Српско хемијско друштво

Клуб младих хемичара Србије

ПРВА КОНФЕРЕНЦИЈА МЛАДИХ ХЕМИЧАРА СРБИЈЕ

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17.15-18.00	**Maria-Cristina Todasca:** *European Young Chemists' Network (EYCN)*
18.00	**Коктел** – *Клуб ТМФ - III спрат*

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Секције Хемијска анализа и **Наука о метеријалима**
(ХА П01-ХА П32 и НМ П01-НМ П18)

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Предавања по позиву -– *Средњи амфитеатар (СА)*

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(ХС П01-ХС П22, ХН П1, БХ П01-БХ П15, ИХ П01-ИХ П04 и ТХ П01-ТХ П08)

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Затварање Конференције

The European Young Chemists' Network

Maria-Cristina Todasca
European Young Chemists' Network

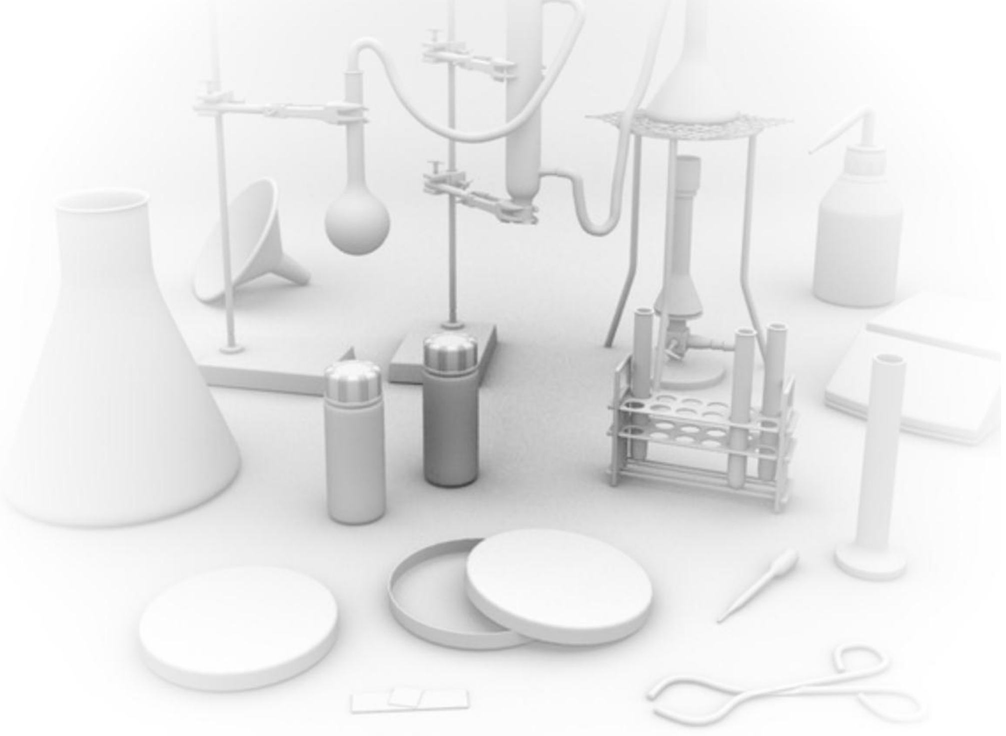
The European Young Chemists' Network (EYCN - www.eycn.eu) is the younger members division of the European Association for Chemical and Molecular Sciences (EuCheMS). Every chemist under 35 within the EuCheMS framework is part of EYCN.

EYCN was founded in 2006. The idea of the European Young Chemists Network (EYCN) within EuCheMS appeared during several young scientist meetings inner Europe in the past. At the brink of the 1st European Chemistry Congress 2006 in Budapest in (Hungary) a paper was written about "Aims, Tasks and Goals of EYCN".

In March 2007 Jens Breffke (Germany) and Csaba Janaky (Hungary) invited all societies to send their young representatives to Berlin in order to set the rules of EYCN. Only three weeks later the Excecutive Committee of EuCheMS confirmed these Rules. EYCN was now the official youth division of EuCheMS. The Network brings together young chemists within the EuCheMS framework.

The aims of EYCN are to promote the exchange of information among chemists in European industry, academia, professional institutions and European government bodies. Also, to open a communication gate for all areas of chemistry within Europe and also to the rest of the world, and form an organized and united opinion to represent the European voice in science and education. To provide the platforms to generate and expand new ideas that contribute to the future role of chemistry and molecular sciences in the European society, and additionally to bridge the gap between academics and industry by organizing shared activities, promoting discussion and handover of experience at an informal level. The EYCN presents chemistry as part of daily life.

КРАТКИ ИЗВОДИ РАДОВА



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Предавања по позиву

ХС ПП 1

Totalna sinteza (–)-atrop-abisomicina C

Filip J. Bihelović i Radomir N. Saičić
Hemijski fakultet, Univerzitet u Beogradu

(–)-Atrop-abisomicin C je prirodni antibiotik izolovan iz aktinomiceta marinskog soja *Verrucosispora* AB 18-032. Usled njegove jedinstvene i kompleksne strukture, kao i novog mehanizma dejstva, ovaj molekul postao je atraktivna sintetička meta organskih hemičara. Sinteza koja je postignuta u okviru naše istraživačke grupe zasnovana je na četiri ključna koraka, a započinje stereoselektivnom aldolnom reakcijom borovog enolata acilovanog oksazolidinona na optički aktivan norcitronelal. Novorazvijeni metod za zatvaranje prstenova, iskorišćen za sintezu potpuno funkcionalizovanog abisomicinskog cikloheksanskog prstena, zasnovan je na istovremenoj dvostrukoj katalizi - kombinaciji organokatalize sa katalizom prelaznim metalom (paladijumom). Ključna transanularna eterifikacija ostvarena je adicijom hidroksilne grupe na trostruku vezu, uz katalizu zlatom, dok je konverzija nastalog bicikličnog intermedijera u triciklično spiro-tetronatno jezgro ostvarena ozračivanjem UV-svetlom, u prisustvu katalitičke količine baze. Sinteza atrop-abisomicina C je kompletirana formiranjem jedanaestočlanog prstena, koristeći veoma efikasnu *Nozaki-Hiyama-Kishi*-jevu makrociklizaciju.
Naš pristup sintezi abisomicina C komplementaran je dvema prethodno opisanim sintezama, omogućavajući tako sintezu različitih analoga, bez značajnijih promena u reakcionim uslovima.

Total synthesis of (–)-atrop-abyssomicin C

Filip J. Bihelović and Radomir N. Saičić
Faculty of Chemistry, University of Belgrade

(–)-Atrop-abyssomicin C is a naturally occurring antibiotic isolated from the marine *Verrucosispora* AB 18-032 actinomicetes. Its unique, complex structure and novel mechanism of action made it an attractive target for synthetic chemists. The synthesis accomplished by our research group was based on four key steps, starting with boron enolate mediated aldol addition of the acylated oxazolidinone to the optically active norcitronellal. A newly developed method for ring closure used for the synthesis of a fully functionalized abyssomicin's cyclohexane core was based on a dual catalysis – combination of organocatalysis with transition metal (palladium) catalysis – in a single step procedure. The essential transanular etherification was achieved through a gold promoted hydroxyl group addition to the triple bond, while conversion of the produced bicyclic intermediate to the tricyclic spiro-tetronate core was effected by irradiation with UV-light, in presence of a catalytic amount of a base. The synthesis of atrop-byssomicin C was completed by the formation of the eleven membered ring via highly efficient Nozaki-Hiyama-Kishi macrocyclization.
Our synthetic approach is complementary to the two previously reported ones, and also allows for the synthesis of various analogues without significant changes in reaction conditions.

Financial support was provided by the Ministry of education, science and technological development of the Republic of Serbia (Project No. 172027).

БХ ПП2

Ispitivanje bioaktivnosti srebra elektroforetske srebro/hidroksiapatit/lignin prevlake u simuliranoj telesnoj tečnosti

Sanja Eraković, Ana Janković, Ivana Z. Matić*, Zorica D. Juranić*, Maja Vukašinović-Sekulić, Tatjana Stevanović**, Vesna Mišković-Stanković
*Tehnološko-metalurški fakultet, Univerzitet u Beogradu, Beograd, Srbija, *Institut za Onkologiju i Radiologiju Srbije, Beograd, Srbija, **Département des sciences du bois et de la forêt, Université Laval, Québec, Canada*

Kompozitne hidroksiapatit (HAP) prevlake na titanu imaju široku upotrebu u proizvodnji implanta za tvrda tkiva zahvaljujući svojoj izuzetnoj biokompatibilnosti i otpornosti prema koroziji. Potencijalnu primenu u medicini ima dodavanje prirodnog polimera lignina (Lig) u kompozitnu prevlaku. Glavni problem implanta u telu jeste post-operativna infekcija koja ugrožava imuni sistem pacijenta. U cilju spečavanja infekcije, srebro (antibaktericidan agens, ali netoksičan za ljudske ćelije) je upotrebljeno na površini kompozitne prevlake. Ag/HAP/Lig prevlaka na titanu dobijena je postupkom elektroforetskog taloženja pri konstantnom naponu. Bioaktivnost i koroziona stabilnost Ag/HAP/Lig prevlake ispitane su uranjanjem iste u simuliranu telesnu tečnost (SBF) na 37 °C. Nakon 7 dana uzorak je ispitan EIS, SEM, FE SEM, XRD i ATR-FTIR analizama, dok su antimikrobno svojstvo i citotoksičnost procenjeni metodom preživljavanja u rastvoru i MTT testom, respektivno. Formiranje karbonatnog apatitinog filma (nakon uranjanja u SBF) na površini prevlake potvrđuje potencijalnu bioaktivnost.

Investigation of silver bioactivity of electrodeposited silver/hydroxyapatite/lignin coatings in simulated body fluid

Sanja Eraković, Ana Janković, Ivana Z. Matić*, Zorica D. Juranić*, Maja Vukašinović-Sekulić, Tatjana Stevanović**, Vesna Mišković-Stanković
*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, *Institute of Oncology and Radiology of Serbia, Belgrade, Serbia, **Département des sciences du bois et de la forêt, Université Laval, Québec, Canada*

Composite coatings on titanium, based on hydroxyapatite (HAP) have been widely utilized due to their exceptional biocompatibility and corrosion resistance for manufacturing of hard tissue implants. Addition of natural biopolymer lignin (Lig) in composite HAP coatings has potential for medical use. The main problem of implant materials inside the body is post-surgical infection that challenges the host immune response. To prevent infections silver (antbactericidal agent, but nontoxic toward human cells) was implemented on composite coating surface. The Ag/HAP/Lig coating was obtained by electrophoretic deposition using constant voltage method. Our goal was to investigate the bioactivity and corrosion stability of Ag/HAP/Lig coating by soaking in simulated body fluid (SBF) at 37 °C. After 7 days the sample was characterized by EIS, SEM, FE SEM, XRD and ATR-FTIR analysis, while antimicrobial property and cytotoxicity were evaluated by liquid challenge method in buffer solution and by MTT test, respectively. Newly formed carbonated apatite film (after SBF immersion) on the coating surface confirmed its potential bioactivity.

ХС ППЗ

Novi meridionalni Ru(II)-terpiridin kompleksi: sinteza, karakterizacija, aktivaciona kinetika i interakcija sa derivatima guanina

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Veoma malo je poznato u literaturi o antitumorskoj aktivnosti kompleksa koji sadrže tridentatni ligand u meridionalnoj geometriji kao funkcionalna jedinjenja. Imajući to u vidu razvili smo seriju novih jedinjenja opšte formule $[Ru(mtl)(chel)(X)][Y]_n$ (mtl=2,2′,6′2″-terpiridin(tpy) ili supstituisan tpy; chel=*N*-*N* ili *N*-*O* helatni ligand; X=Cl ili dmso-S; Y=Cl ili PF_6; *n* zavisi od prirode helatnog liganda i liganda X) kao potencijalne antitumorske agense. Proizvodi su karakterisani elementalnom analizom, UV-Vis, IR i uglavnom 1D i 2D NMR spektroskopijom. Dva proizvoda, $[Ru(tpy)(en)(dmso)]^{2+}$ i $[Ru(tpy\text{-}Cl)(dach)(dmso)]^{2+}$, karakterisana su u čvrstom stanju pomoću rendgensko-strukturne analize. Takodje, ispitivali smo njihovo hemijsko ponašanje u vodenom rastvoru kao i interakcije sa derivatima guanina: 9-Metilguanin (9MeG) i Guanozin-5′-monofosfat (5′-GMP) koristeći NMR spektroskopiju i UV-Vis spektrofotometriju.

New meridional Ru(II)-terpyridine complexes: synthesis, characterization, activation kinetics and interaction with guanine derivatives

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Very little is known in the literature for the antitumor activity of complexes bearing a tridentate ligand in meridional geometry as functional compounds. Thus, we developed a series of new compounds of the general formula $[Ru(mtl)(chel)(X)][Y]_n$ (mtl=2,2′,6′2′′-terpyridine (tpy) or substituted tpy; chel=*N*-*N* or *N*-*O* chelating ligands; X=Cl or dmso-S; Y=Cl or PF_6; *n* depends on the nature of chel and X) as potential antitumor agents. The products were fully characterized by elemental analysis, UV-Vis, IR and mainly by 1D and 2D NMR spectroscopy. Two products, $[Ru(tpy)(en)(dmso)]^{2+}$ and $[Ru(tpy\text{-}Cl)(dach)(dmso)]^{2+}$, were also characterized in solid state by X-ray crystallography. We have studied also their chemical behaviour in aqueous solution and the interactions with the guanine derivatives: 9-Methylguanine (9MeG) and Guanosine-5′-monophosphate (5′-GMP) using NMR spectroscopy and UV-Vis spectrophotometry.

Acknowledgments: This work was performed within the frame of COST Action CM1105. Regione FVG (Project "Nuove Terapie e Farmaci Antitumorali"), Fondo Trieste, Fondazione Beneficentia Stiftung, the Ministry of Science and Technological Development of the Republic of Serbia (Project No. 172011), and the Slovenian Research Agency (Project J1-4131) are gratefully acknowledged for financial support. A. R. is grateful to the bilateral Italian–Serbian project "C.S.I.U.T" for a research fellowship at the University of Trieste.

ХА ПП4

Hemijski sastav i antinociceptorno dejstvo etarskog ulja biljne vrste *Ferula ovina*

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U ovom radu je ispitivano antinociceptorno dejstvo etarskog ulja nadzemnog dela biljne vrste *Ferula ovina* (Boiss.) Boiss. (Umbelliferae) iz Irana, koristeći hot plate i tail immersion metode za ispitivanje centralne, a test abdominalnog grčenja za ispitivanje periferne analgezije kod miševa. Pri najvećoj dozi ulje pokazuje jaku perifernu analgetsku aktivnost tako što za 92,4 % smanjuje broj grčeva izazvanih sirćetnom kiselinom. Sa druge strane, ulje pokazuje umerenu centralnu analgetsku aktivnost sa 55.8 % inhibicije u tail immersion testu. Ovi zanimljivi rezultati naveli su nas da izvršimo detaljnu analizu sastava ovog ulja. GC i GC-MS analizom identifikovano je 120 sastojaka. Glavni sastojci su α-pinen (18,0 %), limonen (14,3 %) i mircen (13,5 %). U ulju je takođe pronađeno više retkih estara borneola. Strukture ovih jedinjenja potvrđena su sintezom, a jedno od njih (bornil *p*-metoksibenzoat) je novi prirodni proizvod.

Ovaj rad je finansiralo *Ministarstvo prosvete i nauke* (Projekat 172061).

Chemical composition and antinociceptive properties of the essential oil of *Ferula ovina*

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In this work we assessed the antinociceptive activity of the essential oil of the aerial parts of *Ferula ovina* (Boiss.) Boiss. (Umbelliferae), collected in Iran, using the hot plate and tail immersion methods for central and the abdominal writhing test for peripheral analgesia in BALB/c mice. In the highest applied dose, the oil showed a strong peripheral analgesic activity by causing a 92.4 % decrease in the number of writhes induced by acetic acid. On the other hand, the oil exerted only moderate central analgesic activity, reaching 55.8 % of inhibition in the tail immersion test. These interesting results provoked us to perform detailed compositional analyses of the oil. GC and GC-MS analyses allowed the identification of 120 constituents. The major constituents of this oil were α-pinene (18.0 %), limonene (14.3 %) and myrcene (13.5 %). The oil also contained a number of rare esters of borneol. The structures of these esters were corroborated by synthesis. Bornyl p-methoxybenzoate turned out to be a new natural compound.

ХС ПП5

Sinteza potencijalnog antiproliferativnog steroidnog derivata

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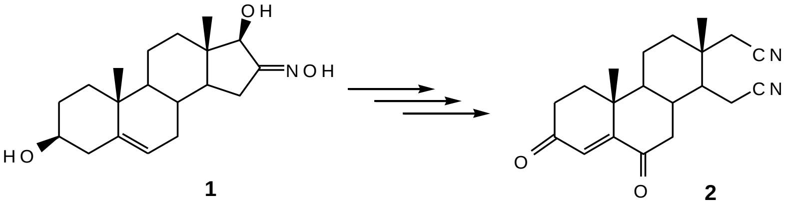
Polazeći od 3β,17β-dihidroksi-16-hidroksiiminoandrost-5-ena (**1**) sintetizovan je 3,6-diokso-16,17-sekoandrost-4-en-16,17a-dinitril (**2**) u sedam sintetskih faza. Ispitana je antiproliferativna aktivnost jedinjenja **2** na pet tumorskih (humani adenokarcinom dojke ER+, MCF-7, humani adenokarcinom dojke ER-, MDA-MB-231, adenokarcinom prostate, PC3, karcinom grlića materice HeLa, humani adenokarcinom kolona, HT-29) i jednoj zdravoj (fibroblasti pluća, MRC-5) ćelijskoj liniji. Jedinjenje **2** je pokazalo snažan uticaj na HeLa i MDA-MB-231 ćelije.



Synthesis of potential antiproliferative steroid derivative

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Starting from 3β,17β-dihydroxy-16-hydroxyiminoandrost-5-ene (**1**) 3,6-dioxo-16,17-secoandrost-4-ene-16,17a-dinitrile (**2**) was synthesized in seven steps. The antiproliferative activity of compound **2** on five tumor (human breast adenocarcinoma ER+, MCF-7, human breast adenocarcinoma ER-, MDA-MB-231, prostate cancer, PC3, cervical cancer, HeLa, human colon adenocarcinoma, HT-29) and one healthy (lung fibroblasts, MRC-5) cell line was evaluated. Compound **2** showed a strong influence on HeLa and MDA-MB-231 cells.

The work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172021*).*

Саопштења

Хемијска анализа

ХА О1

Kvantifikacija ukupnih fenola, antocijana, flavonoida i određivanje antioksidativne aktivnosti različitih ekstrakata aronije (*Aronia melanocarpa*)

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Analizirana je aronija (*Aronia melanocarpa*) koja raste u Srbiji. Određen je sadržaj ukupnih fenola (TP), ukupnih antocijana (TA), ukupnih flavonoida (TF) kao i relativna antioksidativna aktivnost različitih ekstrakata aronije. Posmatran je uticaj primenjenog ekstrakcionog sredstva na dobijene vrednosti ispitivanih parametara. Korišćena ekstrakciona sredstva se razlikuju po polarnosti: voda, metanol, 60 % metanol$_{(aq)}$ i metanol zakišeljen hlorovodoničnom kiselinom. Sadržaj ukupnih fenola je određen Folin-Ciocalteau-ovom metodom. Dobijene vrednosti se nalaze u opsegu 493 do 1637 mg galne kiseline/100 g FW (*eng.* fresh weight). Sadržaj antocijana i flavonoida je određen spektrofotometrijski i dobijene vrednosti za antocijane su od 65 do 435 mg cijanidin-3-glukozida/100 g FW, a za flavonoide od 65 pa do 137 mg kvercetina/100 g FW. Antioksidativna aktivnost je određena primenom spektrofotometrijskog DPPH (2,2-difenil-1-pikrilhidrazil) testa i izražena je kao sposobnost uklanjanja radikala (*eng.* radical scavenging activity, RSA, %). Dobijene vrednosti se nalaze u opsegu od 12,8 do 75,4 %. Dobijeni rezultati pokazuju da postoji razlika u TP, TA, TF i antioksidativnoj aktivnosti u zavisnosti od upotrebljenog ekstrakcionog sredstva.

Total phenols, anthocyans, flavonoids and the antioxidant activity of different solvent extracts of Aronia (*Aronia melanocarpa*)

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Aronia or black chokeberries (*Aronia melanocarpa*), grown in Serbia, were analyzed in this study. The aim was to determine the total phenol (TP), anthocyan (TA) and flavonoid (TF) content, as well as the antioxidant activity of different solvent extracts of Aronia. We investigated the influence of different extraction solvents on the mentioned parameters. The used extraction solvents had different polarity: water, methanol, 60 % methanol$_{(aq)}$ and methanol acidified with HCl. The content of total phenols was determined by Folin-Ciocalteu's method. The obtained values ranged from 493 to 1637 mg gallic acid/100 g FW (fresh weight). Total anthocyans and flavonoids of Aronia extracts were determined spectrophotometrically. The amount of anthocyans ranged from 65 to 435 mg cyanidin-3-glucoside/100 g FW, whereas the flavonoids ranged from 65 to 137 mg quercetin/100 g FW. The antioxidant activity of Aronia extracts was assessed by a spectrophotometric DPPH (2,2-diphenyl-1-picrylhydrazyl) assay. The results are expressed as radical scavenging activity (% RSA) and ranged from 12.8 to 75.4 %. The results indicate that there is a difference in TP, TA, TF values and antioxidant activity in dependence of the solvent used for extraction.

XA O2

Hemometrijski pristup utvrđivanju geografskog porekla voćnih rakija

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Vrednosti odnosa stabilnih izotopa kiseonika i ugljenika u etanolu iz rakije mogu da ukažu na geografsko poreklo uzorka rakije. Metodom masene spektrometrije odnosa izotopa (IRMS) analizirano je 11 vrsta voćnih rakija poreklom sa severa Srbije, centralne Srbije i iz Makedonije. Sve voćne rakije su pripremljene od voća, na tradicionalan način. Time je formirana baza podataka za vrednosti odnosa stabilnih izotopa ugljenika ($^{13}C/^{12}C$), koja ukazuje na autentičnost. Vrednosti odnosa $^{18}O/^{16}O$ pokazale su se kao veoma korisne za određivanje geografskog porekla. Hemometrijski pristup, odnosno, grafičko poređenje rezultata zavisnosti $^{13}C/^{12}C$ i $^{18}O/^{16}O$ omogućilo je klasifikaciju uzoraka rakije prema njihovom geografskom poreklu.

Ovi rezultati su deo projekata No. 172012, No. 172014 i No. 31055 finansiranih od strane Ministarstva nauke i tehnološkog razvoja Republike Srbije, kao i projekta No. 114-451-2707/2012-01, finansiranog od strane Pokrajinskog sekretarijata za nauku i tehnološki razvoj Vojvodine.

Chemometrics approach in determining the geographical origin of fruit brandies

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The ratio values between stable isotopes of oxygen and carbon in ethanol from brandy may indicate the geographical origin of the brandy sample. 11 species of fruit brandies originating from the Northern Serbia, Central Serbia and Macedonia were analyzed by the method of isotope ratio mass spectrometry (IRMS). All fruit brandies are prepared in the traditional way. Therefore, a data base was formed for the ratio values in stable isotopes of carbon ($^{13}C/^{12}C$) indicating authenticity. $^{18}O/^{16}O$ ratio values proved to be very useful in determining the geographical origin. The chemometric approach or a graphical comparison of the results of the dependence between $^{13}C/^{12}C$ and $^{18}O/^{16}O$ allowed the classification of the samples of brandy according to their geographical origin.

These results are the part of the project No. 172012, No. 172014 and No. 31055 supported by the Ministry of Science and Technological Development of the Republic of Serbia, and the project No. 114-451-2707/2012-01, financially supported by the Provincial Secretariat for Science and Technological Development of Vojvodina.

XA O3

Parametri lipofilnosti u QSRR analizi 1,2-*O*-izopropiliden derivata aldoheksoza

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Retencioni parametri oslikavaju složene fizičko-hemijske osobine molekula i u mnogim slučajevima mogu biti upotrebljeni kao alternativni parametri lipofilnosti. Budući da su supstituisani 1,2-*O*-izopropiliden derivati aldoheksoza fiziološki aktivni, u radu je pomoću QSRR metode ispitana mogućnost primene njihovih retencionih parametara (R_M^0 i C_0) dobijenih tankoslojnom hromatografijom na normalnim fazama, za predikciju njihove lipofilnosti. Binarne mobilne faze sačinjavali su diluent cikloheksan i modifikatori aceton, dioksan i tetrahidrofuran, a stacionarnu fazu silika-gel. Radi formiranja modela zavisnosti između retencije i lipofilnosti ispitivanih molekula, određeni su njihovi *in silico* deskriptori lipofilnosti (Clog*P*, logP_{ChDr}, AClog*P* i Mlog*P*). Analiza korelacije je pokazala da statističku značajnost imaju kvadratne zavisnosti između C_0 i Clog*P* vrednosti ($r > 0{,}90$), dok se R_M^0 u ovom slučaju ne može predstaviti kao hromatografski parametar lipofilnosti s obzirom na niske korelacije sa log*P* parametrima ($r < 0{,}80$). Validnost postavljenih modela potvrđena je i korelisanjem eksperimentalnih i predviđenih C_0 vrednosti.

