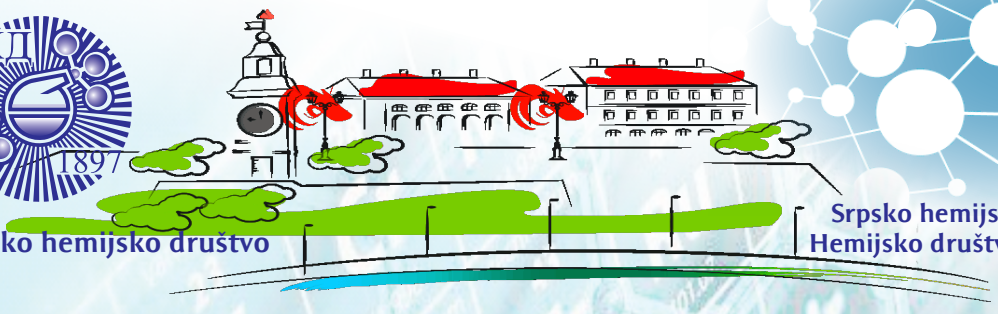

Srpsko hemijsko društvo

Srpsko hemijsko društvo
Hemijsko društvo Vojvodine

55. savetovanje Srpskog hemijskog društva

KRATKI IZVODI RADOVA

55th Meeting of the Serbian Chemical Society

Book of Abstracts

Novi Sad 8. i 9. juni 2018.
Novi Sad, Serbia, June 8-9, 2018

Srpsko hemijsko društvo

Serbian Chemical Society

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Hemijsko društvo Vojvodine

Serbian Chemical Society
Chemical Society of Vojvodina

55. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA

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SADRŽAJ / CONTENTS

Plenarna predavanja / Plenary Lectures

PP 1

Palladium and platinum N-heterocyclic carbene complexes: from catalysis to nanomaterials

Ernesto de Jesús Alcañiz
Organic and Inorganic Chemistry Department, Chemistry Research Institute "Andrés M. del Río", Universidad de Alcalá, Campus Universitario, 28871 Alcalá de Henares, Spain

The introduction of N-heterocyclic carbene ligands (NHCs) in the chemistry of transition metals two decades ago has contributed to significant advances in palladium-promoted cross-couplings and other transition-metal catalyzed reactions.[1] In this presentation, we will summarize some recent developments of our group in three main areas:

a) *Cross-coupling reactions in aqueous-phase.*[2] We developed several years ago efficient conditions for the coupling of organoalkoxysilanes and aryl bromides in water. The challenging activation of inactivated and sterically hindered aryl chlorides was further achieved by using NHC ligands functionalized with ionic groups. Implications of the use of water in mechanistically relevant aspects of these reactions will be discussed.

b) *Water-soluble metal nanoparticles stabilized by hydrophilic NHC ligands.*[3] Thermal decomposition of alkyl Pd and Pt NHC complexes furnished an organometallic approach to the controlled synthesis of metal nanoparticles. These nanoparticles were stable and highly soluble in water as a result of the coordination of hydrophilic NHC ligands to their surface. The mechanism of formation and the characterization of the surface of these nanoparticles by liquid and solid-state NMR spectroscopy will be discussed.

c) *Recovery* of *molecular weight-enlarged catalysts using nanofiltration membranes*.[4] For being attractive for industry, Pd loadings used in C-C coupling reactions should be reduced from the typical mol% range to the ppm or ppb level.[5] We have attained Pd consumptions at the ppm level in Heck-Mizoroki reactions thanks to the recovery of molecular weight-enlarged catalysts using nanofiltration membranes. The high recovery rate was based on the use of NHC catalysts. The NHC complexes act as slow-delivering reservoirs of ligand-free Pd species (which are the true active catalyst). At the end of the reaction, the ligand-free Pd species are trapped again by the NHC ligands, avoiding their degradation to Pd black.

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PP 2 text rada / full text

Intensification of bulk crystal growth by magnetic fields: from lab-scale to commercial size equipment

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**Crystal Technology Consulting, Helga Hahnemann Str. 57, 12529 Schönefeld*

In the bulk crystal growth, there is a strong need for a cost-effective technology that can improve the ingot quality and increase the yield. For a successful process, it is important i.a. to control the level of impurities and thermal stress in the crystal. One approach is to perform process intensification by application of magnetic fields. Within the framework of KRIST*MAG*® project (2005-2008), Leibniz Institute for Crystal Growth with several partners developed the first internal heater magnet module for simultaneous generation of heat and traveling magnetic field in the hot zone. Up to now, this concept has been successfully further developed and applied on 10 furnaces for the growth of various semiconductors: Si, Ge, GaAs, (Hg,Cd)Te *etc.*, from lab scale up to the industrial size equipment. It is guarded by 18 patents and honored by two innovation prizes. The main idea of KRIST*MAG*® concept is to generate Lorentz forces in the melt with intensity, direction and spatial distribution as required. Such volume force can be used to e.g. stir the melt, reduce the turbulences in the melt, flatten solid/liquid (s/l) interface, homogenize dopand distribution, remove impurities from the (s/l) interface etc. The overview of very encouraging numerical results will be presented and the strengths and the bottlenecks of the KRIST*MAG*® concept will be discussed.

Intenziviranje rasta kristala iz rastopa pomoću magnetnih polja: od laboratorijskog nivoa do industrijskog postrojenja

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**Crystal Technology Consulting, Helga Hahnemann Str. 57, 12529 Schönefeld*

U oblasti proizvodnje kristala iz rastopa postoji kontinuirana potreba za razvojem efikasne tehnologije za poboljšanje prinosa i kvaliteta kristala. Za uspešan proces rasta, neophodno je kontrolisati nivo nečistoća i termalna naprezanja u kristalu. Jedan od mogućih pristupa je intenziviranje procesa rasta primenom magnetnih polja. U okviru KRIST*MAG*® projekta (2005-2008), Leibniz Institute for Crystal Growth sa nekoliko partnera razvio je prvi interni grejno-magnetni modul za simultanu proizvodnju toplote i putujućeg magnetnog polja u zoni rasta kristala. Do sada, ovaj koncept je praktično realizovan u 10 postrojenja za rast različitih kristala (npr. Si, Ge, GaAs, (Hg,Cd)Te), od laboratorijskog nivoa do postrojenja industrijske veličine. Tehnologija je zaštićena sa 18 patenata uz osvojene dve nagrade za inovaciju. Osnovna karakteristika KRIST*MAG*® koncepta je mogućnost generisanja Lorencovih sila u rastopu sa željenim intenzitetom, pravcem i prostornom raspodelom. Takve sile se mogu koristiti za npr. bezkontaktno mešanje i smanjenje turbulencija u rastopu, ravnanje kristalizacionog fronta, homogenizaciju raspodele primesa, odnošenje nečistoca sa kristalizacionog fronta itd. U ovom radu biće predstavljen pregled vrlo ohrabrujućih numeričkih rezultata uz diskusiju prednosti i ograničenja KRIST*MAG*® tehnologije.

PP 3

Wetting and evaporation of solvents from nanostructured surfaces, fundamentals of evaporation profile based chemical analysis

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The evaporation of liquid droplets from controlled surfaces represents a sweet spot at the intersection of fundamental physical chemistry with practical applications[1]. We are particularly fascinated by the opportunities created by evaporation phenomena for simple, robust analytical applications. In the course of this work we introduced the concept of evaporation profile based analytics earlier[2]. Preliminary results in this field were achieved on buckypaper, a highly versatile porous macroscopic form of carbon nanotubes that can be prepared by simple filtration. These studies have directed our attention to the importance of engineering the surface of the evaporation substrate in a more controlled way. In this talk I will introduce the concept of the evaporation profile, then discuss a few examples of wetting and evaporation phenomena from non-buckypaper surfaces as well.

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Predavanja po pozivu / Invited Lectures

PPP 1

Chemical composition of buckwheat as revealed by the use of nuclear beams

Ivan Kreft
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The aim of this review is to present some modern approaches and methods of analyzing buckwheat plants and buckwheat materials to elucidate the factors of their technological and nutritional value. This is required in order to develop novel high-quality functional and other food products, based on the variability of properties of common and Tartary buckwheat plants. The principles and potential use of micro-proton induced X-ray emission (micro-PIXE), synchrotron-based micro-X-ray fluorescence (micro-XRF) and inductively coupled plasma-mass spectrometry (ICP-MS) hyphenated with pulsed laser ablation (LA) are presented.

Buckwheat plants consist of different parts, organs, tissues and cells. There are often considerable differences in structure and chemical composition, not only between the major plant parts but also between and within individual tissues.

Some differences emerge during the plant development process. During germination, there is metabolic transformation in an embryo and a plantlet, which impacts the relative distribution of elements and metabolites, and the digestibility, availability for humans when consumed as a food. During the growth and development some substances, for example starch, are degraded, while others, for example fagopyrin in the case of buckwheat, are synthesised. Ecological and agrotechnical factors, most notably UV-B radiation, influence the structure and composition of buckwheat plants, thereby provoking the synthesis of secondary metabolites, especially flavonoids. Structural and compositional features of plant parts are fundamentally connected to the physiological role of structures and compounds and are also associated with plant metabolism and reproduction.

PIXE (proton induced X-ray emission) research in our group was initiated using the van de Graaff particle accelerator to accelerate protons. X-ray emission, characteristic for elements in the sample, and proportional to the concentration of elements (e.g. sulphur) was used for elemental quantification. Over the years the micro-PIXE technique was improved and a better lateral discrimination in screening the elemental composition was obtained. In the last ten years significant progress has been made in the development and application of various 2D imaging techniques, to be used in complex biological systems like buckwheat grain. Lateral resolution and sensitivity have been much improved. The capabilities of the PIXE technique were greatly extended for different applications with the development of the focused proton beam - micro-PIXE. The magnetic quadrupole lenses are generally used to focus the proton beam down to the sub-micrometer level. By rastering the focused proton beam over the sample, and by the scoring of the induced X-ray fluorescence (XRF), spatially resolved element distribution maps of the samples can be obtained. The advantage of micro-PIXE over other 2D imaging techniques is in its wide elemental range (from sodium (Na) to uranium (U)), high elemental sensitivity (sub-micron spatial resolution) and fully quantitative element concentration analysis.

PPP 2

Jonske tečnosti - primena u farmaciji i biotehnologiji

Milan Vraneš, Aleksandar Tot, Snežana Papović, Sanja Belić, Jovana Panić, Slobodan Gadžurić

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U poslednjih nekoliko godina, jonske tečnosti (JT) su u samom fokusu najperspektivnijih grana nauke i tehnologije. JT nisu pronašle primenu samo u fundamentalnim istraživanjima, već su važni kandidati za rešavanje osnovnih izazova i problema savremenog društva, kao što je efikasno dobijanje čiste energije, tretman nuklearnog otpada, razvoj novih katalizatora, ekstrakcija i razdvajanje biološki aktivnih molekula. Ovo predavanje se fokusira na primenu metodologije JT u rešavanje suštinskih farmaceutskih problema, kao što su niska rastvorljivost i posledično smanjena bioraspoloživost farmaceutskih jedinjenja, pojava polimorfizma, koja ozbiljno umanjuje efikasnost komercijalno dostupnih lekova. Razvoj strategija za korištenje JT kao nosača farmaceutskih aktivnih jedinjenja su izuzetno obećavajući i imaju široku perspektivu. Isto tako, sinteza jonskih tečnosti kombinovanjem katjona i anjona sa različitim farmkološkim ulogama pruža odgovore na neke od najvećih izazova savremene farmaceutske industrije.

Ovaj rad je finanijski potpomognut od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije u okviru projekta ON172012.

Ionic liquids: Pharmaceutical and biotechnological applications

Milan Vraneš, Aleksandar Tot, Snežana Papović, Sanja Belić, Jovana Panić, Slobodan Gadžurić

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In the past several years, ionic liquids (ILs) have been at the cutting edge of the most promising science and technology. ILs not only have found applicationsin classical areas of knowledge but also are important candidates to solve classical problems within several societal challenges, such as clean and efficient energy, treatment of high-level nuclear waste, development of new catalysts, extraction and separation of biologically active compounds. This lecture focuses on the application of IL methodologies to solve critical pharmaceutical problems, in particular, the low solubility and thus bioavailability of pharmaceutical compounds and the presence of polymorphs, which severely hamper the efficacy of important commercially available drugs. The development of strategies to use ILs as carriers of pharmaceutical active compounds is an extremely promising and wide avenue. Further, the synthesis of liquid liquids through the discerning combination of cations and anions with several distinct pharmaceutical roles provides answers to some of today's pharmaceutical industrial challenges.

This work was financially supported by the Ministry of Education, Science and Technological Development of Serbia under project contract ON172012.

PPP 3

Tečna biogoriva: značaj, trenutno stanje proizvodnje i predstojeći izazovi

Nataša L. Đurišić-Mladenović
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Biogoriva predstavljaju tečna ili gasovita goriva proizvedena iz različitih izvora biomase, koja se primenjuju u motorima sa unutrašnjim sagorevanjem vozila. Potraga za alternativnim motornim gorivima, uključujući i razvoj procesa za proizvodnju biogoriva, započela je tokom ’70-tih godina 20. veka sa pojavom prve naftne krize, kada je energetska sigurnost najrazvijenijih zemalja sveta bila dovedena u pitanje. Pored toga što utiču na smanjenje zavisnosti od uvoza nafte, biogoriva se koriste danas u razvijenim zemljama i radi dekarbonizacije energetskih izvora sa krajnjim ciljem smanjenja zagađenja životne sredine, globalnog zagrevanja i klimatskih promena. U radu će biti dat pregled različitih biogoriva i njihove proizvodnje, postojeće relevantne regulative i stanja trenutne proizvodnje konvencionalnih i naprednih biogoriva u EU. Takođe biće predstavljeni izazovi koji se nameću u pogledu proizvodnje i korišćenja biogoriva u bliskoj budućnosti u odnosu na druge alternative koje se razvijaju u sektoru saobraćaju. Dodatno, posebna pažnja će biti posvećena trenutnoj situaciji u Srbiji u odnosu na mogućnosti uvođenja biogoriva u sektor transporta i obaveza preuzetih sa dobijanjem statusa kandidata za članstvo u EU.

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Liquid biofuels: importance, current state of production and challenges

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Biofuels represent liquid or gaseous fuels produced from biomass sources with intention to be used in internal combustion engines of vehicles. The search for alternative transportation fuels including development of processes for biofuel production started in the 1970s with the first oil crises, when some of the most developed countries raised concerns about their energy security. Apart reducing the fossil fuel import dependence, biofuels are included today in energy mix of developed countries also in order to contribute to decarbonization of the energy sources towards mitigation of the environmental pollution, global warning and climate changes. This study summarizes some facts on various types of biofuels, existent legislation and current production of conventional and advanced biofuels in the EU, as well as challenges in front of biofuel production and utilization in the near future. Additionally, special attention is given to the current situation in Serbia regarding possibilities to include biofuels in transport in accordance to obligations accepted as the candidate country for the EU membership.

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PPP 4

Prirodni pigmenti u funkciji antioksidanata

Jelena J. Vulić, Jasna Čanadanović-Brunet, Gordana Ćetković, Vesna Tumbas-Šaponjac
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Tokom oksidacionih procesa, antioksidanti imaju važnu ulogu u održivosti hrane i sprečavanju nastajanja negativnih metaboličkih produkata u ljudskom organizmu. Humani organizam je zaštićen od negativnog dejstva reaktivnih oksidativnih vrsta enzimima (superoksid dismutaza, katalaza i glutation peroksidaza), kao i prirodnim antioksidantima. Takođe, antioksidativna jedinjenja umanjuju ili potpuno inhibiraju formiranje sekundarnih procesa peroksidacije lipida. Prirodni pigmenti (fenolna jedinjenja, karotenoidi, betalaini, itd.) pored svoje antioksidativne aktivnosti, utiču i na boju, aromu i teksturu prehrambenih proizvoda. Poznato je da mnoga polifenolna jedinjenja imaju antioksidativna svojstva, a naučne studije su ukazale i na njihove pozitivne efekte u prevenciji i lečenju mnogih bolesti. Takođe, karotenoidi (β-karoten, lutein, likopen i izozeaksantin), narandžasto-žuti pigmenti, zahvaljujući strukturnim karakteristikama pokazuju i antioksidativnu aktivnost. Betalini su N-heterociklični ljubičasti i žuti pigmenti. Pored toga što daju boju prehrambenim proizvodima, imaju antiupalno i detoksifikaciono delovanje, i štite od prevremenog starenja.. Mehanizmi delovanja prirodnih pigmenata zavise od njihove hemijske strukture.

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Antioxidant functions of natural pigments

Jelena J. Vulić, Jasna Čanadanović-Brunet, Gordana Ćetković, Vesna Tumbas-Šaponjac
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During oxidation processes, antioxidants play an important role in food quality and prevent the formation of negative metabolic products in the human organism. The human body is protected against the negative effect of reactive oxidative species by enzymes (superoxide dismutase, catalase and glutathione peroxidase), as well as by natural antioxidants. Also, antioxidant compounds reduce or completely inhibit secondary lipid peroxidation processes. Natural pigments (phenolic compounds, carotenoids, betalaines, etc.), in addition to their antioxidant activity, also affect the color, flavor and texture of food products. It is well known that many polyphenolic compounds have antioxidant properties, and scientific studies have also indicated their positive effects in the prevention and treatment of many diseases. Also, carotenoids (β-carotene, lutein, lycopene and isohexanthin), orange-yellow pigments, due to their structural characteristics, show antioxidant activity. Betalains are N-heterocyclic violet and yellow pigments. In addition to food coloring, they have anti-inflammatory, detoxification and antiaging activity. Mechanism of their actions is correlated to their structure–activity relationships.

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Saopštenja / Contributions

Analitička hemija / Analytical Chemistry

AH P 01

Određivanje sadržaja metala i metaloida u medu metodom induktivno spregnute plazme optičke emisione spektrometrije (ISP-OES)

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Med je prirodni proizvod velike nutritivne vrednosti sa širokom terapeutskom primenom. Kompleksnog je sastava i u ljudskoj ishrani važan izvor esencijalnih, ali zahvaljujući brojnim antropogenim izvorima, nažalost i toksičnih elemenata. Cilj ovog rada je bio određivanje sadržaja esencijalnih i toksičnih elemenata u 20 unifloralnih i multifloralnih medova iz različitih područja Republike Srbije, sakupljenih u periodu od 2015. do 2017. god. Uzorci su za analizu pripremani metodom mikrotalasne digestije, a sadržaj metala i metaloida (Al, As, Cd, Cr, Cu, Fe, K, Mg, Mn, Na, Ni, Pb, Se, Si, Zn) je određivan metodom ISP-OES. Rezultati su pokazali da koncentracija esencijalnih elemenata (K, Fe, Mg, Mn, Na, Se, Si, Zn) zavisi od geografskog porekla, u prvom redu sastava zemljišta, ali i uslova pčelinje paše. Sadržaj toksičnih elemenata je u okviru dozvoljenih granica i vezen za antropološka zagađenja. Rezultati ovog rada su pokazali kako sadržaj elemenata u medu zavisi od brojnih, prirodnih i antropogenih faktora, te da je zbog izuzetne važnosti esencijalnih, ali i ozbiljnih štetnih efekata koji toksični elementi imaju po ljudsko zdravlje, važno kontrolisati njihovu koncentraciju.

Determination of metals and metaloids in honey using inductively coupled plasma - optic emission spectrometry (ICP-OES)

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Honey is a natural product with high nutritive value and wide therapeutic applications. It has a complex composition and it is an important source of essential, but due to numerous anthropogenic sources, also toxic elements. The aim of this paper was to determine the content of essential and toxic elements in 20 unifloral and multifloral honey samples from different areas of Serbia, collected in the period from 2015 to 2017. The samples were prepared by microwave acid-assisteddigestion, and content of selected metals and metaloids (Al, As, Cd, Cr, Cu, Fe, K, Mg, Mn, Na, Ni, Pb, Se, Si, and Zn) was determined by ICP-OES. The results showed that concentration of essential elements (K, Fe, Mg, Mn, Na, Se, Si, and Zn) depends on the geographic origin, primarily the composition of the soil, but also on the conditions of the bee pasture. The concentrations of toxic elements were mainly within a permissible limits. The results of this work have shown that the content of elements in honey depends on many natural and anthropogenic factors, and because of the crucial importance of essential and the serious harmful effects of toxic elements in human health, it is important to control their concentration.

AH P 02

ATR-FTIR/Hemometrija kao moćni alat u analizi droga baziranih na heroinu

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Heroin je jedna od najstarijih i najpoznatijih opojnih droga, čija upotreba datira od davnina. Srbija se nalazi na tzv. „Balkanskoj ruti droga“ i preko njene teritorije se najčešće krijumčari heroin iz Avganistana. Najveća količina zaplenjenog heroina je u formi baze i u smešama sa razblaživačima, kao što su paracetamol, kofein, dekstroza i saharoza. Cilj ovog rada je bio doći do pouzdane procedure za brzu identifikaciju/kvantifikaciju komponenti u heroinskim smešama pomoću ATR-FTIR i hemometrijske analize (PCA, CA i PLS). PCA diskriminiše uzorke u funkciji sastava tj. mešavine heroina sa paracetamolom, kofeinom i dekstrozom, bez prepoznavanja mešavine sa saharozom. Varijable unutar spektra podataka saharoze ne doprinose značajno klasifikaciji faktora. Klasterska klasifikacija analiziranih uzoraka može biti izuzetno korisna, demonstrirajući mogućnosti ATR-FTIR tehnike, za predviđanje tipa heroinske smeše, s obzirom da ih diferencira prema komponentama sa kojima se meša. Istovremeno, nije uspela bilo kakva diferencijacija zasnovana na količini heroina u mešavinama.

ATR-FTIR/Chemometrics aspowerful tool in analysis of heroin based drug mixtures

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Heroin is one of the oldest and most famous among narcotic drugs, whose abuse dates back to ancient times. Serbia is located on the so-called "Balkan route of drugs," and heroin from Afghanistan usually passes through Serbia. The largest quantities of seized heroine is mostly in the form of base and in the mixtures with diluents, such as paracetamol, caffeine, dextrose and sucrose. The aim of this study was to produce a reliable procedure for rapid identification/quantification of components in the heroin based mixtures by ATR-FTIR associated with chemometrics methods (PCA, CA and PLS). The PCA discriminates the samples according to the different compounds *i.e.* the mixtures of heroin with paracetamol, caffeine and dextrose, without recognizing the mixture with sucrose. The variables of sucrose spectral data do not contribute significantly to classification of factors. The cluster classification of analysed samples could be extremely useful, demonstrating the possibilities of the ATR-FTIR technique to predict the kind of particular heroin mixture, since it differentiates mixtures according to their adulterants or diluents content. At the same time, no differentiation based on the quantity of heroin in the mixtures succeeded.

AH P 03 **text rada / full text**

HPLC određivanje herbicida u vodi nakon degradacije sa hlor-dioksidom

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Predmet i cilj ovog rada su bili ispitivanje degradacije herbicida (atrazin, terbutilazin i prometrin) sa hlor-dioksidom. Optimizacija degradacije je prvo proučavana u dejonizovanoj vodi i nakon toga u realnom uzorku vode (savska voda). Optimizacija je ispitivana u uslovima svetla i mraka, sa različitim dozama hlor-dioksida, posle različitih vremenskih perioda degradacije i pri različitim pH-vrednostima rastvora. Efikasnost degradacije herbicida je praćena pomoću HPLC-DAD. Procenat i vreme degradacije su se povećavali sa povećanjem koncentracije hlor-dioksida. Najbolja efikasnost degradacije prometrina postignuta je tretiranjem sa 10 ppm hlor-dioksida, nakon 24 h od početnog tretmana, i iznosila je 78%. U slučaju atrazina i terbutilazina, najbolja efikasnost degradacije postignuta je tretiranjem sa 10 ppm hlor-dioksida, nakon 6 h od početnog tretmana, pri pH 3,00 i iznosila je 47 i 58%. Degradacija herbicida prometrina i terbutilazina u vodi iz reke Save, koristeći hlor-dioksid koncentracije 10 ppm, imala je manju efikasnost u poređenju sa degradacijom u dejonizovanoj vodi usled prisustva organskih supstanci u rečnoj vodi.

HPLC determination of herbicides in water after degradation by chlorine dioxide

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The degradation of triazine herbicides (atrazine, terbuthylazine and prometrine) by chlorine dioxide was investigated in this paper. Optimization of degradation was first studied in deionized water and then in real water system (Sava river water). Optimization was performed under light and dark conditions, with different concentration of chlorine dioxide, at different periods of degradation and at different pH values of solutions. Degradation efficiency of herbicides was followed using HPLC with photodiode array detection (DAD). Percent of degradation and time of degradation were increased with increasing of chlorine dioxide concentration. The best degradation efficiency of prometrine with yield of 78 % was achieved by treatment with 10 ppm of chlorine dioxide, after 24 h of initial treatment under light condition. In the case of atrazine and terbuthylazine, the best efficiency of degradation yielded 47 and 58 % and was achieved by treatment with 10 ppm of chlorine dioxide, after 6 h of initial treatment and at pH of 3.00. Degradation of herbicides prometrine and terbuthylazine, in Sava river water, using concentration of chlorine dioxide of 10 ppm, had smaller efficiency in comparison with degradation in deionized water due to presence of organic substances in river water.

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AH P 04 text rada / full text

Optimizacija postupka ekstrakcije polifenola iz pogače konzumnog suncokreta

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U radu je ispitana efikasnost različitih ekstrakcionih tehnika za izdvajanje polifenolnih jedinjenja iz pogača suncokreta. Poređene su maceracija, ekstrakcija uz intenzivno mešanje, ultrazvučna i mikrotalasna ekstrakcija. Takođe su poređene ekstrakcione osobine različitih rastvarača za izdvajanje polifenolnih jedinjenja, uključujući aceton, etanol i metanol u koncentracijama od 40, 60 i 80 %. Utvrđeno je da se najveći prinos dobija primenom ultrazvučne tehnike ekstrakcije u trajanju od 60 min na 30 °C, uz primenu 80 % etanolnog rastvora kao ekstragensa.

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Optimization of extraction process of polyphenols from sunflower cake

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The paper examines the efficiency of various extraction techniques for isolating polyphenol compounds from sunflower cake. Maceration, extraction with intense mixing, ultrasonic and microwave extraction were compared. The extraction efficiency of different solvents for isolation of polyphenolic compounds, including acetone, ethanol and methanol at concentrations of 40, 60, and 80 %, were also compared. It has been found that the highest yield is obtained by using the ultrasonic extraction for 60 min at 30°C with the application of 80 % ethanol solution as extragens.

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AH P 05 **text rada / full text**

Tečno-čvrsta ekstrakcija izabranih pesticida na bazi jonskih tečnosti za direktnu analizu zemljišta i sedimenata

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Zagađenje zemljišta pesticidima i njihovim degradacionim produktima je globalni problem zagađenja životne sredine. Kao alternativa metodama koje se najviše koriste za ekstrakciju pesticida iz zemljišta predložena je ekstrakcija dvofaznim vodenim sistemima (DVS) na bazi jonskih tečnosti i K_3PO_4 za sledeću smešu pesticida: imidakloprid (IMI), acetamiprid (ACE), linuron (LIN) i tebufenozid (TBF). Uticaj jonske tečnosti na ekstrakciju pesticida je proučavan sa 1-metil-3-oktilimidazolium-hloridom [omim][Cl] i 1-butil-3-metilpirolidinium-dicijanamidom [bmpyr][DCA]. Optimizovani su ekstrakcioni parametri koji obuhvataju sastav DVS, udeo K_3PO_4, vreme ekstrakcije i centrifugiranja da bi se pesticidi maksimalno uklonili iz tri različita uzoraka zemlje. Efikasnost ekstrakcije je veća za [bmpyr][DCA] i K_3PO_4 od [omim][Cl] i K_3PO_4 a metoda pokazuje dobru linearnost ($R^2 > 0,99$), vrednost prinosa veća od 80,68 % i limit detekcije u opsegu od 0,2 µg/g do 0,51 µg/g.

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Liquid-solid extraction of the selected pesticides based on ionic liquids for direct analysis of soil and sediments samples

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Soil contamination of pesticides and their degradation products is a global environmental pollution problem. As an alternative to the currently used extraction methods, aqueous biphasic systems (ABS) composed of ionic liquids (ILs) and K_3PO_4 are here proposed for the simultaneous extraction the mixture of pesticides: imidacloprid (IMI), acetamiprid (ACE), linuron (LIN) and tebufenozide (TBF). The influence of IL on the pesticide extraction was investigated using 1-methyl-3-octylimidazolium chloride [omim][Cl] and 1-butyl-3-methylipyrrolidinium dicyanamide [bmpyr][DCA]. Extraction conditions such as composition of ABS, percentages of K_3PO_4 using ABS, extraction and centrifugation time was optimized so to reach the maximal removal of the pesticides from the three different soils sample. The extraction efficiency of [bmpyr][DCA]+K_3PO_4 was generally better than that for [omim][Cl]+K_3PO_4 procedure showing good linearity ($R^2 > 0.99$) with recovery higher than 80.68 % and limits of detection between 0.2 µg/g and 0.51 µg/g.

