) 1668.9 ng/ml (RSD=1.50%) and 8.56 ng/ml (RSD=0.29%), cadmium (Cd) 18.87 (RSD=3.52%) ng/ml and 0.062 ng/ml (RSD=2.87%), chromium (Cr) 9.59 ng/ml (RSD=1.49%) and 8.66 ng/ml (RSD=1.54%), mercury (Hg) 37.85 ng/ml (RSD=0.012%) and 13.5 ng/ml (RSD=0.03%), talium (Tl) 0.32 ng/ml (RSD=2.65%) and 0.05 ng/ml(RSD=2.43 %). The samples were analyzed by ICP – OES (ICP – OES, iCAP 6500 Duo, Thermo Scientific, UK) and ICP - MS (ICP-MS, iCAP Qc, Thermo Scientific, UK) instruments.

HŽS-P-4

Suncokretova ljuska kao biosorbent za uklanjanje teških metala iz vodenih rastvora

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U ovom radu ispitivane su mogućnosti primene ljuske semenki suncokreta kao biosorbenta za uklanjanje teških metala poput Pb, Ni, Cd i Cu iz vodenih rastvora, kao i upotreba inovativne analitičke tehnike, spektroskopije laserski indukovane plazme (LIBS) za procenu efikasnosti adsorpcije. Ono što izdvaja LIBS tehniku u odnosu na standardne spektrohemijske metode kakva je npr. ICP-OES, jeste to što u LIBS-u nema klasične pripreme uzoraka, ne upotrebljavaju se agresivne hemikalije i što je najvažnije nema hemijskog otpada. Biosorbent dobijen od suncokretove ljuske korišćen je za određivanje efikasnosti adsorpcije teških metala u zavisnosti od pH vrednosti simuliranog uzorka otpadne vode kao i vremena kontakta sorbenta sa uzorkom. Vrednosti dobijene referentnom ICP-OES metodom upoređene su sa rezultatima LIBS metode i postignuto je dobro slaganje.

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Removal of heavy metals from aqueous solutions by using sunflower husk as biosorbent

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In this work, the possibilities of using sunflower seed husk as a biosorbent for removing heavy metals such as Pb, Ni, Cd, and Cu from aqueous solutions, as well as the use of innovative analytical techniques, laser-induced plasma spectroscopy (LIBS) to assess adsorption efficiency, were investigated. What makes the LIBS technique superior from the standards of spectrochemical methods such as ICP-OES, is that in LIBS there is no classical sample preparation, no aggressive chemicals are used and most importantly there is no chemical waste. The biosorbent obtained from sunflower husk was used to determine the adsorption efficiency of heavy metals depending on the pH value of the simulated wastewater sample as well as the contact time of the sorbent with the sample. The values obtained by the reference ICP-OES method were compared with the results obtained by the LIBS method and a good agreement was achieved.

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HŽS-P-5

Predviđanje koeficijenta zadržavanja teških metala iz otpadnih voda kompleksirajuće-mikrofiltracionim procesom u prisustvu aminokiselina primenom veštačkih neuronskih mreža

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Kombinovani kompleksirajuće-mikrofiltracioni proces omogućava selektivnost razdvajanja jona teških metala upotrebom različitih agenasa kao npr. derivata celuloze u prisustvu aminokiselina. U radu su za predviđanje koeficijenta zadržavanja jona teških metala odabrana dva modela veštačkih neuronskih mreža (neuronska mreža sa propagacijom greške unazad (BPNN) i neuronska mreža sa opštom regresijom (GRNN)). Korelacionom analizom je utvrđeno da najveći uticaj na izlaznu veličinu ima prva energija jonizacije, molarnе mase metala i kompleksirajućeg agensa i pH vrednost, kao i da dolazi do kompeticije između kompleksirajućeg agensa i aminokiselina za vezivanje metala. Odabrani kriterijumi performansi modela kao što su koeficijent determinacije, indeks slaganja i srednja apsolutna greška u procentima pokazala su da je BPNN model uspešniji u predviđanju i u granicama prihvatljivog.

Prediction of the retention coefficient of heavy metals from wastewater by complexing-microfiltration process in the presence of amino acids using artificial neural networks

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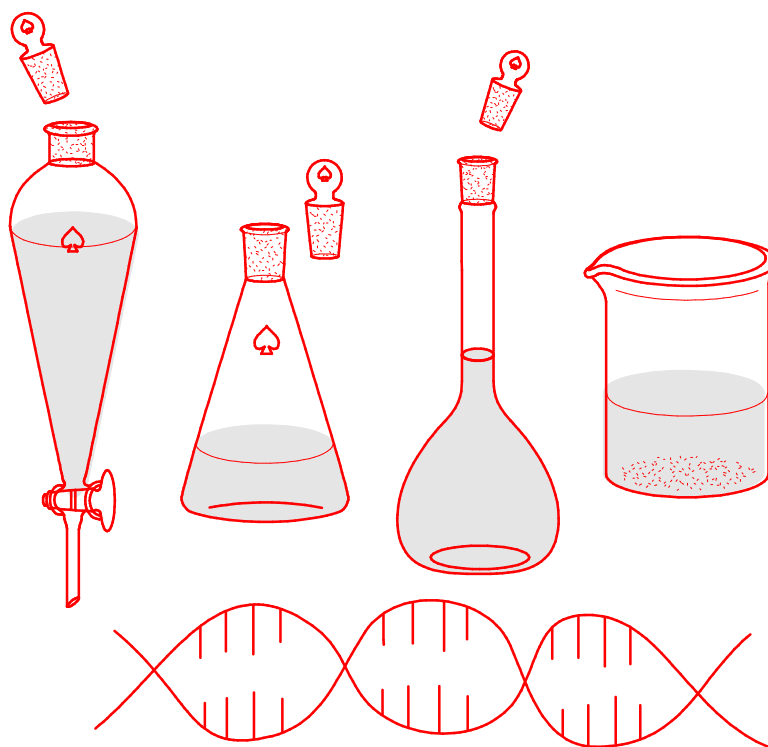
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The combined complexing-microfiltration process enables the selectivity of the separation of heavy metal ions using different agents such as e.g. cellulose derivatives in the presence of amino acids. In this paper, two models of artificial neural networks (Backpropagation Neural Network (BPNN) and General Regression Neural Network (GRNN)) were selected to predict the retention coefficient of heavy metal ions. Correlation analysis determined that the first ionization energy, molar mass of metal and complexing agent and pH value have the greatest influence on the output value, as well as that there is competition between the complexing agent and amino acids for metal binding. Selected model performance criteria such as the coefficient of determination, the index of agreement, and the mean absolute percent error showed that the BPNN model was more successful in predicting and within acceptable limits.

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Biohemija

Biochemistry



BH-U-1

Fluorescentno obeležavanje albumina govedeg seruma fikocijanobilinom korišćenjem Trautovog reagensa

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Fikobiliproteini (FBP) se koriste kao fluorescentni obeleživači zahvaljujući fluorescentnim, kovalentno vezanim, tetrapirolnim hromoforima. U ovom radu predlažemo novu metodu za fluorescentno obeležavanje proteina hromoforom FBP-a fikocijanina, fikocijanobilinom (PCB). Korišćenjem Trautovog reagensa (TR), sulfhidrilne grupe su uvedene u albumin govedeg seruma (BSA), modifikacijom lizinskih ostataka proteina. TR je uspešno modifikovao BSA u svim ispitivanim molarnim odnosima. Povećanje molarnog odnosa TR-a indukovalo je veće strukturne promene BSA-a. PCB se kovalentno vezao za uvedene sulfhidrilne grupe na pH 9. Povećanjem molarnog odnosa TR-a dolazi do pojačavanja fluorescentnog signala. Korišćenjem BSA kao model proteina, pri 50 puta većem molarnom odnosu TR-a postiže se zadovoljavajući nivo pojačavanja fluorescentnog signala, koji ne narušava previše strukturu proteina. Predloženom metodom moguće je fluorescentno obeležiti bilo koji protein od interesa.

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Fluorescent labeling of bovine serum albumin with phycocyanobilin using Traut's reagent

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Phycobiliproteins (PBP) are extensively used as fluorescent probes due to highly fluorescent, covalently bound, tetrapyrrole chromophores. A new method for covalent attachment of phycocyanin's chromophore, phycocyanobilin (PCB), is proposed. We exploited Traut's reagent (TR) to introduce sulfhydryl groups in the bovine serum albumin (BSA), by modifying its lysine residues. TR successfully modified BSA under all tested molar ratios of reagent per mole of BSA. The higher degree of modification by TR induces more profound alterations of BSA structure. PCB was covalently attached to introduced sulfhydryl groups at pH 9 at 20-fold ratio. An increase in the molar ratio of TR per mole of BSA leads to amplification of fluorescent signal of PCB-modified BSA. Using BSA as a model protein, a 50-fold molar excess of TR seems to be the optimal choice for balancing between a satisfactory level of signal amplification and the adverse effect on protein structure. The method could be used for labeling virtually any protein.

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BH-P-2

Antimikrobni i fotokatalitički potencijal nanočestica srebra sintetisanih pomoću ekstrakta biljke *Salvia verticillata* L.

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Cilj ove studije bio je da se proceni antimikrobna i fotokatalitička aktivnost nanočestica srebra sintetisanih upotrebom ekstrakta nadzemnog dela biljke *Salvia verticillata* L.. Takođe, određeni su i najpovoljniji uslovi za njihovu sintezu. Dobijene nanočestice srebra su okarakterisane UV-Vis spektrofotometrijom i infracrvenom spektroskopijom sa Furijeovom transformacijom (FT-IR). UV-Vis podaci potvrdili su formiranje nanočestica i pokazali pik apsorpcije na 427 nm. Funkcionalne grupe jedinjenja prisutnih u ekstraktu takođe su potvrđene u nanočesticama primenom FT-IR, ukazujući da su fenolna jedinjenja ekstrakta biljke odgovorna za stabilizaciju nastalih nanočestica. Dobijene nanočestice srebra pokazale su izraženu antibakterijsku aktivnost sa vrednostima minimalne inhibitorne koncentracije (MIK) manjim od 39,1 µg/mL kod većine testiranih bakterija. Takođe, nanočestice su pokazale dobru katalitičku efikasnost u redukciji kongo crvene boje natrijum-borhidridom. Rezultati ove studije sugerišu da sintetizovane nanočestice imaju obećavajuća antimikrobna i katalitička svojstva.

The antimicrobial and photocatalytic potential of synthesized silver nanoparticles using *Salvia verticillata* L. plant extract

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This study aimed to evaluate the antimicrobial and photocatalytic activity of silver nanoparticles synthesized using *Salvia verticillata* L. aerial part extract. Optimal conditions for their biosynthesis were also determined. The obtained silver nanoparticles were characterized by UV-Vis spectrophotometry and Fourier Transform Infra-Red (FT-IR) spectroscopy. The UV-Vis data confirmed the formation of nanoparticles and showed a strong absorbance peak at 427 nm. Functional groups of compounds present in the extract were also detected in nanoparticles using FT-IR, which indicates that phenolic compounds from the plant extract are responsible for the stabilization of formed nanoparticles. The obtained silver nanoparticles showed pronounced antibacterial activity, with MIC less than 39.1 µg/mL in most of the tested bacteria. The nanoparticles also exhibited a good catalytic efficiency in the reduction of Congo red dye with NaBH₄. The findings of this study suggest that synthesized nanoparticles possess promising antimicrobial and catalytic properties.

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BH-U-3

Katinoni kao stimulatori 5-HT_{2A}R receptora: Definisane bioaktivne konformacije 3-D QSAR profila kao načina za razumevanje njihovog ponašanja kao zloupotrebljivanih droga i dizajn anti-katinona

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Katinoni su poznate zloupotrebljavane droge sa slabo poznatom farmakologijom. Farmakološki profil komercijalno dostupnih katinona ispitivan je na nivou 5-HT_{2A} receptora, molekulskim dokovanjem, pomoću AutoDock Vina, i 3-D QSAR modelima pomoću Open3DQSAR. Potom su 3-D QSAR modeli sumirani u univerzalni SAR model, korišćen za dizajn inovativnih anti-katinona, potencijalnih blokatora dejstva katinona čija je farmakologija procenjena na nivou receptora pomoću molekulskog dokovanja. Dobijena pravila za dizajn antikatinona pružaju mogućnost za dalju sintezu i biološku evaluaciju.

Cathinones as 5-HT_{2A}R stimulators: Definition of bioactive conformations and 3-D QSAR profiles as a pathway for understanding their behavior as abusing drugs and design of anti-cathinones

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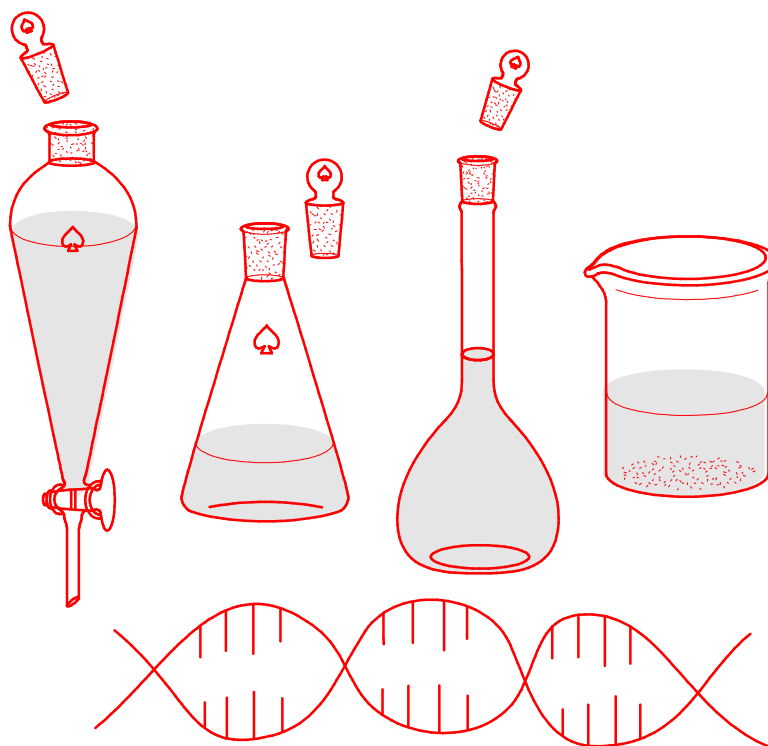
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Cathinones are known abusing drugs with pharmacology fairly known. Commercially available cathinones' pharmacodynamics profiles were elaborated on the 5-HT_{2A}R level with the aid of AutoDock Vina-based molecular docking and Open3DQSAR-based 3-D QSAR studies. Following, 3-D QSAR models were summarized in universal SAR models, further used to design innovative anti-cathinones, with the potential potency to block cathinones' action and pharmacology assessed using molecular docking. The obtained design rules provided the opportunity for further synthesis and biological evaluation.

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Hemija i tehnologija makromolekula

Chemistry and Technology of Macromolecules



HTM-U-1

Kinetika i modelovanje procesa uklanjanja odabranih tekstilnih boja iz otpadnih voda

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Zbog velike količine boja koje se oslobađaju nakon bojenja i štampanja tekstilnih materijala, otpadne vode tekstilne industrije postale su ozbiljan ekološki problem. Iz tog razloga, naučnici neprestano rade na poboljšanju postojećih i razvoju novih metoda za prečišćavanje voda. Imajući na umu da otpadne vode tekstilne industrije obično sadrže nekoliko različitih boja; važno je da se razvije metoda koja će delotvorno ukloniti sve prisutne boje, a istovremeno biti jednostavna i isplativa. U velikom broju ovih metoda koriste se umreženi polimeri, posebno oni prirodni dobijeni iz obnovljivih izvora. Ovaj rad ispituje mogućnost korišćenja modifikovanog hitozana za prečišćavanje otpadnih voda tekstilne industrije. Ispitivanja su izvedena u simuliranoj otpadnoj vodi, a kao model boje korišćene su boje C.I. Acid Orange 7, C.I. Basic Red 1 i njihova mešavina.. Eksperiment je postavljen pod optimalnim pH uslovima za svaku boju kako bi se dobili podaci o ravnoteži na 15 °C, 25 °C, 35 °C i 50 °C od 1 h do 24 h. Utvrđeno je da je najveća efikasnost sorpcije postignuta na 35 °C tokom 24 sata. Za ispitivanje kinetike sorpcije boja korišćeni su Weberov i Morisov model difuzije unutar čestica i Elovičev model. Dobijeni rezultati pokazuju da ovi hidrogelovi imaju izvanrednu sposobnost sorpcije boje C.I. Basic Red 1, bez obzira na sastav otpadnih voda, te bi se daljom modifikacijom mogli koristiti za uklanjanje svih boja.

Kinetics and modeling of the process of removing selected textile dyes from wastewater

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Due to the large number of dyes released after dyeing and printing textile materials, wastewater from the textile industry has become a severe environmental problem. For this reason, scientists are constantly working to improve existing and develop new methods for water purification. Bearing in mind that the wastewater of the textile industry usually contains several different colors, it is essential to develop a method that will effectively remove all the colors present while being cost-effective and simple. Many of these methods use crosslinked polymers, especially natural ones obtained from renewable sources. This paper examines the possibility of using modified chitosan for wastewater treatment in the textile industry. The tests were performed in simulated wastewater, and C. I. Acid Orange 7, C.I. Basic Red 1, and their mixture were used as a dye model. The experiment was set up under optimal pH conditions for each color to obtain equilibrium data at 15 °C, 25 °C, 35 °C, and 50 °C from 1 h to 24 h. The highest sorption efficiency was found to be achieved at 35 °C for 24 hours. Weber and Morris's model of diffusion within particles and the Elovich model were used to examine the kinetics of color sorption. The results obtained show that these hydrogels have an excellent ability to sorb the color of C.I. Basic Red 1, regardless of the composition of wastewater, and further modification could be used to remove all colors.

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HTM-P-2

Sinteza multifunkcionalnih kuglica hitozana za prečišćavanje otpadnih voda

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Otpadne vode iz industrije sadrže velike količine zagađujućih materija veoma štetnih po životnu sredinu, a koje se razlikuju po strukturi, veličini molekula, otrovnosti i mogućnosti biorazgradnje. Za tretman otpadnih voda i uklanjanje zagađujućih materija najčešće se koristi sorpcija. Ispituju se različiti materijali za sintezu sorbenata, a trenutno se intenzivno radi na razvoju sorbenata na bazi hitozana. Prisustvo primarnih amino grupa, neotrovnost, dobijanje iz obnovljivih sirovina i bezbednost prilikom rukovanja su glavni razlozi za primenu hitozana za prečišćavanje otpadnih voda. Kapacitet uklanjanja i mogućnost višekratne upotrebe sorbenata na bazi hitozana se može povećati različitim modifikacijama hitozana. Cilj ovog rada bio je sinteza multifunkcionalnih kuglica na bazi modifikovanog hitozana namenjenih za prečišćavanje otpadnih voda. Modifikacija hitozana je izvedena dodatkom amonijumovih soli (glicidil trimetilamonijum-hlorida, 3-hloro-2-hidroksipropil trimetilamonijum-hlorida i tetradecil trimetilamonijum-bromida). Kako bi se dodatno poboljšala mehanička svojstva, kuglice su sintetisane u prisustvu natrijum alginata, odnosno karboksimetil celuloze. Kapacitet sorpcije sintetisanih kuglica je ispitan u rastvoru boje C.I. Acid Orange 7.

Synthesis of multifunctional chitosan beads for wastewater treatment

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Industrial wastewater contains large amounts of pollutants that are very harmful to the environment, and which differ in structure, molecule size, toxicity, and biodegradability. Sorption is most often used for wastewater treatment and the removal of pollutants. Various materials are being investigated for the synthesis of sorbents, while intensive work is currently being done on the development of chitosan-based sorbents. The presence of primary amino groups, non-toxicity, obtained from renewable raw materials, and safety during handling are the main reasons to use chitosan for wastewater treatment. The removal capacity and the possibility for repetitive use of chitosan-based sorbents can be increased by various modifications of chitosan. This work aimed to the synthesis of multifunctional beads based on modified chitosan for wastewater treatment. Chitosan modification was performed by ammonium salts (glycidyl trimethylammonium chloride, 3-chloro-2-hydroxypropyl trimethylammonium chloride, and tetradecyl trimethylammonium bromide). To further improve the mechanical properties, the beads were synthesized in the presence of sodium alginate or carboxymethyl cellulose. The sorption capacity of the synthesized beads was examined by the removal of C.I. Acid Orange 7 from an aqueous solution.

Acknowledgements: *"This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200135)"*

HTM-P-3

Detekcija i identifikacija mikroplastike iz sedimenata međunarodnih reka u Srbiji

Sanja Šešlija*, Milan Radovanović**, Sanja Sakan*, Pavle Spasojević***, Maja Marković***,
Melina Kalagasidis Krušić**, Dragana Đorđević*

Poslednjih decenija mikroplastika je prepoznata kao jedan od glavnih zagađivača životne sredine. Nastaje kao posledica postepene degradacije/fragmentacije većih čestica plastike usled izloženosti različitim faktorima životne sredine kao što su UV zračenje, vetar, vodene struje, mikroorganizmi, itd. Jedan od najvećih izazova u rešavanju problema mikroplastike jesu metode za njenu detekciju i identifikaciju. Zbog raznovrsnosti mikroplastike, postoji potreba za poboljšanjem postojećih i/ili razvojem novih metoda kako bi se ustanovila najpouzdanija metoda za analizu mikroplastike iz različitih uzoraka. Cilj ovog rada bio je utvrđivanje polaznih osnova za razvoj efikasne metoda za detekciju i identifikaciju vrste mikroplastike koja se može naći u sedimentima međunarodnih reka Srbije. Iz uzoraka sedimenata reka najpre je uklonjena organska materija primenom Fentonovog reagensa, nakon čega je urađeno razdvajanje čestica mikroplastike na osnovu gustine. Supernatanti su izdvojeni i filtrirani, a dobijeni filtrati korišćeni za detekciju čestica mikroplastike primenom optičke mikroskopije. Sa ciljem utvrđivanja strukture, detektovane čestice su dalje ispitane primenom energetske-dispersivne spektroskopije i infracrvene spektroskopije sa Furijeovom transformacijom (FTIR).