Ovi rezultati su deo projekata No. 172012, No. 172014 i No. 31055 finansiranih od strane Ministarstva nauke i tehnološkog razvoja Republike Srbije, kao i projekta No. 114-451-2707/2012-01, finansiranog od strane Pokrajinskog sekretarijata za nauku i tehnološki razvoj Vojvodine.

Lipophilicity Parameters in QSRR Analysis of 1,2-*O*-Isopropylidene Derivatives of Aldohexoses

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Retention parameters reflect the complex physical and chemical properties of molecules and in many cases can be used as the alternative lipophilicity parameters of various compounds. Since the 1,2-*O*-isopropylidene aldohexose derivatives are physiologically active molecules, in this study the possibility of application of its retention parameters R_M^0 and C_0 for prediction of its lipophilicity was examined using QSRR analysis. Retention parameters were obtained by NP TLC in the solvent systems cyclohexane/ acetone, cyclohexane/dioxane, and cyclohexane/tetrahydrofuran and silica gel as stationary phase. *In silico* descriptors of lipohilicity of examined molecules (Clog*P*, logP_{ChDr}, AClog*P* i Mlog*P*) were correlated with R_M^0 and C_0. It was found that R_M^0 can't be used as an lipophilicity parameter for examined molecules because of low correlations ($r < 0{,}80$). Statistically significant square dependence was obtained between C_0 and Clog*P* ($r > 0{,}90$) and confirmed by optimal correlations between $C_0^{exp.}$ and $C_0^{pred.}$ values, thus C_0 can be considered as an alternative lipophilicity parameter of examined derivatives in applied chromatographic systems.

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ХА П01

Hinoni kao hemijsko oružije stonoge *Julus terestris*

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Stonoge (klasa Diplopoda) su značajni predstavnici zemljišnog ekosistema, pre svega zbog razgradnje organske materije. Većina stonoga izlučuje sekret iz odbrambenih žlezda kada se uznemire. Prema hemijskom sastavu odbrambenih sekreta možemo ih podeliti na jedinke koje izlučuju *p*-krezol (red Callipodida), cijanovodonik (red Polydesmida), spirociklične alkaloide (red Polyzoniida), hinone (redovi Spirobolida, Spirostreptida Julida) i alkaloide glomerin i homoglomerin (red Glomerida)[1]. Cilj našeg rada je bio da se okarakteriše hemijski satav odbrambenog sekreta do sada neanalizirane vrste *Julus terestris* (Berlese, 1884) i da se rezultati uporede sa dosadašnjim[2]. Odbrambeni sekret je dobijen metilen-hloridnom ekstrakcijom celih jedinki i analiziran je uz pomoć instrumentalnih tehnika (GC-FID, GC-EI-MS, GC-CI-MS i 1D i 2D NMR). Ukupno devet hinonskih i hidrohinonskih derivata je okarakterisano. Strukture prisutnih hidrohinona su dodatno potvrđene silanizovanjem sa BSTFA, pri čemu su identifikovani odgovarajući trimetilsilil derivati. Rezultati su potvrdili pretpostavku da su jedinke iz familije Julidae „hinonske stonoge“.

Quinones as chemical weapons in julid millipede *Julus terestris*

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Millipedes (Class Myriapoda) have important role in the terrestrial ecosystem because of their function in the breakdown of organic matter. When disturbed, most millipedes discharge fluids from defensive glands. According to the chemical composition of defensive secretions millipedes can be divided in those discharging *p*-cresol (order Callipodida), hydrocyanide (order Polydesmida), spirocyclic alkaloids (order Polyzoniida), quinones (orders Spirobolida, Spirostreptida, and Julida) and alkaloids glomerin and homoglomerin (order Glomerida)[1]. The aim of our study was to characterize, for the first time, the chemical composition of defensive secretions of *Julus terestris* (Berlese, 1884) and to compare the results with literature[2]. Defensive secretion was obtained by whole body extraction in methylene chloride and analyzed by GC-FID, GC-EI-MS, GC-CI-MS and 1D and 2D NMR instrumental techniques. Total of nine benzoquinone and hydroquinone derivatives were identified. Strucutes of hydroquinones confirmed by BSTFA derivatization. The results confirmed the hypothesis that Julida are "quinone millipedes".

Acknowledgment: The authors acknowledge financial support of the Ministry of Education and Science of the Republic of Serbia (Project No. 172036).

[1] Secret weapons: defenses of insects, spiders, scorpions, and other many-legged creatures, Thomas Eisner, Maria Eisner and Melody Siegler, London, England 2005.

[2] Lj. Vujisić, S. Makarov, B. Ćurčić , B. Ilić, V. Tešević, D. Gođevac, I. Vučković, S. Ćurčić, B. Mitić, *J Chem Ecol* 2011 (**37**) 1358-1364

ХА П02

Одређивање садржаја As, Cd и Pb у намирницама са шпанског тржишта

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Циљ рада је одређивање садржаја три токсична елемента (As, Cd, Pb) у одабраним намирницама са шпанског тржишта. Такође садржаји ова три тешка елемента одређивани су и у различитим врстама хране за бебе (такође са шпанског тржишта). Након киселинске дигестије узорака у микроталасном систему, извршена је анализа добијених раствора помоћу атомског апсорпционог спектрофотометра са графитном киветом. Концентрација олова и арсена у два узорка хране за бебе на бази рибе била је изнад максимално дозвољене концентрације. У свим осталим намирницама садржај испитиваних елемената је испод максимално дозвољених вредности прописаних европском регулативом. Резултати испитивања су поређени са доступним подацима првенствено оним који се односе на намирнице са српског тржишта ради упоредне процене њихове хемијске безбедности.

Захвалност: Резултати презентовани у овом раду добијени су у оквиру билатералног пројекта "Напредне хроматографске и масено спектрометријске технике у анализи хемијске безбедности хране", финансираног од стране Министарства просвете, науке и технолошког развоја, Републике Србије, којим руководи Проф. Б. Шкрбић.

Determination of trace element contents in selected foodstuff collected from market in Spain

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The purpose of the study was to determine the concentration levels of three toxic elements (As, Pb, Cd) in selected foodstuffs collected from the Spanish market. Also the levels of these three heavy elements were determined in different types of baby food from Spain. The samples were analyzed after the microwave acid digestion by atomic absorption spectrometer with graphite furnace. In general the observed concentrations were well below the maximum levels set by the current European regulations except in the case of two baby food samples based on fish in which Pb and As were found at higher levels. The results were compared with available data primarily those referring to the Serbian foodstuffs in order to comparatively assess their chemical safety status.

Acknowledgment: The results presented here are obtained within the bilateral project "Advanced chromatographic and mass spectrometric techniques in food chemical safety analysis" supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia coordinated by Prof. B. Škrbić.

ХА П03

Viscosity of the binary systems nicotine with poly(ethylene glycol)s

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Viscosity data of the two binary systems nicotine + PEG200 and nicotine + PEG400 have been measured in temperature range 288.15-333.15 K with temperature step 5K, and at atmospheric pressure. The measurements were performed on Anton Paar SVM 3000 digital viscometer. Based on the corresponding data, viscosity deviations ($\Delta\eta$) were determined and fitted by the Redlich-Kister polynomial equation.

Viskoznost binarnih sistema nikotina sa polietilen glikolima

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Eksperimentalno su određene vrednosti viskoznosti dva binarna sistema nikotin + PEG200 i nikotin + PEG400 u temperaturnom intervalu 288.15–333.15 K sa korakom 5 K, i na atmosferskom pritisku. Eksperimentalna merenja su izvršena na digitalnom viskozimetru Anton Paar SVM 3000. Na osnovu odgovarajućih eksperimentalnih podataka, izračunate su vrednosti promene viskoznosti ($\Delta\eta$), i korelisane Redlich-Kister polinomom.

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XA П04

Skrining i distribucija antioksidative aktivnosti između kože, mesa i semena četiri vrste grožđa iz Srbije

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Plod grožđa sadrži supstance koje pokazuju visoku antioksidativnu aktivnost. Analizirana je antioksidativna aktivnost različitih delova kožice, mesa i osušenog semena ploda grožđa. Korišćeno grožđe je iz Srbije, a ispitivane su četiri sorte: *Rhine Riesling*, *Cabernet Franc*, *Merlot* i *Prokupac.* Kao ekstrakciono sredstvo za osušeno seme je korišćen rastvor 80 % metanola, a za meso i kožicu apsolutni metanol. Antioksidativna aktivnost je određivana DPPH (2,2-difenil-1-pikrilhidrazil) esejom, a dobijene vrednosti su prikazane kao sposobnost (aktivnost) uklanjanja radikala (*eng.* radical scavenging activity, RSA, %). Dobijene vrednosti za antioksidativnu aktivnost semena se kreću u opsegu od 36,71 % do 40,71 %, mesa od 14,89 % do 19,99 %, a kožice od 14,26 % do 70,76 %. Cilj ove studije bio je da se odredi distribucija antioksidativne aktivnosti u različitim delovima ploda srpskog grožđa.

Screening and distribution of antioxidative activity between skin, pulp and seed of four grape varieties (*Vitis vinifera* L.) from Serbia

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Grape fruit is rich in ingredients that show high antioxidative activity. We analyzed antioxidative activity of different parts of grape fruit: skin, pulp and dried seed. Under view of this study were four varieties of Serbian grape: *Rhine Riesling*, *Cabernet Franc*, *Merlot* and *Prokupac*. For extraction of dried grape seed were used 80 % methanol and for pulp and skin it was absolute methanol. Antioxidant activity was screened using DPPH (2,2-diphenyl-1-picrylhydrazyl) assay and determinate values were expressed as radical scavenging activity, RSA, %. Grape seed antioxidative activity rating from 36.71 % to 40.71 % of RSA, for pulp it was from 14.89 % to 19.99 % and for skin from 14.26 % to 70.76 %. The aim of this study was to determine distribution of antioxidant activity in different parts of Serbian grape fruit.

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ХА П05

Elektrohemijska karakterizacija i određivanje karbamazepina kao farmaceutskog standarda i u tableti Galepsin® na elektrodi od zlata

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Anodno ponašanje karbamazepina (KBZ), antikonvulzivnog leka, proučavano je cikličnom voltametrijom na elektrodi od zlata u 0.1 mol dm^{-3} fosfatnom puferu pri pH 7.0. Uočena je linearna koncentraciona zavisnost oksidativnog pika na +1.10 V za standard KBZ-a u opsegu koncentracija 1×10^{-6}–4×10^{-4} mol dm^{-3}. Takođe, KBZ je detektovan pri koncentraciji od 1.0×10^{-8} mol dm^{-3}, što predstavlja najniže detektovanu koncentraciju primenom voltametrijskih tehnika. KBZ u tableti Galepsin® je kvantitativno je determinisan i dobijeni rezultati potvrđeni su primenom HPLC metode. U poređenju sa nemodifikovanom elektrodom od zlata, modifikacija elektrode pomoću bovin serum albumina rezultirala je smanjenjem vrednosti pika oksidativnih struja sto je posledica vezivanja leka za serum. Elektrohemijski odgovor KBZ-a nakon modifikacije elektrode od zlata ugljeničnim nanotubama ukazuje da je nemodifikovana elektroda od zlata bolji katalizator.

Electrochemical characterization and determination of carbamazepine as pharmaceutical standard and as a content of tablet Galepsin® on gold electrode

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The anodic behavior of carbamazepine (CBZ), an anticonvulsant drug, has been studied on gold electrode in 0.1 mol dm^{-3} phosphate buffer of pH 7.0 using cyclic voltammetry. It has been found that the value of the oxidative peak of pure CBZ at +1.10 V is a linear function of the concentration in a range from 1×10^{-6} to 4×10^{-4} mol dm^{-3}. Thus, CBZ has been detected in the concentration of 1.0×10^{-8} mol dm^{-3}, which is among the lowest that have been reported for this drug using voltammetric techniques. CBZ as a content of tablet Galepsine® has been quantitatively determined and the obtained results have been checked by high performance liquid chromatography. In comparison with the unmodified gold electrode, the modification with bovine serum albumine has resulted in a decrease of the oxidative current peaks as a consequence of the CBZ-serum binding. The effects on the electrochemical response of CBZ resulting from the modification of gold electrode with multiwalled carbon nanotubes suggest that bare gold electrode is even better catalyst.

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ХА П06

Fenolni profil i međusobni odnos sadržaja pojedinačnih fenola u kakaou

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Kakao je bogat izvor polifenola. U ovom radu je ispitan fenolni sastav komercijalno dostupnih kakaa, kao i međusobni odnos sadržaja pojedinačnih fenola u njima. Zastupljenost fenolnih jedinjenja opada u nizu: protokatehinska kiselina>epikatehin≥katehin>procijanidin B2>procijanidin B1. Sadržaj epikatehina se kreće u intervalu od 0,045-0,140 mg/g, katehina 0,033 0,184 mg/g, procijanidina B1 ND(nije detektovano)-0,029 mg/g, B2 ND-0,148 mg/g i protokatehinske kiseline 0,100-0,252 mg/g. Međusobnim upoređivanjem sadržaja fenolnih jedinjenja došlo se do zaključka da postoji dobra korelacija između epikatehina i procijanidina B1 (R^2=0,865), katehina (R^2=0,822), procijanidina B2 (R^2=0,746) i niska korelacija između epikatehina i protokatehinske kiseline (R^2=0,381). Kod katehina, takođe, je dobra korelacija sa procijanidinom B2 (R^2=0,836), epikatehinom (R^2=0,822), procijanidinom B1 (R^2=0,733), dok je slaba korelacija sa protokatehinskom kiselinom (R^2=0,028).

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Cocoa phenolic profiles and the correlation of individual phenolic constituents

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Cocoa products are a rich source of polyphenols. The present study investigates the phenolic composition of several commercially available cocoa powders. The relative abundance of individual components as measured by HPLC given in a decreasing order of value was: protocatechuic acid>epicatechin≥catechin>procyanidin B2>procyanidin B1. The amount of epicatechin was in the range 0.045-0.140 mg/g, whereas the quantity of catechin ranged from 0.033 to 0.184 mg/g, B1 from not detected (ND) to 0.029 mg/g, B2 from ND to 0.148 mg/g and protocatechuic acid from 0.100 to 0.252 mg/g. When individual polyphenols detected in cocoa powders are plotted against each other in scatter plots, epicatechin concentrations were strongly correlated to the concentrations of B1 (R^2=0.865), catechin (R^2=0.822), B2 (R^2=0.746), and, to a lesser extent, to the amount of protocatechuic acid (R^2=0.381). In the case of catechin and the other three polyphenols, strong correlations were also observed: B1 (R^2=0.733), epicatechin (R^2=0.822), B2 (R^2=0.836). Only a weak correlation was found between the amounts of catechin and protocatechuic acid (R^2=0.028).

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ХА П07

Hemijski sastav različitog bobičastog voća iz Srbije

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Najznačniji proizvodi Srbije su divlje i kultivisane sorte bobičastog voća, koje sadrže veliki broj bioaktivnih jedinjenja. U okviru ovog istraživanja cilje je bio definisati polifenolne profile devet različitih uzoraka bobičastog voća (malina, kupina, dud i jagoda). Sadržaj ukupnih polifenola određen je uz pomoć Folin-Ciocalteu reagensa, a ukupni antocijani su određeni spektrofotometrijskim merenjem na različitim pH vrednostima. Količina ukupnih polifenola u bobičastom voću varira od 135,30 mg ekv. galne kiseline koliko je pronađeno u 100 g zamrznutog duda do 375,03 mg ekv. galne kiseline koliko sadrži 100 g zamrznute kupine. Najveći sadržaj ukupnih antocijana pronađen je u uzorku kupine (96,94 mg ekv. cijanidin-3-glukozid/100 g zamrznutog voća), dok je namanja količina antocijana (5,39 mg ekv. cijanidin-3-glukozid/100 g zamrznutog voća) određena u uzorku maline (sorta Žuti Miker). Dvanaest polifenolnih jedinjenja i *cis, trans*-abscisinska kiselina su kvantifikovani korišćenjem tečne hromatografije kuplovane sa hibridnom masenom spektrometrijom (UHPLC- MS/MS Orbitrap).

Zahvalnost: Ovaj rad je podržan od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, Projekat br. 172017

Chemical composition of different berries harvested in Serbia

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The most important products of Serbia are wild or cultivated berries which contain many bioactive components. Taking into account the importance of the antioxidant capacity exhibited by polyphenolics, the purpose of this study was to determine the polyphenolic profiles of nine different berries (raspberry, blackberry, mulberry, and strawberry). The amount of total phenolics was determined according to the Folin-Ciocalteu procedure. Total anthocyanin content was estimated by a pH differential method. Liquid chromatography coupled with a hybrid mass spectrometer (UHPLC- MS/MS Orbitrap) was used for a study of the phenolic components of berries. The total phenolics in berries ranged from 135.30 mg GAE/100 g frozen weight (mulberry) to 375.03 mg GAE/100 g frozen weight (blackberry). The highest content of total anthocyanins was found in blackberry (96.94 mg cyn-3-glu/100 g frozen weight), whereas Yellow Meeker contained the lowest amount of anthocyanins (5.39 mg cyn-3-glu/100 g frozen weight). Twelve polyphenolic compounds and *cis,trans*-abscisic acid were quantified using the available standards.

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ХА П08

Određivanje koncentracije platine u listovima listopadnog drveća sa područja Beograda

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Automobilski katalizatori se koriste u auto industriji za smanjenje emisije zagađujućih materija kao što su ugljen(II)-oksid, oksidi azota i nesagoreli ugljovodonici. Tokom rada katalizatora, kao rezultat abrazije njihove površine, platina se oslobađa u životnu sredinu i deponuje se pored saobraćajnica, na obližnjoj vegetaciji, zemljištu kao i u vodotokovima. U ovom istraživanju vršeno je određivanje koncentracije platine u listovima listopadnog drveća četiri biljne vrste (divlji kesten, lipa, breza i platan) sa područja Beograda. Uzorci su sakupljani u julu 2009. godine sa dva lokaliteta – Karađorđev park i Studentski park. Svi uzorci su oprani bidestilovanom vodom pre mikrotalasne digestije. Merenje koncentracije platine je vršeno metodom indukovano spregnute plazme sa masenom spektrometrijom (ICP-MS). Preliminarno dobijeni rezultati ukazuju da su listovi divljeg kestena i lipe podesniji za biomonitoring platine emitovane u životnu sredinu, dok su platan i breza manje pogodni bioindikatori.

Zahvalnica: Istraživanja su realizovana u okviru naučnih projekata Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, broj: OI 172007, III 43007 i OI 173028.

Platinum concentration in deciduous tree leaves from the Belgrade urban area

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The automobile catalyst converters, used in car industry, reduce the emission of pollutants, such as carbon monoxide, nitrogen oxides and unburned hydrocarbons. During the utilisation of converters, as a result of abrasion of the catalyst surface, platinum is released into environment and deposited along roadways, on adjecent vegetation and soil and in water resources. This research focus was on the analysis of the platinum in deciduous tree leaves of four common urban species (horse chestnut, linden, birch and Norway maple) from the Belgrade urban area. The samples were collected in July 2009 from two locations – Karađorđev Park and Studentski Park. All the samples were washed with bidistilated water before microwave digestion. The measurement of platinum concentration was performed by inductively coupled plasma mass spectrometry (ICP-MS). The preliminary results indicate that leaves of horse chestnut and linden could be a better choice in biomonitoring of platinum concentration in the environment while Norway maple and birch are less suitable biomonitors.

ХА П09

Hemijski sastav etarskog ulja gomolja biljne vrste *Helianthus tuberosus* L. (Asteraceae)

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Rod *Helianthus* L. (porodica Asteraceae) obuhvata oko 50 jednogodišnjih i višegodišnjih vrsta suncokreta. *Helianthus tuberosus* L. (Jerusalimska artičoka) se gaji u Evropi i drugim delovima sveta kao industrijska i ukrasna biljka. Etarsko ulje nadzemnih delova ove vrste je analizirano još 1982. godine, ali, do sada, se nijedno istraživanje nije bavilo određivanjem sastava etarskog ulja gomolja. U ovom radu smo opisali prvu GC i GC-MS analizu hidrodestilovanog etarskog ulja gomolja Jerusalimske artičoke. Iz svežeg biljnog materijala, koji je sakupljen u jugoistočnoj Srbiji ili kupljen, dobijena je mala količina ulja (0,0014-0,0021 %). Identifikovano je ukupno sto devedeset i pet sastojaka, što čini 77-89 % ulja. Glavni sastojci su bili *β*-bisabolen (18,8-25,2 %), undekanal (0-10,4 %), *α*-pinen (0,7-6,2 %), kauran-16-ol (0-5,7 %), 2-pentilfuran (0-4,7 %) i (2*E*)-tetradecenal (0-4,0 %). Nekoliko jedinjenja sa ograničenom prirodnom rasprostranjenošću, koja su karakteristična za *Helianthus* spp. su, takođe, detektovana: seskviterpen-heliantol A (1,4-1,7 %) i prenilovani acetofenoni-desmetoksiencekalin (tr-0,2 %), izomer desmetoksiencekalina (0-tr), dihidroeuparin (0-1,9 %), euparin (0-0,2 %) i eupatoriohromen (0-0,3 %). Etarsko ulje podzemnog i nadzemnog dela dele samo isti glavni sastojak – *β*-bisabolen.

Ovaj rad je finansiralo Ministarstvo prosvete, nauke i tehnološkog razvoja (Projekat 172061).

Chemical Composition of Tuber Essential Oil from *Helianthus tuberosus* L. (Asteraceae)

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The genus *Helianthus* L. (Asteraceae) comprises about 50 annual and perennial sunflower species. *Helianthus tuberosus* L. (Jerusalem artichoke) is cultivated in Europe and other parts of the world as a crop and ornamental plant. The volatile oils of the aerial parts of H. tuberosus were analyzed in 1982, but no study has been carried out to date to determine the constituents of the tuber essential oil. Herein, we describe the first analysis by GC and GC-MS of the hydrodistilled essential oil of the Jerusalem artichoke tubers. The fresh plant material, collected in Serbia and a commercial sample, yielded only a small amount of the oil (0.0014-0.0021 %, w/w). One hundred-ninety five constituents were identified in total, representing 77-89 % of the oil. The main constituents were *β*-bisabolene (18.8-25.2 %), undecanal (0-10.4 %), α-pinene (0.7-6.2 %), kauran-16-ol (0-5.7 %), 2-pentylfuran (0-4.7 %) and (2*E*)-tetradecenal (0-4.0 %). Several rare compounds characteristic for *Helianthus* sp. were also detected: helianthol A (1.4-1.7 %), desmethoxy encecalin (0-0.2 %), isomer desmethyl encecalin (0-tr), dihydroeuparin (0-1.9 %), euparin (0-0.2 %) and eupatoriochromene (0-0.3 %). The tuber essential oil and the aerial parts one share a common major component - *β*-bisabolene.

ХА П10

Određivanje polifenolnog profila i geografskog porekla livadskog meda iz Srbije

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Med je prirodan slatki proizvod koji prave pčele. To je, u suštini, vodeni rastvor šećera, pre svega glukoze i fruktoze, ali i drugih supstanci, kao što su organske kiseline, aminokiseline, proteini, minerali, polifenolna jedinjenja i dr. Polifenolna jedinjenja, uglavnom fenolne kiseline i flavonoidi, mogu biti potencijalni biomarkeri za botaničko i geografsko poreklo meda. Cilj ovog istraživanja bio je da se ispita mogućnost određivanja geografskog porekla 58 uzoraka polifloralnih medova iz različitih regiona Srbije, na osnovu njihovog polifenolnog profila. Analiza glavnih komponenata je primenjena za klasifikaciju meda prema sadržaju polifenolnih jedinjenja. Kvalitativni i kvantitativni polifenolni profil meda određen je tehnikom tečne hromatografije u kombinaciji sa hibridnim linearnim jon trap/Orbitrap masenim spektrometrom. Fenoli su identifikovani i kvantifikovani korišćenjem dostupnih standarda. Abscisinska kiselina, biljni hormon, koja je prisutna u cvetnom nektaru i medu, takođe je identifikovana i kvantifikovana.

Zahvalnost: Ovaj rad je podržan je od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, Projekat br. 172017.

Phenolic profiles and the geographical origin of Serbian polyfloral honeys

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Honey is a natural sweet food produced by honeybees. It essentially represents an aqueous solution of saccharides, primarily glucose and fructose, and other substances, such as organic acids, amino acids, proteins, minerals, polyphenolic compounds and other chemicals. Polyphenolic compounds, mainly phenolic acids and flavonoids, were recognized as possible biomarkers for botanical and geographical origin of honey. The goal of this study was to investigate the possibility of determining the geographical origin of 58 polyfloral honey samples from different regions of Serbia, based on their phenolic profiles. Principal Component Analysis (PCA) was applied to classify honey according to their polyphenolic content. Qualitative and quantitative content of polyphenols was determined using liquid chromatography coupled with a hybrid linear ion trap/Orbitrap mass spectrometer. Phenolics were identified and quantified using the available standards. Abscisic acid, a plant hormone known to be present in floral nectar and honey, was also identified and quantified.