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Fizička hemija / Physical Chemistry

FH P 01

Hromatografska karakterizacija derivata aminogvanidina primenom micelarne tečne hromatografije

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Aminogvanidin i njegovi derivati se intenzivno proučavaju zbog sposobnosti da inhibiraju toksična dejstva karbonilnih proizvoda u kasnom stadijumu neenzimskog glikolizovanja proteina, kako *in vitro*, tako i *in vivo*. Pored toga, derivati aminogvanidina pokazuju različite biološke aktivnosti. Imajući u vidu biološki značaj aminogvanidina i njegovih derivata pripremljeno je šest različitih aminogvanidinskih adukata sa piridoksalom, salicilnom kiselinom i 2-acetilpiridinom. Njihovi retencioni parametri određeni su primenom micelarne tečne hromatografije na tankom sloju cijano-modifikovanog silika gela. Kao pokretna faza korišćen je vodeni rastvor surfaktanta (natrijum dodecilsulfat, odnosno, cetil trimetil amonijum bromid) iznad kritične micelarne koncentracije uz dodatak 15 % v/v acetonitrila. Ispitan je uticaj anjonskog i katjonskog surfaktanta na retenciju. Izračunati su koeficijenti raspodele micela-voda kao mera za solubilizacionu sposobnost micelarnih rastvora i procenu efikasnosti postupka u kojem se primjenjuje površinski aktivna materija.

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Chromatographic characterization of aminoguanidine derivatives using micellar liquid chromatography

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Aminoguanidine and its derivates are extensively studied because of their ability to inhibit the toxic effects of carbonyl products that ascend during the end-phases of non-enzymatic protein glycation, both in vitro and in vivo. Furthermore, aminoguanidine derivatives exhibit variety of biological activities. Having in mind the biological importance of aminoguanidine and its derivates, six different aminoguanidine adducts with pyridoxal, salicyl acid and 2-acetylpyridine were prepared. Their retention parameters were determined by micellar liquid chromatography on thin layers of cyano modified silica gel. Mobile pases were an aqueous solutions of surfactant (sodium dodecylsulfate or hexadecyl trimethyl ammonium bromide) above its critical micellar concentration with 15 % addition of acetonitrile. The influence of anionic and cationic surfactant to the retention was investigated. The micelle-water partition coefficient were calculated as a measure for the solubilization capacity of micellar solutions and evaluation the efficiency of a process where surfactants are applied.

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FH P 02

Hidrataciona svojstva i uticaj D-fruktoze na ukus vodenih rastvora aktivnih komponenti gorke narandže (*Citrus aurantium*)

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Citrus aurantium (gorka narandža) i njeni ekstrakti suvog voća i kore se već godinama koriste kao tradicionalno lekovito bilje, za stimulisanje varenja, poboljšanje cirkulacije i funkcije jetre. Aktivne komponente gorke narandže, alkaloidi *p*-sinefrin i *p*-oktopamin, su agonisti α- i β-adrenergičkih receptora. Strukturno su slični neurotransmiterima epinefrinu i norepinefrinu, pa se široko primenjuju kao sredstva za regulisanje telesne mase. S obzirom na to da ovi alkaloidi imaju gorak ukus, a ulaze u sastav različitih sportskih suplemenata ili tradicionalnih slatkih proizvoda (marmelada), u ovom radu ispitavane su njihova hidrataciona svojstva u vodenim rastvorima kao i uticaj D-fruktoze na ukus. U cilju ispitivanja interakcija između sinefrin-hidrohlorida/oktopamin-hidrohlorida i vode, primenjena su volumetrijska i viskozimetrijska merenja kao i molekulska dinamika (MD) i radijalna funkcija raspodele (RDF). Dobijeni rezultati i poređenja sa strukturno sličnim fenalkilaminima-HCl, ukazuju na to da uvođenje hidrofobne metil (-CH_3) grupe u strukturu povećava gorčinu molekula, kao i da dovodi do značajne razlike u hidrataciji molekula.

Zahvalnica: *Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (Projekat br. ON172012).*

Hydration properties and the influence of D-fructose on the taste of bitter orange (*Citrus aurantium*) active components in aqueous solutions

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Citrus aurantium (bitter orange) and its dry fruit and peal extracts have been used as traditional medicinal herbs for years, to stimulate digestion, improve circulation and liver function. Active components of bitter orange, alkaloids *p*-synephrine and *p*-octopamine, are α- and β-adrenoceptor agonists. Due to structurally similar to neurotransmitters epinephrine and norepinephrine, there are widely used as weight loss agents. Since these two alkaloids have bitter taste and are part of various sports supplements or some traditional sweet products (marmalades), this paper examines their hydration properties in aqueous solutions and the effect of D-fructose on quality taste. In order to investigate the interactions between sinephrine hydrochloride/octopamine hydrochloride and water, volumetric and viscometric measurements, as well as molecular dynamics (MD) and radial distribution function (RDF) were applied. The obtained results and comparisons with structurally similar phenalkylamines-HCl indicate that the introduction of a hydrophobic methyl (-CH_3) group into the structure increases the bitterness of the molecules, and leads to a significant difference in the hydration of the molecules.

FH P 03

Optimizacija elektrolita za litijum-jonske baterije

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Elektroliti na bazi jonskih tečnosti (JT) i laktona (*β*-butirolaktona, *γ*-butirolaktona, *γ*-valerolaktona, *δ*-valerolaktona i *ε*-kaprolaktona (BBL, GBL, GVL, DVL, EKL, respektivno)) su ispitane u cilju optimizacije elektrolita za litijum-jonske baterije (LIB) niske zapaljivosti, visoke termičke stabilnosti i visoke provodljivosti. Ispitana su fizičko-hemijska svojstva elektrolita koji sadrži LiTFSI dodatu u binarnu smešu koju čine JT 1-etil-3-metilimidazolijum *bis*(trifluorometilsulfonil)imid ([C_2C_1im][TFSI]) i lakton koji je pokazao najoptimalnija svojstva, GBL. Elektrolit LiTFSI/C_2C_1imTFSI/GBL je testiran na TiO_2 nanotubama kao anodnim materijalom. U cilju poboljšanja bezbednosnih svojstava LIB, elektrohemijska svojstva LiTFSI/C_2C_1imTFSI/GBL upoređena su sa LiTFSI/C_2C_1imTFSI elektrolitom koji sadrži JT bez prisustva GBL. Ćelija sa LiTFSI/C_2C_1imTFSI/GBL elektrolitom pokazuje bolje elektrohemijske performanse posle 350 ciklusa punjenja-pražnjenja.

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Lithium-ion battery electrolytes with improved safety features

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Electrolytes based on ionic liquid (IL) and lactones (*β*-butyrolactone, *γ*-butyrolactone, *γ*-valerolactone, *δ*-valerolactone and *ε*-caprolactone (BBL, GBL, GVL, DVL, EKL, respectively)) are investigated as optimal electrolytes for lithium-ion batteries (LIBs) that can combine low flammability, high thermal stability and high conductivity. Physicochemical properties of 1-ethyl-3-methylimidazolium *bis*(trifluoromethylsulfonyl)imide ([C_2C_1im][TFSI]) and GBL are investigated, which has shown the most optimal properties. Electrolyte LiTFSI/C_2C_1imTFSI/GBL was used for cycling TiO_2 nanotube arrays electrode as Li-ion anode material. In an attempt to realize LIBs with enhanced safety, herein is investigated electrochemical properties of the LiTFSI/C_2C_1imTFSI/GBL and compared with LiTFSI/C_2C_1imTFSI. There is shown that LiTFSI/C_2C_1imTFSI/GBL electrolyte displayed a higher current efficiencies in after 350 full (dis-)charge cycles.

FH P 04

FTIR i DFT ispitivanje građenja vodonično vezanih kompleksa između odabranih benzamida i acetonitrila

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U ovom radu će biti ispitano građenje vodonične veze između N-H grupe odabranih benzamida i acetonitrila kao proton akceptora. Praćenjem promene intenziteta pika koji potiče od N-H trake u IR spektru amida biće procenjena konstanta stabilnosti vodonično vezanih kompleksa. Korišćenjem DFT (Density functional theory) metode proračuna urađena je geometrijska optimizacija i izračunavanje IR spektara monomera i vodonično vezanih kompleksa amida. Kombinovanjem spektroskopski dobijenih podataka sa rezultatima DFT proračuna dobiće se detaljniji uvid u geometriju i jačinu veza u ispitivanim vodonično vezanim kompleksima.

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FTIR and DFT study of hydrogen bonded complexes formation between selected benzamides and acetonitrile

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This study reports investigation of hydrogen bond formation between N-H group from selected benzamides and acetonitrile as proton acceptor. Constant of stability of hydrogen bonded complexes will be estimated through observed changes in N-H adsorption band intensity in IR spectrum of amides. DFT (Density functional theory) computation method has been used for geometry optimization and frequency calculation for monomers and hydrogen bonded complexes of amides. By combining spectroscopic data with results of DFT calculations a more detailed insight into geometry and bond strength of investigated hydrogen bonded complexes will be obtained.

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FH P 05 text rada / full text

Uticaj niskofrekventnog magnetnog polja (10-1000 Hz) na respiracionu aktivnost ćelija kvasca Saccharomyces cerevisiae

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Veoma popularna tema današnjice je ispitivanje električnog, magnetnog i elektromagnetnog polja na različite mikroorganizme, jer pomenuta fizička polja potencijalno deluju kao faktori stresa i tako utiču na njihovo preživljavanje, ponašanje i metabolizam. U ovom radu ispitivan je uticaj niskofrekventnog magnetnog polja sa konstantnim intervalom skeniranja od 10 do 1000 Hz na respiraciju ćelija kvasca, Saccharomyces cerevisiae. Eksperimenti su rađeni u pet ponavljanja i kumulativna potrošnja O_2 i produkcija CO_2 praćena je pomoću Micro-Oxymax® respirometra . U svih pet ponavljanja, ćelije koje su bile izložene magnetnom polju pokazale su manju kumulativnu potrošnju kiseonika u poređenju sa uzorcima van magnetnog polja i nekonzistentnu produkciju CO_2. Rezultati su obrađeni uporednim jednosmernim T-testom, koji je pokazao da postoje statistički značajne razlike u kumulativnoj potrošnji O_2 između kontrolnih ćelija i onih izloženih magnetnom polju, što nije slučaj sa kumulativnom produkcijom CO_2. Iako su dodatna ispitivanja neophodna da se objasni nekonzistentnost produkcije CO_2, dobijeni rezultati ovih inicijalnih eksperimenata predstavljaju dobru osnovu za dalja istraživanja u ovoj oblasti.

Influence of the low frequency 10-1000 Hz magnetic field on Saccharomyces cerevisiae respiration activity

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The effects of electric, magnetic or electromagnetic fields on different microbes have become a very popular topic nowadays, mostly because the fields could potentially affect the survival of the microbial cells as well as their behavior and metabolism. In this paper the influence of the magnetic field with constant low frequency scan regime from 10 to 1000 Hz on yeast cells S. cerevisiae respiration activity was examined using Micro-Oxymax® respirometer. Experiments were performed in five replicates. All five experiments showed lower cumulative O_2 consumption in magnetic field exposed samples, compared to the control sample and inconsistent cumulative CO_2 production. The paired two sample one-tail T-test showed statistically significant differences between control and magnetic field sample for cumulative O_2 consumption, but not for the CO_2 production. Even though additional experiments are neccesary to clarify the differencies in CO_2 production, these preliminary findings strongly suggest that obtained results represent a good basis for further investigations in this field.

Elektrohemija / Electrochemistry

EH P 01

Elektrohemijsko ispitivanje inkluzionih kompleksa odabranih sukcinimida sa β-ciklodextrinom i (2-hidroksipropil)-β-ciklodekstrinom

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Formiranje kompleksa između odabranih sukcinimida sa β-ciklodextrinom i (2-hidroksi-propil)-β-ciklodekstrinom je potvrđeno ATR spektralnom analizom. Voltametrijom sa pravougaonim impulsima je uočen dobro definisan pik na potencijalu E_p = ~60 mV i više struje na potencijalu pika za oba inkluziona kompleksa svih odabranih sukcinimida u poređenju sa prethodno ispitanim čistim sukcinimidaima. To ukazuje da kompleksiranje sukcinimida sa ciklodekstrinima poboljšava njihovu elektro aktivnost.

The electrochemical investigation of inclusion complexes of the selected succinimides with β-cyclodextrin and (2-hydroxypropyl)-β-cyclodextrin

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The complex formation between selected succinimides and β-cyclodextrin and (2-hydroxy-propyl)-β-cyclodextrin was confirmed with ATR spectral analysis. The SWV measurements reveal well defined peak at potential E_p = ~ 60 mV and the higher currents at E_p for both inclusion complex of the succinimides comparing to succinimides. It indicates that the complexation of succinimides improves their electrooxidation ability.

EH P 02

Elektrohemijska sinteza i karakterizacija kopolimera polianilina i *m*-aminobenzoeve kiseline

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Kopolimerizacija anilina i *m*-aminobenzoeve kiseline ostvarena je elektrohemijskim postupkom u uslovima konstantne gustine struje od 1,0 mA cm^{-2} (galvanostatski). Kao elektrolit za sintezu korišćen je vodeni rastvora 1,0 mol dm^{-3} HCl sa dodatkom anilina i *m*-aminobenzoeve kiseline različitog odnosa koncentracija. Prisustvo karboskilne grupe u meta položaju uslovljava povećanje potencijala kopolimerizacije, drugačiju morfologiju i elektrohemijsko ponašanje kopolimera u poređenju sa polianilinom. Kopolimer polianilina i *m*-aminobenzoeve kiseline dobijen kopolimerizacijom iz rastvora koji je sadržao istu količinu anilina i *m*-benzoeve kiseline od 1.0 mol dm^{-3} pokazuje, za razliku od polianilina, elektrohemijsku aktivnost u neutralnoj sredini.

Electrochemical synthesis and characterization of poly(aniline-co-(*m*-aminobenzoic acid)

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Galvanostatic electrochemical syntheses of poly(aniline-co-(*m*-aminobenzoic acid)) was performed at graphite electrode at constant current density of 1.0 mA cm^{-2}. Aqueous electrolyte used for synthesis was consisted of: 1.0 mol dm^{-3} HCl and different amounts of aniline and *m*-aminobenzoic acid. The presence of the meta positioned carboxylic group in *m*-aminobenzoic acid had influenced higher co-polymerization potential, different morphology and electrochemical behavior of copolymers compared to polyaniline. Poly(aniline-co-(*m*-aminobenzoic acid)) obtained from electrolyte with an equal amount of aniline and *m*-aminobenzoic acid exhibits electrochemical activity in neutral electrolyte which can be related to proton exchange process.

EH P 03

Elektroforetski taložene biokeramičke kompozitne prevlake sa gentamicinom za biomedicinsku namenu u formi koštanih implantata

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Sposobnost osteointegracije i izvanredna biokompatibilnost hidroksiapatita (HAP) u kombinaciji sa dobrim mehaničkim i antimikrobnim svojstvima hitozana (CS) uz dodatak antibiotika gentamicina (Gent) omogućava dobijanje biokompatibilnih prevlaka sa poboljšanom biološkom funkcijom. U cilju povećanja biokompatibilnosti i bioaktivnosti titanskih (Ti) implantata, izvršena je modifikacija površine Ti nanošenjem biokeramičke HAP/CS/Gent prevlake postupkom elektroforetskog taloženja (EPD). Taloženje je izvedeno u jednom stupnju, iz trokomponentne vodene suspenzije pri konstantnom naponu. Karakterizacija dobijenih prevlaka je izvršena primenom infracrvene spektroskopije sa Furijeovom transformacijom (FT-IR) i skenirajuće elektronske mikroskopije (FE-SEM). Citotoksičnost dobijenih prevlaka je ispitana MTT testom, a primenom testa u suspenziji verifikovana je antibakterijska aktivnost. Dobijeni rezultati su potvrdili formiranje nove kompozitne prevlake HAP/CS/Gent sa velikim potencijalom za upotrebu u biomedicini.

Electrodeposited bioceramic composite coating loaded with gentamicin for biomedical use as hard tissue implants

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The ability of osseointegration and excellent biocompatibility of hydroxyapatite (HAP) combined with good mechanical and antimicrobial properties of chitosan (CS) with the addition of antibiotic gentamicin (Gent), enabled the production of biocompatible coatings with improved biological function. In order to increase the biocompatibility and bioactivity of titanium (Ti) implants, Ti surface was modified by applying the bioceramic HAP/CS/Gent coating using electrophoretic deposition process (EPD). Deposition was carried out in one step from a three-component aqueous suspension (HAP/CS/Gent) at constant voltage. The obtained coatings were characterized by Fourier transform infrared spectroscopy (FT-IR), and field emission scanning electron microscopy (FE-SEM). The cytotoxicity of the obtained coatings was evaulated by MTT assay, and the antibacterial activity was verified using test in suspension. Results obtained confirmed the formation of a new HAP/CS/Gent composite coating with future prospect for biomedical use.

EH P 04

Trokomponentne bioaktivne prevlake sa gentamicinom elektroforetski taložene na titanu

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Elektroforetsko taloženje je efikasna elektrohemijska metoda za dobijanje višekomponentnih biokeramičkih prevlaka na metalnom supstratu. Za formiranje biomaterijala za koštane implantate, najbolji rezultati su dobijeni kod prevlaka koje predstavljaju kombinaciju mineralne faze i polimera. U cilju dobijanja bioaktivnih prevlaka na titanu primenom elektroforetskog taloženja, urađena je optimizacija uslova taloženja iz trokomponentne vodene suspenzije hidroksiapatita (HAP), hitozana (CS) i antibiotika gentamicina (Gent), pri različitim konstantnim vrednostima napona i vremena taloženja. Karakterizacija prevlaka je izvršena primenom rendgenske difrakcione analize (XRD) i rendgenske fotoelektronske spektroskopije (XPS). Citotoksičnost dobijenih prevlaka je ispitana MTT testom, dok je antibakterijska aktivnost prevlake sa gentamicinom potvrđena primenom testa u suspenziji. Na osnovu dobijenih rezultata, potvrđeno je da trokomponentna biokompatibilna prevlaka HAP/CS/Gent ima veliki potencijal za upotrebu u biomedicini.

Three-component bioactive coatings with gentamicin electrophoretically deposited on titanium

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Electrophoretic deposition is a suitable method for obtaining multicomponent bioceramic coatings on titanium (Ti). For hard tissue implants, the best results are achieved for the coating composed of mineral phase and a polymer. First step in producing bioactive coatings on Ti using electrophoretic deposition process was the optimization of deposition parameters for three-component aqueous suspension, containing hydroxyapatite (HAP), chitosan (CS) and gentamicin (Gent), at constant values of applied voltages and different deposition times. The coatings obtained were characterized by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Cytotoxicity of the coatings was evaluated by MTT assay, and the antibacterial activity of gentamicin loaded coating was verified using test in suspension. Based on the experimental results, the formation of a new HAP/CS/Gent composite coating with future prospect for biomedical use was confirmed.

EH P 05

Uticaj sadržaja hitozana na bubrenje, otpuštanje i biološka svojstva hidrogelova srebro/polivinil-alkohol/hitozan/grafen

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U ovom radu su sintetisani hidrogelovi srebro/polivinil-alkohol/hitozan/grafen (Ag/PVA/CHI/Gr) sa nanočesticama srebra dobijenim elektrohemijskim putem, *in situ* redukcijom Ag^+ jona u matrici hidrogela. Prisustvo nanočestica srebra je dokazano metodom ultraljubičaste-vidljive spektroskopije, a zatim je ispitivana kinetika bubrenja i otpuštanja srebra u fosfatnom puferu koji imitira fiziološke uslove. Pokazano je da gelovi sa većim sadržajem hitozana sadrže i veću koncentraciju nanočestica srebra, ispoljavaju veći stepen bubrenja i sporiji profil otpupštanja srebra tokom 28 dana. MTT testom citotoksičnosti je dokazana netoksičnost uzoraka sa i bez srebra. Antibakterijska aktivnost prema sojevima *Escherichia coli* i *Staphylococcus aureus* je ispitana agar-difuzionom metodom i testom u suspenziji. Najjaču antibakterijsku aktivnost su ispoljili hidrogelovi sa većim sadržajem hitozana, što ukazuje na sinergijsko dejstvo sa nanočesticama srebra. Konačno, može se konstatovati da Ag/PVA/CHI/Gr hidrogelovi imaju dobar potencijal za biomedicinske primene kao aktivne antibakterijske obloge za rane.

The influence of chitosan content on swelling, release and biological properties of silver/poly(vinyl-alcohol)/chitosan/graphene hydrogels

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In this work, we synthesized silver/poly(vinyl-alcohol)/chitosan/graphene (Ag/PVA/CHI/Gr) hydrogels with silver nanoparticles obtained by electrochemical route, by *in situ* reduction of Ag^+ ions in the hydrogel matrix. The presence of silver nanoparticles was confirmed by ultraviolet-visible spectroscopy, after which the kinetics of swelling and silver release were investigated in phosphate buffer which imitates physiological environment. It was shown that gels with higher chitosan content also contain higher concentration of silver nanoparticles, exhibit higher swelling degree and slower silver release profile over 28 days. MTT test of cytotoxicity was used to prove non-toxicity of the samples with and without silver. The antibacterial activity against *Escherichia coli* and *Staphylococcus aureus* strains was evaluated using disc-diffusion method and test in suspension. Hydrogels with higher chitosan content exhibited the strongest antibacterial activity, indicating synergistic effect with silver nanoparticles. In summary, the Ag/PVA/CHI/Gr hydrogels manifested good potential for biomedical applications as active antibacterial wound dressings.

EH P 06

Proučavanje elektrohemijskog ponašanja livenih Cu-Au legura tokom termomehaničke obrade

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U ovom radu primenjena je kompleksna termomehanička obrada u cilju postizanja optimanlnih mehaničkih osobina livenih Cu-Au legura. Termomehanička obrada obuhvatala je: hladno valjanje, termičku obradu sa kaljenjem i žarenje na različitim temperaturama. Elektrohemijsko ponašanje Cu-Au legura u svim stadijumima termomehaničke obrade analizirano je u 0,1 M rastvoru NaOH merenjem potencijala otvorenog kola i cikličnom voltametrijom. U zavisnosti od primenjene termomehaničke obrade dobijene su i različite mikrostrukture, koje su uslovile različite mehaničke i elektrohemijske osobine legura.

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A study of electrochemical behavior of cast Cu-Au alloys during thermo-mechanical processing

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Complex thermo-mechanical processing, applied in order to optimize mechanical properties in cast Cu-Au alloys is described in this paper. The thermo-mechanical processing included: cold working, heat treatment with quenching and annealing at different temperatures. Electrochemical behavior of cast Cu-Au alloys in all stages of thermomechanical process was studied in 0.1 M NaOH by open circuit potential measurement and cyclic voltammetry. Depending on applied thermo-mechanical processing conditions, a wide range of microstructures were obtained, causing a wide range of mechanical and electrochemical properties of the alloys.

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EH P 07

Adsorpcija i inhibitorska svojstva oksaprozina na AA 2024

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Oksaprozin, 3-(4,5-difeniloksazol-2-il)propanska kiselina, pripada klasi nesteroidnih antiinflamatornih lekova sa analgetskim i antipiretičkim dejstvom. Kako je ustanovljeno da formira kompleksna jedinjenja sa različitim metalima cilj ovog istraživanja je ispitivanje potencijalne adsorpcije oksaprozina na površini aluminijuma sa ciljem inhibicije korozije metala. Oksaprozin, kao sintetisan lek, a takođe i kao aktivna komponenta Duraprox® tableta je adsorbovan na površini AA 2024 u molekulskom i jonskom obliku (dobijen neutralizacijom karboksilne grupe). Ispitivan je uticaj različitih koncentracija oksaprozina kao i temperature na inhibitorska svojstva. Korozija aluminijumske legure 2024 je ispitana u 3 mas% rastvoru NaCl metodama linearne voltametrije i spektroskopije elektrohemijske impedancije. Merenja impedancije su pokazala da se oksaprozin adsorbuje na površini metala i na taj način sprečava direktan kontakt elektrolita sa površinom metala. Sa Tafelovih dijagrama je ustanovljeno da se oksaprozin ponaša kao anodni inhibitor, jer nije ustanovljena značajna promena katodnih gustina struje.

Adsorption and corrosion inhibition properties of oxaprozin on AA 2024

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Oxaprozin, 3-(4,5-diphenyl-1,3-oxazole-2yl)-propanoic acid, belongs to the class of non-steroidal anti-inflammatory drugs (NSAIDs) with analgesic and antipyretic properties. Since it was observed that it forms complex compounds with various metals, the goal of this research was to investigate its potential adsorption on aluminium surface hence providing corrosion inhibition properties. Oxaprozin, as synthesized drug, as well as active component of Duraprox® tablets, was adsorbed on AA 2024 surface in molecular or ionic forms (obtained by neutralization of carboxyl group). Influence of different drug concentrations and temperatures on its corrosion inhibition properties was tested. Corrosion of aluminium alloy 2024 in 3 wt. % NaCl solution was investigated using electrochemical impedance spectroscopy and linear sweep voltammetry. Electrochemical impedance spectroscopy measurements showed that oxaprozin was adsorbed on aluminium surface therefore providing protection from electrolyte. Tafel polarization technique revealed that oxaprozin behaves as anodic inhibitor, since no change in cathodic current was observed.

EH P 08 text rada / full text

Elektrohemijsko ponašanje bakra u prisustvu macerata hmelja

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Primena biljnih ekstrakata za inhibiciju korozije metala i legura je predmet mnogobrojnih naučnih istraživanja. U ovom radu su prikazani rezultati ispitivanja elektrohemijskog ponašanja bakra pri oksidaciji u rastvoru 0,5 mol/dm^3 NaCl u odsustvu i prisustvu macerata hmelja različitih koncentracija. Elektrohemijsko ponašanje bakra ispitivano je metodom merenja potencijala otvorenog kola i metodom ciklične voltametrije. Istraživanje primenom ciklične voltametrije pokazuje da se na anodnim polarizacionim krivama pojavljuju tri strujna pika koji odgovaraju adsorpciji anjona i formiranju hlorida bakra i oksida bakra. Vrednost gustine struje strujnih pikova koji su povezani sa reakcijama formiranja jedinjenja bakra opada sa dodatkom macerata hmelja u elektrolit u koncentracijama većim od 10 ml/l, što ukazuje na to da macerat hmelja ima inhibitorsko dejstvo na te reakcije.

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Electrochemical behaviour of copper in the presence of hops macerate

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The use of plant extracts to inhibit the corrosion of metals and alloys is the subject of numerous scientific researches. In this paper the results of the examination of electrochemical behaviour of copper during its oxidation in a solution of 0.5 mol/dm^3 NaCl in the absence and presence of hops macerate of different concentrations are presented. The electrochemical behaviour of copper was examined by measuring the open circuit potential and by the cyclic voltammetry method. The study using cyclic voltammetry shows that three current peaks corresponding to adsorption and the formation of copper chloride and copper oxide occur on anodic polarization curves. The value of the current density of current peaks corresponding to the formation of copper compounds decreases with the increase in the concentration of hops macerate in the electrolyte over 10 ml/l, which indicates an inhibitory effect.

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Hemijsko inženjerstvo / Chemical Engineering

HI O 1 text rada / full text

Experimental determination and modeling of the sunflower oil ozonization process

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Ozonization is a significant reaction in vegetable oil chemistry since the ozonization products are involved in therapeutical application because of its antimicrobial effect. Information on the standard preparation procedures of ozonized sunflower oil is limited. The development of an adequate technology for the effective production of ozonized oil was carried out on the laboratory level. The purpose of this study was to establish an experimental setup using two different types of apparatus in order to optimize the ozonization process. Within the first procedure, the reaction was carried out inside a bubble reactor, while following the second procedure the reaction was performed inside an absorption column. The second procedure gave better results regarding the content of ozonized products in the final sample. It was concluded that the ozonization process should be carried out in a packed-bed absorption column.

Eksperimentalno određivanje i modelovanje procesa ozonizacije suncokretovog ulja

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Reakcije ozonizacije imaju značajnu ulogu u hemiji jestivih ulja uzimajući u obzir da se ozonizovani proizvodi koriste u medicinske svrhe zbog njihovog antimikrobnog dejstva. Informacije o standardnim postupcima pripreme ozonizovanog suncokretovog ulja u dostupnoj i relevantnoj literaturi su ograničene. Razvijanje adekvatne tehnologije za efektivnu proizvodnju ozonizovanog ulja odrađeno je na laboratorijskom nivou. Cilj ovog istraživanja bio je postavljanje dva različita tipa aparature u cilju optimizacije procesa ozonizacije. U okviru prve procedure, reakcija se odvijala u reaktoru s barbortiranjem, dok se u okviru druge procedure reakcija odvijala u apsorpcionoj koloni. Druga procedura je pokazala bolje rezultate po pitanju sadržaja ozonizovanih proizvoda u finalnom uzorku. Shodno tome, zaključeno je da proces ozonizacije treba da se odvija u kontinualnom sistemu koji uključuje apsorpcionu kolonu s pakovanim slojem.

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HI P 01

Upotreba dva oblika otpadnih vlakana polipropilena kao filtarskog materijala u tretmanu zauljenih voda

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Za istraživanja prikazana u ovom radu bila su na raspolaganju vlakna polipropilena koja se javljaju kao otpad pri proizvodnji tepiha, prosečne debljine 40 μm (PP). Pored toga dostupan je bio otpadni polipropilen od džakova koji se koriste kao ambalaža za povrće. Poprečni presek ovog materijala je pravougaonik širine 1 mm i debljine 100 μm (PPDJ). Permeabilnost oba sloja bila je u jednakom opsegu od 0,18 do 5,5 10^{-9} m^2. Eksperimenti su realizovani na poluindustrijskom uređaju kapaciteta 100 l/h. Brzina fluida je varirana u rasponu 19-60 m/h. Model zauljena voda je pripreman tako što je u vodu za piće dispergovano mineralno ulje P1. Mešanjem je prosečna veličina kapi održavana u opsegu od 10 μm. Analiza rezultata rađena je preko izlazne koncentracije ulja u vodi kao i preko kritične brzine v_k. Pri najvećoj permeabilnosti materijal PP ostvaruje v_k od 50 m/h dok materijal PPDJ ostvaruje jednaku vrednost v_k za manju permeabilnost i to od 2,5 10^{-9} m^2 pri kojoj je pad pritiska veći.

