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KRATKI IZVODI RADOVA

56th MEETING OF THE SERBIAN CHEMICAL SOCIETY

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Niš 7. i 8. juni 2019.

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above titles of Abstracts.

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Hemija i tehnologija makromolekula Chemistry and Technology of Macromolecules

Medicinska hemija / Medicinal Chemistry

Plenarna predavanja / Plenary Lectures

PP 1

Photochemical synthesis, chirality and detection of the building blocks of life

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What is responsible for the emergence of life's homochiral biopolymers – DNA/RNA and proteins – where all the constituent monomers exhibit the same handedness?
Based on in-situ observations and laboratory studies, we propose that this handedness occurs when chiral biomolecules are synthesized asymmetrically through interaction with circularly polarized light (cpl) in interstellar space.[1] Previous experimental results on the asymmetric photolysis of amino acids,[2] as well as the absolute asymmetric synthesis from achiral interstellar ice precursor molecules,[3] revealed polarization- and energy-controlled induced enantiomeric enrichments.
Our recent research has shown that the central chiral unit of RNA, ribose, forms readily under simulated comet conditions (Fig. 1) and this has provided new insights into the accessibility of precursors of genetic material in interstellar environments.[4] The significance of our research arises due to the current lack of experimental demonstration that amino acids and sugars can simultaneously and asymmetrically be synthesized by a universal physical selection process. In my presentation, I will therefore highlight a few significant results on our on-going cometary ice simulation experiments, the chiroptical properties of targeted sugar and amino acid molecules in the UV using circularly polarized synchrotron light and present future strategies towards furthering understanding the origin of asymmetric prebiotic molecules.

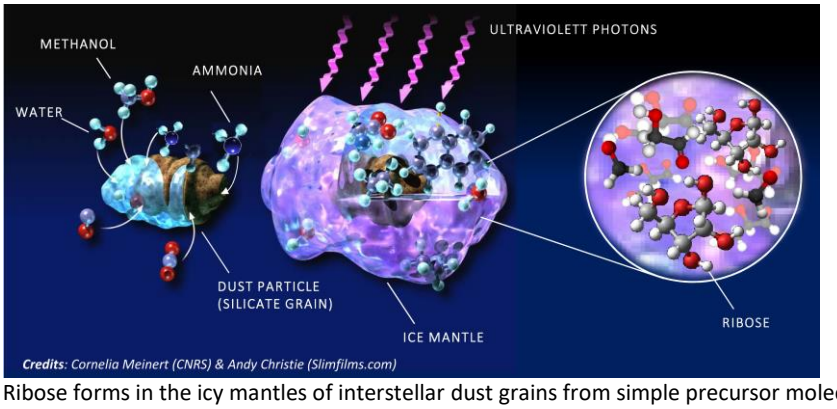

Fig. 1. Ribose forms in the icy mantles of interstellar dust grains from simple precursor molecules (water, methanol, and ammonia) under high energy radiation

Support by the European Research Council under the EU's HORIZON 2020 research & innovation programme [grant agreement 804144] is gratefully acknowledged.

1. C. Meinert et al., *Phys. Life Rev*. **8**, 307 (2011).
2. C. Meinert et al., *Angew. Chem. Int. Ed*. **53**, 210 (2014).
3. P. de Marcellus et al., *Astrophys. J. Lett*. **727**, L27 (2011); P. Modica et al., *ApJ* **788**, 79 (2014).
4. Meinert C. et al., *Science* **352**, 208 (2016).

PP 2

Analytical studies of fragrant raw materials. A quest for their odor active constituents

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The determination of the most important olfactory contributors of a fragrant natural raw material can be an extremely long and complex task which requires the combination of very efficient analytical techniques. Indeed, the characterization of these components is often difficult since the main contributors are usually strongly potent odorants contained only in trace amounts, and therefore, their identification requires an exhaustive analysis of the whole mixture. Consequently, there is still a lack of accurate knowledge about the main odoriferous constituents for many natural raw materials, and this situation is paradoxical when it concerns materials widely used for their odorant properties in the flavor and fragrance industry.

This presentation will describe several examples of analytical investigations based on Gas Chromatography-Olfactometry (GC-O) and focused on the determination of the main odorant contributors of fragrant raw materials such as *Helichrysum italicum*, Atlas cedarwood, frankincense, and vetiver essential oils. In some cases, the syntheses of some of the key odorants and their analogues permitted to confirm their identification and to propose new ingredients for the perfume industry.

Predavanja po pozivu / Invited Lectures

PPP 1

Lekovito bilje – nepresušni izvor novih biološki aktivinih prirodnih proizvoda

Marija S. Genčić
Departman za hemiju, Prirodno-matematički fakultet, Univerzitet u Nišu, Srbija

Tokom istorije arsenal farmaceutskih preparata koji je bio dostupan ljudima u mnogome se oslanjao na lekovito bilje. Otkrivanje bioloških aktivnih jedinjenja iz biljaka je često olakšano dostupnošću etnofarmakoloških podataka o njihovoj upotrebi jer oni daju nagoveštaj o postojanju jedinjenja u datim biljnim vrstama koja mogu biti terapeutski efikasna. Tokom godina ovaj pristup odabira biljnih vrsta za ispitivanja pokazao se veoma svrsishodnim jer je čak 80 % lekova koji potiču iz biljaka dobijeno iz onih vrsta koje imaju etnomedicinsku upotrebu za stanja koja su identična ili veoma srodna stanjima za koja se propisuju odgovarajuća čista aktivna jedinjenja izolovana iz njih. Međutim, neke od poznatih lekovitih biljaka se iznova proučavaju kako sa fitohemijskog, tako i sa farmkološkog aspekta. Stoga se nameće pitanje: Da li je ovo neprekidno proučavanje pojedinih lekovitih biljaka opravdano ili predstavlja gubljenje vremena i resursa? Napredak modernih tehnika analize, metoda razdvajanja i sintetskih metoda, kao i razvoj testova za ispitivanje bioloških aktivnosti, omogućili su ponovni procvat hemije prirodnih prozvoda u poslednjih nekoliko decenija. Sve gore navedeno zajedno sa mogućom promenom profila sekundarnih metabolita kod nekih biljnih vrsta (do koje može doći usled različitih genetičkih i/ili ekoloških faktora), značajno povećava mogućnost nalaženja novih biološki aktivnih prirodnih proizvoda i kod biljnih vrsta koje su prethodno dobro proučene. U ovom radu prikazaćemo rezultate nekih od naših istraživanja dobro proučenih lekovitih biljaka (oman, smilje, kantarion, itd.) gde je njihovo ponovno ispitivanje dovelo do identifikacije novih prirodnih proizvoda.

Medicinal plants – a continuing source of new bioactive natural products

Marija S. Genčić
Department of Chemistry, Faculty of Sciences and Mathematics, University of Niš, Serbia

Historically, the human pharmaceutical armamentarium has been significantly indebted to medicinal plants. An advantage in the context of discovery of bioactive molecules from medicinal plants is that often, well documented ethnopharmacological information about the traditional use is available, which can provide hints for the existence of compounds that could be therapeutically effective in humans. Over the years this classical knowledge-based approach of plant selection turned out to be quite beneficial as even 80 % of plant-derived drugs originate from plants that have ethnomedical use identical or related to the indications for which the respective pure compounds are prescribed. However, some medicinal plants have been studied and restudied from both phytochemical and pharmacological standpoints. Thus, questions arise: Could this continuing re-examination of medical plants be justified or is it just a waste of time and valuable resources? Advances in analytical techniques, separation, and synthetic methods, as well as, bioassay development have helped to push forward the research in natural products over the last few decades. With all these foregoing developments and plausible changes in plant secondary metabolites profiles (that could be triggered by various genetic and/or ecological factors), the chance of finding new bioactive molecules is considerably increased even from these well-studied medicinal plants. Herein we will present some of our studies on medicinal plants (elecampane, immortelle, St John's wort, *etc*.) where their re-examination led to the identification of new or novel natural products.

PPP 2

Primena taktičke kombinacije organokatalizovane aldolne reakcije i reduktivnog aminovanja u sintezi iminošećera značajnih za medicinu

Zorana Ferjančić
Univerzitet u Beogradu - Hemijski fakultet, Studentski trg 12-16, 11158 Beograd, Srbija

Iminošećeri su klasa alkaloida koja je privukla pažnju naučne zajednice zbog svoje interesante i obećavajuće biološke aktivnosti. Ova jedinjenja pokazuju antiviralnu, antidijabetsku i antitumornu aktivnost, što ukazuje na njihov visok terapeutski potencijal za lečenje različitih bolesti. Nekoliko biološki aktvinih iminošećera je enantioselektivno sintetisano primenom organokatalitičke aldolne reakcije i reduktivnog aminovanja kao ključnih koraka (svainsonin, 1-deoksinodžirimicin, 4-*epi*-fagomin, 2,5-dideoksi-2,5-imino-D-altritol i aza-galakto-fagomin). Ova taktička kombinacija reakcija omogućava efikasno gradjenje optički čistih heterocikala, sa tri konsekutivna stereocentra definisane apsolutne stereohemije.

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

Application of tactical combination of organocatalytic aldol reaction and reductive amination in the synthesis of medicinally important iminosugars

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Iminosugars are a class of alkaloids that has attracted considerable attention from the scientific community, due to their interesting and promising biological activity. Since these compounds display antiviral, antidiabetic and anticancer activity, they have therapeutic potential for treatment of various diseases. Several biologically active iminosugars were enantioselectively synthesized utilizing a sequence of organocatalytic aldol reaction and reductive amination as key steps (swainsonine, 1-deoxygalactonojirimycin. 4-*epi*-fagomine, 2,5-dideoxy-2,5-imino-D-altritol and aza-galacto-fagomine). This tactical combination of reactions allows for an expedient entry into optically pure heterocycles with three consecutive stereocenters of defined absolute stereochemistry.

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

PPP 3

150 година периодног система елемената

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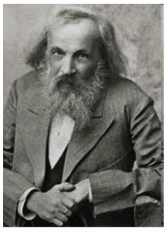

Dmitri Mendeleev
1834 – 1907

Lothar Meyer
1830 - 1895

Децембра 2017. године, на 74. пленарном састанку Генералне скупштине УН, 2019. година је проглашена Међународном годином периодног система елемената (International Year of the Periodic Table of Chemical Elements - IYPT 2019). На тај начин обележава се 150 година од када је Димитриј Мендељејев, фебруара 1869. године, објавио свој чланак у Часопису Руског физичко-хемијског друштва, и у њему презентовао периодни закон и периодни систем елемената. Због тога периодни систем неизоставно повезујемо са овим руским научником, као човеком који га је открио. Оно што чини периодни систем су, ништа друго него природне особине елемената - Мендељејев је то само установио и елементе на основу њих систематизовао. Истине ради, треба рећи и да је, иако је данас познат под именом Мендељејева, независно и скоро истовремено (чак и неколико година раније), готово истоветни периодни систем открио и Лотар Мајер. Ово је само једно од многих истовремених и независних научних открића која су се десила у историји науке, али да би на питање ко је у ствари први открио периодни систем одговорило, треба знати и шта је претходило том открићу.

150 years of the Periodic system of elements

Aleksandar Dekanski
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On December 20, 2017, during its 74th Plenary Meeting, the United Nations (UN) General Assembly 72nd Session has proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements (IYPT 2019). In this way we celebrate the 150th anniversary of the publication of the article by Dimitri Mendeleev (February 1869) in which he presented the periodic law and periodic system of elements. Since then, the periodic system has been inextricably linked with the Russian scientist, as the man who created it. However, the term "created" can hardly be accepted as accurate. Perhaps it is better to say that the system was "discovered" because what makes this system are the natural characteristics of the elements - Mendeleev only systematized the elements on the bases of these features. But that's not exactly true! For the sake of truth, it should also be said that almost simultaneously (even several years earlier) and independently, an almost identical periodical system "was discovered" by Lothar Meyer. To answer the question of who discovered the periodic system first, this text talks what preceded its discovery. This is just one of many simultaneous and independent scientific discoveries that have occurred in the history of science.

PPP 4

Smrt antibiotika: Da li zemljišni mikroorganizmi još uvek mogu nešto da ponude?

Jasmina Nikodinović-Runić
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Antibiotici predstavljaju lekove koji spasavaju život i koji su revolucionirali medicinu, počevši od otkrića penicilina 1928. godine. Od otkrića penicilina, za kliničku primenu je razvijen veliki broj efikasnih antibiotika, čija je primena uvek ograničavana pojavom rezistentnih sojeva. Trenutno se suočavamo sa problemom panrezistentnih patogena otpornih na antibiotsku terapiju, a sa vrlo malo potencijala za razvoj novih terapeutika koji bi zamenili antibiotike prema kojima mikroorganizmi postaju sve rezistentniji.
Mikrobiološki resursi, posebno zemljišni izolati, tradicionalno su nenadmašiv izvor jedinjenja za razvoj novih lekova. Sa razvojem sofisticiranih funkcionalnih testova, i fenotipskih pretraživanja u kojima se koriste cele ćelije ili model organizmi, a u kombinaciji sa genomskim i *in silico* pristupima, ovi resursi, pogotovu sojevi roda *Streptomyces*, i dalje će nastaviti da daju doprinos u smislu novih bioaktivnih jedinjenja, što je pokazano na primeru pretraživanja sojeva zbirke zemljišnih izolata Laboratorije za molekularnu genetiku i ekologiju mikroorganizama (IMGGI, UB).

The death of antibiotics: Do soil microorganisms still have something to offer?

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Antibiotics are essential life-saving drugs that revolutionized medicine, starting with the discovery of penicillin in 1928. Since the discovery of penicillin, a number of highly effective antibiotics have been discovered and developed for clinical use in the treatment of bacterial infections. However, at present we are facing the threat of 'super-bugs' resistant to antibiotic therapy with very little in the pharmaceutical pipeline to replace the antibiotics to which microorganisms are becoming resistant.
On the other side, microorganisms have been, for decades, one of the most important sources for the discovery of new antibiotics. With the development of sophisticated functional screens in combination with genomic and *in silico* approaches, soil microorganisms and communities still hold the promise for the delivery of novel bioactive scaffolds. The highlights of the screen of a number of soil isolates, mainly *Streptomyces* spp. from the Laboratory for Microbial Molecular Genetics and Ecology (IMGGE, UB) provide such evidence.

Acknowledgements: *This work was funded in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 173048).*

PPP 5

Amiloidi: biohemija, biotehnologija i medicina

Natalija Đ. Polović
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Nativni proteini podležu konformacionim promenama koje vode do pogrešnog uvijanja polipeptida, agregiranja i inaktivacije čak i prilikom čuvanja u blagim uslovima. Amiloidni fibrili predstavljaju najstabilniju strukturu polipeptida i perspektivni su kandidati za upotrebu u biotehnologiji (kao biomaterijali, adsorbenti, potencijalni katalizatori itd.). Depoziti amiloida su detektovani u tkivima i učestvuju u razvoju mnogih neurodegenerativnih i sistemskih oboljenja, kao što su: Alchajmerova i Parkinsonova bolest, šećerna bolest tip 2, reumatoidni artritis itd.
Tokom ovog predavanja biće objašnjeni principi na kojima počiva ravnoteža između uvijenih, razvijenih i pogrešno uvijenih polipeptida (termodinamička hipoteza, mehanizam uvijanja, teorija energetskog reljefa). Biće diskutovane strategije destabilizovanja nativnih proteina i dobijanja amiloidnih fibrila na primerima ovalbumina i lizozima. Biće prikazane metode koje se koriste za praćenje formiranja amiloida sa posebnim akcentom na infracrvenu spektroskopiju. Na kraju, biće prikazani rezultati upotrebe amiloidnih vlakana kao adsorbenata teških metala i niskomolekulskih zagađivača iz životne sredine.

Ovaj rad je finanijski potpomognut od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije u okviru projekta 172049.

Amyloids: biochemistry, biotechnology and medicine

Natalija Đ. Polović
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Native proteins are marginally stable, so even if stored in mild conditions, they undergo structural rearrangements that subsequently lead to their misfolding, aggregation and inactivation. Amyloid fibrils are the most stable form of polypeptides and are promising candidates for use in biotechnology (as biomaterials, adsorbents, potential catalysts etc.). Amyloid deposits are main or contributing cause to many neurodegenerative disorders and systemic diseases, such as Alzheimer's and Parkinson's diseases, diabetes mellitus type 2, rheumatoid arthritis etc.
In this lecture, an overview of principles underlying protein folding-unfolding-misfolding equilibria will be given (thermodynamic hypothesis and energy landscapes theory). As examples of amyloid fibril formation, destabilization of ovalbumin and lysozyme will be discussed. Details of methodologies used for monitoring of amyloid fibrillation will be provided with the emphasis on infrared spectroscopy. Finally, results of amyloid fibrils usage in the removal of heavy metal pollutants and low molecular weight contaminants from environmental water will be presented.

This work has been supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Grant No. 172049.

PPP 6

Kakva je priroda vezivanja BF_4^-, NO_3^- i ClO_4^- za komplekse Cu(II) sa Žirarovim T hidrazidom? Kada mogu nastati binuklearni kompleksi?

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Četiri kompleksa, [Cu**L**Cl]BF_4, [Cu**L**Cl]NO_3, [Cu_2**L**$_2Cl_2$]$(BF_4)_2$ i [Cu**L**Cl]ClO_4, sa istim [Cu**L**Cl]$^+$ fragmentom (**L**=(*E*)-*N*,*N*,*N*-trimethyl-2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene) hydrazinyl)ethan-1-amin) su okarakterisani metodom difrakcije X-zraka. Na osnovu dužina veza, formule kompleksa su napisane tako da je [Cu**L**Cl]$^+$ unutrašnja sfera kompleksa, a $BF4^-$, $NO3^-$ i $ClO4^-$ pripadaju spoljašnjoj sferi. Proračuni zasnovani na Teoriji funkcionala gustine, u kojoj je disperzija korigovana na ne-lokalan način, na strukturama dobijenim difrakcijom X-zraka, su izvedeni u cilju razjašnjavanja prirode interakcija anjona sa Cu(II) jonom. Rezultati različitih analiza, kao što su dekompozicija interakcione energije, indeks nekovalentnih interakcija, model nezavisnog gradijenta i kvantna teorija atoma u molekulima, pokazuju da su anjoni u mononuklearnim kompleksima slabo koordinovani, dok je $BF4^-$ u binuklearnom kompleksu kontra jon, elektrostatički vezan za unutrašnju sferu. Takođe, proračuni objašnjavaju činjenicu da je samo kompleks [Cu_2**L**$_2Cl_2$]$(BF_4)_2$ binuklearni sa mostnim Cl^- jonima. Ova studija pokazuje da se nedoumice oko koordinacionog broja u realnim kristalnim strukturama kompleksa mogu otkloniti detaljnom analizom elektronske gustine.

What is the nature of binding of BF_4^-, NO_3^- and ClO_4^- to Cu(II) complexes with Girard's T hydrazine? When can binuclear complexes be formed?

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Four complexes, [Cu**L**Cl]BF_4, [Cu**L**Cl]NO_3, [Cu_2**L**$_2Cl_2$]$(BF_4)_2$ and [Cu**L**Cl]ClO_4 having the same [Cu**L**Cl]$^+$ moiety, (**L**=(*E*)-*N*,*N*,*N*-trimethyl-2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene) hydrazinyl)ethan-1-amin), were characterized by single crystal X-ray diffraction methods. According to the bond distances, the formulas have been written such that [Cu**L**Cl]$^+$ is the inner sphere, while $BF4^-$, $NO3^-$ and $ClO4^-$ belong to the outer sphere. Non-local density-dependent dispersion corrected Density functional theory (DFT) calculations on the X-ray structures have been performed to rationalize interactions of anions to the Cu(II) ion. Results of analysis based on energy decomposition, Non-Covalent Interactions Index, Independent Gradient Model analysis, and Quantum Theory of Atoms in Molecules revealed that in mononuclear complexes, anions are weakly coordinated, while in binuclear complex, $BF4^-$ is counter-anion, electrostatically bonded to the inner sphere. Furthermore, DFT calculations rationalized the fact that only complex [Cu_2**L**$_2Cl_2$]$(BF_4)_2$ is binuclear with bridging Cl^- ions. The present study shows that ambiguity about actual coordination number in the real crystal structures of coordination compounds can be solved with thorough analysis of the electron density.

Saopštenja / Contributions

Analitička hemija / Analytical Chemistry

AH O 1 text rada / full text

Potentially toxic elements in cultivated rose hip - quantification by ICP-AES method

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Serbia is rich in wild species of rose hip and some of them like *Rosa canina* are used as rootstocks for conventional and organic fruit production. The fruits of wild rose - rose hips are the most commonly used to make jams, jellies, pies, stews, tea and wine. The aim of the study was the quantification of selected potentially toxic metals (Al, As, Cr, Cu, Ni, Pb and Zn) as well as one non-metal (B) in cultivated rose hip samples from two areas, by means of inductively coupled plasma atomic emission spectroscopy (ICP-AES) analysis. Elements As, Cr and Pb were below the limit of detection in both seed and mesocarp of all studied samples. The highest and lowest mass fraction values were measured for Zn (19.5 mg/kg) and Cu (0.572 mg/kg). The mesocarp of sample from Valjevo area had the highest concentration of B, whereas the highest content of Cu, Ni and Zn was found in the seed of samples from Prijepolje area. Statistical analysis revealed significant differences in the elements's mass fraction values between seed and mesocarp ($p<0.001$).

Potencijalno toksični elementi u gajenom šipurku – određivanje sadržaja ICP-AES metodom

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Srbija je bogata divljim vrstama šipurka, a neke od njih, kao što su *Rosa canina*, koriste se kao podloge za konvencionalnu i organsku proizvodnju. Plod divlje ruže - šipurak se najčešće koristi za pravljenje džemova, želea, pita, variva, čaja i vina od divljeg voća. Cilj rada bio je određivanje sadržaja odabranih potencijalno toksičnih metala (Al, As, Cr, Cu, Ni, Pb i Zn) kao i jednog nemetala (B), u uzorcima gajenog šipurka sa dve lokacije,tehnikom induktivno spojena plazma atomska emisiona spektroskopija (ICP-AES). Elementi As, Cr i Pb bili su bili ispod granice detekcije u semenkama i mezokarpu ispitivanih uzoraka. Najveća i najmanja koncentracija, izražena kao maseni udeo, izmerena je za Zn (19,5 mg//kg) odnosno Cu (0,572 mg/kg). Mezokarp uzorka sa područja Valjeva imao je najveću koncentraciju B, dok je najveći sadržaj Cu, Ni i Zn detektovan u semenkama uzoraka sa područja Prijepolja. Statističkom analizom su utvrđene značajne razlike u masenim udelima elemenata između semena i mezokarpa u ispitivanim uzorcima šipurka ($p<0,001$).

AH P 1

Dobijanje polimernih sorbenata za selektivnu sorpciju UV-filtera cinamatnog tipa

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Molekulsko obeležavanje predstavlja tehnologiju usmerenu ka stvaranju selektivnih vezivnih mesta u polimernom matriksu polimerizacijom u prisustvu željenog molekula – templata [1]. Nakon polimerizacije i uklanjanja templata, u polimeru ostaju vezivna mesta po veličini i naelektrisanju komplementarna templatu. UV-filteri predstavljaju strukturno raznovrsnu grupu jedinjenja koja se primenjuju u zaštiti kože od štetnog sunčevog zračenja. Povećana upotreba sredstava za zaštitu od sunčevog zračenja ima za posledicu sve veće prisustvo ovih jedinjenja u životnoj sredini [2]. Određivanje UV-filtera se najčešće zasniva na hromatografskim ili spektroskopskim metodama, nakon izdvajanja željene klase jedinjenja iz uzoraka, najčešće primenom ekstrakcije čvrstom fazom (SPE). Pronalaženje novih sorbenata koji mogu selektivno izdvojiti UV filtere iz realnih uzoraka može umnogome olakšati i ubrzati određivanje ovih jedinjenja. U ovom radu sintetisana je serija polimera koristeći cinamatne UV-filtere kao template. Optimizovani su uslovi vezivanja UV-filtera za sintetisane polimere u cilju potencijalne primene dobijenih polimera pri ekstrakciji čvrstom fazom. Kao rastvarači ispitani su acetonitril i smeše acetonitril/voda i metanol/voda (*V*/*V*: 9/1 i 8/2). Pokazano je da polimeri koji u svom sastavu sadrže divinilbenzen (DVB) vezuju UV-filtere bolje od polimera koji sadrže etilenglikol-dimetakrilat (EDMA). Prisustvo funkcionalnog monomera i tehnike polimerizacije imaju mali uticaj na kapacitet vezivanja. Najveći kapacitet vezivanja cinamatnih UV-filtera imao je polistiren-(ko-divinilbenzen) polimer iz rastvora metanol/voda=9/1.

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Preparation of polymer sorbents for selective sorption of cinnamate UV-filters

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Molecular imprinting is a technology for creating selective binding sites in a polymeric matrix by polymerization in the presence of the target compound - the template [1]. The template can be washed out from the polymer and the resulting molecularly imprinted polymer (MIP) is capable of selectively rebinding the target compound from a sample matrix. UV-filters represent structurally diverse group of compounds used in sun protection creams [2]. Determination of the UV-filters is mostly based on chromatographic or spectroscopic methods, after SPE. Our research focus was the synthesis of MIPs using cinnamon UV filters as templates; binding to MIPs as SPE sorbents was optimized. Acetonitrile, acetonitrile/water, and methanol/water were used as solvents (*V*/*V*: 9/1 and 8/2). It was shown that MIPs containing DVB bind UV-filters better than MIPs containing EDMA. The presence of a functional monomer and a polymerization technique have little effect on the binding capacity. The highest binding capacity of cinnamate UV-filters had a polystyrene (co-DVB) polymer from a methanol/water mixture 9/1.

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AH P 2

Određivanje veštačkog zaslađivača neotama u rečnim sedimentima

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Veštački zaslađivači predstavljaju emergentne zagađujuće materije u životnoj sredini. Decenijama se koriste kao aditivi u ishrani i farmaceutskim proizvodima, zbog čega su široko rasprostranjeni u prirodnim vodama, usled nepotpunog prečišćavanja otpadnih voda. Međutim, pojedini zaslađivači, poput neotama, poseduju visok afinitet za adsorpciju na sedimentu prilikom raspodele u sistemu voda-sediment. Zbog toga je u ovom radu razvijen i optimizovan postupak pripreme uzoraka sedimenata metodom ultrazvučne ekstrakcije za određivanje tragova neotama. Nakon predtretmana, rečni sedimenti (2 g) su ekstrahovani pomoću dihlormetana (3×5 cm^3) u ultrazvučnom kupatilu u trajanju od 3×5 min. Dobijeni ekstrakti su analizirani metodom tečne hromatografije sa tandem masenom spektrometrijom. Razvijena metoda je primenjena na uzorke sedimenata iz nekoliko reka u Srbiji – Tise, Morave, Save i Dunava. Po prvi put su dobijeni podaci o stepenu zagađenosti sedimenata u Srbiji veštačkim zaslađivačem neotamom, detektovanom u koncentracijama od 2 do 48 μg g^{-1}.

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Determination of artificial sweetener neotame in river sediments

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Artificial sweeteners are known as emerging pollutants in the environment. For decades they have been used as food and pharmaceutical additives, which is why they are widespread in natural waters, due to incomplete wastewater treatment. However, some sweeteners, such as neotame, possess a high sorption affinity and partition to sediment in the water-sediment system. Therefore, in this paper, a method for the sediment sample preparation using an ultrasonic extraction for determination of neotame traces was developed and optimized. After pre-treatment, river sediments (2 g) were extracted using dichloromethane (3×5 cm^3) in an ultrasonic bath for 3×5 min. The obtained extracts were analyzed by liquid chromatography with tandem mass spectrometry. The developed method was applied to sediment samples from several rivers in Serbia – the Tisza, the Morava, the Sava and the Danube. For the first time, data on the contamination level of sediments in Serbia with artificial sweetener neotame (in the concentration range from 2 to 48 μg g^{-1}) were obtained.