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ХА П11

Korelisanje ravnoteže tečno-tečno ne idealnih binarnih sistema sa NRTL modelom

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NRTL model sa tri različita temperaturno zavisna parametra korišćen je za korelisanje ravnoteže tečno-tečno za sisteme alkohola sa jonskom tečnošću: 1–butyl-2,3-dimethylimidazolium tetrafluoroborate ([bmmim][BF4]). Različiti temperaturno zavisni parametri NRTL modela su testirani za pet eksperimentalnih podataka binarnih sistema.

Correlation of liquid-liquid equilibria of non-ideal binary systems by NRTL model

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NRTL (Non-Random Two-Liquid) model with three different forms of temperature dependant parameters was used to correlate the liquid – liquid equilibrium data for systems of alcohols with ionic liquid: 1–butyl-2,3-dimethylimidazolium tetrafluoroborate ([bmmim] [BF4]). Different temperature dependences of NRTL parameters were tested on five literature experimental liquid – liquid equilibrium data for binary systems.

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ХА П12

Ravnoteža tečnost-tečnost tečnih polietilen glikola sa jonskom tečnošću $[P_{6,6,14}]^{+}[NTF_2]^{-}$

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Tokom poslednjih nekoliko godina pojavile su se dve osnovne teme istraživanja: “green meets toxic” i “green meets green”. Prva razmatra primenu rastvarača koji ne štete okolini u toksičnim organskim jedinjenjima koja su od velikog praktičnog i industrijskog značaja. Druga tema je vezana za ponašanje tečne faze u rastvorima “zelenih”, ekološki održivih supstanci. U ovom radu će biti predstavljeni ravnotežni tečnost-tečnost podaci za sisteme PEG 200+$[P_{6,6,14}]^{+}[NTf_2]^{-}$ i PEG 400+$[P_{6,6,14}]^{+}[NTf_2]^{-}$. Ispitivan je uticaj katjona, anjona i dužine lanca polimera PEG na mešljivost posmatranih sistema, kao i interakcije u rastvorima – vodonične i jon-dipol veze.

Ovi eksperimenti su prvi korak ka ispitivanju mogućnosti upotrebe posmatranih rastvora (PEG+jonska tečnost) kao potencijalnih dugotrajnih hibridnih materijala ili kombinovanih rastvarača kod kojih se mogu podešavati termofizičke osobine i / ili moć rastvorljivosti.

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Liquid-liquid equilibria in liquid polyethylene glycol and ionic liquid $[P_{6,6,14}]^{+}[NTf_2]^{-}$

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In the last years, research follows two main issues, defined by the slogans: “green meets toxic” and “green meets green”. The first issue considers the potential use of ambient friendly solvents for toxic organic compounds of industrial and practical importance. The other is related to liquid phase behavior in solutions of ecologically sustainable substances.

Liquid-liquid phase behaviors of the binary solutions of trihexyltetradecyl phosphonium $[P_{6,6,14}]^{+}$ ionic liquid having bistriflamide $[NTf_2]^{-}$ anion and its solutions with poly(ethylene glycol) (PEG) of average molecular mass (Mw) 200 and 400 were studied. The impact of cation, anion and of PEG polymer chain length on the studied phase behavior was investigated and discussed in the terms of the important interactions – hydrogen bonds and ion-dipole – in the solutions.

This study is a first step to explore the possibilities to use the studied (PEG+ionic liquid) solutions as potential sustainable hybrid materials or combined (mixed) solvents of tunable thermophysical properties and/or solvent power.

ХА П13

Validacija metode za određivanje sadržaja ^{90}Sr u uzorcima voda

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U ovom radu navodi se primer izveštaja validacije metode za određivanje sadržaja ^{90}Sr u vodi (nestandardna metoda koja je modifikovana i koja se koristi u Laboratoriji za radijaciona merenja Laboratorije za zaštitu od zračenja i zaštitu životne sredine).
Validacija je potvrđivanje ispitivanjem i pružanje objektivnog dokaza da su zadovoljeni pojedinačni zahtevi za predvidjenu specifičnu upotrebu. Obuhvata provere koje se izvode kako bi se obezbedilo da karakteristike metode budu razumljive i da se demonstrira da je metoda naučno opravdana u uslovima njene primene.
Određivanje sadržaja ^{90}Sr u uzorcima voda, vrši se prema metodi koja obuhvata radiohemijsko izdvajanje itrijuma ^{90}Y iz uzorka i merenje njegove aktivnosti nakon uspostavljanja radioaktivne ravnoteže sa ^{90}Sr. Na osnovu dobijenih rezultata određuje se aktivnost ^{90}Sr.

Validation of method for the determination of ^{90}Sr in water samples

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An example of validation report for the determination of ^{90}Sr in water (non-standard method that has been modified and used in the laboratory for radiation measurement of laboratory for radiation protection and environmental protection) is presented in this paper.
Validation is the confirmation by examination and provision of objective evidence that they meet the individual requirements stipulated for a specific use.
Determination of ^{90}Sr content in water samples is performed according to the method which implies radiochemical separation of ^{90}Y from the sample and measuring its activity after the establishment of radioactive equilibrium with ^{90}Sr.

ХА П14

SMT protokol za određivanje frakcija fosfora primenom mikrotalasa

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Fosfor igra važnu ulogu u procesu eutrofikacije, koja predstavlja jedan od glavnih problema zagađenja vode. Kako bi sprečili negativan uticaj fosfora, važno je pratiti njegovu koncentraciju u sedimentima, znati u obliku kojih jedinjenja je prisutan i u kolikoj meri je biodostupan. Jedna od najvažnijih procedura koja se koristi u ovu svrhu je metoda sekvencijalne ekstrakcije. SMT (The Standards, Measurements and Testing) procedura omogućava izdvajanje pet frakcija fosfora i sadrži tri odvojene faze. Modifikovana mikrotalasna sekvencijalna ekstrakcija primenjena je na četiri različita uzorka zemljišta i na referentni materijal (BCR684). Sa ciljem da se faze ekstrakcije svedu na manji vremenski interval mućkanje od šesnaest sati zamenjeno je mikrotalasnim tretmanom primenom tri različite snage od 100, 200 i 300W i tri ekstrakciona vremena od 10, 20 i 30 minuta. Rezultati dobijeni primenom konvencionalne i modifikovane SMT procedure pokazali su veliko slaganje, uz znatnu redukciju vremena ekstrakcionih koraka. Takođe, primenom BCR684 referentnog materijala omogućena je validacija metode. Ovaj rad je finansiran u okviru Projekta broj 17030 od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije.

SMT procedure for the determination of phosphorus fractions using microwaves

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Phosphorus plays an important role in eutrophication of freshwater, one of the primary water pollution problems. Important way to stop negative influence of phosphorus is the monitoring of its partitioning in sediments and one of the most important procedure is the method of sequential extraction. The Standards, Measurements and Testing procedure (formerly BCR) has been proved to be a useful tool for the study of phosphorus extraction in freshwater sediments. The SMT extraction protocol consists of determination five phosphorus fractions in three separated extraction steps. Phosphorus fractions were extracted from four different samples and reference material (BCR684). With the aim to accelerate the steps in determination of phosphorus forms, sixteen hours of shaking has been replaced by microwave treatment on three different strengths of 100, 200 and 300W and extraction time for 10, 20 and 30 minutes. Our results have shown great similarity with those obtained using the conventional SMT procedure, but with significantly reduced treatment times. Also, using the reference material BCR-684 allowed validating the simplified microwave-assisted method.

ХА П15

Identifikacija metil estara 2-hidroksi-3-metilkarboksilnih kiselina - *headspace* sastojka cvetova biljne vrste *Galanthus nivalis* L. (Amaryllidaceae)

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Detaljnom analizom hemijskog sastava *headspace* sastojaka svežih, nepovređenih cvetova biljne vrste *Galanthus nivalis* L. (Amaryllidaceae), visibaba, metodama GC i GC/MS utvđeno je prisustvo metil estara 2-hidroksikarboksilnih kiselina, koji su poznati po tome da daju miris apsolutima biljaka čak iako su prisutni u tragovima, pa su zato vrlo cenjeni u industriji parfema. U cilju potvrde identiteta, pomenuti biljni sastojci su sintetisani koristeći dva različita sintetska pristupa. Stereospecifični pristup podrazumevao je diazotovanje i hidrolizu ʟ-aminokiselina do odgovarajućih ʟ-α-hidroksikiselina, dok je drugi pristup uključivao adiciju HCN na odgovarajući aldehid i hidrolizu dobijenog cijanhidrina. U oba slučaja dobijene α-hidroksikiseline su esterifikovane etarskim rastvorom diazometana. Jedan od *headspace* sastojaka visibabe je identifikovan kao jedan od dijastereomera metil-2-hidroksi-3-metilheksanoata (**1**). Jedinjenje **1**, koje predstavlja novi sekundarni metabolit prisutan u biljnom svetu, sintetisano je iz 2-metilvaleraldehida u gramskim količinama (ukupan prinos 55 %) u cilju potpune spektralne karakterizacije i testiranja mirisnih osobina.

Ovaj rad je finansiralo Ministarstvo prosvete, nauke i tehnološkog razvoja RS (Br. Projekta 172061).

Identification of methyl esters of 2-hydroxy-3-methylcarboxylic acids – headspace constituents of intact *Galanthus nivalis* L. (Amaryllidaceae) flowers

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Detailed GC and GC/MS analyses of the headspace constituents of intact *Galanthus nivalis* L. (Amaryllidaceae), snowdrop, flowers revealed, among others, the presence of a number of methyl esters of 2-hydroxycarboxylic acids, that are known to be olfactively important trace components of some flowers absolutes, highly valued in perfumery. In order to corroborate the tentative mass spectral identification of these headspace constituents, a synthesis of several methyl esters of different α-hydroxycarboxylic acids was performed, utilising two different synthetic approaches. The stereospecific one involved the diazotisation and hydrolysis of ʟ-amino acids to the corresponding ʟ-α-hydroxycarboxylic acids, whereas the other approach included the addition of HCN to an aldehyde and the hydrolysis of the obtained cyanohydrin. In both cases the obtained α-hydroxycarboxylic acids were esterified by ethereal diazomethane. One of the headspace constituents was shown to be the diastereisomerically pure methyl 2-hydroxy-3-methylhexanoate (**1**). Compound **1**, which can be regarded as a new plant secondary metabolite, was obtained in gram quantities starting from 2-methylvaleraldehyde (total yield 55 %), in order to perform its full spectral characterisation and for further testing of its biological activity and olfactory properties.

ХА П16

Novi estri dugolančanih *n*-alkohola sa izobutanskom i izovalerijanskom kiselinom iz etarskog ulja biljne vrste *Scandix pecten-veneris* L. (Apiaceae)

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Isparljivi metaboliti ove biljne vrste prethodno su analizirani dva puta, kada je identifikovano samo po ukupno 12 i 10 sastojaka, pa smo odlučili da izvršimo detaljnu analizu etarskog ulja nadzemnih delova i korena *S. pecten-veneris* iz jugoistočne Srbije (ukupno 7 uzoraka). Glavni sastojci ulja su bili alkani tridekan (8,5-52,8 %), pentadekan (1,3-23,5 %) i seskviterpen β-kariofilen (0,1-18,5 %). Uočeno je i prisustvo 14 sastojaka (do 0,9 %) za koje je, na osnovu analize njihovih masenih spektara, pretpostavljeno da su trikozanil-, heneikozanil-, tri-, tetra-, penta-, heksa-, hepta- i oktadecil-pentanoati i -butanoati. U cilju potvrde njihove strukture izvršili smo sintezu 17 estara izobutanske, izovalerijanske i 2-metilbutanske kiseline sa odgovarajućim *n*-alkoholima. Svi sintetisani estri (od kojih je 9 potpuno novih, a 13 je po prvi put detektovano kao prirodni biljni proizvod) su spektralno okarakterisani (IR, MS, NMR) i GC ko-injektirani sa etarskim uljem. Izuzev tri-, penta- i heptadecil 2-metilbutanoata, ostali sintetisani estri su prisutni u analiziranom etarskom ulju biljne vrste *S. pecten-veneris*.

Zahvalnica: Ovaj rad je finansiralo Ministarstvo prosvete i nauke (Projekat 172061).

New esters of long chain alcohols and isobutanoic and isovaleric acids from the essential oil of *Scandix pecten-veneris* L. (Apiaceae)

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Since the volatiles of this plant species have been the subject of only two previous studies, that identified 12 and 10 constituents in total, we decided to perform a more detailed analysis of the aerial parts and roots essential oil of *S. pecten-veneris* from Southeastern Serbia (in total 7 samples). Among one hundred-twentynine constituents identified by GC (FID) and GC/MS, tridecane (8.5-52.8 %), pentadecane (1.3-23.5 %) and β-caryophyllene (0.1-18.5 %) were found to be the most abundant ones. The analysis also pointed to the presence of 14 additional minor compounds (up to 0.9 %), that were, according to their mass spectral fragmentation, tentatively identified as the isomeric tricosanyl-, heneicosanyl-, tri-, tetra-, penta-, hexa-, hepta- and octadecyl pentanoates and butanoates. In order to corroborate the tentative identification of these esters a synthesis was undertaken of 17 esters of isobutanoic, isovaleric and 2-methylbutanoic acids with appropriate alcohols. All synthesized esters (of which 9 entirely new and 13 found for the first time as plant secondary metabolites) were spectrally characterized (IR, MS, NMR) and separately GC co-injected with the essential oils. Except for tri-, penta- and heptadecyl 2-methylbutanoates, all other synthesized compounds were detected in the analyzed oils of *S. pecten-veneris*.

ХА П17

Isparljivi sekundarni metaboliti biljne vrste *Senecio vernalis* Waldst. & Kit.

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Senecio vernalis Waldst. & Kit. (žutenika), porodica Asteraceae, je biljna vrsta rasprostranjena u Aziji i jugoistočnoj Evropi. O hemijskom sastavu njenog etarskog ulja postoji ograničeni broj podataka u literaturi. U ovom radu izvršena je detaljna hemijska analiza isparljivih metabolita nekoliko populacija ove vrste u cilju utvrđivanja potencijalnog postojanja različitih hemotipova ove vrste u Srbiji. Analizom (GC i GC-MS) 8 uzoraka suvih nadzemnih delova i korenova (4 različite populacije) identifikovano je ukupno 60 sastojaka koji predstavljaju 95,5-99,4 % ukupnog ulja. Glavni isparljivi sastojci nadzemnih delova svih populacija su bili monoterpeni *α*-pinen (26,7-38,5 %) i *β*-pinen (23,0-24,8 %), dok su glavni sastojci ulja korena bili ili α-humulen (40,9-57,0 %, tri uzorka) ili nonakozan (33,3 %, jedan uzorak). Na osnovu sastava, moguće je zaključiti da se biosinteza i/ili akumulacija isparljivih metabolita veoma razlikuje od organa do organa. Ovo je dodatno potvrđeno aglomerativnom hijerarhijskom klaster analizom (AHC) i analizom glavne komponente (PCA) podataka za 30 etarskih ulja (18 taksona ovog roda) su izvršene korišćenjem četiri različitih promenljivih.

Zahvalnica: Ovaj rad je finansiralo Ministarstvo prosvete i nauke (Projekat 172061).

Volatile secondary metabolites of *Senecio vernalis* Waldst. & Kit.

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Senecio vernalis Waldst. & Kit., Asteraceae, (local Serbian name: žutenika) is a plant species widely distributed in Asia and SE Europe. However, limited data on the chemical composition of the corresponding essential oil exist. For this reason, detailed chemical analyses of the volatile secondary metabolites of several populations of *S. vernalis* were conducted in order to provide an insight into the chemotypification of this species in Serbia. Analyses (by GC and GC-MS) of 8 essential oils hydrodistilled from dry above-ground parts and roots of *S. vernalis* (4 different populations) enabled the identification of 60 different constituents, representing 95.5-99.4 % of the total oils. The most abundant constituents of the oils obtained from the above-ground parts (all populations) were α-pinene (26.7-38.5 %) and β-pinene (23.0-24.8 %), whereas the most dominant constituents of the rhizome oils were either α-humulene (40.9-57.0 %, 3 samples) or nonacosane (33.3 %, 1 sample). Hence, the biosynthesis and/or accumulation of volatile metabolites in *S. vernalis* is strongly plant organ dependent. This was additionally corroborated by agglomerative hierarchical cluster analysis (AHC) and principal component analysis (PCA). Both AHC and PCA analyses of 30 different essential oils (18 different *Senecio* taxa; data from the literature and the present study) were performed using four different types of variables.

ХА П18

Novi diarilheptanoid iz kore drveta *Alnus glutinosa* subsp. *glutinosa*

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Rod *Alnus* pripada familiji Breza. Rod je podeljen na tri podroda i obuhvata oko 30 vrsta (u zavisnosti od autora). Jedna od vrsta je i *Alnus glutinosa* subsp. *glutinosa,* drvo koje doseže i 30 m visine, a može se naći u većini evropskih zemalja kao i u jugozapadnoj Aziji. Još od ranije je poznato da jedinjenja izolovana iz vrsta *Alnus* poseduju različite biološke aktivnosti kao što su: antivirusna, antitumorska, antibakterijska, kao i mnoge druge aktivnosti zbog kojih su ova jedinjenja značajna u prevenciji i lečenju različitih bolesti. U ovom radu smo ispitali sastav kore drveta *Alnus glutinosa* subsp. *glutinosa*. Biljni materijal je uzorkovan u junu 2009. godine u okolini Prijepolja u Srbiji. Nakon ekstrakcije i hromatografije na koloni silikagela, čisti diarilheptanoidi su izolovani uz pomoć preparativnog HPLC-a. Pored već poznatih diarilheptanoida, oregonina, platifilozida, rubranozida A, rubranozida B, hirsutanonola, hirsutenona i acerozida VII, izolovano je i jedno novo jedinjenje. Struktura novog jedinjenja je identifikovana pomoću sledećih instrumentalnih metoda: ^{1}H NMR, ^{13}C NMR, UV i MS. Ovaj rad proističe iz istraživanja na projektu 172053 koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije.

A new diarylheptanoid from the bark of *Alnus glutinosa* subsp. *glutinosa*

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Alnus is a genus of the family *Betulaceae* with 3 subgenera and around 30 species (depending on the authors). One of them is *Alnus glutinosa* subsp. *glutinosa*, a tree up to 30 m tall, which can be found in most European countries and southwest Asia. Previous studies report compounds isolated from *Alnus* species possessing a broad spectrum of biological activities: antiviral, anticancer, antibacterial and other making these compounds interesting in the prevention and treatment of different diseases. In this work we investigated the composition of the bark extract of *Alnus glutinosa* subsp. *glutinosa.* Plant material was collected in June 2009 near the town Prijepolje in Serbia. After extraction and silica gel fractionation, pure diarylheptanoids were isolated by preparative HPLC. Alongside with the known diarylheptanoids, oregonin, platyphylloside, rubranoside A, rubranoside B, hirsutanonol, hirsutenone, and aceroside VII, a new compound was also isolated. The structure of the new diarylheptanoid was elucidated by ^{1}H NMR, ^{13}C NMR, UV and MS. This work is part of the project no. 172053, financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia.

ХА П19

Ispitivanje retencionog ponašanja N-(fenil-supstituisanih)-2-cijanoacetamida na RP-18 i CN HPTLC nepokretnim fazama

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Ispitivano je retenciono ponašanje deset N-(fenil-supstituisanih)-2-cijano-acetamida hromatografijom na tankom sloju. Korišćena su dva tipa HPTLC stacionarnih faza RP-18 i CN, svaka sa dve mobilne faze voda-acetonitril i voda-metanol u različitom odnosu rastvarača. Diskutovan je uticaj supstituenta, stacionarne i mobilne faze na retenciju. Na osnovu linearne zavisnosti između R_M vrednosti i zapreminskog udela organskog rastvarača, ϕ, u mobilnoj fazi izračunate su R_M^0 vrednosti ispitivanih supstanci. Razlike, ΔR_M^0, u korelaciji su sa Hanšovom konstantom supstituenta.

Zahvalnica: Rezultati su deo projekta OI172028 koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije.

Investigation of retention behavior of N-(substituted-phenyl)-2-cyano acetamides using RP-18 and CN HPTLC stationary phases

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The retention behavior of ten N-(substituted phenyl)-2-cyano-acetamides was studied by thin-layer chromatography on RP-18 and CN stationary HPTLC phases with two binary mobile phases, namely water-acetonitrile and water-methanol containing different proportions of organic solvent. The effect of substituent on retention, as well as stationary and mobile phases was discussed. Linear relationships were obtained between R_M values and volume fraction of organic solvents, ϕ, allowing calculation of R_M^0 for investigated compounds. Differences, ΔR_M^0, are in good correlation with Hansch substituent constant.

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XA П20

Korelacija sadržaja ukupnih fenolnih jedinjenja i antocijana sa relativnom antioksidativnom aktivnošću srpskih vina

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Vino i grožđe sadrže veliki broj polifenolnih jedinjenja koja imaju potencijalno povoljan efekat na zdravlje ljudi, pa su zbog toga u žiži interesovanja poslednjih par godina. Polifenolna jedinjenja imaju antimikrobno, antiinflamatorno, antimutageno, antitumorsko i antioksidativno dejstvo. Cilj ovog ispitivanja bio je da se odredi sadržaj ukupnih fenolnih jedinjenja, ukupnih antocijana kao i relativna antioksidativna aktivnost (RAA) u uzorcima vina. RAA vina određena je pomoću DPPH reagensa standardnom metodom sa malim izmenama. Sadržaj ukupnih fenolnih jedinjenja i antocijana upoređen je sa RAA. Ispitivano je 5 crvenih i 5 belih vrsta vina napravljenih od grožđa koje je gajeno u blizini Beograda (u eksperimentalnom dobru u Radmilovcu koje je u vlasništvu Poljoprivrednog fakulteta Univerziteta u Beogradu, Srbija). Sadržaj ukupnih polifenola u ispitivanim vinima je u rasponu od 0,240 do 2,840 g ekv. galne kiseline/l. Antocijani su nađeni samo u crvenim vinima, a najveći sadržaj ukupnih antocijana nađen je u vinu Merlot (0,310 g ekv. cijanidin-3-glukozida/l). Regresiona korelaciona analiza je korišćena kako bi se odredio odnos RAA i ukupnih polifenola i antocijana. RAA dobro koreliše sa ukupnim sadržajem polifenolnih jedinjenja (r = 0,929).

Correlation of total phenolic and anthocyanin contents with the radical scavenging activity of Serbian wines

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Wine and grapes contain a number of polyphenolics which contribute to the beneficial effect on human health and due to that have attracted much attention in the recent years. Polyphenolic compounds possess antimicrobial, anti-inflammatory, antimutagenic, antitumor and antioxidant activity. The aim of this study was the determination of the total phenolic (TPC) and total anthocyanin contents (TAC) in wine, as well as radical scavenging activity (RSA). RSA of different wines was determined with a DPPH reagent using a slightly modified standard methodology. The content of total phenolics and anthocyanins was compared with RSA. Five red and five white wines made from grape cultivars grown in the vicinity of Belgrade (experimental orchard of Radmilovac, property of the Faculty of Agriculture, University of Belgrade, Serbia) were investigated. TPC ranged from 0.240 to 2.840 g GAE/l of wine. Anthocyanins were found only in red wines and the highest TAC was found in Merlot wine (0.310 g cyn-3-glu/l of wine). A correlation analysis was used to explore the relationships between RSA, TPC and TAC. RSA is a relatively highly correlated with TPC ($r = 0.929$).

ХА П21

Micelarna tankoslojna hromatografija Šifovih baza

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Cilj rada je primena micelarne tankoslojne hromatografije u ispitivanju hromatografskog ponašanja biološki aktivnih Šifovih baza. Prvo je izvršena optimizacija hromatografskog sistema. Primenjena su dva sistema: kada je surfaktant u mobilnoj fazi i kada je stacionarna faza impregnirana surfaktantom. Određena je optimalna koncentracija SDS - a (*sodium dodecil sulphate*) i odnos SDS - a i organskog rastvarača u mobilnoj fazi. Optimizovan je postupak impregniranja stacionarne faze (silika-gela) različitim koncentracijama SDS a. Primenjene su uzlazna i horizontalna tehnika micelarne tankoslojne hromatografije. Ispitivan je uticaj dužine poluživota micela na hromatografsko ponašanje Šifovih baza, kao i uticaj dodatka elektrolita u mobilnu fazu. Diskutovano je hromatografsko ponašanje Šifovih baza i mogući mehanizmi odvajanja u oba hromatografska sistema.