Detection and identification of microplastics from the sediments of international rivers in Serbia

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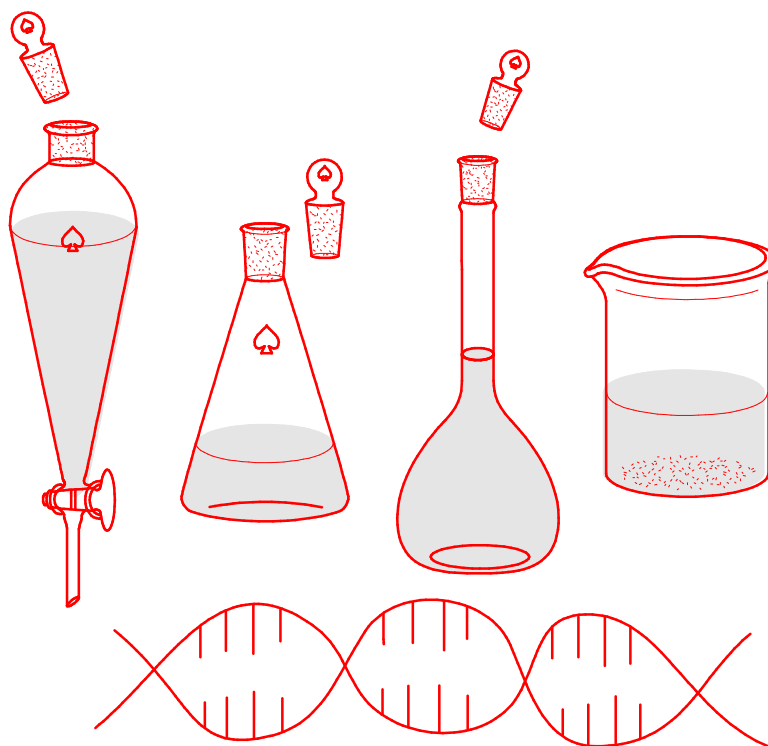
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Microplastics have been recognized as one of the main pollutants of the environment in recent decades. It is formed as a result of gradual degradation/fragmentation of larger plastic particles due to exposure to the different environmental factors such as UV radiation, wind, water currents, microorganisms, etc. One of the biggest challenges in solving the problem of microplastics is the method for their detection and identification. Due to the diversity of microplastics, there is a need to improve existing and/or develop new methods to determine the most reliable method for the analysis of microplastics from different samples. This study was aimed to set the ground for development of efficient method for detection and identification of the microplastics from the sediments of international rivers in Serbia. The sediment samples were firstly treated with Fenton's reagent to remove the organic matter, after which the density separation of microplastics has been performed. The collected supernatants were filtered and used for detection of the microplastics applying optical microscopy. The structure of the detected particles was examined by means of Energy-dispersive spectroscopy (EDS) and Fourier-transform infrared spectroscopy (FTIR).

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Medicinska hemija

Medicinal Chemistry



MH-U-1

Derivati pirazolona: sinteza, antioksidativna aktivnost i molekularni doking sa S i M^{pro} proteinima virusa SARS-CoV-2

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Seriya pirazolonskih derivata dobijena je u reakcijama 5-metil-2,4-dihidro-3H-pirazol-3-ona sa odgovarajućim aromatičnim aldehydima. Sva ispitivana jedinjenja pokazala su odličnu sposobnost *in vitro* inhibicije DPPH radikala, pri čemu je najbolji rezultat dobijen za jedinjenje sa kateholskom farmakoforom ($IC_{50} = 2,63 \pm 0,02 \mu M$). Trenutna globalna situacija prouzrokovana korona virusom motivisala nas je da ispitamo potencijal vezivanja dobijenih jedinjenja sa spajk proteinom (PDB: 6VSB) i M^{pro} proteazom (PDB: 6LU7) virusa SARS-CoV-2. Ovi proteini su značajni zbog njihove velike uloge u procesu vezivanja za ćelijske receptore čoveka, zbog čega se mogu smatrati metama delovanja molekula koji mogu sprečiti to vezivanje, odnosno dalju reprodukciju. Afiniteti vezivanja nekih od dobijenih jedinjenja sa trimernim S proteinom, kao i sa M^{pro} proteazom su uporedivi sa rezultatima dobijenim za lekove kao što su hlorokin, lopinavir i remdesivir.

Pyrazolone derivatives: synthesis, antioxidant activity, and binding to S and M^{pro} proteins of SARS-CoV-2 inferred by molecular docking

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A series of pyrazolone derivatives was obtained in the reactions of 5-methyl-2,4-dihydro-3H-pyrazol-3-one with selected aromatic aldehydes. All compounds expressed excellent *in vitro* scavenging activity against DPPH radical, where the best inhibition potency was found for compound bearing catechol pharmacophore ($IC_{50} = 2.63 \pm 0.02 \mu M$). The emerging global situation with coronavirus motivated us to perform molecular docking analysis of synthesized compounds with SARS-CoV-2 S protein (PDB: 6VSB) and M^{pro} protease (PDB: 6LU7). These proteins were specifically targeted due to their involvement in virus binding to the host human cells and reproduction processes. Therefore, they can be considered targets of action of the molecules which can stop that binding. The binding affinities of some of the investigated compounds with trimeric S protein as well as with M^{pro} protease are comparable with the results obtained for drugs such as chloroquine, lopinavir, and remdesivir.

Acknowledgement: This research was supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-9/2021-14/200122 and 451-03-9/2021-14/200378).

MH-P-2

Interakcije novosintetisanih rutenijum-tpy kompleksa sa DNK i HSA

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Predstavljena je sinteza i karakterizacija serije novih rutenijum(II) kompleksa **1-7**, opšte formule $mer-[RuL_3(N-N)Cl]Cl$, gde je $L = 2,2':6',2''$ -terpiridin (tpy) ili $4'$ -(4-hlorfenil)- $2,2':6',2''$ -terpiridin; $N-N = o$ -benzohinondiimin, 2,3-naftohinondiimin, 4,4'-dimetil-2,2'-bipiridin ili 2,2'-bipiridin-4,4'-dikarboksilna kiselina. Spektrofotometrijski i spektrofluorimetrijski proučavane su interakcije sintetisanih kompleksa sa DNK, primenom interkalirajućeg agensa etidijum-bromida i agensa vezivanja za manji žleb DNK lanca Hoechst 33258, kao i ispitivanjem promene u viskoznosti rastvora DNK. Takođe, ispitivan je afinitet vezivanja kompleksa **1-7** za albumin humanog porekla (HSA). Za preciznije određivanje načina vezivanja za HSA praćena je sposobnost kompleksa da zameni markere eozin Y i ibuprofen na njihovim mestima vezivanja za HSA spektrofluorimetrijskom metodom. U cilju boljeg razumevanja interakcija ispitivanih kompleksa sa biološki važnim molekulima, izvršena su *in silico* modelovanja ukotvljavanjem (*molecular docking*).

Interactions of newly synthesized ruthenium-tpy complexes with DNA and HSA

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The synthesis and structural characterization of a series of new ruthenium(II) complexes **1-7**, with a general formula $mer-[RuL_3(N-N)Cl]Cl$, where $L = 2,2':6',2''$ -terpyridine (tpy) or $4'$ -(4-chlorophenyl)- $2,2':6',2''$ -terpyridine; $N-N = o$ -benzoquinonediimine, 2,3-naphthoquinone diimine, 4,4'-dimethyl-2,2'-bipyridine or 2,2'-bipyridine-4,4'-dicarboxylic acid, are presented. Biomolecular interactions of the complexes with calf thymus DNA (CT DNA) were studied spectrophotometrically and spectrofluorimetrically using an intercalating agent ethidium bromide and by the minor groove binder Hoechst 33258, and by viscosity measurements. Additionally, the binding affinity of complexes **1-7** toward human serum albumin (HSA) was described. To elucidate their HSA binding sites, displacement reactions with the established site markers Eosin Y and Ibuprofen were monitored by spectrofluorimetry. To better understand the interactions between the ruthenium complexes and CT-DNA/HSA, molecular docking studies were performed.

Acknowledgement: Serbian Ministry of Education, Science and Technological Development (Agreements No. 451-03-9/2021-14/200122 and 451-03-9/2021-14/200378)

MH-P-3

Hemoinformatička analiza hinolinskih derivata aromatičnih i heterocikličnih sulfonamida kao inhibitora karboanhidraze I i II

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Karboanhidraza (CA) je metaloenzim cinka koji katalizuje fiziološku reakciju konverzije ugljen-dioksida do bikarbonatnog jona i tako utiče na pH homeostaze. Cilj ove studije je bio da se primenom 2D-QSAR modela odrede najvažniji strukturni deskriptori hinolinskih derivata sulfonamida koji utiču na njihovu CA I i CA II inhibitornu aktivnost. Molekularnim dokingom pokušao se objasniti mehanizam inhibicije CA I i CA II enzima najpotentnijim jedinjenjima. U ovoj studiji, set od 42 sulfonamida sa eksperimentalno određenim pKi vrednostima, je korišćen za 2D-QSAR analizu inhibicije CA I i CA II enzima. Dobijen je najbolji 2D-QSAR model za CA I enzim sa vrednostima R2 (0,9393), Q2 (0,9069) i Rpred2 (0,8066). Primenom iste procedure dobijen je 2D-QSAR model sa vrednostima R2 (0,9558), Q2 (0,9123) i Rpred2 (0,7154) sa odličnim mogućnostima predviđanja inhibicije CA II enzima. Odabrani 2D deskriptori (nArX, nThiazoles, SsssCH, SsssN, SaaN, NssCH2) za CA I enzim, kao i 2D deskriptori (Psi_i_ls, SRW05, nS(=0)2, nArX, nPyridines, SaaS) za CA II imaju značaj u objašnjenju bioloških i farmakoloških osobina važnih za inhibiciju karboanhidraze. Ova studija pruža korisne informacije za dizajn snažnijih i selektivnijih inhibitora enzima CA I i CA II za lečenje glaukoma, epilepsije, ishemične kardiomiopatije i Alchajmerove bolesti.

Chemoinformatics investigation of quinoline derivatives of aromatic and heterocyclic sulfonamides as inhibitors of carbonic anhydrase I and II

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Carbonic anhydrase (CA) is a zinc metalloenzyme that catalyzes the physiological reaction of the conversion of carbon dioxide to bicarbonate ions and thus affecting pH homeostasis. The aim of this study was to use 2D-QSAR models to determine the most critical structural descriptors of quinoline sulfonamide derivatives that affect their CA I and CA II inhibitory activity. Furthermore, to elucidate the mechanism of inhibition of CA I and CA II enzymes with the most potent compounds, molecular docking was performed. In this study, a set of 42 sulfonamides with experimentally determined pKi values was used for the 2D-QSAR analysis of CA I and CA II enzyme inhibition. The best 2D-QSAR model for CA I enzyme with values R2 (0.9393), Q2 (0.9069), and Rpred2 (0.8066) was obtained. By using the same procedure, a 2D-QSAR model with values R2 (0.9558), Q2 (0.9123), and Rpred2 (0.7154) was obtained, with the excellent capability of predicting CA II inhibition. Selected 2D descriptors (nArX, nThiazoles, SsssCH, SsssN, SaaN, NssCH2) for CA I enzyme, as well as 2D descriptors (Psi_i_ls, SRW05, nS(=0)2, nArX, nPyridines, SaaS) for CA II, had significance in explaining biological and pharmacological properties important for inhibition of carbonic anhydrase. This study provides valuable insight for designing more potent and selective CA I and CA II enzyme inhibitors to treat glaucoma, epilepsy, ischemic cardiomyopathy, and Alzheimer's disease.

MH-U-4

Ključni intermedijeri u sintezi protulaktona A

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Protulakton A¹ je prirodni proizvod koji je izolovan 2010. godine iz morske gljive *Aspergillus sp. SF-5044*. Ostvarena je višefazna sinteza ključnih intermedijera za novu sintezu protulaktona A (Scheme 1), polazeći iz D-galaktoze. Pored toga, ispitana je *in vitro* antiproliferativna aktivnost novosintetizovanih alkohola **4**, **5** i **6**.

Key intermediates in protulactone A synthesis

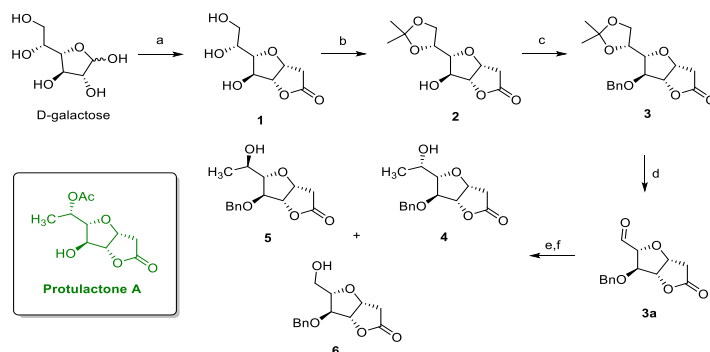
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Protulactone A¹ is a natural product that was isolated in 2010 from the sea fungus *Aspergillus sp. SF-5044*. In this paper, the synthesis of key intermediates for the novel synthesis of this natural product was achieved (Scheme 1), starting from D-galactose. In addition, the *in vitro* antiproliferative activity of newly synthesized alcohols **4**, **5**, and **6** were investigated.



Scheme 1. a) Meldrum's acid, ^tBuNH₂, DMF, 44–46 °C, 5 days, 54%; b) 2,2-DMP, *p*-TsOH×H₂O, acetone, rt, 2 h, 95%; c) BnBr, Ag₂O, CH₂Cl₂, rt, 29 h, 85%; d) H₃IO₆, EtOAc, 45 min, 85%; e) 1.0 M MeMgBr, PhMe, 0 °C → rt, 21 h; f) NaBH₄, MeOH, 13% of **4**, 7% of **5**, 3% of **6**.

Acknowledgement: The work was supported by a grant from the Ministry of Education, Science and Technological Development (Grant No. 451-03-9/2021-14/200125), and (in part) by research projects from the Serbian Academy of Sciences and Arts (Grants No. 01-2019-F6501-2019-F65

¹ J. H. Sohn, H. Oh, *Bull. Korean Chem. Soc.*, 31 (2010) 1695.

MH-U-5

Novi defenilovani analog kardiobutanolida: sinteza, antiproliferativna aktivnost i SAR ispitivanja

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U ovom saopštenju želimo da prikazemo sintezu (Scheme 1)² i antiproliferativnu aktivnost jedinjenja **1**, novog defenilovanog analoga kardiobutanolida. Takođe, detaljno će biti ispitan uticaj konfiguracije na C-6 (**2**), prisustvo fenil grupe (**5**), kao i efekat sternih ograničenja (**4**, **6**) na antitumorsku aktivnost.

A novel dephenylated cardiobutanolide analogue: synthesis, antiproliferative activity and SAR study

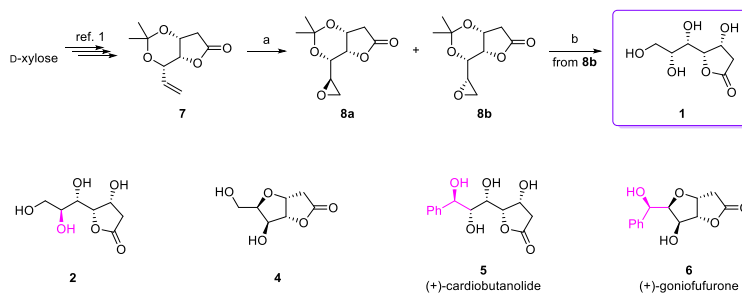
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Herein, we report on the synthesis (Scheme 1)¹ and antitumour activity of compound **1**, a new dephenylated cardiobutanolide analogue. Furthermore, the influence of configuration at C-6 (**2**), presence of phenyl group (**5**) and the effects of steric constrains (**4**, **6**) on antitumour activity will be discussed in detail.



Scheme 1. Reagents and conditions (a) mCPBA, EtOAc; (b) 0.05 M H₂SO₄, EtOAc.

Acknowledgment: The work was supported by a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-9/2021-14/200125), and (in part) by research projects from the Serbian Academy of Sciences and Arts (Grants No. 01-2019-F6501-2019-F65 and F-130).

² I. Kovačević, M. Popsavin, M. V. Rodić, V. Kojić, V. Popsavin, *Tetrahedron Lett.* **60** (2019) 684–687.

MH-P-6

Sinteza i antitumorska aktivnost defenilovanih 5,7-di-*O*-metil analoga goniofufurona

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(+)-Goniofufuron i (–)-goniofufuron su stiril-laktoni sa značajnom citotoksičnom aktivnošću. U ovom radu je ostvarena sinteza njihovih defenilovanih derivata sa 5,7-di-*O*-metil funkcionalnim grupama (*Scheme 1*). Pored toga, ispitana je preliminarna *in vitro* antiproliferativna aktivnost novosintetizovanih analoga.

Synthesis and antitumour activity of dephenylated 5,7-di-*O*-methyl goniofufurone analogues

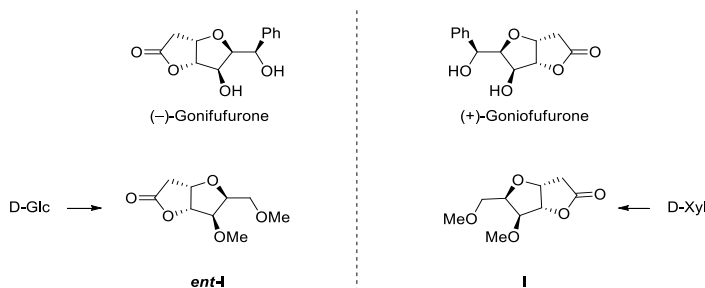
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(+)-Goniofufurone and (–)-goniofufurone are styryl lactones with potent cytotoxic activities. Herein we want to report the synthesis of dephenylated derivatives of these styryl lactones with *O*-methyl functional groups (*Scheme 1*). In addition, the preliminary *in vitro* antiproliferative activity of newly synthesized analogues was investigated.



Scheme 1. Structures of (+)-goniofufurone, (–)-goniofufurone and dephenylated 5,7-di-*O*-methyl analogues.

Acknowledgement: The work was supported by a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-9/2021-14/200125), and (in part) by research projects from the Serbian Academy of Sciences and Arts (Grants No. 01-2019-F6501-2019-F65 and F-130).

MH-P-7

Sinteza, citotoksičnost i SAR analiza novih analoga (–)-murikatacina

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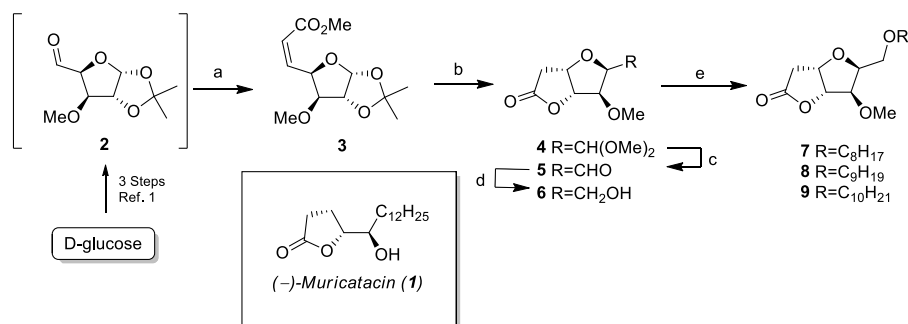
(–)-Murikatacin (**1**) je prirodni proizvod koji pokazuje značajnu antitumorsku aktivnost. U ovom radu je ostvarena sinteza novih 8-oksa analoga (–)-murikatacina **7–9** sa furano-furanonskim sistemom prstenova i metoksi grupom u položaju C-5 (Scheme 1), polazeći iz D-glukoze³. Ispitana je citotoksična aktivnost prema 9 malignih i jednoj zdravoj ćelijskoj liniji i biće predstavljeni rezultati SAR analize.

Synthesis, cytotoxicity and SAR analysis of novel (–)-muricatacin analogues

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(–)-Muricatacin (**1**) is natural product with significant antitumor activity. In this work, the synthesis of novel 8-oxa analogues of (–)-muricatacin **7–9** with a furano-furanone ring system and methoxy group in position C-5 was achieved starting from D-glucose (Scheme 1)¹. Cytotoxic activity was examined against 9 malignant and one healthy cell line. Also, the results of the SAR analysis will be presented.



Scheme 1. Reagents and conditions: (a) Ph₃P:CHCO₂Me, MeOH, 0°C, 0.5 h then rt, 1.5 h; (b) 2.5% H₂SO₄/MeOH, reflux, 2 h, NaHCO₃, rt, 1 h; (c) 9:1 TFA/H₂O, rt, 1 h; (d) NaBH₄, MeOH, rt, 1.5 h; (e) C₈H₁₇Br for **7**, C₉H₁₉Br for **8**, C₁₀H₂₁Br for **9**, Ag₂O, AgOTf, Et₂O, reflux.

Acknowledgment: The work was supported by a grant from Ministry of Education, Science and Technological Development (Grant No. 451-03-9/2021-14/200125), and (in part) by research projects from the Serbian Academy of Sciences and Arts (Grants No. 01-2019-F6501-2019-F65 and F-130).

³ J. Francuz, M. Popsavin, S. Djokić, V. Kojić, T. Srdić-Rajić, M. V. Rodić, D. Jakimov, V. Popsavin, *Med. Chem. Commun.* **9** (2018) 2017–2027.

MH-P-8

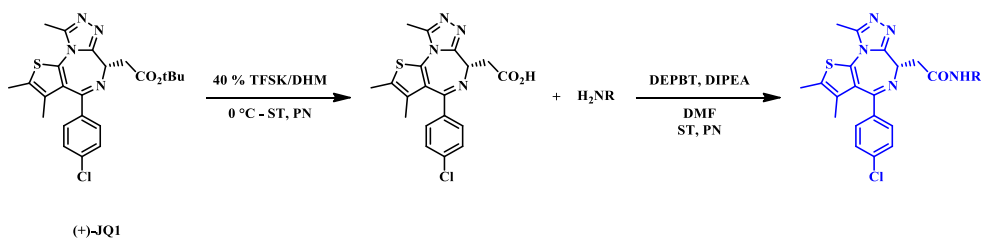
Sinteza i biološko profilisanje (+)-JQ1 amida kao BET inhibitora

Mladen Koravović, Gordana Tasić, Anand Mayasundari*, Fatemeh Keramatnia*, Marcus Fischer*, Zoran Ranković*, Milena Simić, Vladimir Savić

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BET proteini su epigenetski biološki targeti koji regulišu ekspresiju gena i uključeni su u patogenezu kancera. Jedan od inhibitora ovih proteina koji je opisan u literaturi je derivat tienotriazolodiazepina (+)-JQ1. Cilj ovog rada bio je dalje unapređenje osobina (+)-JQ1 derivatizacijom estarske grupe (Shema 1). U toku ovog istraživanja sintetisano je više amidnih analoga od koji je jedan pokazao 16 puta veću aktivnost u TR-FRET testu u odnosu na (+)-JQ1.



Shema 1. Derivatizacija estarske grupe

Zahvalnica: Ovo istraživanje finansirano je od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije kroz Ugovor sa Univerzitetom u Beogradu - Farmaceutskim fakultetom broj: 451-03-9/2021-14/200161.