Two form of waste polypropylene fiber as filter media for oily water treatment

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For the research presented in this paper, polypropylene fibers that appear as waste in the production of carpets, with an average thickness of 40 μm (PP), were available. Additionally, there was a waste polypropylene from bags that are used as vegetable packaging. The cross-section of this material is a rectangle of 1 mm wide and 100 μm thick (PPDJ). Experiments were conducted on a pilot plant capacity of 100 L/h. The bed permeability was changed in a same range from 0.18 to $5.5 \cdot 10^{-9}$ m^2. Superficial velocity was varied from 19 to 60 m/h. The model of oily water is prepared by dispersing mineral oil P1 in the tap water. Average droplet size of dispersed phase was 10 μm and kept constant with mixing process. The results were analysed over the effluent concentration of oil in water and critical velocity, v_k. For higher bed permeability of PP material critical velocity was reached 50 m/h, while for PPDJ material similar critical velocity was achieved with higher pressured drop over lower bed permeability of $2.5 \cdot 10^{-9}$ m^2.

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HI P 02

Mikrobiološka aktivnost vodenih i etanolnih ekstakata belog luka (*A. sativum* L.) i emulzija sa inkapsuliranim ekstraktima

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Antibakterijska aktivnost ekstrakta belog luka ispitivana je na rast *Staphylococcus aureus* i *Escherichia coli*. Minimalne inhibitorne koncentracije (MIC) i minimalne baktericidne koncentracije (MBC) vodenih i etanolnih ekstrakata tri sorte belog luka: NSPBL-70, *Labud* i *Bosut* određene su mikro-dilucionom metodom. Rezultati ukazuju na razlike u antimikrobnom delovanju u zavisnosti od sorte luka, kao i od vrste rastvarača upotrebljenog za ekstrakciju. Vodeni ekstrakt pripreman od sorte *Labud,* pokazao je najmanju MIC (56,82 µl/ml), za oba ispitivana soja bakterija, dok su odgovarajuće MBC bile 227,27 µl/ml. Delovanje etanolnog ekstrakata belog luka na rast *E.coli* ne zavisi od sorte belog luka, dok se za inhibiciju rasta *S.aureus* izdvojio kao najbolji etanolni ekstrakt NSPBL-70. Voda-u-ulju emulzije sa inkorporiranim ekstraktom belog luka nisu pokazale uticaj na rast ispitivanih bakterija. Liofilizovani vodeni i etanolni ekstrakti belog luka pokazali su delovanje na inhibiciju rasta *E. coli* u koncentraciji, redom, 63 i 250 µg/ml, i *S. aureus* u koncentraciji 31 i 125 µg/ml, sa MBC od 125 i većom od 250 µg/ml za oba ispitivana soja.

Microbiological activity of water and ethanol garlic extracts (*A. sativum* L.) and emulsions with incapsulated extracts

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Antibacterial activity of garlic extracts was explored by examining the influence on growth of *Staphylococcus aureus* and *Escherichia coli*. The minimum inhibitory (MIC) and minimum bactericidal (MBC) concentrations of three varieties of garlic were used for extracts preparation: NSPBL-70, *Labud* and *Bosut*, determined using micro-dilution method, indicate that there are differences in results depending on the garlic variety, as well as the extraction solvents. *Labud* water garlic extract had shown the smallest MIC (56.82 µl/ml), for both examined bacteria strains, while the corresponding MBC was 227.27 µl/ml. The effect of ethanol garlic extract on the growth of *E. coli* does not depend on the variety of garlic, while for growth inhibition of *S. aureus*, the best result showed NSPBL-70 ethanol extract. Water-in-oil emulsion with encapsulated garlic extract did not show activity on the bacterial growth. Lyophilized aqueous and ethanol garlic extracts showed inhibition of *E. coli* at concentrations of 63 and 250 µg/ml and *S. aureus* at concentrations of 31 and 125 µg/ml, respectively, with MBC of 125 and >250 µg/ml for both examined strains.

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HI P 03

Primena Pd-Cu-ugljeničnog nanoreaktora u procesu denitracije vode

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Specifična morfologija ugljeničnih nanocevi (UNC) intenzivno je proučavana u oblasti katalize. Unutrašnji kanali nanocevi često su ciljana mesta za smeštaj aktivne faze katalizatora i kao takvi istovremeno predstavljaju hemijske nanoreaktore. Cilj rada je ispitivanje aktivnosti i selektivnosti katalizatora na bazi UNC, sa Pd-Cu aktivnom fazom smeštenom unutar nanocevi (efekat "skučenog prostora"), u reakciji denitracije vode. Pozicioniranje aktivne metalne faze unutar nanocevi potpomognuto je njihovim prethodnim cepanjem na kratke fragmente postupkom katalitičke oksidacije. U cilju detaljnijeg ispitivanja efekta "skučenog prostora" takođe su ispitane performanse katalizatora sa metalnim nanočesticama koje su se našle deponovane na spoljašnjim zidovima UNC. Iako su rezultati katalitičkih testova ukazali na lošije performanse enkapsuliranih nanočestica u odnosu na one prisutne na spoljašnjoj površini UNC, superiorna stabilnost nanoreaktora može se izraziti u vidu ukupnog pada katalitičke aktivnosti od samo 4 % nakon četiri uzastopna radna ciklusa. Prema tome, primena ovakvog nanoreaktora na bazi UNC može biti opravdana sa aspekta radnog (životnog) veka nanokatalizatora u njemu.

Application of Pd-Cu-carbon nanoreactor in water denitration process

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The unique morphology of carbon nanotubes (CNTs) has been intensively examined in the field of catalysis, in therms of both mother-catalysts and as usefull support for new catalysts preparation. However, the carbon nanotube, carrying a catalyst active phase in its interior, can be also considered as a chemical nanoreactor. The aim of this work was to examine the activity and selectivity of Pd-Cu active phase located inside the carbon nanotubes (confinement effect) in water denitration reaction. Positioning of the active metal phase exclusively inside the CNTs was promoted by previous CNTs cutting (*via* catalytic oxidation). In order to examine the effect of encapsulated metal more precisely, the catalytic behavior of metal nanoparticles deposited on the CNT exterior walls was also tested. Although the results of catalytic tests revealed the hindering effect of encapsulated metal nanoparticles compared to their externally deposited counterparts, the superior stability of the confined catalyst can be portrayed as a total activity drop of only 4 % after four consecutive runs. Thus, the application of the CNT-based nanoreactor might find a justification when the nanocatalyst durability is concerned.

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Modeling of mixture densities using PC-SAFT equation of state

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PC-SAFT equation of state is used for correlation of thermodynamic properties and phase equilibrium of both pure components and mixtures. In this work PC-SAFT equation of state was applied to binary mixtures for the correlation of densities in temperature range T=288-15-323.15 K and at atmospheric pressure. Calculation of densities was performed for two binary mixtures of tetrahydrofurane, with 1-butanol or 2-butanol, respectively. The results show that PC-SAFT model density predictions increasingly deviate from the experimental value with increasing the fraction of alcohol in the mixture. This can be explained by increasing impact of hydrogen bonds on density.

Modelovanje gustina binarnih smeša korišćenjem PC-SAFT jednačine stanja

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PC-SAFT jednačina stanja koristi se za korelisanje termodinamičkih osobina i fazne ravnoteže kako čistih komponenti tako i njihovih smeša. U ovom radu PC-SAFT jednačina stanja primenjena je na binarnim smešama za korelisanje gustina u temperaturnom opsegu T=288-15-323.15 K i pri atmosferskom pritisku. Izračunavanje gustina izvedeno je za dve binarne smeše sa hidrofuranom i 1-butanolom, odnosno 2-butanolom, redom. Rezultati pokazuju da predvidjanje gustina pomoću PC-SAFT modela sve više odstupa od eksperimentalnih vrednosti sa povećanjem udela alkohola u smeši. To se može objasniti povećanim uticajem vodoničnih veza na gustine.

HI P 05 text rada / full text

Viscosity modeling of binary mixtures ethyl butyrate + n-alcohol

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Modeling of viscosity of three binary ethyl butyrate + n-alcohol mixtures was done using predictive UNIFAC-VISCO and ASOG-VISCO models. Group contribution based models are suitable for obtaining quick evaluations of thermophysical properties under different conditions of temperature, pressure and composition. The significance of the predictive approach is that the mixture viscosity could be calculated from the pure component data and the interaction parameters between functional groups present in the system. However, having in mind the fact that correlative models often lead to better results, the viscosity data were also correlated by Teja-Rice, Grunberg-Nissan, McAllister, Eyring-UNIQUAC and Eyring-NRTL models. Correlative models involve interaction parameters (one or more) obtained by some optimization technique. These models require some experimental data in order to establish the value of an interaction parameter specific for each mixture for the defined temperature and pressure. All correlative models for investigated mixtures give very good results with percentage deviations within 2 %. Predictive models can be used to calculate viscosity of investigated systems only on higher temperatures.

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Modelovanje viskoznosti binarnih smeša etil butirat + n-alkohol

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Modelovanje viskoznosti tri binarne etil butirat + n-alkohol smeše urađeno je koristeći prediktivne UNIFAC-VISCO i ASOG-VISCO modele. Modeli doprinosa grupa su pogodni za brzo izračunavanje termofizičkih veličina pri različitim uslovima temperature, pritiska i udela. Njihov značaj je u tome što se viskoznost smeše može izračunati samo iz podataka za čiste komponente i interakcione parametre između funkcionalnih grupa prisutnih u sistemu. Međutim, imajući u vidu da korelativni modeli uglavnom daju bolje rezultate, podaci za viskoznost su takođe korelisani Teja-Rice, Grunberg-Nissan, McAlister, Eyring-UNIQUAC i Eyring-NRTL modelima. Korelativni modeli koriste interakcione parametre (jedan ili više), dobijene nekom od optimizacionih tehnika. Ovi modeli zahtevaju eksperimentalne podatke da bi se odredile vrednosti interakcionih parametara posebne za svaku smešu za definisane uslove temperature i pritiska. Svi korelativni modeli za ispitivane smeše daju veoma dobre rezultate sa vrednostima procentualnih odstupanja do 2 %. Prediktivni modeli mogu da se koriste za računanje viskoznosti ispitivanih sistema uglavnom na višim temperaturama.

Tekstilno inženjerstvo / Textile Engineering

TI O 1 text rada / full text

Uticaj sadržaja hemiceluloza na sorpciju vlage i efektivnu relativnu dielektričnu propustljivost alkalno modifikovane tkanine od jute

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U ovom radu je proučavan uticaj alkalnog modifikovanja na hemijski sastav, tj. sadržaj hemiceluloza, sorpciju vlage i na efektivnu relativnu dielektričnu propustljivost tkanina od jute. U tom cilju, tkanina od jute je modifikovana sa NaOH (1 %, 5 % i 17,5 %) na sobnoj temperaturi u toku različitog vremena (5 i 30 min). U odnosu na nemodifikovanu, alkalno modifikovane tkanine imaju niži sadržaj hemiceluloza i povećanu sorpciju vlage. Sa sniženjem sadržaja hemiceluloza, i povećanjem sorpcije vlage, rastu vrednosti efektivne relativne dielektrične propustljivosti ispitivanih tkanina.

The influence of the content of hemicelluloses on moisture sorption and effective relative dielectric permeability of alkali modified jute woven fabrics

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In this investigation, the influence of alkali modification conditions on the chemical composition, i.e. content of hemicelluloses, moisture sorption and effective relative dielectric permeability of jute woven fabric were studied. In that purpose, jute woven fabric has been alkali modified with NaOH solution (1 %, 5 % and 17.5 %) at room temperature for different periods of time (5 and 30 min). Compared to the unmodified, the alkali modified fabrics have lower hemicelluloses content and higher moisture sorption. With decreasing the content of hemicelluloses, and increasing the moisture sorption, values of effective relative dielectric permeability of investigated jute woven fabrics increased.

TI O 2 text rada / full text

Protein-odbijajuća i antioksidativna svojstva bioaktivnih prevlaka na bazi TEMPO oksidisanih celuloznih nanofibrila i hitozana

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U ovom radu, filmovi od regenerisane celuloze (RC) su naslojeni sa TEMPO oksidisanim celuloznim nanofibrilima (TOCN) i hitozanom (CS) metodom rotirajućeg diska. Hitozan je ili pomešan sa TOCN (TOCN+CS) i naslojen na RC film tehnikom rotirajućeg diska ili nanesen na RC/TOCN dvoslojni film propumpavanjem njegovog vodenog rastvora, pH vrednosti 5,5, preko površine filma. Protein-odbijajuća svojstva ispitivanih prevlaka određena su *in situ*, u kontinualnom toku goveđeg serumskog albumina (BSA) primenom kvarc-kristal mikrovage sa praćenjem disipacije (QCM-D). Antioksidativna svojstva TOCN, CS i TOCN+CS amfoterne mešavine su određena metodom inhibicije radikala 2,2'-azino-bis(3-etil-benzotiazolin-6-sulfonske kiseline). Prevlaka sa poboljšanim protein-odbijajućim svojstvima je dobijena upotrebom TOCN+CS amfoterne mešavine, ali sa druge strane TOCN+CS amfoterna mešavina je pokazala slabija antioksidativna svojstva u poređenju sa TOCN i CS.

Protein-repellent and antioxidative properties of bioactive coatings based on TEMPO oxidized cellulose nanofibrils and chitosan

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In this work, regenerated cellulose (RC) films was coated with TEMPO oxidized cellulose nanofibrils (TOCN) and chitosan (CS) by means of subsequent spin-coated deposition. The chitosan was either mixed with the TOCN (TOCN+CS) and deposited on the RC film by spin-coating or deposited on the RC/TOCN bilayer film by pumping its aqueous solution at pH 5.5 over the surface of the film. The protein-repellent properties of investigated coatings were evaluated *in situ* using a continuous flow of bovine serum albumin (BSA) by means of quartz crystal microbalance with dissipation (QCM-D). Antioxidative activity of TOCN, CS and their amphoteric mixture was determined using the 2,2'-azino-bis(3-ethyl-benzothiazoline-6-sulfonic acid) radical scavenging assay. Coating with improved protein-repellent properties was obtained using TOCN+CS amphoteric mixture, but on the other hand TOCN+CS amphoteric mixture showed weaker antioxidative properties in comparison to TOCN and CS.

Uticaj koncentracije 1,2,3,4-butantetrakarboksilne kiseline na in situ sintezu nanočestica Cu_2O/CuO na pamučnoj tkanini i njenu antibakterijsku aktivnost

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U ovom radu je ispitana mogućnost *in situ* sinteze nanočestica Cu_2O/CuO na pamučnoj tkanini prethodno modifikovanoj 1,2,3,4-butantetrakarboksilnom kiselinom (BTCA) različitih koncentracija sa ciljem postizanja antibakterijske zaštite. Utvrđeno je da se većom koncentracijom BTCA postiže bolja sorpcija Cu^{2+}-jona iz rastvora $CuSO_4$ i veći sadržaj nanočestica nakon redukcije. Prisustvo nanočestica na pamučnoj tkanini dokazano je FESEM analizom. XPS i XRD analizama je ustanovljeno da sintetisane nanočestice predstavljaju smešu Cu_2O i CuO. Dobijeni tekstilni nanokompoziti obezbeđuju odličnu antibakterijsku zaštitu prema Gram-negativnoj bakteriji *E. coli* i Gram-pozitivnoj bakteriji *S. aureus* koja zavisi od količine sintetisanih nanočestica Cu_2O/CuO.

The influence of 1,2,3,4-butantetracarboxylic acid on in situ synthesis of Cu_2O/CuO nanoparticles on the cotton fabric and its antibacterial activty

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This study discusses the possibility of *in situ* synthesis of Cu_2O/CuO nanoparticles on the cotton fabric pre-treated with 1,2,3,4-butantetracarboxylic acid (BTCA) of different concentrations with an aim to obtain antibacterial protection. It was found that BTCA of higher concentration ensured larger Cu^{2+}-ions uptakes from $CuSO_4$ solution and total amounts of nanoparticles after reduction. The presence of nanoparticles on the cotton fabric was proved by FESEM analysis. XPS and XRD analyses revealed that nanoparticles existed as a mixture of Cu_2O and CuO. Nanocomposite provided excellent antibacterial protection against Gram-negative bacterium *E. coli* and Gram-positive bacterium *S. aureus,* which depends on the amount of synthetized Cu_2O/CuO nanoparticles.

TI P 02 text rada / full text

Uticaj koncentracije 1,2,3,4-butantetrakarboksilne kiseline na in situ sintezu nanočestica Cu_2O/CuO na pamučnoj tkanini i njenu antibakterijsku aktivnost

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Nauka o materijalima / Material Science

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Homogenization effect on microstructure Al-Mg-Si alloy containing low-melting point elements

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The subject of this study has been an investigation of the homogenization temperature effect on the microstructure of Al-Mg-Si alloy containing low-melting point Pb and Bi elements. The results of the characterization show that homogenization at temperatures lower than 500 °C requires extraordinary long in order to initiate β-AlFeSi -> α-AlFe(Mn)Si transformation, necessary for good extrdability of the alloy ransformation, necessary for good extrudability of the alloy. In addition, precipitation of β-Mg_2Si phase takes place, decreasing the alloy's aging potential during the further processing. High-temperature homogenization not only results in complete β-AlFeSi -> α-AlFe(Mn)Si transformation and dissolution of β−Mg_2Si phase but expected Pb and Bi escape to the specimen surface does not occur.

Effekat homogenizacije na mikrostrukturu Al-Mg-Si legure koja sadrži nisko-topive elemente

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Predmet ovog rada je bilo ispitivanje i karakterizacija uslova homogenizacionog žarenja na mikrostruktu Al-Mg-Si legure legirane nisko-topivim metalima Pb i Bi. Rezultati pokazuju da homogenizacija na temperaturama nižim od 500 °C zahteva izuzetno duga vremena žarenja da bi došlo do β-AlFeSi -> α-AlFe(Mn)Si transformacije, neophodne za sposobnost legure za presovanje. Dodatno, dolazi do izdvajanja β-Mg_2Si faze, čime se smanjuje sposobnost legure za starenje u daljoj preradi. Visoko-temperaturna homogenizacija ne samo da rezultuje u potpunoj β-AlFeSi -> α-AlFe(Mn)Si transformaciji i rastvarnju β-Mg_2Si faze, već i ne dolazi do očekivanog gubitka Pb i Bi usled izdvajanja na površini uzoraka.

NM P 01 text rada / full text

Uticaj akumulativnog spajanja valjanjem (ARB) i konvencionalnog valjanja (CR) na korozionu stabilnost AA5083 legure

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Ispitivan je uticaj stepena i načina deformacije na korozionu stabilnost legure AA5083 koja je procesirana konvencionalnim valjanjem (CR) i akumulativnim spajanjem valjanjem (ARB). Koroziona stabilnost je praćena standardnim elektrohemijskim metodama, spektroskopijom elektrohemijske impedancije (EIS) i polarizacionim merenjima. Utvrđeno je da je gustina struje korozije (j_{corr}) manja za najmanje jedan red veličine kod ARB višeslojnih uzoraka. Veći stepen deformacije indukovao je bolju korozionu stabilnost CR jednoslojnih, kao i ARB višeslojnih uzoraka. Rezultati pokazuju da je ukupna impedancija ARB višeslojnih uzoraka više nego udvostručena u odnosu na CR jednoslojne uzorke kao rezultat višeslojne strukture i prisustva oksidacionog filma između slojeva. Značajno veći polukrugovi na Nyquist-ovim dijagramima za ARB uzorke ukazuju na povećanu korozionu stabilnost, koja raste sa porastom stepena deformacije. Eksperimentalni rezultati pokazuju da način i stepen deformacije imaju veliki uticaj na korozionu stabilnost AA5083 legure.

Ovaj rad je finansiralo Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije, projekat TR 34018.

Influence of accumulative roll bonding (ARB) and conventional cold rolling (CR) on the corrosion stability of AA5083 alloy sheets

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The influence of the degree of deformation and applied processing route on the corrosion stability of AA5083 alloy sheets processed by conventional rolling (CR) and accumulative roll bonding (ARB) has been studied. The corrosion stability was evaluated by standard electrochemical methods, electrochemical impedance spectroscopy (EIS) and potentiodynamic measurements. It was found that the corrosion current density (j_{corr}) is smaller for at least one order of magnitude for ARB multilayer samples. Higher degree of plastic deformation induced better corrosion stability, for both CR monolayer and ARB multilayer samples. Results showed that the overall impedance value of ARB samples was more than doubled compared to the CR samples as a result of the multilayered structure and the presence of oxidation film between the layers. Significantly larger semicircles in Nyquist plots for ARB samples indicate increase of corrosion stability, with increasing the number of ARB cycles. Experimental results showed that applied processing route and the degree of deformation have a major impact on the corrosion stability of the AA5083 alloy.

This work was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, under contract No. TR 34018.

NM P 02

Fizičko-hemijska karakterizacija ostataka sa arheometalurškog lokaliteta Ružana (Srbija)

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Arheometalurški lokalitet Ružana je jedan od, u skorije vreme otkrivenih, lokaliteta u blizini Bora (Srbija), na kome su otkriveni ostaci metalurških peći i metaluških šljaka, koji dodatno potvrđuju postojanje obojene metalurgije u praistorijskim zajednicama Istočne Srbije.
U radu su prikazani rezultati hemijske, rentgenostrukturne i EDXRF analize ostataka metalurških šljaka sa ovog lokaliteta. Rezultati hemijske analize pokazali su dominantno prisustvo železa i silicijuma u ispitivanim uzorcima, što dokazuje činjenicu da se železo u periodu Bronzanog doba nije eksploatisalo i topilo, odnosno nije bilo od značaja metalurzima tog vremena. U najvećem broju uzoraka utvrđeno je prisustvo sledećih dominantnih faza: magnetit/maghemit, kristobalit i kvarc.

Physical and chemical characterization of the remains from archaeometallurgical locality Ruzana (Serbia)

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The archaeometallurgical site Ruzana is a recently discovered site in the vicinity of Bor (Serbia), where remains of metallurgical furnaces and metallurgical slags have been discovered, which further confirm the existence of non-ferrous metallurgy in the prehistoric communities of Eastern Serbia.
The paper presents the results of chemical, X-ray and EDXRF analysis of metallurgical slag residues from this site. The results of chemical analysis showed the dominant presence of iron and silicon in the investigated slag samples, which proved the fact that iron was not exploited or smelted in the Bronze Age, i.e. the metallurgists of the time had no interest in iron. In the majority of samples, the presence of the following dominant phases was determined: magnetite/maghemite, cristobalite and quartz.

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NM P 03

Termička i mikrostrukturna karakterizacija mesinga i broze

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U ovom radu su prikazani rezultati termičke i mikrostrukturne karkterizacije livenih legura Cu sa Zn, Sn, Pb, Al i Ag. Istraživanja koja su izvršena u okviru ovog rada bila su usmerena na merenje toplotne difuzivnosti i određivanje toplotne provodljivosti i specifične topolote primenom metode svetlosnog pulsa (Discovery Xenon Flash, DXF-500), kao i određivanje termijskih karakteristika legura korišćenjem metode diferencijalno skenirajuće kalorimetrije (DSC) i utvrđivanje strukturnih karakteristika primenom optičke mikroskopije (LOM) i skenirajuće elektronske mikroskopije sa energetskom difrakcijom X-zraka (SEM – EDS).

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Thermal and microstructural characterization of brass and bronze

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This paper presents the results of the microstructural and thermal analysis of as-cast Cu alloys with Zn, Sn, Pb, Al and Ag. The investigations were focused on the measurements of thermal diffusivity and determination of thermal conductivity and specific heat capacity using the flash method of light pulse (Discovery Xenon Flash, DXF-500), as well as determination of the thermal properties of the alloys using the DSC method, and the determination of structural characteristics by using optical microscopy (LOM) and scanning electron microscopy with X-ray energy diffraction (SEM - EDS).

Acknowledgment: This work was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Projects ON 172037).

NM P 04

Uticaj funkcionalizacije višeslojnih ugljeničnih nanocevi na toplotnu stabilnost kompozita na osnovu poli(laktida)

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Poli(laktid) (PLA) se smatra ekološki prihvatljivom alternativom za polimere na bazi nafte, ali usled relativno loših mehaničkih svojstava i toplotne stabilnosti, njegova primena je ograničena za mnoge oblasti. Shodno tome, sve veća pažnja je posvećena istraživanju kompozita na osnovu PLA i multifunkcionalnih nanomaterijala, kao što su ugljenične nanocevi. Cilj ovog rada je da se ispita uticaj modifikacije višeslojnih ugljeničnih nanocevi na toplotna svojstva kompozita na osnovu PLA. U tu svrhu izvršena je funkcionalizacija nanocevi gama zračenjem i hemijski, oksidacijom azotnom i sumpornom kiselinom. Toplotna svojstva sintetisanih kompozita analizirana su metodom diferencijalne skenirajuće kalorimetrije i termogravimetrijskom analizom. Na osnovu rezultata dobijenih DSC metodom zaključeno je da vrednosti temperature topljenja i temperature prelaska u staklasto stanje rastu sa porastom udela nanocevi u kompozitnim materijalima. Rezultati TGA analize potvrđuju da inkorporacija malih količina funkcionalizovanih nanocevi može značajno poboljšati toplotnu stabilnost kompozita na osnovu PLA i ugljeničnih nanocevi.

Autori žele da se zahvale Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (projekti III45022 i III45020) za finansijsku podršku.

The influence of multi-wall carbon nanotubes functionalization on the thermal stability of composites based on poly(lactide)

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Poly(lactide) (PLA) is environmentally friendly alternative for petroleum based polymers, but due to the relatively poor mechanical properties and thermal stability, the use of this polimer is limited for many applications. Consequently, increasing attention is paid to the investigation of composites based on PLA and multifunctional nanomaterials, such as carbon nanotubes. The aim of this work was to investigate the influence of multi-wall carbon nanotubes modification on the thermal properties of composites based on PLA. For this purpose, functionalization of nanotubes was performed either by gamma irradiation or chemically by oxidation with nitric and sulfuric acid. Thermal properties of synthesized composites were analyzed by differential scanning calorimetry and thermal gravimetric analysis. From DSC results it was concluded that the values of glass transition and melting temperatures increased with an increasing nanotubes content in composites. The TGA analysis confirm that the incorporation of a small quantity of functionalized nanotubes can significantly improve the thermal stability of the PLA composites with carbon nanotubes.

NM P 05

Strukturna i morfološka karakterizacija praha Ti-Mo mešanih oksida za fotokatalitičke primene

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Binarni poluprovodnički mešani TiO_2-MoO_3 sistem ima potencijal da pokaže visoku fotokatalitičku aktivnost u razgradnji organskih zagađujućih materija u otpadnim vodama. U ovom radu ispitani su optimalni uslovi za mehanohemijsku pripremu mešanog oksidnog $2TiO_2$-MoO_3 praškastog fotokatalizatora. Strukturna i morfološka karakterizacija dobijenog materijala urađena je korištenjem rendgenostrukturne difrakcije, skenirajuće elektronske mikroskopije, energetski disperzivne i Raman spektroskopije.

Structure and morphology characterization of Ti-Mo mixed oxide powder for photocatalytic applications

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The binary semiconductor TiO_2-MoO_3 mixed system has a potential of exhibiting the high photocatalytic activity in degradation of the organic pollutants from wastewaters. In this work, the optimal conditions of mechanochemical preparation of the mixed oxide $2TiO_2$-MoO_3 powder photocatalyst were explored. The structure and morphology characterization of the obtained material was performed by X-ray diffraction, scanning electron microscopy, energy dispersive and Raman spectroscopy.

NM P 06

Identifikacije pigmenata i veziva u istorijskim slikama primenom neinvazivnih tehnika

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Identifikacija matriksa istorijskih slika je veoma kompleksan zadatak jer se slike najčešće sastoje od velikog broja hemijskih jedinjenja koja potiču od pigmenata i slikarskih medijuma. Zbog navedene složenosti, identifikacija upotrebljene palete pigmenata je otežana i u nekim slučajevima skoro nemoguća, te bi postojanje odgovarajuće baze podataka pigmenata, veziva i slikarskih medijuma bilo veoma korisno. Cilj ovog rada je formiranje baze podataka upotrebom neinvazivnih tehnika u identifikaciji pigmenata, veziva i njihove smeše (tehnika jajčane tempere/ulja). Pripremljeni uzorci (40 u jajčanoj tehnici i 27 u tehnici ulja) su ispitani sledećim metodama: infracrvena spektrometrija sa Furijeovom transformacijom (DRIFT), rendgenska fluorescirajuća spektrometrija (XRF), kolorimetrija i multispektralna analiza. Rezultati prezentovani u ovom radu predstavljaju važan resurs za dalji razvoj analitičkih neinvazivnih metoda, zasnovan na analizi prednosti i mana svake od upotrebljenih tehnika.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja na finansijskoj podršci (Projekat III45008).