Micellar thin layer chromatography of Schiff bases

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The aim of this study was to investigate the chromatographic behaviour of biologicaly active Schiff bases under condition of micellar thin layer chromatrography. The optimization of chromatographic conditions was done. We applied two chromatographic systems: surfactant present in the mobile phase and impregnation of stationary phase by molecules of surfactant. The optimal concentration of SDS (*sodium dodecyl sulphate*) and ratio of SDS and organic solvent in the mobile phase was determined. The procedure for impregnation of stationary phase (silica-gel) with different concentrations of SDS was optimized. Vertical and horizontal tehnique of micellar thin layer chromatrography were applied. Also, we investigated the influence of duration half-life of micelles, on chromatographic behavior of Schiff bases, as well as an addition of electrolyte in mobile phase. We discussed the chromatographic behavior of the Schiff bases and possible separation mechanisms in both chromatographic systems.

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ХА П22

Elektrohemijsko ponašanje biološki aktivnih kompleksa Pt(IV) sa edda tipom liganada

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Redukcioni potencijali savremenih antitumorskih lekova su značajni farmakološki parametri koji direktno utiču na mehanizam delovanja istih. Bitnu ulogu u medicinskoj neorganskoj hemiji zauzimaju platinski kompleksi koji podležu *in vivo* redukciji iz višeg u niže oksidaciono stanje, Pt(IV) → Pt(II), što ih čini pogodnim za različita elektrohemijska ispitivanja.

Pt(IV) kompleksi sa *n*-propil i *n*-butil estrima *(S,S)*-etilendiamin-*N,N'*-di-2-(3-cikloheksil)propanske kiseline pokazali su bolju citotoksičnu aktivnost (IC_{50} = 3,1; 8,3 µM) u odnosu na cisplatinu (IC_{50} = 67,0 µM). Redukcioni potencijali oba kompleksa imaju relativno visoke vrednosti (-776; -701 mV) ukazujući na dvoelektronski proces praćen gubitkom odgovarajućih aksijalnih liganada.

Određivanje redukcionih potencijala predstavlja jedan od načina odabira najboljeg kandidata za dalja istraživanja među različitim organometalnim jedinjenjima.

Ovo istraživanje je podržano od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, br. projekata 172035 i 172030.

Electrochemical behavior of biologically active Pt(IV) complexes with edda type ligands

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Reduction potentials of novel antitumor drugs are significant pharmacological parameters which directly influence on a drug's mechanism of action. Great role in medicinal inorganic chemistry have platinum complexes which undergo *in vivo* reduction from higher to lower oxidation states, Pt(IV)→Pt(II), that makes them suitable for various electrochemical studies.

Pt(IV) complexes with *n*-propyl and *n*-butyl esters of (*S,S)*-ethylenediamine *N,N'*-di-2-(3-cyclohexyl)propanoic acid showed higher cytotoxic activity (IC_{50} = 3.1; 8.3 µM) than cisplatin (IC_{50} = 67.0 µM). Reduction potentials of both complexes (-776; -701 mV) are relatively high indicating on two electronic process followed by the loss of corresponding axial ligands. The spotted differences in reduction potentials are shifted toward lower values as the length of alkyl chain increases.

Determining reduction potentials presents one way for selecting the best candidate for further investigations among different organometallics compounds.

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ХА П23

Korelacija radikalskog kapaciteta i fenolnog sastava dve vrste lignikolnih gljiva: *Coriolus versicolor* (L. ex Fr.) Quel i *Flammulina velutipes* (Curt. ex Fr.) Krast

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Lignikolne gljive (ph. Basidiomycota) su značajni prirodni izvori bioaktivnih metabolita od medicinskog značaja. Stoga su u ovom radu analizirane autohtone gljive sa teritorije Srbije (Fruška gora) i Bosne i Hercegovine (Banja Luka) u cilju ispitivanja njihovog radikalskog kapaciteta (Radical Scavenging Capacity, RSC). Analizirani su vodeni (H_2O) i etanolni ekstrakti (EtOH) gljiva: *Coriolus versicolor* i *Flammulina velutipes* DPPH$^{\bullet}$ i OH$^{\bullet}$ testom. Najveću aktivnost pokazali su H_2O ekstrakti vrste *C. versicolor* u oba testa (EC50=4,32μg/mL za DPPH test, EC50=0,36 μg/mL za OH test), kao i EtOH ekstrakti iste vrste (EC50=16,59 μg/mL za DPPH test, EC50=0.91 μg/mL za OH test), dok su ekstrakti *F. velutipes* bili znatno slabiji. Pri tome su EtOH ekstrakti ove jestive gljive bili duplo jači od H_2O u DPPH testu (EC50=45,40, EC50=86;67μg/mL) ili približnih vrednosti u OH testu (EC50=52;32, EC50=50;94 μg/mL). Ukupni sadržaj fenola u ekstraktima utvrđen Folin-Ciocalteu-ovim reagensom (48,05 mg ekv. galne kiseline/g s.m. akt vrste *C. vesicolor*) pokazao je visoku linearnu korelaciju sa RSC (r^2=0;99) za H_2O ekstrakte *C. versicolor,* dok je kod *F. velutipes* korelacija bila mnogo manja. HPLC detekcijom dobijeno je da obe vrste sadrže galnu i protokatehinsku kiselinu, dok je *F.velutipes* sadržala i kafenu kiselinu. Vrsta *C. versicolor* je ispoljila izuzetan RSC, pa bi se mogla upotrebiti kao značajan izvor prirodnih antioksidanasa u budućnosti, dok bi se *F.velutipes* mogla preporučiti u svakodnevnoj ishrani.

Correlation between radical scavenging capacity and phenolic content of two lignicolous fungi: *Coriolus versicolor* (L. ex Fr.) Quel and *Flammulina velutipes* (Curt. ex Fr.) Krast

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Lignicolous fungi (ph. Basidiomycota) are important natural sources of bioactive metabolites with medicinal effects. Hence, autochthonous fungi from Serbia (Fruška Gora Mountain) and Bosnia and Herzegovina (Banja Luka) were analyzed for their radical scavenging capacity (RSC). Aqueous and ethanolic extracts of two fungal species: *Coriolus versicolor* and *Flammulina velutipes* were analyzed using DPPH$^{\bullet}$ and OH$^{\bullet}$ assay. The highest activity was shown by aqueous extracts of *C. versicolor* in both tests (EC50=4.32 μg/ml for DPPH$^{\bullet}$ assay, EC50=0.36 μg/ml for OH$^{\bullet}$ assay), as well as ethanolic extracts of the same species (EC50=16.59, EC50=0.91 μg/mL respectively), while extracts of F. velutipes were much weaker. Ethanolic extracts of this edible mushrooms were twice as stronger than aqueous in DPPH$^{\bullet}$ assay (EC50=45.40, EC50=86.67μg/mL respectively), or approximate value in the OH$^{\bullet}$ assay (EC50=52.32, EC50=50.94 μg/mL respectively). Total phenol content in the examined extracts determined with the Folin-Ciocalteu reagent (48.05 mg galic acid equivalents/ g d.e. act. species *C. versicolor*) showed high linear correlation with RSC (r^2=0.99) for H_2O extracts of *C. versicolor,* while the same for *F. velutipes* was lower. HPLC detection showed that both analyzed fungi contain gallic acid and protochatechuic acid, while *F. velutipes* contains caffeic acid, also. The species *C. versicolor* exhibited excellent RSC and could be used as important source of natural antioxidants in the future, while *F. velutipes* could be recommended in common nutrition.

ХА П24

Hemijska karakterizacija i antiinflamatorna aktivnost metanolnog ekstrakta i etarskog ulja šišarki vrste *Juniperus macrocarpa* Sibth. et Sm.

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Cilj prikazanih ispitivanja bila je hemijska karakterizacija i određivanje antiinflamatorne aktivnosti metanolnog ekstrakta i etarskog ulja šišarki vrste *Juniperus macrocarpa*. LC-MS/MS metodom određen je sadržaj 44 odabrana fenolna jedinjenja, pri čemu su najzastupljeniji bili flavonoidi amentoflavon i apigenin, kao i protokatehinska kiselina. GC-MS analiza etarskog ulja pokazala je jednostavan terpenski sastav, sa monoterpenskim ugljovodonicima kao najzastupljenijima i α-pinenom kao dominantnim sastojkom (47,8 %). Antiinflamatorna aktivnost određena je *ex vivo* metodom koja je zasnovana na određivanju sposobnosti inhibicije produkcije medijatora inflamacije koji nastaju u metabolizmu arahidonske kiseline delovanjem enzima COX-1 i 12-LOX. Etarsko ulje šišarki *J. macrocarpa* pokazalo je veću sposobnost inhibicije produkcije 12-HHT, TXB_2, PGE_2 i 12-HETE metabolita (IC_{50} = 216, 229, 530 i 253 nL/mL, redom), u odnosu na ekstrakt (12-HHT, 2,25 mg/mL i 12-HETE, 5,3 mg/mL), koji je ispoljio i snažnu proinflamatornu aktivnost prema produkciji PGE_2. Dobijeni rezultati ukazuju na moguću primenu šišarki *J. macrocarpa* kao izvora fenolnih jedinjenja i antiinflamatornih agenasa.

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Chemical characterization and anti-inflammatory activity of the methanol extract and essential oil of the cones of *Juniperus macrocarpa* Sibth. et Sm.

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The aim of the present study was a detailed chemical characterization and a determination of the anti-inflammatory activity of the methanol extract and essential oil of the cones of *Juniperus macrocarpa*. The content of 44 phenolics in the extract was determined using LC-MS/MS, and the dominant compounds were found to be the flavonoids amentoflavone and apigenin, as well as protocatechuic acid. GC-MS analysis of the essential oil revealed a simple terpene composition, with monoterpene hydrocarbons as predominant, and α-pinen as the most abundant compound (47.8 %). Anti-inflammatory activity was determined as the potential to inhibit the production of inflammation mediators, which are formed in the arachidonic acid metabolism in COX-1 and 12-LOX pathways. The essential oil showed markedly higher inhibitor potential of 12-HHT, TXB_2, PGE_2 and 12-HETE (IC_{50} = 216, 229, 530, 253 nL/mL, respectively), compared to the extract (12-HHT, 2.25 and 12-HETE, 5.3 mg/mL), which also showed strong proinflammatory activity towards the production of PGE_2. The obtained results make the cones of *J. macrocarpa* a new source of phenolics and anti-inflammatory agents.

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ХА П25

Uticaj protičnih rastvarača na elektronske absorpcione spektre izomernih piridin karboksilnih kiselina *N*-oksida

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UV apsorpcioni spektri pikolinske kiseline *N*-oksida, nikotinske kiseline *N*-oksida i izonikotinske kiseline *N*-oksida snimljeni su u 10 protičnih rastvarača u opsegu od 200-400 nm. Položaji maksimuma apsorpcije (λ_{max}) bili su najniži za pikolinsku kiseline *N*-oksid, a najviši za izonikotinsku kiselinu *N*-oksid. Da bi se analizirao uticaj ratvarača, apsorpcione frekvence su korelisane Kamlet-Taftovom jednačinom, kojom se uticaj polarnosti/polarizabilnosti, proton-donorskog i proton-akceptorskog dejstva rastvarača može kvantitativno izraziti. Navedena jednačina je upotrebljena u obliku $\nu_{max} = \nu_0 + s\pi^* + a\alpha + b\beta$, gde je ν_{max} apsorpciona frekvenca ($1/\lambda_{max}$), π^* je mera polarnosti i polarizabilnosti rastvarača, α predstavlja sposobnost rastvarača da bude donor protona u vodoničnoj vezi, a β predstavlja sposobnost rastvarača da bude akceptor protona u vodoničnoj vezi. Korelacija spektroskopskih podataka je izvedena pomoću višestruke linearne regresione analize i diskutovani su uticaji protičnih rastvarača na položaj apsorpcionih makismuma ispitivanih jedinjenja.

The effects of protic solvents on the electronic absorption spectra of isomeric pyridine carboxylic acid *N*-oxides

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The ultraviolet absorption spectra of the carboxyl group of three isomeric pyridine carboxylic acids *N*-oxides (picolinic acid *N*-oxide, nicotinic acid *N*-oxide and isonicotinic acid *N*-oxide) were measured in 10 protic solvents in the wavelength range from 200 to 400 nm. The position of the absorption maxima (λ_{max}) of the investigated acids showed that the ultraviolet absorption maximum wavelengths of picolinic acid *N*-oxide are at the shortest, and those of isonicotinic acid *N*-oxide acid are the longest wavelengths. In order to analyze the solvent effects, the ultraviolet absorption frequencies of the electronic transitions of the carboxylic group of the acids were correlated using a total solvatochromic equation of the form $\nu_{max} = \nu_0 + s\pi^* + a\alpha + b\beta$, where ν_{max} is the absorption frequency ($1/\lambda_{max}$), π^* is a measure of the solvent polarity/polarizability, α represents the scale of solvent hydrogen bond donor acidities and β represents the scale of solvent hydrogen bond acceptor basicities. The correlation of the spectroscopic data was carried out by means of multiple linear regression analysis. The solvent effects on the position of ultraviolet absorption maxima of these acids were discussed.

ХА П26

Antioksidativna sposobnost ekstrakata *Geranium macrorrhizum* L.

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Određivan je sadržaj ukupnih fenola, ukupnih flavonoida kao i antioksidativna aktivnost DPPH metodom ekstrakata zdravca (*Geranium macrorrhizum* L.). Kao rastvarači za ekstrakciju korišćeni su metanol, etanol, aceton i etil-acetat. Metanolni ekstrakt lišća i metanolni ekstrakt rizoma pokazao je najveći sadržaj fenolnih jedinjenja i flavonoida kao i najveću antioksidativnu sposobnost. Antioksidativna sposobnost ekstrakata opada u nizu: metanol > etanol > aceton > etil-acetat. Visoka vrednost korelacionog koeficijenta je nađena za sadržaj ukupnih fenola i antioksidativnu sposobnost. Rezultati pokazuju da se zdravac može koristiti kao dobar izvor prirodnih antioksidanasa.

Antioxidant power of *Geranium macrorrhizum* L. extracts

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Total phenolic content, total flavonoid content and DPPH antioxidant assay of *Geranium macrorrhizum* L. extracts were determined. Methanol, ethanol, acetone and ethyl acetate were used as extraction mediums. Methanol extracts of Geranium macrorrhizum leaves and rhizome showed highest phenol and flavonoid content and antioxidant activities. Antioxidant potency of extracts decreases in the following order of extraction mediums: methanol > ethanol > acetone > ethyl acetate. A high correlation was found between total phenol content and DPPH antioxidant assay. The results suggest that Geranium macrorrhizum may be used as potent natural source of antioxidants.

ХА П27

Promena sadržaja lekovitih sastojaka i antioksidativne aktivnosti aromatičnog lekovitog bilja tokom obrade u fabrici čaja

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Ovim istraživanjem određene su promene sadržaja lekovitih sastojaka (ukupni fenoli i etarsko ulje) i promene antioksidativnog delovanja odabranog lekovitog bilja tokom njihove prerade u fabrici čajeva. U ispitivanom aromatičnom lekovitom bilju detektovano je smanjenje sadržaja etarskog ulja do koga je došlo tokom obrade sirovog neusitnjenog u fino usitnjeni biljni materijal. Preradom kamilice sadržaj etarskog ulja, koji je u neobrađenom materijalu iznosio 0,46 %, se smanjuje do iznosa od 0,30 %. Utvrđeno je i da se sadržaj etarskog ulja žalfije tokom obrade smanjuje za 6 %. Sadržaj ukupnih fenola u neobrađenom biljnom materijalu kamilice iznosi 14,8 mg GAE/g. Sadržaj ukupnih fenola u herbi žalfije iznosi 44,0 mg GAE/g. Ukupan sadržaj fenola tokom obrade kamilice se smanjio za 12,9 %, dok je ovaj gubitak kod žalfije mnogo veći i iznosi 32,4 %. Antioksidativna aktivnost ispitivanih lekovitih biljaka tokom prerade u fino usitnjeni materijal takođe opada, što je u skladu sa gubitkom sadržaja ukupnih fenola i etarskog ulja.

Changes in the content of health benefit compounds and antioxidant activity of two herbal drugs during their processing in the tea factory

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The present study was undertaken to determine the changes in the content of some health benefit compounds (total phenols and essential oils) and changes in the antioxidant activity of selected medicinal herbs during their processing in a tea factory. A decrease in the content of essential oils in the investigated aromatic herbal drugs was detected during their processing in the tea factory. During the processing of *Matricaria chamomilla* the content of the essential oil changed from 0.46 %, determined in the raw material, to 0.30 %, determined in finely cut plant material of *M. chamomilla*. For the finely cut *Salvia officinalis* material the content of the essential oil decreased for 6 % in comparison to the content of the oil in the raw material. The content of total phenols in the raw plant material was measure to be 14.8 mg GAE/g for *M. chamomilla* and 44.0 mg GAE/g for *S. officinalis*. During the industrial processing of *M. chamomilla* (the production of *M. chamomilla* finely cut herbal drug) loss of total phenols was determined to be 12.9 %, whereas in the case of *S. officinalis* it was much higher, 32.4 %. The antioxidant activity of the two investigated herbal drugs also decreased during the processing of the finely cut materials in the tea factory, and this is in agreement with the decrease of the total phenols and the amount of the essential oils.

XA П28

Korelacija između različitih *in vitro* antioksidativnih testova i sadržaja pojedinačnih fenola, ukupnih fenola i flavonoida voćnih infuz čajeva

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U radu je ispitana korelacija između antioksidativne aktivnosti, koja je izražena različitim metodama (DPPH, ABTS, FRAP, RP), i sadržaja pojedinačnih fenolnih jedinjenja, kao i ukupnih fenola i flavonoida. Odnos je izražen pomoću Pirsonovog koeficijenta korelacije. Dobra korelacija postoji između tri primenjene metode (DPPH, FRAP i RP) i kreće se u intervalu od 0,538 do 0,950 za prag značajnosti $p<0,05$. Takođe, dobra, pozitivna korelacija (0,421-0,841) postoji između sadržaja galne kiseline (GA), rutina (RT), (+)-katehina (CC), (-)-epikatehina (ECC) i procijanidina B1 i antioksidativne aktivnosti izražene DPPH, FRAP i RP metodom. U slučaju sadržaja kafene kiseline (CA), procijanidina B2 i (-)-epigalokatehina (EPGC) i antioksidativne aktivnosti postoji slaba korelacija (0,077-0,333). Pozitivna linerana zavisnost postoji i kod fenola (0,556-0,635). Bolja korelacija je u slučaju flavonoida (0,684-0,809), što ukazuje da su flavonoidi jedna od glavnih komponenti odgovornih za antioksidativnu aktivnost voćnih infuz-čajeva.

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Correlations among different *in vitro* antioxidant assays and individual and total phenolic and flavonoid contents of fruit tea infusions

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The Pearson's correlation coefficients among antioxidant assays (DPPH, ABTS, FRAP, RP) and individual and total phenolic and flavonoid contents were calculated. Significant positive correlations among four assays for fruit teas were observed (ranging from 0.538 to 0.950, $p<0.05$), especially among DPPH radical scavenging activity, ferric reducing antioxidant power (FRAP) and reducing power (RP). These findings suggest that the compounds which could scavenge DPPH radicals in fruit teas are capable of reducing ferric ions. Moreover, gallic acid (GA), rutin (RT), (+)-catechin (CC), (-)-epicatechin (ECC) and procyanidin B1 contents exhibited strong positive correlations with three antioxidant assays (DPPP, FRAP, RP) ranging from 0.421 to 0.841. Results obtained for caffeic acid (CA), procyanidin B2 and (-)-epigallocatechin (EPGC) showed low positive correlation (0.077-0.333). Correlation between antioxidant capacities and total phenolic (0.556-0.635), and total flovonoid contents (0.684-0.809) is also positive, and in the case of total flavonoid content indicated that the flavonoid could be one of the main components responsible for antioxidant activities of these beverages.

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ХА П29

Ekstrakti Coffeeberry, značajne komponente i antioksidantna aktivnost

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Tečni ekstrakti Coffeeberry, ploda biljke *Coffea arabica* su dobijeni primenom 99,85 % metanola kao ekstrakcionog sredstva. Ekstrakcija je izvršena primenom ultrazvuka i postupkom maceracije. U ovako dobijenim ekstraktima određeni su sadržaji ukupnih fenola, ukupnih flavonoida i sadržaj kofeina, kao i antioksidativno delovanje i redukujući kapacitet. U metanolnom ekstraktu koji je dobijen postupkom maceracije određen je nešto veći sadržaj ukupnih fenola i flavonoida, što je u korelaciji sa nešto boljim antioksidativnim delovanjem ovog ekstrakta. U ovom ekstraktu sadržaj ukupnih fenola, određen primenom Folin-Ciocalteu testa, iznosio je 6,635 mg GAE/g, sadržaj ukupnih flavonoida određen kolorimetrijskom metodom, 4,913 mg EK/g, a sadržaj kofeina 2,89 %. Antioksidantna aktivnost, ispitana primenom DPPH testa, okarakterisana je IC_{50} vrednošću od 1,44 mg/ml. Redukujući kapacitet je ispitan metodom po Oyaiz-u, i upoređen je sa redukujućim kapacitetom vitamina C.

Coffeeberry extracts, main compounds and the antioxidant activity

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Liquid extracts of Coffeeberry, fruit of *Coffea arabica*, were obtained using methanol (99.85 %) as extraction solvent. Ultrasound and maceration were applied to perform the extraction. Obtained extracts were analyzed to determine antioxidative activity, reducing capacity and total phenols, total flavonoids and caffeine contents. Methanolic extract obtained by maceration showed some higher values in content of total phenols and flavonoids. Higher content of these compounds was in correlation with higher antioxidant activity. Folin-Ciocalteu method was used to determine total phenolics content, and colorimetric method was used to evaluate total flavonoids content. For this extract obtained values were 6.635 mg GAE/g, and 4.913 mg EK/g, respectively. The measured content of caffeine was 2.89 %. Antioxidant activity, analyzed using DPPH assay, showed IC_{50} value of 1.44 mg/ml. Reducing capacity of sample was determined according to the method of Oyaiz and was compared with the reducing capacity of vitamin C.

ХА П30

Uloga termičke analize u kontroli kvaliteta tablete Enalaprila

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Enalapril tablete se koriste za lečenje hipertenzije i kongestivne srčane insuficijencije. Njihova stabilnost zavisi od vrste pomoćnih supstanci, metode proizvodnje i skladištenja (temperatura i vlaga). Enalapril tablete za ispitivanje su proizvedene u dozama od 10 mg i 20 mg metodom mokre granulacije odnosno direktne kompresije. Metodom visokopritisne tečne hromatografije (HPLC) nađeno je da stabilnost tableta proizvedenih mokrom granulacijom ne ispunjava zahteve Farmakopeje SAD 30 (USP#30).

Enalapril u vodenom rastvoru se razlaže na enalaprilat i diketopiperazin. Kako se sadržaj vode u tabletama ne može odrediti pomoću HPLC, a i za kontrolu kvaliteta farmaceutskih proizvoda redovno se koriste metode termičke analize, tablete su ispitane i simultanom termogravimetrijskom/diferencijalnom skenirajućom kalorimetrijskom metodom (TG/DSC). Termički podaci pokazuju da su tablete proizvedene mokrom granulacijom termički manje stabilne i njihov sastav se razlikuje. Sadržaj vode u ovim tabletama je veći i podržava pretpostavku da vlaga ubrzava raspadanje. Termičke promene počinju isparavanjem vode. Zatim sledi izdvajanje maleinske kiseline i eliminacija etil grupe na oko 130 °C. DSC krive tableta proizvedenih direktnom kompresijom su veoma slične, što ukazuje na njihov skoro identičan sastav. Nasuprot tome, tablete koje se proizvode mokrom granulacijom pokazuju različite DSC otiske. Ovi nalazi su u skladu sa podacima dobijenim metodom HPLC.

The role of thermal analysis in quality control of Enalapril tablets

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Enalapril tablets are used for treatment of hypertension and congestive heart failure. Their stability depends on the type of excipients, the method of production and storage conditions (temperature and moisture). For study, enalapril tablets of 10 mg and 20 mg dosage were produced by wet granulation and direct compression. It was found by high performance liquid chromatography (HPLC) that the stability of the tablets produced by wet granulation does not meet the United States Pharmacopeia 30 (USP#30) requirements.

Enalapril in aqueous solution degrades to enalaprilat and diketopiperazine. As water content in tablets cannot be determined by HPLC, and thermal methods of analysis are regularly used for quality control of pharmaceuticals, tablets were tested by means of simultaneous thermogravimetry/differential scanning calorimetry (TG/DSC). Thermal data show that tablets produced by wet granulation are thermally less stable and their composition is more different. The water content of these tablets is higher therefore supports the proposition that moisture accelerates the decomposition. The thermal changes begin with water evaporation and are followed by maleic acid evolution and ethyl group elimination at around 130 °C. DSC curves of tablets produced by direct compression are very similar, referring to their almost identical composition. In contrast, tablets produced by wet granulation show very different DSC patterns. These findings are in accordance with the data obtained by HPLC.