Synthesis and biological profiling of (+)-JQ1 amides as BET inhibitors

Mladen Koravovic, Gordana Tasic, Anand Mayasundari*, Fatemeh Keramatnia*, Marcus Fischer*, Zoran Rankovic*, Milena Simic, Vladimir Savic

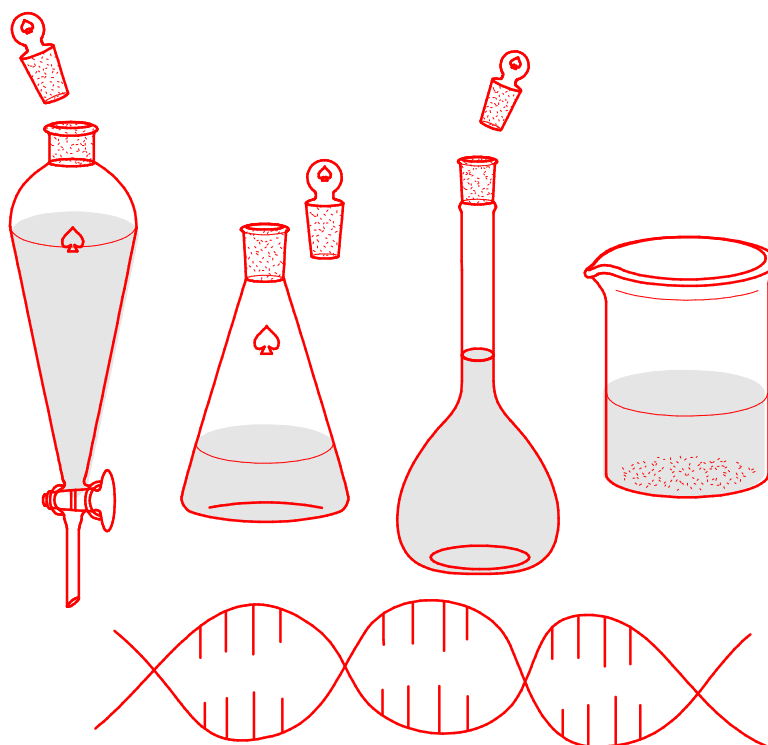
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*St. Jude Children's Research Hospital, Department of Chemical Biology and Therapeutics, Memphis, TN 38105, USA

BET proteins are epigenetic biological targets that regulate gene expression and are involved in cancer pathogenesis. One of BET inhibitors described in the literature is thienotriazolodiazepine derivative (+)-JQ1. The aim of this research was to further improve the properties of (+)-JQ1 by ester group derivatization (Scheme 1). During the research several amide analogs were synthesized and one of them had 16 fold greater activity in TR-FRET assay compared to (+)-JQ1.

Organska hemija

Organic Chemistry



OH-P-1

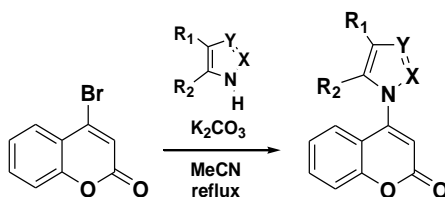
Sinteza i antikancerski potencijal 4-azolilkumarina

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**Institut za onkologiju i radiologiju Srbije, Pasterova 14, 11000 Beograd, Srbija*

Kumarini su heterociklična jedinjenja veoma rasprostranjen u prirodi. Kao privilegovana struktura, ovaj molekul se nalazi i u velikom broju sintetskih derivata sa značajnom biološkom aktivnošću. Posebno su interesantni hibridi koji sadrže dve farmakofore, od kojih je jedna kumarin. Cilj ovog istraživanja bio je sinteza serije jednostavnih novih 4-azolil kumarina i evaluacija njihove *in vitro* citotoksičnosti prema humanim kancerskim ćelijskim linijama HeLa, K562, MCF-7 i MDA-MB-453.



Synthesis and anticancer potential of 4-azolylcoumarins

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Coumarins are heterocyclic compounds widely distributed in nature. As a privileged structure, coumarin is also found in a large number of synthetic molecules with important biological activity. Particularly interesting compounds are coumarin-containing hybrids, compounds with two or more pharmacophores. The aim of this work was preparation of simple novel azolyl-coumarin hybrids and evaluation of their cytotoxic effect on human cancer cells, HeLa, K562, MDA-MB-453 and MCF-7.

Acknowledgement: This research was funded by the Ministry of Education, Science and Technological Development, Republic of Serbia through Grant Agreement with University of Belgrade-Faculty of Pharmacy No: 451-03-9/2021-14/200161.

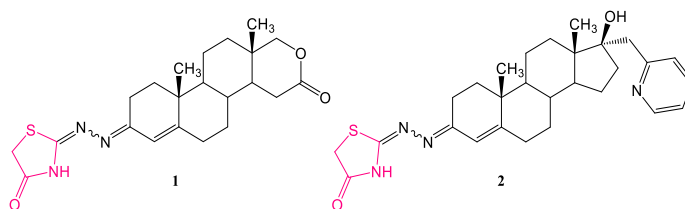
OH-P-2

Sinteza i *in silico* ADME analiza novih steroidnih tiazolidinonskih derivata

Tijana Šestić, Marina Savić, Jovana Ajduković

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

Heterociklična jedinjenja se smatraju značajnim strukturama u medicinskoj hemiji zbog širokog spektra farmakoloških primena. Inkorporacija heterocikličnih prstenova u steroidno jezgro predstavlja korisnu strategiju za razvoj novih antikanceranih agenasa.¹ Među heterocikličnim derivatima, tiazolidinoni su prepoznati kao široko primenjivana farmakofora.² Uzimajući u obzir farmakološki potencijal tiazolidinona i steroida, sintetizovani su novi androstanski tiazolidinonski derivati (**1** i **2**) iz tiosemikarbazona kao prekursora. Nova jedinjenja su okarakterisana spektroskopskim podacima. *In silico* fizičko-hemijska ispitivanja su izvedena pomoću web alatke SwissADME, gde su parametri za oba jedinjenja u optimalnom opsegu, što ukazuje da poseduju željena svojstva leka.

**Synthesis and *in silico* ADME analysis of new steroid thiazolidinone derivatives**

Tijana Šestić, Marina Savić, Jovana Ajduković

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

Heterocyclic moieties are considered as privileged structures in medicinal chemistry due to a wide range of pharmacological applications. The incorporation of heterocycles into the steroid nucleus represents a useful strategy for the development of new anticancer agents.¹ Among heterocyclic derivatives, thiazolidinone core has been well recognized as a widely exploited pharmacophore.² Considering pharmacological potential of both thiazolidinones and steroids, herein we present a synthetic route for the production of new androstane thiazolidinone derivatives (**1** and **2**) from thiosemicarbazones as precursors. New derivatives were characterized by spectroscopic data. *In silico* physicochemical properties were determined using the web tool SwissADME, where parameters for both compounds were within the optimal range, suggesting them as drug-like molecules.

1. M. A. Tantawy, M. S. Nafie, G. A. Elmegeed, I. A. I. Ali, *Bioorg. Chem.* **73** (2017) 128-146.
2. M. B. Živković, I. Z. Matić, M. V. Rodić, I. T. Novaković, A. M. Krivokuća, D. M. Sladić, N. M. Krstić, *J. Steroid. Biochem.* **174** (2017) 72-85.

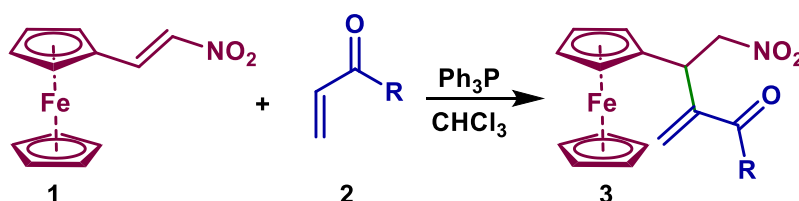
Acknowledgement: *The authors acknowledge financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/200125).*

OH-P-3

Ukrštena Rauhut-Currier-ova reakcija 1-ferrocenil-2-nitroetilena sa vinil-ketonima

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 Kragujevac

Rauhut-Currier-ova reakcija omogućava formiranje nove ugljenik-ugljenik veze između dva različita elektron-deficitarna alkena (Michael-ova akceptora) u prisustvu nukleofilnih katalizatora (Lewis-ove baze).^{1,2} Značaj ove reakcije se ogleda u dobijanju visokofunkcionalnih proizvoda koji mogu da posluže kao supstrati za brojne sintetičke transformacije.¹ Stoga, razvijena je metoda za hemoselektivnu sintezu derivata ferocena **3** Rauhut-Currier-ovim kuplovanjem između α -položaja vinil-ketona **2** i β -položaja nitroalkena **1** u prisustvu trifenilfosfina.



Cross Rauhut-Currier reaction of 1-ferrocenyl-2-nitroethylene with vinyl ketones

Dragana Stevanović, Jovana Bugarinović, Marko Pešić, Ivan Damljanović
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A cross Rauhut-Currier reaction provides a new carbon-carbon bond formation between two different electron-deficient alkenes (Michael acceptors) in the presence of nucleophilic catalysts (Lewis bases).^{1,2} This reaction yields multifunctional compounds that are used for further synthetic transformation.² Herein, a simple method for the chemoselective synthesis of ferrocene-containing derivatives **3** by the Rauhut-Currier coupling between the α -position of vinyl ketones **2** and the β -position of nitroalkene **1** in the presence of triphenylphosphine has been developed.

1. C. E. Aroyan, A. Dermenci, S. J. Miller, *Tetrahedron* **2009**, 65, 4069–4084.
2. P. Xie, Y. Huang, *Eur. J. Org. Chem.* **2013**, 6213–6226.

Acknowledgment: This work was supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-9/2021-14/200122).

OH-P-4

Komparativna studija antioksidativne aktivnosti boja i obojene tkanine: 5-(4-supstituisani fenilazo)-3-piridinijum-6-hidroksi-4-metil-2-piridoni

Aleksandra Mašulović, Aleksandra Ivanovska, Jelena Lađarević *, Julijana Tadić, Luka Matović, Mirjana Kostić*, Dušan Mijin*

Inovacioni centar Tehnološko-metalurškog fakulteta u Beogradu, Karnegijeva 4, Beograd, Srbija
**Tehnološko-metalurški fakultet, Univerzitet u Beogradu, Karnegijeva 4, Beograd, Srbija*

U ovom radu prikazane su sinteza i primena dve azo boje na bazi 6-hidroksi-4-metil-3-piridinijum-2-piridona. Supstituisani piridon dobijen je Guaresi-Torpeovom reakcijom kondenzacije, dok su azo boje sintetisane klasičnim postupkom diazo kuplovanja pri čemu su korišćena dva različito p-supstituisana anilina. Primenom FTIR, ¹H i ¹³C NMR, UV-Vis i masene spektroskopije dobijena jedinjenja su okarakterisana. U zavisnosti od rastvarača i supstituenta, boje se nalaze u ravnoteži dva tautomerna oblika, hidrazonskog i cviterjonskog, za razliku od literaturnih analoga u kojima se navodi hidrazon-azo anjon ravnoteža. Specifična struktura dobijenih boja omogućava bolju rastvorljivost, pre svega u vodi. Primena se sastoji u bojenju vune pri ranije optimizovanim uslovima bojenja. U ovom radu na osnovu predloženog mehanizma vidi se da, pored očekivanih vodoničnih veza, jon-jon interakcije učestvuju u vezivanju boje za tkaninu. Komparativna studija antioksidativne aktivnosti boja i obojenih tkanina urađena je pomoću ABTS metode.

Comparative study of the antioxidant activity of dyes vs. dyestuff: 5-(4-substituted phenylazo)-3-pyridinium-6-hydroxy-4-methyl-2-pyridones

Aleksandra Mašulović, Aleksandra Ivanovska, Jelena Lađarević *, Julijana Tadić, Luka Matović, Mirjana Kostić*, Dušan Mijin*

Innovation Centre, Faculty of Technology and Metallurgy, Belgrade, Serbia **Faculty of Technology and Metallurgy, Belgrade, Serbia*

Herein, we report the synthesis and application of two azo dyes based on 6-hydroxy-4-methyl-3-pyridinium-2-pyridone. The substituted pyridone was synthesized via Guareschi-Thorpe condensation, wherein dyes are obtained by the classical reaction of diazo coupling by using two diversely p-substituted anilines. The characterization of the synthesized compounds was carried out by FTIR, ¹H and ¹³C NMR, UV-Vis and mass spectroscopy. These compounds exist in an equilibrium of two tautomeric forms in solution depending on the solvent as well as on the substituent and are water-soluble. It is worth mentioning that the hydrazone form of the dyes is in equilibrium with the zwitterion form of the dyes unlike the literature analogs existing in the anionic form. The application of the dyes consists of dyeing wool fiber at optimized conditions. The dyeing mechanism is suggested, wherein it revealed that these like dyes utilize ion-ion interactions next to expected hydrogen bonds. A comparative study on the antioxidant activity of the dyes and the dyestuff was conducted using ABTS assay.

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract Nos. 451-03-9/2021-14/200287 and 451-03-9/2021-14/200135).

OH-P-5

DNK interakcije 17-supstituisanih A-modifikovanih androstanskih derivata

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Steroidi čine obimnu i važnu klasu biološki aktivnih policikličnih jedinjenja koja imaju široku primenu u terapijske svrhe. Otkriveno je da uvođenje heteroatoma ili heterocikla u steroidno jezgro, ili zamena jednog ili više atoma ugljenika u molekulu steroida heteroatomom, može dovesti do promene njegovih bioloških aktivnosti. Steroidi koji sadrže heteroatome su široko istraženi i publikovani [1]. Nedavni razvoj u sintezi derivata androstana koji sadrže heterocikle ukazuju da takva jedinjenja mogu da ispolje obećavajuću citotoksičnu aktivnost prema tumorskim ćelijskim linijama [2]. Interakcije 17-supstituisanih A-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.

DNA interactions of 17-substituted A-modified androstane derivatives

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

Steroids constitute an extensive and important class of biologically active polycyclic compounds that are widely used for therapeutic purposes. It was found that introducing a heteroatom or heterocycles into steroid nucleus, or replacing one or more carbon atoms in steroid molecule with a heteroatom, can result in a change in its biological activities. Steroids containing heteroatoms have been widely researched and reported [1]. Recent developments in the syntheses of androstane derivatives containing heterocycles have suggested that such compounds can display promising cytotoxicity against cancer cell lines [2]. Interactions of 17-substituted A-modified androstane derivatives with DNA were examined using UV-Vis and fluorescence spectroscopy. Based on the obtained results, it was found that androstane derivatives stabilize the DNA strand, but they cannot displace ethidium bromide (EtBr) from DNA-EtBr and therefore are not intercalators.

[1] Stulov, S. V.; Misharin A. Y. *Chem. Heterocycl. Compd.* 2013, **48**, 1431.

[2] Ajduković, J. J.; Penov Gaši, K. M.; Jakimov, D. S.; Klisurić, O. R.; S. S. Jovanović-Šanta, Sakač, M. N.; Aleksić, L. D.; Djurendić, E. A. *Bioorg. Med. Chem.* 2015, **23**, 1557.

Acknowledgements: *The authors acknowledge financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/200122 and 451-03-9/2021-14/200125).*

ОН-Р-6

Улога интермолекулских интеракција у супрамолекулој организацији и биолошком препознавању деривата спирохидантоина

Анита М. Лaziћ, Ивана С. Ђорђевић,* Лидија Д. Радовановић, Драган М. Поповић,* Јелена Р. Роган,** Горан В. Јањић,* Немања П. Тришовић

Синтетисан је рацемски дериват спирохидантоина, који поседује тетралинску и 4-метоксибензил-групу, а затим је одређена његова кристална структура. Хијерархијски развој кристалног паковања дискутован је са аспекта кооперативности хомо- и хетерохиралних димерних мотива који одражавају различите интермолекулске интеракције. Специфична структурна карактеристика проучаваног једињења јесу наизменично постављени двоструки слојеви. Велики број контактних фрагмената у окружењу тетралинске групе представља последицу веће контактне површине. Са друге стране, 4-метоксибензил-група обезбеђује већи допринос укупној стабилизацији. Што се тиче фармаколошког потенцијала проучаваног једињења, извршена је симулација везивања молекула за допамински рецептор D3 и ензим IRAK 4 (eng. Interleukin-1 Receptor-Associated Kinase 4). Укупан број аминокиселинских остатака који ступају у интеракцију са 4-метоксибензил-групом је нешто већи од броја аминокиселинских остатака у окружењу тетралинске групе. Услед веће флексибилности, 4-метоксибензил-група се лакше адаптира за успостављање интеракција са биолошким циљевима.

Role of intermolecular interactions in the self-assembly and biorecognition of a spirohydantoin derivative

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A racemic spirohydantoin derivative bearing a tetralin and 4-methoxybenzyl group was synthesized and its crystal structure was determined. The hierarchical development of the crystal packing was discussed through cooperativity of various homo and heterochiral dimeric motifs associated with the presence of different intermolecular interactions. A hallmark structural feature of the investigated compound was alternation of double layers. A larger number of the contact fragments in the environment of the tetralin unit results from its larger contact surface, while the 4-methoxybenzyl unit provides a slightly greater contribution to the overall stabilization. Regarding the pharmacological potential of the investigated compound, we performed a docking study on the dopamine D3 receptor and IRAK 4 (Interleukin-1 Receptor-Associated Kinase 4) enzyme. The total number of amino acid, which interact with the 4-methoxybenzyl unit, was slightly larger than the number of amino acids in the neighborhood of the tetralin unit as a result of its greater flexibility. It made the 4-methoxybenzyl unit more adaptable for interactions with the biological targets.

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200135; 451-03-9/2021-14/200287, 451-03-9/2021-14/200026).

OH-P-7

Sinteza derivata 6,7-dihidro-5H-pirano[3,2-d]tiazol-2-amina

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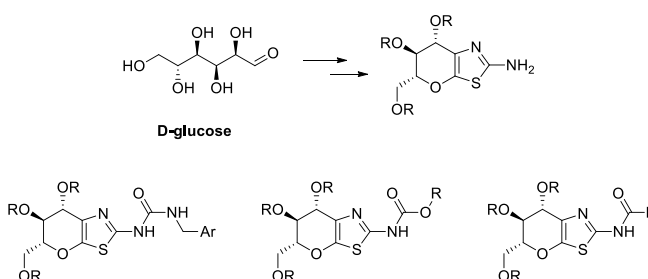
Monosaharidi predstavljaju idealne prekursore u organskoj sintezi: poseduju veliki broj funkcionalnih grupa i stereocentara, dostupni su u velikim količinama, mogu se dobiti iz obnovljive biomase i imaju nisku cenu. Prikazaćemo sintezu derivata 6,7-dihidro-5H-pirano[3,2-d]tiazol-2-amina, polazeći iz D-glukoze, u cilju ispitivanja potencijalne biološke aktivnosti. Željena jedinjenja bi zbog posedovanja šećernog motiva trebalo da imaju veću bioraspoloživost usled lakšeg prolaska kroz ćelijske membrane i bolje rastvorljivosti u fiziološkim uslovima.

Synthesis of 6,7-dihydro-5H-pyrano[3,2-d]thiazol-2-amine derivatives

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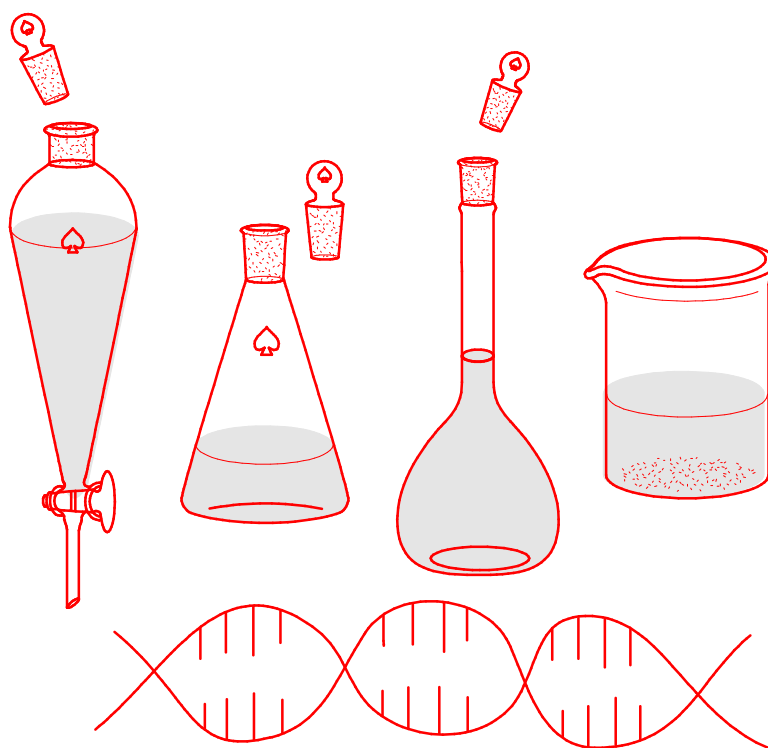
Monosaccharides are ideal substrates in organic synthesis: they are rich in functional groups and stereocenters, they are available in large quantities, they can be obtained from renewable sources and aren't expensive. We present the synthesis of 6,7-dihydro-5H-pyrano[3,2-d]-thiazol-2-amine derivatives in order to investigate their potential biological activity. It is expected that target compounds will have greater bioavailability due to easier transit through cell membranes and better solubility under physiological conditions.



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Teorijska hemija

Theoretical Chemistry



TH-P-1

Korelacija eksperimentalnih podataka sa teorijskim predviđanjem sorpcije jona teških metala na makroporoznom amino-funkcionalizovanom sorbentu

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Decenijama se različiti sorbenti primenjuju za tretman otpadnih voda kontaminiranih jonima teških metala, koji ozbiljno ugrožavaju živi svet. Makroporozni funkcionalni polimeri pokazuju visok afinitet za jone teških metala, pri čemu efikasnost sorpcije i selektivnost direktno zavise od prirode funkcionalnih grupa sorbenta i jona metala. U radu je predstavljena korelacija teorijskih predviđanja i eksperimentalnih podataka dobijenih ispitivanjem sorpcije katjona Cu^{2+} , Co^{2+} , Ni^{2+} i Cd^{2+} u konkurentnim i nekonkurentnim uslovima u vodenom rastvoru na makroporoznom amino-funkcionalizovanom sorbentu poli(glicidil-metakrilat-co-etilen glikol dimetakrilat), PGME-deta. Kvantno-hemijskim proračunima procenjene su energije vezivanja metalnih jona za aktivna mesta sorbenta na model sistemima pojedinačnih fragmenata, metal-ligand, dobijenih statističkom analizom podataka baze kristalnih struktura. Ovakav teorijski pristup pokazao je visok stepen korelacije sa eksperimentalnim podacima u jednodimenzionalnim sistemima.

Correlation of experimental data and theoretical predictions of heavy metal sorption by macroporous amino-functionalized sorbent

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Over the decades, various sorbents have been used in the treatment of wastewater contaminated with heavy metal ions, which seriously endanger the living world. Macroporous functional polymers show a high affinity for sorption of these ions, where sorption efficiency and selectivity directly depend on the nature of the functional groups of sorbent and metal ions. In this study, we performed a correlation of theoretical predictions and experimental data obtained by investigation of Cu^{2+} , Co^{2+} , Ni^{2+} and Cd^{2+} cations sorption under competitive and uncompetitive conditions from aqueous solutions on macroporous amino-functionalized sorbent poly(glycidyl methacrylate-co-ethylene glycol dimethacrylate), PGME-deta. Quantum-chemical calculations estimated the binding energies of metal ions to the active sites of the sorbent, on the model systems of individual fragments, composed of metal ions and ligands, based on statistical analysis of data obtained from crystal structures. By this theoretical approach, the high degree of correlation with experimental data was observed for mono-component system.