Pigments and binders identification in historical paintings by using non-invasive techniques

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The matrix of historical paintings is usually very complex, with numerous chemical compounds originating not only from pigments, but also from binders, ground layers, varnishes, fillers, extenders etc. For conservators and scientists it would be useful to have a reference database of pigments already mixed with other relevant compounds. The subject of this paper is the investigation of the possibility of utilizing non-invasive techniques in the identification of pigment, binder and pigment-binder interactions on egg tempera and oil paintings. In total, over 40 samples of pigments with egg as binder, and 27 samples of pigments with linseed oil as binder, were examined and cross-compared. All samples were characterized by using analytical techniques: DRIFT, XRF, colorimetry and multispectral Imaging. This research also provides a resource for further development of multi-analytical non-invasive methods, by comparing the weaknesses and strengths of the particular characterisation techniques in regard to the identification of an individual pigment.

Neorganska hemija / Inorganic Chemistry

NH P 01

Novi rutenijum–arenski kompleksi sa antiinflamatornim lekovima

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U ovom radu sintetisano je četiri nova arenska kompleksa Ru(II) sa dva nesteroidna antiimflamatorna leka, indometacin i mefenaminskom kiselininom. Kompleksi su sintetisani polazeći od metanolnog rastvora polaznog Ru(II) polusendvič jedinjenja i baznog metanolnog rastvora odgovarajućeg liganda. Strukture novih kompleksa određene su NMR i IC spektroskopijom, kao i masenom spektrometrijom. Pokazano je da se ligandi koordinuju monodentatno preko karboksilnih kiseonika. Citotoksična aktivnost liganada i kompleksa ispitana je na tri ćelijske linije humanog kancera i zdravih humanih fibroblastnih ćelija, korišćenjem MTT metode. IC_{50} vrednosti dobijene na ćelijama leukemije K562 bile su uporedive sa onim za cisplatinu (10.3 μM (cisplatina), 11.9 μM (kompleks **1**) i 13.2 μM (kompleks **3**)). Korišćenjem protočne citometrije pokazano je da ovi kompleksi pri IC_{50} koncentracijama zaustavljaju ćelijski ciklus u S fazi. Merenje produkcije reaktivnih kiseoničnih DCFH-DA metodom potvrdilo je njihov potencijal da povećavaju ROS više od cisplatine.

Novel ruthenium–arene complexes with antiinflamatory drugs

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Two non-steroidal antiinflammatory drugs, indomethacin and mefenamic acid, were coordinated to Ru(II)-arenes to give four new complexes. These four complexes were synthesized by mixing methanolic solution of starting half-sandwich Ru complexes with base solution of ligand in methanol. Structures of complexes were determinated by NMR, IR spectroscopy and mass spectrometry. It was shown that they coordinates monodentatly via carboxylic oxygen. The cytotoxic activity of the ligands and ruthenium complexes was tested in three human cancer cell lines and non-tumour human fetal lung fibroblast cells by MTT assay. The IC_{50} values obtained in leukemia K562 cells, were comparable to cisplatin (10.3 μM (CDDP), 11.9 μM (**1**) and 13.2 μM (**3**)). Flow cytometric analysis of these conplexes**,** showed that at IC_{50} concentrations, they arrested cell cycle progression in the S phase. Measurement of reactive oxygen species (ROS) production, by DCFH-DA staining, confirmed their potential to increase ROS even more than cisplatin.

NH P 02

(Elektro)hemijska karakterizacija novog rutenijum(II) bipiridinskog kompleksa

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Neplatinski kompleksi su opšte poznati kao potencijalni antikancerogeni lekovi i krajnje raznoliki redoks sistemi. U tom smislu opisujemo sintezu i kompletnu karakterizaciju novog rutenijum(II) bipiridinskog kompleksa, $[RuL(bpy)_2]PF_6$ gde L predstavlja O^4-hidrogenpiridin-2,4-dikarboksilat. Takođe je ispitana elektrohemijska i citotoksična aktivnost.
Kompleks je dobijen u reakciji 2,4-piridindikarboksilne kiseline sa ekvimolarnom količinom $[RuCl_2(bipy)_2]$ u etanolu na t. s. Nakon mešanja 3 sata pod refluksom, dodata je ekvimolarna količina NH_4PF_6 i finalni produkt je izolovan kao tamnocrveni talog. Kompleks je okarakterisan pomoću IC, NMR i masene spektrometrije, rendgenske strukturne i elementalne analize. Jedinjenje kristališe u $P2_1/n$ prostornoj grupi. Ru(II) jon je oktaedarski koordinovan za četiri atoma azota dva bipiridinska liganda i po jedan azotov i kiseonikov atom iz O^4-hidrogenpiridin-2,4-dikarboksilata. Elektrohemijsko ispitivanje cikličnom voltametrijom ukazalo je na Ru(II)/Ru(III) transfer elektrona u pozitivnom opsegu elektrodnih potencijala. Na suprotnoj strani potencijala ističu se višestruki, delimično reverzibilni pikovi koji predstavljaju uzastopne redukcije razgranatog bipiridinskog dela. Kompleks je pokazao slabu citotoksičnost samo prema K562 (leukemijskoj) ćelijskoj liniji (IC_{50}=177.63±2.28 μM).

(Electro)chemical characterization of new ruthenium(II) bipyridyl complex

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Non-platinum complexes are well known as potential anticancer drugs and highly diverse redox systems. In that sense, we describe synthesis and full characterization of a new ruthenium(II) bipyridyl complex, $[RuL(bpy)_2]PF_6$ where L represents O^4-hydrogenpyridine-2,4-dicarboxylate. The electrochemical profile and cytotoxic activity are also explored.
The complex was obtained in a reaction of 2,4-pyridinedicarboxylic acid with an equimolar amount of $[RuCl_2(bipy)_2]$ in ethanol at r. t. After stirring for 3 h under reflux, equimolar amount of NH_4PF_6 was addded and the final compound was isolated as dark red precipitate. The complex was characterized by IR, NMR and mass spectrometry, X-ray diffraction analysis and elemental analysis. Compound crystallized in the centro-symmetric space group $P2_1/n$. The Ru(II) ion is octahedrally coordinated by four nitrogen atoms from the two bipyridine ligands, and one nitrogen and one oxygen atom from the O^4-hydrogenpyridine-2,4-dicarboxylate. Electrochemical investigation by cyclic voltammetry pointed out Ru(II)/Ru(III) electron transfer in the positive range of electrode potentials. On the opposite potential side, multiple partially reversible peaks were dominant, representing subsequent reductions of the bulky bipyridyl moiety. The compound showed a moderate cytotoxic activity only for K562 (leukemia) (IC_{50}=177.63±2.28 μM).

NH P 03

Polinuklearni kompleksi srebra(I) sa 1,5-naftiridinom kao efikasni antifungalni agensi

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Sintetisani su i primenom spektroskopskih metoda (^{1}H i ^{13}C NMR, IR, UV-vis) i rendgenske strukturne analize okarakterisani novi polinuklearni kompleksi srebra(I) sa 1,5-naftiridinom (1,5-naph), [Ag(NO_3-*O,O'*)(1,5-naph)]$_n$ (**Ag1**), [Ag(CF_3COO-*O,O'*)(1,5-naph)]$_n$ (**Ag2**) i [Ag(CF_3SO_3-*O*)(1,5-naph)]$_n$ (**Ag3**). U ovim kompleksima, 1,5-naph je mostni ligand između dva Ag(I) jona, dok su za preostala mesta koordinovani anjoni iz polaznih soli srebra(I) koje su se koristile za sintezu odgovarajućih kompleksa. Kompleksi **Ag1-3** inhibiraju rast četiri različite *Candida* vrste, pri čemu su vrednosti minimalnih inhibitornih koncentracija (MIK) između 2,5 i 10,3 μM.

Polynuclear silver(I) complexes with 1,5-naphthyridine as efficient antifungal agents

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Three new polynuclear silver(I) complexes with 1,5-naphthyridine (1,5-naph), [Ag(NO_3-*O,O'*)(1,5-naph)]$_n$ (**Ag1**), [Ag(CF_3COO-*O,O'*)(1,5-naph)]$_n$ (**Ag2**) and [Ag(CF_3SO_3-*O*)(1,5-naph)]$_n$ (**Ag3**) were synthesized and characterized by NMR (^{1}H and ^{13}C), IR and UV-vis spectroscopy and single-crystal X-ray diffraction analysis. In all these complexes, 1,5-naph acts as a bridging ligand between two Ag(I) ions, while the remaining coordination sites are occupied by oxygen atom(s) of the corresponding anion. Complexes **Ag1-3** inhibit the growth of four different *Candida* species with minimal inhibitory concentrations (MIC) between 2.5 and 10.3 μM.

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NH P 04

Kompleksi bakra(II) sa 4,7-fenantrolinom: uticaj polazne bakar(II) soli na strukturu i geometriju kompleksa

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U ovom radu, 4,7-fenantrolin (4,7-phen) korišćen je kao ligand za sintezu kompleksa bakra(II). Ispitivan je uticaj anjona polazne soli bakra(II) (NO_3^- i $CF_3SO_3^-$) na strukturu i geometriju kompleksa. Sintetisani kompleksi bakra(II), $[Cu(NO_3\text{-}O)_2(4,7\text{-phenH})_2](NO_3)_2$ (**1**) i $[Cu(CF_3SO_3\text{-}O)(4,7\text{-phen})_2(H_2O)_2]CF_3SO_3$ (**2**), okarakterisani su primenom elementarne mikroanalize, IR i UV-vis spektroskopije, kao i rendgenske strukturne analize. Kompleks **1** ima kvadratno-planarnu geometriju, dok je geometrija kompleksa **2** kvadratno-piramidalna. Interakcije kompleksa **1** i **2** sa CT DNA su ispitivane primenom elektronske apsorpcione i fluorescentne emisione spektroskopije.

Copper(II) complexes with 4,7-phenanthroline: the influence of the starting copper(II) salt on the complex structure and geometry

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In the present study, 4,7-phenanthroline (4,7-phen) was used as a ligand for the synthesis of copper(II) complexes. In order to investigate the influence of the counter-anion on the copper(II) complex geometry, two CuX_2 salts (X = NO_3^- and $CF_3SO_3^-$) were used as the starting reactants. The characterization of the obtained copper(II) complexes, $[Cu(NO_3\text{-}O)_2(4,7\text{-phenH})_2](NO_3)_2$ (**1**) and $[Cu(CF_3SO_3\text{-}O)(4,7\text{-phen})_2(H_2O)_2]CF_3SO_3$ (**2**) was done on the basis of elemental analysis, IR and UV-Vis spectroscopy, while their crystal structures were determined by single-crystal X-ray diffraction analysis. The coordination geometry around Cu(II) ion in **1** is square planar, while in **2**, it is square pyramidal. The interactions of the complexes **1** and **2** with CT DNA were investigated by electronic absorption and fluoresence emission spectroscopy.

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NH P 05

Sinteza, karakterizacija i katalitička svojstva dinuklearnih kompleksa paladijuma(II) sa benzodiazinima kao mostnim ligandima

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Sintetizovana su tri nova dinuklearna paladijum(II) kompleksa koji sadrže različite benzodiazine kao mostne ligande, $[\{Pd(en)Cl\}_2(\mu\text{-qx})](NO_3)_2$, $[\{Pd(en)Cl\}_2(\mu\text{-qz})](NO_3)_2$ i $[\{Pd(en)Cl\}_2(\mu\text{-phtz})](NO_3)_2$ (en = etilendiamin, qx = hinoksalin, qz = hinazolin i phtz = ftalazin). Kompleksi su okarakterisani na osnovu rezultata elementarne mikroanalize, NMR (^{1}H i ^{13}C), IR i UV-Vis spektroskopije. Primenom ^{1}H NMR spektroskopije ispitivane su reakcije (2,0 < pH < 2,5 i 37 °C) akva derivata dinuklearnih paladijum(II) kompleksa sa Ac-L-Met-Gly i Ac-L-His–Gly dipeptidima. Nađeno je da u svim ispitivanim reakcijama kod ovih dipeptida dolazi do selektivne hidrolize peptidne veze. Ispitivan je uticaj različitih mostnih liganada na katalitička svojstva dinuklearnih paladijum(II) kompleksa.

Synthesis, charcterization and catalytic properties of dinuclear palladium(II) complexes with benzodiazines as bridging ligands

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Three new dinuclear palladium(II) complexes with benzodiazines as bridging ligands, $[\{Pd(en)Cl\}_2(\mu\text{-qx})](NO_3)_2$, $[\{Pd(en)Cl\}_2(\mu\text{-qz})](NO_3)_2$ and $[\{Pd(en)Cl\}_2(\mu\text{-phtz})](NO_3)_2$, have been synthesized and characterized by elemental microanalyses, NMR (^{1}H and ^{13}C) spectroscopy, IR and UV-Vis spectroscopy (en = ethylenediamine, qx = quinoxaline, qz = quinazoline and phtz = phthalazine). These complexes were converted into the corresponding aqua derivatives and their reactions (2.0 < pH < 2.5 and 37 °C) with Ac-L-Met-Gly and Ac-L-His-Gly dipeptides were studied by ^{1}H NMR spectroscopy. It was found that in all these reactions the regioselective hydrolysis of the amide bond in the investigated dipeptides has been occurred. The influence of different bridging ligands on the catalytic properties of dinuclear Pd(II) complexes has been investigated.

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NH P 06

Ispitivanje nukleofilnih supstitucionih reakcija novih platinum(II) i paladijum(II) kompleksa sa biološki relevantnim ligandima

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Iako je cisplatina, cis-$[PtCl_2(NH_3)_2]$, jedan od najviše korišćenih hemioterapeutskih agenasa, pojava toksičnosti i rezistentnosti ograničavaju njegovu kliničku upotrebu.[1] To je dovelo do ispitivanja potencijalne antitumorske aktivnosti kompleksa drugih jona metala, kao što su na primer kompleksi paladijuma. Iz tog razloga kinetička i mehanistička ispitivanja reakcija Pt(II) i Pd(II) kompleksa sa biomolekulima pod fiziološkim uslovima mogu doprineti boljem razumevanju biohemijskih procesa tokom upotrebe kompleksa kao antitumorskih agenasa. Nukleofilne supstitucione reakcije četiri nova Pt(II) i Pd(II) kompleksa $Pd(H_2L^{tBu})Cl]Cl$, $[Pt(H_2L^{tBu})Cl]Cl$, $[Pd(Me_2L^{tBu})Cl]Cl$ i $[Pt(Me_2L^{tBu})Cl]Cl$ (gde je H_2L^{tBu} = 2,6-bis(5-(*tert*-butyl)-1H-pyrazol-3-yl)pyridine i Me_2L^{tBu} = 2,6-bis(5-(*tert*-butyl)-1-methyl-1H-pyrazol-3-yl)pyridine) su izučavane sa biološki značajnim ligandima, kao što su tiourea, L-cistein, L-metionin i guanozin-5'-monofosfat. Kompleksi sa H_2L^{tBu} ligandom su pokazali veću reaktivnost u odnosu na Me_2L^{tBu} komplekse, dok su Pd(II) kompleksi uvek bili znatno reaktivniju u odnosu na Pt(II) analoge.

The study of the nucleophilic substitution reactions of the new platinum(II) and palladium(II) complexes with some bio-relevant ligands

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Although, cisplatin, cis-$[PtCl_2(NH_3)_2]$, is one of the most common chemotherapy drugs, the acquired toxicity and resistance limit its clinical use.[1] This has led to examination of potential antutumor activity of some other metal ion complexes, such as palladium complexes. Therefore, the studies of the kinetics and mechanism of the substitution reaction of Pt(II) and Pd(II) complexes with bio-molecules under physiological conditions can improve understanding of the biochemical processes that occur in the body during their application as antitumor drug.

Nucleophilic substitution reactions of four new Pt(II) and Pd(II) complexes, $[Pd(H_2L^{tBu})Cl]Cl$, $[Pt(H_2L^{tBu})Cl]Cl$, $[Pd(Me_2L^{tBu})Cl]Cl$ and $[Pt(Me_2L^{tBu})Cl]Cl$ (where H_2L^{tBu} = 2,6-bis(5-(*tert*-butyl)-1H-pyrazol-3-yl)pyridine and Me_2L^{tBu} = 2,6-bis(5-(*tert*-butyl)-1-methyl-1H-pyrazol-3-yl)pyridine) with biologically relevant ligands such as thiourea, L-cysteine, L-methionine and guanosine-5'-monophosphate were investigated. The complexes that contain H_2L^{tBu} showed higher reactivity than those with Me_2L^{tBu}, while Pd(II) complexes were always more reactive than their Pt(II) analoques.

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NH P 07

Novi dinuklearni zlato(III) kompleksi: Sinteza, karakterizacija i ispitivanje njihovih interakcija sa DNK/BSA

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Zlato(III) kompleksi, strukturni analozi kompleksa platine(II), sve više se proučavaju zbog potencijalne antikancerogene aktivnosti. Zapravo, zlato(III) jon je izoelektronski sa platina(II) jonom, tako da može da gradi komplekse kvadratno-planarne geometrije, ali i da formira slične DNK produkte kao platina(II). [1][2]

U cilju ovog istraživanja sintetisana je serija novih dinuklearnih Au(III) kompleksa opšte formule $[Au_2(N\text{-}N)Cl_6]$, gde je *N-N* bidentatni ligand (1,4-diaminobutan; 1,6-diaminoheksan ili 1,8-diaminooktan). Pomenuti kompleksi su okarakterisani spektroskopskim tehnikama (IR, UV-Vis, ^{1}H NMR). Interakcije kompleksa i DNK su ispitivane pomoću UV-Vis spektrofotometrije i fluorescentne spektroskopije. Rezultati ispitivanja konkurentnih reakcija između kompleksa zlata(III) i etidijum bromida (EB) prema DNK su pokazali da izučavani kompleksi mogu da zamene EB iz DNK-EB proizvoda interagujući kovalentno ili preko interkalacije. Veliki afinitet kompleksa zlata(III) prema goveđim serum albuminom (BSA) potvrđen je na osnovu dobijenih visokih vrednosti za konstante vezivanja.

New dinuclear gold(III) complexes: Synthesis, characterization and study of their interactions with DNA/BSA

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Gold(III) complexes have been extensively studied as potential anticancer agents because they are structurally very similar to platinum(II) compounds. In fact, gold(III) ion is isoelectronic with platinum(II) ion, so it also forms complexes with square-planar geometry which interact with DNA similar as platinum(II) complexes. [1][2]

In this study we have synthesized a series of new dinuclar gold(III) complexes with general formula $[Au_2(N\text{-}N)Cl_6]$ in which *N-N* is a bidentate ligand (1,4-diaminobutane; 1,6-diaminohexane or 1,8-diaminooctane). These complexes were characterized by spectroscopic techniques (IR, Uv-Vis, ^{1}H NMR). DNA binding studies were performed by UV-Vis spectrophotometry and fluorescence spectroscopy. The results of the study of competitive reactions between gold(III) complexes and etidium bromide (EB) toward DNA have shown that complexes can displace EB from DNA-EB aduct. Also, these experiments confirm that gold(III) complexes interact with DNA covalently or *via* intercalation. High values of binding constants towards bovine serum albumin protein (BSA) indicate good binding affinity, as well.

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NH P 08

Antiproliferativna aktivnost kompleksa $[Co_2Cl_2$ tpmc$](BF_4)_2$, *in vitro*

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Antiproliferativna aktivnost kompleksa $[Co_2Cl_2$tpmc$](BF_4)_2$ je testirana na tumorskim ćelijskim linijama humanog cervikalnog adenokarcinoma (HeLa) i mijeloidne leukemije (K562). Preživljavanje ćelija procenjivano je pomoću MTT kolorimetrijskog testa, nakon 48 h inkubacije sa različitim koncentracijama testirane supstane. Kompleks $[Co_2Cl_2$ tpmc$](BF_4)_2$ je na dozno zavistan način doveo do smanjenja metaboličke aktivnosti HeLa i K562 ćelija. Na osnovu dobijenih podataka, numeričkom analizom, izračunata je IC_{50} vrednost.

Antiproliferative activity of complex $[Co_2Cl_2$ tpmc$](BF_4)_2$, *in vitro*

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The cytotoxic activity of the complex $[Co_2Cl_2$tpmc$](BF_4)_2$ was tested against tumor cell lines human cervix adenocarcinoma (HeLa) and human myelogenous leukemia (K562). Cell survival was determined by MTS test, after 48 h exposure to compound. The complex $[Co_2Cl_2$ tpmc$](BF_4)_2$ has promoted significant decreases in the metabolic activity of the HeLa and K562 cells, which occurred in a dose-dependent fashion. IC_{50} values for compound were obtained by numerical analysis of data obtained.

Hemija životne sredine / Environmental Chemistry

HZS P 01

ZnFe фотокатализатори: Утицај термичког третмана и pH реакционог система на фотокаталитичка својства

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Услед већ доказане фотокаталитичке ефикасности, ZnFe фотокатализатори се све више примењују у области заштити животне средине. Међутим, због високих захтева за фотокатализаторе, као што су активност, селективност, нетоксичност, економичност и стабилност, потреба за њиховим развојем се у последње време намеће као приоритет за будућестудије. Приказана истраживања су усмерена ка структурној и текстуралној карактеризацији ZnFe фотокатализатора, испитивању њихове ефикасности и стабилности у разградњи Родамина Б при сунчевом зрачењу, као и утврђивању утицаја термичког третмана ZnFe фотокатализатора и pH реакционог система на ефикасност. Резултати су показали да су ZnFe мешовити оксиди веома ефикасни у разградњи родамина Б. Поред тога запажен је и утицај pH реакционог система на фотокаталитичку активност која се може објаснити корелацијом различитих текстуралних и структурних својстава фотокатализатора.

ZnFe photocatalysts: The effect of thermal treatment and the pH of the reaction system on the photocatalytic properties

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Due to the proven photocatalytic efficiency, ZnFe photocatalysts have been increasingly used in the field of environmental protection. As a result of high demands, such as activity, selectivity, toxicity, cost and stability, the need for the photocatalyst further development is lately emerging as a priority for future research. The presented study is focused on the structural and textural characterization of the synthesized ZnFe photocatalysts, on their efficiency and stability in the photocatalytic degradation of rhodamine B under solar irradiation, as well as on the determination of the impact of their thermal treatment and the pH of the reaction system on the efficiency. The results showed that the obtained mixed oxides are highly efficient in the rhodamine B degradation. In addition the pH effect of the reaction system in the photocatalytic activity was observed, which can be explained by the correlation of different textural and structural properties of the photocatalysts.

HZS P 02

Ispitivanje mogućnosti primene otpadnog filterskog peska u tretmanu otpadne vode tekstilne industrije

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Tekstilna industrija se odlikuje izrazito zagađenim otpadnim vodama, jer tokom procesa pripreme, bojenja i završne obrade tekstila, značajan udeo neizreagovalih sintetičkih boja završi u efluentu. Tokom protekle decenije izvršena su istraživanja u pravcu pronalaska efikasnog tretmana ovih otpadnih voda, među kojima se heterogeni Fenton proces izdvaja. U ovom radu je ispitivana mogućnost primene otpadnog filterskog peska (OFP), koji nastaje prilikom pripreme vode za piće, kao katalizatora Fenton reakcije. SEM/EDS metoda je ukazala na prisustvo gvožđa (15,73 %) i mangana (46,15 %), koji potvrđuju mogućnost njegove primene. Sprovedena je optimizacija procesa pri različitim pH-vrednostima, inicijalnoj koncentraciji vodonik-peroksida i dozi katalizatora. Primenom centralnog kompozitnog dizajna na 20 proba ustanovljeno je da se najviša efikasnost obezbojavanja (60,71 %) postiže pri pH=3, [H_2O_2]=9,45 mM i [OFP]=0,1 g.

Zahvalnica: *Istraživanje je finansirano od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije (III43005).*

Investigation of the application possibilities of waste filter sand in treatment of textile industry wastewater

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The textile industry has extremely polluted wastewaters, because during preparation, dyeing and finishing processes significant number of synthetic dyes does not react with textile. Over the past decade, research has been carried out to find effective wastewater treatment, among which the heterogeneous Fenton process is distinguished. This paper examines the possibility of the use of waste filter sand (WFS), which occurs during the preparation of drinking water, as a Fenton catalyst. The SEM/EDS method indicated the presence of iron (15.73 %) and manganese (46.15 %), which confirms the possibility of its use. Process optimization was carried out with varying pH values, initial hydrogen peroxide concentration and initial catalyst dose. By applying the central composite design on 20 probes that were established, the optimal values of effluent decolorization (60.71 %) were at pH=3, [H_2O_2]=9.45 mM i [OFP]=0.1 g.

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HZS P 03

Adsorpciona kinetika Cr(VI) na oksidovanim višeslojnim ugljeničnim nanocevima

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Cilj ovog rada bio je ispitivanje adsorpcione kinetike i definisanje mehanizma adsorpcije Cr(VI) na FMWCNT6h. Na osnovu dobijenih podataka izveden je zaključak da se adsorpciona ravnoteža Cr(VI) uspostavlja nakon 2 h. Efikasnost uklanjanja datog metala u stanju ravnoteže iznosila je ≈ 46%. Ispitivanje mehanizma adsorpcije Cr(VI) izvršeno je primenom četiri kinetička modela: Lagergren-ovog modela pseudo-prvog reda, modela pseudo-drugog reda, Elovich-evog modela i Weber-Morris-ovog modela. Eksperimentalno dobijeni rezultati najbolje su se slagali sa modelom pseudo-drugog reda (R^2 = 0,998), što potvrđuje da se adsorpcija Cr(VI) na FMWCNT6h u najvećoj meri može pripisati razvoju hemijskih interakcija na relaciji površina adsorbenta/adsorbat (elektrostatičke interakcije i kompleksiranje). Koristeći Weber Morris-ov model utvrđeno je da je intra-čestična difuzija takođe uključena u adsorpciju Cr(VI). Dodatno, odsečak grafika Weber-Morris-ovog modela, različit od nule, bio je jasan indikator da data pojava, iako spora, nije jedini ograničavajući korak u pogledu brzine ukupnog adsorpcionog procesa Cr(VI).

Adsorption kinetics of Cr(VI) on oxidised multiwalled carbon nanotubes

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The objective of this study was to investigate the adsorption kinetics, as well as to define the adsorption mechanism of Cr(VI) on FMWCNT6h. Based on the obtained data it was concluded that the adsorption equilibrium of Cr(VI) was achieved after 2 h. The removal efficiency of this metal at equilibrium was ≈ 46%. Investigation of the adsorption mechanism of Cr(VI) was carried out using four kinetic models: Lagergren's pseudo-first order model, the pseudo-second order model, Elovich's model and Weber-Morris's model. The experimentally obtained results were in the best agreement with the pseudo-second order model (R^2 = 0.998), indicating that the adsorption of Cr(VI) can mainly be attributed to chemical interactions between the surface of FMWCNT6h and the investigated heavy metal (electrostatic interactions and complexation). Using the Weber-Morris model it was determined that intra-particle diffusion also contributes to the adsorption of Cr(VI). In addition, the nonzero intercepts of the Weber-Morris plot clearly indicated that intra-particle diffusion, although slow, was not the only rate limiting step.

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HZS P 04

Fotokatalitička razgradnja diklofenaka u akvatičnom medijumu primenom nanostrukturne mešavine ZnO/In_2O_3

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Farmaceutska jedinjenja kontinuirano dospevaju u akvatičnu sredinu primarno preko netretiranih ili neadekvatno tretiranih otpadnih voda. Diklofenak je najčešće detektovana aktivna komponenta u vodenim medijumima koja je uključena u prvu *Watch* listu emergentnih polutanata, EU Direktive 2013/39. Cilj rada je bio da se ispita primena novog nanomaterijala ZnO/In_2O_3 za dekompoziciju diklofenaka. Nanomaterijal je pripremljen jednostavnom, mehanohemijskom *solid-state* metodom. Kinetika fotokatalitičke razgradnje diklofenaka je ispitivana u različitim vremenskim intervalima (5-60 min). Nakon 40 min UV izloženosti, 99 % diklofenaka je razgrađeno. Novi sintetisani nanomaterijal pokazuje potencijal za fotorazgradnju diklofenaka u akvatičnoj sredini.

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Photocatalytic degradation of diclofenac in the aquatic medium by nanopowder mixture of ZnO/ In_2O_3

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Pharmaceutical compounds are continuously introduced into aquatic environment primarily through untreated or inadequately treated wastewater. Diclofenac is the most commonly detected active compound in aqueous media that is included in the First Watch List for emerging pollutants, the EU Directive 2013/39. The aim of this study was to examine the use of new ZnO/In_2O_3 nanomaterial for the decomposition of diclofenac. The nanomaterial was prepared by simple, mechanochemical solid-state method. The photocatalytic degradation of diclofenac was studied at different time intervals (5-60 min). After 40 min of UV exposure, 99 % of diclofenac was degraded. The new synthesized nanomaterial shows the potential for photodegradation of diclofenac in the aquatic environment.

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HZS P 05

Efikasnost uklanjanja herbicida fluroksipira iz prirodnih voda primenom novosintetisanog ZrO_2/Fe_3O_4 nanopraha

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U cilju poboljšanja efikasnosti eliminacije herbicida fluroksipira iz vodene sredine ispitana je fotokatalitička aktivnost heterogenog foto-Fentonskog sistema $ZrO_2/Fe_3O_4/H_2O_2$ primenom simuliranog sunčevog zračenja. Nađeno je da povećanje količine ZrO_2 u intervalu od 2 do 11 % (w/w) u novosintetisanim nanoprahovima na bazi Fe_3O_4 dovodi do povećanja efikasnosti uklanjanja ispitivanog herbicida u dva puta destilovanoj vodi. Isto tako ispitivana je efikasnost eliminacije fluroksipira i u prirodnim vodama (podzemna, rečna (Dunav) i pijaća voda) primenom $11ZrO_2/Fe_3O_4/H_2O_2$ (fotokatalizator sa 11 % w/w ZrO_2). Za praćenje efikasnosti uklanjanja polaznog jedinjenja korišćena je UFLC–DAD tehnika.