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AH P 3

Tečno-hromatografsko ispitivanje mogućnosti uklanjanja komercijalne formulacije tiakloprida primenom magnetitom modifikovanih višezidnih ugljeničnih nanocevi

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Ispitivana je mogućnost uklanjanja tiakloprida (TIA) početne koncentracije 2,0 μg mL^{-1} iz rastvora komercijalne formulacije Calypso SC 480 primenom višezidnih ugljeničnih nanocevi modifikovanih sa 2,5 % i 10 % magnetita suspendovanih u vodenoj sredini. Ispitan je i uticaj različitih koncentracija H_2O_2 (21,8 i 43,5 μg mL^{-1}) na efikasnost uklanjanja TIA u pomenutim sistemima. U toku 40 min kontaktnog vremena, za praćenje koncentracije ciljnog analita primenjena je HPLC-DAD tehnika. Oba nanokompozitna materijala su se pokazala kao efikasni adsorbensi, pri čemu dodatkom H_2O_2 može se smatrati da je TIA potpuno uklonjen iz sistema u toku prvih 5 min kontaktnog vremena. Takođe, dobijeni rezultati ukazuju da se pored adsorpcije odigrava i proces degradacije TIA.

Liquid chromatographic investigation of possibility of thiacloprid commercial formulation removal by magnetite modified multiwalled carbon nanotubes

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The possibility of thiacloprid (TIA) removal of the initial concentration 2.0 μg mL^{-1} from the solution of the commercial formulation Calypso SC 480 by multiwalled carbon nanotubes modified with 2.5 % and 10 % magnetite suspended in an aqueous media was investigated. The influence of different concentrations of H_2O_2 (21.8 and 43.5 μg mL^{-1}) on the efficiency of TIA removal in these systems was examined. During the 40 min contact time, the HPLC-DAD technique was used for monitoring the target analyte concentration. Both nanocomposite materials have been shown to be effective adsorbents, while with the addition of H_2O_2, it can be considered that the TIA is completely removed from the system during the first 5 min of the contact time. Also, the obtained results indicate that in addition to adsorption, the process of degradation of TIA takes place.

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AH P 4 text rada / full text

Ispitivanje antioksidativne aktivnosti različitih ekstrakata kupine spektrofotometrijskim testovima

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U radu je ispitana antioksidativna aktivnost različitih ekstrakata pet sorti kupine, primenom spektrofotometrijskih testova: 2,2'-azino-bis(3-etilbenzotiazolin-6-sulfonska kiselina (ABTS), 2,2-difenil-1-pikrilhidrazil radikal (DPPH), redukcija gvožđa (FRAP) i redukciona sposobnost (RP). Najveća antioksiadativna aktivnost zabeležena je u ekstraktima gde je kao rastvarač korišćen 80 % metanol sa 1 % HCl, dok je najmanja aktivnost zabeležena u vodenim ekstraktima. Vrednosti antioksidativne aktivnosti ekstrakata kupine prema ABTS radikal katjonu se kreću u granicama od 0,1960 mmol TE/g do 0,5462 mmol TE/g, dok se prema DPPH radikalu kreću u granicama od 3,33 mmol TE/g do 13,1 mmol TE/g. Vrednosti antioksidativne aktivnosti ovih uzoraka, izražene preko redukcione moći u testovima FRAP i RP, su u intervalu od 17,11 mmol FE/g do 52,6 mmol FE/g, i od 13,3 mmol AAE/g do 31,6 mmol AAE/g. Korelaciona analiza između primenjenih metoda za antioksidativnu aktivnost pokazala je dobru korelaciju između ABTS i DPPH metode, kao i između FRAP i RP metode.

Examination of antioxidant activity of different blackberry extracts by spectrophotometric assays

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The aim of this work was to determine the antioxidant activity of different extracts obtained from five cultivars of blackberry fruits (*Rubus spp*.). The total antioxidant capacities of extracts were measured using four in vitro spectrophotometric methods: 1,1-diphenyl-2-picryl-hydrazyl free radical (DPPH) scavenging activity, 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulphonic acid) (ABTS) radical cation scavenging activity, ferric reducing-antioxidant power (FRAP) and reduction power (RP) Fe(III) to Fe(II). The highest antioxidant activity has been measured in acidified methanol extracts, while the lowest activity has been measured in aqueous extracts. The antioxidant activity measured by the ABTS and DPPH ranged from 0.1960 mmol TE g^{-1} to 0.5462 mmol TE g^{-1} and from 3.33 mmol TE g^{-1} to 13.1 mmol TE g^{-1}. The activity measured by the FRAP and RP ranged from 17.11 mmol FE g^{-1} to 52.6 mmol FE g^{-1} and from 13.3 mmol AAE g^{-1} to 31.6 mmol AAE g^{-1}. Strong correlation has been observed between the DPPH and ABTS method, as well as between the FRAP and RP method.

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AH P 5

Klasifikacija školjki na osnovu sadržaja esencijalnih elemenata i hemometrije

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Cilj ove studije je klasifikacija biološki različitih vrsta školjki na osnovu sadržaja esencijalnih elemenata primenom hemometrije. Sadržaj esencijalnih elemenata kao što su Co, Cr, Cu, Mn, Ni, Se, Zn, i Fe je određen u četiri biološki različite vrste školjki *Ruditapes philippinarum* (Manila clam, MC), *Yesso scallop* (YS), *Tegillarca granosa* (TG) i *Anadara broughtonii* (AB). Analizitani uzorci su kupljeni u Incheonu, Koreja. Sadržaj esenicjalnih elemenata je određen primenom induktivno spregnute plazme kuplovane sa masenom spektrometrijom (ICP-MS) nakon mikrotalasne digestije. Hemometrijske tehnike pokazuju grupisanje ispitivanih uzoraka školjki prema sadržaju esencijalnih elemenata i identifikuju elemente najvažnije za klasifikaciju.

Chemometric characterization of sellfish according to their element composition

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The main aim of current study was classification of four biologically different sellfish species such as bivalve molluscs *Ruditapes philippinarum* (Manila clam, MC), *Yesso scallop* (YS), *Tegillarca granosa* (TG) and *Anadara broughtonii* (AB) bought in the Incheon, South Korea. Content of essencial ellements such as Co, Cr, Cu, Mn, Ni, Se, Zn, and Fe were determined by using inductively coupled plasma mass spectrometry (ICP-MS) after closed-vessel microwave digestion. Chemometrics techniques showed classification of sellfish smaples based on biological species and identified elements most important for classification.

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AH P 6

Analiza elemenata u jezičastim cvetovima kamilice atomskom apsorpcionom spektroskopijom

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Rad povučen

Konzumirane u formi čaja, mnoge lekovite bil[illegible] i raznih oboljenja. Jedan od najčešće kon[illegible] vetova kamilice (*Maricari*[illegible] a dan) je kori[illegible] ovog čaja konz[illegible] dravstveno bezbednog čajno, [illegible] og biljnog materijala. Cilj ovog rada bio je [illegible], naročito sadržaja toksičnih teških metala, u jezičas[illegible] gajene na teritoriji AP Vojvodine, Srbija. Određivanje sadržaja Fe, Zn, [illegible], Cd i Pb je izvedeno primenom atomske apsorbcione spektroskopije. Dobijeni rezultati pokazali su da je biljka bogata mikro elementima, dok prisutrvo teških metala nije detektovano.

Elemental analysis of chamomile ligulate flowers by using atomic absorption spectroscopy

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Withdrawn

Consumed in the form of tea, many medicinal plants have significant role in prevention of numerous diseases. One of the most common herbal tea is made fr[illegible] amomile (*Maricaria chamomilla* L.) flowers. For centuries, 3-4 cups [illegible] en used for promoting digestion or calming gastritis. T[illegible] this tea are consumed daily. In order to [illegible] sary to monitor the compos[illegible] milate elemen[illegible] the plant coul[illegible] study was evaluation of mi[illegible] amomile ligulate flowers from AP Vojvo[illegible], Zn, Cr, Ni, Mn, Cd and Pb was performed by using a[illegible] troscopy. Obtained results demonstrated that this plant is opulent [illegible] elements, while the presence of heavy metals in the investigated sample was not detected.

The present work was carried out within the projects of the Serbian Ministry of Education, Science and Technological Development (Project No. TR31013).

AH P 7

Nano-Fe_2O_3 čestice kao pojačivači voltametrijskog signala u indikaciji teških metala i pesticida

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Nanočestice na bazi oksida gvožđa (NPs) su privukle veliku pažnju imajući u vidu njihove fizičke, posebno magnetne, i hemijske osobine. U ovom istraživanju su nanočestice gvožđe(III)-oksida (Fe_2O_3 NPs) sintetisane jednostavnim hemijskim metodom u čvstom stanju iz dve različite soli, $FeSO_4 \cdot 7H_2O$ i $FeCl_3 \cdot H_2O$, u molskom udelu (1 : 2,5). Veličina NPs od 3 nm i njihov sferni oblik su određeni TEM merenjima. Dobijene NPs su dispergovane u vodi i monodisperzni koloid je okarakterisan UV-Vis i FTIR spektroskopijom, i merenjem zeta potencijala. Voltametrija sa obogaćivanjem i anodnim rastvaranjem i diferencijalana pulsna voltametrija su pokazale poboljšanje u kvantifikaciji odabranih teških metala i pesticida u uzorcima rečnih voda, kroz značajan pojačavajući efekat signala sintetisanih Fe_2O_3 NPs koji je zabeležen u elektrohemijskoj detekciji različitih vrsta važnih zagađivača životne sredine.

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Nano-Fe_2O_3 particles as voltammetric signal amplifiers in sensing of heavy metals and pesticides

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Iron oxide nanoparticles (NPs) has attracted great attention due to their unique physical, especially magnetic, and chemical properties. In this study, the iron(III)-oxide NPs (Fe_2O_3 NPs), were synthesized by a simple solid-state chemical method from two different ion salts, $FeSO_4 \cdot 7H_2O$ and $FeCl_3 \cdot H_2O$, in the molar ratio (1 : 2.5). The NPs size, 3 nm, and their spherical shape were evaluated by TEM measurements. The obtained NPs were dispersed in water and, monodisperse colloid was characterized by UV-Vis and FTIR spectroscopy and zeta potential measurements. Anodic stripping and differential pulse voltammetric measurements were shown improvement in the quantification of selected heavy metal ions and pesticide in river water samples, due to significant amplification effect of synthesized Fe_2O_3 NPs on electrochemical detection signal recorded at electrodes from different carbon materials. This study offers promising results which can lead to the application of iron NPs in the electroanalytical determination of different kinds of serious environmental pollutants.

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AH P 8

Procena zavisnosti između bioraspoloživosti i osobina molekula odabranih antihipertenziva

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Inhibitori enzima koji konvertuje angiotenzin (*ACEI*), blokatori kalcijumovih kanala (*CCB*) kao i antagonisti receptora angiotenzina II (*ARB*), predstavljaju danas često propisivane lekove koji imaju primenu u lečenju hipertenzije, odnosno povišenog krvnog pritiska. Cilj ovog rada bio je da se za dvadeset šest antihipertenzivnih lekova iz tri različite grupe, ACEI, CCB kao i ARB, proceni zavisnost između njihove bioraspoloživosti i fizičko-hemijskih osobina molekula. Za sve ispitivane lekove, primenom softverskih paketa izračunate su vrednosti deskriptora molekula: molekulska masa, volumen, polarna površina kao i različiti deskriptori lipofilnosti (logP vrednosti). Primenom proste linearne regresione analize dobijene su niske vrednosti koeficijenata korelacije ($R < 0,25$) za zavisnosti između podataka o bioraspoloživosti i izračunatih osobina molekula. U nastavku istraživanja, primenom višestruke regresione analize, ispitana je zavisnost bioraspoloživosti i lipofilnosti ispitivanih molekula uz primenu polarne površine, molekulske mase ili volumena kao nezavisno promenljive. Najbolja korelacija ($R = 0,70$) dobijena je primenom višestruke regresione analize između podataka o bioraspoloživosti, lipofilnosti i polarne površine odabranih molekula. Dobijeni rezultati ukazuju na značajnu zavisnost bioraspoloživosti odabranih antihipertenziva i osobina njihovih molekula, u prvom redu njihove lipofilnosti.

The evaluation of relationship between bioavailability and molecular properties of selected antihypertensive drugs

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Angiotensin-converting enzyme inhibitors (ACEI), calcium channel blockers (CCBs) as well as angiotensin II receptor antagonists or blockers (ARBs) are commonly prescribed antihypertensive drugs. The aim of this work was to investigate relationships between bioavailability and calculated molecular properties for twenty-six antihypertensive drugs from different groups, ACEI, CCBs and ARBs. With application of different software packages several molecular descriptors, polar surface area, molecular mass, volume and lipophilicity descriptors (log*P*) of selected antihypertensive drugs were calculated. Simple linear regression analysis showed the low correlation ($R < 0.25$) between bioavailability of selected drugs and their calculated molecular descriptors. Following, multiple linear regression analysis was applied to investigate further correlations between bioavailability, lipophilicity and polar surface area, molecular mass or volume as one additional independent variable. The best correlation ($R = 0.70$) was proven between bioavailability, lipophilicity and polar surface area as the independent variable. The results obtained indicate a important relationship between antihypertensive drugs bioavailability and their molecular properties on the first place their lipophilicity.

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AH P 9 text rada / full text

Degradacija organofosfornog insekticida pomoću hlor-dioksida

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U ovom radu je ispitivana degradacija organofosfornog insekticida (malationa) primenom hlor-dioksida. Degradacija je proučavana u dejonizovanoj vodi. Optimizacija uslova degradacije je ispitivana u uslovima svetlosti, sa različitim dozama hlor-dioksida, posle različitih vremenskih perioda degradacije i pri različitim pH vrednostima rastvora. Ovo je prvo istraživanje gde je degradacija malationa ispitivana upotrebom hlor-dioksida kao degradacionog sredstva. Procenat degradacije je određen pomoću HPLC-DAD, dok su degradacioni proizvodi izolovani i indentifikovani pomoću GC/MS. Rezultati su pokazali da pH ima značajan uticaj na stepen degradacije malationa. Ispitivani insekticid pokazuje dobar stepen degradacije. Vrednost stepena degradacije pri optimalnim uslovima za malation je 97,78 % primenom 5 mg/L hlor-dioksida na pH 7,00 posle 24 h tretmana. Analizom masenih spektara malationa utvrđeno je da su dobijeni degradacioni proizvodi: dietil 2-hidroksisukcinat, dietil fumarat, dimetil hidrogen fosfat, dietil 2-((dimetoksifosforil)tio)sukcinat.

Degradation of organophosphorus insecticide by chlorine dioxide

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In this paper, the degradation of organophosphorus insecticide (malathion) with chlorine dioxide was investigated. Degradation was studied in deionized water. Optimization of degradation conditions was examined under light condition, with different doses of chlorine dioxide, after different degradation times and at different pH values. This is the first study where degradation of malathion was done using chlorine dioxide as a degradation agent. The percentage of degradation was determined by HPLC-DAD, while the degradation products were isolated and identified by GC-MS. The results showed that pH has a significant influence on the degree of degradation. The value of degradation degree determined under the optimal conditions for malathion was 97.78 % using 5 mg/L chlorine dioxide at pH 7.00 after 24 h of treatment. By analyzing mass spectra of malathion, it was found that the resulting degradation products were diethyl 2-hydroxysuccinate, diethyl fumarate, dimethyl hydrogen phosphate and diethyl 2-((dimethoxyphosphoryl)thio)succinate.

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Fizička hemija / Physical Chemistry

FH O 1

Interakcije prelaznih metala sa *N*-metilformamidom kao model sistemom peptidne veze

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Sintetisane su tri nove soli prelaznih metala u cilju proučavanja interakcija sa molekulom *N*-metilformamida (NMF), kao model sistemom peptidne veze. Da bi se izbegle sporedne interakcije između katjona i anjona komercijalno dostupnih soli i dobili relevantni podaci o njihovim interakcijama sa NMF, sintetisane su nove soli sa nekoordinišućim perhloratnim anjonom i NMF kao solvatom. Sintetisane soli su kobalt(II)-perhlorat $Co(ClO_4)_2 \cdot 6NMF$, nikal(II)-perhlorat $Ni(ClO_4)_2 \cdot 6NMF$ i bakar(II)-perhlorat $Cu(ClO_4)_2 \cdot 4NMF$. Njihova struktura je potvrđena rentgeno-strukturnom analizom. Urađena su denzimetrijska, viskozimetrijska, konduktometrijska i spektrofotometrijska merenja rastvora soli u NMF, na temperaturi od 298,15 K i koncentracijama do 0,2 mol dm^{-3}. Spektrofotometrijski podaci, negativne vrednosti prividne molarne zapremine i visoke vrednosti *B*-koeficijenta *Jones-Dole*-ove jednačine ukazuju na snažne jon-dipol interakcije i formiranje kompleksa između molekula NMF i ispitivanih jona, čak i u prisustvu vode.

Ovaj rad je realizovan u okviru projekta ON172012, Ministarstva za nauku, prosvetu i tehnološki razvoj Republike Srbije

Interactions of transition metal ions with *N*-methylformamide as a peptide bond model system

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The three newly synthesized transition metal salts were investigated in order to show the interactions between transition metal ions with *N*-methylformamide (NMF), as a peptide-bond model system. In order to eliminate additional interactions between the cations and anions from commercially available inorganic salts and to obtain the most relevant data for their interactions with NMF, new complex compounds with the *N*-methylformamide and non-coordinating perchlorate anion were synthesized and used for measurements. The salts that were studied are the following: $Co(ClO_4)_2 \cdot 6NMF$, $Ni(ClO_4)_2 \cdot 6NMF$ and $Cu(ClO_4)_2 \cdot 4NMF$. Their structure was confirmed by the X-ray crystallographic data analysis. Density, viscosity, electrical conductivity and spectrophotometric measurements of salt solution in NMF were performed at 298.15 K and in the concentration range from up to ~ 0.2 $moldm^{-3}$. Spectrophotometric data, negative values of apparent molar volumes at infinite dilution of ions and high values of the *B*-coefficient of the Jones-Dole viscosity equation indicate strong ion-dipole interactions and the formation of complexes between NMF molecules and investigated ions, even in the presence of water.

FH P 1 text rada / full text

Isoljavanje i sinergizam pri ekstrakciji salicilne kiseline iz vodenih rastvora

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Ispitivan je uticaj NaCl, KCl i $(NH_4)_2SO_4$ na ekstrakciju salicilne kiseline iz vodenih rastvora dietil-etrom, kao i efekat sinergizma pri ekstrakciji binarnim smešama dietil-etar/1-butanol iz vodenih rastvora koji sadrže NaCl. Konstante isoljavanja za ispitivane soli opadaju u nizu $K_s((NH_4)_2SO_4) > K_s(NaCl) > K_s(KCl)$, a dobijene vrednosti su uporedive sa literaturnim vrednostima koje su dobijene merenjem rastvorljivosti salicilne kiseline. Najveća vrednost koeficijenta sinergizma dobijena je pri ekstrakciji binarnom smešom u kojoj je molski udeo dietil-etra 0,568. Međutim, najefikasnija ekstrakcija salicilne kiseline (najveća vrednost distribucionog koeficijenta) postignuta je pri ekstrakciji binarnom smešom u kojoj je molski udeo dietil-etra 0,778. Razultati dobijeni u ovom radu mogu se koristiti za poboljšanje efikasnosti ekstrakcije salicilne kiseline, što je značajno kod pripreme uzoraka za analizu različitim metodama. Takođe se ovi rezultati mogu koristiti za bolju fizičko-hemijsku karakterizaciju salicilne kiseline.

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Salting-out and synergism in the extraction of salicylic acid from aqueous solutions

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The influence of NaCl, KCl, and $(NH_4)_2SO_4$ on the extraction of salicylic acid from aqueous solutions with diethyl ether, as well as synergic effects in the extraction of salicylic acid with diethyl ether/1-butanol binary solvent mixtures from aqueous solutions containing NaCl, were investigated. The salting-out constants for the salts investigated were ordered as $K_s((NH_4)_2SO_4) > K_s(NaCl) > K_s(KCl)$ and the obtained values are comparable with literature data obtained by the salicylic acid solubility measurements. The highest value of synergic coefficient was obtained for a binary solvent mixture containing 0.568 mole fraction of diethyl ether. However, the most efficient extraction of salicylic acid (highest value of distribution ratio) was achieved with the binary solvent mixture with 0.778 mole fraction of diethyl ether. The results obtained in this study may be used for improving extraction efficiency of salicylic acid which is important in the sample preparation step for its determination by various methods. Also, these results may be used for a better physicochemical characterization of salicylic acid.

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FH P 2 text rada / full text

Uticaj niskofrekventnog magnetnog polja (10-50 Hz) na respiracionu aktivnost ćelija kvasca *Saccharomyces cerevisiae*

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Ispitivanje uticaja električnog, magnetnog i elektromagnetnog polja na mikroorganizme je veoma aktuelni predmet istrazivanja, jer ova fizička polja potencijalno deluju kao faktori stresa i tako utiču na mikrobni metabolizam i preživljavanje. U ovom radu ispitivan je uticaj niskofrekventnog magnetnog polja (MP) sa konstantnim intervalom skeniranja od 10 do 50 Hz na respiraciju ćelija kvasca, *S. cerevisiae*. Eksperiment je rađen u pet ponavljanja i praćen Micro-Oxymax® respirometrom. Kumulativna potrošnja kiseonika je bila manja kod ćelija izloženih MP u svih pet ponavljanja, dok je produkcija CO_2 bila nekonzistentna. Međutim, ove razlike u potrošnji O_2 i produkciji CO_2 su statistički značajne. Iako su dodatna ispitivanja neophodna, dobijeni rezultati ovih inicijalnih eksperimenata predstavljaju dobru osnovu za dalja istraživanja u ovoj oblasti.

Influence of the low frequency magnetic field with scan regime from 10 Hz to 50 Hz on *Saccharomyces cerevisiae* respiration

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The analysis of the electric, magnetic and electromagnetic fields influence on microorganisms is a very popular research topic, since these fields could potentially act as stressors and affect the microbial metabolism and survival. The aim of this work was to investigate the influence of the low frequency magnetic field (MF) with scan regime from 10 Hz to 50 Hz on *S. cerevisiae* respiration. The experiment was performed in five replicates and monitored using the Micro-Oxymax® respirometer. All five experiments showed lower cumulative O_2 consumption in MF exposed samples, compared to the control sample and inconsistent cumulative CO_2 production. However, these differences in O_2 consumption and CO_2 production were statistically significant. Even though additional experiments are necessary, these results strongly suggest that this is a good basis for further investigation in this field.

FH P 3

Imobilizacija enzima za razvoj biokatalitičkih sistema u stabilnim disperzijama

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Imobilizacija enzima ili jedinjenja koja oponašaju enzime predstavlja obećavujući pravac istraživanja koji vodi razvoju novih biokatalizatora sa istom aktivnošću ali smanjenom osetljivošću u odnosu na prirodne enzime. Cilj dosadašnjeg istraživanja bio je razvoj antioksidativnih bionanokompozitnih jedinjenja koja se sastoje od nanocevastih struktura halojzita, protamin - sulfata kao polielektrolita i enzima superoksidne dismutaze.
Nanocevi halojzita poseduju negativno naelektrisanje i dovoljnu stabilnost da formiraju stabilne disperzije. Međutim, njihova otpornost na agregaciju izazvanu solima je prilično niska. Protamin – sulfat se snažno adsorbuje na suprotno naelektrisanu nanocevastu strukturu halojzita, što dovodi do neutralizacije i do preusmeravanja naelektrisanja pri odgovarajućim dozama. Enzim superoksid dismutaza je imobilizovan na protamin-sulfat-funkcionalizovanim nanocevima halojzita preko elektrostatičkih, hidrofobnih i vodoničnih interakcija. Enzimatski testovi su pokazali da enzim superoksid dismutaza zadržava svoju funkciju i pokazuje visoku aktivnost u dismutaciji superoksidnih radikala nakon imobilizacije. Na taj način je dobijena stabilna bionanokompozitna disperzija.

Immobilization of enzymes for development of biocatalytic systems in stable dispersions

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The immobilization of enzymes or enzyme mimicking compounds is a promising research direction towards the development of novel biocatalysts with the same activity, but less sensitivity than the native enzymes. The aim of the previous research was to develop an antioxidant bionanocomposite that consists of halloysite nanotubes (HNT), protamine sulfate polyelectrolyte (PSP) and superoxide dismutase (SOD) enzyme. The HNT possess negative charge and sufficient stability to form stable dispersions, however, their resistance against salt-induced aggregation is rather low. PSP adsorbs strongly on the oppositely charged HNT giving rise to charge neutralization and charge reversal at appropriate doses. The SOD enzyme was immobilized on the PSP-functionalized HNT through electrostatic, hydrophobic and hydrogen bonding interactions. Enzymatic assays revealed that SOD kept its function and showed high activity in superoxide radical dismutation upon immobilization. In this way, a stable antioxidant bionanocomposite dispersion was obtained.

FH P 4

Uloga vode u procesu konverzije kreatina u kreatinin

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U ovom radu ispitan je uticaj strukturne organizacije molekula vode na konverziju biološki aktivnog molekula kreatina u njegov biološki neaktivan oblik, kreatinin. Kreatin je esencijalna, neproteinska aminokiselina koja se u organizmu metaboliše do fosfokreatina, glavnog oblika skladištenja energije. Dodatna suplementacija kreatinom, kojom se dobija više energije tokom vežbanja, ograničena je njegovom slabom rastvorljivošću u vodi i spontanom konverzijom u kreatinin. Na osnovu volumetrijskih i viskozimetrijskih merenja vodenih rastvora ispitivanih supstanci različitih molaliteta u temperaturnom opsegu od 293,15 do 313,15 K, kao i računarskih simulacija (molekulske dinamike I DFT proračuna) proučavane su interakcije između kreatina/kreatinina i vode, njihove *structure making/breaking osobine*, kao i uticaj temperature na njih. Dobijeni rezultati ukazuju na to da je brža konverzija kreatina u kreatinin na povišenim temperaturama posledica smanjenja broja molekula vode u hidratacionoj sferi kreatina, što može da dovede do olakšanog formiranja neutralne forme kreatina i zatim do njegove ciklizacije.

Ovaj rad je realizovan u okviru projekta ON172012, Ministarstva za nauku, prosvetu i tehnološki razvoj Republike Srbije.

The water role in the conversion process of creatine into creatinine

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In this paper, the influence of the structural organization of the water molecule on the conversion of biologically active creatine into its inactive form, creatinine, was examined. Creatine is an essential, non-proteinaceous amino acid that is metabolized to the phosphocreatine, the main energy storage form in the organism. Additional creatine supplementation, which generates more energy during exercises, is limited by its low solubility in water and spontaneous conversion into creatinine. Based on volumetric and viscometric measurements of creatine/creatinine aqueous solutions at different molalities in the temperature range from 293.15 to 313.15 K, as well as on the results of computational simulations (molecular dynamics and DFT calculations), interactions between creatine/creatinine and water, their *structure making/breaking* properties were studied, as well as the temperature influence on them. The obtained results suggest that a faster conversion of creatine into creatinine at a higher temperature can be explained by a decrease of the number of water molecules in the hydration shell of creatine, which may lead to the more favourable formation of creatine neutral form and further cyclization.