This work was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/200026 and 451-03-9/2021-14/200135).

TH-P-2

Jake vodonične veze koordinovanog molekula amonijaka

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Vodonične veze nekoordinovanog (NH/O) i koordinovanog amonijaka (MLNH/O) sa molekulom vode su proučavane analizirajući Kembričku banku kristalografskih podataka (CSD) i koristeći DFT proračune. Podaci iz CSD-a koji pokazuju raspodelu $d_{\text{H}_2\text{O}}$ rastojanja koordinovanog amonijaka pokazuju pik u opsegu od 2.0 - 2.2 Å sa značajnim brojem vodoničnih veza u opsegu od 1.8 - 2.0 Å. DFT proračuni su korišćeni za linearne komplekse srebra(I), kvadratno-planarne komplekse platine(II), tetraedarske komplekse cinka(II), i oktaedarske komplekse kobalta(III), različitih naelektrisanja. Izračunati podaci pokazuju da koordinovani amonijak ima jače vodonične veze od nekoordinovanog, čak i kad je kompleks neutralan. Energija vodonične veze za nekoordinovani amonijak je -2.3 kcal/mol, dok je za koordinovani amonijak u opsegu od -5.5 do -25.0 kcal/mol, zavisino od jona metala i naelektrisanja kompleksa. Energija interakcije je u dobroj saglasnosti sa elektrostatičkim potencijalom (V_s) na interagujućem vodonikovom atomu; pozitivnija V_s vrednost na vodonikovom atomu vodi ka jačim interakcijama.

Strong Hydrogen bonds of coordinated ammonia molecules

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The hydrogen bonds of noncoordinated (NH/O) and coordinated ammonia (MLNH/O) with water molecule were studied by analyzing data in the Cambridge Structural Database (CSD) and by DFT calculations. The data from the CSD on the distribution of hydrogen bond $d_{\text{H}_2\text{O}}$ distances of the coordinated ammonia show peak in the range of 2.0 - 2.2 Å with significant number of hydrogen bonds in the range of 1.8 - 2.0 Å. The DFT calculations were performed on linear complexes of silver(I), square-planar complexes of platinum(II), tetrahedral complexes of zinc(II), and octahedral complexes of cobalt(III), varying the charge of the complexes. The calculated data show that coordinated ammonia has stronger hydrogen bonds than noncoordinated, even for neutral complexes. The hydrogen bond energy for noncoordinated ammonia is -2.3 kcal/mol, while for coordinated ammonia is in the range -5.5 to -25.0 kcal/mol, depending on the metal ion and charge of the complex. The interaction energies correspond well with the electrostatic potential (V_s) values on interacting hydrogen atoms; the more positive V_s values on hydrogen atoms lead to stronger interaction.

This work was supported by the Serbian Ministry of Education, Science and Technological Development (Contract numbers: 451-03-9/2021-14/200168 and 451-03-9/2021-14/200288)

ТН-Р-3

Улога нековалентних интеракција у модификовању особина високоенергетских материјала

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У овом раду смо испитивали утицај нековалентних интеракција на електростатичке потенцијале и осетљивост ка детонацији одабраних високоенергетских молекула. Резултати прорачуна рађених на М06/сс-РVDZ нивоу су показали да водоничне везе значајно утичу на вредности електростатичког потенцијала и осетљивост ка детонацији високоенергетских молекула. У случајевима када високоенергетски молекул игра улогу акцептора водоника, вредности електростатичког потенцијала изнад центара високоенергетских молекула се смањују за 20-25%. Ово даје могућност за коришћење водоничног везивања за модификовање осетљивости високоенергетских молекула.

Истраживање спроведено уз подршку Фонда за науку Републике Србије, ПРОМИС, #6066886, CD-HEM.

Role of non-covalent interactions in modification of properties of high energetic materials

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In this work we studied influence of non-covalent interactions on the electrostatic potentials and impact sensitivity of selected high energetic molecules (HEM). Study was performed using quantum chemical calculations on model systems and crystal structures of selected HEMs. Results of M06/cc-PVDZ calculations showed that hydrogen bonding significantly affects electrostatic potential values and impact sensitivities of HEMs. In cases in which HEM molecules act as hydrogen atom acceptors, electrostatic potential values in the centers of HEM molecules decreases by 20-25%. This gives opportunity for modification of impact sensitivities of HEM molecules.

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

TH-U-4

Steking interakcije između *p*-cimen liganada u polusendvič-jedinjenjima rutenijuma(II)

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Pretraživanje kristalnih struktura arhiviranih u Kembričkoj bazi strukturnih podataka (CSD) urađeno je kako bi se pronašle steking interakcije između *p*-cimen (1-metil-4-izopropilbenzen) liganada u kompleksima prelaznih metala. Najveći broj steking interakcija uspostavljen je između *p*-cimen liganada u polusendvič-jedinjenja rutenijuma(II) sa hloridnim i ligandima koji sadrže azot, u antiparalelnoj orijentaciji. U najzastupljenijoj geometriji uspostavljaju se steking interakcije aromatičnih prstenova, kao i C-H/ π interakcije metil-supstituenata sa aromatičnim prstenovima, dok druga najzastupljenija geometrija uključuje steking i C-H/ π interakcije aromatičnih prstenova sa metil-grupama izopropil-supstituenata. Najzastupljenija geometrija pronađena u CSD odgovara najjačoj izračunatoj interakciji između *p*-cimen liganada model-kompleksa [Ru(*p*-cym)Cl₂(NH₃)]. Energija ove interakcije, izračunata na B97-D2/def2-TZVP nivou teorije, iznosi -7,56 kcal/mol, što je značajno jače od steking interakcije između benzen liganada model-kompleksa [Ru(benzen)Cl₂(NH₃)] (-3,93 kcal/mol). Proračuni pokazuju da prisustvo supstituenata može značajno da poveća jačinu steking interakcija.

Stacking interactions between *p*-cymene ligands in ruthenium(II) half-sandwich compounds

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A search of crystal structures deposited in the Cambridge Structural Database (CSD) was performed in order to find stacking interactions between *p*-cymene (1-methyl-4-isopropylbenzene) ligands of transition metal complexes. The vast majority of stacking interactions were between *p*-cymene ligands in ruthenium(II) half-sandwich compounds with chloride and nitrogen ligands, in antiparallel orientation. The most frequent geometry involves stacking of aromatic rings and C-H/ π interactions of methyl substituents with aromatic rings, while the second most frequent geometry involves stacking and C-H/ π interactions of aromatic rings with methyl groups of isopropyl substituents. The most frequent stacking geometry found in the CSD corresponds to the strongest calculated interaction between *p*-cymene ligands of the model complex [Ru(*p*-cym)Cl₂(NH₃)]. The B97-D2/def2-TZVP energy of this interaction is -7.56 kcal/mol, which is significantly stronger than the stacking between benzene ligands of [Ru(benzene)Cl₂(NH₃)] (-3.93 kcal/mol), showing that the presence of substituents can significantly increase the strength of stacking interactions.

This research was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (contract 451-03-68/2020-14/200168).

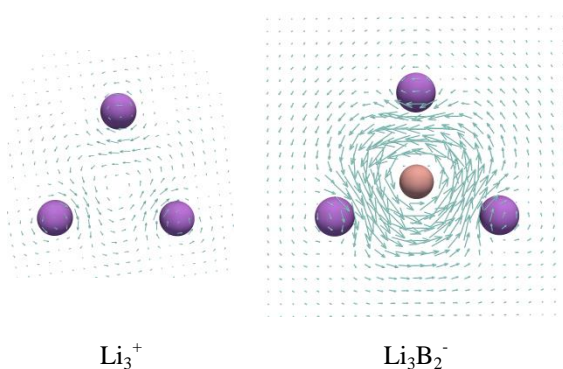
TH-U-5

Podršavanje magnetno indukovanih gustina struja u Li klasterima

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Poznato je da monociklični Li_3^+ i Li_4^{2+} klasteri nisu aromatični. U prisustvu spoljašnjeg magnetnog polja, ovi klasteri pokazuju veoma slabe globalne gustine struja. U ovom radu je pokazano da uvođenje B_2^{2-} jedinice u ove sisteme daje klustere Li_3B_2^- i Li_4B_2 , koji se sastoje iz Li_3/Li_4 prstena između dva atoma bora. Pronađeno je da strukture Li_3/Li_4 u Li_3B_2^- i Li_4B_2 podsećaju na monociklične Li_3^+ i Li_4^{2+} klustere. Sa druge strane, magnetno indukovane gustine struje u Li_3B_2^- i Li_4B_2 , dobijene na M06-2X/CTOCD-DZ/def2-TZVP nivou teorije, suprotno od Li_3^+ i Li_4^{2+} , pokazuju izrazito diatropni karakter. Dobijene gustine struja se mogu direktno povezati sa elektronskom strukturom klastera preko analize virtuelnih prelaza iz popunjenih u nepopunjene molekulske orbitale.

**Modulating the magnetically induced current density in monocyclic Li clusters**

Sladana Đorđević, Slavko Radenković

Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac

It is known that the monocyclic Li_3^+ and Li_4^{2+} clusters are non-aromatic. In the presence of an external magnetic field these clusters show negligibly weak global current densities. In this work we showed that introduction of the B_2^{2-} unit in these systems resulted in stable Li_3B_2^- and Li_4B_2 clusters which consist of Li_3/Li_4 rings sandwiched by two boron atoms. We found that the Li_3/Li_4 rings in Li_3B_2^- and Li_4B_2 remarkably resemble the monocyclic Li_3^+ and Li_4^{2+} clusters. On the other hand, the magnetically induced current densities obtained at the M06-2X/CTOCD-DZ/def2-TZVP level of theory showed that in contrast to Li_3^+ and Li_4^{2+} , the Li_3B_2^- and Li_4B_2 clusters sustain a strong diatropic current density. The observed current densities in the studied clusters can be directly related to their electronic structure by analysing occupied-to-virtual orbital transitions.

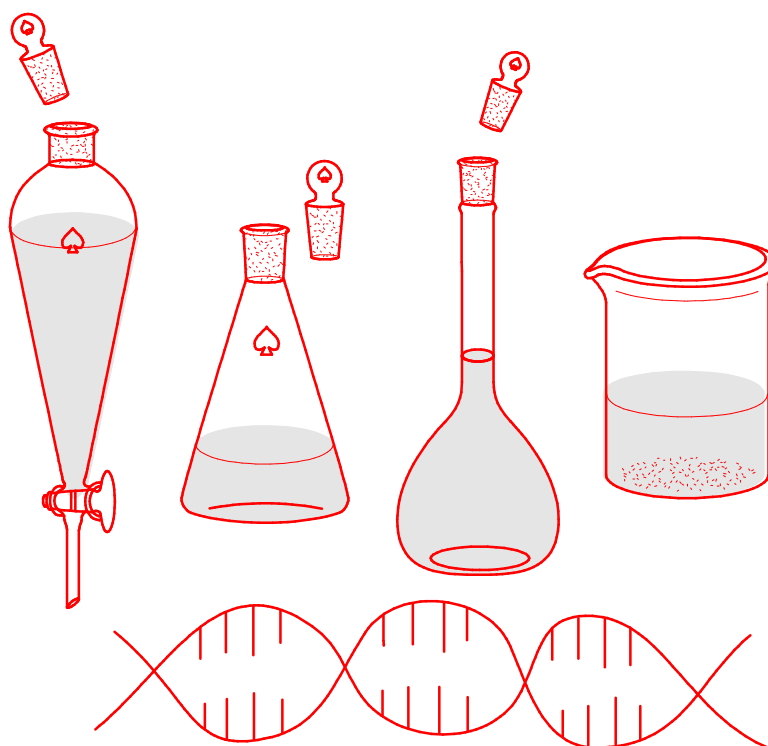
Acknowledgement: This work was supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-9/2021-14/200122).

KNJIGA RADOVA

Proceedings

Analitička hemija

Analytical Chemistry



TR-AH-1

Optimizacija uslova za degradaciju ibuprofena pomoću hlor – dioksida

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Izvod

Ibuprofen (IBP) zbog svoje široke primene, velike konzumacije, relativno brzog metabolizma i eliminacije iz organizma, predstavlja potencionalni rizik po životnu sredinu. Hlor - dioksid, kao jako oksidaciono sredstvo, pokazao se kao dobar reagens za uklanjanje određenih grupa pesticida iz hrane i vode, kao i za degradaciju određenih lekova. Cilj ovog rada bio je da se ispita pod kojim uslovima i u kojoj meri hlor - dioksid može da ukloni IBP u vodi. Ispitivana je degradacija IBP različitih koncentracija (10, 20, 35 i 60 mg/L) sa različitim koncentracijama hlor - dioksida (5, 10 i 15 mg/L) na pH vrednostima 3,00, 7,00 i 10,00 i pri različitim reakcionim vremenima (0,5 h, 1 h, 2 h, 3 h, 6 h, 24 h). Rezultati HPLC - DAD analize su pokazali da je IBP moguće efikasno ukloniti iz vode. Najveća efikasnost degradacije od 99% postignuta je kada je koncentracija IBP u vodi bila 10 mg/L, a rastvor je bio tretiran sa 15 mg/L hlor - dioksida na pH 10,00 posle 24 h tretiranja hlor - dioksidom.

Uvod

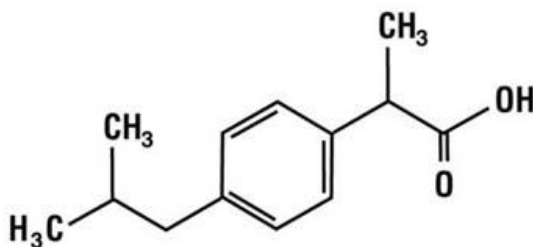
Razvitak farmaceutske industrije kao i sve starija populacija na Zemlji, dovele su do veoma rasprostranjene proizvodnje i upotrebe lekova. Sve to dovodi do stvaranja farmaceutskog otpada. Nastali farmaceutski otpad je veoma opasan i on uključuje farmaceutske proizvode i hemikalije koje su pripremljene a neupotrebene ili hemikalije kojima je istekao rok. Čak i neznatne koncentracije određenih supstanci iz lekova mogu imati štetan efekat na kvalitet kako podzemne tako i nadzeme vode, zemljišta, a samim tim i na ljudsko zdravlje.¹ Danas je u upotrebi oko 4000 različitih bioaktivnih jedinjenja koji se koriste u farmaceutskim preparatima. Postojeće tehnike za tretman otpadnih voda se ne bave u dovoljnoj meri problemom povećanja zagađenosti vodenih sistema usled sve veće upotrebe farmaceutskih preparata i proizvoda za ličnu higijenu. U otpadnim vodama koje izlaze iz fabrika, farmaceutske komponente su i dalje prisutne iz razloga što se ove komponente uklanjaju samo delimično ili se uopšte ne uklanjaju. Koncentracija farmaceutskih preparata u otpadnim vodama se obično kreće od 500 do 5000 ng/L, od 50 do 3000 ng/L po izlasku iz pogona za obradu otpadnih voda i od 1 do 500 ng/L u površinskim vodama.²

Ibuprofen (IBP), poznat još i pod nazivom brufen, prvi put je razvijen i sintetisan 1960. godine od strane britanske farmaceutske kuće Buts (slika 1). Pored toga, IBP je nesteroidni antiinflamatorni lek koji ima veoma široku primenu u lečenju bolova, groznice i upale.^{3,4} IBP se brzo metaboliše i eliminiše preko urina (oko 90%), dok se u potpunosti eliminiše

nakon 24 h. Najčešće se eliminiše preko metabolita ili u obliku konjugata. Simptomi predoziranja su individualni, ali sa dozom većom od 99 mg/kg. Ustanovljena je LD₅₀ vrednost ibuprofena i iznosi 636 mg/kg kod pacova, a 495 mg/kg kod zamoraca.⁵

Zbog raznih akcidenata koji su se desili ili koji imaju potencijal da se dese, težimo da zaštitimo životnu sredinu, kao i samog čoveka. Zato pronalazimo nove i unapređujemo postojeće načine za uklanjanje zagađujućih organskih supstanci i njihovih degaradacionih proizvoda. Jedan od načina za uklanjanje farmaceutskih komponenti je pomoću hlor - dioksida.⁶

Hlor - dioksid je efikasno sredstvo za uništavanje bakterija, virusa, gljivica i drugih patogena i zato je veoma široko rasprostranjen kao dezinfekcijsko sredstvo za prečišćavanje vode za piće i u prehrambenoj industriji.⁷ Kao veoma jak oksidans ($E^{\circ} = 0,936 \text{ V}$), hlor - dioksid može ukloniti ili oksidovati mnoge zagađujuće supstance, uključujući i lekove.⁸ Hlor - dioksid je našao značajnu primenu kao sredstvo za dezinfekciju u prehrambenoj industriji, kao i za dezinfekciju pijaće vode i otpadnih voda.⁹ Cilj ovog rada bio je da se ispituju i odrede optimalni uslovi za degradaciju IBP pomoću hlor - dioksida. Efikasnost degradacije je ispitana primenom tečne hromatografije visokih performansi sa detektorom sa diodnim nizom (HPLC - DAD).



Slika 1. Struktura ibuprofena

Ekperimentalni deo

Materijali

Kao uzorak za proučavanje korišćen je farmaceutski proizvod ibuprofen (IBP; čistoće 99%, proizvođač Hemofarm). U eksperimentima su korišćeni napravljeni rastvori koncentracije 10, 20, 35 i 60 mg/L, pri čemu je ibuprofen dodavan u dejonizovanu vodu. Hlor - dioksid je pripremljen na način opisan u radu Pergal i sar.¹⁰ Kao eluenti za HPLC - DAD analizu korišćeni su acetonitril (AcN >99,9%, Sigma - Aldrich) i 0,1% rastvor mravlje kiseline (HPLC čistoća, Fluka analytical) u ultra čistoj vodi. Uzorci su profiltrirani kroz filtere (Econofilter PTFE 25 mm 0,45 μm , Agilent Technologies).

Priprema uzoraka

Uzorak IBP je rastvoren u metanolu čime je napravljen interni standardi rastvor koncentracije 1000 mg/L. Interni standard je razblažen ultra čistom vodom do željene koncentracije od 10, 20, 35 i 60 mg/L IBP. U cilju optimizacije uslova degradacije, reakcija je praćena na različitim pH vrednostima (3,00; 7,00 i 10,00). pH vrednost je podešavana sa rastvorima natrijum - hidroksida i sumporne kiseline, koncentracija 0,1 mol/L, a određivana je na instrumentu Orion Star A221, Thermo Scientific, pH/mV -

metrom sa staklenom elektrodom. U rastvore IBP nakon podešavanja pH, dodat je hlor - dioksid kao degradaciono sredstvo. U jednu seriju uzoraka dodat je u koncentraciji od 5 mg/L, u drugu seriju u koncentraciji od 10 mg/L i u treću seriju u koncentraciji od 15 mg/L. Degradacija je prekidana sa 0,1 mol/L standardnim rastvorom natrijum - tiosulfata nakon određenog vremenskog perioda: 0,5 h, 1 h, 2 h, 3 h, 6 h i 24 h ibuprofena u dejonizovanoj vodi. Procenat degradacije određivan je pomoću HPLC – DAD tehnike.

HPLC analiza

Stepen degradacije praćen je pomoću HPLC - DAD analize. Korišćen je hromatograf Thermo Ultimate 3000 sa DAD detektorom i kolonom Hypersil Gold aQ C18 (150 mm x 3 mm x 3µm), na 60 °C, dok je temperatura uzorka bila 5 °C. Mobilna faza se sastojala od 0,1% rastvora mravlje kiseline u ultra čistoj vodi (komponenta A) i AcN (komponenta B). Eluiranje je bilo u gradijentnom režimu: 20% - 75% B u 10 min., 75% B od 10 do 12 min. i 75% - 25% B u 12 – 14 min. i 20% B u naredna 3 min. (17 min.). Injektovano je 20 µL uzorka. Detektor je bio podešen na sledeće talasne dužine za IBP: 192, 220, 254 i 263,8 nm. Analiza podataka je izvedena softverom Chromeleon v6.8 (ThermoFisher Scientific, Bremen, Germany). Stepen degradacije određen je prema izrazu opisanom u radu Pergal i sar.¹⁰

Rezultati i diskusija

Efikasnost degradacije je praćena pomoću HPLC - DAD analize na osnovu smanjenja površine pika za IBP nakon degradacije u odnosu na površinu pika IBP pre degradacije.

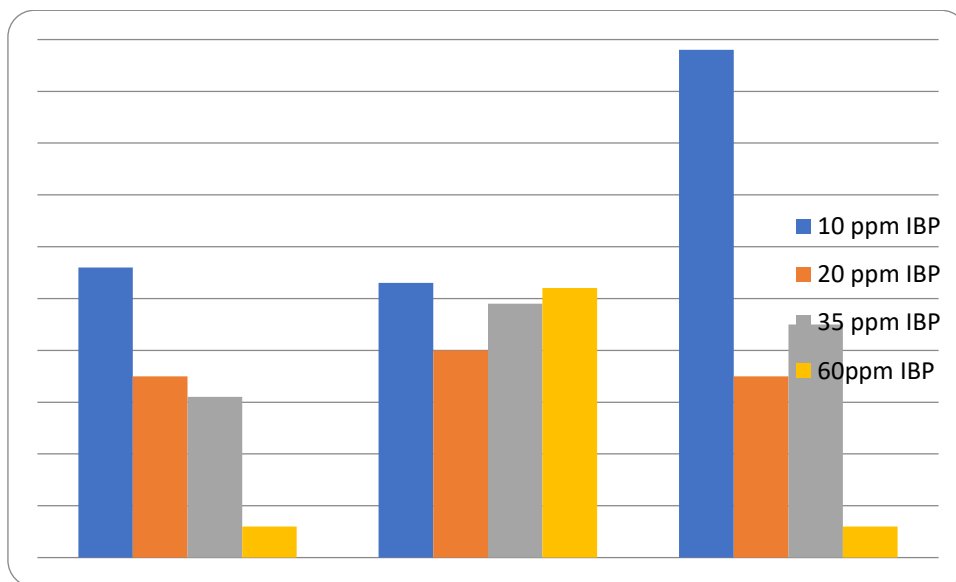
Došlo je do smanjenja signala analiziranog polaza IBP sa vremenom, a samim tim je došlo i do degradacije IBP.

Analizom dobijenih rezultata utvrđeno je da se na svim pH vrednostima najviši procenat degradacije postiže sa 15 mg/L hlor - dioksida (Slika 2).

Analiza na pH 3,00 pokazala je da se najveća efikasnost degradacije (56%) postiže za 10 mg/L IBP. Dobijeni rezultati su pokazali da se sa 20 mg/L IBP postiže manja efikasnost degradacije IBP (35%). Dalje povećanje koncentracije IBP takođe pokazuje još manju efikasnost degradacije odnosno sa 35 mg/L IBP, efikasnost degradacije iznosi 31%, a najniža efikasnost degradacije se postiže za 60 mg/L IBP, samo 6%.