ХА П31

Садржај As, Cd i Pb у основним намирницама потрошачке корпе у Србији

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У раду су представљени резултати испитивања садржаја три веома токсична тешка елемента, арсена (As), кадмијума (Cd) и олова (Pb), у намирницама које су у великом уделу заступљене у потрошачкој копри Србије, као што су хлеб, кромпир, јабуке, млеко, јестиво уље и сл. Након киселинске дигестије узорака у микроталасном систему, извршена је анализа добијених раствора помоћу атомског апсорпционог спектрометра са графитном киветом. У свим намирницама садржај испитиваних елемената је испод максимално дозвољених вредности прописаних важећом националном и европском регулативом. На основу средњих вредности концентрација As, Cd и Pb извршена је процена њиховог дневног уноса коришћењем података о просечној потрошачкој корпи Србије и дневним количинама изабраних намирница. Процењени уноси су далеко испод постојећих привремених толерантних вредности уноса (PTDI-provisional tolerable daily intakes). Највећем уносу испитиваних елемената доприноси хлеб услед велике дневне количине ове намирнице заступљене у домаћој исхрани, при чему је у случају Pb ово последица и значајно већег присуства овог елемента у хлебу у односу на остале анализиране намирнице.

The content of As, Cd, and Pb in main food items of the Serbian market basket

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The study presents the results of the analysis of three highly toxic heavy elements (arsenic (As), cadmium (Cd) and lead (Pb)) in selected foodstuffs that contibute to the average Serbian market basket in large shares, like bread, potatoes, apples, milk, edible oil, etc. The samples were analyzed after the microwave acid digestion by atomic absorption spectrometer with graphite furnace. All samples were in compliance with the relevant national and European regulations. The average element concentrations obtained for particular food item were combined with the the Serbian market basket data on the daily consumption rates to assess dietary intake of these three elements. The calculated intakes were well below the Provisional Tolerable Daily Intakes, so, there was no concern about intake of the heavy elements through different foodstuffs by adult consumers. The higest contribution to the total intakes of all three elements gave the bread due to its highest consumption rate. Moreover, in the case of Pb the significantly higer intake through bread was also a consequence of the markedly higher concentration found.

ХА П32

Sastav voska biljne vrste *Heracleum sphondylium* L. (mečja šapa): jesu li *n*-oktil estri masnih kiselina zaista markeri otpadnih voda u živom svetu?

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Nedavno su Chaler i saradnici[1] *n*-oktil estre viših masnih kiselina označili kao markere gradskih otpadnih voda u ribama i mnogočekinjastim crvima. Fitohemijskim ispitivanjem biljne vrsti *Heracleum sphondylium* L. (Apiaceae) pronađeno je sedam *n*-oktil estara nerazgranatih viših masnih kiselina (C-20 to C-26). Ako se ova jedinjenja javljaju u prirodi, da li onda mogu da budu markeri otpadnih voda? Struktura ovih biljnih metabolita nedvosmisleno je utvrđena GC ko-injektiranjem sintetisanih estara sa ispirkom cvetova. Proučavanjem spektara ovih jedinjenja koji su dali Chaler i sar.[1] utvrđeno je da postoji značajno neslaganje sa našim spektralnim podacima. Verujemo da su markeri koji su pronađeni u biljnom svetu u stvari 2-etilheksil estri i da su pogrešno identifikovani kao *n*-oktil estri.

Ovaj rad je finansiralo Ministarstvo prosvete i nauke (Projekat 172061).

Wax composition of Common Hogweed (*Heracleum sphondylium* L.): Are *n*-octyl esters of alkanoic acids urban wastewater markers in biota?

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n-Octyl esters of higher fatty acids have been recently reported by Chaler *et al.* as markers of urban wastewater in polychaeta and fish[1]. During a phytochemical investigation of wild-growing *Heracleum sphondylium* L. (Apiaceae), seven *n*-octyl straight-chain alkanoates (C-20 to C-26) were detected. If these esters occur naturally can they be recognized as wastewater markers? The identity of the plant metabolites was unambiguously established by GC co-injection of samples of synthesized esters with the inflorescence washings. A closer look at the spectra of these compounds given in Chaler et al.[1] revealed significant discrepancies with our spectral data. We believe that the markers found in biota are in fact 2-ethylhexyl esters, mistakenly identified as *n*-octyl esters.

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1. R. Chaler, L. Cantón, M. Vaquero, J.O. Grimalt, *J. Chromatogr. A*, **1046** (2004) 203-210

ХА П33

3-Metil-2-alkanoni dugog lanaca iz etarskog ulja korena biljne vrste *Inula helenium* L. (Asteraceae)

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Inula helenium L. (Compositae) je višegodišnja biljna vrsta koja se često koristi u srpskoj narodnoj medicini. U ovom radu predstavljamo identifikaciju i sintezu devet novih sastojaka frakcije etarskog ulja korena *I. helenium* sa veoma niskom MIC vrednošću (0.8 μg/mL) protiv bakterije *Staphylococcus aureus*. Identitet ovih jedinjenja, tj. da su to 3-metil-2-alkanoni, je pretpostavljen na osnovu analize masenih spektara ovih jedinjenja (npr. osnovni jon na *m/z* 72). Razlika od 14 amu (jedna CH_2 grupa) između molekulskih jona dva uzastopna jedinjenja u gasnom hromatogramu, razdvojenih za *ca*. 100 RI jedinica, ukazivala je na postojanje C_{11}–C_{19} homologe serije ovih jedinjenja. Ovi 3-metil-2-alkanoni su sintetisani, a koinjekcija dobijenih uzoraka sa pomenutom frakcijom ulja nesumnjivo je potvrdila njihovo prisustvo u ulju. Testirana je mikrobiološka aktivnost sintetisanih 3-metil-2-alkanona. Ovo je prvi put da su 3-metil-2-alkanoni dugog lanca nađeni kao biljni sekundarni metaboliti.

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Long chain 3-methyl-2-alkanones from the root essential oil of *Inula helenium* L. (Asteraceae)

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Inula helenium L. (Compositae) is a perennial herb frequently used in Serbian folk medicine. Herein, we report the identification and synthesis of nine new constituents from a fraction of *I. helenium* root essential oil with a low MIC value (0.8 μg/mL) against *Staphylococcus aureus*. Their possible identity as 3-methyl-2-alkanones was inferred from their mass spectral fragmentation pattern (*e.g*. base peak at *m/z* 72). The difference of 14 amu (one CH_2 group) between the molecular ions of two consecutive compounds in the gas chromatogram, separated by *ca*. 100 RI units, pointed to the existence of a C_{11}–C_{19} homologous series. Such 3-methyl-2-alkanones were synthesized and gas co-chromatography of the obtained compounds with the fraction in question unequivocally corroborated the original assumptions. The synthetic 3-methyl-2-alkanones were also screened for *in vitro* antimicrobial activity. This is the very first report of long chain 3-methyl-2-alkanones as plant secondary metabolites.

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Хемијска ситеза

XC O4

,,Up-conversion" luminescencija u Tm^{3+}/Yb^{3+}-$GdVO_4$

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Glavni cilj ovog rada je proučavanje,,up-conversion" luminescencije u seriji Tm^{3+}/Yb^{3+}-ko-dopiranih uzoraka $GdVO_4$ koji su sintetisani metodom u čvrstom stanju. Koncentracije Yb^{3+} jona su iznosile 3, 6 i 9 mol %, dok je koncentracija Tm^{3+} jona bila konstantna i iznosila je 3 mol %. Difraktogrami koji su dobijeni nakon XRD analize potvrđuju formiranje čiste faze $GdVO_4$ kod svih sintetisanih uzoraka. Kvantitativna EDX analiza dokazala je uspešno ugrađivanje Tm^{3+} i Yb^{3+} jona u matricu $GdVO_4$. Sa slika koje su dobijene na skenirajućem elektronskom mikroskopu može se videti da su uzorci sastavljeni od deformisanih (nepravilnih) sfernih čestica prečnika od 1.4 μm do 8.4 μm. ,,Up-conversion" emisioni spektar sniman je na sobnoj temperaturi sa talasnom dužinom ekscitacije na 980 nm. Utvrđeno je da svi naši uzorci pokazuju ,,up-conversion" emisiju u tri različita dela spektra: jake emisije su uočene na 475 nm koja odgovara ${}^1G_4 \rightarrow {}^3H_6$ prelazu i na 800 nm koja odgovara ${}^3H_4 \rightarrow {}^3H_6$ prelazu, dok je emisija u crvenom delu spektra oko 650 nm veoma slaba i odgovara ${}^1G_4 \rightarrow {}^3F_4$ prelazu. Pokazano je da je konverzija bliskog-infracrvenog zračenja u emisiju plave svetlosti veoma efikasna u svim sintetisanim sistemima. Utvrđeno je da krive vremena života emisije pokazuju eksponencijalno ponašanje za sve uzorke.

Up-conversion luminescence in Tm^{3+}/Yb^{3+}-$GdVO_4$

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The main aim of this work was to study up-conversion luminescence in a series of Tm^{3+}/Yb^{3+}-co-doped $GdVO_4$ samples synthesized by the solid state method. The concentration of the Yb^{3+} ions were 3, 6 and 9 mol %, while the concentration of Tm^{3+} ions was fixed (3 mol %). XRD patterns for all synthesized samples confirmed a successfull formation of a pure $GdVO_4$ phase. Quantitative EDX analysis confirmed a successful doping of Tm^{3+} and Yb^{3+} ions into the $GdVO_4$ matrix. SEM images show that the samples are composed from deformed (iregular) spherical particles with an average diametar size in the range of 1.4 μm to 8.4 μm. Up-converted emission spectra were recorded at room temperature under excitation of 980 nm. It was found that all our samples exhibit up-conversion emission in three different spectral regions: the strong emissions are observed at 475 nm and 800 nm corresponding to ${}^1G_4 \rightarrow {}^3H_6$ and ${}^3H_4 \rightarrow {}^3H_6$ transitions, respectively, while emission in the red region around 650 nm is very weak and is due to the ${}^1G_4 \rightarrow {}^3F_4$ transition. It was concluded that conversion of near-infrared radiation into blue emission proved to be very effective in all synthesized systems. It was found that emission decay curves for all samples exibit a single exponential behavior.

XC O5

Ispitivanje reakcija monofunkcionalnog $[M(dien)Cl]^{n+}$ kompleksa (M = Au(III), Pt(II) i Pd(II)) sa dipeptidima koji sadrže L-histidin

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Primenom ^{1}H NMR spektroskopije, ispitivane su reakcije monofunkcionalnog $[M(dien)Cl]^{n+}$ kompleksa (M = Au(III), Pt(II) i Pd(II)), gde je dien tridentatno koordinovani dietilentriamin, sa dipeptidima L-histidil-glicinom (L-His-Gly) i glicil-L-histidinom (Gly-L-His). Sve reakcije su izvođene u vodenom rastvoru u pD oblasti $3.50 \leq pD \leq 5.50$ i na sobnoj temperaturi. Nađeno je da se u ispitivanim reakcijama, u zavisnosti od položaja L-histidina u bočnom nizu dipeptida i pD vrednosti reakcione smeše, formiraju različiti reakcioni proizvodi. Dobijeni rezultati su poređeni sa odgovarajućim literaturnim podacima za reakcije ovih kompleksa sa strukturno sličnim peptidima.[1-3]

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A study of the reactions of the monofunctional $[M(dien)Cl]^{n+}$ complex (M = Au(III), Pt(II) and Pd(II)) with L-histidine-containing dipeptides

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The course of the reactions between the monofunctional $[M(dien)Cl]^{n+}$ complex (M = Au(III), Pt(II) and Pd(II)), in which dien is tridentate coordinated diethylenetriamine, with L-histidine-containing dipeptides, namely L-histidyl-glycine (L-His-Gly) and glycyl-L-histidine (Gly-L-His), was studied by application of ^{1}H NMR spectroscopy. All reactions were performed in aqueous solution at $3.50 \leq pD \leq 5.50$ and at ambient temperature. Depending on the L-histidine position in the dipeptide side chain and solution pD, different reaction products were observed. The data obtained from this study were compared with those for the reactions of these complexes with structural similar peptides.[1-3]

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1. M. Wienken, B. Lippert, E. Zangrando, L. Randaccio, *Inorg. Chem.*, **31** (1992) 1983.
2. U. Rychlewska, B. Warżajtis, B. Đ. Glišić, M. D. Živković, S. Rajković, M. I. Djuran, *Dalton Trans.*, **39** (2010) 8906.
3. T. G. Appleton, F. J. Pesch, M. Wienken, S. Menzer, B. Lippert, *Inorg. Chem.*, **31** (1992) 4410.

XC O8

Ispitivanje mehanizma fenilselenoeterifikacije linalola

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Mehanizam fenilselenoeterifikacije linalola ispitivan je kinetičkim studijama ciklizacije UV/VIS spektrofotometrijski koristeći neke baze (piridin, trietilamin, hinolin, piperidin) i neke kiseline ($SnCl_2$, $CoCl_2$) kao katalizatore. Pokazano je da je u prisustvu baza intramolekulska ciklizacija olakšana usled vodinične veze baze i OH grupe alkenola. DFT studije pokazuju da je favorizovano nastajanje THF prstena.

Mechanistic investigation of phenyselenoetherification of linalol

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The mechanism of phenylselenoetherification of linalol using some bases (pyridine, triethylamine, quinoline, piperidine) and some acids ($SnCl_2$, $CoCl_2$) as catalysts was examined through studies of kinetics of the cyclization, by UV-VIS spectrophotometry. It was demonstrated that the intramolecular cyclization is facilitated in the presence of bases caused by the hydrogen bond between base and alkenol OH-group. DFT study (B3LYP/6-311+G**) show, that the formation of THF ring is favored.

ХС П01

Sintetički ekvivalent enolata hidroksiacetona

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Alilovanjem strukturno različitih aldehida i ketona pomoću 4-(bromometil)-1,3-dioksol-2-ona u prisustvu indijuma diastereoselektivno nastaju ciklični enol-karbonati, koji su zapravo zaštićeni oblik *anti-α,β*-dihidroksiketona. Ovi proizvodi se mogu deprotektovati u slobodne dihidroksiketone pomoću vodenog rastvora živa(II)-nitrata, pri čemu se zadržava inicijalna *anti*-konfiguracija ili se mogu pod blagim reakcionim uslovima prevesti u ciklične karbonate, još jedan oblik zaštićenih *anti-α,β*-dihidroksiketona. Na taj način naš pristup predstavlja dobru metodu za dobijanje aldola hidroksiacetona.

Synthetic equivalent of a hydroxyacetone enolate

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***Facultu of Pharmacy, University of Belgrade;*
****Faculty of Science, University of Novi Sad*

Indium promoted allylation of structurally different aldehides and ketones with 4-(bromometil)-1,3-dioksol-2-one diastereoselectively affords enol carbonates, which are, in fact, protected form of *anti-α,β*-dihydroxyketones. These products can be deprotected to free dihidroxyketones with aqueous mercuric nitrate with retention of the initial *anti* configuration or transformed under mild conditions into the corresponding cyclic carbonates, another protected form of *anti-α,β*-dihydroxyketones. This makes our reaction as a useful approach to obtain hydroxyacetone aldols.

ХС П02

Conformational preferences of 2-[(2-hydroxyethyl)sulfanyl]-4-oxo-4-(2,4-diisopropylphenyl)-butanoic acid phenylamide. The NMR/MD study

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Title molecule, recently prepared in our laboratory comprises the pharmacophoric pattern of the BH3 domain inhibitors. Such compounds were extensively studied as the antiproliferative agents. In this communication we present its conformational preferences in the solvents of different polarity and HBD/HBA abilities. NOESY spectra of compound were recorded in DMSO-d_6 and $CDCl_3$. NOESY cross-peaks and coupling constants were processed by NAMFIS analysis and results compared with the conformational assembly and the free-energy surfaces of compound obtained by molecular dynamics simulations in the corresponding explicit solvents. Adaptive biasing force was used to map free-energy surfaces. Janocchio program was used for the NAMFIS analysis, molecular dynamics simulations (30 ns, each) were performed in NAMD 2.9 using CHARMm22 force field on the multi-node Linux cluster. Conformations of the compound were generated by OMEGA program.

Acknowledgement: This work was supported by Ministry of Education and Science of Republic of Serbia, under Grant 172035. The computational work reported makes use of results produced by the High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE), a project co-funded by the European Commission (under Contract No 261499) through the Seventh Framework Programme HP-SEE (http://www.hp-see.eu/).

Proučavanje preferentnih konformacija fenilamida 2-[(2-hidroksietil)sulfanil]-4-okso-4-(2,4-diizopropilfenil)butanske kiseline simulacijama molekulske dinamike i NMR spektroskopijom

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Proučavani molekul ima elemente farmakofore inhibitora BH3 domena. Takvi molekuli su antiproliferativni agensi. U ovoj komunikaciji su predstavljene preferentne konformacije jedinjenja u rastvaračima različite polarnosti i sposobnosti stvaranja vodoničnih veza. Informacije dobijene iz NOESY i ^{1}H NMR spektara su poređene sa površinama potencijalne energije izračunatim simulacijama molekulske dinamike u različitim eksplicitnim rastvaračima.

ХС П03

Sinteza 2,5-bis(4-amidinofenil)tiofenskih derivata submikromolarnih inhibitora metaloproteaze botulinum neurotoksina serotipa A

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Botulinum neurotoksini (BoNTs), koje čini familija sa sedam serotipova (A-G), su najletalniji otrovi poznati čoveku. Aktivnost metaloproteaze, kratkog niza (LC) toksina je odgovorna za izazivanje potencijalno smrtonosne paralize povezane sa bolešću botulizmom. U ovom radu opisani su potentni analozi novog jedinjenja, BoNT serotip A LC inhibitora 2,5-bis(4-amidino-fenil)tiofena (K_i = 10.88 μM). Sintetičke modifikacije polaznog jedinjenja uključuju simultanu zamenu terminalnih bis-amidinskih grupa sekundarnim aminskim i sistematsko vezivanje 4-amino-7-hlorhinolinskih supstituenata za dobijanje derivata sa Ki vrednostima u opsegu od 0.302 μM do 0.889 μM .

The synthesis of 2,5-bis(4-amidinophenyl)thiophene derivatives providing submicromolar-range inhibition of the botulinum neurotoxin serotype A metalloprotease

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Botulinum neurotoxins (BoNTs), composed of a family of seven serotypes (categorized A-G), are the deadliest of known biological toxins. The activity of the metalloprotease, light chain (LC) component of the toxins is responsible for causing the life-threatening paralysis associated with the disease botulism. Herein we report significantly more potent analogs of novel, lead BoNT serotype A LC inhibitor 2,5-bis(4- amidinophenyl)thiophene (K_i = 10.88 μM). Specifically, synthetic modifications involved simultaneously replacing the lead inhibitor's terminal bis-amidines with secondary amines and the systematic tethering of 4-amino-7-chloroquinoline substituents to provide derivatives with Ki values ranging from 0.302 μM to 0.889 μM.

Acknowledgement: This research was supported by the Ministry of Education and Science of Serbia (grant no. 172008) and NATO's Public Diplomacy in the framework of Science for Peace project SfP983638.

ХС П04

Rutenijum(II)-arenski kompleksi sa metil-pikolinskim ligandima: sinteza i karakterizacija

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Organometalna jedinjenja intenzivno se proučavaju kao potencijalni lekovi za hemoterapiju kancera. Tokom dve decenije mnogo je radova publikovano o kompleksima rutenijuma, a neki od njih rezultovali su vrlo efikasnim antikancerogenim lekovima kao što su NAMI-A i KP1019. Tokom proteklih nekoliko godina publikovali smo seriju Ru(II)-arenskih kompleksa sa funkcionalizovanim piridinskim derivatima koordinovanim monodentatno ili bidentatno. U reakciji polaznog kompleksa $[(\eta^6\text{-}p\text{-cymene})RuCl_2]_2$ sa 3- i 6-metilpikolinskom kiselinom dobijeni su kompleksi opšte formule $[(\eta^6\text{-}p\text{-cymene})Ru(L^{1,2})Cl]$. Kompleksi su okarakterisani elementalnom analizom, masenom spektrometrijom, IC i NMR spektroskopijom. Na osnovu ovako dobijenih podataka, zaključeno je da su ligandi L^1 i L^2 bidentatno koordinovani preko piridinskog azota i deprotonovanog kiseonika karboksilne grupe vezane za piridinski prsten. Kompleksi imaju karakterističnu "piano-stool" geometriju, u kojoj arenski ligand predstavlja sedište, a helatni ligand zajedno sa hloridnim ligandom noge u ovoj pseudooktaedarskoj geometriji.

Zahvalnost: Ovaj rad je podržan je od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, Projekat br. 172017

Ruthenium(II) arene-complexes with methyl-picolinate ligands: synthesis and characterization

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Organometallic compounds are extensively studied class of anticancer chemotherapy drug candidates. For two decades, there were many publications on the subject of ruthenium complexes and some of them resulted in very active anticancer drugs like NAMI-A and KP1019. Over the past couple of years we have reported a series of Ru(II)-arene complexes with functionalized pyridines coordinated in a monodentate or bidentate way. Reaction of starting compound $[(\eta^6\text{-}p\text{-cymene})RuCl_2]_2$ with 3- and 6-methylpicolinic acid afforded the complexes of general formula $[(\eta^6\text{-}p\text{-cymene})Ru(L^{1,2})Cl]$. The complexes were characterized by elemental analysis, mass spectrometry, IR and NMR spectroscopies. According to these data, ligands L^1 i L^2 coordinate in a bidentate fashion via pyridine nitrogen and deprotonated oxigen of carboxylic group attached to the pyridine ring. These complexes have typical "piano-stool" geometry, where arene ligand forms seat and the chelating ligand along with chlorido ligand are the legs of the piano stool.

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ХС П05

Esterifikacija fenolnih kiselina katalizovana lipazom B iz *Candida antarctica*

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U ovom radu ispitana je mogućnost primene imobilisane lipaze B iz *Candida antarctica* (Novozyme 435) u sintezi estara fenolnih kiselina. Struktura fenolne kiseline pokazala se kao veoma bitan faktor u reakciji esterifikacije, pa su najveći prinosi ostvareni sa cimetnom kiselinom, koja ima najjednostavniju strukturu od ispitivanih kiselina. Pored efekta acil donora na prinos reakcije, ispitan je i efekat acil akceptora, koji se pokazao kao manje uticajan. Pokazalo se i da je početni molarni odnos reaktanata jako bitan faktor u reakciji esterifikacije. Najveći prinos, od 89 %, ostvaren je u reakciji između cimetne kiseline i etanola, pri molarnom odnosu 1:3. Pri većem početnom molarnom odnosu reaktanata, etanol se pokazao kao inhibitor. Najveći prinos je ostvaren sa *n*-butanolom, 50 %. Prinosi ostvareni u reakciji esterifikacije cimetne kiseline aromatičnim alkoholom su zanemarljivi.

Esterification of phenolic acids catalyzed by lipase B from *Candida antarctica*

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Immobilized lipase from *Candida antarctica* (Novozyme 435) was assayed for the synthesis of various phenolic acid esters. The effect of the acid type proved to be a very significant factor in esterification reactions and the highest reaction yields were obtained with cinnamic acid, which had the simplest structure of all employed acids. The effect of the acyl acceptor on the esterification yield was also investigated, but it was found to be less significant. The initial molar ratio of the substrates was a very important factor in the esterification reaction catalyzed by lipase B. The highest esterification yield, 89 %, was obtained in ethyl cinnamate synthesis, when the initial 1:3 molar ratio was employed. When higher initial molar ratios of the substrates were used, ethanol caused a deactivation of the enzyme. The highest esterification yield was obtained with *n*-butanol, 50 %. The yields of esters of aromatic alcohol were negligible.

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ХС П06

Novi aminohinolinski benzotifeni kao inhibitori botulinum neurotoksina tipa E

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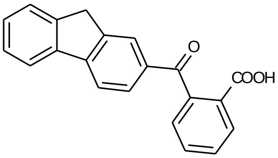
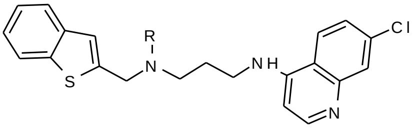
Botulinum neurotoksini su proteini koje luči bakterija *Clostridium botulinum*. Predstavljaju najjače poznate biološke neurotoksine. Gotovo sve slučajeve botulizma kod čoveka izazivaju serotipovi A, B i E. Serotip E pokazuje visoku toksičnost i izrazito brzo delovanje, ali je najmanje proučen. Do sada je otkriven samo jedan nepeptidni molekul (NSC-77053) koji se ponaša kao inhibitor, zbog čega se sve više teži ka sintetisanju malih molekula koji će moći da se primene za lečenje BoNT/E intoksikacije. U okviru naših istraživanja, sintetisani su novi aminohinolinski derivati benzotiofena, koji pokazuju trenutno najviši procenat *in vitro* inhibicije BoNT/E.



NSC-77053



BoNT/E LC % inhibicije: 52,5 (20 μM)

New aminoquinoline derivatives of benzothiophene as inhibitors of botulinum neurotoxin type E

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Clostridium botulinum neurotoxins (BoNTs) are one of the most poisonous biological substances known to humans. Almost all human cases of botulism are caused by serotypes A, B and E. Although it is highly potent and blocks neurotransmission faster compared to all other serotypes, serotype E has yet to be investigated. Until now, only one non-peptide inhibitor (NSC-77053) for botulinum neurotoxin serotype E was discovered. There is an urgent need to develop new small molecules that can be used for treating BoNT/E intoxication. Here we report the synthesis of new aminoquinoline derivatives of benzothiophene with currently highest *in vitro* inhibitory potency against BoNT/E light chain.