FH P 5

Fizičko-hemijska i elektrohemijska karakterizacija elektrolita za litijum-jonske baterije

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Elektrolit na bazi jonske tečnosti (JT) je ispitan u cilju optimizacije elektrolita za litijum-jonske baterije (LIB) niske zapaljivosti, visoke termičke stabilnosti i visoke provodljivosti. Ispitana su fizičko-hemijska svojstva i zapaljivost elektrolita koji sadrži litijumovu so LiTFSI dodatu u jonsku tečnost 1,3-dietilimidazolijum *bis*(trifluorometilsulfonil)imid ([C_2C_2im][TFSI]). Elektrolit LiTFSI/C_2C_2imTFSI je testiran na TiO_2 nanotubama kao anodnim materijalom. U cilju poboljšanja bezbednosnih svojstava litijum-jonskih baterija, elektrohemijska svojstva LiTFSI/C_2C_2imTFSI upoređena su sa LiTFSI/C_2C_1imTFSI elektrolitom koji sadrži drugu jonsku tečnost, kao i sa elektrolitom koji sadrži komercijalni organski rastvarač, *γ*-butirolakton, GBL (LiTFS/[C_2C_2im][TFSI]/GBL). Ćelija sa LiTFSI/C_2C_1imTFSI/GBL elektrolitom pokazuje bolje elektrohemijske performanse posle 150 ciklusa punjenja-pražnjenja i nakon izlaganja na povišenoj temperaturi, T = 328,15 K.

Ovaj rad je realizovan u okviru projekta ON172012, Ministarstva za nauku, prosvetu i tehnološki razvoj Republike Srbije.

Physicochemical and electrochemical characterisation of electrolyte for lithium-ion batteries

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Electrolyte based on ionic liquid (IL) is investigated as the optimal electrolyte for lithium-ion batteries (LIBs) that can combine low flammability, high thermal stability and high conductivity. Physicochemical properties of the electrolyte after addition of LiTFSI in 1,3-diethylimidazolium *bis*(trifluoromethylsulfonyl) imide ([C_2C_2im][TFSI]) are investigated. Electrolyte LiTFSI/C_2C_2imTFSI was used for cycling TiO_2 nanotube arrays electrode as anode material. In an attempt to realize LIBs with enhanced safety, herein are investigated electrochemical properties of the LiTFSI/C_2C_1imTFSI and compared with LiTFSI/C_2C_1imTFSI as well with electrolyte containing the commercial organic solvent, *γ*-butyrolactone, GBL (LiTFSI/[C_2C_1im][TFSI]/GBL). It was shown that LiTFSI/C_2C_1imTFSI/GBL electrolyte displayed higher current efficiencies after 150 full charge-discharge cycles and after cell exposure to elevated temperature, T = 328.15 K.

Elektrohemija / Electrochemistry

EH O 1 text rada / full text

Bimetalni nanokatalizatori kontrolisanog oblika za anodne reakcije u gorivnim galvanskim spregovima

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Sve veće potrebe za proizvodnjom energije iz obovljivih izvora, uslovile su intenzivna istraživanja u pravcu korišćenja ekološki prihvatljivih goriva. Oksidacijom vodonika u gorivnim spregovima postiže se proizvodnja energije na ekološki prihvatljiv način, a umesto vodonika mogu se koristiti i mali organski molekuli, poput mravlje kiseline koji su bezbedniji za upotrebu i transport. Njihova oksidacija u anodnom delu polimer elektrolitnog gorivnog sprega zahteva upotrebu plemenitih metala kao katalizatora, jer mogu da omoguće njihovu dehidrogenaciju kao početni stupanj reakcije. Kao do sada najbolji katalizatori za oksidaciju mravlje kiseline pokazali su se bimetalni PtAu katalizatori, zahvaljujući geometrijskom efektu zlata na platinu kojim se favorizuje direktni mehanizam oksidacije i izbegava stvaranje reakcionog intermedijara CO koji se ponaša kao katalitički otrov. U ovom radu PtAu katalizatori na aktiviranom ugljeniku sintetizovani su mikroemulzionim postupkom, sa uticajem aditiva kojim je izmenjen oblik čestica, čime je dodatno poboljšana njihova katalitička sposobnost.

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Shape controlled bimetallic nanocatalysts for anodic reactions in fuel cells

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Ever rising needs for renewable energy, in order to decrease pollution and exploitation of limited fossil resources, have caused intensive research on the use of eco friendly fuels. Hydrogen electrooxidation in fuel cells is a promissing process of zero-emission energy production from a renewable source. Furthermore, using small organic molecules (SOMs) such as formic acid, instead of hydrogen, makes this process safer and fuel transportation easier to manage. Oxidation of SOMs in fuel cells requires a noble metal as catalyst, capable of enabling dehydrogenation of SOM as an initial step of the reaction. Bimetallic PtAu catalysts are the best catalysts for formic acid oxidation so far, due to the ensemble effect of Au on Pt which favors the direct oxidation of formic acid, avoiding the formation of CO that acts as a catalytic poison. In this reseach carbon supported PtAu nanocatalysts were synthesized by a microemulsion method, in presence of a capping agent that affected the particle shape, which made further improvement in catalytic performance of these nanoparticles.

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EH O 2

Elektroforetsko taloženje antibakterijske kompozitne prevlake hidroksiapatita sa hitozanom, grafenom i gentamicinom

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U ovom radu su ispitivane kompozitne prevlake koje se sastoje od hidroksiapatita (HAP), hitozana (CS) i grafena (Gr), sa i bez gentamicina (Gent) dobijene postupkom elektroforetskog taloženja (EPD). Taloženje je izvedeno u jednom koraku iz četvorokomponentne vodene suspenzije (HAP/CS/Gr/Gent) pri konstantnom naponu na titanskim (Ti) pločicama. Uticaj Gr i Gent je detaljno istražen primenom različitih fizičko-hemijskih i bioloških analiza. Karakteristike dobijenih HAP/CS/Gr i HAP/CS/Gr/Gent prevlaka ispitivane su infracrvenom spektroskopijom sa Furijeovom transformacijom (FT-IR), skenirajućom elektronskom mikroskopijom (FE-SEM), rendgenskom fotoelektronskom spektroskopijom (XPS) i rendgenskom difrakcionom analizom (XRD). Ispitivanja antibakterijske aktivnosti prema *Escherichia coli* i *Staphylococcus aureus* izvršena su metodom agar difuzije i testa u suspenziji, a citotoksičnost MTT testom na ćelijskim linijama MRC-5 i L929. Dobijeni rezultati ukazali su na veliki potencijal elektroforetski istaloženih kompozita za medicinske primene.

Electrophoretic deposition of antibacterial composite hydroxyapatite coating with chitosan, graphene and gentamicin

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In this work composite coatings consisting of hydroxyapatite (HAP), chitosan (CS) and graphene (Gr), with and without gentamicin (Gent) produced by electrophoretic deposition process (EPD) were investigated. Deposition was performed in a single step from the four-component aqueous suspension (HAP/CS/Gr/Gent) at a constant voltage on titanium (Ti) plates. The influence of Gr and Gent has been thoroughly explored using various physico-chemical and biological analyses. The characteristics of the obtained HAP/CS/Gr and HAP/CS/Gr/Gent coatings were investigated using Fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), X-ray photoelectron analysis (XPS) and X-ray diffraction (XRD) techniques. Antibacterial efficacy assays against *Escherichia coli* and *Staphylococcus aureus* were performed by agar diffusion method and in suspension testing, while cytotoxicity was elucidated using MTT test toward MRC-5 and L929 cell lines. Obtained results pointed out high potential of electrodeposited composites for medical applications.

EH O 3

Novi materijali za obloge za rane sa elektrohemijski sintetisanim nanočesticama srebra

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Nauka i inženjerstvo biomaterijala u poslednje vreme pokazuju sve veću težnju ka pronalaženju novih materijala za obloge za rane, gde su naročito važna poboljšana svojstva kao što su apsorpciona moć, mehanička svojstva i niska adhezivnost. Umrežene matrice hidrogelova su odlični potencijalni nosači za kontrolisano otpuštanje antibakterijskih agenasa, kao što su nanočestice srebra. Hitozan je posebno interesantna komponenta obloga za rane, zbog svoje prirodne antibakterijske aktivnosti i sposobnosti stabilizacije nanočestica. Cilj ovog rada je priprema novih obloga za rane na bazi polivinil-alkohola i hitozana sa elektrohemijski sintetisanim nanočesticama srebra, u obliku hidrogela. Dobijene su sferne nanočestice srebra, prečnika oko 5-10 nm, što je potvrđeno UV-vidljivom spektroskopijom i transmisionom elektronskom mikroskopijom. Bubrenje i otpuštanje srebra je praćeno u fosfatnom puferu koji imitira fiziološke uslove, dok je antibakterijska aktivnost potvrđena na bakterijskim sojevima *Staphylococcus aureus* i *Escherichia coli*. Dobijeni netoksični hidrogelovi (što je utvrđeno MTT testom) imaju izuzetan potencijal za primene kao obloge za rane nove generacije.

Novel wound dressing materials containing electrochemically synthesized silver nanoparticles

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Recently, the biomaterials science and engineering fields have seen a shift towards novel hydrogel materials, especially for wound dressing applications where improved properties, such as high sorption ability, good mechanical properties and low adhesiveness are of utmost importance. The cross linked hydrogel matrices are excellent potential carriers for controlled release of antibacterial agents, such as silver nanoparticles (AgNPs). Chitosan is an especially attractive option for wound dressing applications, because of its intrinsic antibacterial activity and the ability to stabilize AgNPs. The aim of this work is the production of poly(vinyl alcohol) and chitosan based hydrogel matrices with electrochemically synthesized AgNPs for wound dressing materials applications. The obtained AgNPs were spherical with 5-10 nm diameters, as confirmed by UV-visible spectroscopy and transmission electron microscopy. The swelling and release behaviors of AgNP-embedded hydrogels were evaluated in phosphate buffer, mimicking physiological environment, and the antibacterial activity was confirmed against both *Staphylococcus aureus* and *Escherichia coli*. The obtained non-toxic hydrogel materials (as affirmed by MTT test) have excellent potential to be used as novel antibacterial wound dressings.

EH P 1

Elektrohemijski sintetizovani kompoziti sa inkorporiranim antibakterijskim agensima

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Elektrohemijske metode su korišćene za sintezu različitih kompozita namenjenih za medicinsku primenu kao antibakterijske prevlake za koštane titanske implantate ili kao visoko efikasni antibakterijski hidrogelovi za ubrzano zarastanje rana. Elektroforetskim taloženjem (EPD) u jednom koraku pri konstantnom naponu, uspešno je dobijena kompozitna prevlaka na bazi hidroksiapatita (HAP), hitozana (CS) i gentamicina (Gent) iz vodene suspenzije na titanu. Sadržaj gentamicina je kvantifikovan pomoću tečne hromatografije sa ultravioletnom (UV) detekcijom. Prevlaka HAP/CS/Gent je pokazala dobru antibakterijsku aktivnost protiv *Staphylococcus aureus* i *Escherichia coli*, što ukazuje na visok potencijal za biomedicinske primene. Biokompatibilni nanokompozitni hidrogel polivinil-alkohol/hitozan/grafen (PVA/CHI/Gr) sa nanočesticama srebra (AgNPs) dobijen je *in situ* elektrohemijskom sintezom u matrici nabubrelih hidrogelova PVA/CHI/Gr. Otpuštanje srebra je praćeno tokom 28 dana, a dobijeni profili ukazuju na postepeno kontrolisano otpuštanje tokom ovog perioda. Antibakterijska aktivnost prema *S.aureus* i *E.coli* je potvrđena testom u suspenziji i agar-difuzionom metodom.

Electrochemically synthesized composites with incorporated antibacterial agents

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Electrochemical methods were used for the synthesis of various composites intended for medical use as antibacterial coatings for bone titanium implants or as highly effective antibacterial hydrogels for accelerated wound healing. Electrophoretic deposition (EPD) in a single step at the constant voltage was successfully used to obtain composite coating based on hydroxyapatite (HAP), chitosan (CS) and gentamicin (Gent) from an aqueous suspension on titanium. Gentamicin content was quantified by liquid chromatography with ultraviolet (UV) detection. HAP/CS/Gent coating exhibited good antibacterial activity against *Staphylococcus aureus* and *Escherichia coli,* indicating the high potential for biomedical applications. Biocompatible poly(vinyl alcohol)/chitosan/graphene (PVA/CHI/Gr) nanocomposite hydrogel loaded with silver nanoparticles (AgNPs) was produced by *in situ* electrochemical synthesis in the pre-swollen PVA/CHI/Gr hydrogel matrix. Silver release was monitored for 28 days and the obtained profiles indicate slow controlled release over chosen time period. Antibacterial activity against *S.aureus* and *E.coli* was confirmed by in suspension testing and by disc-diffusion method.

EH P 2

Uticaj termomehaničke obrade na elektrohemijsko ponašanje sinterovanih bakar-zlato legura

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Sinterovane Cu-Au legure podvrgnute su kompleksnoj termomehaničkoj obradi koja je obuhvatala: predzavršno valjanje, rastvorno žarenje sa kaljenjem, završno valjaje i žarenje ispod i iznad temperature rekristalizacije. Vršeno je merenje potencijala otvorenog kola i primenjena je metoda ciklične voltametrija u 0,1 M rastvoru NaOH, u cilju analize elektrohemijskog ponašanja sinterovanih Cu-Au legura nakon različitih stadijuma termomehaničke obrade. Primenjena termomehanička obrada uslovila je promene u mikrostrukturi, što je uticalo i na promene u elektrohemijskom ponašanju sinterovanih Cu-Au legura. Završno valjani uzorci pokazali su najbolju korozionu postojanost u odnosu na ostale termomehanički obrađene uzorke.

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The influence of thermo-mechanical treatment on the electrochemical behavior of sintered copper-gold alloys

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Sintered Cu-Au alloys were subjected to the complex thermo-mechanical treatment, which included: pre-final rolling, solution annealing followed with quenching, final rolling and annealing under and above the recrystallization temperature. The open circuit potential measurements were performed and the cyclic voltammetry method was applied in a 0.1 M NaOH solution in order to analyze the electrochemical behavior of sintered Cu-Au alloys after different stages of thermo-mechanical treatment. The applied thermo-mechanical treatment caused changes in the microstructure, which also influenced the changes in electrochemical behavior of sintered Cu-Au alloys. Finally rolled samples had the best corrosion resistance compared to the other thermo-mechanically treated samples.

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EH P 3

Elektrohemijsko ponašanje čelika u prisustvu macerata kestena

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U ovom radu su prikazani rezultati ispitivanja elektrohemijskog ponašanja čelika X180CrMo12-1 pri oksidaciji u rastvoru 0,3 mol/dm^3 NaCl u odsustvu i prisustvu macerata kestena različitih koncentracija. Elektrohemijsko ponašanje čelika ispitivano je metodom merenja potencijala otvorenog kola i metodom ciklične voltametrije. Rezultati merenja potencijala otvorenog kola pokazuju da su vrednosti potencijala otvorenog kola pozitivnije u odnosu na vrednost potencijala otvorenog kola bez dodatka macerata kestena. Na voltamogramu dobijenom bez prisustva macerata kestena nema jasno definisanih strujnih pikova već samo jedan vrlo širok i nizak strujni talas u širokoj oblasti potencijala pre nego što dođe do naglog porasta gustine struje, i jedan strujni pik na povratnom delu voltamograma. Sa dodatkom macerata kestena vrednosti gustine struje su niže u odnosu na vrednosti gustine struje bez dodatka macerata kestena. Niže vrednosti gustine struje u prisustvu macerata kestena ukazuju na to da macerat kestena pokazuje inhibitorsko dejstvo.

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Electrochemical behaviour of steel in the presence of chestnut macerate

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This paper presents the results of the investigation of electrochemical behaviour of steel X180CrMo12-1 during oxidation in a solution of 0.3 mol/dm^3 NaCl in the absence and in the presence of chestnut macerate of various concentrations. Electrochemical behaviour of steel was tested by the method of measuring the open circuit potential and the cyclic voltammetry method. Results of the open circuit potential measurements show that the values of the open circuit potential are more positive than the value of the open circuit potential without the addition of chestnut macerate. On the voltammogram obtained without the chestnut macerate there are no clearly defined current peaks, but only one very wide and low current wave in a wide range of potentials before a sudden increase in current density, and one current peak at the reverse part of the voltammogram. With the addition of chestnut macerate, the value of the current density is lower than the value of the current density without the addition of chestnut macerate. Lower values of the current densities in the presence of chestnut macerate suggest that chestnut macerate exhibits an inhibitory effect.

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EH P 4

Analiza prisustva inhibitora u alkalnom rastvoru natrijum-karbonata na elektrohemijsko ponašanje hladno deformisane bakarne zice

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U ovom radu je ispitivan uticaj 1M vodenog rastvora Na_2CO_3, sa i bez dodataka inhibitora, želatina i kalijum-etil-ksantata u različitim koncentracijama na koroziono ponašanje hladno deformisane bakarne žice (ε=87, 95 i 99 %). Merene su vrednosti potencijala otvorenog (POK) kola i primenjena je metoda ciklične voltametrije (CV). Merenja POK pokazuju stalni porast pre uspostavljanja konstantne vrednosti. Na voltamogramima zapažaju se dva anodna pika, koji pokazuju da postoji oksidacija bakra do Cu_2O i CuO. Rezultati ukazuju da stepen deformacije između 87 i 99 % nema bitan uticaj na vrednosti POK. Pokazan je pozitivan uticaj želatina u zaštiti od korozije. Međutim, povećanje koncentracije želatina ponovo dovodi do ubrzanja korozionih procesa. Kalijum-etil-ksantat u rastvoru 1M Na_2CO_3 menja mehanizam procesa pri anodnoj polarizaciji. Složeni procesi adsorpcije i desorpcije kalijum-etil-ksantata na površini bakra dovode do formiranja zaštitnog oksidacionog sloja na površini electrode.

Analysis of the presence of inhibitors in the alkaline sodium carbonate solution on the electrochemical behavior of cold-deformed copper wire

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In this paper the influence of 1M aqueous Na_2CO_3 solution with and without additional inhibitors, gelatin and potassium ethyl xanthate at different concentrations, on the corrosion behavior of cold worked copper wire (ε=87, 95 i 99 %) was tested. The values of the open circuit potential (OCP) were measured and a cyclic voltammetry (CV) method was used. OCP measurements show steady increase before establishing a constant value. The voltammograms indicated two anode peaks, showing that oxidation of copper to Cu_2O and CuO occurs. The results indicated that the degree of deformation between 87 and 99 % does not have a significant effect on the OCP value . A positive effect of the gelatin on the corrosion protection was shown. However, increasing gelatin concentrations again leads to acceleration of the corrosion processes. Potassium ethyl xanthate in 1M Na_2CO_3 solution changes the mechanism during the anode polarization. Complex processes of adsorption and desorption of potassium ethyl xanthate on the copper surface lead to the formation of a protective oxidation layer at the electrode surface.

Hemijsko inženjerstvo / Chemical Engineering

HI O 1 text rada / full text

Eksperimentalna merenja i teorijske simulacije binarnih sistema alkohola i ugljovodonika

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Eksperimentalne i teorijske metode korišćene su za proučavanje dve smeše, 1-heksanola sa n-heksanom i cis-3-heksen-1-ola sa n-heksanom. Eksperimentalne tehnike su korišćene za određivanje dopunskih zapremina i promene viskoznosti za temperaturni opseg od 288.15K do 318.15K. Podaci o dopunskoj molarnoj zapremini ukazuje na slično ponašanje dva alkohola, 1-heksanola i cis-3-heksen-1-ola u smešama sa n-heksanom. Eksperimentalni podaci su u skladu sa simulacijom molekularne dinamike ovih smeša, pokazujući sličan broj vodoničnih veza u dve smeše. Eksperimentalni podaci o promeni viskoznosti pokazuju značajnu razliku između dve smeše, odstupanje je značajno veće za smešu cis-3-heksen-1-ol i n-heksan, što ukazuje na jaču interakciju u binarnoj smeši cis-3-heksen-1-ola i nheksana. Ovi eksperimentalni podaci su u skladu sa kvantno-hemijskim proračunima energija interakcija na molekulskom nivou. Naime, izračunate energije interakcije pokazuju da je interakcija između jednostrukih i dvostrukih veza jača, nego interakcija između dve jednostruke veze.

Experimental measurements and theoretical simulations of alcohol and hydrocarbon binary systems

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Experimental and theoretical methods were used to study two mixtures, 1-hexanol with n-hexane and cis-3-hexen-1-ol with n-hexane. The experimental technics were used to determine excess molar volume and viscosity deviations in the temperature range from 288.15K to 318.15K. The data of excess molar volume indicate similar behavior of the two alcohols, 1-hexanol and cis-3-hexen-1-ol in mixtures with n-hexane. The experimental data are in accordance with molecular dynamics simulation of these mixtures, showing similar number of hydrogen bonds in the two mixtures. The experimental data of viscosity deviations show difference of the two mixtures, where the deviation is significantly larger for cis-3-hexen-1-ol and n-hexane mixture, indicating stronger interactions within cis-3-hexen-1-ol and n-hexane binary mixture. These experimental data are in accordance with quantum chemical calculations on interactions energies. Namely, calculated interaction energies show that interaction between single and double bonds are stronger, than interactions between two single bonds.

HI P 1

Uporedna analiza postupaka dobijanja ekstrakata bogatih saponinima iz semena *Trigonella foenum-graceum* L. natkritičnom ekstrakcijom

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Grčko seme je dostiglo tendenciju rasta u proizvodnji, zahvaljujući širokoj primeni u tradicionalnoj medicini od davnina, shodno svojim bioaktivnostima. Najveći doprinos bioaktivnosti grčkog semena, pripisan je saponinima, kao jedinjenjima od interesa. Mnoge ekstrakcione tehnike su analizirane u dobijanju ekstrakata, međutim natkritična ekstrakcija je pokazala tehniku koja najviše obećava, sa prednošću dobijanja čistih ekstrakata, efikasnošću dobijanja ekstrakata za kraće vreme i bez daljih potreba za prečišćavanjem. U cilju dobijanja ekstrakata bogatih saponinima, natkritična ekstrakcija je primenjena na više procesnih uslova. Radi poređenja sastava saponina u dobijenim ekstraktima, natkritična ekstrakcija je praćena konsekutivnim izvođenjem Sokslet ekstrakcije. Prinosi ekstrakata, kao i njihovi sastavi su bili determinisani i analizirani pri različitim procesnim uslovima pritiska i temperature. Praćena je kinetika natkritične ekstrakcije, koja predstavlja dinamiku ekstrakcije i masenog transfera ekstrahovanog materijala kroz matricu biljke s vremenom ekstrakcije.

Comparative analysis of methods in aim to obtain saponins rich extracts from *Trigonella foenum-graecum* seeds L. by supercritical fluids

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Fenugreek seed has reached growing interest in implementation, applied in traditional medicine for its benefitial health effects during the centuries. It has been found that saponins, which occur abundantly in fenugreek take mostly main role in their activity. Numerous extraction techniques were applied to enable the obtaining the extracts, but supercritical fluid extraction has shown the most promising technique with the advantages to obtain extract free of organic solvents, much faster without necessity to employ the steps of further purification. In aim to enable extracts rich in saponins supercritical extraction was applied in several process conditions. Supercritical extraction was consequently followed by Soxhlet extraction, in comparison to saponins content in obtained extracts. The yields of extract as well as its composition were determined and analyzed at different process conditions of pressure and temperature. Kinetics of the SC-CO_2 extraction from fenugreek presenting hydrodynamic of extraction and dynamic of mass transfer through extraction time, was presented and analyzed.

HI P 2 text rada / full text

Istovremeno modelovanje gustine i viskoznosti sistema sa etil butiratom

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Eksperimentalne vrednosti viskoznosti i gustine pet binarnih tečnih smeša sa etil butiratom, određene pri atmosferskom pritisku i u temperaturnom opsegu, korišćene su za testiranje Eyring modela, zajedno sa Peng-Robinson jednačinom stanja i van der Waals pravilom mešanja, za izračunavanje ovih svojstava. Dobijeni rezultati su analizirani u smislu primenjenog pristupa i modela. Rezultati korelisanja gustine korišćenom jednačinom stanja su odlični, sa vrednostima procentualnih odstupanja ispod 0,01 %, dok su za korelisanje viskoznosti primenjenim modelom vrednosti uglavnom manje od 4,5 %.

Simultaneous modeling of density and viscosity of the systems with ethyl butyrate

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Experimental values of viscosities and densities of five binary liquid mixtures with ethyl butyrate, determined at atmospheric pressure and in a temperature range, were used to test Eyring model, coupled with the Peng-Robinson equation of state and van der Waals mixing rule, for calculating these properties. The obtained results were analyzed in terms of the applied approach and model. Results of density correlation with used equation of state are excellent, with values of percentage deviations below 0.01 %, while for viscosity correlation, with applied model, values are mostly lower than 4.5 %.

HI P 3 text rada / full text

Volumetric properties modeling of binary mixtures by Prigogine-Flory-Patterson (PFP) and Extended Real Association Solution (ERAS) models

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In this work, excess molar volume, V^E, of two previously published binary systems, dimethyl adipate+1-butanol and dimethyl adipate+2-butanol were correlated with two models, Prigogine-Flory-Patterson (PFP) and Extended Real Association Solution (ERAS).
Volumetric coefficients, thermal expansion coefficient, α, and isothermal compressibility, κ, were calculated from density, speed of sound and isobaric heat capacity data. Isobaric molar heat capacities, C_p, at all temperatures for 2-butanol were obtained by correlation of literature data using Jovanović et al. model, while heat capacities for dimethyl adipate were predicted with Kolskà *et al.* model.
PFP and ERAS models were used for analysis of molecular interactions present in the investigated solutions.

Modelovanje volumetrijske osobina binarnih smeša korišćenjem Prigogine-Flory-Patterson (PFP) i Extended Real Association Solution (ERAS) modela

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U ovom radu, dopunske molarne zapremine, V^E, dva prethodno objavljena binarna sistema, dimetil adipat+1-butanol i dimetil adipat+2-butanol korelisane su sa dva modela, Prigogine-Flory-Patterson (PFP) i Extended Real Association Solution (ERAS) modelom.
Volumetrijski koeficijenti, koeficijent termalne ekspanzije, α, i izotermalne kompresibilnosti, κ, izračunati su preko podataka za gustinu, brzine zvuka i izobarske toplotne kapacitivnosti. Izobarski molarni toplotni kapaciteti, C_p, na svim temperaturama za 2-butanol dobijeni su korelisanjem literaturnih podataka koristeći Jovanović *et al.* model, dok su toplotni kapaciteti za dimetil adipat dobijeni preko Kolskà et al. modela.
PFP i ERAS modeli primenjeni su za analizu molekulskih interakcija prisutnih u datim smešama.

HI P 4 text rada / full text

Ispitivanje dinamike granulacije praškastih materijala u fluidizovanom sloju

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U ovom radu izvršeno je eksperimentalno ispitivanje procesa mokre granulacije u fluidizovanom sloju u cilju pronalaženja optimalnih uslova izvođenja procesa i sastava veziva kojim će se ostvariti željena dinamika razvoja granula. Ispitivanje je izvršeno u šaržnom sistemu, a korišćeno je kukuruzno brašno kao polazni materijal. Izvršeno je 10 eksperimenata u kojima je kao vezivno sredstvo korišćen rastvor saharoze različitih koncentracija: 20, 30, 35 i 40 %. Temperatura je održavana konstantnom tokom procesa granulacije i iznosila je 40-50°C. Uzorci su iz sloja uzimani u jednakim vremenskim intervalima od 3 min. Dinamika granulacije ispitivana je određivanjem tri različita faktora (nasipne gustina, vlažnosti i raspodele veličine čestica) za svaki od uzoraka. Utvrđeno je da nasipna gustina kontinualno opada tokom izvođenja procesa granulacije, dok u fazi sušenja ostaje konstantna. Raspodela veličina čestica je pokazala da srednji prečnik projektovane površine ravnomerno raste tokom procesa. Poređenjem sva tri ispitivana faktora pokazano je da se najbolji kvalitet granula postiže korišćenjem 35 % rastvora saharoze kao vezivnog sredstva.