Efficiency of the removal of herbicide fluroxypyr from environmental waters using newly synthesized ZrO_2/Fe_3O_4 nanopowder

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In order to improve the efficiency of the elimination of fluroxypyr from the aqueous media the photocatalytic activity of the heterogeneous photo-Fenton system $ZrO_2/Fe_3O_4/H_2O_2$ was investigated using simulated solar radiation. It was found that with increasing the amount of ZrO_2 in the range from 2 to 11 % (w/w) in newly synthesized Fe_3O_4 nanopowders leads to an increase the efficiency of the removal of the selected herbicide in double distilled water. The efficiency of the elimination of fluroxypyr was also investigated in environmental waters (groundwater, river (Danube) and drinking water) using $11ZrO_2/Fe_3O_4/H_2O_2$ (photocatalyst with 11 % w/w ZrO_2). For monitoring the efficiency of degradation of the parent compound UFLC–DAD technique was used.

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HZS P 06

Bioakumulacija teških metala i mineralni sadržaj u uzorcima divljih vrsta jestivih pečuraka sa područja južne Srbije

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U ovom radu je prikazano određivanje sadržaja esencijalnih i toksičnih metala u uzorcima divljih vrsta jestivih pečuraka i površinskog sloja zemljišta, obzirom da predstavljaju popularni delikates u mnogim zemljama. Sadržaj metala u uzorcima pečuraka i zemljišta sa više različitih lokacija, određen je ICP-OES i ICP-MS metodama, nakon pripreme uzoraka mokrom digestijom. Procenjen je doprinos dnevnom unosu esencijalnih elemenata (Cu, Zn, itd.) kao što su bioakumulacioni potencijal i eventualni negativni uticaj na ljudsko zdravlje. Sadržaj 21 makro i mikro elementa, uključujući i elemente u tragovima analiziran je u divljim jestivim pečurkama (*Chantarelus cibarius* i *Boletus edulis*) i zemljištu prikupljenih sa nekoliko različitih lokacija na teritoriji južne Srbije. Koncentracije nekih toksičnih metala (Cd, Cr i Pb) kreću se u untervalu 0,11-1,85, 0,14-1,91 i 1,37-18,2 $\mu g \cdot g^{-1}$ u *Chantarelus cibarius*, i 0,09-0,57, 0,35-1,97 i 2,16-89 $\mu g \cdot g^{-1}$ u *Boletus edulis*. Sve analizirane vrste pečuraka predstavljaju bioekskluzore olova (BFC<1). *Chantarelus cibarius* bioakumulira Cd i Cu (BFC > 1), dok *Boletus edulis* bioakumulira Cd i Zn (BFC > 1). Obe vrste pokazuju bioakumulacionu sposobnost cinka i bakra. Poznavanje sadržaja teških metala u uzorcima divljih jestivih pečuraka važno je za javno zdravlje zbog činjenice da se neke pečurke često konzumiraju, a poseduju bioakumulatorne sposobnosti. Na osnovu rezultata analiziranih pečuraka sa teritorije južne Srbije, može se zaključiti da one predstavljaju izvor esencijalnih minerala i ne predstavljaju toksikološki rizik za ljudsko zdravlje.

Bioacumulation of heavy metals and mineral contents in wild growing mushrooms species from area of South Serbia

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Investigation of the level of essential and toxic metals of wild edible mushrooms species and top soil was performed in this study, as wild growing mushrooms have been a popular delicacy in many countries. The metal content of mushroom and soil samples from 5 different sampling sites was determined using ICP-OES and ICP-MS method. It was also intended to evaluate the contribution of mushrooms to the daily intake of essential elements (Cu, Zn, *etc.*), such as the bioaccumulation potential of these mushrooms and potential negative impact on human health. The contents of 21 minerals and trace elements were analysed in wild edible mushrooms (*Chantarelus cibarius* and *Boletus edulis*) collected from different location in South-East Serbia were analysed by ICP-MS. Element concentrations for toxic metals copper, Cd, Cr, Ni and Pb were 25.7-43.9, 0.11-1.85, 0.14-1.91, 1.15-4.75 and 1.37-18.2 $\mu g \cdot g^{-1}$ in *Chantarelus cibarius* and 12.2-34.8, 0.09-0.57, 0.35-1.97, 0.20-0.58 and 2.16-89 $\mu g \cdot g^{-1}$ in *Boletus edulis*. All of the analysed mushroom species were bioexclusors of lead (BFC < 1). *Chantarelus cibarius* bioaccumulated cadmium and copper (BFC > 1), while *Boletus edulis* bioaccumulated cadmium and zinc (BFC > 1). Both species showed bioaccumulation ability for zinc and for copper. Knowledge of heavy metal contents of wild growing mushrooms is important for public health due the fact that some mushrooms are widely consumed in many countries. Our study showed that analysed mushrooms represent a major source of essential minerals for human health and that consumption of these mushrooms does not represent a toxicological risk for human.

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HZS P 07

Indirektna fotoliza i fotokatalitička efikasnost novosintetisanih ZrO_2/Fe_3O_4 nanoprahova u razgradnji ceftriaksona primenom simuliranog sunčevog zračenja

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Ceftriakson (β-laktamski antibiotik, M_r = 554,58 g/mol, CAS No 104376-79-6, $C_{18}H_{16}N_8Na_2O_7S_3$), predstavnik treće generacije cefalosporinskih antibiotika, se koristi za lečenje različitih infekcija uključujući respiratorni trakt, urinarni sistem, kao i infekcije karlične šupljine. Dugotrajna izloženost ceftriaksonu predstavlja rizik za vodeni ekosistem i zdravlje čoveka. U ovom radu proučavana je kinetika indirektne fotolize ceftriaksona u prisustvu H_2O_2, kao i uticaj koncentracije H_2O_2 na efikasnost razgradnje primenom simuliranog sunčevog zračenja (SSZ). Isto tako, koprecipitacionom metodom sintetisana su tri ZrO_2/Fe_3O_4 nanopraha sa različitim masenim odnosom ZrO_2 prema Fe_3O_4 (2 %, 7 % i 11 %). Nakon toga, ispitana je efikasnost fotokatalitičke razgradnje ceftriaksona u prisustvu novosintetisanih ZrO_2/Fe_3O_4 nanoprahova u prisustvu H_2O_2 i primenom SSZ.

Indirect photolysis and photocatalytic efficiency of newly synthesized ZrO_2/Fe_3O_4 nanopowders in degradation of ceftriaxone under simulated solar irradiation

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Ceftriaxone (β-lactam antibiotic, M_r = 554.58 g/mol, CAS No 104376-79-6, $C_{18}H_{16}N_8Na_2O_7S_3$), as the third generation cephalosporin antibiotic is used for treating various infections including respiratory tract, urinary system and pelvic cavity infection. Long-term exposure to ceftriaxone will induce the potential risk to the aquatic ecosystem and the health of human being. In this study the kinetics of indirect photolysis of ceftriaxone in the presence of H_2O_2, as well as the influence of concentration of the H_2O_2 on the degradation efficiency using simulated solar irradiation (SSI) were studied. Also, three ZrO_2/Fe_3O_4 nanopowders with different mass ratio ZrO_2 to Fe_3O_4 (2 %, 7 %, and 11 %) were synthesized using co-precipitation method. Thereafter, the efficiency of photocatalytic degradation of ceftriaxone in the presence of newly synthesized ZrO_2/Fe_3O_4 nanopowders in the presence of H_2O_2 using SSI was studied.

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HZS P 08

Uticaj strukture odabranih aktivnih komponenata lekova i pesticida na reaktivna i adsorpciona svojstva u prisustvu ZrO_2: DFT i MD studija

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Reaktivna svojstva aktivnih komponenti lekova (4-amino-6-hlorbenzen-1,3-disulfonamid i amitriptilin) i pesticida (sulkotrion i fluroksipir) su ispitana upotrebom proračuna na bazi teorije funkcionala gustine (DFT) i simulacija molekulske dinamike (MD). Na osnovu proračuna energije disocijacije veze za abstrakciju vodonika, DFT proračuni su korišćeni za identifikaciju delova molekula koji su podložni oksidaciji. U okvirima formalizma prirodnih prelaznih orbitala, vremenski zavisni DFT proračuni su omogućili ispitivanje ekscitacija koje najviše doprinose apsorpciji zračenja od strane ispitanih molekula. Analizom radijalnih distributivnih funkcija, rezultati MD simulacija su dali uvid u interakcije ispitanih molekula i vode. Adsorpciona svojstva korišćenog fotokatalitičkog materijala posmatrana su na osnovu interakcija između reprezentativne model površi ZrO_2 i ispitanih molekula.

Influence of structure of selected pharmaceutical active components and pesticides to reactive and adsorption properties in presence of ZrO_2: DFT and MD study

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Reactive properties of active components in frequently used pharmaceuticals (4-amino-6--chloro-1,3-benzenedisulfonamide and amitriptyline) and pesticides (sulcotrione and fluroxypyr) have been computationally investigated by density functional theory (DFT) calculations and molecular dynamics (MD) simulations. Based on the bond dissociation energies for hydrogen abstraction, DFT calculations have been used for identification of molecule sites sensitive towards the oxidation. In the framework of natural transition orbital formalism, time dependent DFT calculations enabled study of excitations that are principally responsible for the absorption of radiation by the investigated molecules. By analysis of radial distribution functions, MD simulations gave an insight into the interactions of studied molecules with water. Adsorption properties of used photocatalytic material have been examined based on the interactions between representative model surface of ZrO_2 and studied molecules.

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HZS P 09

Fotokatalitička razgradnja amitriptilina primenom kuplovanih cink-kalaj-oksid nanoprahova

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Kuplovanje poluprovodnika je jedna od metoda za povećanje efikasnosti fotokatalitičke razgradnje, koje nastaje kao posledica povećanja opsega apsorpcije zračenja i razdvajanja naelektrisanja, smanjenja rekombinacije naelektrisanja, kao i sprečavanja fotokorozije. Dve serije kuplovanih ZnO/SnO_2 su sintetisane mehano-hemijskom metodom u dva molarna odnosa 1:1 i 2:1 i kalcinisane na određenoj temperaturi u opsegu od 500 do 700 °C. Fotokatalitička aktivnost ZnO/SnO_2 nanoprahova je ispitana u fotorazgradnji amitriptilina, tricikličnog antidepresiva iz klase dibenzocikloheptadiena, primenom simuliranog sunčevog zračenja. Dobijeni rezultati su upoređeni sa efikasnošću komercijalnog fotokatalizatora TiO_2 Degussa P25 i kao najefikasniji se pokazao ZnO/SnO_2 u molarnom odnosu 2:1 koji je kalcinisan na 700 °C. Određena je i njegova optimalna koncentracija koja iznosi 1,0 mg/cm^3.

Photocatalytic degradation of amitriptyline using coupled zinc-tin-oxide nanopowders

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Semiconductor coupling is one of the methods used for increasing photocatalytic degradation efficiency as a result of increasing of the irradiation absorption and the separation of charge carriers, the reduction of charge recombination, and the prevention of photocorrosion. Two series of coupled ZnO/SnO_2 were synthesized by a mechanochemical method in two molar ratios 1:1 and 2:1 and calcined at a specific temperature in the range of 500 °C to 700 °C. Photocatalytic efficiency of ZnO/SnO_2 nanopowders was investigated in photodegradation of amitriptyline, a tricyclic antidepressant from the dibenzocycloheptadiene class, using simulated solar irradiation. The obtained results were compared with the efficiency of the commercial TiO_2 Degussa P25 photocatalyst and the ZnO/SnO_2 in the 2:1 molar ratio which was calcined on 700 °C has shown the highest efficiency. Its optimal loading was also determined, which is 1.0 mg/cm^3.

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HZS P 10

Poboljšanje fotokatalitičke efikasnosti komercijalnog TiO_2 dodatkom NiO za produkciju vodonika primenom simuliranog sunčevog zračenja

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Metodom mokre impregnacije sintetisana su četiri NiO/TiO_2 materijala sa različitim masenim odnosom NiO prema TiO_2 (3,5; 7,0; 24,5 i 38,5 %). Ispitana je fotokatalitička efikasnost ovih materijala za generisanje vodonika iz vodenog rastvora metanola u prisustvu simuliranog sunčevog zračenja (I_{UV} = 2,264 × 10^{-3} W/cm^2; I_{vis} = 1,656 W/cm^2). Sadržaj vodonika nastalog tokom fotorazlaganja metanol/vode utvrđen je upotrebom gasnog hromatografa sa detektorom toplotne provodljivosti. Za sve sintetisane NiO/TiO_2 materijale ustanovljena je veća fotokatalitička efikasnost u poređenju sa komercijalnim TiO_2 P25 katalizatorom. Utvrđen je optimalni maseni odnos NiO prema TiO_2 i analiziran je doprinos u širokom opsegu koncentracija fotokatalizatora i metanola na ukupnu efikasnost nastanka vodonika.

Improving the photocatalytic efficiency of commercial TiO_2 by adding NiO for hydrogen production using simulated solar radiation

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Four NiO/TiO_2 materials with a different mass ratio of NiO to TiO_2 (3.5; 7.0; 24.5 i 38.5 %) were synthesised by wet impregnation method. The photocatalytic efficiency of these materials for generating hydrogen from an aqueous solution of methanol in the presence of simulated solar radiation (I_{UV} = 2.264 × 10^{-3} W/cm^2; I_{vis} = 1.656 W/cm^2) was investigated. The content of hydrogen formed during the photodecomposition of methanol/water was determined using a gas chromatograph equipped with a thermal conductivity detector. For all synthesised NiO/TiO_2 materials higher photocatalytic efficiency was found compared to the commercial TiO_2 P25 catalyst. The optimum mass ratio of NiO to TiO_2 was determined, and the contribution of a wide range of photocatalyst and methanol concentrations to the overall efficiency of hydrogen production was analysed.

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HZS P 11

Uticaj fulerenola na fotokatalitičku razgradnju nikosulfurona primenom TiO_2 Hombikat pod dejstvom simuliranog sunčevog zračenja

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Nikosulfuron (2-[(4,6-dimetoksipirimidin-2-il)karbamoilsulfamoil]-*N*,*N*-dimetilpiridin-3-karboksamid) je selektivni sistemični sulfonilurea herbicid namenjen suzbijanju jednogodišnjih travnih i nekih širokolisnih korova u poljima kukuruza, pirinča, citrusnog voća, krompira, kao i u vinogradima. Stabilnost nikosulfurona je ispitana u prisustvu simuliranog sunčevog zračenja bez i uz dodatak različitih zapremina fulerenola (FNP), pri čemu nije uočena značajnija razgradnja. Nakon toga je, u prisustvu simuliranog sunčevog zračenja, ispitana aktivnost TiO_2 Hombikat (TiO_2) različitih masenih koncentracija (0,5, 1,0 i 2,0 mg/cm^3). Dobijeni rezultati ukazuju da sa povećanjem masene koncentracije TiO_2 do 1,0 mg/cm^3 efikasnost fotokatalitičke razgradnje nikosulfurona raste, pri čemu dalje povećanje nema uticaja. Ispitan je i uticaj dodatka različitih zapremina FNP pri svim masenim koncentracijama TiO_2.

Influence of fullerenol on the photocatalytic degradation of nicosulfuron using TiO_2 Hombikat under simulated sunlight

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Nicosulfuron (2-[(4,6-dimethoxypyrimidin-2-yl)carbamoylsulfamoyl]-*N*,*N*-dimethylpyridine -3-carboxamide) is a selective systemic sulfonylurea herbicide used to control annual grasses and some broad-leaved weeds in corn, rice, citrus, potatoes, and vines field. The stability of nicosulfuron was tested under simulated sunlight without and with different volumes of fullerenol (FNP), whereby no significant degradation was observed. After that, the activity of TiO_2 Hombikat (TiO_2) was studied at different loadings (0.5, 1.0 and 2.0 mg/cm^3) under simulated sunlight. The obtained results indicated that with increase of TiO_2 loading to 1.0 mg/cm^3 efficiency of nicosulfuron photocatalytic degradation was enhanced, wherein the further increase has no effect. In addition, the influence of different volumes of FNP at all TiO_2 loadings was investigated.

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Uticaj pH na vezivanje jona teških metala na površinu lignoceluloznih biosorbenata

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Poslednjih decenija je iskazan značajan trud u ispitivanju novih, jeftinijih i efikasnijih materijala za adsorpciju jona teških metala iz vode prirodnim materijalima, većinom agroindustrijskim otpadom, koji je lako dostupan u velikim količinama. Najveći izazov za istraživače je izbor odgovarajuće biomase iz tako velikog broja jeftinih biomaterijala. Zbog toga je neophodno svaki potencijalni biosorbent ispitati detaljno, utvrditi adsorpcioni kapacitet i optimalne uslove adsorpcije, kako bi se ovi materijali mogli uspešno primenjivati u praksi.
U ovom radu je ispitana adsorpciona sposobnost izluženih rezanaca šećerne repe za vezivanje jona bakra, nikla, hroma i kadmijuma pri različitim pH vrednostima rastvora. Rezultati su pokazali da izluženi rezanci šećerne repe imaju mnogo bolje adsorpcione karakteristike za jone bakra u ispitanim opsezima pH u odnosu na jone drugih teških metala. Adsorpciju jona bakra je najbolje izvoditi na pH 4. Za jone nikla i kadmijuma pH vrednost nema veći uticaj na adsorpciju u ispitivanom opsegu pH. Za jone hroma, najveći adsorpcioni kapacitet se postiže na najnižoj pH vrednosti (pH 1), ali je zbog velikog utroška kiseline ipak pogodnije adsorpciju izvoditi na pH 2.

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The influence of pH on the binding of heavy metal ions to the surface of lignocellulosic biosorbents

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Recently, significant efforts have been made to find new, cheaper and more efficient materials for adsorption of heavy metal ions from water. Researchers are investigating natural materials, mostly agro-industrial waste that is easily accessible in large quantities. The greatest challenge for the researchers is the selection of the appropriate biomass from such a large number of cheap biomaterials. Therefore, it is necessary to investigate potential biosorbents in order to determine the adsorption characteristics and optimal conditions for practical application.
In this paper, the adsorption ability of sugar beet shreds to bond copper, nickel, chromium and cadmium ions at different pH values of water was studied. Results showed that sugar beet shreds have much better adsorption capacity for copper ions compared to other metal ions. Adsorption of copper ions is the best to perform at pH 4. In that case, the decrease of residual concentration of metal ions is not only due to adsorption. For nickel and cadmium ions the pH has not influence on adsorption in investigated pH range. For chromium ions, the highest adsorption capacity is achieved at the lowest pH (pH 1), but due to the high acid consumption it is recommended to perform it at pH 2.

HZS P 13 text rada / full text

Istovremeno uklanjanje odabranih pesticida iz vode primenom ugljeničnog materijala dobijenog iz kokosove ljuske

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U ovom radu ispitivana je mogućnost primene aktiviranog ugljeničnog materijala dobijenog iz kokosove ljuske kao adsorbensa za uklanjanje pesticida različite polarnosti (imidakloprid, acetamiprid, karbendazim, simazin, linuron) iz vode. Adsorpcija pesticida iz vodenog rastvora je rađena u šaržnom sistemu i ispitivan je uticaj različitih parametara na efikasnost uklanjanja pesticida u cilju optimizacije uslova za njihovo što efikasnije vezivanje za ispitivani adsorbens. Rezultati su pokazali da se ravnoteža uspostavlja nakon 180 min, a da je efikasnot uklanjanja najveća u intervalu pH-vrednosti od 3,5 do 6. Dobijeni podaci su fitovani pomoću dva ravnotešna adsorpciona modela - Lengmirovom i Frojndlihovom izotermom. Bolje slaganje je postignuto primenom Lengmirove izoterme, te su primenom ovog ravnotežnog modela određeni adsorpcioni kapaciteti za svaki pesticid posebno. Na osnovu dobijenih rezultata može se zaključiti da ugljenični materijal sintetisan iz kokosove ljuske ima dobar potencijal za primenu u prečišćavanju otpadnih voda zagađenih pesticidima.

Simultaneous removal of selected pesticides from aqueous solutions by coconut shell activated carbon

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The removal of different polarity pesticides (imidaclopride, acetamipride, carbendasim, simazine, linuron) from aqueous solutions using coconut shell-derived activated carbon as an adsorbent was investigated. The experiments were performed in a batch system and the influence of various experimental parameters on the removal of pesticides was observed, with the aim of optimization of the conditions for their efficient binding for the investigated adsorbent. The results showed that the adsorption equilibrium was established within 180 min, and the maximum adsorption occurred in the pH range of 3.5 to 6. The obtained data were fitted using two equilibrium adsorption models – Langmuir and Freundlich isotherm. The adsorption equilibrium data fit the Langmuir equation, and the adsorption capacities for particular pesticide were also estimated by this equation. According to the obtained results, it can be concluded that coconut shell-derived activated carbon has a great potential for application in the treatment of pesticide contaminated wastewaters.

Biohemija / Biochemistry

Metaboličke promene tokom životnog ciklusa kukuruznog plamenca *Ostrinia nubilalis* (Hübner, 1796) – aktivnost citrat sintaze i laktat dehidrogenaze

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U cilju ispitivanja prelaska iz aerobnog u anaerobni metabolizam tokom dijapauze kukuruznog plamenca *Ostrinia nubilalis*, u homogenatima celih lutki, nedijapauzirajućih i dijapauzirajućih gusenica merene su aktivnosti citrat sintaze (CS) i laktat dehidrogenaze (LDH). Dijapauzirajuće gusenice su istovremeno bile izložene niskim temperaturama (5°C, -3°C i -16°C). Najveća aktivnost CS je izmerena u grupi nedijapauzirajućih gusenica, dok je aktivnost LDH bila niska u ovoj grupi. Nasuprot tome, izmerena aktivnost CS je bila statistički značajno niža kod dijapauzirajućih gusenica izloženih niskim temperaturama, dok je aktivnost LDH bila povećana, posebno nakon izlaganja gusenica temperaturi od -3°C. Dobijeni rezultati su u skladu sa početnom pretpostavkom da se u hipometaboličkom stanju dijapauze smanjuje intenzitet katabolizma ugljenih hidrata i sinteza piruvata, u odnosu na aktivni razvoj karakterističan za nedijapauzirajuće gusenice.

Metabolic changes during the life cycle of the European corn borer *Ostrinia nubilalis* (Hübner, 1796) – the activity of citrate synthase and lactate dehydrogenase

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In order to explore aerobic-anaerobic shift in metabolism during diapause of European corn borer *Ostrinia nubilalis*, we measured activities of citrate synthase (CS) and lactate dehydrogenase (LDH) in the whole body homogenates of pupae, non-diapausing and diapausing caterpillars. Diapausing larvae were also exposed to low temperatures (5°C, -3°C, -16°C). The highest activity of CS was measured in the group of non-diapausing caterpillars, while the activity of LDH was low in this group. Conversely, measured CS activity was significantly lower in diapausing caterpillars exposed to low temperatures, while LDH activity was increased, especially after the exposure to -3°C. These results are in accordance with the initial assumption that the less intensive catabolism of carbohydrates and synthesis of pyruvate are the typical characteristics of the hypometabolic state of diapause, in comparison to non-diapausing actively developing caterpillars.

BH P 01

Posttranslacione modifikacije (PTM) epitopa glavnih alergena kikirikija nastale kao rezultat prečišćavanja

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Alergije na kikiriki su zastupljene kod velikog procenta svetske populacije, i mogu izazvati kako blage tako i ozbiljne simpotome. Ara h 1, Ara h 2, Ara h 3 i Ara h 6 su alergeni kikirikija sa dobro okarakterisanim IgE epitoplima, ali se malo zna o uticaju PTM na njihove osobine. Naš cilj je bio da proučimo PTM koje se nalaze na epitopima pomenutih prečišćenih proteina korišćenjem bottom-up metoda u proteomici.
Najveći broj modifikacija sadrži Ara h 2 (14), dok se kao najčešće javljaju hidroksilacija Pro, dehidratacija i deamidacija (N, Q). Naši rezultati su pokazali da epitopi alergena kikirkija jesu nosioci PTM, koje bi mogle da utiču na njihovu alergenost i digestibilnost. U cilju boljeg razumevanja potencijalnih uticaja modiikacija na alergenost neophodno je detljnije proučiti ovaj fenomen i na drugačije pripremljenim ekstraktima kikirikija.

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Post-translational modifications (PTMs) of major peanut allergen epitopes occurring as a result of purification process

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Peanut allergy affects a large portion of world population causing reactions ranging from mild to severe. Seed storage proteins Ara h 1, Ara h 2, Ara h 3 and Ara h 6 are peanut allergens, with well characterized IgE epitopes but little is known about PTMs effect on their properties. Our aim was to investigate PTMs present on known epitopes of said purified proteins using bottom-up proteomcs methods.
Out of the 4 allergens, Ara h 2 has the highest number of PTMs (14), while the most common are hydroxylation Pro, dehydration and deamidation (N, Q). Peanut allergen epitopes are indeed carriers of PTMs that could affect protein allergenicity and digestibility. Further investigation on peanut extracts prepared in different ways is necessary in order to fully understand the impact protein modifications could have on their allergenic potential.

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BH P 02

Kompleksi derivata izatina i njihovo antimikrobno dejstvo

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Derivati izatina su se u novije vreme pokazali kao jedinjenja korisna u farmakologiji, jer ispoljavaju širok spektar dejstava kao sto su antivirusna, antitumorna, antibakterijska, antituberkulozna, antigljivična, antikonvulzivna. Reč je o jedinjenjima koja nastaju reakcijom izatina i primarnih amina i spadaju u grupu Šifovih (Schiff) baza. Kao deo serije istraživanja koje se bavi derivatima izatina, sintetisani su i njihovi kompleksi sa metalima. Ispitana je njihova antimikrobna aktivnost, pomoću bujon - mikrodilucione metode, na kojoj se može zasnovati i mogućnost njihove primene.

The complexes of isatin derivatives and their antimicrobial acitivity

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The isatin derivatives have recently shown the potential to be used in pharmaclogy because of their activities such as antiviral, anticancer, antibacterial, antituberculosis, antifungal and anticonvulsive. These compounds belong to the group of Schiff bases and they are synthesized by the reaction of isatin and primary amines. As a part of the series of investigation that deals with the isatin derivatives, their complexes with metals were synthesized. Their antimicrobial activity was examined using the broth micro-dilution method, which could provide the ground for the application of these compounds.

Hemija i tehnologija hrane / Chemistry and Technology of Food

HTH O 1

Ispitivanje mogućnosti procene neorganskih oblika azota u zemljištu metodama DRIFT spektroskopije i hiperspektralnog fotografisanja

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U ovom radu ispitivane su mogućnosti procene amonijačnog i nitratnog oblika azota u zemljištu korišćenjem metoda difuziono refleksione infracrvene spektroskopije (DRIFT) i hiperspektralnog snimanja. Uzorci zemljišta su tretirani NPK đubrivom poznatog sastava i izvršeno je kvantitativno određivanje količine amonijačnog i nitratnog oblika azota klasičnim mokrim metodama hemijske analize. Spektri uzoraka zemljišta su snimljeni u srednjoj oblasti infracrvenog zračenja (4000-400 cm^{-1}). Uzorci zemljišta su takođe fotografisani hiperspektralnom kamerom u opsegu od 400-1000 nm. Od dobijenih spektara i fotografija formirane su 2D i 3D matrice podataka na koje su primenjene metode multivarijantne analize. Analizom glavnih komponenata utvrđeno je da je moguće razdvajati uzorke zemljišta sa određenim nivom neorganskog oblika azota. Takođe selekcijom piksela procenjene su spektralne oblasti od interesa za hiperspektralno određivanje amonijačnog azota.

Examination of possibility of estimation of inorganic forms of nitrogen in soil using DRIFT spectroscopy and hyperspectral imaging

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In this study, the possibility of assessing the ammonium and nitrate form of nitrogen in the soil was investigated using diffuse reflectance infrared spectroscopy (DRIFT) and hyperspectral imaging. Soil samples were treated with NPK fertilizer of known composition. Quantitative determination of the ammonium and nitrate nitrogen forms was carried out by classical wet methods of chemical analysis. IR spectra of the soils were recorded in the middle infrared radiation region (4000-400 cm^{-1}). Soil samples were also photographed with a hyperspectral camera in the range of 400-1000 nm. Data matrices were formed from the obtained spectra and images and the multivariate methods of analysis were applied. Principal component analysis showed that it is possible to separate soil samples using certain level of inorganic nitrogen. Also, by pixel selection, spectral regions of interest for the hyperspectral determination of ammonium nitrogen were estimated.