This research was supported by NATO's Public Diplomacy Division in the framework of Science for Peace project SfP983638 and the Ministry of Education and Science of Serbia (Grant No. 172008).

ХС П07

Sinteza i strukturna karakterizacija kompleksa Cu(II) sa piridoksalaminogvanidinom

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Još od 1950, kada je prvi put dokazana njegova biološka aktivnost, aminogvanidin (AG) je postao tema brojnih istrazivanja. Danas važi za jednog od najmoćnijih inhibitora „karbonilnog stresa“ i stvaranja dijabetskih komplikacija. Međutim, zbog neželjene farmakološke aktivnosti samog AG, njegove Šifove baze sa aromatičnim jedinjenjima predložene su kao jednako efikasni, a ujedno i sigurniji agensi. Među ovim Šifovim bazama izdvaja se ona sa piridoksalom (PLAG), jednom od formi vitamina B_6. Pored ispitivanja biološke aktivnosti PLAG, nedavno je, radovima Leovca i sar., počelo i proučavanje koordinacionih sposobnosti ovog jedinjenja.

U ovom radu opisana je sinteza novog kompleksa Cu(II) sa PLAG, koordinacione formule $[Cu(PLAG–H)N_3]$, koji je okarakterisan elementalnom analizom, IR spektrima i konduktometrijskim merenjem, kao i rendgeno-strukturnom analizom. Ovo je prvi primer kompleksa u kome je PLAG koordinovan u monodeprotonovanoj formi, koja nastaje deprotonacijom ranije okarakterisane zwitter-jonske forme liganda. Kvadratno-planarno okruženje Cu(II) realizovano je tridentanom ONN koordinacijom PLAG, preko atoma kiseonika fenolne OH-grupe i atoma azota azometinske i imino grupe aminogvanidinskog fragmenta, i atoma azota N_3^- jona na četvrtom koordinacionom mestu.

Synthesis and structural characterization of Cu(II) complex with pyridoxalaminoguanidine

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Since 1950, when its first significant biological activity was proven, aminoguanidine (AG) has been an interesting research subject. Nowadays, AG is one of the most poverful inhibitors of „carbonyl stress“ and various diabetic sequelae. However, AG has been also shown to have undesired pharmacological activities and therefore its Schiff bases containing aromatic moieties have been suggested as equally efficient, but more safe agents. Among them, the one with pyridoxal (PLAG), as one of the forms of vitamine B_6, stands out. Beside the examination of biological activity of PLAG, recently, the study of its coordination abilities has been started, by Leovac et al.

Here we describe the synthesis of a novel Cu(II) complex with PLAG, of the formula $[Cu(PLAG–H)N_3]$, which is characterized by elemental analysis, IR spectra, conductometric measurements and X-ray analysis. We emphasize that this is the first complex in which PLAG is coordinated as monoanion, formed by the deprotonation of previously characterized zwitter-ion of this ligand. Square-planar environment of Cu(II) is achieved by tridentate ONN coordination of PLAG, *via* oxygen atom of the phenolic OH-group and nitrogen atoms of azomethine and imino groups of the aminoguanidine fragment, while the fourth coordination site is occupied by N atom of azide anion.

ХС П08

Proučavanje solvatohromnog ponašanja 2,6-bis[(*E*)-2-(3-etoksi-4-hidroksifenil)etenil]piridina

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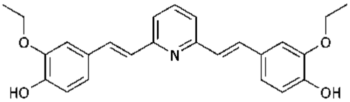
U ovom radu, novi solvatohromni indikator 2,6-bis[(*E*)-2-(3-etoksi-4-hidroksifenil)etenil]piridin sintetisan je reakcijom kondenzacije 2,6-lutidina i etilvanilina i okarakterisan FTIR, ^{1}H, ^{13}C i 2D NMR spektroskopijom. Njegovi apsorpcioni spektri određeni su u setu odabranih rastvarača i u binarnim smešama etanol–voda i aceton–voda. Efekti dipolarnosti/polarizabilnosti rastvarača i vodoničnog vezivanja između molekula rastvarača i rastvorene supstance na pomeranje apsorpcionih maksimuma interpretirani su korišćenjem modela linearne korelacije energije solvatacije (LSER) Kamlet–Tafta i Katalana. Zadovoljavajuće korelacije apsorpcionih maksimuma proučavanog indikatora sa Kamlet–Taftovom i Katalanovom skalom rastvarača pokazale su da izabrani modeli dobro opisuju LSER. Efekat koji najviše određuje solvatohromno ponašanje proučavanog indikatora potiče od interakcija sa rastvaračima različite dipolarnosti/polarizabilnosti.

Zahvalnica Autori se zahvaljuju Ministarstvu za prosvetu i nauku Republike Srbije za finansijsku pomoć prilikom izrade ovog rada (Projekat 172013).



Slika 1. Hemijska struktura 2,6-bis[(E)-2-(3-etoksi-4-hidroksifenil)etenil]piridina
Figure 1. Chemical structure of 2,6-bis[(E)-2-(3-ethoxy-4-hydroxyphenyl)ethenyl]pyridine

On the solvatochromic behaviour of 2,6-bis[(*E*)-2-(3-ethoxy-4-hydroxyphenyl)ethenyl]pyridine

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In this work, a novel solvatochromic probe 2,6-bis[(*E*)-2-(3-ethoxy-4-hydroxyphenyl)ethenyl]pyridine was synthesized via a condesation reaction between 2,6-lutidine and ethyl vanilin and further characterized by FTIR, ^{1}H, ^{13}C and 2D NMR spectroscopy. Its absorption spectra were recorded in a set of selected solvents and binary mixtures of ethanol–water and acetone–water, respectively. Effects of solvent dipolarity/polarizability and solvent–solute hydrogen bonding on the absorption maxima shifts were interpreted using the well-established linear solvation energy relationships (LSER) of Kamlet–Taft and Catalán, respectively. The reasonable correlations of the absorption maxima of the probe with the Kamlet–Taft and Catalán solvent parameter set indicated that the selected models described its LSER correctly. The most dominant effect on the solvatochromic behaviour of the probe resulted from interactions with solvents of a different dipolarity/polarizability.

ХС П09

Синтеза и карактеризација Никал(II) комплекса са несиметричним пентадентатним, H_3pd3a лигандом

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У овом раду извршена је синтеза комплекса никла(II) са несиметричним пентадентатним pd3a лигандом (pd3a је скраћеница од пропандиамин-*N,N,N′*-триацетато јона). Поменути лиганд је хелат едта-типа који у себи садржи шесточлани 1,3-пропандиамински прстен и петочлане ацетатне прстенове. Синтетисани пентадентат може имати три могућа различита изомера: *цис*-поларни, *цис*-екваторијални и *транс*-екваторијални. Карактеризација синтетисаног комплекса $K[Ni(pd3a)(H_2O)]\cdot 3H_2O$ извршена је применом IR и UV спектроскопије. Дискутована је кристална структура *цис*-поларног комплекса калијум(1,3-пропандиамин-*N,N,N′*-триацетато(аква))никла(II)трихидрата $K[Ni(pd3a)(H_2O)]\cdot 3H_2O$.

Аутори се захваљују на финансијској подршци Министарству науке и просвете Републике Србије (Пројекат бр. III41010).

Synthesis and characterization of Nickel(II) complex with unsymmetrical pentadentate, H_3pd3a ligand

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In this report we have been synthesized complexes of nickel(II) with unsymmetrical pentadentate pd3a ligand (pd3a stands for propanediamine-*N,N,N´*-triacetate ion). Mentioned ligand represent chelate of edta-type which contains 6-membered 1,3-propanediamine ring and 5-membered acetate rings. Synthesized pentadentate may have three possible different isomers: *cis*-polar, *cis*-equatorial and *trans*-equatorial. Characterization of the synthesized complex $K[Ni(pd3a)(H_2O)]\cdot 3H_2O$ was performed by using IR and UV spectroscopy. We discussed crystal structure of the *cis*-polar potassium(1,3-propanediamine-*N,N,N'*-triacetato(aquo))nickelate(II)trihydrate, $K[Ni(pd3a)(H_2O)]\cdot 3H_2O$ complex.

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ХС П10

Uticaj rastvarača na azo–hidrazon tautomeriju kod tiazolilazo piridonskih boja

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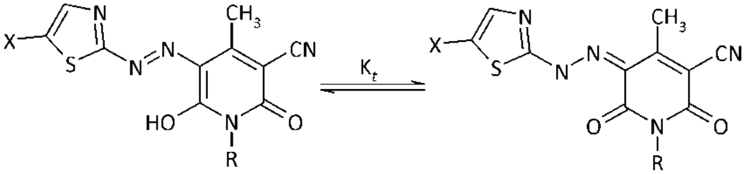
U ovom radu sintetisana su sledeća jedinjenja: 5-(tiazolilazo)- i 5-(2-nitrotiazolilazo)- 4-metil-6-hidroksi-3-cijano-2-piridon kao i 1-etil-5-(tiazolilazo)- i 1-etil-5-(2-nitrotiazolilazo)-4-metil-6-hidroksi-3-cijano-2-piridon. Sva jedinjenja okarakterisana su temperaturom topljenja, FT-IR, ^{1}H i ^{13}C NMR spektroskopijom. Apsorpcioni spektri svih jedinjenja određeni su u dvadeset rastvarača različite polarnosti u opsegu talasnih dužina 350–600 nm. Efekti polarnosti rastvarača, kao i proton-donorskih i proton-akceptorskih interakcija sa ispitivanim molekulima na pomeranje apsorpcionih maksimuma proučavani su metodom linearne korelacije solvatacionih energija (LSER), odnosno Kamlet-Taft-ovom i Catalán-ovom jednačinom.

Zahvalnica Autori se zahvaljuju Ministarstvu za prosvetu i nauku Republike Srbije za finansijsku pomoć prilikom izrade ovog rada (Projekat 172013).



Slika 1. Azo–hidrazon tautomerija kod tiazolilazo piridonskih boja (X = H, NO_2; R = H, C_2H_5)
Figure 1. Azo–hydrazone tautomerism of thiazolyl pyridone dyes (X = H, NO_2; R = H, C_2H_5)

Solvent effects on azo–hydrazone tautomerism of thiazolylazo pyridone dyes

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In this work, 5-(thiazolylazo) and 5-(2-nitrothiazolylazo)-4-methyl-6-hydroksy-3-cyano-2-pyridone as well as 1-ethyl-5-(2-thiazolylazo) and 1-ethyl-5-(2-nitrothiazolylazo)-4-methyl-6-hydroksy-3-cyano-2-pyridone have been synthesized. All compounds have been characterized by melting point, FTIR, ^{1}H and ^{13}C NMR spectroscopy. Absorption spectra have been recorded in twenty solvents of different polarity in the range from 350 to 600 nm. Effects of solvent dipolarity/polarizability and solvent–solute hydrogen bonding interactions on the absorption maxima shift have been analyzed by means of linear solvation energy relationship (LSER) concepts proposed by Kamlet-Taft and Catalán, respectively.

ХС П11

Sinteza i karakterizacija kompleksa Au(III) sa ligandom R_2edda-tipa

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Nakon otkrića cisplatine koja je uspešno korišćena u terapiji za razne tipove tumora, nastala je potreba za sintezom novih lekova, odnosno kompleksa metala, koji ne bi izazivali negativne sporedne efekte. Zlato(III) ima hemiju sličnu platini(II) (izoelektronski su, d^8-sistem, grade kvadratno-planarne komplekse), pa bi njegova jedinjenja mogla da pokazuju sličan model vezivanja za DNK, kao cisplatina.

Kompleks $[AuCl_2\{(S,S)\text{-}i\mathrm{Bu}_2\mathrm{eddip}\}]PF_6$ - dihloro(*O,O′*-diizobutil-(*S,S*)-etilendiamin-*N,N′*-di-2-propanoat)zlato(III)-heksafluorofosfat je dobijen u reakciji $[(S,S)\text{-}H_2i\mathrm{Bu}_2\mathrm{eddip}]Cl_2$ i Na_2AuCl_4 uz dodavanje rastvora LiOH (1:1:2) u metanolu. U dobijeni crveni rastvor se zatim doda čvrst NH_4PF_6. Rastvor je uparavan na vakuumu, a dobijeni žuti proizvod je ispran vodom. Pretpostavljena struktura kompleksa potvrdjena je IC i NMR spektroskopijim, masenom spektrometrijom i elementalnom analizom.

Dalja istraživanja biće zasnovana na sintezama novih kompleksa zlata(III) sa ligandima R_2edda-tipa i ispitivanju njihove antitumorske aktivnosti.

Ovo istraživanje je podržano od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, br. projekta 172035.

Synthesis and characterization of a gold(III) complex with R_2edda-type ligand

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After the discovery of cisplatin, which is succesfuly used in treatment of various types of cancers, a need for synthesis of new metal-based drugs arised, that would have less negative side effects. Gold(III) has similar chemistry to platinum(II) (isoelectronic, d^8-system, square-planar complexes), so its compounds could show a model of binding to DNA, similar to cisplatin.

The complex $[AuCl_2\{(S,S)\text{-}i\mathrm{Bu}_2\mathrm{eddip}\}]PF_6$ - dichloro(*O,O′*-diisobutyl-(*S,S*)-ethylenediamine-*N,N′*-di-2-propanoate)gold(III)-hexafluorophosphate is obtained in a reaction of $[(S,S)\text{-}H_2i\mathrm{Bu}_2\mathrm{eddip}]Cl_2$ and Na_2AuCl_4, with addition of LiOH (1:1:2) in methanol. Solid NH_4PF_6 is added in the resulting red solution. The solution is then evaporated under vacuum, and the yellow product is washed with water. The proposed structure is confirmed *via* IR and NMR spectroscopy, mass spectrometry and elemental analysis. Further investigations will be based on syntheses of new gold(III) complexes with R_2edda-type ligands and assessment of their antitumor activity.

ХС П12

Selenociklizacija 5-metil-5-(4-metil-pent-3-enil)-imidazolidin-2,4-diona i njegovih N(3)-metil i benzil derivata

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Hidantoinsko jezgro se javlja u mnogim biološki aktivnim jedinjenjima čiji farmaceutski značaj je pre svega poznat po njihovoj antimikrobnoj, antitumorskoj i antikonvulzivnoj aktivnosti[1,2].
U ovom radu ispitivana je reakcija ciklizacije 5-metil-5-(4-metil-pent-3-enil)-imidazolidin-2,4-diona sa fenilselenil halogenidima u acetonitrilu na sobnoj temperaturi. Azotov atom je u funkcionalnoj grupi sa drugim nukleofilnim atomima koji mogu dovesti do konkurentnih reakcija i stvaranja različitih heterocikla[3]. Pronađeno je da je petočlani laktam glavni proizvod u ovoj reakciji. Ispitivan je uticaj kontrajona iz selenskog reagensa kao i prisustvo Lewis-ovih kiselina na regio i stereohemijski tok ciklizacije. U slučaju N(3)-alkilovanih derivata reakcije su mnogo čistije.

Selenocyclization of 5-methyl-5-(4-methyl-pent-3-enyl)-imidazolidine-2,4-dione and its N(3)-methyl and benzyl derivatives

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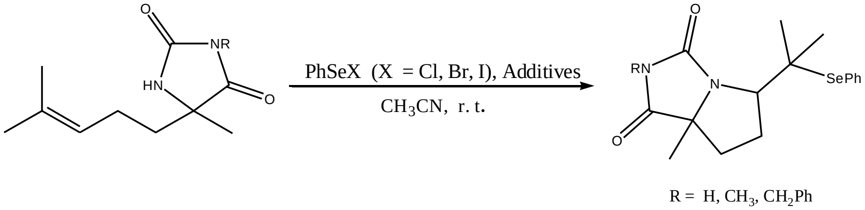
The hydantoin moiety occurring in various biologically active compounds represents a pharmaceutical importance most notably known due to their antimicrobial, anticancer and anticonvulsant activity[1,2].
The cyclization reaction of 5-methyl-5-(4-methyl-pent-3-enyl)-imidazolidine-2,4-dione with phenylselenyl halogenides in acetonitrile at ambient temperature was investigated. The nitrogen atom is incorporated in a functional group with other nucleophylic atoms which can give rise to competitive reactions leading to different heretocycles[3]. It was found that the five-membered lactam is the major product. The influence of the nature of counterion of selenilating agent as well as the presence of some Lewis acids on reactivity and regiochemical and stereochemical outcome of the cyclization was studied. In the case of N(3)-alkylated derivatives much cleaner reactions were observed.



R = H, CH$_3$, CH$_2$Ph

1. J. C. Thenmozhiyal, P. T. Wong, W. Chui, *J. Med. Chem.*, **47** (2004) 1527
2. A. Volonterio, C. R. de Arellano, M. Zanda, *J. Org. Chem.*, **70** (2004) 2161
3. A. Toshimitsu, K. Terao, S. Uemura, *J. Org. Chem.*, **52** (1987) 2018

ХС П13

Ternerni kompleksi cinka sa 2,2’-dipiridilaminom i polikarboksilatima benzena

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Zbog primene kao mikroporozni materijali, zatim u medicini i katalizi, itd.[1], ternerni kompleksi prelaznih metala sa polikarboksilatima benzena (BPC) od velikog su značaja u koordinacionoj hemiji. U ovom radu sintetisana je nova serija Zn-kompleksa sa BPC i aromatičnim diaminskim ligandom 2,2’-dipiridilaminom (dipya). Kao BPC ligandi korišćeni su anjoni 1,2-benzendikarboksilne (pht), 1,3-benzendikarboksilne (ipht), 1,4--benzendikarboksilne (tpht) i 1,2,4,5-tetrakarboksilne (pyr) kiseline.

Kompleksna jedinjenja [Zn(dipya)(pht)] (**1**), [Zn(dipya)(ipht)] (**2**), [Zn(dipya)(tpht)]·H_2O (**3**) i [Zn_2(dipya)$_2$(pyr)] (**4**) dobijena su reakcijom izmene liganada na sobnoj temperaturi kao beli mikrokristalni prahovi, nerastvorni u vodi, etanolu i DMSO. Kompleksi **1**-**4** su okarakterisani elementarnom i TG/DSC analizom, kao i FT-IR spektroskopijom. BPC su koordinirani kao mostovni bis-monodentatni ili asimetrični bis-helatni ligandi, a dipya kao helatni ligand. Na osnovu rezultata TG/DSC analize, pretpostavljeni su mehanizmi razlaganja i izračunata je entalpija dehidratacije kompleksa **3**. Termička stabilnost kompleksa opada u nizu: **2** > **4** > **3** > **1**.

Ternary zinc complexes with 2,2’-dipyridylamine and benzene polycarboxylates

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Ternary transition metal complexes containing benzene polycarboxylates (BPC) are of great interest in coordination chemistry because of their application in medicine, catalysis, as microporous materials etc.[1]. In this investigation a series of new Zn complexes with BPC and aromatic diamine ligand 2,2’-dipyrydilamine (dipya) has been synthesized. The anions of 1,2-benzenedicarboxylic (pht), 1,3-benzenedicarboxylic (ipht), 1,4-benzenedicarboxylic (tpht) and 1,2,4,5-benzenetetracarboxylic (pyr) acid were used as BPC ligands.

The compounds with the formulae [Zn(dipya)(pht)] (**1**), [Zn(dipya)(ipht)] (**2**), [Zn(dipya)(tpht)]·H_2O (**3**), and [Zn_2(dipya)$_2$(pyr)] (**4**) were obtained by ligand exchange reaction at room temperature as white microcrystalline powders, insoluble in water, ethanol and DMSO. The complexes **1**-**4** have been characterized by elemental and TG/DSC analysis and FT-IR spectroscopy. The BPCs are coordinated as bridging, bis-monodentate or asymmetric bis-chelate ligands, while dipya is coordinated as chelate ligand. Based on TG/DSC results, decomposition mechanisms were assumed and the dehydration enthalpy of **3** was calculated. Thermal stability of the complexes decreases in the order: **2** > **4** > **3** > **1**.

1. J. A. McCleverty, T. J. Meyer, *Comprehensive Coordination Chemistry II*, 2nd Edition, Elsevier, 2005.

ХС П14

Sinteza i struktura kompleksa nikla(II) sa bidentatnim S-metilizotiosemikarbazonom 2-acetilpiridina

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Koordinaciona hemija izotiosemikarbazida i njegovih derivata izotiosemikarbazona počela je da se razvija tek sa radovima Leovca i sar, koji su oborili dotadašnja uverenja da isti ne grade komplekse sa metalima. Ova grupa liganada se po pravilu koordinuje preko azometinskog i izotioamidnog atoma azota, što predstavlja osnovnu razliku u koordinacionoj hemiji tiosemi- i analognih izotiosemikarbazona.

U ovom radu opisana je sinteza, struktura i fizičko-hemijska karakterizacija kompleksa nikla(II) sa S-metilizotiosemikarbazonom 2-acetilpiridina (HL) koordinacione formule $[Ni(HL)_2(NCS)_2]$. Nikal(II) se nalazi u oktaedarskom okruženju šest atoma azota, koje je ostvareno koordinacijom dva molekula HL i dva tiocijanatna jona. Ono što izdvaja kompleks $[Ni(HL)_2(NCS)_2]$ od svih do sada strukturno okarakterisanih kompleksa sa HL, jeste bidentatna koordinacija oba molekula liganda u neutralnoj formi. Oba molekula HL se koordinuju preko azometinskog i piridinskog atoma azota, zbog čega nekoordinovani izotioamidni fragment zadržava amido formu, koju ima i slobodan ligand. Prema našem znanju kompleks $[Ni(HL)_2(NCS)_2]$ predstavlja jedan od pet dokazanih slučajeva odsustva koordinacije izotioamidnog atoma azota izotiosemikarbazonskih liganada.

Synthesis and structure of Ni(II) complex with bidentate 2-acetylpyridine S-methylisothiosemicarbazone

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Faculty of Sciences, University of Novi Sad

Development of coordination chemistry of isothiosemicarbazide and its derivatives — isothiosemicarbazones — has started with papers of Leovac *et. al*, which disapproved current beliefs that aforementioned do not form metal complexes. This group of ligands, as a rule, coordinates *via* azomethine and isothioamide nitrogen atoms, which presents the fundamental difference in coordination chemistry of thiosemi- and analogous isothiosemicarbazones.

This paper describes synthesis, structure and physico-chemical characterization of nickel(II) complex with 2-acetylpyridine S-methylisothiosemicarbazone (HL) of the coordination formula $[Ni(HL)_2(NCS)_2]$. Nickel(II) is situated in an octahedral environment of six nitrogen atoms, which is achieved by coordination of two HL molecules and two thiocyanate anions. Bidentate coordination of both ligand molecules in neutral form makes complex $[Ni(HL)_2(NCS)_2]$ distinctive from all hitherto structurally characterized complexes with HL. Both HL molecules are coordinated *via* azomethine and pyridine nitrogen atoms, due to which uncoordinated isothisemicarbazide moiety retains its amido form, also present in neutral ligand. According to our knowledge, the complex $[Ni(HL)_2(NCS)_2]$ is one of the five cases where absence of coordination of isothioamide nitrogen atom is unequivocally proven, taking all isothiosemicarbazide-based ligands into account.

ХС П15

Rutenijum(II)-bipiridil kompleks kao PDT agens

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Poslednjih godina, velika istraživanja su usmerena ka polju fotodinamičke terapije (PDT), pri čemu se ćelije kancera tretiraju foto-aktivnim lekom. Na ovaj način se neželjeni efekti mogu drastično smanjiti, što omogućava aplikaciju većih doza leka. Princip dejstva fotodinamičke terapije podrazumeva aplikaciju fotoaktivnog agensa, uz osvetljenje lokalnog tumora svetlosću određene talasne dužine, nakon čega se molekuli PDT agensa pobuđuju iz osnovnog stanja u ekscitovano singletno stanje, odakle se može fluorescencijom direktno vratiti u osnovno stanje. Posebnu grupu kompleksa čine jedinjenja rutenijuma opšte formule $[Ru(bpy)_2(L\text{-}L)]^{2+}$, L-L predstavlja helatni N,N-ligand. U ovu grupu jedinjenja spada i rutenijum(II)-bipiridil kompleks sa (*S,S*)-etilendiamin-*N,N'*-di-2-(3-cikloheksil)propanoat dietil estrom kao ligandom. Ovaj kompleks je dobijen u reakciji između *cis*-$[RuCl_2(bpy)_2]$ i odgovarajućeg liganda. Reakcija se odvija uz refluks, u smeši rastvarača, $EtOH/H_2O$. Željeni kompleks precipitira nakon dodatka NH_4PF_6. Ovaj kompleks je okarakterisan elementalnom analizom, IC, NMR i ES-MS spektroskopijom i svi spektralni podaci su u skladu sa pretpostavljenom strukturom.

Ovaj rad je finansiran od strane Ministarstva prosvete, nauke i tehnološkog razvoja projekat broj 172035.