Investigation of the dynamics of fluidized bed granulation process

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In this paper, experimental investigation of the dynamics of the process of fluidized bed granulation was performed, in order to find optimal process conditions and binder concentration to achieve the desired granules development. The experiments were performed in batch system using corn flour as starting material. Ten experiments were performed in which sucrose solution of different concentrations (20, 30, 35 and 40 %) was used as binder. The temperature of the system was kept constant during the granulation process and amounted to 40-50°C. Samples were taken from the fluidized bed at time intervals of 3 min. The dynamics of granulation was examined by determining three different factors (bulk density, moisure content and particle size distribution) for each of the samples. It has been found that bulk density continuously decreases during the granulation process, while in the drying phase it remains constant. Particle size distribution has shown that the average diameter of the projected surface increases uniformly during the process. By comparing all of the three investigated factors, it was shown that the best quality of granules is achieved using 35 % sucrose solution .

HI P 5

Novi senzor na bazi MWCNT za određivanje oksifluorfena tehnikom diferencijalne pulsne striping voltametrije

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Elektroda od staklastog ugljenika (GC) modifikovana pomoću MoO_2-MWCNT je primenjena kao elektrohemijski senzor za određivanje koncentracije oksifluorfena u modelnim vodenim rastvorima pomoću tehnike diferencijalne pulsne striping voltametrije (DPSV). Po prvi put je ispitivana elektrohemijska detekcija ovog intenzivno korišćenog herbicida u troelektrodnom sistemu. Komercijalno dostupne MWCNT su hemijski impregnirane sa natrijum-molibdat dihidratom i nanešene na GC koja je korišćena kao radna elektroda. Pretpostavlja se da su strukturne i elektronske/elektrohemijske karakteristike dobijenog materijala odgovorne za poboljšani elektrodni odziv u slučaju detekcije oksifluorfena. Pravilna raspodela MoO_2 u strukturi MWCNT je potvrđena TEM mikroskopom. Oksifluorfen je određivan pomoću DPSV u rasponu koncentracija od 2,5 do 34,52 ng cm^{-3}, sa r^2 = 0.998 i granicom detekcije od 1,52 ng cm^{-3}, dok relativna standardna devijacija (RSD) nije prelazila 2.4 % što ukazuje na relativno dobru preciznost razvijene metode sa potvrđenom reproduktivnošću. U laboratorijskom istraživanju potvrđen je novi pristup u brzoj i pouzdanoj detekciji oksifluorfena.

Novel MWCNT based sensor for oxyfluorfen determination by the differential pulse stripping voltammetry

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A glassy carbon electrode modified with MoO_2-MWCNTs was constructed and applied as electrochemical sensor for the determination of oxyfluorfen in model aqueous solutions by the means of differential pulse stripping voltammetry (DPSV). For the first time, this widely used herbicide was electrochemically investigated in three electrode system. As a working electrode agent, commercially available MWCNTs were chemically impregnated by the sodium molybdate dihydrate. It is supposed that structural and electronical/electrochemical features of the obtained material are responsible for enhanced electrodic response in the case of oxyfluorfen sensing. Proper distribution of MoO_2 in the structure of MWCNTs was confirmed by TEM. Oxyfluorfen was determined by DPSV in the concentration range from 2.5 to 34.52 ng cm^{-3}, with r^2 = 0.998 and the limit of detection of 1.52 ng cm^{-3}, while the relative standard deviation (RSD) did not exceed 2.4 % which indicates a relatively good precision of the developed method with confirmed reproducibility. A novel approach in rapid and reliable oxyfluorfen detection is confirmed in laboratory study.

Tekstilno inženjerstvo / Textile Engineering

TI O 1 text rada / full text

Naslojavanje TEMPO oksidisanim celuloznim nanofibrilima kao novi pred-tretman za poboljšanje antibakterijskih svojstava viskozne tkanine funkcionalizovane hitozanom

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Osnovni cilj ovog rada je dobijanje viskozne tkanine funkcionalizovane hitozanom sa poboljšanim antibakterijskim svojstvima. Radi poboljšanja interakcija viskozne tkanine sa hitozanom, viskozna tkanina je naslojena TEMPO oksidisanim celuloznim nanofibrilima (TOCN) pre funkcionalizacije sa hitozanom. Tkanina je okarakterisana pomoću elementalne analize, merenjima zeta potencijala, sadržaja funkcionalnih grupa, prekidne jačine i antibakterijske aktivnosti. Naslojavanjenje tkanine TOCN-om je poboljšalo njena mehanička i antibakterijska svojstva.

Coating with TEMPO oxidized cellulose nanofibrils as novel pre-treatment for improving antibacterial properties of viscose fabric functionalized with chitosan

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The main objective of this study was to obtain viscose fabric functionalized by chitosan with improved antibacterial properties. In order to improve interactions between viscose fabric and chitosan, viscose fabric was coated with TEMPO oxidized cellulose nanofibrils (TOCN) before functionalization with chitosan. Fabric was characterized using elemental analysis and zeta potential measurements. Functional group content, breaking strength and antibacterial activity were also evaluated. Coating of fabric with TOCN improved its mechanical and antibacterial properties.

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TI O 2 text rada / full text

Uticaj alkalnog tretmana na strukturu, sorpciju vlage i zapreminsku električnu otpornost tkanina od jute

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Tkanina od jute je tretirana rastvorom NaOH različitih koncentracija u toku 5 min, što je dovelo do smanjenja sadržaja hemiceluloza i povećanje sorpcije vlage. Analiza rezultata dobijenih difrakcijom rendgenskih zraka pokazala je da tkanine sa manjim sadržajem hemiceluloza imaju manji indeks kristaliničnosti i da nakon mercerizovanja, dolazi do konverzije celuloze I_β u cellulozu II. Manje vrednosti zapreminske električne otpornosti nakon alkalnih tretmana mogu se povezati sa smanjenjem sadžaja hemiceluloza i indeksa kristaliničnosti i povećanjem sorpcije vlage. Povećan stepen konverzije celuloze I_β u celulozu II dovodi do povećanja zapreminske električne otpornosti mercerizovanih tkanina.

Effect of the alkali treatment on the structure, moisture sorption and volume electrical resistivity of woven jute fabrics

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Woven jute fabric was treated with NaOH solution of different concentrations for 5 min to obtain jute fabrics with gradually decreased content of hemicelluloses and increased moisture sorption. With increasing the concentration of NaOH the crystallinity index decreased; in the case of NaOH concentration ≥ 10 % the conversion from cellulose I_β to cellulose II occurred. The obtained decrease of the volume electrical resistivity after the alkali treatments can be attributed to the changes in hemicelluloses content, crystallinity index and moisture sorption. Increased conversion from cellulose I_β to cellulose II leads to an increase in the volume electrical resistivity of the mercerized jute fabrics.

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Uticaj oksidacije na strukturu i površinsko naelektrisanje pamučne pređe

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U ovom radu ispitivan je uticaj oksidacije kalijum-permanganatom ($KMnO_4$) različite koncentracije, na strukturu, soprciona svojstva i površinsko naelektrisanje pamučne pređe. Oksidacija pamuka je vršena na konstantnoj pH tokom 1 sata. Nakon oksidacije uzorci su isprani, osušeni i okarakterisani sa aspekta promene morfologije, sorpcionih svojstava, sadržaja COOH grupa i površinskog naelektrisanja. Rezultati su pokazali da je oksidacija najkoncentrovanijim rastvorom $KMnO_4$ dovela do značajnog povećanja sadržaja COOH grupa u uzorku (oko 6 puta), što je uticalo na povećanje sadržaja vlage kao i redukciju ceta potencijala u baznoj sredini. Ovim rezultatima je pokazano da se $KMnO_4$ može uspešno koristiti za oksidaciju pamuka u cilju poboljšanja sorpcionih svojstava.

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Influence of oxidation on the structure and surface charge of cotton yarn

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In this work, an influence of oxidation with potassium permanganate ($KMnO_4$) of different concentration, on the structure, sorption properties and surface charge of cotton yarn was investigated. Cotton oxidation was performed at constant pH during 1 hour. After the oxidation, samples were washed, dried and characterized from the aspect of change in morphology, sorption properties, COOH group content and surface charge. The results have shown that oxidation with the most concentrated solution of $KMnO_4$ led to significant increase of COOH group content in the sample (around 6 times), which thus led to increment of moisture sorption as well as reduction of zeta potential in basic range. These results confirmed that $KMnO_4$ could be successfully used for cotton oxidation with aim to improve sorption properties.

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TI P 2

Poređenje metoda za merenje propustljivosti vazduha tekstilnih materijala

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Propustljivost vazduha tekstilnih materijala definiše se količinom vazduha koji pri konstantnom pritisku u jedinici vremena prođe kroz jedinicu površine materijala. Ovaj parametar se često koristi za ocenjivanje performansi odevnih tekstilnih materijala i tehničkog tekstila kao što su tkanine za vazdušne jastuke, jedra i padobrane, i industrijski tekstilni filteri. U stručnoj praksi, koja ne uključuje obavezno naučna istraživanja, neophodno je da se sva testiranja tekstilnih materijala vrše prema normama propisanim važećim standardima. Propustljivost vazduha tekstilnih materijala najčešće se ispituje standardnim metodama ASTM D737 i ISO 9237. Vrlo često se dešava da se kvantifikovane vrednosti ispitivanog svojstva tekstilnog materijala razlikuju u zavisnosti od upotrebljenog uređaja, odnosno primenjene standardne metode. Zbog toga je u okviru ovog istraživanja izvršeno poređenje rezultata propustljivosti vazduha grupe DL pletenina, koji su dobijeni primenom dva različita uređaja i dve standardizovane (ASTM D737 i ISO 9237) metode. Poređenjem dve grupe rezultata propustljivosti vazduha DL pletenina uočene su razlike u vrednosti ovog parametra kod svih ispitivanih pletenina. Ipak, zapažen je isti trend u pogledu uočenih razlika u propustljivosti vazduha pletenina, što je potvrđeno visokom vrednošću koeficijenta korelacije (r=0,98).

Rad u okviru projekta MPNT (OI-171029)

Comparison of methods for measurement of air permeability of textile materials

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The air permeability of textile fabrics is defined as the air passed over a surface under a certain pressure difference in a unit time. Air permeability is often used in evaluating the performance of clothing textiles and technical textiles such as air bags, sail cloth, parachutes sails and industrial textile filters. In practice, which does not have to include scientific research, it is necessary that all tests of textile materials are carried out according to the standards. In the case of air permeability, the most commonly used standard methods are ASTM D737 and ISO 9237 standards. The values of the tested property of a textile material vary very often depending on the device used and method applied. In this research, a comparison of the results of air permeability of some plain knitted fabrics was made, which were obtained using two different devices according to ASTM D737 and ISO 9237 methods. The results obtained indicated the differences in the values of air permeability for all the knitted fabrics. However, the same trend was observed in terms of the observed differences which was confirmed by the high value of the correlation coefficient (r=0.98).

Within the Project MPNT (OI-171029)

Nauka o materijalima / Material Science

NM O 1

Optička i fotokatalitička svojstva hibridnih materijala

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Vezivanje malih bezbojnih organskih molekula (derivati benzena) za površinu oksida velikog energetskog procepa (TiO_2, CeO_2, Al_2O_3, itd.) dovodi do formiranja kompleksa sa prenosom naelektrisanja koji apsorbuju u vidljivom, očiglednijem spektralnom opsegu. Transmisiona elektronska mikroskopija, analiza difrakcije X-zraka, adsorpcione-desorpcione izoterme azota, i različite spekroskopske tehnike su korišćene za detaljnu karakterizaciju sintetisanih materijala. Takodje, proračuni zasnovani na teoriji elektronske gustine su korišćeni za odredjivanje energetskog procepa različitih neorganskih/organskih hibrida. Posebna pažnja je posvećena fotokatalitičkim svojstvima sintetisanih hibridnih materijala. Fotokatalitička degradacija organskih boja i nastajanje vodonika su korišćeni za testiranje performansi površinski modifikovanih oksida velikog energetskog procepa derivatima benzena u oksidacionim i redukcionim katalitičkim reakcijama indukovanim svetlošću, respektivno.

Optical and photocatalytic properties of hybrid materials

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The attachment of small colorless organic molecules (benzene derivatives) to the surface of wide-band-gap oxides (TiO_2, CeO_2, Al_2O_3, *etc.*) leads to the formation of interfacial charge transfer (ICT) complexes and appearance of absorption in more obvious visible-light spectral region. Comprehensive characterization of the synthesized materials involving transmission electron microscopy, X-ray diffraction analysis, nitrogen adsorption-desorption isotherms, and various spectroscopic techniques were performed. The density functional theory (DFT) calculations with periodic boundary conditions were performed in order to estimate the energy gaps of various inorganic/organic hybrids. Special attention was paid to the photocatalytic ability of the synthesized inorganic-organic hybrids. The photodegradation of different organic dyes and hydrogen production was used to test the photocatalytic performance of surface-modified wide-band-gap oxides with benzene derivative in oxidation and reduction light-driven processes, respectively.

NM P 1

Chemical modification of nanocellulose for nanocomposites

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Nanocellulose (NC) has attracted a great deal of interest in the nanocomposite science due to its availability, biodegradability and renewability. Nanoscale dimensions, high surface area, unique morphology, low density, and impressive mechanical properties, together with possibility of modification give nanocellulose a great potential as reinforcement agent in composites. However, some of the major disadvantage of the NC-reinforcing filler represents its polar and hydrophilic nature, which inhibit homogeneous dispersion in nonpolar polymer matrices. In order to improve the interfacial interaction/reactivity between nanocellulose and polymer matrix, cellulose nanocrystals were modified with fatty acids residues containing reactive vinyl groups as active centres involved in copoly-merisation reaction with unsaturated polyester resins. Two methods of NC modification are performed: direct esterification with oleic acid, linseed, or sunflower oil fatty acids, and esterification/amidation with maleic acid/ethylene diamine (MA/EDA) bridging group followed by amidation with methyl ester of fatty acids.

Hemijska modifikacija nanoceluloze za primenu u nanokompozitima

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Nanoceluloza (NC) privlači veliko interesovanje u nauci o nanokompozitima, zahvaljujući svojoj dostupnosti, biodegradabilnosti i obnovljivosti. Nanodimenzije, velika specifična površina, jedinstvena morfologija, mala gustina i impresivna mehanička svojstva, zajedno sa mogućnostima modifikacije daju nanocelulozi veliki potencijal za primenu kao ojačavajućeg agensa u kompozitima. Međutim, neki od glavnih nedostataka nanoceluloze za primenu kao ojačavajućeg sredstva predstavljaju njena polarna i hidrofilna priroda koja onemogućava njenu homogenu disperziju u nepolarnim polimernim matriksima. U cilju poboljšanja interfazne interakcije/reaktivnosti između nanoceluloze i polimernog matriksa, nanokristalna celuloza je modifikovana ostacima masnih kiselina koje sadrže reaktivne vinilne grupe kao aktivne reaktivne centre koji su uključeni u reakciju kopolimerizacije sa nezasićenim poliestarskim smolama. Dve metode modifikacije nanoceluloze su primenjene: direktna esterifikacija oleinskom kiselinom i masnim kiselinama lanenog i suncokretovog ulja, kao i esterifikacija/amidovanje preko tzv. linkera koji sadrži ostatke maleinske kiseline i etilen-diamina (MA/EDA), a zatim amidovanje metil estrima masnih kiselina.

NM P 2

Abnormalni rast zrna u AA5182 leguri: uticaj deformacije i temperature žarenja

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U ovom radu prikazani su rezultati sistematičnih ispitivanja uticaja parametara termo-mehaničke prerade (TMP) Al-Mg legure AA5182 na pojavu abnormalnog rasta zrna (AGG). AGG predstavlja razvoj mikrostrukture koju karakteriše pojava velikih zrna okruženih finijim, tj. obrazovanje bimodalne distribucije veličine zrna. Sklonost legure prema AGG ograničava temperaturu žarenja, sposobnost oblikovanja u toplom stanju i pogoršava mehanička svojstva. TMP je uključila hladno valjanje sa redukcijama u opsegu 40-85 % i rekristalizaciono žarenje 1h u temperaturnom intervalu 350-520 °C ili izotermalno žarenje na 480 °C pri različitim vremenima. Mikrostruktura je karakterizovana optičkom mikroskopijom u polarizovanom svetlu i u FEG SEM-u. Rezultati pokazuju da povećanje stepena redukcije pomera početak abnormalnog rasta zrna ka nižim temperaturama. Abnormalan rast zrna i mobilnost granica zrna pokazali su izraženu anizotropiju, ukazujući na uticaj oblika i distribucije disperzoida, kao i Zenerovo blokiranje granica zrna.

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Abnormal grain growth in AA5182 alloy: Influence of deformation and annealing temperature

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This study investigated the effect of parameters of thermo-mechanical processing (TMP) of Al-Mg alloy AA5182 on the occurrence of abnormal grain growth (AGG). AGG represents development of microstructure of large grains surrounded by finer, *i.e.* bimodal grain size distribution. The propensity of alloy toward AGG severely limits the annealing temperature range, capability for hot forming and deteriorates mechanical properties. TMP included cold rolling with reductions ranging 40-85 % followed by isochronal anneal (1h) in temperature range 350-520 °C or isothermal treatment at 480 °C for various times. The microstructure was characterized by optical microscopy in polarized light and in FEG SEM. The results showed that the increase in the degree of reduction lowers annealing temperature at which the onset of AGG takes place. AGG and grain boundary mobility showed strong anisotropy indicating the influence of shape and distribution of dispersoids as well as Zenner pinning.

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NM P 3

Termijska analiza procesa oksidacije prirodnog minerala milerita

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Sulfidi nikla česti su pratioci sulfidnih minerala bakra. Sa aspekta pirometalurške proizvodnje bakra, nikl spada u onečišćujuće, toksične komponente. U cilju boljeg poznavanja faznih promena tokom procesa oksidacije, urađena je DTA-TG analiza prirodnog minerala milerita. Termijska analiza rađena je u temperaturnom intervalu 25-1000 °C pri različitim brzinama zagrevanja. Konstruisani su dijagrami stabilnosti faza Ni-O-S sistema na nekoliko karakterističnih temperatura. Komparativnom analizom dobijenih rezultata predložen je reakcioni mehanizam razlaganja milerita na povišenim temperaturama u atmosferi vazduha.

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Thermal analysis of the natural mineral milerite oxidation process

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Sulfides of nickel are frequent followers of sulphide based copper minerals. From the aspect of pyrometallurgical copper production, nickel belongs to polluting, toxic components. In order to better understanding the phase changes during the oxidation process of the natural mineral milerite DTA-TG analysis was done. Thermal analysis was performed in temperature interval 25-1000 °C at various heating rates. Phase stability diagrams of the Ni-O-S system were constructed at some characteristic temperatures. Based on comparative analysis of the obtained results a reaction mechanism for the decomposition of milerite at elevated temperatures in the air atmosphere was proposed.

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NM P 4

Uticaj termomehaničke obrade na svojstva EN AW-6060 aluminijumske legure

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Eksperimentalno ispitivanje je izvršeno na aluminijumskoj leguri EN AW-6060. Ispitivanje je uključivalo promene različitih osobina legure pod uticajem termomehaničke obrade (TMO). Ispitivana je tvrdoća, mikrotvrdoća i elektroprovodljivost u funkciji intenziteta deformacije korišćene pre ili posle termičke obrade starenjem. Deformisani uzorci upoređivani su sa onim koji su prošli samo kroz termičku obradu starenjem radi analize samog uticaja primenjene deformacije. Uticaj deformacije, pre i posle starenja, doveo je do porasta vrednosti tvrdoće i mikrotvrdoće, dok su vrednosti elektroprovodljivosti opale. Određen broj uzoraka je izdvojen i detaljnije analiziran uz pomoć, optičke i skenirajuće elektronske mikroskopije. Hemijski sastav precipitata kao i njihova distribucija u mikrostrukturi ispitivana je uz pomoć energetsko disperzivne spektroskopije uz pomoć funkcije mapiranja prisutnih elemenata u mikrostrukturi.

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The influence of thermomechanical treatment on the properties of the EN AW-6060 aluminium alloy

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Aluminum alloy EN AW-6060 was used for experimental study. The experimental study included changes in different properties of alloys under the influence of thermomechanical treatment (TMT). Hardness, micro-hardness and electrical conductivity were investigated as a function of deformation intensity, before and after the aging treatment. In order to pinpoint the influence of deformation only, the samples were compared to those which were subjected to aging treatment exclusively. The deformation, in both cases caused an increase in hardness and micro-hardness values while electrical conductivity decreased. Some representative samples were chosen and further investigated by the means of optical and scanning electron microscopy. Energy dispersive spectroscopy was used to investigate the chemical composition of precipitates and EDS mapping feature for the analysis of distribution of alloying elements in the microstructure of alloys.

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Neorganska hemija / Inorganic Chemistry

NH O 1

Srebro(I) kompleksi sa piridinkarboksilatnim ligandima: sinteza, strukturna karakterizacija i antimikrobna aktivnost

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Sintetisani su i strukturno okarakterisani kompleksi srebra(I) sa piridinkarboksilatnim ligandima, [Ag(py-2py-*N,N'*)(NO_3-*O*)]$_n$ (**1**), [Ag(py-2metz-*N,N'*)(NO_3-*O*)]$_n$ (**2**), [Ag(py-2py-*N,N'*)(CH_3CN-*N*)]BF_4 (**3**), [Ag(py-2tz-*N,N'*)$_2$]BF_4 (**4**) i [Ag(py-2metz-*N,N'*)$_2$]BF_4 (**5**), py-2py je dimetil[2,2'-bipiridin]-4,5-dikarboksilat, py-2metz je dimetil 6-(4-metiltiazol-2-il)piridin-3,4--dikarboksilat i py-2tz je dimetil 6-(tiazol-2-il)piridin-3,4-dikarboksilat. Antimikrobna aktivnost kompleksa **1 – 5** i piridinkarboksilata korišćenih za njihovu sintezu je ispitivana *in vitro* prema panelu bakterijskih i *Candida* spp. sojeva. Većina sintetisanih kompleksa pokazuje značajnu aktivnost prema *Candida* sojevima, dok ligandi nisu aktivni.

Silver(I) complexes with pyridinecarboxylate ligands: synthesis, structural characterization and antimicrobial activity

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New silver(I) complexes, [Ag(py-2py-*N,N'*)(NO_3-*O*)]$_n$ (**1**), [Ag(py-2metz-*N,N'*)(NO_3-*O*)]$_n$ (**2**), [Ag(py-2py-*N,N'*)(CH_3CN-*N*)]BF_4 (**3**), [Ag(py-2tz-*N,N'*)$_2$]BF_4 (**4**) & [Ag(py-2metz-*N,N'*)$_2$]BF_4 (**5**), py-2py is dimethyl [2,2'-bipyridine]-4,5-dicarboxylate, py-2metz is dimethyl 6-(4-methylthiazol-2-yl)pyridine-3,4-dicarboxylate and py-2tz is dimethyl 6-(thiazol-2-yl)pyridine--3,4-dicarboxylate, were synthesized and structurally characterized. Antimicrobial activity of complexes **1** – **5**, along with that of pyridinecarboxylates used for their synthesis, were evaluated *in vitro* against a panel of bacterial and *Candida* spp. strains. Most of the synthesized complexes show significant anti-*Candida* activity, while the corresponding ligands are not active.

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NH P 1

Strukturna karakterizacija proizvoda reakcija bakar(II) soli i 1,7-fenantrolina

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Izvedene su reakcije između ekvimolarnih količina CuX_2 soli (X = NO_3^- i $CF_3SO_3^-$) i 1,7-fenantrolina (1,7-phen) u etanolu na sobnoj temperaturi. U ovim reakcijama ne dolazi do koordinacije 1,7-phen liganda za Cu(II) jon, pri čemu su 1,7-HphenNO_3 (**1a** i **1b**) i 1,7-HphenCF_3SO_3 (**2**) dobijeni kao konačni proizvodi. Ova jedinjenja su okarakterisana primenom spektroskopskih metoda i rendgenske strukturne analize. Dobijeni rezultati su poređeni sa rezultatima dobijenim za reakcije istih soli bakra(II) sa 4,7-fenantrolinom, u kojima nastaju $[Cu(NO_3)_2(4,7\text{-Hphen})_2](NO_3)_2$ i $[Cu(CF_3SO_3)(4,7\text{-phen})_2(H_2O)_2]CF_3SO_3$ kompleksi [1].

Structural characterization of the products formed in the reactions between copper(II) salts and 1,7-phenanthroline

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The reactions between equimolar amounts of CuX_2 (X = NO_3^- and $CF_3SO_3^-$) and 1,7-phenanthroline (1,7-phen) were performed in ethanol at room temperature. In these reactions, no coordination of 1,7-phen to the Cu(II) ion was observed and only 1,7-HphenNO_3 (**1a** and **1b**) and 1,7-HphenCF_3SO_3 (**2**) were formed as the final products. These compounds were characterized by spectroscopic and X-ray diffraction techniques. The obtained results were compared with those for the reactions between these two copper(II) salts and 4,7-phenanthroline, resulting in the formation of $[Cu(NO_3)_2(4,7\text{-Hphen})_2](NO_3)_2$ and $[Cu(CF_3SO_3)(4,7\text{-phen})_2(H_2O)_2]CF_3SO_3$ complexes [1].

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1. N. Lj. Stevanović, T. P. Andrejević, A. Crochet, T. Ilic-Tomic, N. S. Drašković, J. Nikodinovic-Runic, K. M. Fromm, M. I. Djuran, B. Đ. Glišić, *in preparation*

NH P 2

Pikolinato-rutenijum(II) arenski i bipiridil kompleksi: sinteza i karakterizacija

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Poslednjih godina Ru(II) kompleksi se ispituju kao potencijalni prolekovi u fotodinamičkoj i fotoaktivacionoj terapiji. U cilju poboljšanja aktivnosti sintetisanih polusendvič kompleksa Ru(II) sa derivatima pikolinske kiseline, izmenili smo arenski deo kompleksa bipiridinom. Citotoksičnost ovih kompleksa nije poboljšana, ali sledeći korak u istraživanju je ispitivanje fotoaktivnosti ovih bipiridinskih kompleksa na šta upućuje prisustvo bipiridinskog liganda. Sintetisano je tri Ru(II)-toluen kompleksa i tri odgovarajuća Ru(II)-bipiridin kompleksa sa pikolinskom kiselinom i njenim 4-karboksilato i 5-karboksilato derivatima. Ovih šest kompleksa je sintetisano polazeći od etanolnih rastvora $[Ru(\eta^6\text{-toluene})Cl(\mu\text{-}Cl)]_2$ ili $[RuCl_2(bpy)_2]$ uz dodatak odgovarajućeg pikolinskog liganda (1:1 mol), u toku par sati mešanja na sobnoj temperaturi, odnosno uz refluks, redom. Svi dobijeni kompleksi okarakterisani su NMR i IC spektroskopijom, kao i rendgensko strukturnom analizom. Svi bipiridin Ru(II) kompleksi kao i aren-pikolinski kompleksi kristalisali su u $P2_1/n$ prostornoj grupi, dok je Ru(II)-toluen kompleks sa 5-karboksilatnim derivatom pikolinske kiseline, kristalisao u P-1 prostornoj grupi simetrije. Najbolju aktivnost prema MDR Colo 320 ćelijskim linijama, pokazao je kompleks $[Ru(\eta^6\text{-toluene})(pic)Cl]$ sa IC_{50}=84.84 ± 4.79 μM.