HTH P 01

Kombinovani pristup pri utvrđivanju funkcionalnih karakteristika aronije (*Aronia melanocarpa)*: određivanje hemijskog sastava i biološkog potencijala

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Osnovni cilj prikazanog istraživanja je bio karakterizacija hemijskog sastava i biološke aktivnosti subkritičnih vodenih ekstrakata različitih delova aronije (lišće, peteljke, plod). U cilju određivanja biološke aktivnosti određena su enzim-inhibitorna i antiproliferativna svojstva ispitivanih ekstrakata. Enzim-inhibitorna aktivnost je određena u odnosu na holinesterazu i elastazu. Antiproliferativna svojstva ekstrakata su testirana na tri različite ćelijske linije: A-549; LS-174T i HeLa. Sadržaj ukupnih fenola je određen spektrofotometrijski. Ekstrakt lišća se odlikovao najvišim sadržajem ukupnih fenola (131.53 mg EHK/g), dok je nešto niži sadržaj određen u ekstraktima peteljke (49.96 mg EHK/g) i ploda (13.88 mg EHK/g). Ekstrakt ploda je pokazao najveći sposobnost inhibiranja holineseteraze i elastaze. Takođe, ekstrakt ploda zajedno sa ekstraktom lišća je pokazao i značajni citotokisčni efekat.

Combining multidirectional perspectives to explain functional properties of aronia (*Aronia melanocarpa)*: Chemical content and biological propensities

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The present study is aimed to characterize subcritical water extracts obtained from different plant parts (leaves, stems and berries) of *Aronia melanocarpa* in terms of biological and chemical fingerprints. For biological fingerprints, enzyme inhibitory and antiproliferative properties were investigated. Enzyme inhibitory effects were tested against cholinesterase and elastase. Antiproliferative properties were detected on three cell lines (lung carcinoma (A-549); human colorectal adenocarcinoma (LS-174T) and human cervix adenocarcinoma (HeLa)). For chemical fingerprints, total phenolic components were determined by spectrophotometric technique. Explored leaves extracts contained the highest level of total phenolics (131.53 mg CAE/g), followed by stems (49.96 mg CAE/g) and berries (13.88 mg CAE/g). Extract prepared from berries showed the strongest cholinesterase and elastase inhibitory activity. Similarly, the leaves and berries extracts showed considerable cytotoxic effects against tested cell lines. The study demonstrated possible utilization of plants and plant waste and their exploitation by green and safe technology.

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HTH P 02

Razlikovanje uzoraka suncokretovog ulja od ulja koštice kajsije i šljive primenom GC-MS metode

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Hladno ceđena ulja različitih biljnih vrsta postaju sve popularnija, kako na svetskom, tako i na domaćem tržištu, jer pored specifične arome sadrže i nutritivne komponente koje imaju pozitivno dejstvo na zdravlje čoveka. Međutim, zbog povišene cene, ovakvi proizvodi podložni su falsifikovanju i mešanju sa jeftinijim sastojcima. U ovom radu ispitan je stepen sličnosti između lipidnih profila hladno ceđenih ulja semena suncokreta i koštica kajsije i šljive, primenom GC-MS metode u kombinaciji sa multivarijantnom analizom. Tri uzorka jestivog ulja suncokreta (dva uzorka hladno ceđenog, S1 i S2, i jedan uzorak rafinisanog suncokretovog ulja, S3), dva uzorka hladno ceđenog ulja koštice kajsije (A1 i A2) i jedan uzorak hladno ceđenog ulja koštice šljive (P) dobijeni su sa Katedre za inženjerstvo konzervisane hrane, Tehnološkog fakulteta Novi Sad. Uzorci ulja derivatizovani su primenom rastvora reagensa TMSH (trimetilsulfonijum-hidroksid) u metanolu, analizirani na gasnom hromatografu, a potom su eluirajuće uljne komponente identifikovane primenom masene spektrometrije, poređenjem karakterističnih fragmentacija eluirajućih komponenata sa NIST14 i WILEY7 bibliotekama masenih spektara. Koristeći hijerarhijsku klaster analizu, kao multivarijantnu istraživačku metodu, utvrđen je visok stepen sličnosti između uzoraka hladno presovanih ulja koštica voća – kajsije i šljive, kao i mogućnost njihovog razlikovanja od botanički različitog hladno ceđenog ulja semena suncokreta.

Differentiation of sunflower oil samples from apricot and plum seed oil using the GC-MS method

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Cold-pressed oils of various plant species are becoming more and more popular both in the world and in the domestic market, because they contain, in addition to specific aromas, nutritional components that have a positive effect on human health. However, due to the increased price, such products are often subjected to adulteration and mixing with cheaper ingredients. In this paper, the degree of similarity between lipid profiles of sunflower oil and apricot and plum seed oils was examined, using the GC-MS method in combination with multivariate analysis. Three samples of edible oil of sunflower seeds (two samples of cold-pressed, S1 and S2, and one sample of refined sunflower oil, S3), two samples of cold-pressed apricot seed oil (A1 and A2) and one sample of cold-pressed plum seed oil (P) were obtained from the Department of Conservation of Food Engineering, Faculty of Technology Novi Sad. Oil samples were derivatized using a TMSH reagent solution (trimethylsulfonium hydroxide) in methanol, analyzed on a gas chromatograph, and then the eluting oil components were identified using mass spectrometry, by comparing characteristic fragmentation of the eluting components with NIST14 and WILEY7 mass spectra libraries. Using a hierarchical cluster analysis, as a multivariate exploratory data analysis tool, a high degree of similarity was found between samples of cold pressed fruit seed oils (apricot and plum), as well as the possibility of distinguishing them from botanically different cold-pressed sunflower seed oil.

HTH P 03

Uticaj dodatka etarskog ulja korijandera na mikrobiološku stabilnost barenih kobasica

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U ovom radu ispitan je uticaj dodatka etarskog ulja korijandera (CEO) na vrednost pH i mikrobiološku stabilnost barenih kobasica tokom 60 dana čuvanja. Proizvedene su 3 grupe kobasica: sa dodatkom CEO (0,075 i 0,150 µl/g) i kobasice kontrolne grupe. Mikrobiološki kvalitet kobasica praćen je preko: ukupnog broja aerobnih mezofilnih bakterija, *Salmonella* spp., *E. coli* i *L. monocytogenes*. Tokom 60 dana čuvanja u svim ispitanim uzorcima došlo je do značajnog smanjenja vrednosti pH. Dodatak etarskog ulja korijandera uticao je statistički značajno ($p<0,05$) na redukciju kolonija aerobnih mezofilnih bakterija. *Salmonella* spp., *E. coli* i *L. monocytogenes* ni u jednoj od ispitanih kobasica nisu izolovani. Rezultati ovoga rada ukazuju na značajan uticaj etarskog ulja korijandera na povećanje antimikrobne aktivnosti i produženje održivosti barenih kobasica.

The effect of coriandrum essential oil on the microbial stability of cooked pork sausages

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The effect of coriandrum essential oil (CEO) on the pH value and microbial stability of cooked pork sausages during 60 days of storage was evaluated. Sausages with two concentrations of CEO (0.075 and 0.150 µl/g) and control were prepared. The following microbial analyses were performed: total number of aerobic mesophilic bacteria *Salmonella* spp., *E. coli* and *L. monocytogenes*. Significant decrease of pH values was observed in all sausages after 60th day of storage. The addition of SEO significantly ($p<0.05$) reduced the growth of mesophilic bacteria in cooked pork sausages. For all examined sausages, *Salmonella* spp., *E. coli*, and *L. monocytogenes* were not detected. Hence, the results of this study showed significant antimicrobial activity of coriandrum essential oil and potential of its utilization in production of cooked pork sausages in order to prolong their shelf life.

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Hemija i tehnologija makromolekula
Chemistry and Technology of Macromolecules

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Hidrolitička degradacija i citotoksičnost razgranatih PCL poliestara sa različitim brojem grana

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Poli(ε-kaprolakton), PCL, razgranate strukture sa jasno definisanom arhitekturom, privlači sve veću pažnju kao nova vrsta biomaterijala. Spora degradacija linearnih PCL-a usled relativno visokog stepena kristaliničnosti može biti unapredjena sintezom razgranatih PCL polimera koji poseduju manju kristaliničnost. Razgranati PCL poliestri sa različitim brojem grana i dužinom grana PCL-a oko 5000 g/mol su uspešno sintetisani polimerizacijom otvaranja prstena ε-CL u masi, inicirane hidroksilnim grupama višefunkcionalnih alkohola (sa tri, četiri i šest -OH grupa), katalisane $Sn(Oct)_2$. Hidrolitička degradacija je testirana na različitim pH vrednostima, u fosfatnom puferu (pH 7,4) i u rastvoru HCl-a (pH 1,0) na 37 °C, tokom pet nedelja. Degradacija je praćena gravimetrijski, GPC i FTIR analizom. Sintetisani razgranati PCL poliestri su bili relativno stabilni tokom abiotske hidrolize na pH 7,4, dok je efikasna hidrolitička degradacija postignuta u kiseloj sredini. Za testove citotoksičnosti su korišćene normalne ćelije fibroblasta (MRC5), dok je procena embriotoksičnosti izvedena *in vivo* pomoću zebra-ribice (*Danio rerio*) modela. Testirani materijali nisu pokazali toksične efekte.

Hydrolytic degradation and cytotoxycity effects of star-shaped PCL polyesters with different number of arms

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Star-shaped poly(ε-caprolactone), PCL, polyesters with well defined architecture have been attracting more and more interest as a new type of biomaterials. Slow biodegradation rate of linear PCL due to the relatively high degree of crystallinity, could be significantly improved by application of their branched counterparts, with reduced crystallinity. Star-shaped PCL polyesters with different number of PCL arms and fixed PCL arms length (about 5000 g/mol) were successfully synthesized through the ring-opening polymerization (ROP) of ε-CL in bulk, initiated by hydroxyl groups of multifunctional alcohols (with three, four and six -OH groups), catalyzed by $Sn(Oct)_2$. Hydrolytic degradation was tested at different pH values, including phosphate buffer solution (pH 7.4) and HCl solution (pH 1.0) at 37 °C over five weeks. Degradation rate was followed gravimetrically, by GPC and FTIR analysis. Synthesized star-shaped PCL polyesters were quite stable against abiotic hydrolysis at pH 7.4, while the effective hydrolytic degradation was achieved in HCl solution. For the cytotoxicity tests normal human fibroblasts (MRC5) were used, while embriotoxicity assessment has been performed *in vivo* using the zebrafish (Danio rerio) model. There were no toxic effects of tested materials.

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HTM P 01

Sinteza kopolimera na osnovu laktida i polidimetilsiloksana

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Polilaktid (PLA) i polidimetilsiloksan (PDMS) se primenjuju u različitim granama industrije, pre svega zahvaljujući svojoj biorazgradivosti ili superhidrofobnosti. Neka od njihovih manje poželjnih svojstava, kao što je krtost PLA i neadekvatne mehaničke osobine PDMS, mogu biti prevaziđene formiranjem njihovog kopolimera. Cilj ovog rada je iskorišćenje dobrih osobina PLA i PDMS radi formiranja superhidrofobnog biorazgradivog elastomernog materijala. Tri-blok kopolimeri na bazi PDMS i PLA su sintetisani u dihlormetanu kao rastvaraču u prisustvu trifluorometan sulfonske kiseline kao katalizatora za katjonsku polimerizaciju laktida iniciranu –OH grupama PDMS-a. Variranjem molskog udela PDMS i laktida varirana je molska masa dobijenih blokova redom 4000, 6000 i 8000 g mol^{-1}. Infracrvenom spektroskopijom je potvrđeno da je do polimerizacije laktida došlo inicijacijom –OH grupama PDMS. Određivanjem OH broja potvrđena je dobra kontrola molske mase dobijenog kopolimera. DSC analizanom su ispitana termička svojstva dobijenih kopolimera i kao rezultat ustanovljeno je da ona zavise od molske mase i dužine blokova polilaktida. Kao konačna primena ovog kopolimera razmatrana je mogućnost formiranja superhidrofobnog biorazgradivog premaza koji bi trebalo da bude nosač za agrikulturne komponente za zaštitu i ishranu poljoprivrednih kultura.
Autori žele da se zahvale Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (projekti III45022) za finansijsku podršku.

Synthesis of copolymers based on lactide and polydimethilsiloxane

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The use of polylactide (PLA) and polydimethylsiloxane (PDMS) as separate materials is very wide in various branches of the industry. However, their mechanical properties, such as brittleness of PLA, or inadequate mechanical properties of the PDMS, can be overcome by making their copolymer. The aim of this work was to take advantage of PLA and PDMS in order to obtain superhydrophobic biodegradable elastomeric materials. A three-block copolymers based on PDMS and PLA were synthesized in dichloromethane, in the presence of trifluoromethane sulfonic acid as catalyst, for cationic polymerization of lactide initiated by –OH groups of PDMS. By varying the molar ratio of PDMS and lactide, the molar mass of the resulting blocks varies, ranging from 4000, 6000 and 8000 g mol^{-1}. Infrared spectroscopy confirmed that lactide polymerization was initiated by -OH groups of PDMS. Determination of the OH number of the copolymer confirmed good control of the molar mass of the obtained material. DSC analysis examined the thermal properties of the resulting copolymers which showed that they depend on the molar mass and the length of the blocks of polylactides. As the ultimate application of this copolymer, a superhydrophobic biodegradable coating is considered, which should be a carrier for agricultural components for the protection and nutrition of agricultural crops.

HTM P 02

Epoksidni nanokompoziti na bazi gline modifikovane poli(amidoaminom)

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Poslednjih godina gline su našle veliku primenu kao nanopunioci za pripremu višefunkcionalnih polimernih nanokompozita (NK). Za značajno poboljšanje termičkih, mehaničkih, barijernih i antikorozivnih svojstava polimernih NK neophodno je postići uniformnu raspodelu (eksfolijaciju) nanoslojeva gline u polimernoj matrici. Površinska modifikacija gline dovodi do porasta rastojanja između slojeva (interkalacija) i poboljšava kompatibilnost gline i polimera. U ovom radu ispitan je uticaj sadržaja (0,5–3 mas.%) organo-modifikovane gline na strukturu, propustljivost vodene pare, mehanička i antikorozivna svojstva epoksidnih NK na bazi diglicidil-etra bisfenola A. Komercijalni poli(amidoamin) je istovremeno korišćen kao modifikator gline i umreživač epoksidne smole. SEM i TEM analize su detektovale obrazovanje interkalarne/eksfolirane strukture u NK. Dodatak krutih čestica gline u epoksidnu matricu je povećao modul sačuvane energije u oblasti gumolikog ponašanja i temperaturu ostakljivanja, dobijeno DMA-om. Test istezanja je potvrdio porast zatezne čvrstoće pri kidanju i maksimalnog izduženja kod NK. Test propustljivosti je pokazao da se barijerni efekat gline u NK povećao sa porastom sadržaja gline. Najveći stepen korozione zaštite na čeliku je postignut korišćenjem NK sa 0,5 mas.% gline, pokazano EIS analizom.

Epoxy nanocomposites based on polyamidoamine modified clay

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In recent years clays were frequently applied as a nanofillers for multifunctional polymer nanocomposites (NC). In order to improve thermal, mechanical, barrier and anticorrosion properties of polymer NC it is necessary to achieve uniform distribution (exfoliation) of clay nanolayers in the polymer matrix. The surface modification of clay increases distance between stacked layers (intercalation) and serves as a compatibilizer between the clay and the polymer. In this study, the effect of loading (0.5–3 wt%) of organo-modified clay on structure, water vapor permeability, mechanical and anticorrosion properties of epoxy NCs based on diglycidyl ether of bisphenol A has been investigated. The commercial polyamidoamine was simultaneously applied as a clay modifier and curing agent for epoxy resin. The SEM and TEM analyses detected formation of an intercalated/exfoliated structure in NCs. The addition of rigid clay particles in epoxy matrix increased storage moduli in rubbery state and glass transition temperature, shown by DMA. The tensile test confirmed that ultimate tensile strenght and elongation at break of NC were increased. The permeability test showed that barrier effect of clay in NCs was improved by increasing clay loading. The highest degree of corrosion protection of steel was achieved by using NC with 0.5 wt% clay, revealed by EIS.

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Chitosan-based films for application in food industry

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Excessive use of synthetic food packaging polymers has led to a serious ecological problem, due to its non-biodegradability. Consequently, large amounts of waste are generated daily. For this reason, scientists' attention is focused on the development of biodegradable films based on polysaccharides.
In this work, films of chitosan (Ch) and poly(vinyl alcohol) (PVA) were prepared by solvent/casting method. Although PVA is a synthetic polymer, it is biocompatible, biodegradable and non-toxic, and addition of PVA can lead to the improvement of the Ch films properties. It has been found that with the increase of PVA content, the tensile strength of the films decreased and elongation at break increased, while the PVA content did not have a significant effect on the thermal properties. Also, Ch/PVA films have relatively high water vapor permeability, indicating that Ch/PVA films could be used as edible films, but further modifications have to be made in order to meet all the criteria required for the use as food packaging material.

Primena filmova na bazi hitozana u prehrambenoj industriji

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Prekomerna upotreba sintetskih polimera za pakovanje hrane je dovela do ozbiljnog ekološkog problema, jer takva pakovanja nisu biorazgradiva. Samim tim, dnevno se stvaraju velike količine otpada koji ugrožava životnu sredinu. Upravo iz tog razloga, pažnja naučnika je usmerena na razvoj biorazgradivih filmova na bazi polisaharida.
U ovom radu pripremljeni su filmovi hitozana (Ch) i poli(vinil alkohola) (PVA) metodom izlivanja iz rastvora i otparavanjem rastvarača. Iako je PVA sintetski polimer, on je biokompatibilan, biodegradabilan i netoksičan, a njegova primena dovodi do poboljšanja svojstava Ch filmova. Utvrđeno je da se sa povećanjem sadržaja PVA smanjuje zatezna čvrstoća filmova i povećava izduženje pri kidanju, dok sadržaj PVA nema značajan uticaj na termička svojstva. Takođe, Ch/PVA filmovi imaju relativno visoku propustljivost vodene pare. Navedena svojstva ukazuju da se ovi filmovi mogu koristiti kao jestivi, ali da je neophodna dalja modifikacija kako bi se zadovoljili svi kriterijumi za pakovanje hrane.

HTM P 04 text rada / full text

Glucose-sensitive chitosan/PVA microbeads with the potential application for the controlled release of insulin

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The aim of this research is to prepare glucose-sensitive microbeads that could imitate the function of pancreas in glucose level control and release of insulin in controlled manner. The microbeads were synthetized with chitosan (Ch) and poly (vinyl alcohol) (PVA) and crosslinked by boric acid and sodium tripolyphosphate. Swelling of hydrogels was studied in distilled water, PBS buffer and glucose/PBS solution, with concentration of glucose ranging from normoglycemic (100 mg dL^{-1}) to extremely hyperglycemic (400 mg dL^{-1}).
Ch/PVA hydrogels were found to be glucose-sensitive, but some of them have shown to be unsuitable for controlled insulin delivery, because they had a higher swelling degree in lower-concentration glucose solutions. The sample with Ch:PVA=5:1 ratio was chosen as most suitable to be used for controlled release of insulin due to the higher swelling degree with the increase of glucose concentration in solutions and was used for the preliminary insulin release test. The UV/VIS spectrophotometry revealed that insulin was released during 48 h, indicating that these hydrogels may potentially be used for the treatment of *Diabetes mellitus* and that further research in that area is necessary.

Mikrogelovi hitozana i PVA osetljivi na glukozu sa potencijalnom primenom za kontrolisano otpuštanje insulina

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Predmet ovog rada je sinteza hidrogelova osetljivih na glukozu koji mogu da kontrolisano otpuste glukozu i na taj način imitiraju funkciju pankreasa u kontroli nivoa glukoze. Hidrogelovi hitozana (Ch) i poli(vinil alkohola) (PVA) su sintetisani u obliku sfernih čestica umreženih bornom kiselinom i natrijum-tripolifosfatom. Ispitano je bubrenje dobijenih hidrogelova u destilovanoj vodi, fosfatnom puferu (PBS) i rastvoru glukoze u PBS-u, pri čemu je koncentracija glukoze varirana od normoglikemijske (100 mg dl^{-1}), do izrazito hiperglikemijskih koncentracija (400 mg dl^{-1}).
Utvrđeno je da su Ch/PVA hidrogelovi osetljivi na glukozu, ali pojedini su nepovoljni za kontrolisano otpuštanje insulina jer dostižu veći stepen bubrenja u rastvorima glukoze niže koncentracije. Kao najbolji za upotrebu u kontrolisanom otpuštanju insulina pokazao se uzorak sa odnosom Ch:PVA=5:1 zahvajujući većem stepenu bubrenja sa porastom koncentracije glukoze, pa je on korišćen za preliminarno ispitivanje otpuštanja insulina. UV/VIS spektrofotometrijom je utvrđeno da se insulin otpušta tokom 48 h, što ukazuje da se ovi hidrogelovi potencijalno mogu koristiti za lečenje *Diabetes mellitus* i da je neophodno sprovesti dalja istraživanja u toj oblasti.

HTM P 05

Dizajn svojstava hibridnih mreža hidrogelova na bazi kazeina i poli(metakrilne kiseline)

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Istraživanje je sprovedeno sa ciljem dizajna i ispitivanja svojstava hibridnih hidrogelova na bazi kazeina i poli(metakrilne kiseline) (PMAA). Osnovna ideja odnosi se na unapređenje svojstava PMAA hidgrogelova, koje se ostvaruje kroz sinergetski efekat nakon dodatka kazeinske komponente. Interakcije između proteina i suprotno naelektrisanih polielektrolita mogu biti dominantno elektrostatičke, vodonične i/ili hidrofobne i predstavljaju veoma složen fenomen. Parametri bubrenja, dinamičko-mehanička i morfološka svojstva sintetisanih hidogelova ispitana su u zavisnosti od stepena neutralizacije metakrilne kiseline, koncentracije kazeina i umreživača. Utvrđeno je da upravo različite interakcije usostavljene u sistemu dovode do formiranja različitih strukturnih oblika kazeina (od micela do razvijenih lanaca), što u velikoj meri utiče na svojstva dobijenih materijla.

The design properties of casein-poly(methacrylic acid) hybrid hydrogel networks

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The aim of the present study was to design and evaluate the properties of hybrid hydrogels based on casein and poly(methacrylic acid) (PMAA). The guiding principle of the research was the improvement of the single PMAA hydrogels performance by coupling its basic properties with casein. The interactions between proteins and oppositely charged polyelectrolytes could be dominantly electrostatic, hydrogen and/or hydrophobic and represent very complex phenomenon. The swelling, dynamic-mechanical and morphological properties of obtained hybrid networks were investigated as functions of the neutralization degree of methacrylic acid and the concentrations of casein and crosslinker. It was shown that the domination of different interactions between components leads to diverse forms of casein macromolecules (from micelles to unfold chains) and dictates the properties of the material in general.

HTM P 06

Novi kompozitni materijali na bazi bio-obnovljivih nezasićenih poliestarskih smola i otpadnog poli(etilen teraftalata)

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U ovom radu su prvi put ispitani novi kompozitni materijali na bazi nezasićenih poliestarskih smola (NPS), dobijenih iz bio-obnovljivih izvora, i otpadnog poli(etilen teraftalata) (PET). Ojačavajuće čestice PET-a su dobijene postupkom aminolize (1,6-diamino heksan i 3,6-dioksa-1,8-diaminooktan) vlakana otpadnog PET-a. Amino funkcionalizovani PET je dalje modifikovan itakonil hloridom radi uvođenja dvostruke veze na površinu PET-a. Kompoziti su pravljeni umrežavanjem smole sa dimetil itakonatom u prisustvu čestica PET-a (3, 6 i 9 mas%). Dobijeni rezultati su pokazali da dodatak PET čestica dovodi do poboljšanja mehaničkih karakteristika. Ipak, pri većem udelu PET-a dolazi do smanjenja mehaničkih karakteristika usled aglomerizacije PET čestica. Kompozitni materijali su imali niže vrednosti koeficijenta termalnog širenja i više vrednosti temperature ostakljivanja usled većeg umreženja. Ovi rezultati su ukazali na dobru kompatibilnost između NPS i funkcionalizovanih čestica PET-a.

New composite materials from bio-based unsaturated polyester resins and waste poly(ethylene terephthalate)

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In this work new composites obtained from fully bio-based unsaturated polyester resin (UPR) and waste poly(ethylene terephthalate) (PET) were studied for the first time. Reinforcing PET particles were prepared throughout aminolysis of waste PET fibers with diamines (1,6-diaminohexane and 3,6-dioxa-1,8-diaminooctane). The amino functionalized PET was further modified using itaconyl chloride to introduce double bond functionality to the PET surface. The composites were prepared by crosslinking the UPR in the presence of functionalized PET particles (3, 6 and 9 wt%), using dimethyl itaconate as reactive diluent. The results showed that the incorporation of the PET particles led to the increase in mechanical properties. However, higher PET loading caused a decrease in the mechanical properties of the composites because of the PET particle agglomeration. The composites showed lower coefficient of thermal expansion, and an increase of the glass transition temperature due to the higher degree of crosslinking. These observations indicate a good compatibility between the UPR and functionalized PET particles.

Medicinska hemija / Medicinal Chemistry

MH P 01

Uticaj kompleksa rutenijuma(II) sa trifluoperazinom na oksido-redukcione procese u ćelijama humane leukemije

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Kompleks rutenijuma(II) sa trifluoperazinom TF.2H[$RuCl_3(DMSO)_3$], gde je TF.2H protonovani trifluoperazin, u koncentracijama 10 i 15 μM, ispitan je na oksido-redukcione procese na proteinima i lipidima (sadržaj karbonilnih (CO) grupa i malondialdehida (MDA)) i aktivnost enzima antioksidativne odbrane (superoksidne-dismutaze (SOD) i katalaze (CAT)) u zdravim humanim ćelijama HS-5, kao i ćelijama humane leukemije THP1, K562 i Hel. Primenom 10 μM kompleksa zabeležena je povećana aktivnost SOD i CAT, kao i veći sadržaj MDA i slobodnih CO grupa u THP1 ćelijama. U koncentraciji od 15 μM kompleks povećava aktivnost SOD za 37 % u odnosu na kontrolnu grupu u Hel ćelijama, u kojima izaziva i najveće oštećenje proteina praćenjem sadržaja CO grupa. Povećan sadržaj MDA primenom obe koncentracije kompleksa rutenijuma posledica je visokog procenta lipidne peroksidacije u ćelijama kancera, dok u HS-5 ćelijama ima zaštitni efekat. Sadržaj MDA i povećana aktivnosti SOD primenom kompleksa u svim tretiranim ćelijama u odnosu na kontrolnu grupu, rezultat je veće produkcije reaktivnih kiseoničnih vrsta i oksidativnog stresa, što dovodi do nekroze i apoptoze ćelijskih linija humane leukemije.

The effect of ruthenium(II) complex with trifluoperazine on the oxidation-reduction processes in human leukemic cells

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Ruthenium(II) complex with trifluoperazine TF.2H [$RuCl_3(DMSO)_3$], where TF.2H is protonated trifluroperazine, applied in concentrations of 10 and 15 μM, are investigated on the oxidation-reduction processes in proteins and lipids (carbonyl (CO) group and malondialdehyde content (MDA)) and activities of enzymes antioxidative defenses (superoxide dismutase (SOD) and catalase (CAT)) in normal human cells HS-5 and human leukemic cells, THP1, K562 and Hel. Using 10 μM of the complex is increased activity of SOD and CAT, as well as higher content of MDA and free CO groups in THP1 cells. Ruthenium complex increased 37 % of the SOD activity in compared to the control group in concentration of 15 μM and shows high damage on CO groups of proteins in Hel cells. The higher MDA level by applying both concentrations of the ruthenium complex results from a great degree of lipid's peroxidation in cancer cells, while in HS-5 cells it has protective effect. Content of MDA and increased activity of SOD by the complex in all treated cells compared to the control group is the result of higher production of reactive oxygen species and oxidative stress, which leads to necrosis and apoptosis in cell lines of human leukemia.

MH P 02

Dobijanje i antiproliferativna aktivnost 7-*O*-metil-7-*epi*-goniofufurona

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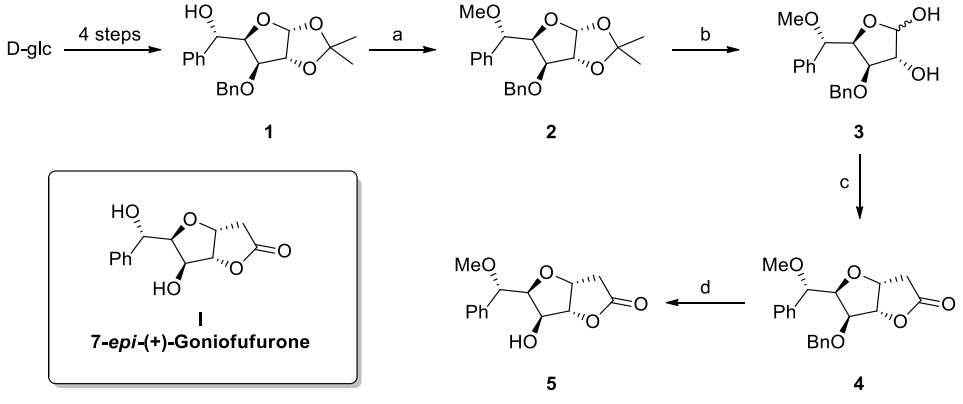
Ostvarena je višefazna sinteza 7-*O*-metil derivata 7-*epi*-(+)-goniofufurona (**I**) (jedinjenje **5**) koji pokazuje značajnu antiproliferativnu aktivnost. Benzilni alkohol **1**, koji se lako dobija iz D-glukoze, preveden je u željeni analog **5** četvorofaznom sekvencom koja je prikazana na reakcionoj shemi. Ispitana je *in vitro* antiproliferativna aktivnost dobijenog analoga na nekoliko odabranih malignih ćelijskih linija, kao i na normalnim ćelijama fetalnih fibroblasta pluća (MRC-5).