Ruthenium(II)-bipyridyl complex as PDT agens

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In recent years, large studies have focused on the field of photodynamic therapy (PDT), in which the cancer cells are treated with photo-activated drugs. In this way, side effects can be reduced and this may allow for higher dosages of drugs. The principle of PDT involves the administration of the photoactive agens followed by local illumination of the tumor with light of appropriate wavelength to activate the specific drug. Upon illumination, the PDT agent is excited from its ground state to a singlet excited state, from where it may decay directly back to the ground state (fluorescence). A special group of ruthenium complexes are compounds of the general formula $[Ru(bpy)_2(L\text{-}L)]^{2+}$, L-L represent chelating N,N-ligand. This group of compounds includes ruthenium(II)-bipyridyl complex with (*S,S*)-ethylenediamine-*N,N'*-di-(3-cyclohexyl)propanoate diethyl ester as ligand. This complex was obtained in reaction between *cis*-$[RuCl_2(bpy)_2]$ and appropriate ligand. Reaction takes place under reflux in $EtOH/H_2O$ solution. Desirable complex precipitate after addition of NH_4PF_6. This complex is characterized by elemental analysis, IC, NMR, ES-MS spectroscopy and all spectral data are consistent with the proposed structure.

This work was supported by the Ministry of Education, Science and Technology Development, project No. 172035.

ХС П16

Uticaj delimične modifikacije strukture na aktivnost diazahrizenskih inhibitora filovirusa

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Ebola (EBOV) i Marburg (MARV) filovirusi su visoko infektivni patogeni, uzročnici smrtonosne hemoragične groznice kod ljudi i ne-humanih primata. Pronađeni su obećavajući kandidati za vakcine koje pružaju imunitet protiv infekcije filovirusima. Međutim, sporadična priroda i brzo širenje zaraze iziskuju razvoj malih molekula sa trenutnim antviralnim dejstvom. U kratkoj studiji ispitan je uticaj delimične modifikacije strukture dva poznata diazahrizenska inhibitora EBOV-a na antiviralnu aktivnost (prema EBOV i MARV virusima) i na inhibitorom posredovanu toksičnost. Sintetisana su tri analoga diazahrizena, od kojih je jedan visoko efikasan i pokazuje IC_{50} vrednosti od 0,696 ± 0,13 μM prema EBOV, odnosno 2,76 ± 0,21 μM prema MARV infekciji, sa malo ili nimalo ispoljene toksičnosti.

The Impact of a Limited Structural Modification on the Activity of Diazachrysene-Based Filovirus Inhibitors

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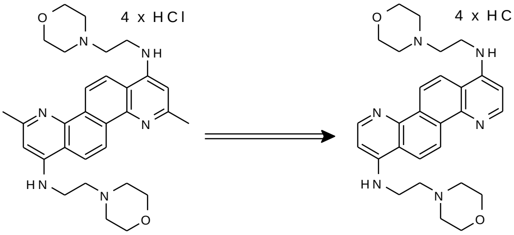
Ebola (EBOV) and Marburg (MARV) filoviruses are highly infectious pathogens causing deadly hemorrhagic fever in humans and non-human primates. Promising vaccine candidates providing immunity against filoviruses have been reported. However, the sporadic nature and swift progression of filovirus disease underlines the need for the development of small molecule therapeutics providing immediate antiviral effects. Herein we describe a brief structural exploration of two previously reported diazachrysene (DAAC)-based EBOV inhibitors. Specifically, three analogs were prepared to examine how slight substituent modifications would affect inhibitory efficacy and inhibitor-mediated toxicity during not only EBOV, but also MARV cellular infection. Of the three analogs, one was highly efficacious, providing IC_{50} values of 0.696 ± 0.13 μM and 2.76 ± 0.21 μM against EBOV and MARV infection, respectively, with little or no associated cellular toxicity.



EBOV: 53% inhibicije na 20 μM

EBOV: IC_{50} = 0.69 ± 0.13 μM

MARV: IC_{50} = 2.76 ± 0.21 μM

This research was supported by NATO's Public Diplomacy Division in the framework of Science for Peace project SfP983638 and the Ministry of Education and Science of Serbia (Grant No. 172008).

ХС П17

Enzymatic synthesis of L-ascorbyl linoleate

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Polyunsaturated fatty acid ascorbyl esters are liposoluble antioxidants with high nutritive value. Hence, these esters are eligible for usage in food and cosmetics as additives. In this case, lipase-catalyzed synthesis is method of choice because it can be conducted under mild reaction conditions and it is stereospecific. Aim of this research was optimization of key reaction parametars – vitamin C concentration, substrates molar ratio, enzyme loading, and initial water content for lipase-catalyzed esterification of vitamin C with linoleic acid in acetone as reaction media. Maximum yields were achieved at 0.2 M of vitamin C, ascorbic/linoleic acid molar ratio 1:4, lipase loading 7 g/l, and initial water content 0.07 %(v/v). Highest conversions were obtained at 50 mM of L-ascorbic acid, while at 3 g/l of immobilized lipase highest specific yields (mmole of ester per mass of enzyme) were achieved. Obtained results are promissing, being comparable to those achieved in previous researches with activated acyl donors and/or more expencive solvents.

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Enzimska sinteza L-askorbil-linolata

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Askorbil-estri polinezasićenih masnih kiselina su liposolubilni antioksidansi sa velikom nutritivnom vrednošću, što ih čini pogodnim aditivima za primenu u prehrambenoj i kozmetičkoj industriji. Mogu se dobiti u stereospecifičnim rekcijama katalizovanim lipazama pod blagim reakcionim uslovima. Cilj ovog rada bila je optimizacija najznačajnijih faktora – koncentaracije L-askorbinske kiseline, molskog odnosa supstrata, koncentracije enzima i početnog sadržaja vode za esterifikaciju vitamina C linolnom kiselinom katalizovanu lipazom u acetonu kao reakcionom medijumu. Maksimalni prinosi postignuti su pri koncentraciji vitamina C od 0,2 M, molskom odnosu askorbinske prema linolnoj kiselini 1:4, koncentraciji lipaze od 7 g/l i početnom sadržaju vode od 0,07 %(v/v). Najviše konverzije dobijene su pri najmanjim ispitivanim koncentracijama vitamina C – 50 mM, dok su najveći specifični prinosi (količina estra po masi enzima) ostvareni sa 3 g/l imobilisane lipaze. Postignuti prinosi su uporedivi sa rezultatima ranijih studija sa aktiviranim acil donorima i/ili skupljim organskim rastvaračima, pa predstavljaju dobru osnovu za dalja ispitivanja.

ХС П18

New method for synthesis of dilithium terephthalate

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Recently, it has been discovered that dilithium terephthalate (Li_2tpht) shows enhanced thermal stability over conventional anode materials for Li-ion batteries[1]. This investigation compares two ways of synthesis of the mentioned compound. The first one was described by Kaduk[2] and the other approach presents a new procedure. According to Kaduk, Li_2tpht is obtained by precipitation from an aqueous suspension containing Li_2O and terephthalic acid (H_2tpht) in a molar ratio 1:1. The new method is based on a simple grinding of Li_2CO_3 and H_2tpht in an agate mortar. Both samples were characterized by FTIR spectroscopy, TG/DSC and XRD analysis. The obtained results are compared and discussed.

Novi postupak sinteze litijum-tereftalata

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Nedavno je otkriveno da litijum-tereftalat (Li_2tpht) pokazuje veću termičku stabilnost u poređenju sa konvencionalnim anodnim materijalima u litijum-jonskim baterijama[1]. U ovom radu upoređena su dva postupka sinteze pomenutog jedinjenja. Prvi postupak opisan je od strane Kaduka[2], dok drugi pristup predstavlja nov postupak. Prema Kaduku, Li_2tpht dobijen je taloženjem iz vodene suspenzije koji sadrži Li_2O i tereftalnu kiselinu (H_2tpht) u molskom odnosu 1:1. Novi postupak zasnovan je na jednostavnom mlevenju reaktanata, Li_2CO_3 i H_2tpht, u ahatnom avanu. Oba uzorka okarakterisana su pomoću FTIR spektrokopije, TG/DSC i XRD analize. Dobijeni rezultati su međusobno upoređeni i diskutovani.

1. M. Armand, S. Grugeon, *Nature Mater.* **8**, 120-125 (2009).
2. J. A. Kaduk, *Acta Crystallogr.* **B56**, 474-485 (2000).

ХС П19

Novi aminohinolinski derivati kao inhibitori Botulinum neurotoksina

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Botulinum neurotoksini (BoNT) zbog svoje velike toksičnosti i lakoće proizvodnje predstavljaju potencijalno veliku pretnju kao agensi koji se mogu koristiti u bioterorizmu. Za sad ne postoji odobren farmakološki pristup u lečenju od intoksikacije botulinum neurotoksinima, iz čega proizilazi potreba za razvojem jedinjenja koja bi našla primenu u tretmanu ovog oboljenja. 4-Amino-7-hlorohinolinski derivati su poznati inhibitori BoNT, i u ovom radu smo ispitivali kako određene strukturne promene utiču na aktivnost potencijalnih inhibitora. Sintetisali smo derivate koji u položaju C4 aromatičnog jezgra imaju supstituente sa različitim sternim i elektronskim osobinama. Rezultati će biti diskutovani.

New aminoquinoline derivatives as inhibitors of Botulinum neurotoxin

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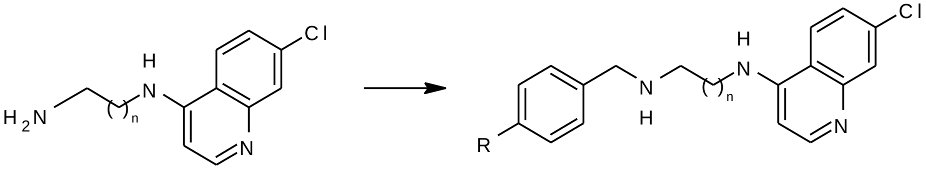
Naturally occurring botulinum neurotoxins (BoNTs) are the most potent of bacterial toxins. Due to their ease of dissemination and lethality BoNTs are classified as major threats to use as a dangerous biological weapon. Presently, there is no approved pharmacological approach for the treatment of intoxication caused by botulinum neurotoxins. 4-Amino-7-chloroquinoline derivatives are known inhibitors of BoNTs. To further investigate the potential of 4-amino-quinoline molecules as a multitarget compounds, we synthesized several new derivatives with different steric and electronic properties. The results will be discussed.



Acknowledgement: This research was supported by the Ministry of Education and Science of Serbia (grant no. 172008) and NATO's Public Diplomacy in the framework of Science for Peace project SfP983638.

ХС П20

Aldolni pristup enantioselektivnoj sintezi (-)-oseltamivir fosfata

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Formalna sinteza (-)-oseltamivir fosfata (tamiflu^{TM}) je urađena polazeći od (*S*)-glutaminske kiseline. Ova sinteza kao ključne reakcije obuhvata dve aldolne reakcije, kojima se formiraju C-C veze. Prva aldolna reakcija je enantioselektivna i formiraju se dva nova stereocentra. U drugoj aldolnoj reakciji pimenjuje se enolegzo ciklizacija dialdehida, pri čemu se zatvara cikloheksenski prsten sa željenom regiohemijom.

An aldol approach to the enantioselective synthesis of (-)-oseltamivir phosphate

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Formal synthesis of (-)-oseltamivir phosphate (tamiflu^{TM}) was accomplished starting from (*S*)-glutamic acid. The synthesis comprised two carbon-carbon bond forming reactions, using two aldol reactions as key steps. The first aldol reaction is enantioselective and results in formation two stereocenters. The second carbon-carbon bond formation – cyclohexene ring closure - using an enolexo aldolization of a dialdehyde resulted in the formation of product with the desired regioselectivity.

ХС П21

Uticaj supstituenata na intramolekulski transfer naelektrisanja kod novih antikonvulzivnih derivata sukcinimida

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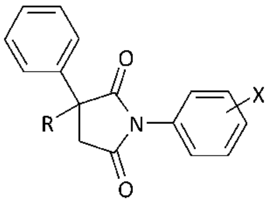
Imajući u vidu farmakološki značaj derivata sukcinimida, u ovom radu sintetisani su novi *N*-aril-2-fenil- i *N*-aril-2,2-difenilsukcinimidi (Slika 1) i određeni su njihovi apsorpcioni maksimumi u oblasti od 200 do 400 nm u dvanaest rastvarača različitih polarnosti. Uticaj supstituenata na arilnom prstenu na apsorpcione spektre proučavanih jedinjenja interpretiran je upotrebom DFT metoda. Rezultati kvantnohemijskih proračuna pokazuju da supstituenti određuju karakter ICT prelaza od kojeg potiču najintenzivnije apsorpcione trake.

Zahvalnica Autori se zahvaljuju Ministarstvu prosvete i nauke Republike Srbije na finansijskoj pomoći prilikom izrade ovog rada (Projekat 172013).



Slika 1. Hemijska struktura N-aril-2-fenil- i N-aril-2,2-difenilsukcinimida
Figure 1. Chemical structure of N-aryl-2-phenyl and N-aryl-2,2-diphenylsuccinimide
(R = H, C_6H_5; X = H, 4-CH_3, 4- CH_3O, 4-NO_2, 4-OH, 4-CN, 4-$COCH_3$, 4-F, 4-Cl,4-Br, 4-I, 3-OH, 3-Cl, 3-CN)

Substituent effect on intramolecular charge transfer of new anticonvulsant succinimide derivatives

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Regarding the pharmacological importance of succinimide derivatives, new *N*-aryl-2-phenyl and *N*-aryl-2,2-diphenylsuccinimide have been synthesized (Figure 1) and their absorption maxima have been determined in the region from 200 to 400 nm in twelve solvents of different polarity. Effects of substituent on the aryl ring on the the absorption spectra of the investigated compounds have been interpreted using DFT method. Results of the quantum chemical calculations have demonstrated that substituents determine character of ICT transitions from which the most intense absorption bands originate.

ХС П22

Sinteza jodotimola i ispitivanje njihove antimikrobne aktivnosti

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Timol je jedinjenje prirodnog porekla, pripada biljnim monoterpenoidima i poznato je da poseduje antimikrobnu aktivnost.
Cilj ovog rada je sinteza jodotimola i poređenje njihove antimikrobne aktivnosti u odnosu na polazno jedinjenje- timol. Elektrofilnom aromatičnom supstitucijom dobijeni su monojod, dijod timol i proizvod kondenzacije dva mola timola vezanih preko joda (smeša A). Jodovanjem benziltimola (C) dobijena je smeša monojod- i dijodbenziltimola (smeša B). Izolovanje sintetisanih jedinjenja izvršeno je korišćenjem "Fleš" hromatografije i TLC, a identifikacija je postignuta upotrebom GC-MS i NMR spektroskopije. Antimikrobna aktivnost određivana je agar-difuzionim metodom na šest bakterijskih i jednom gljivičnom soju. Pokazano je da sintetisani jodotimoli imaju slabije antimikrobno dejstvo u odnosu na timol.

Ovaj rad je proistekao iz istraživanja na projektu broj 172041 koje finansira Ministarstvo nauke.

Synthesis of iodothymol and determination of its antibacterial activity

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Thymol belongs to plant monoterpenoids and It shows antimicrobial activity.
The aim of this paper is synthesis of iodothymols and comparison of their antimicrobial activity with the starting compound-thymol. Thymol monoiodide, diiodide and condensation product of two moles of thymol connected via iodine (mixture A) were synthetised by electrophilic aromatic substitution. Indirect thymol iodation via benzylthymol (C) resulted in mixture of benzylthymol monoiodide and diiodide (mixture B). The isolation of the synthesized compounds was conducted using "Flash" chromatography and TLC. Identification was achieved using GC-MS and NMR spectroscopy. Antimicrobial activities of A, B and C were determined using agar-diffusion method on six bacterial and one fungal strains.
Results show that iodothymols exhibit lower antimicrobial activity than thymol.

Acknowledgement: Our work has been supported by Scientific Research Grant from the Ministry of Science (Serbia) No 172041.

Биохемија и биотехнологија

БХ О10

Ispitivanje mogućnosti primene mikroemulzija i mikroemulzija sa inkorporiranim lipazama kao detergenata za uklanjanje fleka trigliceridnog porekla

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U radu je ispitan detergentni učinak mikroemulzija Lutensol® XP 80/amil alkohol/izooktan/50 mM fosfatnu pufer u uklanjanju trigliceridnih fleka kao i potencijalni doprinos *C. rugosa* lipaze i lipaza prisutnih u sirovom enzimskom ekstraktu *P.aeruginosa* san-ai inkorporiranih u ove mikroemulzije njihovom detergentnom učinku. Na model reakciji hidrolize *p*-nitrofenil-butirata ispitivan je uticaj odnosa vodene i uljane faze u mikroemulziji, odnosa surfaktanta i kosurfaktanta u pseudoemulgatoru, masenog udela pseudoemulgatora u mikroemulziji kao i uticaji pH vrednosti i temperature na aktivnost lipaza u datim mikroemulzijama. Takođe je ispitana stabilnost lipaza u mikroemulzijama. Testovi pranja izvođeni na belim pamučnim krpicama onečišćenim trioleinskim flekama pokazali su da je primenom mikroemulzija u količini od svega 5 g/g tkanine već u toku prvog pranja moguće ukloniti 91 % prvobitno prisutne trioleinske fleke, što je značajno više u odnosu na rastvor komercijalnog detergenta kojim je postignut stepen uklanjanja fleke od oko 61 %. Doprinos lipaza nije primećen nakon prvog testa pranja. Nakon drugog pranja, mikroemulzija koja je sadržala *P. aeruginosa* lipaze pokazala je za oko 3 % veći detergentni učinak u odnosu na mikroemulziju bez lipaza.

Investigation of possible application of microemulsions and microemulsions with incorporated lipases as detergents for triglyceride fatty soil removal

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Efficiency of Lutensol® XP 80/amyl alcohol/isooctane/50 mM phosphate buffer microemulsions, microemulsions with C. rugosa lipase and lipases present in crude extract obtained from P. aeruginosa–san-ai, respectively in triolein fatty soil removal from cotton fabrics was tested as a model detergency. Using hydrolysis of p-nitrophenyl-butyrate as model reaction, influence of water to oil and surfactant to cosurfactant ratio, pseudoemulgator concentration, pH and temperature on lipases activity in microemulsions was investigated. Stability of lipases i microemulsions was also tested. Model detergency tests carried on 6x6 cm white cotton fabric cloths stained with triolein showed that using only 5g of microemulsions per gram of fabric approximately 91 % of initial triolein stain can be removed as compared with 61 % of initial soil removal achieved using solution of commercial laundry detergent. Lipases contribution to detergency of microemulsions was not observed after first washing cycle. After second washing cycle microemulsions which contained P. aeruginosa san-ai lipases achieved around 3 % better trioelin soil removal from cotton fabric than microemulsions with no enzymes.

БХ О11

Uticaj fikocijanobilina iz *Spirulina*-e na humane eritrocite: *in vitro* studija

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Fikocijanobilin (PCB) je plava tetrapirolna hromofora fikocijanina (PC), glavnog proteina prokariotske i filamentozne cijanobakterije *Spirulina*-e. PC pokazuje izražena antioksidativna, antiinflamatorna i imunomodulatorna svojstva, kao i obećavajuće antikancerogeno delovanje. Većina nabrojanih efekata pripisuje se upravo PCB-u. Cilj ovog rada je bio da preliminarno ispitamo efekte prisustva PCB-a u sistemskoj cirkulaciji, na primeru njegovog delovanja na humane eritrocite. Spin-label EPR studijom je utvrđeno da PCB ne utiče na fluidnost plazmine membrane eritrocita. Određivanja aktivnosti ključnih enzima antioksidativne odbrane, nakon inkubiranja hemolizata sa hromoforom, pokazala su da PCB značajno, i to inhibitorno, deluje samo na seleno-protein glutation peroksidazu (smanjuje aktivnost za oko 20 %). Rezultati spektroskopskih studija sugerišu vezivanje PBC-a za hem u hemoglobinu (tzv. plavo pomeranje i smanjenje intenziteta Soretove trake u UV-VIS spektrima), bez većeg uticaja na konformaciju i stabilnost molekula (sličnost fluorescentnih i istovetnost CD spektara hemoglobina u prisustvu PCB-a, u poređenju sa kontrolnim uzorcima). Fundamentalni (biohemijski) i primenjeni (fotodinamska terapija) značaj opisanih nalaza biće ukratko diskutovan.

The effect of phycocyanobilin from *Spirulina* on human erythrocytes: *in vitro* study

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****Center for multidisciplinary studies, University of Belgrade, Serbia*

Phycocyanobilin (PCB) is blue tertrapyrrol chromophore of phycocyanin (PC), a major protein of prokaryotic and filamentous cyanobacteria Spirulina. PC shows a pronounced antioxidant, antiinflammatory and immunomodulatory properties, as well as promising anticancer activity. Most of the mentioned effects are ascribed to PCB. The aim of this study was to preliminary examine the effects of PCB presence in the systemic circulation, on the example of its impact on human erythrocytes. Spin-label EPR study showed that PCB does not affect the erythrocyte plasma membrane fluidity. Determinations of the activities of key antioxidant enzymes, after hemolysate incubation with chromophore, showed a significant, and inhibitory effect on the selenium protein glutathione peroxidase only (reduced activity by about 20 %). Results of spectroscopic studies indicated binding of PCB to the heme in hemoglobin (blue shift and decrease in Soret band intensity in the UV-VIS spectra), without a significant influence on the conformation and stability of the molecule (similarity of fluorescent and comparability of the CD spectra of hemoglobin in the presence of PCB, in comparison with control samples). Fundamental (biochemical) and applied (photodynamic therapy) significance of described findings will be briefly discussed.

БХ О12

Kolagenazna aktivnost proteaza lateksa smokve

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Smokva (*Ficus carica*) je biljna vrsta koja se vekovima koristi u ishrani i medicini. Lateks smokve predstavlja bogat izvor različitih formi cistein proteaza poznatih pod opštim nazivom ficin. Cilj ove studije je detekcija i bazična karakterizacija kolagenaza lateksa smokve.

Kolagenaze lateksa smokve ispoljavaju različite osobine u odnosu na ficin, uključujući molekulsku masu (oko 45 kDa) i profile pH optimuma (pH 7,0, pH 9,0 i pH 4,0). Postoje kisele, neutralne i bazne forme kolagenaza lateksa smokve. Inhibitori cistein proteaza inhibiraju samo 15 % kolagenolitičke aktivnosti, PMSF dovodi do 30 % inhibicije, dok pepstatin inhibira 20 % aktivnosti. Kolagenaze su potpuno stabilne u blago kiselim, neutralnim i baznim uslovima (pH 6-10). Kolagenaze lateksa smokve su aktivne nakon tretmana na 80 °C, bez obzira na prisustvo cisteina kao aktivatora cistein proteaza, ali dolazi do naglog pada aktivnosti nakon inkubacije na 90 °C.

Kolagenaze lateksa smokve ne pripadaju samo klasi cistein proteaza, već dominantno drugim klasama proteaza (serin i aspartat proteazama). Ova studija predstavlja do sada prvi izveštaj o detekciji i bazičnoj karakterizaciji kolagenaza lateksa smokve.

Zahvalnica: Ovaj rad je finansiran od strane Ministarstva za prosvetu i nauku Republike Srbije (Projekat 172049).

Collagenolytic activity of fig latex proteases

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Ficus carica, the common fig, is widely used for centuries as food and medicine. Fig latex is a source of different forms of cysteine proteases known under common name ficin. The aim of the study was to detect and basically characterize fig latex collagenases.

Fig latex collagenases display different properties then fig latex ficin proteases, regarding molecular weight (around 45 kDa) and pH optima profiles (pH 7.0, pH 9.0 and pH 4.0). There are acidic, neutral and basic forms of collagenases in the fig latex. Cysteine protease inhibitors inhibited only 15 % of collagenolytic activity, PMSF treatment cause 30 % of inhibition; Pepstatin A inhibited 20 % of activity, while EDTA did not have any effect on collagenolytic activity. Collagenases are completely stable in slight acidic, neutral and basic conditions (pH 6-10). Fig latex collagenases are active after treatment at 80 °C, regardless of the presence of cysteine as activator of cysteine proteases, but massively lost the activity if incubated at 90 °C.

Fig latex collagenases belong not just to cysteine protease family but mainly to different classes of proteases (serin and aspartic proteases). To the best of our knowledge, this is the first report about detection and basic characterization of fig latex collagenases.

Acknowledgement: This work is supported by the Ministry of Education and Science, Republic of Serbia (Grant No. 172049).