Analiza na pH 7,00 pokazala je da se najefikasnija degradacija od 53% postiže za 10 mg/L IBP. Za 20 mg/L IBP procenat degradacije je iznosio 40%. Za 35 i 60 mg/L IBP efikasnosti degradacija su nešto bolje nego za 20 mg/L i iznosile su redom 49% i 52%.

Analiza na pH 10,00 pokazala je da se 10 mg/L, IBP razgrađuje čak 99%. Degradacijom koncentrovanijih rastvora IBP, efikasnosti degradacije su se smanjivale i to za 20 mg/L IBP 35%, 35 mg/L IBP 45% i 60 mg/L IBP samo 6%. Na osnovu dobijenih rezultata može se zaključiti da bazna sredina pogoduje procesu degradacije IBP, kao i visoka koncentracija hlor-dioksida.



Slika 2. Efikasnost degradacije za različite koncentracije IBP sa 15 mg/L hlor - dioksida na različitim pH vrednostima

Zaključak

Proučavana je degradacija leka IBP u dejonizovanoj vodi tretmanom sa različitim koncentracijama hlor - dioksida koje su iznosile 5, 10 i 15 mg/L. Degradacija IBP je ispitivana na tri različite pH vrednosti (3,00; 7,00; 10,00), u različitim vremenskim intervalima od 0 - 24 h.

Iz analiziranih rezultata zaključeno je da se degradacija IBP odigravala na svim pH vrednostima, ali da pH utiče na sam tok reakcije. Najveća efikasnost degradacije IBP postignuta je na pH 10,00 pri koncentraciji IBP od 10 mg/L sa 15 mg/L hlor - dioksida i iznosila je 99%. Rezultati su pokazali da povećanje koncentracije hlor - dioksida od 5 do 15 mg/L doprinosi većoj efikasnosti degradacije IBP. Takođe, rezultati su pokazali da smanjenje koncentracije IBP, kao i povećanje pH vrednosti od 3,00 do 10,00 doprinosi povećanju efikasnost degradacije.

Zahvalnica: Ovaj rad je finansiran od strane Ministarstva Prosvete, Nauke i Tehnološkog Razvoja Republike Srbije (451-03-9/2021-14/200026; 451-03-9/2021-14/200168). Zahvaljujemo se i TwinOxide RS d.o.o za dostupnost preparata "TWINS".

Optimization of conditions for degradation of ibuprofen using chlorine dioxide

Due to ibuprofen (IBP) wide application, high consumption, relatively fast metabolism and elimination from the organism, it represents a potential risk for our environment. Chlorine dioxide, as a strong oxidizing agent, has been shown to be a good reagent for removing certain groups of pesticides from food and water, as well as for degradation of certain drugs. The aim of this study was to find optimal conditions for IBP removal from water using chlorine dioxide. Degradation of IBP of different concentrations (10, 20, 35 and 60 mg/L) with different concentrations of chlorine dioxide (5, 10 and 15 mg/L) at pH values of

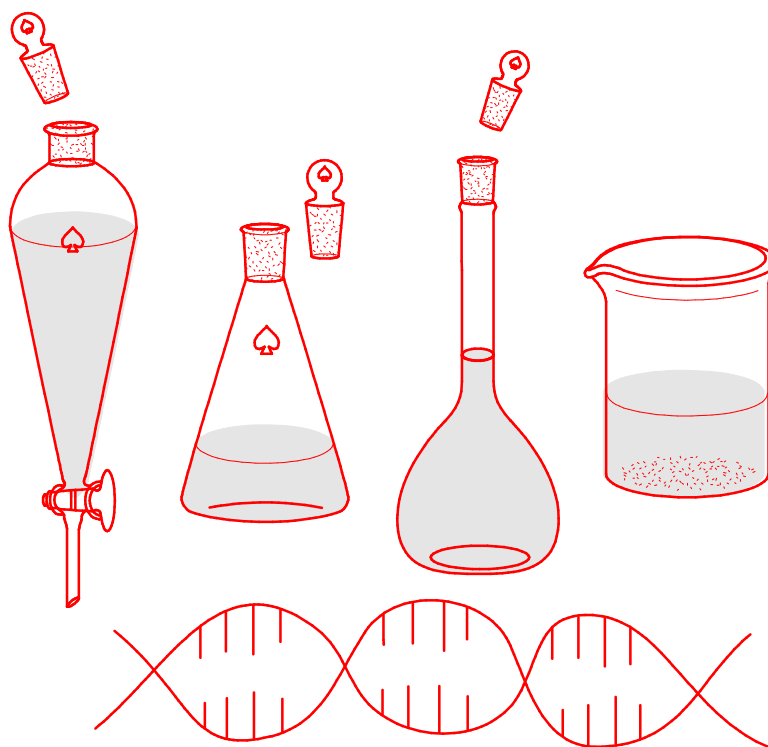
3.00, 7.00 and 10.00 and at different reaction times (0.5 h, 1 h, 2 h, 3 h, 6 h, 24 h), was investigated. The results of HPLC - DAD analysis showed that IBP can be effectively removed from water. The highest degradation efficiency of 99% was achieved when the concentration of IBP in water was 10 mg/L, and the solution was treated with 15 mg/L of chlorine dioxide at pH 10.00 after 24 h of chlorine dioxide treatment.

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Elektrohemija

Electrochemistry



TR-EH-1

Corrosion Rate of Stainless Steel Tubes Calculated by Electrochemical Frequency Modulation

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Introduction

The use of high energy, ionizing radiation in nuclear medicine is now pervasive and routine. The interaction of gamma radiation with aqueous solutions produces different kinds of reducing and oxidizing agents. Reducing agents represent e^-_{aq} , $H\bullet$ and H_2 while oxidizing agents represent H_2O_2 , $\bullet OH$, O_2 , O_2^- and HO_2 [1]. Production of such species under gamma irradiation, there may affect the rates or mechanisms of corrosion attack modes.

In recent times, electrochemical frequency modulation (EFM) has caught the attention of corrosion scientists as a rapid and non-destructive technique for the instantaneous determination of corrosion rate. The advantage of the EFM technique is the fact that the measurement can be completed in a short time period [2]. The EFM technique offers an excellent [alternative](#) for the analysis of electrochemical corrosion behavior of metals compared with contemporary techniques like potentiodynamic polarization, linear polarization, electrochemical impedance spectroscopy and weight loss. This technique provides measurements of corrosion rate directly without knowledge of the Tafel constants. Even though the Tafel constants are not required, it measures them and a change in Tafel constant may indicate a change in corrosion mechanism. The theory behind the technique is the same Butler-Volmer kinetics that underpins all corrosion rate measurements. It is a small signal ac technique where two sine waves (at different frequencies) are applied to the cell simultaneously.

In our work, we used the EFM technique to calculate the corrosion rate on stainless steel samples in saline and under gamma radiation.

Methods

Stainless steel tubes used in this study were AISI 304 purchased from different companies. Their composition was determined by x-ray fluorescence spectrometer for elemental analysis Analyticon Instruments gmbh XL3-101210. Three types of tubes with dimensions of fi 0.5 mm and 100 mm length were prepared for the electrochemical tests.

Prior to each measurement, the samples were ground using a carbide emery papers ranging 600 grit size, subsequently rinsed by bidistilled water and acetone, and finally dried at room temperature.

Electrochemical measurements were performed using a Gamry potentiostat/galvanostat model 750 ZRA.

Electrochemical experiments were carried out at room temperature in saline purchased from Hemofarm A.D, in an electrolytic cell with an AgCl reference electrode tip placed

close to the working electrode to minimize ohmic resistance. The working electrode was a stainless steel tube while the platinum plate (20 mm x 80mm) was a counter electrode. After immersion in bidistilled water and saline for ten days samples have been analyzed. The second group of samples was tested after irradiation by gamma rays obtained by ^{60}Co in bidistilled water and saline. The delivered dose of the radioactive source was 25 kGy. Samples immersed in saline for ten days were marked with Roman numerals and with letter S (S I, S II, and S III) (Table 1); while the samples that were aged in saline and additionally irradiated were marked with Roman numerals and the letters FG (S I-FG, S II-FG, and S III-FG).

The EFM data have been analyzed using the Gamry Echem Analyst software v561.

Table 1. Composition (wt.%) of different 304 SS tubes from x-ray fluorescence spectrometer for elemental analysis Analyticon Instruments gmbh XL3-101210

Sample	Element / wt.%								
	Mo	Cu	Ni	Mn	Cr	V	Si	P	Fe
S I	0.11	0.19	8,04	1.10	17.56	0.18	0.40		72.39
S II			7.85	1.28	18.40		0.53	0.053	71.831
S III	0.06		9.12	1.63	17.48		0.58		71.04

Results and discussion

The response to the appropriate excitation of a material with a voltage of the appropriate frequency is a graph of the change in current in a given time interval, as shown in Figure 1. EFM chart in Figure 1 shows the I vs. t chart for all of the data collected. The number of cycles (16) is chosen that it is neither small due to uncertainty nor large so that the measurement does not take too long. The maximum number of cycles with a given device is 255. For the EFM analysis, the data from the first cycle is not used but the device itself adds this number given that it should not be taken into account when setting the parameters. A frequency spectrum of an EFM current response, illustrating the different harmonic and intermodulation frequencies, is depicted in Figure 2.

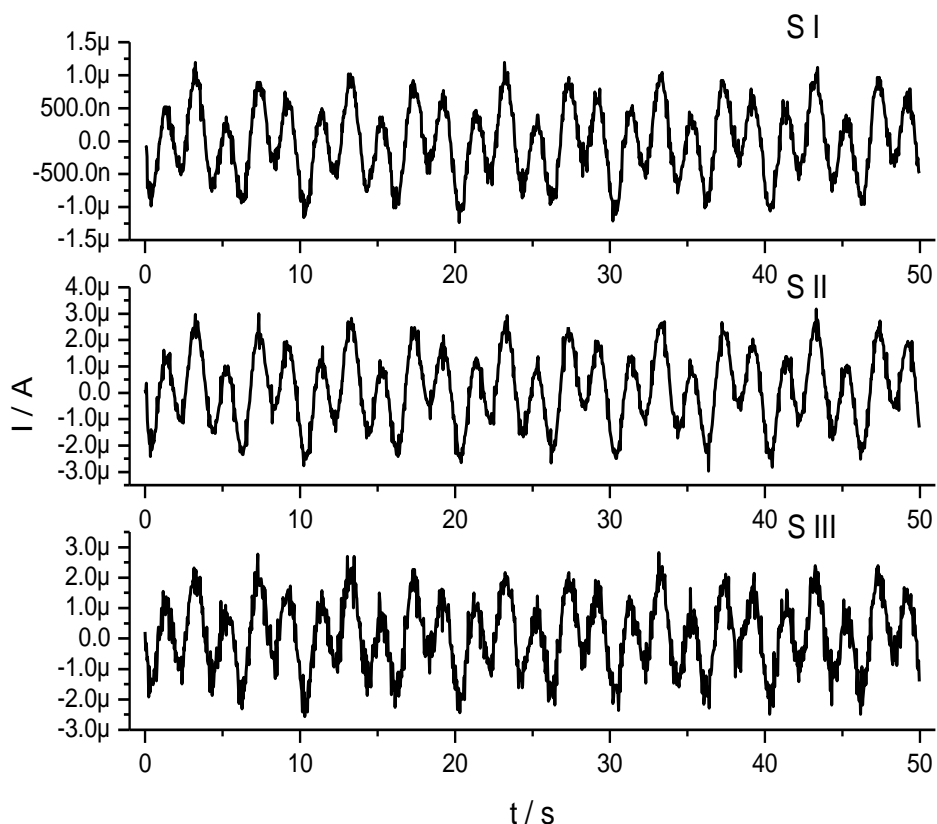


Figure 1. Current I vs. time t for sample I, II, and III

The baseline frequency was 0.1 Hz with four cycles, the multipliers were 2 and 5 and the amplitude was 10 mV. Harmonic current responses at ω_1 , $2\omega_1$, $3\omega_1$ and ω_2 , $2\omega_2$, $3\omega_2$ as well as intermodulation frequencies like $2\omega_1 \pm \omega_2$ and $2\omega_2 \pm \omega_1$ caused that bandwidth Δf of the EFM measurement was $0.1 < \Delta f \text{ (Hz)} < 1.5$.

The currents obtained at certain frequencies such as 0.2 Hz and 0.5 Hz as well as 0.3 Hz and 0.7 Hz have equal values, which agree with the claims Bosch et al. can be seen in Figures 2 and 3 [3].

The chosen frequencies were considered a reasonable compromise of some arguments. The harmonics and intermodulation frequencies should not influence each other and the frequency should be as low as possible to avoid the influence of the capacitive behavior of the electrochemical double layer. Also, the frequency should be as large as possible to reduce the time needed to accomplish a measurement.

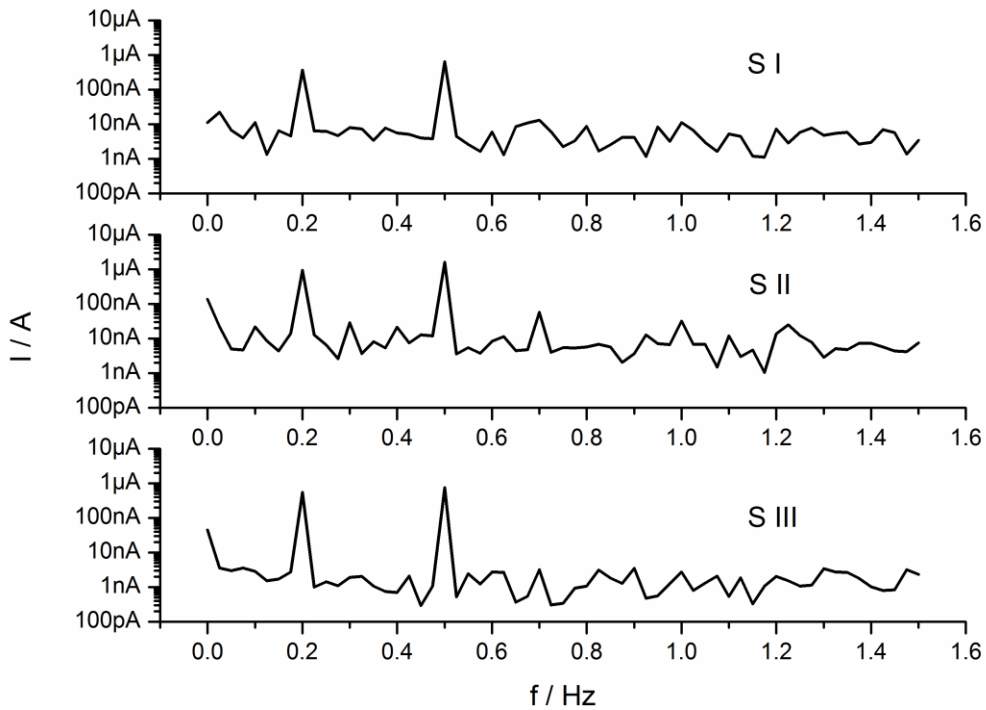


Figure 2. Current I vs. frequency f plot for samples I, II, and III.

Figure 2 shows results obtained from samples that were immersed in saline for ten days and analysed using a perturbation signal with an amplitude of 10 mV for both frequencies. On sample S II two peaks can be seen at 0.3 Hz and 0.7 Hz which are missing in the other two samples. In the S II-FG sample, four additional peaks appear compared to the S I-FG and S III-FG samples. These peaks are positioned at 0.3 Hz, 0.4 Hz, 0.7 Hz and 1 Hz. From the given figures 2 and 3, it can be seen that sample S II is more susceptible to corrosion and much more if it is exposed to chloride ions and gamma radiation.

Assuming that the cathodic reaction is under diffusion control the results of the analysis are given in Figure 4. In Figure 4, the corrosion rate of samples S I, S II, and S III under various influences of the corrosive environment is shown.

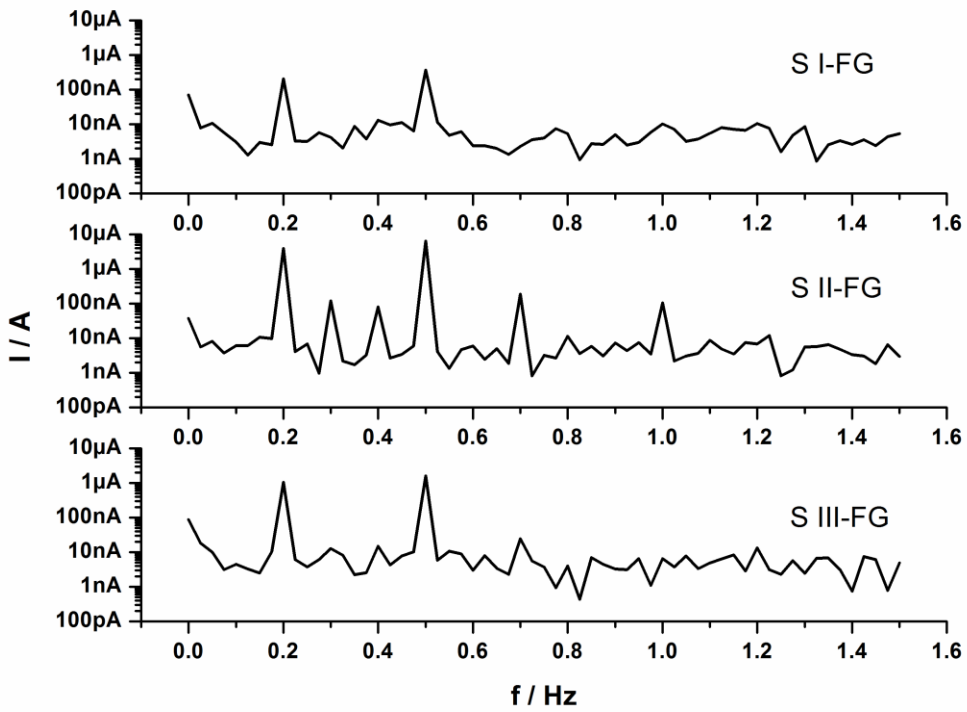


Figure 3. Current I vs. frequency f plot for samples I, II, and III.

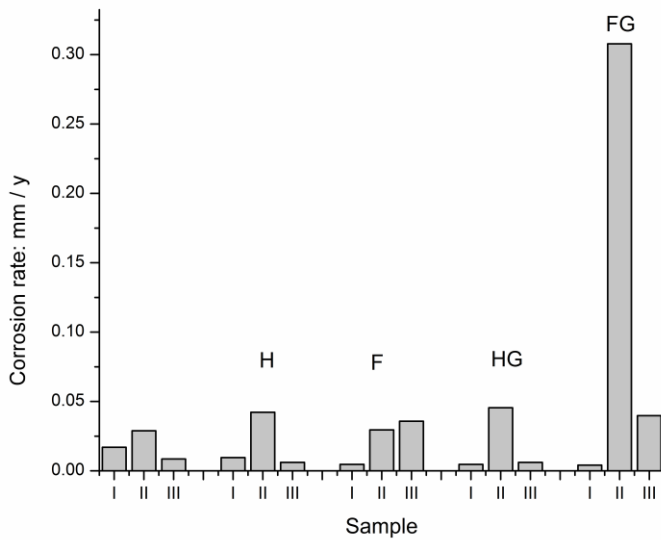


Figure 4. Corrosion rate in mm/yr for samples S I, S II and S III under various influences of the corrosive environment (the S mark has been omitted for clarity).

The sample marked as S II shows a significant influence of chloride ions on corrosion rate but a dramatic increase in the corrosion rate can be seen when sample S II simultaneously was immersed in saline and irradiated with gamma rays.

The composition of tubes determined by x-ray fluorescence spectrometer is presented in table 1. It is obvious that the content of macroelements in all samples is similar, but sample S II shows a lack of some elements, such as Mo, Cu and V. Also, this sample contains a small amount of phosphorus, while the two other samples do not have the same element.

Conclusion

A corrosive environment containing chloride ions is detrimental to materials such as stainless steel. A slight increase in the corrosion rate in material immersed in saline occurs due to a low concentration of NaCl in the solution. Gamma irradiation increases the oxidizing nature of the aqueous solutions used in this study through the production of H_2O_2 , $\bullet OH$, O_2 , O_2^- and HO_2 species which with Cl^- account for the observed positive corrosion potential shift for sample S II. The lack of certain elements like Mo in stainless steel, as in the case with sample S II (Table 1), can result in reduced corrosion resistance of materials.

Acknowledgements

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Brzina korozije cevi od nerđajućih čelika izračunata pomoću elektrohemijske frekvencione modulacije

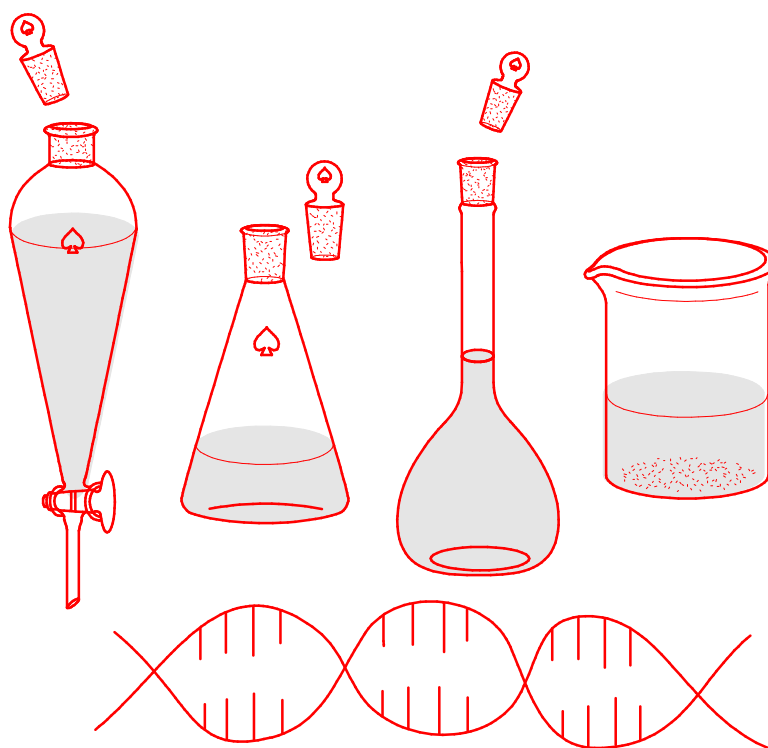
Nerđajući čelici su omiljeni materijali u nuklearnoj medicini zbog jednostavnog održavanja (brisanje, dekontaminacija, itd.). Otpornost na rđanje ovih materijala je smanjena usled istovremenog delovanja hloridnih jona i jonizujućeg zračenja. Brza i nedestruktivna tehnika merenja korozije, kao što je elektrohemijska frekvenciona modulacija (EFM), korisna je za brzu procenu materijala koji moraju biti otporni na rđanje. Tri različite cevi od nerđajućeg čelika su analizirane pomoću EFM metode i Gamry potencioštata / galvanostata, i izračunate su njihove brzine korozije. Uzorak označen kao S II, koji ne sadrži Mo u svom sastavu pokazuje veću brzinu korozije u odnosu na uzorke koji sadrže Mo ako je istovremeno izložen hloridnim jonima i gama zračenju. Ovaj rezultat je u sagalsnosti sa sastavom nerđajućeg čelika dobijenim rentgenskim fluorescentnim spektrometrom koji pokazuje nedostatak bakra i vanadijuma u tragovima, uključujući molibden.