Reagents and conditions: (a) NaH, MeI, DMF, 0 °C→rt, 2 h, 94%; (b) 90% aq TFA, rt, 0.5 h, 99%; (c) Meldrum's acid, Et_3N, DMF, 46 °C, 68 h, 47%; (d) H_2-Pd/C, MeOH, 24 h, 68%.

Synthesis and antiproliferative activity of 7-*O*-methyl-7-*epi*-goniofufurone

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A multi-step synthesis of 7-*O*-methyl derivative of 7-*epi*-(+)-goniofufurone (**I**) (compound **5**) that shows a significant antiproliferative activity, has been achieved. Benzylic alcohol **1**, which is readily obtained from D-glucose, was converted to the desired analogue **5** by the four-step sequence outlined in the reaction scheme. I*n vitro* antiproliferative activity of analogue **5** was evaluated against several malignant cell lines, and against a single normal cell line (foetal lung fibroblasts, MRC-5).

Acknowledgement: *This work was supported by a research grant from the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 172006), and (in part) by a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).*

MH P 03

N-supstituisani 4-aminohinolini dugog niza kao novi quorum sensing inhibitori kod *Seratia marcescens*

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Razvoj bakterijske rezistencije prema antibioticima može izazvati globalnu zdravstvenu krizu. Iz tog razloga je neophodno razviti nov pristup u tretmanu bakterijskih infekcija. Quorum-sensing (QS) je složen sistem međubakterijske komunikacije koji kontroliše glavne virulentne karakteristike uključujući kretanje i formiranje biofilmova (BF). Razvoj malih molekula koji ometaju QS je nova perspektivna strategija u borbi protiv bakteriskih infekcija, sa smanjenom pojavom rezistencije. *S. marcescens* je pathogen prisutan u bolnicama, posebno je prisutna kod kateterskih i urinarnih infekcija i infekcija površinskih rana.

Po prvi put je opisana anti-QS aktivnost kod *S. marcescens* serije novih derivata 4-aminohinolina (4-AQ). Najaktivniji derivati su 4-AQ dugog niza koji inibiraju BF do 70 % pri 50 μM koncentraciji i imaju IC_{50} = 20 μM i pokazuju jaku inhibiciju rojevitog kretanja pri 50 μM koncentraciji. Jedinjenja ne pokazuju baktericidnu aktivnost (MIC ≥ 4 mM) i nisu toksični do koncentracije od 100 μM na modelu nematode *Caenorhabditis elegance*.

Zahvalnica: *Ova istraživanja su podržana od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat br. ON172008 i ON 173048) i CRP – ICGEB Research Grants Programme 2016 (projekat br. CRP/SRB16-02).*

N-substituted long-chain 4-aminoquinolines as new quorum sensing inhibitors in *Seratia marcescens*

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Developing of a bacterial resistance to clinically used antibiotics could evolve into a global health crisis. For that reason, new and innovative strategies for antibacterial treatment is urgently required. Quorum-sensing (QS) is sophisticated density-dependent communication system responsible for controlling most of bacterial virulence characteristics, including motility and biofilm formation (BF). Developing of small molecules that interfere with QS is one of the new promising strategies to combat bacterial infections, with low possibility to develope resistance. *S. marcescens* is a nosocomial pathogen, particularly involved in catheter-associated bacteremia, urinary tract infections and wound infections.

We described, for the first time, the series of a highly active new 4-aminoquinoline (4-AQ) derivatives with anti-QS activity in *S. marcescens*. The most active long chain 4-AQ show up to 70 % of BF inhibition at 50 μM concentration and $BICF_{50}$ = 20 μM. Also, derivatives showed strong inhibition of swarming when applied at 50 μM. Compounds did not show bactericidal activity (MIC ≥ 4 mM) and are not toxic at concentrations up to 100 μM in nematode *Caenorhabditis elegance*.

Acknowledgments: *This research were supported by the Ministry of education, science and technological development of the Republic of Serbia (project ON172008 and ON 173048) and CRP – ICGEB Research Grants Programme 2016 (grant No CRP/SRB16-02).*

MH P 04

Sinteza i *in vitro* antitumorska aktivnost novih mimetika goniofufurona sa tiofenskim prstenom na položaju C-7

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Ostvarena je višefazna sinteza novih mimetika (+)-goniofufurona (**1**) sa tiofenskim prstenom umesto fenil grupe u položaju C-7 polazeći iz D-glukoze (Shema 1). Ispitana je *in vitro* citotoksična aktivnost novosintetizovanih mimetika prema odabranim tumorskim ćelijskim linijama, kao i prema jednoj normalnoj ćelijskoj liniji (fetalni fibroblasti pluća, MRC-5).

Synthesis and *in vitro* antitumour activity of new goniofufurone mimics with thiophene ring at the C-7 position

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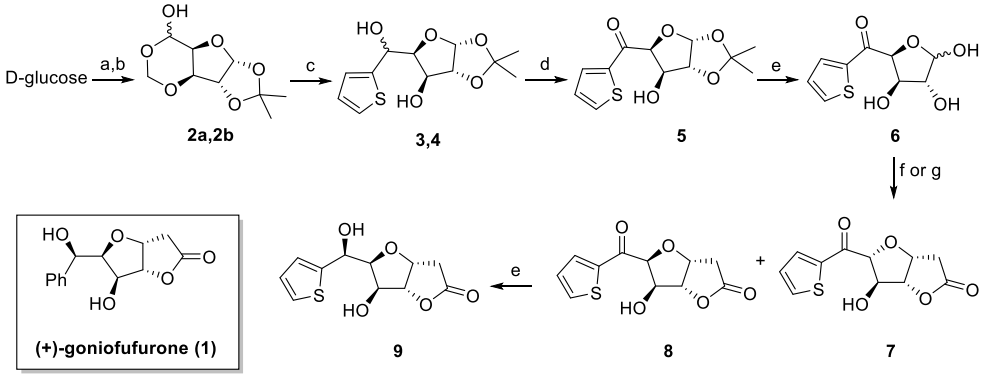
Multiphase synthesis of (+)-goniofufurone (**1**) mimetics with thiofene ring instead of phenyl group at the C-7 position is completed using D-glucose as a starting compound (Scheme 1). *In vitro* cytotoxicity of newly synthetized analogues against eleven human tumour cell lines and against a single normal cell line (MRC-5) was evaluated.



Scheme 1. Reagents and conditions: (a) conc. H_2SO_4, anh. Me_2CO, ≤10 °C→rt, (b) H_5IO_6, anh. EtOAc, rt; (c) C_4H_3SMgBr, anh. THF, 0 °C→rt., (d) AcCl, Py, rt; (e) 90 % TFA, 0 ºC→rt.; (f) Meldrum's acid, DMF, Et_3N, 46−48 °C; (g) MCMP, aps. MeOH, rt; (e) L-tartaric acid, $NaBH_4$, anh. THF, ↓↑.

The work was supported by the Ministry of Education, Science and Technological Development (Project 172006).

MH P 05

Sinteza i antiproliferativna aktivnost 7-*O*-cinamoil 4,6-di-*O*-benzilovanih analoga (–)-kleistenolida

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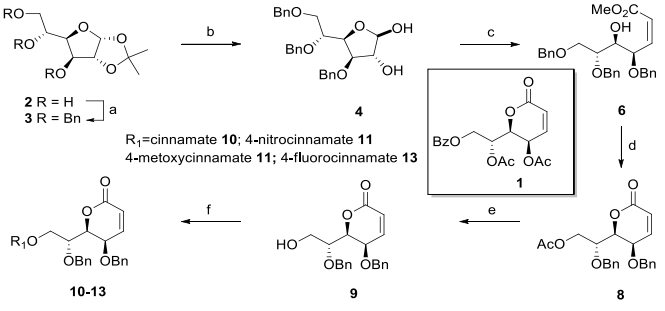
Ostvarena je sinteza 7-O-cinamoil derivata 4,6-dibenzilovanih analoga (**10**–**13**) prirodnog proizvoda (−)-kleistenolida (**1**) primenom višefazne sintetičke sekvence koja je prikazana na reakcionoj shemi. Ključnu fazu sinteze predstavlja (*Z*)-selektivna Wittig-ova olefinacija laktola **4** sa stabilizovanim ilidom MCMP. Ispitana je antiproliferativna aktivnost sintetizovanih analoga (**8**–**13**) prema panelu humanih tumorskih ćelijskih linija.



Reagents and conditions: (a) BnBr, NaH, DMF, 0 °C, rt; (b) aq 50% TFA, rt; (c) (*i*) $NaIO_4$, MeOH, rt; (*ii*) MCMP, rt; (d) (*i*) TsOH, CH_2Cl_2, rt; (*ii*) Ac_2O, AcOH, $FeCl_3$, rt; (e) TsOH, MeOH, rt; (f) cinnamic acid, DCC, DMAP, CH_2Cl_2, rt.

Synthesis and antiprolifetive activity 7-*O*-cinnamoyl 4,6-di-*O*-benzylated analogues of (–)-cleistenolide

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Synthesis of 7-O-cinnamoyl derivatives of 4,6-dibenzylated analogues of natural product (−)-cleistenolide (**1**) has been achieved through a multi-step sequence outlined in the reaction scheme. The key step of the synthesis was a (*Z*)-selective Wittig olefination of **4** with a stabilized ylide, MCMP. Synthesized analogus (**8**–**13**) were evaluated for their antiproliferative activity against a panel of human tumour cell lines.

Acknowledgement*: The work was supported by a grant from the Ministry of Education, Science and Technological Development (Project 172006).*

MH P 06

Sinteza, kristalna i molekulska struktura novog analoga kleistenolata

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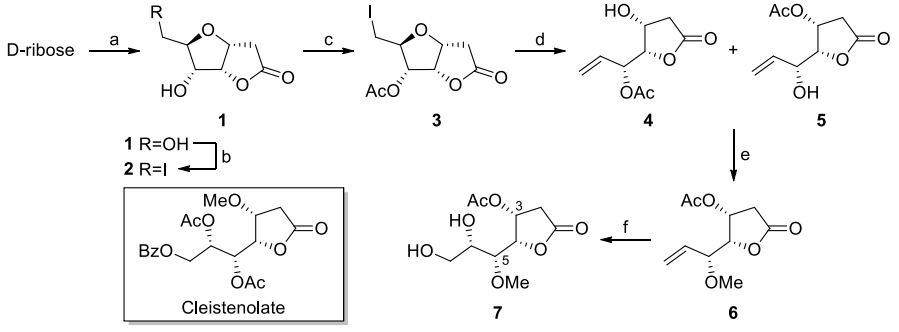
Kleistenolat je prirodni proizvod izolovan iz listova subtropske biljke *Cleistochlamys kirkii* (Benth.) Oliv., Annonaceae.[1] U ovom saopštenju želimo da prikažemo asimetričnu sintezu, kristalnu i molekulsku strukturu analoga kleistenolata **7** sa zamenjenim funkcionalnim grupama na položajima C-3 i C-5, polazeći od komercijalno pristupačne D-riboze (Shema 1).



Scheme 1. (a) Meldrum's acid, $^{t}BuNH_2$, dry DMF; (b) I_2, Imidazole, Ph_3P, dry THF; (c) AcCl, DMAP, dry CH_3CN; (d) Zn dust, dry THF; (e) Ag_2O, MeI, AgOTf, dry Et_2O (from **4** or **5** or **4**+**5**); (f) 2.5 wt% OsO_4, NMO, 10:1 Me_2CO/H_2O.

Synthesis, crystal and molecular structure of a novel cleistenolate analogue

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Cleistenolate is a natural product isolated from leaves of subtropical plant *Cleistochlamys kirkii* (Benth.) Oliv., Annonaceae.[11] Herein, we present asymmetric synthesis as well as crystal and molecular structure of a cleistenolate analogue **7** with exchanged functional groups at the C-3 and C-5 positions, starting from the commercially available D-ribose (Scheme 1).

Acknowlegdement: *The work was supported by a grant from Ministry of Education, Science and Technological Development (Project 172006).*

1. S. S. Nyandoro, J. J. E. Muniss, A. Gruhonjic, S. Duffy, F. Pan, R. Puttreddy, J. P. Holleran, P. A. Fitzpatric, J. Pelletier, V. M. Avery, K. Rissanen, M. Erdélyi, *Journal of Natural Products* **80** (2017) 114–125.

MH P 07 text rada / full text

Zavisnost između osobina molekula lekova koji imaju antihipertenzivno dejstvo i njihovog vezivanja za proteine plazme

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Hipertenzija, odnosno povišeni krvni pritisak danas predstavlja jedno od veoma čestih hroničnih oboljenja i antagonisti receptora angiotenzina II (*ARBs*), inhibitori enzima koji konvertuje angiotenzin (ACEI) i blokatori kalcijumovih kanala (CCBs) predstavljaju često propisivane lekove za sniženje pritiska. Cilj rada bio je da se za dvadesetšest lekova koji imaju antihipertenzivno dejstvo iz tri različite grupe (deset ACEI, sedam *ARBs,* devet CCBs) ispita odnos osobina molekula i vezivanja za proteine plazme. Za sve ispitivane antihipertenzive, primenom softverskih paketa izračunate su vrednosti molekulskih deskriptora: polarna površina, molekulska masa, volumen i različiti deskriptori lipofilnosti (logP). Primenom proste linearne regresione analize najbolja zavisnost (R^2 = 0,72) dobijena je između podataka o vezivanju za proteine plazme odabranih molekula i njihovih milogP vrednosti. U nastavku istraživanja ispitana je zavisnost polarne površine, molekulske mase, volumena i vezivanja za proteine plazme. Najbolja korelacija dobijena je primenom višestruke regresione analize između podataka o vezivanju za proteine plazme, lipofilnosti i polarne površine odabranih molekula (R^2 = 0,76; P < 0,05). Dobijeni rezultati ukazuju na značajnu zavisnost osobina molekula i vezivanja za proteine plazme za lekove koji imaju antihipertenzivno dejstvo i pripadaju različitim grupama.

The relationship between molecular properties of different selected antihypertensive drugs and their plasma protein binding

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**Faculty of Medicinal Science, University of Kragujevac, Serbia*

Hypertension is today one of the most common chronic diseases and angiotensin II receptor antagonists/blockers (ARBs), angiotensin-converting enzyme inhibitors (ACEI) or calcium channel blockers (CCBs) are commonly prescribed antihypertensive drugs. The aim of this work was to investigate twenty-six antihypertensive drugs from different groups (ten ACEI, seven ARBs, nine CCBs) for relationships between literature available plasma protein binding data and their molecular properties. The molecular descriptors, polar surface area, molecular mass, volume and lipophilicity descriptors (log*P*) of selected antihypertensives were calculated using software packages. Simple linear regression analysis showed the best correlation (R^2=0.72) between plasma protein binding of selected drugs and their lipophilicity descriptor milog*P*. Following, multiple linear regression analysis was applied to investigate further correlations between other calculated molecular properties and plasma protein binding data. The best correlation was established between plasma protein binding data and milog*P* with the polar surface area as the independent variable (R^2=0.76; P<0.05). The results obtained indicate a significant association between plasma protein binding and molecular properties of antihypertensive drugs from different groups.

Acknowledgments: *This work was supported in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia as a part of Projects TR34031.*

MH P 08

Sinteza i antitumorski potencijal pentacikličnih androstanskih D-homo laktona

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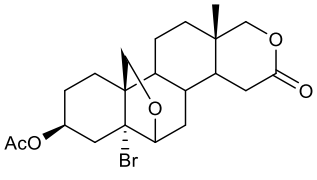
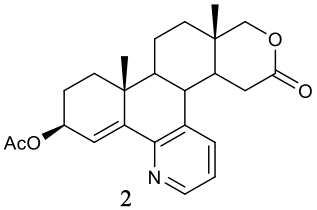
U cilju dobijanja selektivnih antitumorskih agenasa sintetizovani su novi pentaciklični androstanski D-homo laktoni. Kao polazna jedinjenja upotrebljeni su C-6 derivatizovani steroidi. Polazeći od 5α-bromo-6β-hidroksi androstanskog D-homo laktona dobijen je 6,19-premošćeni derivat **1**, sa kondenzovanim tetrahidrofuranskim prstenom. Kada je kao polazno jedinjenje upotrebljen androstanski derivat sa C-6 keto grupom dobijen je B-kondenzovani piridinski derivat **2**. Ispitivanje oralne bioraspoloživosti novih jedinjenja je izvršeno poređenjem sa pravilima Lipinski-og, Veber-a i Oprea-e. Takođe je ispitana antiproliferativna aktivnost na šest tumorskih i jednoj zdravoj humanoj ćelijskoj liniji. Dalje je u cilju utvrđivanja molekulskih osnova antiproliferativne aktivnosti urađen virtuelni skrining upotrebom ChemMapper3D.



1



2

Synthesis and antitumor potential of androstane pentacyclic D-homo lactones

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In order to obtain selective antitumour compounds, pentacyclic steroidal D-homo lactones were synthesized. C-6 derivatized steroidal compounds were used as starting compounds. 6,19-Bridged steroid **1**, containing tetrahydrofuran ring, was synthesized from 5α-bromo-6β-hydroxy androstane derivative. Starting from C-6 keto derivative, B-condensed androstane pyridine derivative **2** was obtained. Oral bioavailability of these compounds was assessed by comparing calculated molecular properties with the criteria for Lipinski, Veber and Oprea rules. Antiproliferative activity was tested against six cancer and one healthy human cell line. In order to investigate molecular basics of antiproliferative activity, virtual screening using ChemMapper3D was conducted.

Authors would like to thank the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 172021) for financial support.

MH P 09

Potencijalno antimetastatsko i antiproliferativno dejstvo derivata benzotiazola na ćelije embrionalnog humanog teratokarcinoma NT2/D1

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Naše istraživanje u oblasti sinteze novih derivata benzotiazola i njihove antiproliferativne aktivnosti na ćelije tumora, nastavili smo ispitivanjem uticaja ovih jedinjenja na proliferaciju NT2/D1 ćelija embrionalnog humanog teratokarcinoma. NT2/D1 ćelije predstavljaju pogodan model za testiranje potencijalnih citoreduktivnih terapeutika jer imaju patofiziološke osobine testikularnih tumora i pokazuju ekstremnu osetljivost na citotoksične agense.[1] Derivati benzotiazola smanjuju proliferaciju NT2/D1 ćelija *in vitro* indukujući masovno odlepljivanje ćelija sa podloge praćeno apoptozom. Gubitak sposobnosti za adheziju, koji nije praćen apoptozom, predstavlja rizik za metastatsko širenje tumora.[2] U tom kontekstu, ispitali smo i pokazali značajno smanjenje migratornog i invazivnog potencijala, kao i inhibiciju formiranja i rasta kolonija NT2/D1 ćelija posle tretmana derivatima benzotiazola.

Potential antimetastatic and antiproliferative activity of benzothiazole derivatives against NT2/D1 embryonal human teratocarcinoma cell line

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Our research towards the investigation of new benzothiazole derivatives' antiproliferative properties and possible mechanism of anticancer activity continued with an examination of their influence on embryonal human teratocarcinoma cell line NT2/D1. NT2/D1 cells with pathophysiological features of testicular tumors and extreme sensitivity to cytotoxic agents, present suitable model system for testing potential cytoreductive therapeutics.[1] Novel benzothiazole derivatives decreased cell viability and proliferation *in vitro*, inducing massive cell detachment followed by apoptosis. The loss of cell anchorage not followed by apoptosis could lead to metastasis.[2] Consequently, we examined and showed significant inhibition of NT2/D1 cells' migration and invasion, as well as colony forming and colony growing suppression after treatment with benzothiazole derivatives.

Acknowledgment: *This research was supported by the Ministry of Education, Science and Technological Development of Serbia (grant no. 172008)*

1. H. Burger, K. Nooter, A. W. M. Boersma, C. J. Kortland, G. Stoter, *Br. J. Cancer* **77** (1998), 1562.
2. C. D. Simpson, K. Anyiwe, A.D. Schimmer, *Cancer Lett*. **272** (2008), 177.

MH P 10

Odnos strukture i reaktivnosti i biološka aktivnost kamfor derivata *bis*-pirazolpiridinskih kompleksa Rh(III)

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Kinetički inertni kompleksi prelaznih metala, kao što su Rh(III) kompleksi, privlače sve veću pažnju za razvoj potencijalnih farmakoloških sredstava za lečenje bolesti zbog njihove inertnosti i stabilnosti [1]. 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. Kao dodatak urađena su DFT izračunavanja.

Navedeno istraživanje je finansiski pomoglo Ministarstvo prosvete, nauke i tehnološkog ražvoja projekat broj 172011.

Structure–reactivity relationship and biological activity of the camphor-derived of the bis-pyrazolylpyridine Rh(III) complexes

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Kinetically-inert transition metal complexes, such as Rh(III) complexes have attracted increasing attention as leading scaffolds for the development of potent pharmacological agents for disease treatment due to their inertness and stability [1]. Therefore we have designed and fully characterized a two new Rh(III) complexes with camphor-derived of the *bis*-pyrazolylpyridine ligands.The substitutive reactions with biomolecules were studied and the interaction ability with CT-DNA and protein bovine serum albumin were examed. The impact of the metal complex on cytotoxicity was tested by MTT assay on HCT-116 line. As well as DFT calculation was performed.

1. S. Medici, M. Peana, V-M. Nurchi, J. Lachowicz, G. Crisponi, M-A. Zoroddu, *Coord. Chem. Rev*., **284** (2015) 329-350.

Organska hemija / Organic Chemistry

OH P 01

Od monosaharida do polifunkcionalizovanih ketona

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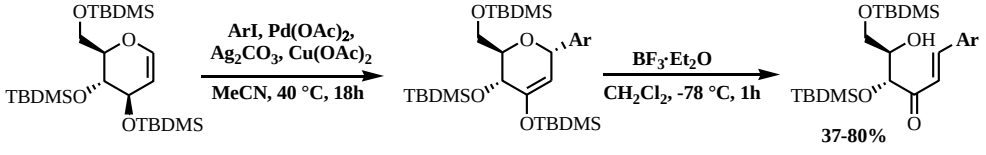
U ovoj studiji prikazana je reakciona sekvenca koja omogućuje dobijanje visoko funkcionalizovanih ketona polazeći iz monosaharidnih derivata. Primenom Hekove reakcije[1] na glikale i naknadnim otvaranjem dihidropiranskog prstena u prisustvu bor-trifluorida dobijaju se hiralni polifunkcionalizovani ketoni koji mogu biti korisna polazna jedinjenja u sintezi složenih molekula.



From monosaharids to polyfunctionalised ketones

Predrag Jovanović, Dragiša Obradović, Gordana Tasić, Milena Simić, Miloš Jovanović, Miloš Petković, Vladimir Savić
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In this report we describe the reaction sequence for the synthesis of highly functionalised ketones, starting from monosaccharide derivatives. Heck reaction is utilised to derivatise glycals followed by dihydropyran ring opening in the presence of boron trifluoride diethyl etherate. This gives access to polyfunctionalized ketones which can be useful starting compounds in the synthesis of complex molecules.

Acknowledgements: *This research was supported by the Ministry of Education, Science, and Technological development of Serbia (Grant 172009)*

1. Hou-Hua Li, Xin-Shan Ye, *Org. Biomol. Chem.*, **2009**, 7, 3855–3861.

OH P 02

Cikloadicione reakcije β-ketoestara na fuleren C_{60}

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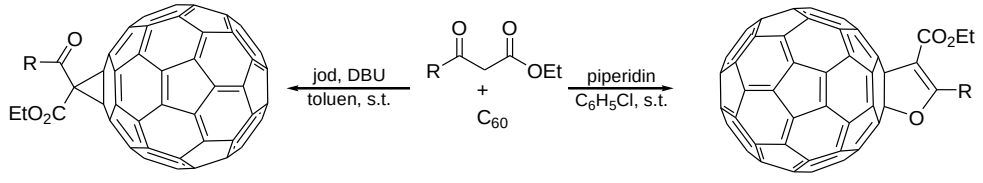
U cilju dobijanja novih derivata fulerena koji se mogu primeniti za dobijanje materijala i biološki aktivnih molekula, proučavane su cikloadicione reakcije različitih β-ketoestara i C_{60}. Tokom ovih istraživanja utvrđeno je da se u zavisnosti od primenjenih reakcionih uslova dobijaju strukturno različiti proizvodi.[1,2] Metanofulereni, poznati kao Bingel-ovi adukti, dobijeni su reakcijom fulerena i β-ketoestara u prisustvu joda i 1,8-diazabiciklo[5,4,0]undec-7-ena (DBU) u toluenu na sobnoj temperaturi. Kada se reakcija izvodi sa piperidinom kao bazom u hlorbenzenu na sobnoj temperaturi dobijeni su dihidrofuranofulereni.



metanofuleren ***dihidrofuranofuleren***

Cycloaddition reactions of β-keto esters on the fullerene C_{60}

Jovana Jakšić*, Zorana Tokić-Vujošević**, Aleksandra Mitrović*,
Jasmina Nikodinović-Runić***, Dragana Milić*, Veselin Maslak*
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***University of Belgrade-Faculty of Pharmacy, Vojvode Stepe 450, Belgrade, Serbia,*
****Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Vojvode Stepe 444a, Belgrade, Serbia*

In order to develop new derivatives of fullerenes which could be used as new materials and bioactive compounds, we have explored cycloadition reactions of the fulerene with different β-keto esters. During these studies it was found that different reaction conditions resulted in formation structurally different products.[1,2] Methanofullerenes, known as Bingel adducts, were prepared in the reaction of the fullerene and β-keto esters in the presence iodine and 1,8-diazabicyclo [5,4,0]undec-7-ene (DBU) in toluene at room temperature. When reactions were performed with piperidine as a base in chlorobenzene at room temperature, C_{60}-fused dihydrofuran derivatives were obtained.

1. J.-F. Nierengarten, D. Felder, J.-F. Nicoud, *Tetrahedron Lett.* **1998,** *39,* 2747
2. S. Chen, Z.-J. Li. X. Gao, *J. Org. Chem.* **2016**, *81*, 121

OH P 03

Sinteza novih steroidnih *N*-heterocikala

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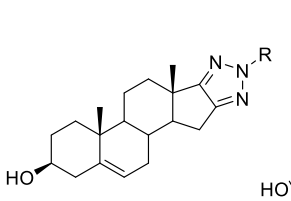
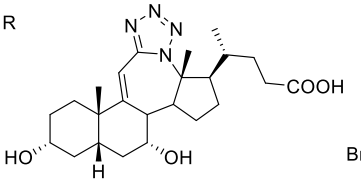
Veliki broj značajnih prirodnih i sintetskih steroida sadrže jedan ili više heterociklični prsten kondenzovan sa steroidnim skeletom ili formiran modifikacijama bočnog niza. Pošto poseduju značajan potencijal za primenu u farmaciji, steroidi koji sadrže azot interesantan su cilj u organskoj sintezi.
U ovom radu predstavljene su sinteze novih steroidnih derivata tetrazola, triazola i oksazolina. Jedinjenja **1** i **2** dobijena su iz dehidrepiandrosterona, dok su jedinjenja **3** i **4** sintetisana polazeći od holne kiseline.
Strukture svih jedinjenja prikazanih u ovom radu potvrđene su spektroskopskom analizom.



1 R = Me
2 R = Bu



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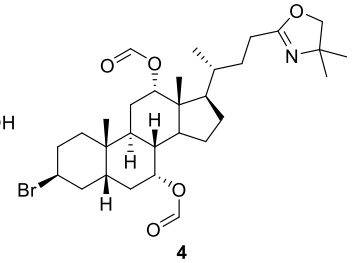

4

Syntheis of some new steroidal *N*-heterocycles

Dušan Đ. Škorić, Andrea R. Nikolić, Srđan I. Bjedov, Marija N. Sakač, Janoš J. Čanadi
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Many important naturally occurring and synthetic steroids contain one or more heterocyclic rings, fused to steroidal skeleton or formed by modifications of the side chain. Due to their great potential in pharmaceutical application, such nitrogen containing steroidal compounds are very interesting targets for synthetic chemists.
In this work we present the synthesis of some new steroidal tetrazole, triazole and oxazoline derivatives. Compounds **1** and **2** are obtained from dehydroepiandrosterone while compounds **3** and **4** were synthesized from cholic acid.
Structures of all compounds reported in this work were confirmed by spectroscopic analysis.

Realizacija ovog rada finansirana je iz sredstava projekata OI 172021

OH P 04

Intramolekulski prenos naelektrisanja kod derivata 5-ariliden-3-supstituisanih-2,4-tiazolidindiona

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Derivati tiazolidin-2,4-diona (TZD) privlače značajnu pažnju istraživača zbog različitih sintetičkih mogućnosti, brojnih farmakoloških svojstava i bioloških aktivnosti. Uticaj supstituenata i rastvarača na intramolekulski prenos naelektrisanja (ICT) kod 5-ariliden-3-metil-2,4-tiazolidindiona i 5-ariliden-3-fenil-2,4-tiazolidindiona je proučavan pomoću eksperimentalne i teoretske metodologije. Uticaj rastvarača i supstituenata na ICT je procenjen korišćenjem LSER i LFER metoda primenjenih na eksperimentalne podatke. Eksperimentalni rezultati su interpretirani uz pomoć *ab initio* MP2 i TD-DFT metoda. Dodatna TD-DFT izračunavanja su urađena da bi se kvantifikovala efikasnost ICT omogućavajući da se definiše razdaljina prenosa (D_{CT}), količina prenešenog naelektrisanja (Q_{CT}), i razlika između dipolnih momenata osnovnog i pobuđenog stanja (μ_{CT}). Nađeno je da i supstituenti i rastvarači imaju uticaj na promenu elektronske gustine, odnosno veličinu konjugacije i na karakter intramolekulskog prenos naelektrisanja..