Picolinate-ruthenium(II) arene and bipyridil complexes: synthesis and characterization

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In recent years Ru(II) complexes have been investigated as potentially good prodrugs that can undergo photodynamic therapy (PDT) or photoactivated chemotherapy (PACT). In order to improve the activity of the synthesized half-sandwich Ru(II) complexes with the derivatives of picolinic acid, we changed the arene part of these complexes with bipyridine. Activity against cancer cell line was not better, but the next step in the study would be the examination of the photoactivity of these bipyridine complexes, as that is indicated by the presence of bipyridine ligand. We have synthesized three Ru(II)-toluene complexes and three coresponding bipyridine Ru(II) complexes with picolinic acid, and its 4-carboxylic and 5-carboxylic derivatives. These six complexes were synthesized using ethanol solution of starting $[Ru(\eta^6\text{-toluene})Cl(\mu\text{-}Cl)]_2$ or $[RuCl_2(bpy)_2]$ and corresponding picolinate ligand (1:1 mol) and stirring at r.t. or refluxing, respectively. All complexes were characterized by NMR and IR spectroscopy, as well as X-ray crystalography. All bipyridine ruthenium complexes and arene/picolinic complex crystallized in the centro-symmetric space group $P2_1/n$, while Ru(II)-toluene with 5-carboxylic derivate of picolinic acid crystallized in triclinic crystal systems in space group P-1. The best activity against MDR-Colo 320 cell lines, had simple $[Ru(\eta^6\text{-toluene})(pic)Cl]$ with IC_{50}=84.84 ± 4.79 μM.

NH P 3

Organorutenijumski(II)-halido kompleksi sa derivatima benzimidazola: sinteza i uporedna citotoksična studija

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Kompleksi rutenijuma predstavljaju najperspektivniju alternativu kompleksima platine koji se decenijama unazad koriste kao antikancerogeni lekovi. Stoga opisujemo sintezu i kompletnu karakterizaciju šest novih kompleksa [(η^6-*p*-cymene)RuX($L_{1,2}$)] gde je HL_1= 1*H*-benzimidazol-2-karboksilna kiselina, HL_2= 5-hloro-1*H*-benzimidazol-2-karboksilna kiselina, a X= Cl^-, Br^-, I^-. Citotoksičnost kompleksa je ispitana na ćelijskim linijama K562 i MRC-5.
Ru(II) kompleksi su dobijeni u reakciji dva ekvivalenta HL_1, odnosno HL_2 sa ekvimolarnom količinom [(η^6-*p*-cymene)$RuX_2]_2$ u etanolu na sobnoj temperaturi. Nakon četvoročasovnog mešanja, izolovan je finalni proizvod u vidu žuto-narandžastog taloga. Kompleksi su okarakterisani pomoću IC, NMR i MS spektrometrije, elementalne analize i rendgenske strukturne analize za [(η^6-*p*-cymene)RuI(L_1)] koji kristališe u $P2_1/n$ prostornoj grupi. Ru(II) jon je oktaedarski koordinovan za imidazolski atom azota i karboksilatni kiseonik potvrđujući konformaciju stolice tipičnu za ovaj tip kompleksa. Kompleksi sa I^- ligandom pokazuju umerenu, ali selektivnu citotoksičnost prema K562 (IC_{50} ([(η^6-*p*-cimen)RuI(L_1)]) =53.9±2.2 μM i IC_{50} ([(η^6-*p*-cimen)RuI(L_2)]) =83.97±3.85 μM).

Organoruthenium(II)-halido complexes with benzimidazole derivatives: synthesis and comparative cytotoxic study

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Ruthenim complexes are the most promising alternative to platinum complexes which have been utilized as anticancer drugs decades ago. Thus we describe synthesis and full characterization of six new complexes [(η^6-*p*-cymene)RuX($L_{1,2}$)], where HL_1= 1*H*-benzimidazole-2-carboxylic acid, HL_2= 5-chloro-1*H*-benzimidazole-2-carboxylic acid, and X= Cl^-, Br^-, I^-. Cytotoxicity of the complexes was studied on K562 i MRC-5 cell lines.
Ru(II) complexes were obtained in a reaction of two equivalents of HL_1 or HL_2 with equimolar amount of [(η^6-*p*-cymene)$RuX_2]_2$ in ethanol at r.t. After four-hour long stirring, the final product was isolated in a form of a yellow-orange precipitate. The complexes were characterized by IR, NMR and MS spectrometry, elemental analysis and X-ray diffraction analysis for [(η^6-*p*-cymene)RuI(L_1)], crystallizing in the $P2_1$/n space group. The Ru(II) ion is octahedrally coordinated for imidazole nitrogen atom and carboxylate oxygen confirming ''piano stool'' conformation typical for this type of complexes. Complexes with I^- ligand show moderate but selective cytotoxicity towards K562 (IC_{50} ([(η^6-*p*-cimen)RuI(L_1)])= =53.9±2.2 μM and IC_{50} ([(η^6-*p*-cimen)RuI(L_2)]) =83.97±3.85 μM).

NH P 4

Interakcije kompleksa Rh(III) sa DNK/protein; Ispitivanje citotoksičnosti kompleksa

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Kompleksi prelaznih metala se dugo primenjuju kao farmakološki agensi u medicini. Kompleksi Rh(III) zbog svoje inertnosti i stabilnosti privlače sve veću pažnju kao potencijalni farmakološki agenasi u terapiji bolesti. U okviru ovog istraživanja sintetisali smo i okarakterisali novi kompleks Rh(III) sa ligandom derivatom bis-piridilpiridina i ligandom 1,2,4-triazolom. Kompleks je okarakterisan elementarnom mikroanalizom, kao i spektroskopskim metodama (IR, UV-Vis, ^{1}H i ^{13}C NMR, ESI). Ispitivana je kinetika supstitucionih reakcija ovog kompleksa sa biološki važnim ligandima (5'-GMP, GSH i L-Met). Urađena su i ispitivanja sposobnosti interakcije datog kompleksa sa CT-DNK korišćenjem Uv-Vis spektrofotometrije, fluorescentne spektroskopije, merenjem viskoznosti i ,,docing''. Pored interakcija sa CT-DNK, urađene su i interakcije sa albumin serum proteinom (BSA). Citotoksičnost kompleksa metala je ispitana.

Interactions of the Rh (III) complex with DNA / protein; Testing the cytotoxicity of the complex

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Transition metal complexes have long been used as pharmacological agents in medicine. Complexes of Rh(III), due to their inertness and stability, attract increasing attention as potential pharmacological agents in the treatment of diseases. Within this study, we synthesized and characterized a new Rh(III) complex with a ligand derivative of bis-pyridylpyridine and a ligand of 1,2,4-triazole. The complex was characterized by elemental microanalysis, as well as spectroscopic methods (IR, UV-Vis, ^{1}H and ^{13}C NMR, ESI). Substitution reactions kinetics of this complex with biologically important ligands (5'-GMP, GSH and L-Met) were examined. Analysis of the interaction capabilities of this complex with CT-DNA were performed using Uv-Vis spectrophotometry, fluorescence spectroscopy, and viscosity measurement and docing. In addition to interactions with CT-DNA, interactions with albumin serum proteins (BSA) were also performed. The cytotoxicity of the metal complex was tested.

NH P 5

Dinuklearni kompleksi srebra(I) sa *N,N',N'',N'''*-tetrakis(2-piridilmetil)-1,4,8,11--tetraazaciklotetradekanom: sinteza, karakterizacija i biološka aktivnost

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U ovom radu, *N,N',N'',N'''*-tetrakis(2-piridilmetil)-1,4,8,11-tetraazaciklotetradekan (tpmc) kao makrociklicni ligand sa 2-piridilmetil grupama je korišćen za sintezu kompleksa srebra(I). Različite AgX soli (X = $CF_3SO_3^-$, CF_3COO^- i BF_4^-) su korišćene za sintezu u cilju ispitivanja uticaja kontra-anjona na nuklearnost, stabilnost i biološku aktivnost kompleksa. Sintetisani kompleksi srebra(I) su okarakterisani primenom različitih spektroskopskih metoda, ciklične voltametrije i rendgenske strukturne analize. Ovi kompleksi pokazuju značajnu antimikrobnu aktivnost prema različitim sojevima bakterija i gljiva.

Dinuclear silver(I) complexes with *N,N',N'',N'''*-tetrakis(2-pyridylmethyl)--1,4,8,11-tetraazacyclotetradecane: synthesis, characterization and biological evaluation

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In this study, *N,N',N'',N'''*-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane (tpmc) as a macrocyclic ligand with pendant 2-pyridylmethyl groups was used for the synthesis of silver(I) complexes. Different AgX salts (X = $CF_3SO_3^-$, CF_3COO^- and BF_4^-) were used for the synthesis in order to investigate the influence of a counter-anion on nuclearity, stability and biological activity of the complexes. The synthesized complexes were characterized by different spectroscopic techniques, cyclic voltammetry and single-crystal X-ray diffraction analysis. All investigated complexes show remarkable antimicrobial activity against different bacterial and fungal strains.

NH P 6

(Hlorofenil)terpiridin Ru(II) kompleksi: Sinteza, kinetika supstitucionih reakcija sa biomolekulima i interakcije sa DNA i BSA

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Sa ciljem da ispitamo uticaj aromatičnosti helatnih liganada na reaktivnost Ru(II) polipiridil kompleksa, sintetisali smo dva nova Ru(II) kompleksa [Ru(Cl-Ph-tpy)(phen)Cl]Cl (**1**) i [Ru(Cl-Ph-tpy)(*o*-bqdi)Cl]Cl (**2**) (gde je phen = 1,10-fenantrolin i *o*-bqdi = *o*-benzohinondiimin).[1] Kompleksi su okarakterisani pomoću elementalne analize i različitih spektroskopskih metoda, kao što su IR, UV-Vis i (1D i 2D) NMR, dok je njihova molekulska struktura u čvrstom stanju utvrđena pomoću rendgenske strukturne analize. Kinetika i mehanizam reakcije kompleksa **1** i **2** sa biološki relevantnim ligandom 5'-GMP ispitivani su pomoću UV-Vis spektroskopije. Proučavane su interakcije kompleksa sa CT DNA, kao i kompetitivne reakcije interkalirajućeg agensa etidijum bromida (EB). Pored toga, ispitivan je afinitet kompleksa prema goveđem serum albuminu (BSA), i određene su konstante vezivanja.

(Chlorophenyl)terpyridine Ru(II) complexes: Synthesis, kinetics of the substitution reactions with small biomoleculs and DNA/BSA binding studies

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In order to gain more insight into the influence of chelating ligand's aromaticity on the reactivity of Ru(II) polypyridyl complexes, we synthesized two new Ru(II) complexes [Ru(Cl-Ph-tpy)(phen)Cl]Cl (**1**) and [Ru(Cl-Ph-tpy)(*o*-bqdi)Cl]Cl (**2**) (where phen = 1,10-phenanthroline and *o*-bqdi = *o*-benzoquinonediimine).[1] The new complexes were fully characterized by elemental analysis and various spectroscopic techniques, such as IR, UV-Vis and (1D and 2D) NMR, whereas their molecular structure in solid state was determined by single crystal X-ray diffraction analysis. The kinetics and the mechanism of the reaction of complexes **1** and **2** with the biologically more relevant 5'-GMP ligand were studied by UV-Vis spectroscopy. The interaction of complexes **1** and **2** with CT DNA was studied, and a competitive study of the intercalative agent ethidium bromide (EB) was performed. Furthermore, the affinity toward bovine serum albumin (BSA) was investigated, and their binding constants were determined.

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NH P 7

Novi zlato(III) kompleksi: Sinteza, karakterizacija i ispitivanje interakcija sa 5'-GMP, GSH i L-Met

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Farmakološke karakteristike kompleksa zlata poznate su još od kraja 19. veka. Ova jedinjenja najčešće su korišćena u lečenju reumatoidnog artritisa. Poslednjih decenija kompleksi zlata su ispitivani zbog raznolikosti primene, koja pre svega obuhvata upotrebu kao potencijalnih antikancerogenih i hemioterapeutskih agenasa.[1] Zlato(III) kompleksi zbog sličnosti sa kompleksima platine, su pokazali obećavajuće antikancerogene, citotoksične i antitumorske karakteristike.[2] U okviru ovog istraživanja sintetisana su dva nova zlato(III) kompleksa opšte formule $[Au(N\text{-}N)Cl_2]$, gde je *N-N* bidentatni ligand (4,7-difenil fenantrolin ili 2,9-dimetil fenantrolin). Pomenuti kompleksi su okarakterisani spektroskopskim tehnikama (IR, UV-Vis, ^{1}H NMR). Ispitivana je kinetika supstitucionih reakcija ovih kompleksa sa biološki važnim ligandima kao što su guanozin-5'-monofosfat (5'-GMP), glutationa (GSH) i L-metionin (L-Met), korišćenjem stopped-flow uređaja. Takođe, ispitivane su interakcije kompleksa i DNK pomoću UV-Vis spektrofotometrije, fluorescentne spektroskopije i na osnovu promene viskoziteta. Istovremeno, kao i interakcije sa govođim serum albuminom (BSA).

New gold(III) complexes: Synthesis, characterization and study of their interactions with 5'-GMP, GSH and Met

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The pharmacologic properties of gold compounds have been known since the end of 19th century. They have been used for different studies, even though they are usually used for the treatment of rheumatoid arthritis. In the last decade gold complexes have received increased attention due to the variety of their applications. Primary, they have been investigated as potential anticancer and chemotherapeutic agents.[1] It is well known that gold(III) complexes are very similar to platinum(II) compounds, so they could exhibit prospective anticancer, cytotoxic and antitumor properties.[2] In this study we have synthesized two new gold(III) complexes with general formula $[Au(N\text{-}N)Cl_2]$ in which *N-N* is a bidentate ligand (4,7-diphenyl-1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline). These complexes were characterized by spectroscopic techniques (IR, UV-Vis, ^{1}H NMR). Kinetic of the substitution reactions between complexes and biological important molecules, such as guanosine-5'-monophosphate (5'-GMP), glutathione (GSH) and L-methionine (L-Met), were performed by stopped-flow technique. Also, we performed DNA binding studies using UV-Vis spectrophotometry, fluorescence spectroscopy and viscosity measurements, as like as interaction with bovine serum albumine (BSA).

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NH P 8

Sinteza i antifungalna aktivnost kompleksa cinka(II) sa aromatičnim heterocikličnim jedinjenjima koja sadrže azot u prstenu

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Novi kompleksi cinka(II), $[ZnCl_2(qz)_2]$ (**1**), $[ZnCl_2(1,5\text{-naph})]_n$ (**2**) i $[ZnCl_2(4,7\text{-phen})_2]$ (**3**), (qz = hinazolin, 1,5-naph = 1,5-naftiridin i 4,7-phen = 4,7-fenantrolin) sintetisani su u reakcijama $ZnCl_2$ i odgovarajućeg *N*-heterocikličnog liganda u 1 : 2 molskom odnosu u etanolu na sobnoj temperaturi. Sintetisani kompleksi cinka(II) su okarakterisani primenom elementalne mikroanalize, NMR, IR i UV-Vis spektroskopije i rendgenske strukturne analize. Na osnovu disk-difuzione metode, utvrđeno je da kompleksi **1 – 3** pokazuju dobru antifungalnu aktivnost prema dva *Candida* soja (*C. albicans* i *C. parapsilosis*), pri čemu nisu toksični na normalnoj ćelijskoj liniji fibroblasta pluća (MRC-5).

Synthesis and antifungal activity of zinc(II) complexes with aromatic nitrogen-containing heterocycles

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New zinc(II) complexes, $[ZnCl_2(qz)_2]$ (**1**), $[ZnCl_2(1,5\text{-naph})]_n$ (**2**) and $[ZnCl_2(4,7\text{-phen})_2]$ (**3**), (qz = quinazoline, 1,5-naph = 1,5-naphthyridine and 4,7-phen = 4,7-phenanthroline) were synthesized by the reactions of $ZnCl_2$ and the corresponding *N*-heterocyclic ligand in 1 : 2 molar ratio in ethanol at room temperature. The characterization of the synthesized zinc(II) complexes was done by the elemental analysis, NMR, IR and UV-Vis spectroscopy, while their crystal structures were determined by a single-crystal X-ray diffraction analysis. In agar disc-diffusion assay, complexes **1 – 3** showed good antifungal activity against two *Candida* strains (*C. albicans* and *C. parapsilosis*). These complexes were not toxic on the normal human fibroblast cell line (MRC-5).

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NH P 9

Strukturna analiza i antimikrobna aktivnost kompleksa srebra(I) sa 1,10-fenantrolinskim ligandima

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Sintetisani su novi kompleksi srebra(I), $[Ag(1,10\text{-phen})_2]CF_3COO{\cdot}H_2O$ (**Ag1**) i $\{[Ag(5,6\text{-epoxy-1,10-phen})]CF_3COO\}_2$ (**Ag2**), 1,10-phen je 1,10-fenantrolin i 5,6-epoxy-1,10-phen je 5,6-epoksi-5,6-dihidro-1,10-fenantrolin, u reakcijama $AgCF_3COO$ i odgovarajućeg *N*-heterocikličnog liganda u 1 : 1 molskom odnosu u etanolu. Kompleksi **Ag1** i **Ag2** su okarakterisani primenom spektroskopskih metoda i rendgenske strukturne analize. Sintetisani kompleksi pokazuju selektivnu aktivnost prema ispitivanim *Candida* sojevima, pri čemu su vrednosti minimalnih inhibitorskih koncentracija između 0,8 i 12,5 μg/mL.

Structural analysis and antimicrobial activity of silver(I) complexes with 1,10-phenanthroline based ligands

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New silver(I) complexes, $[Ag(1,10\text{-phen})_2]CF_3COO{\cdot}H_2O$ (**Ag1**) and $\{[Ag(5,6\text{-epoxy-1,10-phen})]CF_3COO\}_2$ (**Ag2**), 1,10-phen is 1,10-phenanthroline and 5,6-epoxy-1,10-phen is 5,6-epoxy-5,6-dihydro-1,10-phenanthroline, were obtained from the reactions of $AgCF_3COO$ and the corresponding *N*-heterocyclic ligand in 1 : 1 molar ratio in ethanol. The **Ag1** and **Ag2** complexes are characterized by spectroscopic methods and a single-crystal X-ray diffraction analysis. The synthesized complexes showed selectivity towards four different *Candida* species with minimal inhibitory concentrations between 0.8 and 12.5 μg/mL.

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NH P 10

Sinteza, karakterizacija i ispitivanje reakcija novih mononuklearnih kompleksa platine(II) sa DNK

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Poslednjih godina intenzivno se izučavaju interakcije kompleksa prelaznih metala sa DNK. U skladu sa tim, u ovom radu sintetisana su dva nova mononuklearna Pt(II) kompleksa, [Pt(Me_2-mal-*O,O'*)(phen-epoxy)] i [Pt(cbdca-*O,O'*)(phen-epoxy)] (phen-epoxy = 5,6-epoksi-5,6-dihidro-[1,10]fenantrolin; Me_2-mal = anjon dimetilmalonske kiseline i cbdca = anjon ciklobutan-1,1-dikarboksilne kiseline). Kompleksi su okarakterisani na osnovu rezultata IR, UV-Vis i NMR (^{1}H i ^{13}C) spektroskopije. Interakcije kompleksa sa DNK su ispitivane *primenom UV-Vis i fluorescentne spektroskopije. Rezultati ispitivanja su pokazali da ovi* kompleksi interaguju sa DNK i da mogu istisnuti etidijum-bromid (EtBr) iz DNK-EtBr.

Synthesis, characterization and study of the interactions of new mononuclear platinum(II) complexes with DNA

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Recent years have witnessed a great deal of attention in the studies on the interaction of transition-metal complexes with DNA. In accordance to this, in the present study two new mononuclear Pt(II) complexes, [Pt(Me_2-mal-*O,O'*)(phen-epoxy)] and [Pt(cbdca-*O,O'*)(phen-epoxy)] (phen-epoxy = 5,6-epoxy-5,6-dihydro-[1,10]phenanthroline, Me_2-mal = anion of 2,2-dimethylmalonic acid, cbdca = anion of cyclobutane-1,1-dicarboxylic acid), have been synthesized. These complexes were characterized by IR, UV-Vis and NMR (^{1}H i ^{13}C) spectroscopic techniques. The binding of these complexes to DNA was investigated by UV-Vis and fluorescence spectroscopy. The obtained results of this study showed that these complexes interact with DNA and that they can displace ethidium bromide (EtBr) from DNA-EtBr adduct.

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NH P 11

Sinteza praha nanočestica srebra

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Nanočestice plemenitih metala (NPs) od velikog su interesa zbog svojih izvanrednih optičkih, hemijskih i fizičkih svojstava[1]. Nanočestice srebra (Ag NPs) privukle su posebnu pažnju zbog njihove primene u različitim oblastima. Ag NPs čestice najčešće se dobijaju redukcijom jona Ag^+ u vodenim rastvorima. Međutim, koloidne disprezije su stabilne samo pri niskim koncentracijama metala i teško je dobiti prah NPs iz njihovih disperzija. U literaturi je objavljena sinteza praha Ag NPs primenom skroba metodom iz čvrstog stanja[2]. U ovom radu je predstavljena sinteza praha Ag NPs redukcijom jona Ag^+ jonima citrata, hemijskom reakcijom komponenata u čvrstom stanju, odnosno mehaničko-hemijskim postupkom. Sintetisani prah Ag NPs analiziran je fizičko-hemijskim metodama, SEM, UV-Vis i FTIR spektroskopijom, kao i merenjem zeta potencijala. Dobijene NPs čestice su sfernog oblika, prosečnog prečnika 20 nm i negativnog površinskog naelektrisanja.

Solid-state synthesis of silver nanoparticles

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Noble metal nanoparticles (NPs) have attracted attention due to their remarkable optical, chemical and physical properties[1]. Silver NPs (Ag NPs) are of particular interest because of their wide applications, in different areas. The most often Ag NPs were obtained by chemical reduction of Ag^+ ions in aqueous solutions. However, colloidal dispersions are stable only in low metal concentration, and it is very difficult to obtain solid NPs from dispersion. Recently, the solid-state method was reported for Ag NPs synthesis[2] using starch. Here we presented a citrate-capped Ag NPs successfully prepared by solid-state chemical reaction. The Ag NPs were synthesized by the mechanochemical process. Powdered materials were characterized by SEM, UV-Vis and FTIR spectroscopy and, zeta potential measurements. The obtained NPs were spherical, with an average diameter of 20 nm and negative surface charge.

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Hemija životne sredine / Environmental Chemistry

HZS P 1

Identifikacija degradacionih produkata malationa nastalih primenom plazme na atmosferskom pritisku

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U ovom radu opisan je razvoj instrumentalne metode za određivanje proizvoda degradacije organofosfatnog pesticida malationa. Za razgradnju malationa u cilju dekontaminacije poljoprivrednih otpadnih voda koje se potom mogu ponovo koristiti za zalivanje, primenjen je izvor plazme na atmosferskom pritisku - plazma mlaz. Polazni rastvor malationa i uzorci tretirani plazma mlazom su analizirani korišćenjem LTQ XL linearnog jonskog trapa, kao masenog spektrometra. Na osnovu rezultata MS^n analize odabrane su reakcije fragmentacije dobijenih degradacionih produkata malationa. Uz tečno-hromatografsku analizu, ove reakcije su zatim korišćene za identifikaciju i praćenje malationa i odabranih produkata degradacije u tretiranim uzorcima. Kao dominantni produkti razgradnje identifikovani su dietil-2-merkaptosukcinat (*m/z* 229), kao i malaokson (*m/z* 315) koji se dalje degraduje u dimetilfosfonat (*m/z* 111). Takođe je utvrđeno postojanje degradacionih proizvoda (*m/z* 127, 273 i 293) koji su prisutni u manjem obimu. Na osnovu dobijenih rezultata predložen je put razgradnje malationa i nastanak degradacionih prozvoda.

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Identification of malathion degradation products produced by atmospheric pressure plasma

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This paper describes the development of an instrumental method for determination of degradation products of organophosphate pesticide malathion. For degradation of malathion, an atmospheric pressure plasma jet was applied, for the purpose of decontamination of agricultural wastewater, which can then be re-used for watering. Initial malathion solution and samples treated with atmospheric pressure plasma were analyzed using the LTQ XL linear ion trap as a mass spectrometer. Based on the results of MS^n analysis, fragmentation reactions of obtained malathion degradation products were selected. Using liquid chromatography, these reactions were then used to identify and track malathion and selected degradation products in the treated samples. The dominant degradation products were identified as diethyl-2-mercaptosuccinate (*m/z* 229), and malaoxon (*m/z* 315), which further degrades to dimethyl phosphonate (*m/z* 111). Additional degradation products (*m/z* 127, 273 and 293), present to a lesser extent, were also determined. Based on the obtained results, the pathway of malathion degradation and formation of degradation products was proposed.

HZS P 2

Ispitivanje adsorpcionih performansi i antimikrobnog potencijala nanočesticama srebra modifikovane montmorilonitne gline

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U ovom istraživanju ispitivan je adsorpcioni potencijal nanočesticama srebra (nčAg) modifikovane sirove montmorilonitne gline (Gl) izvađene iz depozita u okolini Pirota. U cilju dobijanja visokih adsorpcionih performansi adsorbenta Gl-nčAg, izvršena je optimizacija procedure sinteze koja uključuje varijacije vremena, temperature i količine nanetog nanočestičnog srebra (nčAg), korišćenjem metodologije odzivnih površina (response surface methodology - RSM). Najefikasniji adsorbent, dobijen hemijskom redukcijom srebra korišćenjem natrijum borohidrida - Gl-nčAgh detaljno je okarakterisan korišćenjem BET, SEM, FTIR, XRD tehnika i određivanjem tačke nultog naelektrisanja (pHPZC). Dobijeni rezultati su pokazali da u procesu prečišćavanja vode mogu da učestvuju dva sinergistička efekta korišćenjem Gl-nčAgh, uklanjanje zagađivača uz istovremeno smanjenje mikrobiološke kontaminacije koja doprinosi ukupnom poboljšanju kvaliteta vode.

Adsorption performance and antimicrobial potential of nanoparticles of silver modified montmorillonite clay

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In this study, the adsorption potential of raw montmorillonite clay (MC) modified by nanoparticles of silver (npAg) was tested. The clay was extracted from deposits in the vicinity of Pirot. In order to obtain high adsorption performance of the adsorbent MCnpAg, optimization of the synthesis procedure involving variations of the time, temperature and amount of applied nanoparticle silver (npAg) was performed, using the surface surface methodology (RSM). The most efficient adsorbent, obtained by chemical reduction of silver using sodium borohydride – MC-npAgh, was characterized in detail by using BET, SEM, FTIR, XRD techniques and determining the zero-charge point (pHPZC). The obtained results show that two synergistic effects can be involved in the water purification process using MC-npAgh, for the removal of pollutants while minimizing microbiological contamination, which contributes to overall improvement in water quality.

HZS P 3

Praćenje koncentracije n-alkana kao dijagnostička metoda za procenu vremena izlivanja dizel goriva

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Distribucija koncentracije n-alkana, kao i njihov odnos u zemljištu, dobro je poznata metoda za procenu vremena izlivanja dizel goriva na površini zemljišta. U ovom radu ispitivan je uticaj vremenskih uslova i različitih tipova zemljišta na raspodelu n-alkana u tlu tokom vremena. Koncentracije n-alkana su merene tokom perioda od 60 dana, korišćenjem gasne hromatografije. Korišćena su dva tipa zemljišta, odnosno pesak i glina. Prikupljeni su podaci o najpogodnijem sloju tla za praćenje, kao i najpogodnijem dijagnostičkom alatu za identifikaciju vremena izlivanja.

Monitoring of n-alkanes concentration as a diagnosis method for estimating the time of diesel fuel spillage

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The concentration distribution of n-alkanes as well as their relationships in soil, is a well known method for the estimation of the time of the spillage of diesel fuel in a land area. In this work, the influence of weathering conditions and of different soil types on the distribution of n-alkanes in soil over time, was investigated. The n-alkane concentrations were measured over 60 day period, by using gas chromatography. The two soil types were used, namely sand and clay. The information about the most suitable soil layer for the monitoring, as well as the most suitable diagnosis tool for identification of the spillage time, is provided.