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Hemijsko inženjerstvo

Chemical Engineering



TR-HI-1

Termodinamička svojstva i modelovanje međumolekulske interakcije dvokomponentne smeše limonena i hloroforma

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Apstrakt

U cilju proučavanja termodinamičkih svojstava binarne smeše limonen + hloroform eksperimentalno su određene gustine (ρ), viskoznosti (η) i indeksi refrakcije (n_D) za ovu smešu. Eksperimentalna merenja su rađena u opsegu temperatura od 288,15 K do 323,15 K na atmosferskom pritisku, za ceo opseg udela. Na osnovu eksperimentalno dobijenih rezultata izračunate su vrednosti dopunske molarne zapremine V^E , vrednosti promene viskoznosti $\Delta\eta$ i vrednosti promene indeksa refrakcije Δn_D . Za izvedene vrednosti rezultati su dobijeni primenom *Redlich-Kister* polinomske jednačine. Na osnovu ovih rezultata izvedeni su zaključci o međumolekulskim interakcijama u limonen + hloroform binarnom sistemu. Vrednosti dopunske molarne zapremine, kao i vrednosti promene viskoznosti i indeksa refrakcije pokazuju pozitivno odstupanje u celom opsegu molskih udela. Povećanje dopunske molarne zapremine pokazuje da je pakovanje molekula u smeši manje efikasno nego u čistim komponentama.

Uvod

Terpeni su grupa jedinjenja koja su široko rasprostranjena u prirodi, a za industrijske svrhe se dobijaju iz biljaka. Terpeni imaju intenzivnu aromu, a pokazuju antiseptička i terapijska svojstva, pa se zato koriste u farmaceutskoj i prehrambenoj industriji. Jedan je od čestih terpena u prirodi je limonen (1-metil-p-izopropenil-1-cikloheksen) i on je glavni sastojak brojnih esencijalnih ulja iz citrusa (limun, pomorandža, mandarina i grejpfruta). Postoji u dva enantiomera, (R) -, ili d-limonen, i (S) -, ili l-limonen, a enantiomer koji se češće javlja je d-limonen. Ovaj enantiomer se u industriji dobija iz citrusa na dva načina, destilacijom vodenom parom i centrifugalnim odvajanjem. Koristi se često kao dodatak arome i mirisa u prehrambenim proizvodima, a često je i sastojak u proizvodnji proizvoda za čišćenje [1]. Limonen se koristi i u kozmetičkoj industriji, pa se može naći u mnogim parfemima, sapunima i šamponima [2-4].

U hemijskoj industriji postoje postrojenja čija efikasnost zavisi od transportnih svojstava fluida, pa se to odnosi i na postrojenja u kojima se dobija limonen u procesu ekstrakcije iz biljnog materijala, kao i na postrojenja za proizvodnju proizvoda u kojima se koristi limonen. S obzirom da se u procesu dobijanja limonena kao i u procesu proizvodnje proizvoda sa limonenom koriste različite smeše koje u sebi sadrže limonen, važno je

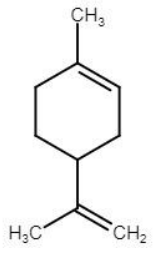
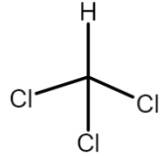
proučavanje termodinamičkih svojstava smeša različitih rastvarača sa limonenom. Termodinamička svojstva čistog limonen su već ispitivana na različitim temperaturama i visokim pritiscima [5].

U ovom radu, eksperimentalno su proučavana termodinamička svojstva binarne smeše limonen + hloroform određivanjem gustine (ρ), viskoznosti (η) i indeksa refrakcije (n_D) ove smeše. Eksperimentalna merenja su rađena za ceo opseg udela, u opsegu temperatura od 288,15 K do 323,15 K na atmosferskom pritisku. Na osnovu eksperimentalno dobijenih rezultata izračunate su vrednosti dopunske molarne zapremine V^E , vrednosti promene indeksa refrakcije Δn_D i vrednosti promene viskoznosti $\Delta \eta$. Za izvedene vrednosti rezultati su dobijeni primenom *Redlich-Kister* (Redlich-Kister) polinomske jednačine. Na osnovu ovih rezultata izvedeni su zaključci o međumolekulskim interakcijama u limonen + hloroform binarnom sistemu.

Eksperimentalni deo

Opis supstanci, kao i hemijska struktura je data u tabeli 1. Eksperimentalna merenja ispitivanih supstanci i njihove smeše su urađena na sledećim instrumentima: gustine su merene na uređaju Anton Paar DSA 5000 digitalnom U-cev vibracionom gustinomeru, merenje viskoznosti je vršeno na automatskom Anton Paar RXA 156 refraktometru, a indeksi refrakcije (n_D) su mereni na digitalnom Stabinger viskozimetru SVM 3000/G2. Pre svakog merenja, svi uređaji su kalibrisani Milipore dejonizovanom vodom i ambijentalnim vazduhom. Sve smeše pripremane su gravimetrijski na Mettler AG 204 digitalnoj vagi sa preciznošću od $1 \cdot 10^{-7}$ kg i sa standardnom nesigurnošću molskog udela manjom od $\pm 1 \cdot 10^{-4}$. Proširene nesigurnosti gustine ($U(\rho)$), viskoznosti ($U(\eta)$) i indeksa refrakcije ($U(n_D)$) sa nivoom pouzdanosti od 95% (faktor pokrivenosti, $k = 2$), su $0,09 \text{ kg} \cdot \text{m}^{-3}$, $0,004 \text{ mPas}$, odnosno $5 \cdot 10^{-5}$.

Tabela 1. Opis ispitivanih supstanci:

Hemijska supstanca	Čistoća	CAS broj	Molarna masa / $\text{g} \cdot \text{mol}^{-1}$	Hemijska struktura
(+)-limonen	0,994	5989-27-5	136,24	
hloroform	0,995	67-66-3	119,38	

Rezultati i diskusija

Eksperimentalna merenja termodinamičkih svojstava (gustina, viskoznost i indeks refrakcije) za izabranu smešu su rađena na osam temperatura ($T = 288,15 \text{ K}, 293,15 \text{ K}, 298,15 \text{ K}, 303,15 \text{ K}, 308,15 \text{ K}, 313,15 \text{ K}, 318,15 \text{ K}, 323,15 \text{ K}$) i na atmosferskom pritisku. Koristeći eksperimentalne podatke za čiste komponente i njihove smeše, računata su dopunske veličine [5].

Dopunska molarna zapremina je računata sledećom jednačinom, pomoću gustina čistih komponenti i gustine smeša.

$$V^E = \sum_{i=1}^N x_i M_i \left[(1/\rho) - (1/\rho_i) \right] \quad (1)$$

gde N predstavlja broj komponenti (u našem slučaju $N = 2$), x_i je molski udeo komponente i u smeši, M_i predstavlja molarnu masu komponente i , ρ je gustina binarne smeše, a ρ_i gustina čistih komponenti i .

Promena viskoznosti ($\Delta\eta$) je računata pomoću sledeće jednačine:

$$\Delta\eta = \eta - \sum_{i=1}^N x_i \eta_i \quad (2)$$

gde η predstavlja viskoznost izmerene smeše, a η_i viskoznost čistih komponenti i .

Vrednosti promene indeksa refrakcije je računata pomoću indeksa refrakcije čistih komponenta i indeksa refrakcije smeše i opisano je sledećom jednačinom:

$$\Delta n_D = n_D - \sum_{i=1}^N x_i n_{Di} \quad (3)$$

gde n_D predstavlja indeks refrakcije smeše, a n_{Di} odnosi na indeks refrakcije čiste komponente i .

Dopunske veličine predstavljene u jednačinama (1) - (3) podešene su pomoću sledeće jednačine koja predstavlja Redlih-Kister (RK) polinomsku jednačinu [6]:

$$Y = x_i x_j \sum_{p=0}^k A_p (2x_i - 1)^p \quad (4)$$

gde Y predstavlja jednu od dopunskih veličina iz gore definisanih jednačina (V^E , Δn_D ili $\Delta\eta$), A_p predstavljaju parametre RK polinoma, koji se optimizuju i određuju pomoću F-testa.

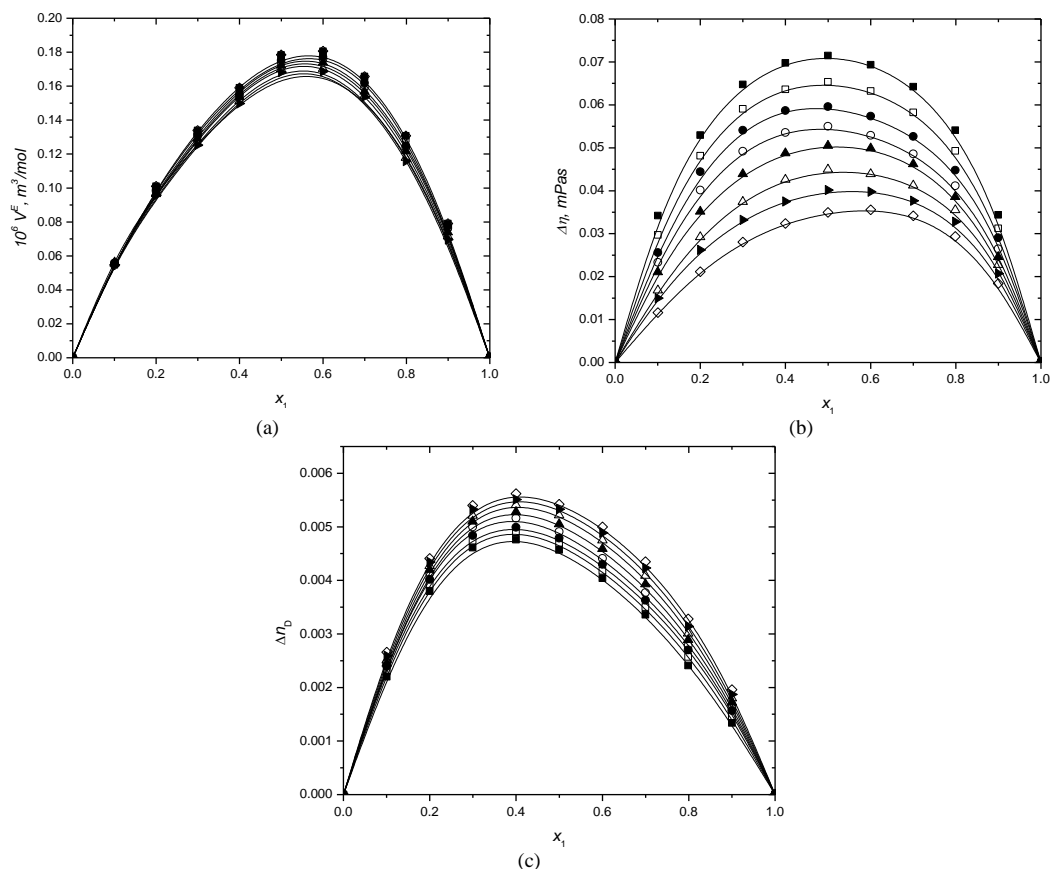
Standardna devijacija je definisana pomoću jednačine:

$$\sigma = \left(\sum_{i=1}^m (Y_{\text{exp},i}^E - Y_{\text{cal},i}^E)^2 / (m - k) \right)^{1/2} \quad (5)$$

gde m predstavlja broj eksperimentalnih podataka, dok k predstavlja broj parametara.

Za ispitivani sistem limonen (1) + hloroform (2), na slici 1 su predstavljeni rezultati merenja, tj vrednosti dopunskih molarnih zapremina (a), promena viskoznosti (b) i promena indeksa refrakcije (c) u funkciji molskog udela limonena (1) u smeši. Simbolima su predstavljeni eksperimentalni podaci, dok linije predstavljaju vrednosti dobijene RK jednačinom (5).

57. savetovanje SHD



Slika 1. Eksperimentalni podaci za (a) dopunsku molarnu zapreminu (V^E), (b) promenu viskoznosti ($\Delta\eta$) i (c) promenu indeksa refrakcije (Δn_D), u funkciji molarnog udela x_1 , za binarnu smešu limonen (1) + hloroform (2) na temperaturama: (■) 288,15 K, (□) 293,15 K, (●) 298,15 K, (○) 303,15 K, (▲) 308,15 K, (△) 313,15 K, (▶) 318,15 K, (◇) 323,15 K; (-) RK jednačina

Analizirajući dobijene vrednosti dopunskih molarnih zapremina (slika 1(a)), može da se uoči da postoji pozitivno odstupanje od idealnog ponašanja i maksimalne vrednosti dostižu se za molski udeo limonena od 0,6. Ovo ukazuje na povećanje zapremine u smeši, što je rezultata strukture molekula (tabela 1). Molekuli u smeši zauzimaju takve konformacije da dolazi do ekspanzije ukupne zapremine. Ova manja gustina pakovanja molekula u smeši, pored geometrije molekula, može biti i posledica slabijih međumolekulskih interakcija. Sa povećanjem temperature, vrednosti molarne dopunske zapremine opadaju što ukazuje na bolje pakovanje molekula u smeši sa porastom temperature.

Promene viskoznosti prikazane na slici 1(b) su pozitivne u celom opsegu molskog udela, sa maksimalnim vrednostima kada je sastav smeše ekvimolaran. Za razliku od vrednosti molarne dopunske zapremine, sa povećanjem temperature, vrednosti promene viskoznosti opadaju.

Na slici 1(c) su prikazane vrednosti promene indeksa refrakcije, koje su takođe pozitivne tokom celog opsega molskog udela. Maksimalne vrednosti se dostižu za molski udeo limonena od 0,4. Slično kao vrednosti molarne dopunske zapremine, a za razliku od promene viskoznosti, vrednosti promena indeksa refrakcije rastu sa povećanjem temperature.

Zaključak

Izmerene eksperimentalne vrednosti termodinamičkih svojstava binarne smeše limonen + hloroform, pokazuju da vrednosti dopunskih molarnih zapremina pozitivno odstupaju od idealnog ponašanja smeše. Promene viskoznosti i promene indeksa refrakcije takođe su pokazale pozitivno odstupanje u celom opsegu molskih udela. Vrednosti dopunskih molarnih zapremina ukazuju na povećanje zapremine u smeši dve komponente, što je rezultat strukture molekula. Manja gustinu pakovanja molekula u smeši u odnosu na čiste komponente, može biti posledica geometrije molekul ili/i slabijih međumolekulskih interakcija. Naši podaci o ponašanju smeše na različitim temperaturama pokazuju trendove na osnovu kojih se može potencijalno predviđati ponašanje i na drugim temperaturama. U cilju dobijanja dodatnih podataka o ponašanju molekula u smeši, u nastavku ovih istraživanja biće urađene molekulske simulacije korišćenjem metode molekulske dinamike. To će omogućiti da se na molekulskom nivou odredi koliko konformacija molekula, a koliko interakcije između molekula utiču na termodinamička svojstva smeše.

Zahvalnica

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Thermodynamic properties and modeling intermolecular interaction of binary mixture of limonene and chloroform

In order to study the thermodynamic properties of the binary mixture limonene + chloroform, the densities (ρ), viscosities (η) and refractive indices (n_D) for this mixture were experimentally determined. Experimental measurements were performed in the temperature range from 288.15 K to 323.15 K at atmospheric pressure, for the entire range of composition. Based on the experimental results, the values of excess molar volume V^E , the viscosity deviation $\Delta\eta$ and the refractive index deviation Δn_D were calculated. Additionally, the excess molar volume and viscosity and refractive index deviations were fitted with the Redlich-Kister polynomial equation. Based on these results, conclusions can be made on intermolecular interactions in the limonene + chloroform binary system. Values of excess molar volume, viscosity and refractive index deviations have shown a positive non-ideal behavior in the entire composition range. An increase in

the values of excess molar volume indicates that the packaging of the molecules in the mixture is less efficient than in the pure components.

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TR-HI-2

Eksperimentalno određivanje gustina linalola, alfa-pinena i beta-pinena na visokom pritisku

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Apstrakt

U cilju smanjenja zagađenja na globalnom nivou poslednjih godina aktuelna je tema zamene fosilnih goriva nekim novim biogorivima. Terpeni, koji su sastavni delovi biljaka, mogu se koristiti u ove svrhe kao dodatak standardnim gorivima. Neke od termodinamičkih svojstva pod uslovima visokog pritiska i određenih temperatura su od velike važnosti za efikasnost motora. U ovom radu su dobijene gustine linalola, alfa-pinena i beta-pinena u temperaturnom intervalu 293.15-413.15 K i na pritiscima do 60 MPa. Na osnovu ovih rezultata utvrđeno je da s porastom temperature pri konstantnom pritisku gustina navedenih terpena opada, dok sa povećanjem pritiska pri konstantnoj temperaturi gustina raste.

Uvod

Terpeni su velika i raznovrsna klasa organskih jedinjenja koje proizvode mnogobrojne biljke, a posebno su zastupljeni kod četinarara. Ova grupa prirodnih hemijskih jedinjenja, predstavljaju veoma povoljne kandidate za aditive goriva. Mogli bi se proizvesti ili iz biomase algi ili razgradnjom drvnih ostataka tokom perioda skladištenja izazvanog bakterijama [1,2]. Terpeni su vrlo dobri kandidati, jer obično ne sadrže kiseonik, za razliku od biodizela i alkohola. Takođe, veoma su povoljni i zbog svojih svojstava kao što su tačka ključanja, tačka paljenja, tačka mržnjenja, niska viskoznost, velika gustina energije. Uopšteno govoreći, terpeni su stekli veliko interesovanje za hemijsku industriju kao alternativni održivi izvori [3]. Predstavljaju prirodni proizvod poznat kao sekundarni metabolit biljke, dobijen ekstrakcijom iz biljaka. Linalool je prirodni terpeniski alkohol koji je prisutan u mnogim cvetajućim i začinskim biljkama, dok se alfa-pinen i beta-pinen nalaze u četinarima. Ovi terpeni imaju mnoštvo komercijalnih primena, većina kojih se bazira na prijatnom mirisu ali može naći i primenu kao dodatak gorivima. Poslednjih godina pridaje se sve veći značaj gorivima visoke energije, niske viskoznosti i efikasnog i čistog sagorevanja, koja mogu koristiti avioni, brodovi, teški kamioni, vojni transporteri [4,5]. Zbog konstantne potrebe za gorivima za transport i rigorozne kontrole zaštite životne sredine, neophodan je razvoj proizvodnje goriva koji bi podrazumevao upotrebu

ekonomski isplativih i obnovljivih sirovina [6,7]. U vazduhoplovnim vozilima uticaj gustine i zapreminske energije upotrebljenih tečnih goriva su najvažniji aspekti pogonskih karakteristika. Veličina ili težina ovih vozila su često ograničena, pa bi trebalo puniti male rezervoare za gorivo sa tečnostima velike gustine energije. Da bi se povećao korisni teret, gorivo treba da ima visoku gustinu energije i nisku viskoznost. Biogoriva sa pomenutim svojstvima treba sintetizovati iz sirovine biomase, uključujući terpen, hemicelulozu, celulozu i lignin. Ponekad, da bi se poboljšala zapreminska energija, terpeni bi se mogli koristiti u smešama sa konvencionalnim gorivima [8]. U ovom radu, eksperimentalno određene gustine linalola, alfa-pinena i beta-pinena. Eksperimentalna merenja su rađena za čiste komponente, u opsegu temperatura od 239.15 K do 413.15 K na pritiscima do 60 MPa. Na osnovu eksperimentalno dobijenih rezultata perioda oscilovanja izračunate su gustine navedenih terpena.

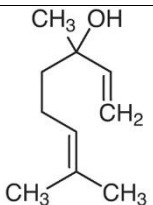
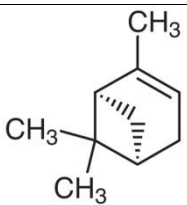
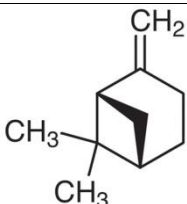
Eksperimentalni deo

Opis supstanci, kao i hemijska struktura je data u tabeli 1. Uređaj na kome je vršeno merenje gustine na visokom pritisku je DMA HP gustinomer proizvođača Anton Paar (Slika 1.a). Ovaj aparat ne poseduje svoj ekran te je povezan sa DMA 5000 (Slika 1.b) uređajem koji se koristi za merenje gustine na atmosferskom pritisku i u kojem je instalirana softverska jedinica kojom se podešavaju željeni procesni uslovi (temperatura i pritisak) na kojima se meri gustina uzorka u mernoj ćeliji DMA HP gustinomera. Od posebnog značaja su gustinomeri sa vibrirajućim elementom čiji se princip rada zasniva na pobuđivanju vibracija čvrstog elementa koji sadrži fluid (ili je okružen njime) i posmatranju njegove rezonantne frekvencije. Tada će frekvencija rezonancije sklopa čvrsto/fluid zavisi od osobina fluida, i posebno, njegove gustine ρ . Veliki broj različitih gustinomera i sa različitim vibrirajućim elementom je razvijen, među kojima vredi istaći: gustinomere sa vibracionom cevi, gustinomere sa vibracionim cilindrom, gustinomere sa zvučnim viljuškama i gustinomere sa vibrirajućom žicom. Detalji o eksperimentalnoj proceduri i načinu rada koji je korišćen u našoj laboratoriji opisani su u prethodnim radovima [9,10]



Slika 1. Uređaji: a) DMA HP i b) DMA 5000

Tabela 1. Opis ispitivanih supstanci:

Hemijska supstanca	Čistoća	CAS broj	Molarna masa g/mol	Hemijska struktura
linalol	97%	78-70-6	154.25	
alfa-pinen	98%	7785-70-8	136.24	
beta-pinen	98%	18172-67-3	136.24	

Eksperimentalna merenja gustine za čiste komponente linalol, alfa-pinen i beta-pinen su rađena na devet temperatura ($T = 293,15 \text{ K}$, $303,15 \text{ K}$, $313,15 \text{ K}$, $323,15 \text{ K}$, $333,15 \text{ K}$, $353,15 \text{ K}$, $378,15 \text{ K}$, $393,15 \text{ K}$, $413,15 \text{ K}$) i u opsegu pritiska od 0.1 MPa do 60 MPa .