Intramolecular charge transfer in 5-arylidene-3-substituted-2,4-thiazolidinedione derivatives

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Thiazolidine-2,4-dione (TZD) derivatives have attracted a significant research interest due to their synthetic diversity, numerous pharmacological properties and biological activities. The substituent and solvent effect on intramolecular charge transfer (ICT) in 5-arylidene-3-methyl-2,4-thiazolidinediones and 5-arylidene-3-phenyl-2,4-thiazolidinediones was studied by means of experimental and theoretical methodology. The solvent and substituent effect on ICT was evaluated using LSER and LFER methods applied on experimental data. The experimental findings were interpreted with the aid of *ab initio* MP2 and time-dependent density functional (TD-DFT) methods. Additional TD-DFT calculations are performed in order to quantify the efficiency of ICT allowing us to define the charge-transfer distance (D_{CT}), amount of transferred charge (Q_{CT}), and difference between dipole moments of the ground and excited states (μ_{CT}). It was found that both substituents and solvents influence the electron density shift, *i.e*. the extent of conjugation, and affect intramolecular charge transfer character in the course of excitation.

OH P 05

Синтеза нових пиколин- и фероцен-функционализованих андростана

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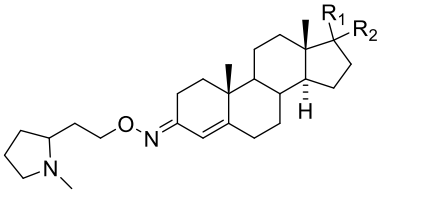
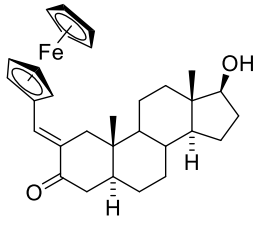
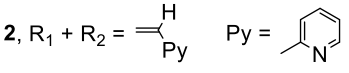
Исцрпним хемијским модификацијама стероидног скелета синтетизовани су многи потентни антинеопластични агенси који би могли циљано деловати на хормон-зависне канцере. Претходни радови указују на значајну цитотоксичну активност стероидних оксима и њихових *O*-алкил деривата према различитим хуманим туморима. Како би се испитао комбиновани ефекат 17-(пиридин-2-ил)метил или (17*E*)-(пиридин-2-ил)метилиден групе и алкилоксимино функције на C-3 на антитуморску активност, синтетизовани су нови A-модификовани 17-супституисани андростански деривати **1** и **2**. Такође, са циљем испитивања биолошког потенцијала конјугата најпотентнијег ендогеног андрогена дихидротестостерона са фероценском фармакофором, синтетизован је (2*E*)-фероценилметилиден дериват **3**.



1, R_1 = 17βOH, R_2 = 17αCH_2Py



3



2, $R_1 + R_2$ =

Synthesis of novel picoline- and ferrocene-functionalized androstanes

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Extensive chemical modifications of the steroid skeleton have been carried out to synthesize many potent antineoplastic agents which could target hormone-dependent cancers. Literature reports indicate prominent cytotoxicity of steroidal oximes and their *O*-alkyl derivatives on various human tumors. In order to evaluate the combined effect of the 17-(pyridin-2-yl)methyl or (17*E*)-(pyridin-2-yl)methylidene group and the alkyloximino function at C-3 on antitumor activity, new A-modified 17-substituted androstane derivatives **1** and **2** were synthesized. In addition, with the goal of investigating the biological potential of a conjugate of the most potent endogenous androgen, dihydrotestosterone, with the ferrocene pharmacophore, its (2*E*)-ferrocenylmethylidene derivative **3** was synthesized.

The authors would like to thank the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 172021) for financial support.

OH P 06

Novi prirodni proizvodi iz voska biljne vrste *Dianthus cruentus* Griseb. (Caryophyllaceae)

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Detaljnim analizama (GH i GH-MS) dietil-etarskog ispirka svežih cvetova biljne vrste *Dianthus cruentus* Griseb. (Caryophyllaceae) identifikovana su ukupno 153 sastojaka. Glavni sastojci ekstrakta su bili dugolančani *n*-alkani - pentakozan (5,0 %), heptakozan (19,5 %) i nonakozan (6,5 %). Sintezom odabranih sastojaka i hemijskim transformacijama uzoraka ekstrakta (transesterifikacija i sinteza dimetil-disulfid (DMDS) derivata), praćenim GH-MS analizom, identifikovane su homologe serije *n*-, *izo*- i *anteizo*- dugolančanih *n*- estara (n-heksil-alkanoata i alkil-benzoata), kao i dugolančanih (*Z*)- i (*E*)-alkena (od C_{23} do C_{35}) sa nekoliko različitih položaja dvostruke veze. Ukupno 55 sastojaka (10 estara i 45 alkena) predstavlja nove prirodne proizvode (od toga deset potpuno novih jedinjenja). Identifikovani novi prirodni proizvodi predstvaljaju moguće hemotaksonomske markere za biljne vrste roda *Dianthus*.

New natural products from the epicuticular wax of *Dianthus cruentus* Griseb. (Caryophyllaceae)

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Detailed GC and GC-MS analysis of a diethyl ether washings of fresh flowers of *Dianthus cruentus* Griseb. (Caryophyllaceae) enabled the identification of 153 constituents. The major identified compounds were long-chain *n*-alkanes - pentacosane (5.0 %), heptacosane (19.5 %) and nonacosane (6.5 %). Detailed analyses, in combination with synthesis and chemical transformations (transesterification and synthesis of dimethyl disulfide adducts), led to the identification of a homologous series of *n*-, *iso*- and *anteiso*- long-chain esters (*n*-hexyl alkanoates and alkyl benzoates) and long-chain (*Z*)- and (*E*)-alkenes (C_{23}–C_{35}) with several different double bond positions. Fifty five of these constituents (eight hexyl esters, two benzoates and forty five alkenes) represented new natural products in Plantae (10 new compounds in general). The identified metabolites appear to be chemotaxonomic markers of *Dianthus* spp.

Acknowledgement: *This work was funded by the Ministry of Education, Science and Technological Development of Serbia (Project 172061 and 45022).*

ОН Р 07

5-Арилиден-2-фероценил-1,3-тиазолидин-4-они: синтеза, електрохемијска карактеризација и антимикробна активност

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Константно интересовање истраживача за синтезу тиазолидинонских деривата, посебно 5-алкенилтиазолидинона, последица је њихове разноврсне биолошке активности.[1] У овом раду биће описана синтеза серије фероценских деривата 5-алкенилтиазолидинона, полазећи од раније описаних 2-фероценил-1,3-тиазолидин-4-она.[2] Knoevenagel-овом кондензацијом ових једињења са бензалдехидом у присуству калијум терц-бутоксида добијени су одговарајући 5-арилиден-2-фероценил-1,3-тиазолидин-4-они. Поред експерименталних детаља биће дата електрохемијска карактеризација, као и резултати антимикробне активности.

1 **2** **3**

Fc = фероценил;
R = *n*-C_4H_9, *n*-C_6H_{13}, *n*-C_8H_{17}, *n*-$C_{11}H_{23}$, *n*-$C_{16}H_{33}$, *p*-$OCH_3C_6H_4CH_2CH_2$, $C_6H_5CH_2$;

5-Arylidene-2-ferrocenyl-1,3-thiazolidin-4-ones: The synthesis, electrochemical characterization and antimicrobial activity

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Permanent researchers' interes in synthesis of thiazolidinones, especially 5-alkenylthiazolidinones, is a consequence of their diverse biological activities.[1] In this work we wish to report on a protocol for the synthesis of a series of ferrocenyl derivatives of 5-alkenylthiazolidinones, starting from 2-ferrocenyl-1,3-thiazolidin-4-ones, recently described by us.[2] The synthesis of 5-arylidene-2-ferrocenyl-1,3-thiazolidin-4-ones was achieved by Knoevenagel condensation of 2-ferrocenyl-1,3-thiazolidin-4-ones with benzaldehyde in the presence of potassium tert-butoxide. In addition of experimental details, ectrochemical characterization and the results of antimicrobial activity also will be presented.

Acknowledgement: *This work was supported by the Ministry of Education, Science and Technological development of the Republic of Serbia (Grant Nos. 172034 and III43004).*

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2. A. Pejović at al., *Eur. J. Med. Chem*. **83** (2014) 57.

OH P 08

Sinteza i karakterizacija fuleropirolidinskih monoadukata i difulerenskih osa povezanih fumarilnim diamidnim mostom

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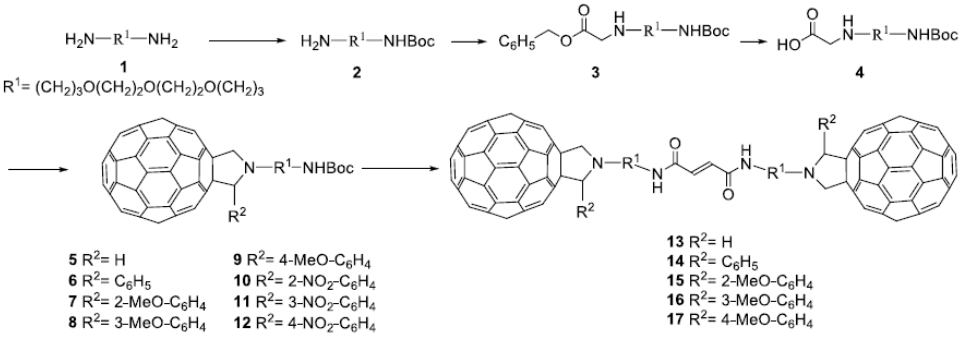
Cilj našeg rada bila je priprema fuleropirolidinskih monoadukata i njihovo povezivanje preko fumarilnog diamidnog mosta, čime nastaju ose sa difulerenskim graničnicima. Boc-zaštićeni 3,4-fuleropirolidini **5-12** dobijeni su korišćenjem standardne Prato-ve metode, koja se bazira na 1,3-dipolarnoj cikloadiciji azometin ilida na C_{60}. Serija *orto*-, *meta*- i *para*-metoksi- i nitrofenil-derivata fuleropirolidina sintetisana je radi proučavanja uticaja položaja supstituenata na osobine jedinjenja. Boc-zaštitna grupa je uklonjena pomoću TFA u svrhe dobijanja difulerenskih osa povezanih diamidnim mostom **13-17**.



Synthesis and characterization of fuleropirolidine monoadducts and dimeric fullerenes axes associated with fumaryl diamide bridge

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Our synthetic strategy was to prepare different fulleropyrrolidine monoadducts, as well as to incorporate some of them into a dumbbell-shaped difullerene derivatives containing fumaryl diamide bridge. Boc-protected 3,4-fulleropyrrolidines **5**-**12** have been synthesized utilizing a standard Prato method, based on the 1,3-dipolar cycloaddition of azomethine ylides to C_{60}. A series of *orto*-, *meta*- and *para*-methoxy- and nitrophenyl-derivatives of fulleropyrrolidine was synthesized to study the effect of the substitution position on their properties. The Boc-protecting group was removed by treatment with TFA giving diamide-based dumbbell type compounds **13-17**.

OH P 09

Sinteza novih derivata pirolidina [3+2] cikloadicijom vinil enona i azometin ilida

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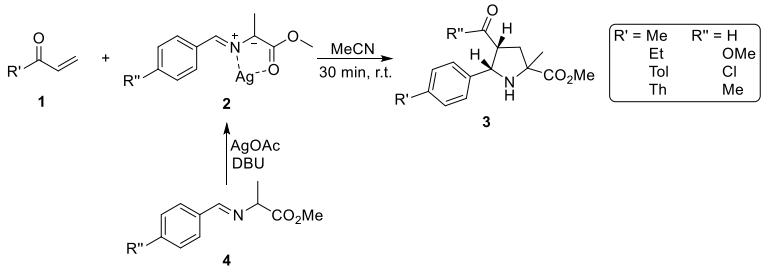
Cikloadicione reakcije su se ustalile kao pogodan metod za sintezu derivata pirolidina, pre svega zbog visoke stereoselektivnosti i dobrih reakcionih prinosa. Pirolidin je čest strukturni fragment prirodnih proizvoda i farmaceutskih preparata, a neretko se njegovi derivati koriste kao gradivni blokovi u sintezi biološki aktivnih molekula.[1] U ovom radu će biti prikazana sinteza serije derivata pirolidina (**3**) ostvarena [3+2] cikloadicijom odgovarajućih enona (**1**) na azometin ilide (**2**) u acetonitrilu kao rastvaraču. Azometin ilidi (**2**) su generisani *in situ* reakcijom aromatičnih α-iminoestara L-alanina (**4**) sa srebro-acetatom (AgOAc) i 1,8-diazabiciklo[5.4.0]undec-7-enom (DBU). Sva dobijena jedinjenja su okarakterisana NMR spektroskopijom.



Synthesis of new pyrrolidine derivatives by [3+2] cycloaddition of vinyl enones and azomethine ylides

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Cycloadditions represent a suitable method for the synthesis of pyrrolidine derivatives, primarily due to high stereoselectivity and good reaction yields. Pyrrolidine is a common structural fragment of natural products and pharmaceuticals, and its derivatives are often used as building blocks in the synthesis of biologically active molecules.[1] In this paper, we will present the synthesis of the pyrrolidine derivatives (**3**), obtained by [3+2] cycloaddition of the corresponding enones (**1**) and azomethine ylides (**2**) in acetonitrile as a solvent. Azomethine ylides (**2**) were generated in situ by the reaction of aromatic α-imino esters of L-alanine (**4**) with silver acetate (AgOAc) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU). All compounds were characterized by NMR spectroscopy.

Acknowledgement: *The authors are grateful to the Ministry of Education, Science and Technological Development of Republic of Serbia (Project number 172034).*

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OH P 10

Mehanistička studija trokomponentne Manihove reakcije i karakterizacija proizvoda

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Trokomponentna Manihova reakcija benzaldehida, supstituisanih anilina i acetofenona/4-jodoacetofenona izvedena je u prisustvu dietanolamonijum hloracetata kao reciklabilnog katalizatora. Pod blagim uslovima, dobijeni su aminokarbonilni proizvodi u dobrim prinosima. U reakcijiama sa 4-jodoacetofenonom, svi dobijeni proizvodi su novosintetisana jedinjenja. Proizvodi su okarakterisani elementalnom analizom, NMR, IR i UV-Vis spektroskopijom. Pored toga, mehanizam reakcije je detaljno ispitan pomoću teorije funkcionala gustine.

Mechanistic study of three-component Mannich reaction and characterization of the products

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Three-component Mannich reaction of benzaldehyde, substituted anilines, and acetophenone/4-iodoacetophenone was performed in the presence of diethanolammonium chloroacetate as recyclable catalyst. Aminocarbonyl products were obtained in good yields under mild conditions. In the reactions with 4-iodoacetophenone five products are newly synthetized compounds. All compounds were characterised using elemental analysis, NMR, IR, and UV-Vis spectroscopy. In addition, the mechanism of the reaction was examined in detail by means of density functional theory.

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Project No. 172016

OH P 11

Upotreba katalizatora na bazi paladijuma na maghemitu u reakcijama dekarbonilovanja aromatičnih aldehida i dehalogenovanja aril-halida

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Dekarbonilovanje, reakcija uklanjanja ugljen-monoksida iz molekula, predstavlja veoma korisnu transformaciju u organskoj sintetičkoj hemiji. Razvijena je praktična metodologija za reakciju dekarbonilovanja različitih aromatičnih i heteroaromatičnih aldehida uz pomoć paladijuma na maghemitu kao katalizatora.[1] Magnetne osobine katalizatora omogućavaju jednostavno i efikasno odvajanje katalizatora od reakcione smeše, uz pomoć eksternog magneta. Katalizator je moguće ponovo upotrebi i do četiri puta bez značajnog gubitka katalitičke aktivnosti. Kao nastavak istraživanja, isti katalizator je upotrebljen i u reakciji dehalogenovanja aril-halida. Ovo istraživanje predstavlja prvu primenu direktno-imobilizovanog pladijuma na maghemitu kao katalizatora za reakcije dekarbonilovanja i dehalogenovanja.

Maghemite-supported palladium as a catalyst for decarbonylation of aromatic aldehydes and dehalogenation of aryl halides

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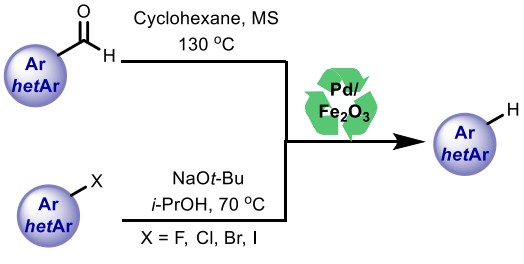

Decarbonylation, a reaction for removal of carbon monoxide from a molecule, represents a valiuable transformation in organic synthetic chemistry. A practical methodology for decarbonylation of a variety of aromatic and heteroaromatic aldehydes using maghemite-supported palladium catalyst has been developed.[1] The magnetic properties of catalyst facilitated an easy yet efficient recovery of the catalyst from the reaction mixture using an external magnet. The catalyst shows high stability and it was found that the catalyst could be reused for up to four consecutive catalytic runs without a significant loss in activity. In addition, the catalyst was also very effective in the dehalogenation of aryl halides. This is the first report on valuable utilization of directly immobilized palladium on maghemite in decarbonylation and dehalogenation reactions.

Acknowledgements: This research was supported by the Ministry of Education, Science, and Technological development of Serbia (Grant No. 172008).

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OH P 12

Biološka aktivnost 3,4-dihidro-2(1H)-hinoksalinona i 3,4-dihidro-1,4-benzoksazin-2-ona

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S ciljem da se otkrije potencijalna terapeutska primena, ispitivana je biološka aktivnost hinoksalinona i 1,4-benzoksazin-2-ona. Na osnovu rezultata ispitivanja zaključili smo da jedinjenja 5, 9-11 pokazuju dobru citotoksičnu aktivnost na HeLa ćelijskim linijama tumora pri čemu je najniža vrednost za IC_{50} (10.46 ± 0.82 µM/mL) izmerena za jedinjenje 10. Takođe, najaktivnija jedinjenja (5, 9-11) pokazala su mnogo bolju selektivnost za MRC-5 ćelijsku liniju (do 17.4) u odnosu na cisplatinu. Ispitivana je, *in vitro,* inhibicija enzima α-glukozidaze i pokazalo se da jedinjenja 10 i 11 pokazuju značajnu vrednost inhibicije enzima za 52.54 ± 0.09 i 40.09 ± 0.49 µM.

Biological evaluation of the 3,4-dihydro-2(1H)-quinoxalinones and 3,4-dihydro-1,4-benzoxazin-2-ones

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In order to investigate new potential therapeutically active agents, we investigated the biological properties of two small libraries of quinoxalinones and 1,4-benzoxazin-2-ones (Fig. 1). The results obtained showed that compounds 5, 9–11 have good cytotoxic activity against HeLa cells where the lowest IC_{50} value (10.46 ± 0.82 µM/mL) was measured for compound 10. Additionally, the most active compounds (5, 9–11) showed much better selectivity for MRC-5 cells (up to 17.4) compared to cisplatin. *In vitro* evaluation of the inhibition of the enzyme α-glucosidase showed that compounds 10 and 11 exert significant inhibition of the enzyme at 52.54 ± 0.09 and 40.09 ± 0.49 µM, respectively.

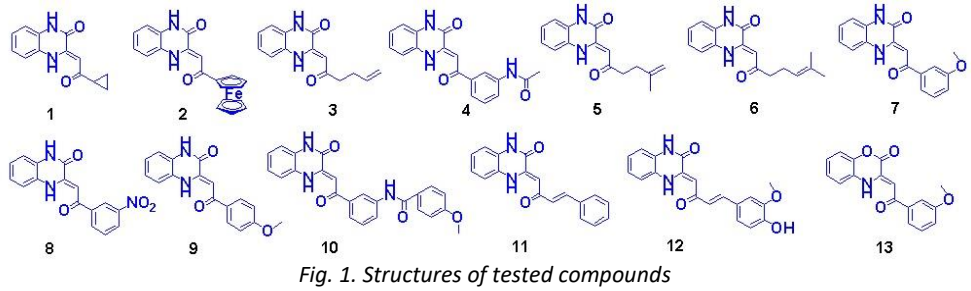

Fig. 1. Structures of tested compounds

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OH P 13

Totalna sinteza (±)-alstoskolarizina A

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Alstoskolarizin A je monoterpenoidni indolski alkaloid, izolovan iz lišća biljke *Alstonia scholaris*, koji u značajnoj meri promoviše proliferaciju i diferencijaciju nervnih matičnih ćelija odraslih jedinki. Pored toga što je biološki aktivan, ovo je veoma interesantan molekul i sa sintetičkog stanovišta, jer poseduje pentacikličnu strukturu i 5 uzastopnih stereocentara. Racemski alstoskolarizin A je sintetisan u 13 koraka, pri čemu je ključna reakcija u ovoj sintezi bila efikasna domino sekvenca, kojom je formiran premošćeni tetracikličan intermedijer, uz nastajanje 3 nove kovalentne veze u jednom koraku: dve C-N i jedne C-C veza.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije za finansijsku podršku (projekat br. 172027).

Total synthesis of (±)-alstoscholarisine

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Alstoscholarisine A is a monoterpenoid indole alkaloid, isolated from the leaves of *Alstonia scholaris,* which significantly promotes proliferation and differentiation of the adult neural stem cells. In addition to its important biological activity, this molecule is also very interesting from a synthetic point of view, as it possess unique pentacyclic structure, with five contiguous chiral centers. Racemic alstoscholarisine A was synthesized in 13 steps. The key step of the synthesis is an efficient domino sequence, used to assemble the bridged tetracyclic core, leading to formation of three covalent bonds in one step: two C-N and one C-C bond.

This work was supported by the Serbian Ministry of Education, Science and Technological Development (Project No. 172027).

OH P 14

Reagensom kontrolisana organokatalizovana aldolna adicija dioksanona na aciklične hiralne α-razgranate aldehide

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S obzirom na to da se u reakciji organokatalizovane aldolne adicije dioksanona na hiralne aldehide javlja fenomen dvostruke asimetrične sinteze, kao i da u literaturi postoje oprečna opažanja po pitanju stereohemijskog ishoda ovih reakcija, želeli smo da utvrdimo da li je aciklična priroda akceptorske komponente od presudne važnosti za stereoselektivnost ovih reakcija. Sintetisan je niz hiralnih, optički čistih aldehida, koji u α-položaju imaju heteroatomni ili ugljenični supstituent. Nađeno je da se aldolne adicije dioksanona na aciklične hiralne aldehide odvijaju uz visok nivo reagensom kontrolisane selektivnosti, nezavisno od toga da li je reč o stereohemijski usklađenom, ili neusklađenom paru reaktanata. Sa cikličnim aldehidima stereohemijski ishod reakcije, kao i usklađenost reaktanata su teže predvidivi, što često rezultuje niskom selektivnošću.

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Reagent-controlled organocatalyzed aldol addition of dioxanone to acyclic chiral α-branched aldehydes

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In the reaction of organocatalytic aldol addition of dioxanone to chiral aldehydes, the phenomenon of double asymmetric induction occurs. As literature data on the stereochemical outcomes of these reactions are contradictory, we undertook a study to find out whether acyclic nature of chiral α-substituted aldehydes could play a decisive role in the stereochemical outcome of these reactions. Several chiral, opticaly pure aldehydes, with carbon or heteroatom substituents in the α-position were synthesized as substrates for this study. Our results showed that aldol addition of dioxanone to acyclic chiral aldehydes proceed with a synthetically useful level of stereoselectivity, regardless of whether a matched or mismatched pair of reactants was employed. With cyclic aldehydes, the stereochemical outcome, as well as the matched pair or reactants, are more difficult to predict, thus resulting in low levels of stereoselectivity.

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Teorijska hemija / Theoretical Chemistry

TH P 01

Derivati 5-ariliden barbiturne kiseline: Eksperimentalno i kvantno-hemijsko proučavanje

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Benzilideni barbiturne kiseline koriste se za sintezu merocijaninskih boja, dizajn $PPAR_\gamma$ liganada, deluju kao antibakterijski agensi, kao inhibitori tirozinaze i privlače veliku pažnju kao nelinearni optički materijali. U cilju objašnjenja solvatohromnog ponašanja, sintetisani su derivati 5-ariliden barbiturne kiseline sa različitim hromoforama i njihovi UV spektri određeni su u organskim rastvaračima različite polarnosti. Uticaj specifičnih i nespecifičnih rastvorak-rastvarač interakcija na pomeranje apsorpcionih maksimuma procenjen je solvatohromnim konceptom Kamlet-Taft-a i Catalàn-a (LSER analiza). Efekat supstituenata na apsorpcione spektre analiziran je pomoću Hammet-ove jednačine (LFER analiza). Kvantno hemijskim proračunima, tačnije TD-DFT metodom su izračunati UV/VIS spektri sintetisanih molekula. Za proračune je korišćen B3LYP funkcional sa 6-311G(d,p) bazis setom. Na osnovu izračunate elektronske gustine u osnovnom i prvom pobuđenom stanju određena su i rastojanja između baricentara transfera naelektrisanja, količina prenetog naelektrisanja pri elektronskom prelazu i razlika dipolnih momenata. Izračunate su i mape molekulskih elektrostatičkih potencijala za sve sintetisane molekule u osnovnom stanju.

5-Arylidene barbituric acid derivatives: Experimental and quantum chemistry study

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Benzylidene barbituric acids are used for synthesizing merocyanine dyes, designing $PPAR_\gamma$ ligands, acting as antibacterial agents, as tyrosinase inhibitors and have attracted great attention as nonlinear optical materials. In order to interpret their different solvatochromic behavior, 5-arylidene barbituric acid derivatives were synthesized with different chromophores, and their UV absorption spectra have been recorded in organic solvents of different polarity. The effect of specific and non-specific solvent–solute interactions on the absorption maxima shifts were estimated by using solvatochromic concept of Kamlet-Taft and Catalàn (*LSER analysis*). Substituent effect on the absorption spectra were analyzed using Hammett equation (*LFER analysis*). UV-Vis spectra of all synthetized molecules were calculated using TD-DFT method, more specifically B3LYP functional with 6-311G(d,p) basis set. From obtained ground and excited state electron densities charge-transfer distances between charge barycenters, amount of transferred charge and associated dipole moments were evaluated. Maps of molecular electrostatic potentials (MEP) were calculated for all molecules in their ground state.

TH P 02

Ab Initio molekulsko dinamički pogled na reakciju dopamina sa hidroksilnim radikalom

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Uloga dopamina je veoma važna i raznovrsna u živim sistemima pa je stoga u cilju boljeg razumevanja neophodno posvetiti značajnu pažnju ispitivanju mehanizama oksidacije koji uključuju dopamin. Analiza antiradikalskog afiniteta dopamina prema hidroksilnom radikalu je ispitivana sa akcentom na utvrđivanju mehanizma reakcije koja se dešava u biološkim sistemima. Upotrebom *ab initio* molekulske dinamike u sprezi sa teorijom funkcionala elektronske gustine i formalizmom Vanijerovih funkcija objašnjen je redosled izmene elektrona i protona između dopamina, molekula vode i hidroksilnog radikala. Ovi rezultati su pokazali da najpre dolazi do prenosa elektrona i to direktno sa fenolnog prstena na hidroksilni radikal što je potom praćeno gubitkom protona sa OH grupe dopamina koji se kasnije posredstvom molekula vode prenosi do hidroksilnog anjona. Prenos elektrona traje oko ~ 50 fs dok je za čitav proces formalnog prenošenja atoma vodonika od dopamina do hidroksilnog radikala potrebno ~ 100 fs.

Ab initio molecular dynamics insights on how dopamine disarms hydroxyl radical

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Diverse and important in vivo role of dopamine indicates that research attention must be provided in order to clarify dopamine-related oxidative mechanisms. Analysis of dopamine antiradical scavenging towards hydroxyl radical is investigated with an accent on determination of a reaction mechanism that takes place in biological systems. Ab initio molecular dynamics calculation were performed within a framework of density functional theory calculations together with Wannier functions formalism in order to elucidate sequence of electron and proton exchange between dopamine, water molecules and hydroxyl radical. These results suggested that the electron gets transferred first, directly from the dopamine phenol ring to the hydroxyl radical followed by dopamine's OH group proton loss which is later transferred towards hydroxyl anion through water molecules. The electron transfer lasted for ~ 50 fs while the whole process of formal hydrogen abstraction from dopamine took ~ 100 fs.

TIMIZOLIRKA

PRODAJNI PROGRAM

HIDROIZOLACIJE

- BITUMENSKI PREMAZI, PASTE I MASE
- BITUMENSKE HIDROIZOLACIONE TRAKE
- BITUMENSKE EMULZIJE

TERMOIZOLACIJE

- EPS TERMOIZOLACIONE PLOČE
- XPS TERMOIZOLACIONE PLOČE
- TERMOAKUSTIČNE -KOMBI PLOČE
- LAKI IZOLACIONI BETON POLITERM
- LEPKOVI ZA FASADE I PRATEĆI MATERIJAL
- FASADNI ZAVRŠNI SLOJEVI

PODNO GREJANJE

- STIROTERMAL - PLOČE ZA PODNO GREJANJE
- OPREMA

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