HZS P 4 text rada / full text

Kvalitet vazduha na teritoriji grada Šapca

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Zagađen vazduh predstavlja značajan faktor rizika za zdravlje ljudi širom sveta. U ovom radu je prikazan kvalitet vazduha na teritoriji grada Šapca tokom 2018. godine. Dobijeni rezultati pokazuju da su koncentracije SO_2 i NO_2, bile ispod zakonom propisanih vrednosti, dok je koncentracija čađi 15 dana tokom godine bila preko maksimalno dozvoljene koncentracije. Proučavanje kvaliteta vazduha u urbanim i industrijskim područjima ima za cilj kontrolu i utvrđivanje stepena zagađenosti vazduha, kao i utvrđivanje trenda zagađenja, kako bi se pravovremeno delovalo ka smanjenju sadržaja štetnih supstanci

Air quality in the territory of the town of Šabac

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Air pollution is an important risk factor for health in Europe and worldwide. This paper presents the quality of air in the territory of the town of Šabac during 2018. The measured values of SO_2 and NO_2 were less than the legally permitted limit, but the concentration of soot was above the limit of 50 $\mu g/m^3$ for 15 days during the examined period. The study of air quality in urban and industrial areas is very important, because it enables us to determine the degree and trend of pollution, with the aim of reducing the content of harmful substances in a time manner.

Ispitivanje upotrebe otpadne biomase za uklanjanje naftnih ugljovodonika iz vodenog rastvora

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Adsorpcija je jedna od najčešće korišćenih tehnika za tretiranje voda zagađenih naftom i njenim derivatima. U radu je ispitivana mogućnost primene otpadne biomase (koštice breskve, agroindustrijskog otpada), kao jeftinog biosorbenta, za uklanjanje nafnih zagađivača iz vodenog rastvora u stacionarnim uslovima. Biosorpcioni eksperimenti su obavljeni u erlenmajerima na na orbitalnom šejkeru u kojima je konstantna količina biosorbenta od 1 g mešana sa 100 ml vode kontaminirane naftnim ugljovodonicima u koncentacijama 4 mg/L, 12 mg/L, 18 mg/L, 24 mg/L, 30 mg/L, 40 mg/L and 80 mg/L. Dobijeni rezultati pokazuju da je otpadna biomasa efikasna u uklanjanju naftnih polutanata iz vodenog rastvora. Biosorpcija je potencijalno alternativna tehnika za prečišćavanje otpadnih voda. Njene glavne prednosti su niska cena, visoka efikasnost i obnovljivost.

Investigations of possibility for petroleum hydrocarbons removal from aqueous solution by waste biomass

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Adsorption is one the best commonly used technique for treatment of petroleum contaminated water. The biosorption potential of waste biomass (peach shell, agro-industrial waste) as a low-cost biosorbent for petroleum hydrocarbon from aqueous solution was explored. Biosorption experiments were carried out using a shake-flask technique with a constant amount of (bio) sorbent of 1 g mixed with 100 ml of water contaminated with petroleum hydrocarbons at concentrations of 4 mg/L, 12 mg/L, 18 mg/L, 24 mg/L, 30 mg/L, 40 mg/L and 80 mg/L. The obtained results show that waste biomass is efficient in the removal of petroleum pollutants from the water solution. Biosorption is a potentially alternative technique for wastewater treatment. Their major advantages are low cost, high efficiency, renewability.

HZS P 6 text rada / full text

Ispitivanje zagađenosti podzemnih voda organskim zagađujućim supstancama

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Podzemne vode su važan prirodni resurs. Analiza kvaliteta podzemnih voda je neophodna za održavanje i očuvanje čitavog ekosistema.

Na termoenergetskom objektu, tokom redovne kontrole kvaliteta vode, uočena je povećana koncentracija organskih zagađujućih supstanci. Cilj ovog rada bio je ispitivanje i praćenje stepena zagađenja podzemnih voda i efikasnost tretmana, koji je korišćen za uklanjanje zagađujućih supstanci. Primena mikrobioloških i fizičko-hemijskih tretmana, organski zagađivači su uklonjeni sa svih mikrolokacija, više od 96 %.

Investigation of groundwater polluted with organic pollutants

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Groundwater is an important natural resource.The analysis of groundwater quality is necessary to maintain and preserve the entire ecosystem.

On a thermal energy facility, during regular water quality control, an increased concentration of organic pollutants has been observed. The aim was to analyze petroleum hydrocarbons and their derivatives, before and after cleaning treatments. The application of microbiological and physical-chemical treatments, organic pollutants were removed from all microlocations, more than 96 %.

HZS P 7

Uticaj odabranih jonskih tečnosti na klijanje i rani rast pšenice, ječma i krastavaca

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U ovom radu ispitan je uticaj novosintetisanih jonskih tečnosti različitih polarnosti, na klijanje i rani rast pšenice, ječma i krastavaca. Praćena je brzina i stepen klijanja datih biljnih vrsta nakon tretmana vodenim rastvorima jonskih tečnosti, dok su parametri rasta praćeni na osnovu sveže i suve mase biljnog materijala, kao i dužine korena i nadzemnog dela. Ukupni sadržaj hlorofila i karotenoida, kao i malonildialdehida (MDA) praćen je kao indikator stresa koje različite biljne vrste trpe pod dejstvom jonskih tečnosti. Iz dobijenih rezultata uočava se pozitivna korelacija između inhibicije rasta biljnih vrsta i polarnosti jonskih tečnosti. Pšenica je najrezistentnija na dejstvo jonskih tečnosti, dok je krastavac najsenzitivniji, ukazujući da na toksičnost značajan uticaj imaju i različite fiziološke i morfološke karakteristike samih biljaka.

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The effect of selected ionic liquids on germination and growth of wheat, barley and cucumber

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In this paper, the influence of newly synthesized ionic liquids with different polarity on germination and growth of wheat, barley and cucumber was investigated. The toxicity effect of ionic liquids was discussed based on results of germination rate, the plant's root and shoot length and measured dry and fresh mass of plants. Also the effects on stress marker (MDA) as well as on biosynthesis of chlorophyll and carotenoids were investigated. From obtained results it was conducted positive correlation between lipophilicity of synthesized ionic liquids and toxicity towards investigated plants. It was shown that wheat is most resistent on influence of ionic liquids. Hence, cucumber was most sensitive, indicating that toxicity is significantly determined by different physiological and morphological background of plants.

HZS P 8 text rada / full text

Mikrobna gorivna ćelija – hemijska i mikrobiološka karakterizacija sedimenta

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Mikrobne gorivne ćelije (Microbial fuel cell-MFC) predstavljaju nove potencijalne izvore energije, preko kojih se generiše električna energija, a među brojnim prednostima je i ta što izostaje emisija štetnih gasova. MFC su vrsta bioloških gorivnih ćelija, sistema koji konvertuju hemijsku energiju u električnu pomoću mikroorganizama. Postoji više načina konstrukcije i među njima se nalaze jednokomorne, dvokomorne i složene MFC. Takođe, mikroorganizmi i supstrati koji se koriste u MFC, koje ti mikroorganizmi obrađuju u hemijskim procesima, mogu da budu različitog porekla i da imaju različite karakteristike. MFC su dobri alternativni izvori energije koji svoju potencijalnu primenu nalaze u industriji biosenzora, sistemima za proizvodnju vodonika ili električne energije i postrojenjima za prečišćavanje otpadnih voda. U ovom radu dat je opis sedimenta korišćenog u sistemu jednokomorne MFC, okarakterisan pomoću mikrobioloških, hemijskih i analitičkih parametara.

Testing microbiological and chemical parametars of the sediment of microbial fuel cell

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Microbial fuel cells (MFCs) represent new potential energy sources through which electricity is generated, and among numerous advantages is that the emission of harmful gases is missing. MFC is a type of biological fuel cell, a system that converts chemical energy into electrical power by microorganisms. These systems can be constructed in many ways so that there are one-chamber, two-chamber and complex MFCs. MFCs are good alternative sources of energy offering possibility of application that can be found in the biosensor industry, hydrogen or electricity production systems and wastewater treatment plants. In this paper, characterization of the sediment used in a single chamber MFC is presented. The sediment used to form the microbial fuel cell is characterized by microbiological, chemical and analytical parameters.

HZS P 9

Nanočestice magnetita kao imobilizacioni matriks za peroksidazu iz rena

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Peroksidaze predstavljaju veliku grupu enzima koji se intenzivno koriste u tretmanu otpadnih voda. Slobodne oblike ovih enzima karakteriše kratko vreme operativne stabilnosti. Primenom postupka imobilizacije povećava se stabilnost enzima, kao i mogućnost njihove regeneracije i ponovne upotrebe. Cilj ovog rada bio je ispitivanje aktivnosti imobilisanog i neimobilisanog enzima peroksidaze dobijenog iz rena (HRP) u vremenskom periodu od mesec dana. Enzim je procesom adsorpcije imobilisan na nanočesticama magnetita (Fe_3O_4) prethodno sintetisanim iz Fe^{2+} i Fe^{3+} sulfatnih soli metodom koprecipitacije na sobnoj temperaturi (25^oC). Aktivnost slobodnog enzima u rastvoru na sobnoj temperaturi iznosila je 3,8 U/ml, pri čemu je enzim nakon dva dana potpuno izgubio svoju aktivnost. Čist magnetit je pokazao veoma slabu katalitičku aktivnost (0,3 U/g). Pri istim reakcionim uslovima, aktivnost imobilisanog enzima je bila dva puta veća (8,0 U/ml) i ostala je nepromenjena tokom celog ispitivanog perioda (mesec dana). Dobijeni rezultati potvrđuju prednost korišćenja magnetita za imobilizaciju enzima, kao i potencijalnu primenu ovakvog enzima u tretmanu fenolnih otpadnih voda.

Magnetite nanoparticles as immobilization matrix for horseradish peroxidase

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Peroxidases represent a large group of enzymes that have been used extensively in wastewater treatment. Free forms of enzymes have short-term operational stability. The immobilization procedure increases the stability of enzymes, as well as possibility of their regeneration and reuse. The aim of this study was to investigate the activity of the immobilized and free peroxidase obtained from horseradish (HRP) during one month. The enzyme was immobilized by adsorption process on magnetite nanoparticles (Fe_3O_4), previously synthesized from Fe^{2+} and Fe^{3+} sulfate salts by co-precipitation method at room temperature (25^oC). The activity of the free enzyme in solution at room temperature was 3.8 U/ml, and after two days, the enzyme completely lost its activity. Pure magnetite has shown very low catalytic activity (0.3 U/g). Under the same reaction conditions, the activity of an immobilized enzyme was twice as high (8.0 U/ml) and remained stable during the whole measuring period (one month). The obtained results of improved activity and stability confirm the advantage of using magnetite nanoparticles for enzyme immobilization, as well as the potential use of this enzyme in phenolic wastewater treatment.

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HZS P 10 text rada / full text

Uklanjanje šestovalentnog hroma iz vode primenom biosorpcije na hitozanu

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U ovom radu ispitivana je mogućnost primene biopolimera hitozana kao adsorbensa za uklanjanje šetvovalentnog hroma iz vode. Adsorpcija je rađena u šaržnom sistemu i ispitivan je uticaj različitih parametara (pH, vreme kontakta, početna koncentracija Cr(VI)) na efikasnost uklanjanja Cr(VI). Rezultati su pokazali da se ravnoteža uspostavlja nakon 60 min, a da je efikasnost uklanjanja najveća u intervalu pH vrednosti od 2.0 do 3.5. Analiza kinetičkih parametara adsorpcije Cr(VI) pokazala je da model pseudo-drugog reda reakcije najbolje opisuje kinetiku adsorpcije za dati sistem. Dobijeni podaci su fitovani pomoću dva ravnotežna adsorpciona modela - Langmirovom i Frojndlihovom izotermom. Bolje slaganje je postignuto primenom Langmirove izoterme i nađeno je da je adsorpcioni kapacitet hitozana 86.1 mg/g. Na osnovu dobijenih rezultata može se zaključiti da hitozan ima dobar potencijal za primenu u prečišćavanju otpadnih voda zagađenih toksičnim metalom hromom.

Removal of hexavalent chromium from aqueous solutions by adsorption on biopolymer chitosan

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Biopolymer chitosan was used as an adsorbent for the removal of hexavalent chromium from aqueous solutions. Batch adsorption experiments were conducted to evaluate the effects of different parameters, such as pH, contact time and initial Cr(VI) concentration, on Cr(VI) removal. The obtained results showed that the adsorption equilibrium was established within 60 min, and the maximum adsorption occurred in the pH range of 2.0 to 3.5. Analysis of kinetic parameters of Cr(VI) adsorption showed that pseudo second-order model described the kinetics fot the investigated system. The data were fitted using two equilibrium adsorption models – Langmuir and Freundlich isotherm. The adsorption equilibrium data fit the Langmuir equation and the maximum adsorption capacity was found to be 86.1 mg/g. According to the presented results, it can be concluded that biopolymer chitosan has a great potential for application in the treatment of chromium contaminated wastewaters.

HZS P 11

Kinetika procesa adsorpcije jona bakra iz vodenih rastvora na glavama suncokreta

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U ovom radu, prikazana je kinetika procesa adsorpcije jona bakra iz vodenih rastvora korišćenjem glava suncokreta kao adsorbensa. U tu svrhu eksperimentalni podaci su modelovani korišćenjem sledećih kinetičkih modela: kinetički model pseudo-prvog reda, kinetički model pseudo-drugog reda, model međučestične difuzije, i Elovich-ev kinetički model. Praćena je promena kapaciteta adsorpcije sa vremenom. Analizom rezultata dobijenih modelovanjem eksperimentalnih podataka navedenim kinetičkim modelima, može se zaključiti da najbolje slaganje sa eksperimentalnim podacima pokazao kinetički model pseudo-drugog reda, sa koeficijentom korelacije R^2 = 0,999. Ovo ukazuje na to da je hemisorpcija mogući mehanizam vezivanja jona bakra na površini glava suncokreta.

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Kinetic study of the adsorption of copper ions from aqueous solutions on the sunflower heads

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In this paper, the kinetics of the adsorption of copper ions from aqueous solutions using sunflower heads as an adsorbent are presented. For this purpose, the experimental data were modeled using the following kinetic models: pseudo-first order kinetic model, pseudo-second order kinetic model, interparticle diffusion model, and Elovich kinetic model. Change in the adsorption capacity with process time was monitored. Analyzing the results obtained by modeling the experimental data with above mentioned kinetic models, it can be concluded that the best agreement with experimental data showed the pseudo-second order kinetic model, with the coefficient of correlation R^2 = 0.999. This indicates that chemisorption is a possible mechanism of binding the copper ions on the surface of the sunflower heads.

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In situ bioremedijacija sedimenta kontaminiranog mineralnim uljem

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Zagađenje vode, zemljišta i sedimenta naftom i njenim derivatima, može se javiti tokom eksploatacije, transporta i skladištenja i predstavlja rizik za životnu sredinu i ljudsko zdravlje. Bioremedijacija je zelena tehnologija kojom se uklanja zagađenje iz kontaminirane životne sredine upotrebom mikroorganizama. U ovom radu su praćene promene u sadržaju mineralnih ulja i aktivnost mikroorganizama koji razgrađuju ugljovodonike tokom procesa bioremedijacije koji je trajao 210 dana. Rezultati ukazuju da mikroorganizmi koji razgrađuju ugljovodonike sa visokom efikasnošću degraduju mineralna ulja. Na osnovu količine mineralnog ulja (smanjena za 63,82 %), stepena degradacije i udela mikroorganizama naftnih degradera u ukupnom broju mikroorganizama, može se zaključiti da su faza adaptacije konzorcijuma i faza intenzivne razgradnje bile u periodu od 0. do 90. dana, praćene dalje sporijom fazom razgradnje u periodu od 90. do 210. dana.

In situ bioremediation of sediment contaminated with mineral oil

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Pollution of water, soil and sediment with petroleum and its products may occur during the exploitation, transportation and storage and it poses a risk to the environment and human health. Bioremediation is a green technology that can remove pollution from contaminated environment using microorganisms. In this paper changes in the content of mineral oil and the activity of hydrocarbon degraders during remediation process that lasted 210 days were monitored. The results indicate that hydrocarbon degrading microorganisms with high efficiency have biodegraded mineral oil. Based on the amount of mineral oil (decreased for 63.82 %), degradation rates and level of hydrocarbon degraders in the total number of microorganisms, we note that the stages of adaptation of the consortium and intensive degradation phases were in the range of 0-90 days, followed by a slower decomposition phase in the period of 90-210 days.

BH P 1

Biohemija / Biochemistry

Identification of novel ligands of human steroid 17α-hydroxylase among modified androstanes and bile acids

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In the present time testing of ligand libraries towards to the range of targets is a standard procedure in the workflow of large pharmaceutical companies and scientific laboratories that design and create effective drugs for various diseases. Today cytochrome P450 enzymes (CYPs) – are important group of drug targets. CYPs are a superfamily of heme-containing enzymes taking part in biotransformation of xenobiotics (including drugs), biosynthesis and metabolism of cholesterol, steroid hormones, fat-soluble vitamins and polyunsaturated fatty acids. Steroid 17α-hydroxylase (CYP17) — is a key human enzyme, taking part in steroid hormone biosynthesis. Mutations of CYP17 gene and changes in CYP17 expression level are associated with congenital adrenal hyperplasia, isolated 17,20-lyase deficiency, polycystic ovary syndrome and Cushing's syndrome. In the present study we performed initial screening of a panel of modified steroids toward human CYP17 to identify novel ligands of the enzyme – perspective high efficient inhibitors.

Recombinant human CYP17 was expressed in the *E. coli* cells, purified and used for the screening of new ligands. *In vitro* screening allowed us to find new CYP17 ligands among modified androstanes and bile acids. All the substances bind in the enzymes' active site like substrates, usually with high or moderate affinity (in comparison to substrates of this enzyme: pregnenolone, progesterone) towards human CYP17, so they could be considered as competitive inhibitors of the enzyme. *In silico* structural insights (docking followed by molecular dynamics simulation) showed that in all cases binding mode of the compounds is quite similar to the binding mode of the "essential" CYP17 ligands, while corresponding "protein-ligand" complexes are quite stable. It was found that long side chain and different modifications does not allow ligand to accept correct pose, which is necessary for hydroxylation.

Analysis of the inhibitory potential of the ligands and identification of possible products of enzymatic reactions are the main tasks of our further work.

Presented results are obtained in the frame of Belarus-Serbia bilateral project „Target-specific screening of new activity modulators of human sterol-hydroxylases" (X18-SRBG002) which is being realized between Institute of Bioorganic Chemistry of NAS of Belarus and University of Novi Sad Faculty of Sciences.

BH P 2

Identification of potential inhibitors of *Pseudomonas aeruginosa* cholesterol oxidase activity

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Pseudomonas aeruginosa is a metabolically versatile bacterium that can cause a wide range of severe opportunistic infections with serious underlying medical conditions. These infections are characterized by an intense neutrophilic response resulting in significant damage to host tissues and often exhibit resistance to antibiotics leading to mortality (Shaan L. Gellatly 2013). One of the main pathogenesis factors of such pathogens is cholesterol oxidases.

Cholesterol oxidase (EC 1.1.3.6) is a flavin adenin dinucleotide (FAD)-dependent enzyme that in most cases catalyzes the oxidation of cholesterol (cholest-5-en-3β-ol) using oxygen as an electron acceptor to form cholest-4-en-3-one (CEO) and hydrogen peroxide (Smith and Brooks 1974).

In current work, we performed new purified recombinant enzyme –the cholesterol oxidase of *Pseudomonas aeruginosa*, described its activity features and conducted an initial screening of the affinity of a series of modified steroids as substrates to the cholesterol oxidase. Our results show some perspective ways to inhibit cholesterol oxidative activity that may slow down the disease spreading or even stop it (Anna Brzostek 2007).

Presented results are obtained in the frame of Belarus-Serbia bilateral project ”Target-specific screening of new activity modulators of human sterol-hydroxylases“ (X18-SRBG002) which is being realized between Institute of Bioorganic Chemistry of NAS of Belarus and University of Novi Sad Faculty of Sciences.

Hemija i tehnologija hrane / Chemistry and Technology of Food

HTH P 1

Spray drying of camel milk induces protein aggregates and Maillard reaction products formation

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Camel milk (CM) powders are nutritious food with many health benefits. We investigated physicochemical properties of CM proteins upon spray drying at six inlet temperatures (190°C - 250°C). Electrophoretic and spectrophotometric analysis revealed occurrence of Maillard reaction upon spray drying. Size exclusion chromatography showed increase in protein Mw and aggregates formation. Spray drying inlet temperatures exerted significant effects on the properties of CM powder proteins. Project was supported by the GA No.172024 of Ministry of Education, Science and Technological Development.

Sušenje kamiljeg mleka raspršivanjem indukuje formiranje proteinskih agregata i Majarovih proizvoda

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Kamilje mleko (KM) u prahu je visoko nutritivno sa brojnim zdravstvenim učincima. U ovoj studiji smo ispitivali fizičko-hemijske osobine proteina KM nakon sušenja raspršivanjem na šest ulaznih temperatura (190°C - 250°C). Elektroforetske i spektrofotometrijske analize su pokazale odigravanje Majarove reakcije tokom sušenja raspršivanjem. Ekskluziona hromatografija je pokazala povećanje Mw proteina i formiranje proteinskih agregata. Ulazna temperatura kod sušenja raspršivanjem ima značajne efekte na fizičko-hemijske osobine proteina KM u prahu. Studija je podržana od strane Ministarstva prosvete, nauke i tehnološkog razvoja, projekat br. 172024.

HTH P 2

Masnokiselinski profil organskog i konvencionalnog semena spelte

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Usled izuzetno povoljnih prehrambenih, medicinskih i agronomskih karakteristika, kao i povoljnog hemijskog sastava semena koje je u skladu sa najsavremenijim nutritionističkim zahtevima, proizvodnja spelte dobija sve veći značaj, naročito u organskoj proizvodnji hrane. Veoma važan nutritivni faktor namirnica predstavlja sadržaj masnih kiselina u njima, neophodnih za pravilno funkcionisanje ljudskog organizma. Cilj ovog rada bio je da GC-FID metodom ispita sadržaj masnih kiselina u organskom i konvencionalnom semenu spelte, poreklom iz 2015 i 2016. godine. Sadržaj masnih kiselina izražen je kao % sadržaj u odnosu na ukupne masne kiseline. Detektovano je deset masnih kiselina. Kod obe vrste semena, u najvećoj količini se nalaze linolna (C18:2n-6) i oleinska (C18:1n-9) kiselina. Najveći udeo polinezasićenih masnih kiselina sadrži seme konvencionalne spelte (59.46 %), dok se u organskom semenu iz 2016. godine nalazio najveći udeo zasićenih (18.33 %) i mononezasićenih masnih kiselina (26.71 %).

Fatty acids profile of organic and conventional spelt seeds

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Due to the extremely favorable nutritional, medical and agronomic characteristics, as well as the favorable chemical composition of seed which is in accordance with the current nutritional requirements, spelt production is gaining increasing importance, especially in organic food production. The fatty acids (FAs) content is a very important nutritional factor. Adequate FAs daily intake is necessary for the proper functioning of the human body. The aim of this paper was to examine fatty acids content in organic and conventional spelt seeds produced during 2015 and 2016 year. GC-FID method was used for FAs determination. FAs content is expressed as % of content in relation to the total fatty acids. Ten fatty acids were detected. Both types of seeds contained linoleic (C18:2n-6) and oleic acid (C18:1n-9) as predominant. Conventional spelt seed possessed higher content of polyunsaturated fatty acids (59.46 %) while organic seed from 2016 contained higher amount of saturated (18.33 %) and monounsaturated fatty acids (26.71 %).

HTH P 3

Određivanje toksičnih elemenata (žive, kadmijuma, olova i arsena) u uzorcima školjki

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Morski plodovi imaju visoku nutritivnu vrednost, ali sa druge strane postoji rizik od kontaminacije toksičnim elementima. Sadržaj As, Cd, Hg i Pb je određen u četiri vrste školjki *Ruditapes philippinarum* (Manila clam, MC), *Yesso scallop* (YS), *Tegillarca granosa* (TG) i *Anadara broughtonii* (AB) kupljene u Incheonu, Koreja. Uzorci su analizirani induktivno spregnutom plazmom - masenom spektrometrijom (ICP-MS) nakon mikrotalasne digestije. Izračunati su dnevni/nedeljni unosi za ove elemente u mg/300 g uzorka. Ukupan sadržaj As (neoganski i organski) u svim vrstama je bio veći od dozvoljenog limita preporučenog od Svetske zdravstvene organizacije (WHO). Procenjeni dnevni unosi ostalih elemenata (Hg, Cd i Pb) su niži od maksimalnih podnošljivih granica (MDI) koje je odredila Evropska agencija za bezbednost hrane (EFSA) što ukazuje da nema rizika za konzumente.

Determination of toxic elements (mercury, cadmium, lead and arsenic) in shellfish samples

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Bivalve molluscs, which include mussels, oysters and clams, have high nutritional value. On the other hand, seafood may also contain harmful contaminants and other undesirable substances such as mercury and persistent halogenated compounds. Four species of bivalve molluscs *Ruditapes philippinarum* (Manila clam, MC), *Yesso scallop* (YS), *Tegillarca granosa* (TG) and *Anadara broughtonii* (AB) were bought in Incheon, Korea, in order to determine content of As, Cd, Hg, and Pb and consequently, to estimate the health hazards associated to dietary intake. The samples were analyzed by inductively coupled plasma mass spectrometry (ICP-MS) after microwave digestion. All species showed As content higher than the maximum tolerable limit specified by EFSA. Estimated daily intake of Hg, Cd and Pb from consumption of 300 g was very low and hence poses no toxicological risk.

Acknowledgments: *This research was financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, project no. 172030 and the European Commision, under the Horizon 2020, FoodEnTwin project grant agreement no. 810752.*

Hemija i tehnologija makromolekula
Chemistry and Technology of Macromolecules

HTM P 1

Uticaj anjona na uklanjanje boja iz otpadnih voda tekstilne industrije

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Otpadne vode tekstilne industrije predstavljaju ozbiljan ekološki problem, jer u sebi sadrže različite boje i toksične supstance koje se upotrebljavaju tokom proizvodnje i bojenja tekstila. Stoga, potrebno je da se ispita mogućnost uklanjanja boja iz otpadnih voda tekstilne industrije jednostavnom metodom sorpcije. Kako se u procesu bojenja tekstila koriste različite soli, u ovim otpadnim vodama često su prisutni anjoni i katjoni koji mogu da utiču na sam proces uklanjanja boja.
U ovom radu analiziran je uticaj nekoliko anjona na uklanjanje boja za tekstil pomoću hidrogelova na bazi hitozana. Korišćeni hidrogelovi su kopolimeri hitozana i metakrilne kiseline dobijeni slobodno-radikalskom polimerizacijom, a kao umreživač je upotrebljen *N,N'*-metilenbisakrilamid. Anjonska boja *C.I. Acid Orange 7* i katjonska boja *C.I. Basic Red 1* su korišćene u model vodama, a uklanjanje boja je izvedeno na dve različite temperature (25 i 50 °C). Uticaj anjona je ispitan dodatkom natrijumovih jedinjenja u rastvore boja (NaCl, CH_3COONa, Na_2CO_3, Na_2HPO_4, NaH_2PO_4, $NaNO_3$, NaOH). Utvrđeno je da hidrogelovi izrazito bubre sa povećanjem pH rastvora. Prisustvo različitih jona utiče na kapacitet sorpcije, a najbolji rezultati su dobijeni kada su u rastvoru prisutne soli NaH_2PO_4 i $NaNO_3$.