Za izračunavanje gustine prema jednačinama:

$$\rho(T, p) = \rho_{\text{voda}}(T, p) + \rho_{\text{voda}}(T, 0.1 \text{ MPa}) \cdot \left[\frac{\tau^2(T, p) - \tau_{\text{voda}}^2(T, p)}{\tau_{\text{voda}}^2(T, 0.1 \text{ MPa}) - \tau_{\text{vakuum}}^2(T)} \right] \quad (1)$$

$$\rho(T, 0.1 \text{ MPa}) = \rho_{\text{dekan}}(T, 0.1 \text{ MPa}) \cdot \left[1 + \frac{\tau^2(T, 0.1 \text{ MPa}) - \tau_{\text{dekan}}^2(T, 0.1 \text{ MPa})}{\tau_{\text{dekan}}^2(T, 0.1 \text{ MPa}) - \tau_{\text{vakuum}}^2(T)} \right] \quad (2)$$

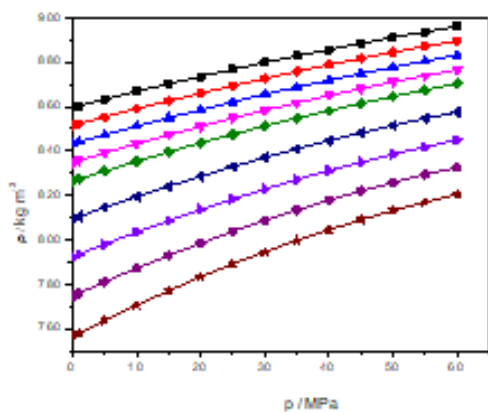
$$\rho(T, p) = \rho_{voda}(T, p) + \rho_{dekan}(T, 0.1MPa) \cdot \left[\frac{\tau^2(T, p) - \tau_{voda}^2(T, p)}{\tau_{dekan}^2(T, 0.1MPa) - \tau_{vakuum}^2(T)} \right] \quad (3)$$

potrebno je, pored perioda oscilovanja U cevi za uzorak, poznavanje i perioda oscilovanja cevi gustinomera za vodu, vakuum i referentni fluid (*n*-dekan) na atmosferskom pritisku, kao i gustine vode i gustina referentnog fluida na atmosferskom pritisku.

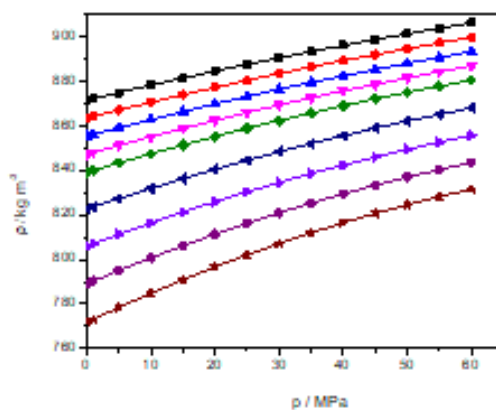
S tim u vezi, najpre su vršena merenja navedenih fluida potrebnih za kalibraciju [9,10].

Rezultati i diskusija

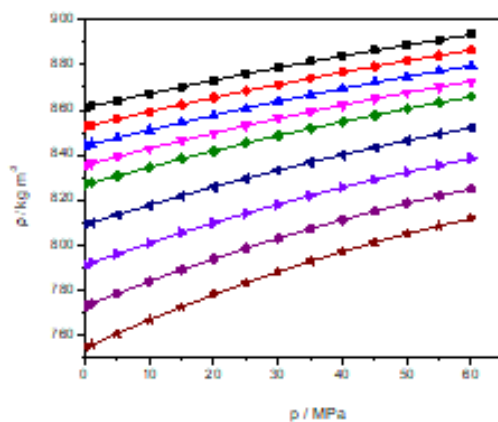
Za čiste komponente linalol, alfa-pinen i beta-pinen na slici 2 su predstavljeni rezultati merenja, tj vrednosti gustina u funkciji pritiska.



(a)



(b)



(c)

Slika 2. Eksperimentalni podaci gustine za (a) alfa-pinen, (b) beta-pinen i (c) linalol, u funkciji pritiska p , na temperaturama: (■) 293.15 K, (●) 303.15 K, (▲) 313.15 K, (▼) 323.15 K, (◆) 333.15 K, (◀) 353.15 K, (▶) 373.15 K, (●) 393.15 K, (★) 413.15 K;

Zaključak

Analizom grafika zavisnosti gustina od pritiska i temperature za odgovarajuće terpene može se jasno videti da s povećanjem pritiska u cevi se povećava i vrednost gustine samog uzorka, dok s povećanjem temperature uzorka vrednost gustine se smanjuje, kao što je i očekivano. Takođe je utvrđeno da pri istim uslovima temperature i pritiska najveću gustinu ima beta-pinen, dok linalol i alfa-pinen imaju veoma slične gustine pri ovim uslovima.

Dobijeni rezultati eksperimentalno određenih gustina dalje mogu koristiti u određivanju volumetrijskih karakteristika, odnosno parametara kao što su koeficijent izotermnog sabijanja, koeficijent izobarskog sabijanja i unutrašnji pritisak. Ovi parametri su veoma značajni u projektovanju motora koji bi koristili navedene terpene kao aditive. Dobijene su niske vrednosti gustina za sva tri termena što predstavlja jedan od bitnih uslova za njihovu upotrebu kao aditivi goriva.

Zahvalnica

Autori se zahvaljuju finansijskoj podršci koju su dobili od strane istraživačkog fonda Ministarstva prosvete, nauke i tehnološkog razvoja, Republike Srbije i Tehnološko metalurškog fakulteta, Univerziteta u Beogradu (br. ugovora 451-03-9/2021-14/200135).

Experimental determination of linalool, α -pinene and β -pinene densities at high pressure

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In order to reduce pollution at the global level in recent years, the main topic is replacing fossil fuels with some new biofuels. Terpenes, which are integral parts of plants, can be used for these purposes as an addition to standard petroleum fuels. Some of

thermodynamic properties under high pressure conditions and moderate temperatures are of significant importance for engine efficiency. In this work, the densities of linalool, α -pinene and β -pinene were obtained in the temperature range 293.15-413.15 K and at pressures up to 60 MPa. Based on these results, it was found that with increasing temperature at constant pressure the density of these terpenes decreases, while with increasing pressure at constant temperature the density increases.

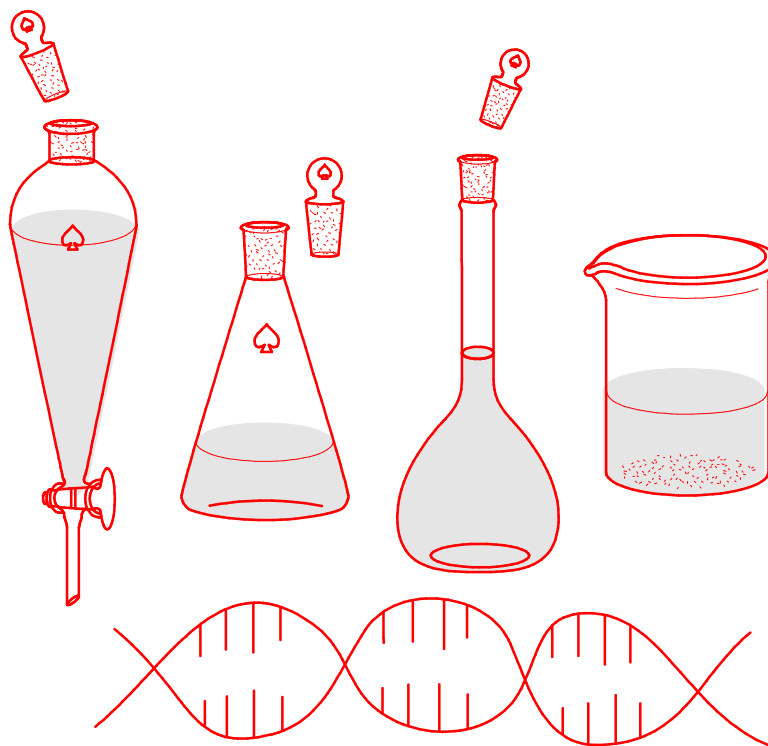
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Tekstilno inženjerstvo

Textile Engineering



TR-TI-2

Sposobnost jednosmernog upravljanja tečnošću glatkih DL pletenina

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Uvod

Pored veličine i oblika (kroja) odevnog predmeta, od ključne važnosti za postizanje adekvatnog termofiziološkog komfora su sposobnost odevnog predmeta da propušta vazduh, paru i toplotu.¹ Pored navedenih parametara, sposobnost tekstilnih materijala da provode tečnost postaje izuzetno važan faktor u uslovima poremećene ravnoteže u termofiziološkoj razmeni između čovečjeg tela i neposredne okoline. U uslovima kada se čovek pojačano znoji usled jače fizičke aktivnosti ili određenih klimatskih uslova okruženja, na površini kože se javlja znoj koji je neophodno brzo ukloniti kako bi se sprečila pojava nelagodnosti. Tečnost se kroz tekstilne materijale prenosi mehanizmima adsorpcije po površini vlakana, odnosno pređa kao i mehanizmom kapilarnog kvašenja. U zavisnosti od hidrofилности površine vlakana, tečnost se zadržava u porama materijala ili se apsorbuje vlaknima.²

Kapilarno kvašenje se može definisati kao makroskopsko kretanje ili prolaz tečnosti kroz kanale (kapilare) uslovljeno geometrijom površine kapilara i međufaznim silama. Kada je reč o tekstilnim materijalima, kapilarno kvašenje predstavlja spontani prolaz tečnosti kroz sistem pora u materijalu, uz prethodno kvašenja površine tekstilnog materijala.³ Tečnost se sa površine tekstilnog materijala kapilarnim silama uvodi u makropore (pore između pređa) koje se prve pune tečnošću, pa se može reći da su one odgovorne za početak prenosa tečnosti kroz materijal. Kada se makropore napune tečnošću, počinje kvašenje mikropora (vazdušni prostori između vlakana u pređi) koje se brzo pune tečnošću i ubrzavaju tok prenosa tečnosti. Drugim rečima, za napredovanje kapilarnog kvašenja kroz tekstilni materijal odgovorne su kapilare manjih dimenzija (pore između vlakana u pređi).⁴ Imajući na umu prethodno rečeno, u okviru ovog rada predstavljeno je istraživanje sposobnosti kapilarnog kvašenja glatkih DL pletenina izrađenih od hidrofилnih (konoplja), hidrofobnih (poliakrilonitril, PAN), i mešavine hidrofилnih/hidrofobnih (konoplja/PAN) vlakana sa ciljem da se ustanovi veza između određenih parametara glatkih DL pletenina (sirovinski sastav, geometrija) i njihove sposobnosti kapilarnog kvašenja.

Materijal i metode

U okviru ovog istraživanja kao eksperimentalni materijal korišćene su tri pletenine: pletenina od 100% konoplje, poliakrilonitrilna (100% PAN) i 50%/50% konoplja/PAN pletenina. Pletenine su bile izrađene uz odgovarajuće kombinovanje konopljine i PAN pređe istih finoća (50 tex) i upredenosti (400 m⁻¹). Konoplja je izabrana pre svega kao hidrofилno vlakno, a zatim zbog svojih pozitivnih aspekata održivosti, i zbog vrlo dobre predispozicije za proizvodnju komfornih proizvoda visoke vrednosti.⁵ Kao hidrofobno

vlakno odabrana su PAN vlakna zbog njihove poroznosti i mekoće. Konstrukcione karakteristike pletenina date su u tabeli 1.

Tabela 1. Konstrukcione karakteristike DL pletenina. ⁶

Parametar (jedinica)		Konoplja	Konoplja/PAN	PAN
Gustina a petlji	D_v^a (cm ⁻¹), (SD)	13,7 (0,6)	13 (0,05)	11 (0,04)
	D_h^b (cm ⁻¹), (SD)	5,5 (0,02)	5,5 (0,02)	6,5 (0,01)
	Površinska ^c (cm ⁻²)	75,4	71,5	71,5
Debljina (mm), (SD)		0,916 (0,03)	1,038 (0,041)	1,181 (0,043)
Površinska masa (g/m ²), (SD)		360 (21,7)	359 (9,5)	376 (9,5)

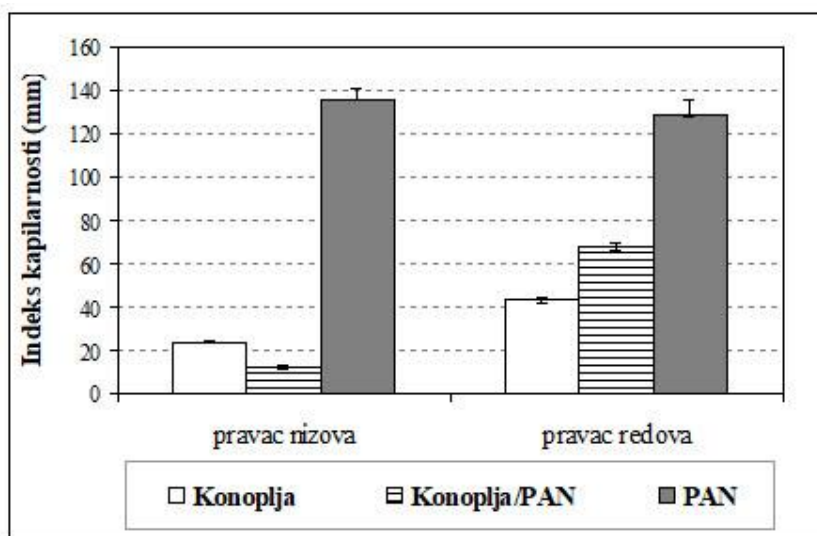
^{a)} vertikalna gustina (broj redova); ^{b)} horizontalna gustina (broj nizova); ^{c)} $D_h \times D_v$

Ispitivanje sposobnosti kapilarnog kvašenja pletenina sprovedeno je standardnim postupkom "test-trake". Za ovu svrhu upotrebljen je eksperimentalni sklop razvijen na Katedri za tekstilno inženjerstvo Tehnološko-metalurškog fakulteta.^{6,7} Eksperiment je sproveden prema nešto modifikovanom standardu ISO 9073-6. Uzorak u obliku trake (50 mm×300 mm) postavlja se na nosač uz predopterećenje na njegovom donjem kraju. Za materijale čija je površinska masa veća od 200 g/m², preporučeno predopterećenje iznosi 10 g. Donji kraj uzorka se uranja u sud sa vodom tako da nivo vode bude iznad postavljenog opterećenja. Kapilarno kvašenje uzorka snima se kamerom i registruje se visina napredovanja tečnosti. Praćeno je kapilarno kvašenje pletenina u pravcu nizova i u pravcu redova. Dobijeni rezultati predstavljaju srednju vrednost tri merenja za svaku pleteninu i za svaki pravac kvašenja. Sposobnost kapilarnog kvašenja pletenina opisana je parametrima: standardni indeks kapilarnosti i maksimalna visina kvašenja. Pletenine sa većim vrednostima ovih parametara imaju prednost u pogledu toplotnog komfora. Statistička analiza dobijenih eksperimentalnih rezultata izvršena je upotrebom ANOVA statistike (analiza varijanse) i Studentovog t-testa. Uticaj sirovinskog sastava pletenina na ispitivane parametre sposobnosti kapilarnog kvašenja statistički je analiziran ANOVA statistikom, pri čemu je za potvrdu ispitivanog efekta neophodno da je vrednost statistike (F) veća od kritične vrednosti statistike (Fcrit), uz uslov da je nivo značajnosti (P) manji od praga značajnosti ($\alpha=0,05$). Uticaj pravca kapilarnog kvašenja statistički je analiziran t-testom, prema kome se u slučaju kada je nivo značajnosti (P) manji od praga značajnosti ($\alpha=0,05$), prihvata hipoteza da su dve nezavisne grupe podataka statistički različite.

Rezultati i diskusija

Standardni indeks kapilarnosti predstavlja visinu napredovanja tečnosti u toku 60 min. Na slici 1, prikazane su vrednosti indeksa kapilarnosti DL pletenina u pravcu nizova i u pravcu redova. Dobijeni rezultati ukazali su na različite vrednosti indeksa kapilarnosti u zavisnosti od sirovinskog sastava ispitivanih pletenina, i pravca kapilarnog kvašenja (izuzev kod poliakrilonitrilne pletenine). Uticaj sirovinskog sastava na brzinu kapilarnog kvašenja pletenina potvrđen je ANOVA statističkom analizom, i to u pravcu redova [$F(130,98) > F_{crit}(5,14)$ za $P(1,12 \times 10^{-5}) < \alpha(0,05)$] i u pravcu nizova [$F(502,38) > F_{crit}(5,14)$ za $P(2,09 \times 10^{-7}) < \alpha(0,05)$]. Najvećim indeksom kapilarnosti okarakterisana je PAN pletenina, kako u pravcu nizova, tako i u pravcu redova. Ovo podrazumeva najbrže kapilarno

kvašenje pletenine u prvih 60 minuta što je posledica hidrofobne prirode PAN vlakana. Najmanjom vrednošću indeksa kapilarnosti odlikuje se konoplja/PAN pletenina u pravcu nizova i konopljna pletenina u pravcu redova. Niži indeks kapilarnosti konopljne pletenine je očekivan zbog hidrofilne prirode celuloznih vlakana, međutim, interesantna činjenica je da je pravcu nizova konoplja/PAN pletenina okarakterisana najnižom vrednošću indeksa kapilarnosti. Ovo se može objasniti uticajem geometrije pletenine na sposobnost kapilarnog kvašenja, s obzirom da je kapilarno kvašenje uslovljeno geometrijom, veličinom i distribucijom mikropora formiranih između vlakana u pređi.⁸ Kapilarnim kvašenjem u pravcu redova pletenine, tečnost putuje duž pređe, time obezbeđuje kontinuitet toka tečnosti a to je preduslov za brže napredovanje tečnosti.³ Kada se kapilarno kvašenje pletenine dešava u pravcu nizova, tok tečnosti nema kontinuitet pa je neophodno da tečnost prelazi sa jednog na susedne slojeve vlakana i usporava se kapilarno kvašenje. U tom smislu, upotreba dve različite pređe kod konoplja/PAN pletenine dodatno je povećala heterogenost toka tečnosti, što objašnjava manji indeks kapilarnosti ove pletenine u odnosu na vrednost indeksa kapilarnosti kod pletenine od konoplje (slika 1).



Slika 1. Indeks kapilarnosti DL pletenina

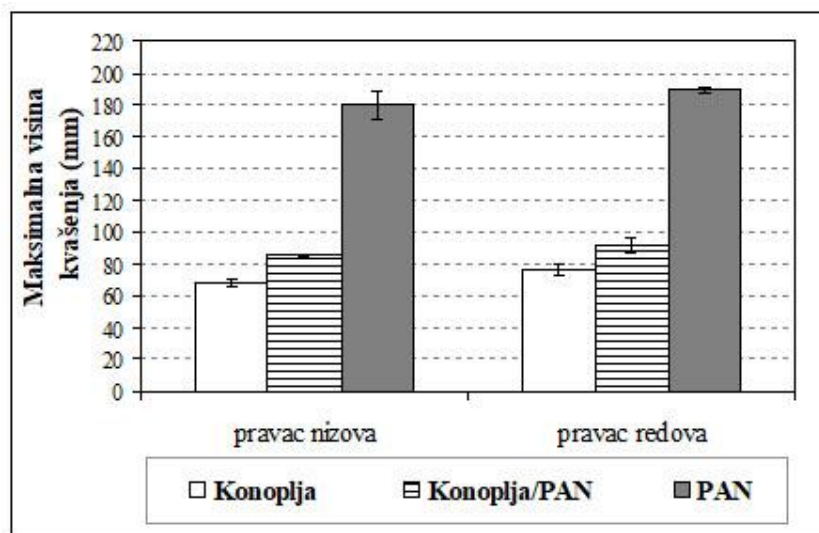
Za konoplja i konoplja/PAN pletenine, statistička analiza (Studentov t-test) je potvrdila različitu sposobnost kvašenja u pravcu nizova i u pravcu redova, dok je PAN pletenina ispoljila slične vrednosti indeksa kapilarnosti u oba pravca (tabela 2).

Tabela 2. Studentov t-test – smer kapilarnog kvašenja (nizovi i redovi), (*statistički značajno za $P < \alpha$, $\alpha = 0,05$)⁶

Parametar (jedinica)	Konoplja	Konoplja/PAN	PAN
$H_{60}^{a)}$ (mm)	0,000*	0,000*	0,462
$H_{max}^{b)}$ (mm)	0,043*	0,306	0,215

a) indeks kapilarnosti; b) maksimalna visina kvašenja

Maksimalna visina kvašenja je visina maksimalnog napredovanja tečnosti do uspostavljanja ravnoteže sa suprotstavljenim gravitacionim silama. Na slici 2 date su vrednosti maksimalne visine kvašenja ispitivanih DL pletenina. Vrednosti maksimalne visine kvašenja bile su uslovljene sirovinskim sastavom pletenina. PAN pletenina je okarakterisana najvećom vrednošću maksimalne visine kvašenja, dok se pletenina od konoplje odlikovala najnižom vrednošću ovog parametra. ANOVA statistička analiza je to potvrdila kako za kapilarno kvašenje u pravcu nizova [$F(121,47) > F_{crit}(5,14)$ za $P(1,4 \times 10^{-5}) < \alpha(0,05)$], tako i kvašenje u pravcu redova [$F(207,7) > F_{crit}(5,14)$ za $P(2,9 \times 10^{-6}) < \alpha(0,05)$]. Hidrofobna priroda PAN vlakana sigurno je obezbedila najveću visinu napredovanja tečnosti kod PAN pletenine, kao i povećanje maksimalne visine kvašenja konoplja/PAN pletenine u odnosu na konopljinu pleteninu. Pored toga, veruje se da je manja visina napredovanja tečnosti konopljine pletenine bila uslovljena i većim makroporama u njoj. Veće makropore sporije se pune tečnošću što usporava i punjenje mikropora tečnošću, odnosno otežava napredovanje tečnosti kroz materijal.



Slika 2. Maksimalna visina kvašenja DL pletenina

Kada se radi o efektu pravca kapilarnog kvašenja pletenina (nizovi ili redovi) na maksimalnu visinu njihovog kapilarnog kvašenja, Studentov t-test je pokazao da razliku u vrednostima maksimalne visine kvašenja u pravcu nizova i u pravcu redova ispoljava samo pletenina koja sadrži isključivo hidrofila (konopljina) vlakana (tabela 2). Ovo se može objasniti činjenicom da je efekat usporavanja toka tečnosti u pravcu nizova pletenine (usled strukturne specifičnosti DL pletenine) najizraženiji kod konopljine pletenine upravo zbog njenih najvećih makropora. Usled manje veličine makropora kod konoplja/PAN i PAN pletenina, obezbeđena je veća dodirna površina između susednih petlji u nizu, a time je olakšano prelaženje tečnosti kroz susedne slojeve vlakana.

Zaključak

Ispitivanjem sposobnosti jednosmernog upravljanja tečnošću DL pletenina izrađenih od hidrofilnih (konoplja), hidrofobnih (poliakrilonitril, PAN), i mešavine hidrofilnih/hidrofobnih (konoplja/PAN) vlakana zapaženi su određeni efekti koje sirovinski sastav i specifična geometrija ove vrste pletenina ima na ispitivane parametre kapilarnog kvašenja: indeks kapilarnog kvašenja i maksimalna visina kvašenja. Dobijeni rezultati ukazali su na različite vrednosti indeksa kapilarnosti u zavisnosti od sirovinskog sastava ispitivanih pletenina, i pravca kapilarnog kvašenja (izuzev kod PAN pletenine). Najvećim indeksom kapilarnosti okarakterisana je PAN pletenina, praćena konoplja/PAN i konopljinom pleteninom, ili obrnuto (konoplja i konoplja/PAN) zavisno od smera kapilarnog kvašenja. Maksimalna visina kvašenja uslovljena je sirovinskim sastavom pletenina, ali i njihovim geometrijskim parametrima, odnosno distribucijom pora u pletenini. PAN pletenina je okarakterisana najvećom vrednošću maksimalne visine kvašenja usled hidrofobne prirode PAN vlakana i manje veličine makropora. Najniža vrednost maksimalne visine kvašenja konopljine pletenine posledica je hidrofilnosti konopljinih vlakana i njene najveće makroporoznosti. Efekat pravca kapilarnog kvašenja pletenina (nizovi ili redovi) na maksimalnu visinu kapilarnog kvašenja uočen je samo kod pletenine od hidrofilnih (konopljinih) vlakana.

Zahvalnica: Rad u okviru MPNT (451-03-68/2020-14/200135)

Unidirectional liquid management properties of plain weft knitted fabrics

In this investigation, an attempt was made to assess the unidirectional liquid management properties of plain knitted fabrics using the wicking test. Two parameters were determined in the wicking tests conducted: capillary index and maximum wicking height. In terms of thermal comfort, higher values of these parameters are desirable. The experimental material included the plain weft knitted fabrics made from pure hydrophilic (hemp), pure hydrophobic (acrylic) and hydrophilic/hydrophobic (hemp/acrylic) fibre blend. The obtained results indicated the differences in the capillary index in respect to the composition of the knitted fabrics and wicking direction (except acrylic knit). The highest capillary index was observed in the acrylic knitted fabric, followed by the hemp/acrylic and hemp knits, or vice versa depending on wicking direction. Maximum wicking height depended on the knit composition. The highest value of the maximum wicking height appeared in the acrylic knit, while the hemp knit exhibited the lowest max wicking height. However, the influence of the wicking direction (wale or course) on the maximum wicking height was confirmed only for the pure hydrophilic (hemp) knitted fabric.

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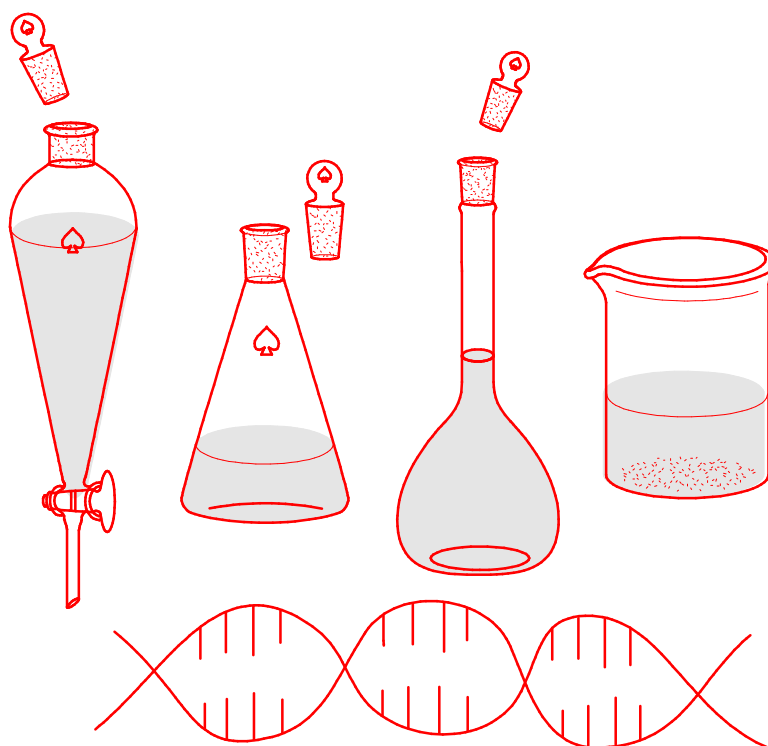
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Hemija životne sredine

Environmental Chemistry



TR-HŽS-1

Chromium(VI) removal from aqueous solutions using powdered coconut shell activated carbon as a low-cost adsorbent

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INTRODUCTION

Most heavy metals, such as Cr (chromium), Pb (lead), Cd (cadmium), Ni (nickel), Cu (copper) and Fe (iron), are extremely toxic above a tolerance limit. These heavy metals in wastewater are not biodegradable and can cause serious harm to human health and ecological environments.¹ One of the top-priority toxic heavy metal in wastewater is chromium.² In natural waters, chromium exists in both trivalent Cr(III) and hexavalent Cr(VI) forms. Cr(VI) is the most toxic one and have the tolerance limit 0.1 mg/L into surface water and 0.05 mg/L in potable water.³

Various methods, such as ion exchange, sedimentation, electrochemical process, cementation, coagulation, adsorption and solvent extraction have been developed for the removal of Cr(VI) and other toxic metals from wastewater.⁴ Among these methods, in some papers,⁵⁻⁸ adsorption has been used as one of the most effective method for the removal of Cr(VI) from aqueous solutions. Characteristics of adsorption, such as low cost, easy to perform, efficient and reversible method with high operating speed, make this method as most commonly used for the removal of Cr(VI) from aqueous solutions.⁹ Several adsorbents, like activated alumina,¹⁰ zeolites,¹¹ natural bisorbents such as chitosan,¹² but also activated carbon¹³ have been used for the removal of Cr(VI) from aqueous solutions. Due to the high cost, commercial activated carbon is not available in less developed countries and there is a considerable attention to produce activated carbon from less expensive and available materials. As a low-cost adsorbent, activated carbon can be produced from materials such as rice husk, seeds husk, tea leaves, sawdust, oil palm shell, coconut husk and coconut shell.¹⁴

Activated carbon is one of the most important adsorbents which is applied in different areas. In these areas it is important to determine and remove low concentrations of some pollutants, such as heavy metals. Very good features of this adsorbent are the main reason why it is used, such as large surface area, porous structure, high adsorption capacity, selective adsorption and low cost. Also, it is important to note that activated carbon has microcrystalline structure with different size and shape of pores, while surface groups plays important role in the adsorption process. Carbon - oxygen surface groups are the most important and they influence the surface characteristics, such as polarity and physico-chemical properties of adsorbent. There are two processes for preparation of activated carbon, chemical activation which involves presence of chemical agents, and physical activation, which involves carbonization.¹⁵⁻¹⁶

For this research, low-cost powdered activated carbon made from coconut shell was used as adsorbent to remove Cr(VI) from aqueous solutions. Characterization of activated carbon, produced from coconut shell, was accomplished using scanning electron microscopy (SEM) and Brunauer-Emmett-Teller (BET) method. The effects of three

adsorption parameters, such as solution pH, contact time and initial Cr(VI) concentration, were investigated with respect to the removal efficiency of Cr(VI) from aqueous solutions. Adsorption equilibrium characteristics were analyzed by using the two adsorption models, namely the Langmuir and the Freundlich isotherms.

EXPERIMENTAL

Coconut shell activated carbon (CSAC) was obtained from Trayal corporation (Kruševac, Serbia). The morphological characteristics and semi-quantitative elemental analyses of the CSAC powder were obtained by SEM microscope VEGA TS 5130 MM (Tescan, Czech Republic) equipped with the INCA PentaFET-x3EDS detector (Oxford Instruments, UK). The porous structure of CSAC was characterized by nitrogen sorption technique at -196°C using Thermo Scientific Surface Analyzer (Thermo Fisher Scientific Inc., USA). The specific surface area of the sample (S_{BET}) was calculated according to the BET method from the linear part of the isotherms.¹⁷ The total pore volume (V_{tot}) was calculated by applying Gurevitsch's rule¹⁸ at the relative pressure $p/p^0 = 0.95$ (p and p^0 represent the equilibrium and saturation pressures of nitrogen at the temperature of adsorption). Micropore volume (V_{micro}) was obtained using the t-plot-method.¹⁹

A stock solution (1000 mg/L) of Cr(VI) was prepared by dissolving $\text{K}_2\text{Cr}_2\text{O}_7$ into deionized water. The pH values of the initial solutions were adjusted by adding HNO_3 (0.1 mol/L) or NaOH (0.1 mol/L). In these experiments, the batch adsorption studies were conducted by mixing 50 mg of the adsorbent material with 25 mL of 10 mg/L Cr(VI) solution at pH 3.1. Then, the liquid mixture was shaken for 180 min at 150 rpm and obtained solutions were filtered using 0.45 μm microporous membrane filter. Determination of initial and residual concentrations of Cr(VI) ions was done by using a 797 VA Computrace polarography system (Metrohm, Switzerland) with the Metrohm's procedure for the voltammetric determination of Cr(VI) ions in water samples (No. 116/3 e). The effects of different experimental parameters, such as pH value (2.0 - 8.0), contact time (0 - 180 min) and initial Cr(VI) concentration (10 - 500 mg/L), were investigated with respect to the removal efficiency of Cr(VI) ions. One of the parameters was changed, while the other parameters were kept constant.

The equilibrium adsorption capacity of Cr(VI) per unit mass of adsorbent, q_e (mg/g), and the removal efficiency of Cr(VI), E (%), were calculated using the equations:

$$q_e = \left(\frac{C_i - C_e}{m} \right) V \quad (1)$$

$$E = 100 \left(\frac{C_i - C_t}{C_i} \right) \quad (2)$$

where C_i and C_e (mg/L) represent initial and equilibrium concentrations of Cr(VI) in the solution, respectively, C_t is the concentration at time t (mg/L), V is the volume of the solution (L), and m is the weight of powdered coconut shell activated carbon (g).

RESULTS AND DISCUSSION

Morphology of the CSAC sample, shown in Fig. 1a and b, revealed particles in the range of less than a μm up to 120 μm in diameter. Particles have irregular shape and sharp edges. A rough texture with a large number of pores in different sizes and shapes, as well as shallow and deep cavities, could be observed on the external surface of CSAC. These cavities and pores on the surface promote adsorption.

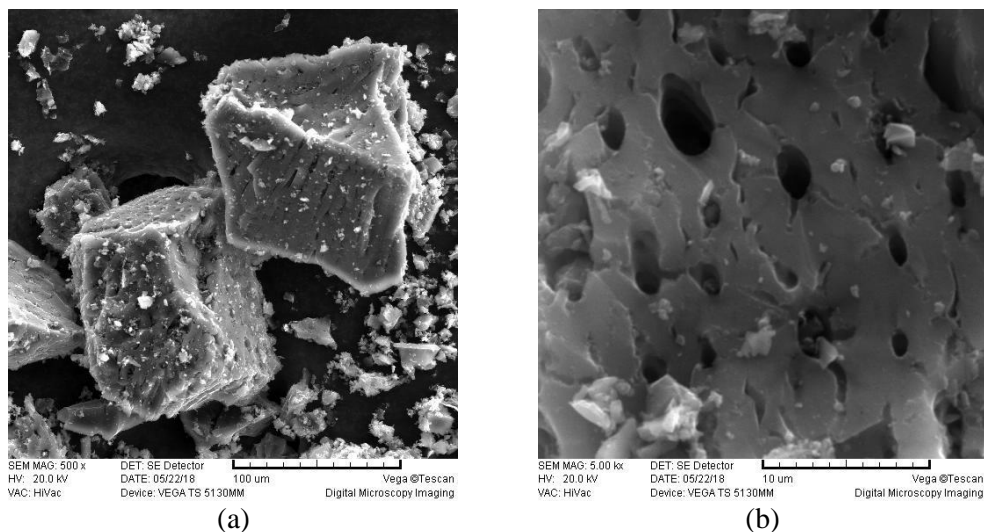


Fig. 1. SEM micrographs of the CSAC adsorbent at (a) 500x and (b) 5000x magnification.

Nitrogen adsorption/desorption isotherms and pore distributions for the CSAC sample are shown in Fig. 2. Specific surface area, S_{BET} , and pore volumes of CSAC, V_{tot} and V_{micro} , obtained from nitrogen adsorption/desorption isotherms, were $1177 \text{ m}^2/\text{g}$, $0.595 \text{ cm}^3/\text{g}$ and $0.397 \text{ cm}^3/\text{g}$, respectively. Considering the pore volume of the sample, nitrogen adsorption showed that CSAC sample is mainly microporous. The most frequent pore diameters, corresponding to the maximum of the pore size distribution curve presented in the insert of Fig. 2, have values of 2.1 and 4.0 nm, with a small fraction of pores with diameter of 5.2 nm.

The adsorption of Cr(VI) ions onto CSAC was strongly dependent on the initial pH of aqueous solutions. The obtained results are shown in Fig. 3a. The effect of initial solution pH was investigated from a range of 2.0 to 8.0, under the precise conditions. As the pH of the solution was increased from 2.0 to 3.5, the removal efficiency of Cr(VI) increased from 76% to 98%, while the maximum adsorption occurred at the pH value 3.1. The effect of pH on the removal efficiency of Cr(VI) can be explained by the adsorbent surface properties and the fact that Cr(VI) ions in the solution can exist in different forms. In acidic medium Cr(VI) exists in two forms, as hydrogen chromate (HCrO_4^-) and dichromate ($\text{Cr}_2\text{O}_7^{2-}$), while in basic solutions Cr(VI) exists in the form of chromate (CrO_4^{2-}). The increase of Cr(VI) adsorption at acidic pH should be due to the electrostatic attraction between positively charged groups of CSAC surface and the HCrO_4^- anion, which is the dominant species at low pH values. At higher pH values, decrease of Cr(VI) adsorption may be explained by the competitive adsorption between CrO_4^{2-} and hydroxyl (OH^-) ions. Thus, the initial pH of 3.1 was selected as the optimum pH value of Cr(VI) solution for all the following experiments.

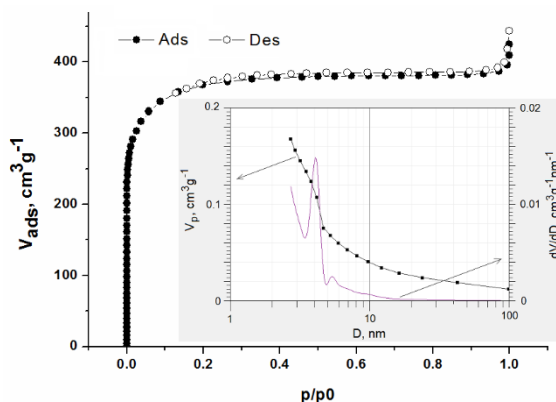


Fig. 2. Nitrogen adsorption/desorption isotherms of the CSAC (Insert: Pore size distribution).

The effect of contact time on Cr(VI) adsorption by CSAC is presented in Fig. 3b. The removal of Cr(VI) increased sharply in the first 10 min, then slowed down from 10 to 60 min, and finally reached equilibrium after 60 min of contact. Such behavior can be explained by the presence of large number of vacant sites at the beginning of the adsorption process. As the time proceeded, the removal of Cr(VI) decreased due to its accumulation on the vacant sites until the removal approached the equilibrium. Further increase in contact time did not influence the removal of Cr(VI). The removal efficiency of Cr(VI) at equilibrium was 98%, while the equilibrium adsorption capacity reached the value of 5 mg/g. In order to ensure the equilibrium, the adsorption time of 120 min was used in further experiments.

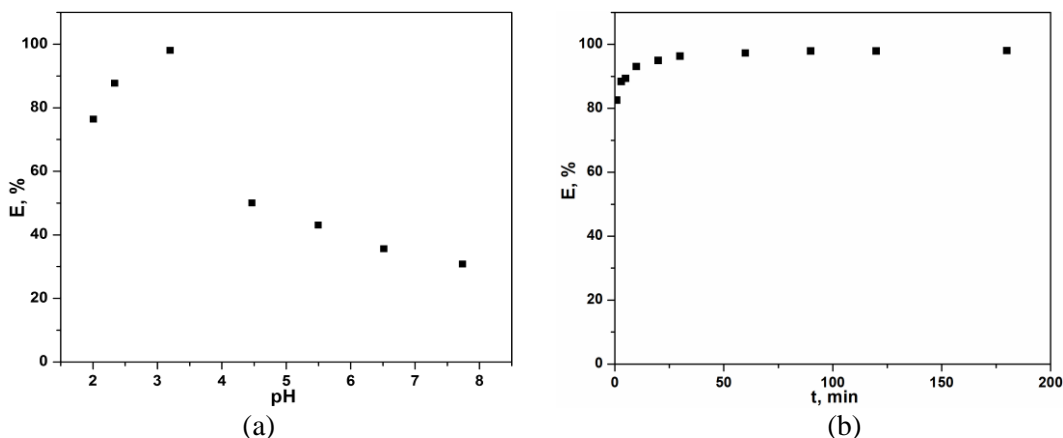


Fig. 3. Effect of (a) initial solution pH and (b) contact time on the removal efficiency of Cr(VI) by CSAC. Conditions: initial Cr(VI) concentration, 10 mg/L; stirring speed, 150 rpm; adsorbent concentration: 2 g/L; pH 3.1

The effect of initial Cr(VI) concentration on the removal efficiency and adsorption capacity of CSAC is shown in Fig. 4a. As can be seen, the removal efficiency of Cr(VI), E , decreased from 98% to 12% and the adsorption capacity, q_e , increased from 5 mg/g to 33 mg/g with increasing the initial Cr(VI) concentration in the aqueous solution from 10 to 500 mg/L. The observed decreased removal efficiency as the function of increased initial

Cr(VI) concentration can be explained by the fact that adsorption sites of CSAC got saturated in the case of higher concentrations. The adsorption capacity increased with increasing the initial Cr(VI) concentration because of the increase in the driving force of the Cr(VI) ions toward the active sites on the CSAC adsorbent.

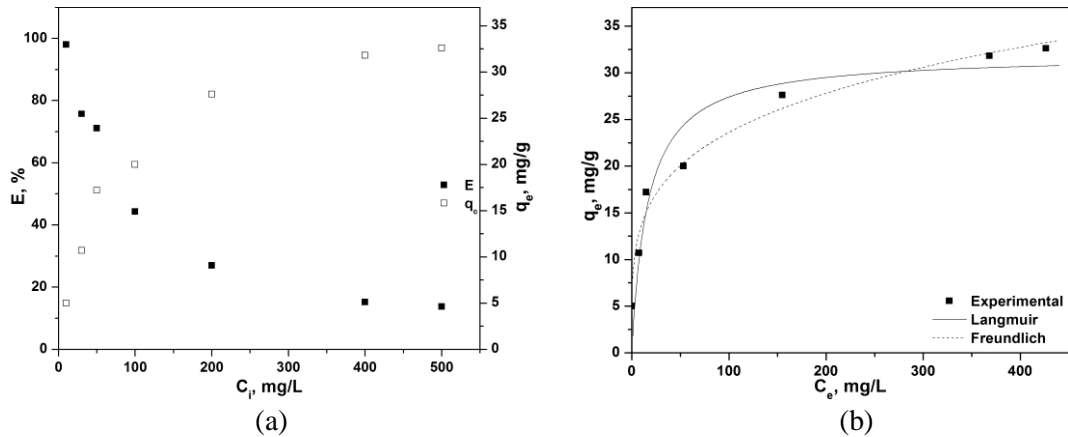


Fig. 4. (a) Effect of initial Cr(VI) concentration on its adsorption by powdered CSAC and (b) Experimental and theoretical isotherm plots for Cr(VI) adsorption. Conditions: initial Cr(VI) concentration, 10 - 500 mg/L; pH, 3.1; contact time, 180 min; stirring speed, 150 rpm; adsorbent concentration: 2 g/L

The experimental data obtained for the adsorption equilibrium of Cr(VI) onto CSAC at different initial Cr(VI) concentrations were analyzed using the two adsorption isotherm models, the Langmuir and the Freundlich, which is shown in Fig. 4b. The closeness between experimental data and isotherm model is determined from the value of the coefficient of determination, R^2 . Besides, the non-linear chi-square analysis, χ^2 , was used to find the better fitting isotherm model. The corresponding isotherm parameters and the determination coefficients, as well as χ^2 values, of these two models are listed in Table 1. Based on the values of the R^2 and the results of chi-square analysis, Cr(VI) adsorption by CSAC can be better described by the Freundlich isotherm compared to Langmuir isotherm. The obtained results suggested that the surface of CSAC adsorbent is heterogeneous and that the adsorption of Cr(VI) occurred through multilayer formation. The value of n , falling in the range from 1 to 10, indicated that Cr(VI) adsorption by CSAC was favorable.

Table 1. Langmuir and Freundlich isotherms for the adsorption of Cr(VI) onto powdered CSAC. Conditions: initial Cr(VI) concentration, 10 - 500 mg/L; pH, 3.1; contact time, 180 min; stirring speed, 150 rpm; adsorbent concentration: 2 g/L

Isotherm model	Parameters	Non-linear fit
Langmuir $q_e = q_m \cdot K_L \cdot C_e / (1 + K_L \cdot C_e)$	q_m (mg/g)	31.9
	K_L (L/mg)	0.061
	R^2	0.948
	χ^2	53.77
Freundlich $q_e = K_F \cdot C_e^{1/n}$	n	4.2
	K_F (mg/g)/(mg/L) ^{1/n}	8.0
	R^2	0.983

* q_m and K_L are the Langmuir constants related to the adsorption capacity and free energy of adsorption, respectively; K_F and n are the Freundlich constants related to the adsorption capacity of adsorbent and adsorption intensity, respectively

CONCLUSION

Removal of the toxic hexavalent chromium from aqueous solutions was possible using CSAC as a low-cost adsorbent. The removal of Cr(VI) was found to be dependent on the pH value, contact time and initial ion concentration. Adsorption was efficient in the pH range of 2.0 to 3.5. The adsorption isotherm data of Cr(VI) onto CSAC were described by Freundlich isotherm equation. CSAC is inexpensive and readily available. Results of the presented study showed that the investigated material could be used as an efficient adsorbent for the removal of Cr(VI) ions from aqueous solutions.

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Uklanjanje hroma(VI) iz vode primenom praškastog ugljeničnog materijala dobijenog iz kokosove ljuske kao jeftinog adsorbenta

Praškast ugljenični materijal proizveden iz kokosove ljuske korišćen je kao adsorbent za uklanjanje Cr(VI) jona iz vodenih rastvora. Karakterizacija adsorbenta rađena je primenom dve analitičke tehnike, skenirajućom elektronskom mikroskopijom (SEM) i BET metodom. Eksperimenti adsorpcije rađeni su u šaržnom režimu, kako bi se istražili uticaji pH rastvora, vremena kontakta i početne koncentracije Cr(VI) jona. Eksperimentalni rezultati su pokazali da je efikasnost uklanjanja Cr(VI) najveća u pH intervalu od 2,0 do 3,5, a da se ravnoteža uspostavlja nakon 60 minuta. Dva ravnotežna adsorpciona modela, Langmirov i Frojndlihov, korišćena su za fitovanje dobijenih podataka. Frojndlihova izoterma je obezbedila najbolju korelaciju za adsorpciju Cr(VI) jona na ugljeničnom materijalu proizvedenom iz kokosove ljuske. Na osnovu dobijenih rezultata može se zaključiti da ugljenični materijal proizveden iz kokosove ljuske predstavlja jeftin i efikasan adsorbent koji bi potencijalno mogao biti korišćen za tretman otpadnih voda koje sadrže toksični Cr(VI).

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