The effect of anions on the removal of dyes from textile industry wastewater

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Textile industry wastewater represents a serious environmental problem because it contains different dyes and toxic substances used during the production and dyeing of textile. Thus, it is necessary to investigate the removal of dyes from wastewater using a simple method such as sorption. Since different salts are used during the dyeing of textile, anions and cations are present in wastewaters and they can affect the process of dye removal.
In this paper, the influence of several anions on the removal of textile dyes was investigated. Chitosan and methacrylic acid-based hydrogels obtained by free-radical polymerization and cross-linked with *N,N*'-methylenebisacrylamide were used as sorbents. Removal of two textile dyes was investigated (anionic dye *C.I. Acid Orange 7* and cationic dye *C.I. Basic Red 1*) at two different temperatures (25 and 50 ° C). The influence of anions on the removal was evaluated using sodium compounds dissolved in dye solutions (NaCl, CH_3COONa, Na_2CO_3, Na_2HPO_4, NaH_2PO_4, $NaNO_3$, NaOH). It has been found that hydrogel degree of swelling increased significantly with the increase of pH of the dye solution. The presence of different ions affected the sorption capacity of hydrogels and the best results were obtained when NaH_2PO_4 and $NaNO_3$ were present.

HTM P 2

Sinteza hibridnih vodorazredivih alkidnih smola

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U ovom radu ispitivan je uticaj dodatka nanočestica silicijum(IV)-oksida na svojstva hibridnih vodorazredivih alkidnih smola. Sinteza vodorazredivih alkidnih smola izvedena je reakcijom direktne poliesterifikacije glicerola, anhidrida ftalne kiseline i modifikovane ricinolne kiseline. Modifikacija ricinolne kiseline izvršena je reakcijom radikalske polimerizacije sa anhidridom maleinske kiseline. Sinteza hibridnih alkidnih smola izvedena je dodavanjem hidrofilnih nanočestica silicijum(IV)-oksida (1, 2 i 5 % na masu alkidne smole) u alkidnu disperziju i tretiranjem ultrazvukom u trajanju od 15 min, pre formiranja filma. Struktura dobijene modifikovane smole potvrđena je FTIR metodom. Za ispitivanje mehaničkih osobina, alkidni film je formiran umrežavanjem sa 2 % (po masi) stirena na 100 °C. Prema rezultatima dobijenim fizičko-mehaničkim ispitivanjima, dobijene alkidne smole su pogodne za različite primene kao premazi. Takođe, rezultati pokazuju da dobijene modifikovane alkidne smole imaju visok sjaj, pokazuju mogućnost dobre adhezije i da im se dodatkom nanočestica povećava tvrdoća, kao i otpornost na metil-etil-keton.

Synthesis of hybrid waterborne alkyd resins

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In this work, the influence of silica nanofiller on the properties of hybrid waterborne alkyd resins was investigated. Synthesis of water dispersible alkyd resins was carried out by direct polyesterification of glycerol, phthalic anhydride, and modified ricinoleic acid. Modification of ricinoleic acid was accomplished by free-radical polymerization of ricinoleic acid and maleic anhydride. The synthesis of hybrid alkyd resins was performed by addition of hydrophilic surface modified silica nanoparticles (1, 2 and 5 % based on alkyd resin weight) in the alkyd dispersion and sonication for 15 minutes. Structures of the obtained modified resins were confirmed by FTIR method. Mechanical properties were assessed for an alkyd film obtained by curing with 2 wt % of styrene at 100 °C. Based on the results of physical-mechanical testing, the obtained alkyds are suitable for various applications as coatings. These results indicate that the obtained films based on modified alkyd resins have a high gloss, good adhesion properties and that the addition of nanoparticles results in a higher value of hybrid film hardness and resistance to methyl ethyl ketone.

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HTM P 3

Light-scattering techniques as a tool for on-line monitoring of artificial gene assembly by thermostable DNA polymerases

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The artificial genes or synthetic DNA is highly demanded by the fast-growing field of synthetic biology [1]. The building of synthetic DNA is a multistage process that includes phosphoramidite synthesis, oligonucleotide preparation, enzymatic gene assembly, and quality control. The results of gene assembly are evaluated by gel electrophoresis and by Sanger sequencing. These procedures add additional efforts and time to the gene synthesis workflow. The ability for real-time monitoring of gene assembly was previously reported by an indirect method using real-time polymerase chain reaction [2]. Since gene assembly is accompanied by the formation of duplex DNA from smaller oligonucleotides we decided to test light-scattering techniques as a direct method for on-line gene assembly monitoring. Our results clearly confirm that oligonucleotide annealing and gene assembly process could be monitored by static/dynamic light-scattering (SLS/DLS) measurements. However, we should state that modern SLS/DLS equipment is not adapted for such tasks, mainly due to the inertia of heating and heat transfer. Therefore, it is necessary to conclude, that if there is an opportunity to overcome the stated problems by a special design of the sample compartment and measuring cell, light-scattering techniques may be considered an alternative method for the optimization of gene assembly methods.

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Medicinska hemija / Medicinal Chemistry

MH O 1 text rada / full text

Molecular properties and bioactivity score of hydroxy-substituted hydrazones

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Hydrazones are compounds possessing diverse biological activities such as analgesic, anti-inflammatory, anticancer, antimicrobial, antibacterial, *etc.* Especially active are the aroylhydrazones of the type R'-CH = N-NH-CO-R obtained by the condensation of aromatic aldehydes and various hydrazides. Different substituents in the molecules of the compounds could improve their pharmacological effect. The presence of a hydroxy group in the molecules of different hydrazones strongly influences the biological activity of the compounds. Novel hydroxy-substituted hydrazone derivatives were designed by inserting the OH-group in both the aldehyde and hydrazide moieties and by varying the position of the substituents. The molecular properties of the compounds, important for drug pharmacokinetics in the human body, were assessed by a method based on group contribution. *In silico* evaluation of the value of logP and the remaining parameters of drug similarity, as well as the topological polar surface area and absorption percentage, were used to find the lead candidates with encouraging properties for further elaboration.

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MH O 2

Sinteza i antiproliferativna aktivnost C-6 epimera kleistenolata

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U ovom radu želimo da saopštimo sintezu C-6 epimera kleistenolata, prirodnog proizvoda izolovanog iz listova subtropske biljke *Cleistochlamys kirkii* (Benth.) Oliv., Annonaceae.[1] Kao polazno jedinjenje primenjena je D-riboza. Pored toga, biće prikazani i rezultati citotoksičnosti **10**, prema nekoliko malignih i jednoj normalnoj ćelijskoj liniji.

Synthesis and antiproliferative activity of C-6 epimer of cleistenolate

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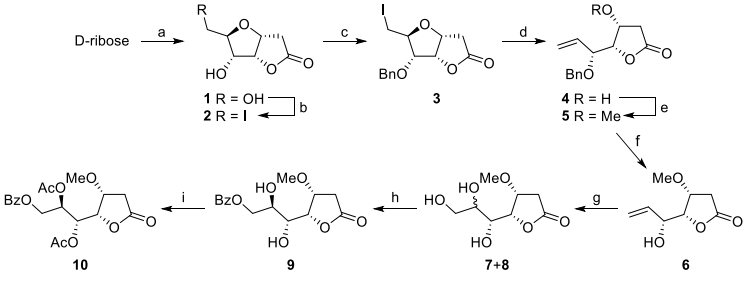
Herein, we present the synthesis of C-6 epimer of cleistenolate, a natural product isolated from the leaves of subtropical plant *Cleistochlamys kirkii* (Benth.) Oliv., Annonaceae.[1] D-ribose was used as a starting material (Scheme 1). Additionally, cytotoxicity of **10** against several malignant human cell lines and one normal cell line will be presented.



Scheme 1. a) Meldrum's acid, ^{t}BuNH$_2$, DMF; b) Ph$_3$P, Imidazole, I$_2$, THF; c) BnBr, Ag$_2$O, AgOTf, CH$_2$Cl$_2$; d) Zn dust, 4:1 THF/H$_2$O; e) MeI, Ag$_2$O, AgOTf, Et$_2$O; f)TiCl$_4$, CH$_2$Cl$_2$; g)2.5 w % OsO$_4$ in ^{t}BuOH, NMO, 10:1 Me$_2$CO/H$_2$O; h) BzCl, CH$_2$Cl$_2$, Py; i) Ac$_2$O, *p*-TsOH·H$_2$O.

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

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MH P 1

Sinteza i citotoksična aktivnost novog defenilovanog analoga (–)-goniofufurona

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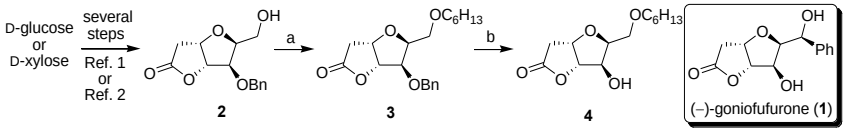
U cilju pronalaženja novih antineoplastičnih agenasa, dizajniran je novi defenilovani analog sintetičkog i vrlo potentnog molekula, (–)-goniofufurona (**1**, *Scheme 1*),[1,2] analog **4**. U ovom radu želimo da saopštimo sintezu analoga **4**, preliminarne rezultate ispitivanja njegove *in vitro* citotoksične aktivnosti prema ćelijama odabranih humanih tumora, kao i odnos strukture i aktivnosti (SAR) novosintetizovanog molekula **4** i ranije dobijenih analoga u našoj laboratoriji.



Scheme 1. Reagents and conditions: (a) $C_6H_{13}Br$, Ag_2O, AgOTf, Et_2O, reflux; (b) H_2, 10 % Pd/C, EtOH, rt.

Synthesis and cytotoxic activity of a new dephenylated (–)-goniofufurone analogue

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In the search for new antineoplastic agents, a new dephenylated analogue of a synthetic and very potent molecule, (–)-goniofufurone (**1**, *Scheme 1*),[1,2] analogue **4**, was designed. Herein we report the synthesis of analogue **4**, along with its effects on the proliferation of selected human tumour cell lines, as well as structure–activity relationship (SAR) of the new analogue **4** and analogues that were previously synthesized in our laboratory.

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

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MH P 2

Sinteza i biološka ispitivanja novih analoga (–)-goniofufurona

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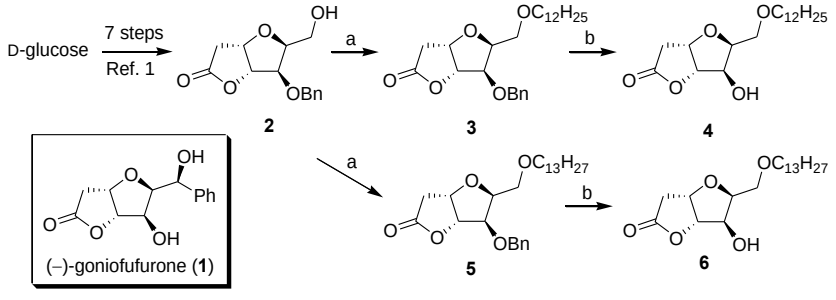
Sintetizovani su novi analozi (–)-goniofufurona (**1**), molekuli **4** i **6**, polazeći od komercijalno dostupne D-glukoze (*Scheme 1*).[1] Furanolaktoni **4** i **6** se mogu smatrati nestirilnim analozima (–)-goniofufurona (**1**), suprotnog enantiomera prirodnog citotoksičnog laktona (+)-goniofufurona. Sintetizovana jedinjenja su podvrgnuta *in vitro* testovima prema velikom broju tumorskih ćelijskih linija, kao i prema normalnim fetalnim fibroblastima pluća. Osim antiproliferativne aktivnosti, biće predstavljeni i rezultati SAR analize.



Scheme 1. Reagents and conditions: (a) $C_{12}H_{25}Br$ for **3**, $C_{13}H_{27}Br$ for **5**, Ag_2O, AgOTf, Et_2O, reflux; (b) H_2, 10 % Pd/C, EtOH, rt.

Synthesis and biological evaluation of novel (–)-goniofufurone analogues

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New (–)-goniofufurone (**1**) analogues, compounds **4** and **6**, were synthesized starting from commercially available D-glucose (*Scheme 1*).[1] Furanolactones **4** and **6** might be considered as non-styryl analogues of (–)-goniofufurone (**1**), the opposite enantiomer of naturally occurring cytotoxic lactone (+)-goniofufurone. Synthesized compounds were evaluated by *in vitro* experiments against a number of tumour cell lines, as well as against normal foetal lung fibroblasts. Apart from antiproliferative activity the results of SAR analysis will be presented.

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

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MH P 3

Promene u HEL ćelijama kao rezultat uticaja kompleksa rutenijuma(II)

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Mnogi kompleksi rutenijuma(II) pokazali su izuzetnu citotoksicnost. U cilju istraživanja mehanizma delovanja ispitan je efekat kompleksa Ru(II) sa N-alkilfenotiazinima na HEL ćelije humane eritroleukemije. Primenom tri kompleksa Ru(II), opšte formule L[$RuCl_3(DMSO)_3$] **(1-3)**, gde je L protonovani hlorpromazin, trifluoperazin ili tioridazin, u koncentraciji 15 μM ispitan je uticaj na oksido-redukcione procese u proteinima i lipidima (sadržaj malondialdehida (MDA) i karbonilnih (CO) grupa) i aktivnost enzima antioksidativne odbrane (superoksidne-dismutaze (SOD), katalaze (CAT) i laktat-dehidrogenaze (LDH)) u HEL ćelijama. Svi kompleksi povećavaju aktivnost SOD, dok kompleks **3** inhibira 40% aktivnost CAT u poređenju sa kontrolnom grupom. Primenom svih kompleksa povećan je sadržaj MDA i CO grupa a rezultat su većeg stepena lipidne peroksidacije i oštećenja proteina. Ukupna aktivnost LDH povećana je primenom svih kompleksa, a kompleks **1** povećava njenu aktivnost 29%. Ovi rezultati ukazuju da kompleksi rutenijuma(II) oksido-redukcionim procesima dovode do apoptoze HEL ćelija.

Changes in the HEL cells as a result of the influence of the ruthenium(II) complexes

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Many ruthenium(II) complexes have shown exceptional cytotoxicity. In order to examine the mechanism of action, the influence of complexes of Ru(II) with N-alkylphenothiazines in the human erythroleukemic cells HEL is examined. The three complexes, general formulae L[$RuCl_3(DMSO)_3$] (**1–3**), where L is protonated chlorpromazine, trifluoperazine or thioridazine, applied in concentration of 15 μM, are investigated on the oxidation-reduction processes in proteins and lipids (content of malondyaldehyde (MDA) and carbonyl groups (CO)) and activities of enzymes antioxidative defenses (superoxide dismutase (SOD), catalase (CAT) and lactate dehydrogenase (LDH)) in HEL cells. The complexes increased the activity of SOD, while complex **1** inhibited 40% of CAT activity compared to the control group. The higher level of MDA and content of CO groups are results from a great degree of lipid's peroxidation as well as great damage on the proteins by applying all complexes. The higher total LDH activity are noted using complexes, while complex **1** increased 29% activities of LDH. All of these results indicate that ruthenium(II) complexes through the oxidation-reduction processes lead to apoptosis of the HEL cell line

Acknowledgements: *This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No 172014).*

MH P 4

Procena antikancerogene aktivnosti novih organokalaj(IV) jedinjenja koja sadrže derivate 2-propanske kiseline

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Dva nova organokalaj(IV) jedinjenja, koja sadrže derivate 2-propanske kiseline, sintetisana su i okarakterisana pomoću standardnih spektroskopskih metoda. *In vitro* antiproliferativna aktivnost ovih jedinjenja ispitana je prema četiri tumorske ćelijske linije: PC3 (prostata), HT-29 (debelo crevo), MCF-7 (dojka) i HepG2 (jetra) pomoću MTT and CV testova. Rezultati ispitivanja ukazuju da sintetisana jedinjenja ispoljavaju izvanrednu antikancerogenu aktivnost prema svim ispitanim ćelijskim linijama i njihova aktivnost je od 54 do 113 puta veća od aktivnosti referentne supstance, cisplatine. Dobijeni rezultati ukazuju na neophodnost daljih *in vitro*/*in vivo* istraživanja sa ciljem ispitivanja mehanizma delovanja ovih potencijalnih antitumorskih agenasa.

The anticancer activity evaluation of novel organotin(IV) compunds containing 2-propanoic acid derivatives

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Two novel organotin(IV) compounds containing 2-propanoic acid derivatives were synthesized and characterized by standard spectroscopic methods. *In vitro* antiproliferative activity of these complexes was investigated *versus* four tumor cell lines: PC3 (prostate), HT-29 (colon), MCF-7 (breast) and HepG2 (hepatic) using MTT and CV assays. The results have shown that that synthesized complexes exhibit remarkable anticancer activity toward all tested cell lines with 54 to 113 fold higher activity than the reference compound cisplatin. The obtained promising results indicate the necessity for further *in vitro*/*in vivo* research with the aim to investigate the mechanism of action of these potencial antitumor agents.

Acknowledgement: *This research was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, [grant number 172035].*

Sinteza i *in vitro* antitumorska aktivnost 3'-amino-D-*ksilo* analoga tiazofurina

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Tiazofurin je sintetički *C*-nukleozid sa značajnom antitumorskom aktivnošću. Višefazna sinteza njegovog analoga 3'-amino-D-*ksilo* analoga **1**, ostvarena je polazeći iz D-glukoze, korišćenjem odabranih 2,5-anhidro šećera kao ključnih intermedijera. Rezultati ispitivanja *in vitro* antiproliferativne aktivnosti jedinjenja **1** prema ćelijskim linijama odabranih humanih tumora, kao i njegov efekat na ćelijski ciklus i apoptozu u K562 ćelijama biće takodje saopšteni i diskutovani.

Synthesis and *in vitro* antitumour activity of 3'-amino-D-*xylo* analogue of tiazofurin

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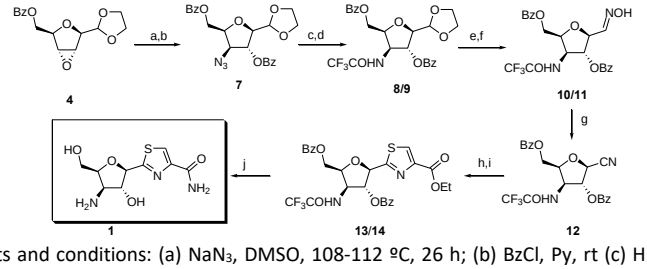
Tiazofurin is a synthetic *C*-nucleoside with significant antitumour activity. A multi-step synthesis of its 3'-amino-D-*xylo* analogue **1** has been achieved starting from D-glucose, by utilizing selected 2,5-anhydro sugars as key intermediates. Herein we report the effect of this compound to the proliferation of certain human tumour cell lines and the results related to its effects on the K562 cell cycle. Its ability to induce apoptosis in the same cell culture will be also presented and discussed.



Scheme 1. Reagents and conditions: (a) NaN_3, DMSO, 108-112 ºC, 26 h; (b) BzCl, Py, rt (c) H_2, 10 % Pd/C, $CHCl_3$ (kat.), EtOH, rt; (d) $(CF_3CO)_2O$, Py, CH_2Cl_2, −10 ºC→ 4ºC; (e) TFA - 6M HCl, +4 ºC→ rt; (f) $NH_2OH{\times}HCl$, NaOAc, EtOH, CH_2Cl_2, rt; (g) MsCl, Py, −15ºC, 0.5 h→, rt; (h) CysEt×HCl, Et_3N, MeOH, rt; (i) $BrCCl_3$, DBU, CH_2Cl_2, 0 °C→ +4 °C; (j) NH_3, MeOH, rt.

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

MH P 6

Divergentna sinteza i antiproliferativna aktivnost (−)-kleistenolida i (−)-5-*epi*-kleistenolida

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Ostvarena je divergentna sinteza prirodnog laktona (−)-kleistenolida (**1**) i njegovog analoga, (−)-5-*epi*-kleistenolida (**7**) polazeći iz monoacetonida D-glukoze (**2**). Jedinjenje **2** je prevedeno u *Z*-olefin **4** višefaznom sintetičkom sekvencom prikazanom na reakcionoj shemi. Ciklizacijom **4** dobija se intermedijer **5** koji je *one-pot* metodom preveden u prirodni proizvod **1**. Intermedijerni *Z*-olefin **4** je, nakon hidrolize, *Mitsunobu*-ove ciklizacije i *one-pot* debenzilovanja/acilovanja, preveden u izomer **7**.

Divergent synthesis and antiproliferative activity of (−)-cleistenolide and (−)-5-*epi*-cleistenolide

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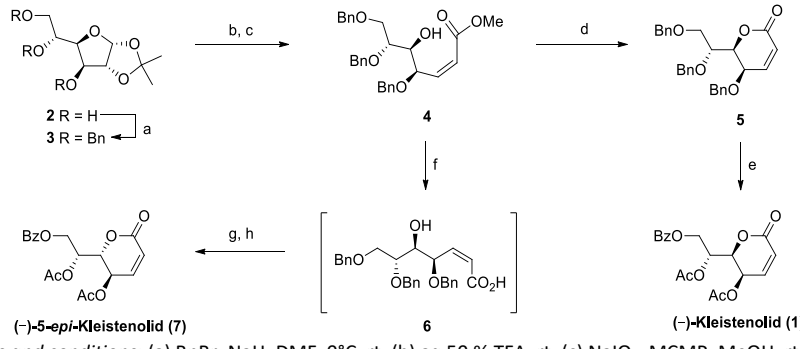
A divergent synthesis of natural product **1** and its analogue (−)-5-*epi*-cleistenolide (**7**) was achieved. Monoacetonide D-glucose (**2**) was converted to the divergent intermediate, *Z*-olefine (**4**), through a multi-step sequence outlined in reaction scheme. Natural products **1** can be accessed from **4** after cyclization and *one-pot* debenzilation/acylation process. *Z*-olefin **4** is converted to the isomer **7** after hydrolysis, *Mitsunobu's* cyclization and the the mentioned *one-pot* method.



Reagents and conditions: (a) BnBr, NaH, DMF, 0°C, rt; (b) aq 50 % TFA, rt; (c) $NaIO_4$, MCMP, MeOH, rt; (d) TsOH, CH_2Cl_2, rt; (e) BzBr, AcBr, $FeCl_3$, CH_2Cl_2, rt; (f) LiBr, Et_3N, aq CH_3CN, rt; (g) Ph_3P, DEAD, EtOAc, rt; (h) BzOH, Bz_2O, AcBr, $FeCl_3$, CH_2Cl_2, rt.

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

MH P 7

Uticaj fenil grupe na antitumorsku aktivnost konformaciono krutih analoga goniofufurona

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****Srpska akademija nauka i umetnosti, Knez Mihajlova 35, Beograd, Srbija*

Defenilovani, konformaciono kruti analog goniofufurona (**3**) sintetzovan je u tri faze polazeći iz komercijalno dostupne D-ksiloze i ispitana je njegova aktivnost prema nekoliko malignih i jednoj normalnoj ćelijskoj liniji. U cilju utvrđivanja uticaja fenil-grupe na antitumorsku aktivnost, dobijene vrednosti su upoređene sa aktivnostima odgovarajućih analoga sa fenil-grupom (**5** i **6**). Rezultati će biti prikazani i diskutovani detaljno.

Phenyl group influence on antitumour activity of conformationally contrainsted gonofufurone analogues

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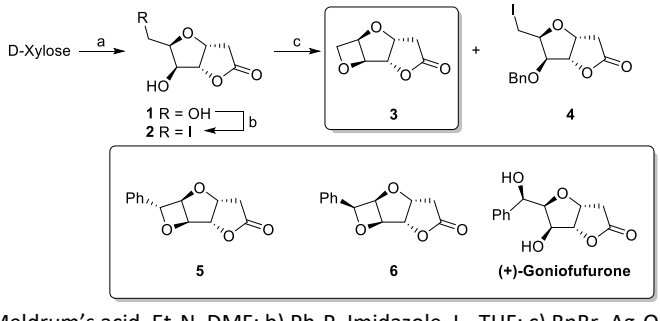
Dephenylated, conformationally constrained goniofufurone analogue (**3**) was synthesized in tree steps starting from commercially available D-xylose and its antitumour activity evaluated against several tumour cell lines and one normal cell line. In order to evaluate the influence of phenyl group on antitumour potential, cytotoxicity of dephenylated analogue was compared to cytotoxicities of previously synthesized analogues with phenyl group (**5** and **6**). The results will be presented and discussed in detail.



Scheme 1. a) Meldrum's acid, Et_3N, DMF; b) Ph_3P, Imidazole, I_2, THF; c) BnBr, Ag_2O, AgOTf, CH_2Cl_2.

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

Organska hemija / Organic Chemistry

OH O 1

Oksidacija 1,4-dihidropiridina katalizovana rekombinantnom bakterijskom lakazom eksprimiranom u *E. coli*

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Lakaze predstavljalju raznoliku klasu enzima koja nalazi primenu od valorizacije otpada do organske sinteze. U ovom istraživanju ispitivane su cele ćelije koje sadrže bakterijsku lakazu kao katalizator u oksidaciji 1,4-dihidropiridina. Ekspresija *cotA* gena iz *Bacillus licheniformis* je izvršena u ćelijama *E. coli* i za nastali biokatalizator je ustanovljeno da ubrzava oksidaciju 1,4-dihidropiridina. Pored toga, ustanovljeno je da „multicopper" oksidaza CueO iz *E. coli* takođe poseduje aktivnost prema oksidaciji 1,4-dihidropiridina. Ekspresioni sistem koji sadrži lakazu iz bakterije *Bacillus licheniformis* zatim je imobilizovan na bakterijskoj nanocelulozi i upotrebljen je kao katalizator u istoj transformaciji. Takav katalizator je bilo moguće ponovo upotrebiti tri puta, nakon čega je njegova aktivnost iznosila 37 % od početne. Navedeno istraživanje predstavlja prvu primenu celih ćelija sa rekombinantnom lakazom u oksidaciji 1,4-dihidropiridina.

Oxidation of 1,4-dihydropyridines catalyzed by recombinant bacterial laccase expressed in *E. coli*

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***IMGGE, University of Belgrade, Vojvode Stepe 444a, Belgrade, Serbia*

Laccases are a versatile class of enzymes with applications ranging from waste valorization to organic synthesis. We have tested whole-cell systems containing bacterial laccase as catalysts in the oxidation of 1,4-dihydropyridines. *E. coli* was used as the expression host for the *cotA* gene from *Bacillus licheniformis*, and the resulting whole-cell catalyst facilitated the oxidation of 1,4-dihydropyridines. It was found that multicopper oxidase CueO from the *E. coli* expression host also possesses catalytic activity in the oxidation of 1,4-dihydropyridines. The whole-cell biocatalyst expressing *Bacillus licheniformis* laccase was subsequently immobilized on bacterial nanocellulose and utilized in the same transformation, retaining 37 % of its original activity after three consecutive catalytic runs. This is the first report of a whole-cell catalytic system containing recombinant laccase for the oxidation of 1,4-dihydropyridines.

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

OH P 1

Sinteza i antiproliferativna aktivnost novih steroidnih tetrazola

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Androstanski derivati koji sadrže heterociklične prstenove kao supstituente u položaju C-17 pokazuju anti-tumorsku aktivnost. Jedan od poznatijih predstavnika C-17 supstituisanih androstanskih derivata jeste abirateron acetat, selektivni inhibitor CYP17A enzima, koji se koristi u tretmanu kancera prostate. Osim što deluju kao inhibitori enzima, derivati slične strukture pokazuju antiproliferativnu aktivnost prema ćelijskim linijama humanih tumora. Uzimajući u obzir navedene činjenice, cilj ovog rada je bio sinteza novih steroidnih derivata koji u položaju C-17 imaju supstituent sa tetrazolskim prstenom, kao i ispitivanje njihove antiproliferativne aktivnosti.

Synthesis and antiproliferative activity of novel steroidal tetrazoles

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Androstane derivatives with tethered heterocyclic groups at position C-17 show anti-cancer activity. Abiraterone acetate, a well-known member of this type of androstane derivatives, is a selective inhibitor of CYP17A enzyme and it is used in the treatment of prostate cancer. Besides the enzyme inhibition, derivatives with similar structure display antiproliferative activity against various cancer cell lines. Bearing in mind these facts, the aim of this study was a synthesis of novel steroidal derivatives with tetrazole ring as a substituent at C-17 position, as well as testing of their anti-proliferative activity.

Realizacija ovog rada finansirana je od strane Ministarstva prosvete, nauke i tehnološkog razvoja (Projekat ON172021).

OH P 2

Sinteza, karakterizacija i antiproliferativna aktivnost novog tetrazolskog derivata henodeoksiholne kiseline

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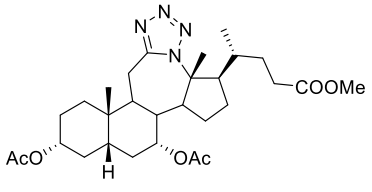
Steroidni molekuli koji sadrže heterociklični prsten u svojoj strukturi ispoljavaju značajno antiproliferativno dejstvo. 1,5-Disupstituisani tetrazoli predstavljaju strukturne analoge *cis*-amidne grupe koji ne podležu metaboličkoj degradaciji[1]. U ovom radu predstavljena je hemijska sinteza tetrazolskog derivata **1** iz holne kiseline. Jedinjenje je pored spektroskopskih tehnika karakterisano i rentgenostrukturnom analizom. U cilju boljeg uvida u osobine jedinjenja **1**, izvršena je analiza pomoću DFT metode.



1

Synthesis, characterization and antiproliferative activity of chenodeoxycholic acid tetrazole derivative

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Steroidal compounds with a heterocyclic ring in their structure are exhibiting strong antiproliferative efects. 1,5-Disubstituted tetrazoles are metabolically stable structural analogs of *cis*-amide groups[1]. In this work we present the chemical synthesis of tetrazole derivative **1** from cholic acid. Besides spectroscopy techniques, the structure of derivative **1** was determined by X-ray diffraction on monocrystal. In order to get a better insight into the characteristics of compound **1**, a computational study was performed using a DFT method.

1. Ostrovskii V. A., et al.; *Russ. Chem Bull.* 61. (768-780) 2012.

OH P 3

Sinteza glukokortikoidnih žučnih kiselina

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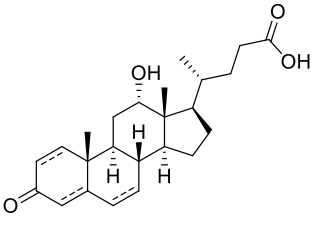
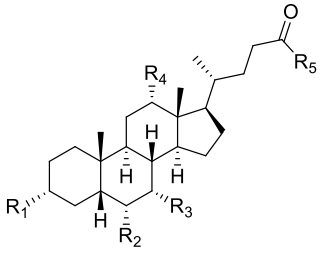
Žučne kiseline (ŽK) su steroidni molekuli koji pored važne uloge koju imaju u digestiji lipida su i značajni signalni molekuli koji aktiviraju brojne receptore (FXR, TGR5, PXR, VDR...) i tako utiču na homeostazu ŽK i glukoze, liponeogenezu, inflamatorne procese i supresiju tumora.[1,2] Pleiotropna aktivnost ovih molekula čini ŽK dobrim supstratima za razvoj potencijalnih farmakoloških agenasa. Ovde želimo da saopštimo sinteze enonskih **1** i oksimino **2** derivata ŽK kao potencijalnih liganada za glukokortikoidni receptor. Detalji sinteze ovih jedinjenja će biti prezentovani.



4-en, 1,4 ili 4,6-dien

1



R_1, R_2, R_3, R_4= -H, -OAc ili =N-OH;
R_5= -OH ili -OCH_3

2

Synthesis of glucocorticoid bile acids

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Bile acids (BAs) are steroidal molecules which beside important role in lipid digestion are also signaling molecules able to activate a number of receptors (FXR, TGR5, PXR, VDR…) and thus affect the BA and glucose homeostasis, liponeogenesis, inflammatory processes and tumor suppression.[1,2] Pleiotropic activity makes bile acid good substrates for developing potential pharmacological agents. Herein we would like to report the synthesis of BA enone **1** and oxime **2** derivatives as potential ligands for the glucocorticoid receptor. Synthesis of these compounds will be presented in detail.

1. Kim, I. *et al.*, *Carcinogenesis*, **28**, (2007) 940.
2. Deuschle, U. *et al.*, *PLoS ONE*, **7**, (2012) e43044 .

***Zahvalnica**: Ovaj rad je finansiran od strane Ministarstva prosvete, nauke i tehnološkog razvoja (Projekat ON172021).*

OH P 4

Proučavanje kristalne strukture i interakcija 5-(3- i 4-supstituisanih)-5-metilhidantoina sa albuminom humanog seruma i DNK

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***Univerzitet u Kragujevc, Prirodno-matematički fakultet, , Radoja Domanovića 12*

U okviru proučavanja uticaja strukture na farmakološku aktivnost derivata hidantoina, 5-(3-metilfenil)-5-metilhidantoin (**1**) i 5-(4-metoksifenil)-5-metilhidantoin (**2**) su sintetisani i potpuno strukturno okarakterisani određivanjem temperature topljenje, FTIR, ^{1}H i ^{13}C NMR spektroskopskim metodama. Određene su njihove kristalne strukture i izvršena je analiza kristalnog pakovanja sa aspekta međumolekulskih interakcija i strukturnih motiva. U kristalnom pakovanju oba jedinjenja uspostavljaju se jake intermolekulske N-H···O vodonične veze između njihovih *R* i *S* izomera. Vezivanje proučavanih jedinjenja za DNK i serum humanog albumina (HSA) proučavano je merenjem gašenja fluerescencije triptofana. Pokazano je da **2** ima viši afinitet vezivanja i za DNK i HSA od **1**. Predstavljeno istraživanje pruža smernice za dizajniranje novih derivata hidantoina sa poboljšanim farmakološkim svojstvima.

Study of the crystal structure and interactions of 5-(3- and 4-substituted)-5-methylhydantoins with human serum albumin and DNA

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***University of Kragujevac, Faculty of Natural Sciences and Mathematics, Radoja Domanovića 12*

Within the framework of the investigation of the structure–activity relationship of hydantoin derivatives, 5-(3-methylphenyl)-5-methylhydantoin (**1**) and 5-(4-methoxyphenyl)-5-methylhydantoin (**2**) were synthesized and structurally characterized by determination of their melting points, FTIR, ^{1}H and ^{13}C spectroscopic techniques. Their crystal structures were determined and the analysis of the crystal packings in terms of the contributing intermolecular interactions and structural motifs was performed. In the crystal packing of both compounds, strong intermolecular N-H···O hydrogen bonds were observed between their *R* and *S* isomers. Binding of the investigated compounds to DNA and to human serum albumin (HSA) was studied by measuring quenching of the fluorescence of tryptophan. It was shown that **2** has a higher binding affinity for both DNA and HSA than **1**. The presented investigation provide guidance for design of novel hydantoin derivatives with improved pharmacological properties.

OH P 5

Sinteza i antiproliferativna aktivnost heterocikličnih estrogenih derivata

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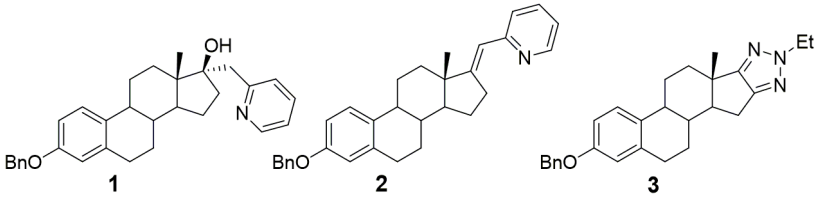
Hemijski modifikovani prirodni estrogeni su poznati antitumorski agensi. Oni se pre svega ističu svojom antiestrogenom aktivnošću, usled koje su neki od njih našli primenu u lečenju estrogen-zavisnih kancera dojke. Međutim, retki su estrogeni derivati koji u svojoj strukturi poseduju heterociklični prsten. Ova strukturna karakteristika kod androgena je osim izuzetne antitumorske aktivnosti, doprinela i poboljšanju njihove selektivnosti prema pojedinim tumorima. Imajući ovo u vidu, u ovom radu su polazeći od benzil-etra estrona sintetisani 17α-pikolil i 17-pikoliniliden derivati **1** i **2**, kao i *N(2)*-supstituisani D-kondenzovani 1,2,3-triazolski derivat **3**. Za odabrana jedinjenja je ispitana antiproliferativna aktivnost na šest tumorskih i jednoj normalnoj ćelijskoj liniji.



Synthesis and antiproliferative activity of heterocyclic estrogen derivatives

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Modified natural estrogens are well known antitumor agents. They have found widespread use in the treatment of breast cancer due to their antiestrogen activity. However, estrogen derivatives with a heterocyclic ring are rare. This structural feature in androgens has contributed to selectivity for specific tumors, in addition to excellent antitumor activity. With this in mind, we have synthesized 17α-picolyl and 17-picolinylidene estrogen derivatives **1** and **2**, as well as a compound with a *N(2)*-substituted D-condensed triazole ring **3**. The starting compound in these syntheses was benzyl ether of estrone. For selected compounds, antiproliferative activity was tested on six tumor and one normal cell line.

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 6

Antioksidantna aktivnost i akutna toksičnost novih nesimetričnih azina sa kumarinskim i još jednim heterocikličnim jezgrom

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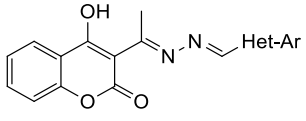
Do sada smo pripremili seriju mešovitih azina kumarina i različitih benzaldehida i ispitivali njihovu akutnu toksičnost i antioksidantnu aktivnost. Zbog činjenice da heterociklična jedinjenja sa sumporom i azotom poseduju širok spektar bioloških aktivnosti, u nastavku našeg rada, osmislili smo, sintetisali i potpuno spektralno okarakterisali niz novih mešovitih azina polazeći od 3-acetil-4-hidroksikumarina i različitih heteroaromatičnih aldehida. Sintetisanim jedinjenjima ispitana je antioksidantna aktivnost i akutna toksičnost na modelu slanovodnih račića *Artemia salina*. Najveću antioksidantnu aktivnost poseduje azin sa pirolskim supstituentom, dok je najmanja aktivnost uočena kod derivata indola. Najveća toksičnost uočena je kod derivata tiofena, dok izohinolin-kumarinski mešoviti azin pokazuje najmanju toksičnost.



Antioxidant activity and acute toxicity of new unsymmetrical azines containing coumarin and one more heterocyclic moieties

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During our previous work, we prepared a series of mixed azines with a coumarin moiety and different benzaldehydes, and tested their acute toxicity and antioxidant activity. Since heterocyclic compounds possess a broad range of biological activities, in the continuation of our work, we designed, synthesized and fully spectrally characterized a series of new mixed azines starting from 3-acetyl-4-hydroxycoumarin and different heteroaromatic aldehydes. The synthesized compounds were evaluated for their antioxidant activities and the acute toxicity in the brine shrimp *Artemia salina* model. Pyrrole-containing azine showed the higest antioxidant activity, while the lowest activity was noted for the indole derivative. The highest toxicity rate was observed for the thiophene derivate, while the isoquinoline-coumarin mixed azine was shown to be the least toxic.

Acknowledgement: This work was funded by the Ministry of Education, Science and Technological Development of Serbia (Projects No. 172061 and 45022).

OH P 7

Синтеза, електрохемијска и антипролиферативна својства нових конјугата стероидних естрогена са фероценом

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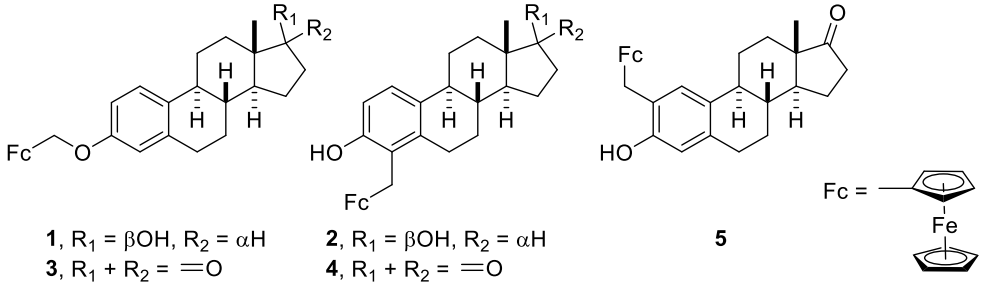
Неки конјугати стероидних хормона са фероценом су до сада испитивани као потенцијални селективни антипролиферативни агенси за хормон-зависне туморе. Овде саопштавамо синтезу нових конјугата стероидних естрогена са фероценом (**1**–**5**) остварену фероценилметиловањем естрадиола или естрона помоћу (фероценилметил)триметиламонијум-јодида. Електрохемијске особине добијених једињења испитане су цикличном волтаметријом. Одређена је цитотоксичност ових једињења за шест туморских и једну нормалну хуману ћелијску линију.



1, R_1 = βOH, R_2 = αH
3, $R_1 + R_2$ = =O
2, R_1 = βOH, R_2 = αH
4, $R_1 + R_2$ = =O
5

Synthesis, electrochemical and antiproliferative properties of novel steroidal estrogen–ferrocene conjugates

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Steroid hormone–ferrocene conjugates have thus far been explored as potential selective antiproliferative agents for hormone-dependent tumors. Herein we report the synthesis of novel steroidal estrogen–ferrocene conjugates **1**–**5** by ferrocenylmethylation of estradiol or estrone using (ferrocenylmethyl)trimethylammonium iodide. Electrochemical properties of the obtained compounds were determined by cyclic voltammetry. Activities of the compounds towards six tumor and one normal human cell line were evaluated.

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

OH P 8

Sinteza novih A-kondenzovanih steroidnih pirazola

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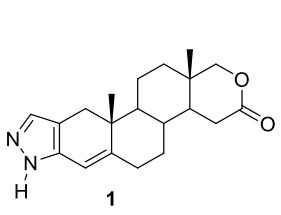
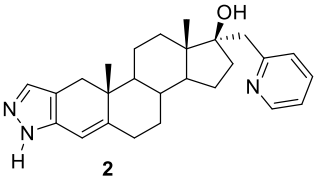
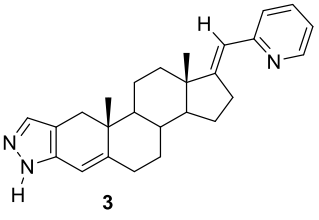
Pirazolski prsten kondenzovan sa steroidnim jezgrom doprinosi biološkoj aktivnosti osnovnog steroidnog molekula. Tako na primer neki od njih imaju značajnu antiproliferativnu aktivnost ili su potentni inhibitori enzima aromataze ili 17α-hidroksilaza/$C_{17,20}$-lijaze. Iz tog razloga mi smo sintetizovali nove A-kondenzovane steroidne pirazole sa D-homo laktonskom (**1**), 17α-(piridin-2-il)metil (**2**)- ili 17(*E*)-(piridin-2-il)metiliden (**3**) funkcijom, kako bi se ispitao njihov antitumorski potencijal. Polazno jedinjenje u ovim višefaznim sintezama je bio dehidroepiandrosteron.



1



2



3

Synthesis of new A-condensed steroidal pyrazoles

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The pyrazole ring condensed with the steroidal core contributes to the biological activity of the primary steroidal molecule. For example, some of them exhibit significant antiproliferative activity or they are potent inhibitors of aromatase or 17α-hydroxylase/$C_{17,20}$-lyase. For this reason, we have synthesized new A-condensed steroidal pyrazoles with D-homo lactone (**1**) or 17α-(pyridine-2-yl)methyl (**2**) or 17(*E*)-(pyridine-2-yl)methylidene (**3**) function in order to examine their antitumor potential. The starting compound in these multistep syntheses was dehydroepiandrosterone.

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 9

Sinteza i spektroskopska analiza 5-(2,4-disupstituisanih fenilazo)-3-cijano-6-hidroksi-4-metil-2-piridona

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U ovom radu sintetisane su tri azo piridonske boje, koje su potom okarakterisane FT-IR i NMR spektroskopijom. UV-Vis apsorpcioni spektri i tautomerija tri 5-(2,4-disupstituisanih fenilazo)-3-cijano-6-hidroksi-4-metil-2-piridona detaljno su analizirani u etru, *N*,*N*-dimetalformamidu, dimetil-sulfoksidu. Jedinjenja u okviru ove serije boja razlikuju se prema prirodi supstituenata u fenilnom jezgru (–Me, –OMe, $–NO_2$). U etru i dimetilsulfoksidu ispitivane boje postoje u hidrazonskom obliku. U rastvoru *N*,*N*-dimetilformamida, kod 5-(2,4-dinitrofenilazo)-3-cijano-6-hidroksi-4-metil-2-piridona, utvrđeno je da postoji ravnoteža između anjonskog i hidrazonskog oblika. Ravnoteža između ova dva oblika analizirana je u binarnim smešama etra i *N*,*N*-dimetilformamida različitih zapreminskih odnosa.

Synthesis and spectroscopic study of 5-(2,4-disubstituted phenylazo)-3-cyano-6-hydroxy-4-methyl-2-pyridones

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In this work, three azo pyridone dyes have been synthesized and analyzed by FT-IR and NMR spectroscopy. UV-Vis absorption spectra, as well as tautomerism of three 5-(2,4-disubstituted phenylazo)-3-cyano-6-hydroxy-4-methyl-2-piridones have been thoroughly analyzed in ether, dimethyl sulfoxide and *N*,*N*-dimethylformamide. The dye molecules have different substituents (-Me, -OMe, $-NO_2$) in the phenyl moiety. In ether and dimethyl sulfoxide, investigated dyes exist in hydrazone form. In *N*,*N*-dimethylformamide 5-(2,4-dinitro phenylazo)-3-cyano-6-hydroxy-4-methyl-2-piridone exhibits hydrazone-azo anion tautomerism. Equilibrium of two tautomeric forms has further been analyzed in binary mixtures of *N*,*N*-dimethylformamide and ether using different solvent ratios.

OH P 10

Optimizacija metode sinteze etilen-diamin-monosirćetne kiseline, H-EDMA

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U ovom radu je optimizirana metoda sinteze etilen-diamin-monosirćetne kiseline (H-EDMA). Literaturni podaci sinteze H-EDMAxHCl, nisu bili reproducibilni u značajnom prinosu te se probalo sa više metoda dobijanja željenog proizvoda.
U više pokušaja modifikacije postupka sinteze (produžena sinteza u dihlormetanu, bez prisustva rastvarača) nastajao je željeni proizvod u izuzetno niskom prinosu i/ili paralelno nastajanje neželjenih višestruko supstituisanih etilen-diaminskih derivata (etilendiamin-disirćetna i trisirćetna kiselina) što je pokušano riješiti zaštitom jedne od dvije amino grupe Boc-zaštitnom grupom, no rezultat je ponovo bio nerazdvojiva smješa proizvoda.
Na osnovu iskustava stečenih prethodnim pokušajima sinteze H-EDMA, dizajnirana je modifikovana metoda sinteze u organskom mediju na sobnoj temperaturi, pri višku etilendiamina i uz sporo dodavanje monohlorsirćetne kiseline koja je rezultirala prinosom od 55 % čistog željenog proizvoda. Na taj način smo dobili H-EDMA kraćom i efikasnijom i ekonomičnijom metodom.

Optimization of the method of synthesis of ethylene-diamine monoacetic acid, H-EDMA

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In this paper, the synthesis of ethylene diamine monoacetic acid (H-EDMA) is optimized. Literary data were not reproducible in significant yield so we tried this synthesis with several methods for the purpose of obtaining of the wanted product.
In several attempts to modify the synthesis process (extended synthesis time in dichloromethane, reacting without the presence of a solvent), the desired product was produced in an extremely low yield and / or several unwanted, multiply substituted ethylene diamine derivatives were formed in the same reaction mixture.
We tried to solve this problem by protecting one of the two amino groups with the Boc-protecting group, but the result was a mixture of products that can not be separated.
Based on the experience gained from previous attempts in the synthesis of H-EDMA, a modified synthetic method in an organic medium at room temperature was developed, with an excess of ethylenediamine, followed by slow addition of monochloroacetic acid which resulted in a yield of 55 % pure desired product.Thus, in this work, we got H-EDMA by shorter, more efficient and more economical method.

This work was derived from the project of bilateral collaboration of MNE and Croatia.

OH P 11

Određivanje sadržaja masnih i aminokiselina u peloidu iz Igala (Crna Gora)

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Termalni mulj (blato) koje nastaje i sakuplja se u priobalju Igala već se tokom dužeg niza decenija koristi za terapeutske i kozmetičke tretmane. U našem radu smo ispitivali sadržaj masnih i aminokiselina u peloidu iz Igala. Za to određivanje su korišćene različite analitičke tehnike poput hromatografskih, elektroforetskih i NMR-tehnika. Peloid iz Igala je blago kiseo sa oko 9 % sadržaja ukupne organske materije. Ukupan sadržaj azota je 0.097 ± 0.004 %, a najvećim dijelom iz četrnaest prisutnih aminokiselina, dok je sadržaj proteina 3.71 ± 0.01 μg/g. Od ukupno trinaest masnih kiselina, pronađenih u peloidu, svega su četiri nezasićene, a među njima najviše ima oleinske. Od polinezasićenih kiselina zastupljena je linoleinska. NMR spektroskopijom potvrđen je značajan udio aromatičnih jedinjenja, uglavnom od aromatičnih aminokiselina.
Dobijeni rezultati definišu peloid iz Igala kao prirodni peloid koji je bogat sadržajem organskih materija. Rezultati koje smo dobili sugerišu da prisustvo velikog broja biološki aktivnih jedinjenja može biti i ključni faktor za balneološku vrijednost Igalskog peloida.

Determination of fatty and amino acids in Igalo bay peloid (Montenegro)

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Ivana Milašević[3], Ljubica Ivanović[3], Dijana Djurović[3], Vjeroslava Slavić[4], Milica Popović[5]
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Thermal mud found at the coast of Igalo has had a long history of therapeutic and cosmetic use. In our work we examined the content and composition of fatty acids and amino acids in the Igalo peloid. For the purpose of this study, different analytical techniques were applied to the collected peloid, including extraction, chromatographic and NMR analysis. Igalo peloid is mildly acidic with close to 9 % (w/w) of total organic matter. Total percent of nitrogen was determined to be 0.097 ± 0,004 %, which among other included fourteen amino acids and protein content of 3.71 ± 0.01 μg/g of wet mass of peloid. Out of thirteen identified fatty acids only four were unsaturated with oleic acid being the most abundant one among them. Only polyunsaturated acid detected in the material was linoleic. NMR spectra indicated presence of aromatic compounds, most lightly aromatic amino acids.
Our results suggest that the presence of many biologically active organic compound may be beneficial for the balneological value of Igalo peloid.

ОН P 12

Нови деривати 1,3,4-тиадиазола изведени из протокатехуинске киселине: Синтеза, антиоксидативна активност, теоријска и електрохемијска студија

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Извршена је синтеза и структурна карактеризација петнаест нових амидних деривата 1,3,4-тиадиазола изведених из протокатехуинске киселине. Такође, синтетизовани су одговарајући имино и амино аналози фенил-супституисаног амидног деривата 1,3,4-тиадиазола ради поређења ефеката структурних промена на способност везивања радикала. Испитан је антиоксидативни потенцијал добијених једињења помоћу DPPH и ABTS тестова, као и коришћењем теорије функционалне густине (DFT) и цикличне волтамерије. Тестирана једињења су показала значајну антиоксидативну активност у поређењу са референтним антиоксидантима аскорбинском киселином и нордихидрогвајаретинском киселином (NDGA). На основу израчунатих термодинамичких параметара и електрохемијских експеримената изведени су закључци о највероватнијем механизму по ком се одвија антиоксидативна активност ових једињења.

Novel 1,3,4-thiadiazole conjugates derived from protocatechuic acid: Synthesis, antioxidant activity, computational study and electrochemistry

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**Faculty of Sciences, University of Novi Sad, Trg D. Obradovića 3, 21000 Novi Sad, Serbia,*
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A series of fifteen novel 1,3,4-thiadiazole amide derivatives containing protocatechuic acid moiety was synthesized and structurally characterized. In addition, the corresponding imino and amino analogues of phenyl substituted 1,3,4-thiadiazole amide derivative were prepared in order to compare effects of the structural changes on radical scavenging activity. The obtained compounds were examined for their antioxidative potential using DPPH and ABTS assays, including density functional theory (DFT) and cyclic voltammetry. The tested compounds showed high antioxidative potential compared to the referent antioxidants ascorbic acid and nordihydroguaiaretic acid (NDGA). Based on the calculated thermodynamic parameters and electrochemistry it can be concluded which mechanism represents the most probable reaction pathway for the radical scavenging activity of examined compounds.

Teorijska hemija / Theoretical Chemistry

TH P 1

Molecular dynamics simulation of ethanol on TiO_2 anatase surface

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In the work molecular dynamics simulation of anatase surfaces and ethanol molecules was investigated. Appropriate force field was developed using q= 2.196 e, σ=1.958 Å, ε=0.6070 kcal/mol parameters for Ti atom, and q= -1.098 e, σ=2.875 Å, ε=0.3319 kcal/mol parameters for O atom. Anatase unit cell containing four titanium atoms and eight oxygen atoms was simulated. Using Amber program package (110), (011), and (101) anatase surfaces with 20x20 unit cells size were developed. Each surface was extended with application of boundary conditions. For molecular dynamics calculations NVT ensemble was used, time step was 0.002 fs for each case. Temperature of 300 K was used for each molecular dynamics simulation.

It was established that (110) anatase surface is characterized by the highest preference of interaction with ethanol molecules. This fact was revealed by the analysis of the calculated energies for the simulated systems and relying on the dependencies of ethanol molecules distances from the surface on simulation time.

The force field that was developed in the work can be used for investigation of interactions between anatase surfaces with other molecules including biomolecules and peptides. Investigations of such kind are especially important in the field of chemical sensors and biosensors for directional synthesis of materials with required sensor properties.

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Nastava i istorija hemije / Education in and History of Chemistry

NIH O 1

Primena onlajn upitnika u nastavi hemije

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Za prikupljanje stavova i mišljenja ispitanika (učenika, studenata, nastavnika...) u okviru pedagoških istraživanja, najefikasniji i najekonomičniji postupak je anketiranje primenom odgovarajućeg upitnika. Upotreba IKT u nastavi je pojednostavila ovaj postupak, jer se mogu kreirati digitalni upitnici koji se distribuiraju internetom i onlajn (online) popunjavaju, korišćenjem nekog digitalnog uređaja. Prednosti su što se takav upitnik pravi bez ikakvih finansijskih investicija, a dostavljanje ispitanicima, pristupanje i popunjavanje je jednostavno. U cilju prikupljanja stavova učenika sedmog razreda o onlajn postavljenim materijalima za učenje nastavne jedinice o rastvorima i rastvaranju, kao i njihovim navikama vezanim za pristupanje internetu, za potrebe istraživanja kreiran je onlajn upitnik. Analiza odgovora učenika je pokazala da skoro svi učenici svakodenevno pristupaju internetu. Više od polovine učenika nikada nisu tražili na internetu sadržaje iz hemije. Učenici su izneli pozitivan stav o onlajn učenju sadržaja iz hemije, ali bi češća primena ovakog načina rada doprinela njihovom većem interesovanju za učenje.

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Implementation of the online questionnaire in chemistry teaching

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A survey with an appropriate questionnaire is the most efficient and economical procedure for collecting data on attitudes and opinions of pupils, students and teachers in educational researches. This process is simplified by using ICT, which enable to create digital questionnaires for online distribution and answering, from different digital devices. The advantages of this kind of questionnaires are related to that there is no need for additional financial investments, and they could be easy delivered to respondents for completing. In order to collect data on attitudes of the seventh grade students associated with the online materials for learning the teaching unit about solutions and dissolution, as well as their habits related to Internet access, an online questionnaire was created for the research purposes. An analysis of student responses has shown that almost all students access the Internet daily. More than half of the students have never searched for the content of chemistry on the Internet. Students have had a positive view of online learning chemistry contents, but more frequently use of this method could contribute to their higher interest.
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