БХ П01

Uticaj različitih izvora ugljenika na rast soja *Lb. johnsonii* NRRL B-2178 pri proizvodnji probiotskog napitka na bazi surutke

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Cilj ovog rada je bio izbor odgovarajućih izvora ugljenika za proizvodnju probiotskog napitka na bazi surutke sojem *Lb. johnsonii* NRRL B-2178.
Selekcija izvora je izvršena primenom specifičnog eksperimentalnog dizajna uz izvođenje minimalnog broja eksperimenata. Istovremena analiza uticaja glavnih eksperimentalnih faktora kao i uticaja njihovih interakcija na željeni odgovor sistema, u ovom slučaju broj ćelija u proizvedenom probiotskom napitku nakon 8 h fermentacije, izvršena je primenom delimičnog faktorijalnog plana u okviru statističkog programa Design Expert 8.
Na osnovu dobijenih rezultata, inulin i saharoza predstavljaju najbolji izbor izvora ugljenika za postizanje maksimalnog broja ćelija *Lb. johnsonii* NRRL B-2178 u proizvodnji probiotskog napitka na bazi surutke. Rezulati dobijeni primenom delimičnog faktorijalnog plana pokazali su da interakcija inulina i saharoze predstavlja glavni faktor za postizanje maksimalnog broja ćelija u probiotskom napitku na bazi surutke. Na osnovu statističke analize proizilazi da je maksimalni rast ćelija (8,1 log CFU/mL) ostvaren obogaćivanjem surutke dodatkom 0,5 g inulina i 0,5 g saharoze.

Influence of different carbon sources on the growth of *Lb. johnsonii* NRRL B-2178 in the production of a probiotic whey-based beverage

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The aim of this study was the selection of appropriate carbon sources for the production of a probiotic whey-based beverage utilizing the microorganism *Lb. johnsonii* NRRL B-2178. Selection of a carbon source was performed by using a specific experimental design and through the least number of experiments. Simultaneous investigation of the main effect of experimental variables and the effect of their interaction on the desired response, which was the highest number of cells in the probiotic whey-based beverage after 8 h of the fermentation, were carried out by fractional factorial design by the statistical software Design Expert 8. Based on the obtained results inulin and sucrose were the best choice of carbon source to obtaining the maximal cell number of *Lb. johnsonii* NRRL B-2178 in probiotic whey-based beverage production. The results obtained from a two-level fractional factorial design showed that the combination of inulin and sucrose were the major factor for the production of maximal cell number. The statistical analysis showed that maximum cell growth (8.1 log CFU/mL) was obtained by enriching the whey by the addition of 0.5 g of inulin and 0.5 g of sucrose.

БХ П02

Proizvodnja sirovog ćelijskog ekstrakta β-galaktozidaze pomoću bakterija mlečne kiseline

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U ovom radu izvršena je optimizacija proizvodnje *β*-galaktozidaza pomoću bakterija mlečne kiseline. Kao najbolji producent među ispitanim bakterijama pokazala se bakterija *Lactobacillus acidophilus.* Najveća aktivnost *β*-galaktozidaze, dobijena je mikroaerofilnom fermentacijom u modifikovanoj MRS podlozi, sa 2,5 % laktoze, na tresilici (150 rpm) u trajanju od 48 h. Kako je enzim intracelularan, u cilju razaranja ćelija i oslobađanja enzima, primenili smo više različitih fizičkih metoda, a daleko najboljom pokazala se metoda vorteksiranja sa kvarcnim peskom (150 μm). Shodno činjenici da enzimi iz mlečnih bakterija mogu biti korišćeni bez dodatnog prečišćavanja, određeni su temperaturni (45 ^{o}C) i pH optimum (6,8) za ovako dobijen preparat.

Production of β-galactosidase crude cell extract from lactic acid bacteria

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In this study, different strains of lactic acid bacteria were screened for β-galactosidase activity. Since among them *Lb. acidophilus* showed highest production potential, optimal conditions for accomplishing high yields of β-galactosidase activity were investigated. Highest specific activity (2.1 IU/ml) was obtained by 2 days shake flask culture fermentation at 37 ^{o}C in modified MRS broth, provided that lactose content was 2.5 %. Different mechanical methods were conducted to release intracellular β-galactosidase activity. Nevertheless, vortexing with quartz sand (150 μm) was proven to be prime choice. In order to characterize crude cell extract, temperature (45 ^{o}C) and pH optimum (6.8) were determined.

Zahvalnica: Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije na finansijskoj podršci u okviru projekata III 46010

БХ П03

Sinteza superapsorbujućih hidrogelova na bazi hitozana

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Superapsorbujući pH-osetljivi hidrogelovi na bazi hitozana su sintetisani jonskim umrežavanjem hitozana (Ch) i itakonske kiseline (IA), nakon čega je nastala Ch/IA mreža umrežena sa metakrilnom kiselinom. Pri sintezi je variran sadržaj metakrilne kiseline i koncentracija umreživača. Ovi hidrogelovi predstavljaju kombinaciju prirodnih i sintetskih polimera sa podesivim bubrenjem. Sastav hidrogelova u velikoj meri utiče na strukturu, mehanička i termička svojstva, morfologiju i kinetiku bubrenja. Ugradnja u hidrogel je potvrđena FT-IR analizom; porozna struktura je dokazana SEM analizom, a topografija hidrogelova je ispitana AFM i IFM mikroskopijom.

Synthesis of a chitosan-based superabsorbing hydrogels

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Superabsorbing pH-sensitive hydrogels were synthesized by ionic crosslinking of chitosan and itaconic acid followed by free radical polymerization and crosslinking with different methacrylic acid and crosslinking agent concentrations. These hydrogels represent a combination of natural and synthetic polymers with tunable swelling. The hydrogel composition greatly affects the hydrogel structure, mechanical and thermal properties, morphology and swelling kinetics. Incorporation of monomers in hydrogels was confirmed by FT-IR analysis; the porous structure was showed by SEM analysis, while topography of hydrogels was determined by AFM and IFM analysis.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije, Projekat br. 172062.

БХ П04

Procena toksičnosti azo boje Reactive Blue 52 nakon elektrohemijskog tretmana

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Tekstilna industrija ispušta veliku količinu otpadnih voda (efluenata) koje sadrže azo boje. Elektrohemijski tretman rastvora reaktivne plave boje (Reactive Blue 52) sa cirkonijumskom elektrodom kroz proces redukcije u 0,1 M Na_2SO_4 elektrolitu dovodi do obezbojavanja. Kako fizički i hemijski testovi sami po sebi nisu dovoljni da se proceni rizik po životnu sredinu od uticaja tretiranih efluenata, primenjen je test akutne toksičnosti na vrsti *Artemia salina*. Testovi su rađeni sa kontrolom i pet razblaženja (6,25 %, 12,5 %, 25 %, 50 %, 100 %), kao i sa tri ponavljanja po razblaženju za sve uzorke. Smrtnost je konstatovana ako se jedinka ne pokrene u periodu od 10 sekundi. Mortalitet je izražena kao procenat smrtnosti i LC_{50} vrednosti su utvrđene za svaki uzorak. Rezultati su smatrani validnim ako smrtnost u kontroli ne prevazilazi 10 %. Proizvodi degradacije praćeni su HPLC tehnikom. Istraživanje je ostvareno u okviru Projekta OI 172030, pod pokroviteljstvom Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije.

Toxicity evaluation of azo dye Reactive Blue 52 after electrochemical treatment

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Textile industry releases a large amount of wastewater (effluent) containing azo dyes. Electrochemical treatment of Reactive Blue 52 dye with zirconium electrode as cathode (reduction) in 0.1 M Na_2SO_4 electrolyte leads to discoloration. As physical and chemical tests alone are not sufficient enough to evaluate the risk to the environment from exposure to treated solution, acute toxicity test was performed using nauplii of *Artemia salina*. Tests were conducted with control and five test dilutions (6.25 %, 12.5 %, 25 %, 50 %, 100 %) with three replicates per dilution for all samples. Endpoint was the mortality of nauplii. They were considered dead if no movement was observed within 10 seconds. Lethality was expressed as the percentage of mortality, and LC_{50} values were determined for each sample. Tests were considered valid if the mortality in the control did not exceed 10 %. Color degradation intermediates were monitored by HPLC method. This research is a part of the project OI 172030, funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia.

БХ П05

Stabilizacija imobilisane lipaze iz *Candida rugosa* tretmanom imobilizata aminokiselinama

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Lipaze su važna klasa katalizatora u farmaceutskoj, kozmetičkoj i prehrambenoj industriji. U industriji lipaze se koriste isključivo u imobilisanom obliku. Enzimi tokom imobilizacije gube deo aktivnosti, a deo aktivnosti se gubi i tokom upotrebe i skladištenja imobilizata. Za primenu imobilisanih enzima neophodan je pravilan odabir nosača za imobilizaciju. Kod nosača sa epoksi grupama, nakon imobilizacije deo epoksi grupa ostaje neproreagovan. Neproreagovale epoksi grupe mogu reagovati sa bočnim lancima u molekulu proteina, čime dolazi do dodatnog pada aktivnosti imobilizata. Uobičajeni način blokiranja epoksi grupa se zasniva na tretmanu imobilizata 2-merkaptoetanolom ili etilendiaminom. U ovom radu, neproreagovale epoksi grupa blokirane su tretmanom aminokiselinama (glicinom, fenilalaninom, argininom i asparaginskom kiselinom). Rezultati pokazuju da fenilalanin i glicin imaju pozitivan efekat na stabilnost imobilisane lipaze, dok sa druge strane, arginin i asparaginska kiselina nemaju nikakav efekat na stabilnost imobilisane lipaze.

Stabilization of immobilized lipase from *Candida rugosa* by amino acid treatment

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Lipases are important catalysts in pharmaceutical, cosmetics and food industry. On industrial scale, lipases are used only in immobilized form. Majority of enzymes lose part of its initial activity during immobilization process, but activity also decreases throughout storage and usage of immobilized lipase. Therefore, adequate immobilization supports are prerequisite for successful application of immobilized enzyme. When it comes to epoxy supports, after immobilization unreacted epoxy groups can interact with side chains of protein, which could result in additional enzyme activity loss. Blocking of epoxy groups is usually performed with 2-mercaptoethanol or ethylenediamine. In this study, treatment of immobilized lipase with different amino acids (glycine, phenylalanine, arginine and aspartic acid) was performed. Phenylalanine and glycine exhibited positive effect on stabilization of immobilized lipase, so this treatment should be examined more thoroughly. On the other hand, arginine and aspartic acid showed no effect on stabilization of immobilized lipase.

Zahvalnica: Autori se zahvalju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije na finansijskoj podršci u okviru projekata III46010 i 172013.

БХ П06

Imunološka karakterizacija rekombinantne beta-1,3-glukanaze iz banane

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Beta-1,3-glukanaza iz banane (*Musa acuminata*) je protein za koji je pokazana IgE reaktivnost kod osoba alergičnih na ovo voće. Nalazi se u pulpi banane i pretpostavlja se ima ulogu u reprodukciji biljke i odbrani od patogena, prvenstveno gljiva.

Svrha ovog rada je imunološka karakterizacija rekombinantne beta-1,3-glukanaze obeležene GST-om na N-terminalnom kraju kako bi se potvrdila sličnost prirodnog i rekombinantnog oblika enzima i eventualna mogućnost upotrebe rekombinantnog enzima u dijagnostici alergija.

Protein je eksprimiran u ćelijama BL21 iz vektora pGEX 4T. Inkluziona tela koja sadrži beta-1,3-glukanazu su intenzivno ispirana sve dok protein od interesa nije postao dominantan. GST-glukanaza je ekstrahovana iz inkluzionih tela rastvorom 2 M uree i prečišćena gel hromatografijom. Urađen je Western blot i pokazana je IgE reaktivnost naspram seruma pacijenata alergičnih na banane. Takođe, pokazana je i reaktivnost naspram zečijeg anti-banana seruma.

Immunological characterization of recombinant beta-1,3-glucanase from banana

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Beta-1 ,3-glucanase is a protein from banana (*Musa acuminata*) which revealed IgE reactivity in persons allergic to this fruit. It is located in the pulp of banana and it is assumed that this protein plays a role in plant reproduction and defense against pathogens, especially fungi.

The purpose of this paper is immunological characterization of recombinant beta-1,3-glucanase with a GST-tagg included in the N-terminal end to confirm the similarity of natural and recombinant forms of the enzyme and the eventual possibility of using the recombinant enzyme in allergy diagnostics.

The protein was expressed in BL21 cells from vector pGEX 4T. The inclusion bodies contain beta-1 ,3-glucanase were extensively washed until the protein of interest has become dominant. GST-glucanase was extracted from inclusion bodies by solution of 2M urea and purified by gel chromatography. Western blot analysis was performed and demonstrated IgE reactivity against serum of banana allergic persons. It also demonstrated the reactivity against rabbit banana anti-serum.

БХ П07

Razvijanje testa za istovremeno određivanje kazeinolitičke i koagulacione aktivnosti proteaza

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Biljne proteaze sve više nalaze primenu u industriji sira. Da bi se neki enzim koji izaziva koagulaciju mleka koristio u industriji sira, potrebno je da ima što manju kazeinolitičku aktivnost i što veću koagulacionu aktivnost. Poređenje ove dve aktivnosti nije moguće usled toga što se koriste različiti testovi za njihovo određivanje i različite jedinice. U difuzionom testu u agaroznom gelu sa inkorporiranim kazeinom dolazi do formiranja prosvetljenih prstenova kazeinskog precipitata oko bunara u koje je nanesen himotripsin. Površine unutrašnjih prstenova linearno koreliraju sa kazeinolitičkom (R^2=0,9859), dok površine spoljašnjih prstenova precipitata linearno koreliraju sa koagulacionom aktivnošću himotripsina (R^2=0,9639). Test je reproducibilan u oba slučaja (p>0,05 za dva nezavisna merenja). Difuzioni test u agaroznom gelu sa inkorporiranim kazeinom može da se koristi za istovremeno određivanje kazeinolitičke i koagulacione aktivnosti enzima. Takođe bi mogao da se upotrebi za rutinsku pretragu velikog broja biljnih ekstrakata u cilju identifikovanja novih potencijalnih enzima koji bi mogli da se koriste za izazivanje koagulacije mleka u industriji sira.

Zahvalnica: Ovaj rad je finansiran od strane Ministarstva za prosvetu i nauku Republike Srbije (Projekat 172049).

Development of simultanous assay for caseinolytic and milk clotting activity determination

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The application of plant proteases in the dairy industry has increased over the years. The possible application of an enzyme with milk clotting properties requires that the enzyme have low caseinolytic but high milk clotting activity. A excact comparison of these two activities is impossible due to the fact that the tests used for their determination have different activity units. In the diffusion test done in an agarose gel with casein incorporated a formation of transparent rings of casein precipitate occurs around the well in which chymotripsin is applied. The areas of the inner rings correlate with the caseinolytic activity in a linear fashion (R^2=0, 9859), while the area of the outer rings of the precipitate correlate with the coagulation activity of chymotrypsin also in a linear fashion (R^2=0, 9639). The reproductivity of the test is valid (p>0.05 for two independent samples). The diffusion test with casein incorporated in the agarose gel can be used to determine the caseinolytic and coagulation activity of an enzyme. The test can also be used to routinely test a large number of plant extracts with the goal of identifying new potential enzymes which can be later used in inducing milk coagulation in the dairy industry.

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БХ П08

Citotoksični i genotoksični efekat 17-pikolil androstanskih derivata

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U radu je ispitivana *in vitro* citotoksična aktivnost dva androstanska derivata: 17α-pikolil-androsta-5-en-3β,4α,17β-triola (**1**) i 5α,6α-epoksi-17α-pikolil-androsta-N-oksid-3β,17β-diola (**2**) na ćelijama humanih tumora i poređena sa delovanjem formestana pri istim uslovima. Oba jedinjenja su značajno smanjila proliferaciju ćelija estrogen-nezavisnog adenikarcinoma dojke (MDA-MB-231 linija), formestan mnogo manje, dok ni jedno od ispitivanih jedinjenja nije značajnije izazivalo smanjenje proliferacije ostalih tumorskih ćelija, kao ni zdravih.

Broj izmena sestrinskih horomatida kod ćelija tretiranih jedinjenjem **1** bilo je veće nego u slučaju netretiranih ćelija, kao i incidencija mikronukleusa (slično kao u slučaju formestana), dok kod jedinjenja **2** takav efekat nije uočen. Proliferacioni indeks je najveći kod ćelija tretiranih jedinjenjem **2**.

The cytotoxic and genotoxic effects of 17- picolyl androstane derivatives

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Here we present the results of the *in vitro* cytotoxicity studies of two androstane derivatives: 17α-picolyl-androst-5-ene-3β,4α,17β-triol (**1**) and 5α,6α-epoxi-17α-picolyl-androstane-N-oxide-3β,17β-diol (**2**) on human tumor cells, and compare them with the effect of formestane in the same conditions. Both compounds significantly decreased proliferation of the estrogen-independent breast adenocarcinoma cells, formestane much less, while neither compound had effect on other tumor or healthy cells proliferation.

The number of the sister chromatid exchanges is greater in cells treated with compound **1** then in case of untreated cells, as well as micronucleus incidence (similarly is for formestane), while in test with compound **2** such effect was not noticed. The proliferation index has the greatest value when cells are treated with compound **2**.

БХ П09

Optimizacija prečišćavanja alergena Mus a 2, Mus a 4 i Mus a 5 iz banane

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Banana (*Musa acuminata*) je postao važan izvor alergena hrane. Pulpa banane sadrži proteine za koje je pokazana IgE reaktivnost sa serumima osoba alergičnih na ovo voće. Do sada je identifikovano 5 alergena banane među kojima su glavni alergeni: hitinaza klase I, oznacen kao Mus a 2, protein slican taumatinu (TLP) oznacen kao Mus a 4 i β-1,3-glukanaza, oznacen kao Mus a 5. Unapređenje dijagnostike alergija na hranu podrazumeva zamenu alergenskih ekstrakata panelom pojedinačnih alergena izolovanih iz datog alergenskog izvora koji mogu naći primenu u kliničkim ispitivanjima.

Svrha istraživanja bila je optimizacija prečišćavanja tri glavna alergena banane.

Optimizovan je proces prečišćavanja proteina jonoizmenjivačkom hromatografijom (Hi Trap SP FF kolona) i reverzno faznom hromatografijom (Supelco C5 kolona). Prečišćavanje proteina je praćeno SDS-PAGE tehnikom. Karakterizacija prečišćenih proteina je urađena izoelektričnim fokusiranjem (IEF), 2D elektroforezom, imunoblotom i N-terminalnim sekvenciranjem. Postupkom u četiri koraka izolovana su sva tri važna alergena banane.

Zahvalnica: Ovaj rad je proistekao iz istraživanja na projektu br. 172049 koji finansira Ministarstvo prosvete i nauke Republike Srbije.

Optimization of Mus a 2, Mus a 4 and Mus a 5 allergens purification from banana fruit

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Banana fruit (Musa acuminata) has become an important food allergen source in recent years. The ripe banana contains proteins which show IgE reactivity with sera from banana allergic patients. Five banana allergens have been identified so far, and the major allergens are an class I chitinase, denoted as Mus a 2, thaumatin like protein (TLP), denoted as Mus a 4, and β-1,3-glucanase, denoted as Mus a 5. Food allergy diagnosis can be improved by using individual allergen components instead of banana allergen extracts, which can be used in clinical trials.

The purpose of this research was to optimize the purification of three major allergens present in the banana fruit.

This allergens were purified by a combination of ion exchange chromatography (Hi Trap SP FF column) and reverse phase chromatography (Supelco C5 column). During purification process proteins were detected by using SDS-PAGE technique. The characterization of the purified proteins was done with the usage of isoelectric focusing (IEF), 2D electrophoresis, immunoblot techniques and N-terminal sequencing. With this four-step procedure we were able to purify all three important banana fruit allergens.

БХ П10

Uticaj masnih kiselina vezanih za humani serum albumin na reaktivnost slobodne tiol-grupe albumina

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Humani serum albumin (HSA) je najznačajniji transporter slobodnih masnih kiselina u serumu, u proseku šest molekula masnih kiselina dugog niza (C13 – C21) vezano je za jedan molekul serum albumina. HSA poseduje jednu slobodnu tiol-grupu koja se nalazi na cistein-34 (Cys34) ostatku i u plazmi predstavlja značajni redukcioni potencijal usled velike zastupljenosti albumina. Kristalografski podaci pokazuju da je izloženost Cys34 tiol-grupe različita ukoliko su za HSA vezani različiti ligandi. U ovom radu ispitana je reaktivnost Cys34 tiol-grupe kada se, za prethodno odmašćeni albumin, vezuje stearinska kiselina (C18:0), odnosno oleinska kiselina (C18:1). Reaktivnost slobodne tiol grupe merena je modifikovanom Elmanovom metodom (sa 5,5'-ditiobis-(2-nitrobenzoevom) kiselinom). Albumin je prethodno odmašćen tretmanom aktivnim ugljem, a potom pod kontrolisanim uslovima inkubiran sa stearinskom kiselinom, odnosno oleinskom kiselinom. Praćena je kinetika reakcije slobodne tiol-grupe i 2 mM Elmanovog reagensa tokom 30 minuta. Reakcioni profili pokazuju da je reaktivnost Cys34 tiol-grupe veća kod albumina zasićenog stearatom u odnosu na odmašćeni albumin (kontrola). Kod albumina zasićenog oleatom tiol-grupa je reaktivnija u odnosu na kontrolu, ali je i reaktivnost tiol grupe u prisustvu oleata statistički značajno veća u odnosu na reaktivnost Cys34 tiol-grupe u prisustvu stearata, što ima značaj pri hvatanju reaktivnih vrsta u različitim patološkim stanjima.

The influence of free fatty acids bound to human serum albumin on the reaction of free thiol group of albumin

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Human serum albumin (HSA) is the most important transporter of free fatty acids in sera, and about six molecules of the long chain fatty acids (C13 – C21) binds to one molecule of serum albumin. HSA has one free thiol group located at cystein-34 (Cys-34) residue, which is very important source of reductive capacity according to HSA abundance in the plasma. Crystallographic studies showed that accessibility of HSA Cys34 residue to oxidation was significantly changed when free fatty acids were attached to HSA. The aim of this study was investigation of the impact of stearic (C18:0) and oleic acid (C18:1) HSA binding on reactivity of Cys34 free thiol group. Free thiol groups were assayed according to modified Ellman's method (with 5,5'-dithiobis-(2-nitrobenzoic acid as reagent)). Reaction kinetics of free thiol and 2mM Ellman's reagent were observed during 30 minutes from start of the reaction. The profile of reaction shows statistically significant difference between reactivity of Cys34 in presence of stearic acid compared to reactivity of Cys34 of fatty acids free HSA which was control sample. Also, the reactivity in presence of oleic acid was greater than control, as well as with stearic acid, which is very important in capturing reactive species in many pathological conditions.

БХ П11

Uticaj vezivanja bakar(II)-jona za HSA na sadržaj slobodne tiol-grupe Cys34

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Humani serum albumin (HSA) je najzastupljeniji protein plazme i važan transporter različitih liganada u cirkulaciji. Pored drugih funkcija koje HSA ima u organizmu, uz ceruloplazmin predstavlja najveći pul bakra u plazmi. HSA je i važan antioksidans plazme zahvaljujući slobodnoj –SH (tiol) grupi Cys34 prisutnoj na površini molekula HSA. Cilj ovog rada bio je da se ispita uticaj vezivanja bakar(II)-jona za HSA na sadržaj slobodne tiol-grupe Cys34. HSA je preinkubiran sa različitim koncentracijama bakar(II)-jona u cilju dobijanja HSA-bakar(II)-kompleksa. Nevezani bakar(II)-jon uklonjen je ultrafiltracijom. HSA-bakar(II) kompleks potom je inkubiran tokom 24^h na 37^0C. Sadržaj vezanih bakar(II)-jona meren je spektrofotometrijski batokuproinskim reagensom (BCS). Sadržaj –SH grupa Cys34 praćen je Ellman-ovim testom. Moguće promene na HSA praćene su snimanjem fluorescentnih spektara, kao i elektroforetski (nativna i SDS). Sadržaj slobodnih –SH grupa Cys34 smanjuje se za oko 13 %. Fluorescentni spektri ne pokazuju značajne razlike između kompleksa HSA-bakar(II) i HSA. Pokretljivost kompleksa nije značajno promenjena u odnosu na HSA, ali je nativnom elektroforezom pokazano da HSA-bakar(II)-kompleks ima oko 10 % više udela dimerske trake. Na osnovu ovih rezultata može se zaključiti da vezivanje bakar(II)-jona za HSA dovodi do smanjenja sadržaja slobodnih tiol grupa Cys34 na površini HSA, bez uticaja na konformaciju i elektroforetsku pokretljivost.

The influence of binding of copper (II) ions to HSA on Cys34 thiol group content

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Human serum albumin (HSA) is the most abundant plasma protein (35-50g/L) and important transporter of various ligands in circulation. Besides ceruloplasmin, HSA is a large pool of bound copper in plasma. HSA is important plasma antioxidant having free thiol group on Cys34 present on its molecule surface. The aim of this study was to examine the influence of binding of copper (II) ions to HSA on Cys34 thiol group content. HSA was pre-incubated with different concentrations of copper (II) ions to obtain HSA-copper (II) complexes. Any unbound copper was removed by ultracentrifugation. Complexes were then incubated during 24^h at 37^0C. Copper (II) content was determined with bathocuproine reagent and the content of free thiol group Cys34 was monitored by Ellman's assay. Possible changes on HSA were monitored by recording fluorescent spectra, as well as by electrophoresis (native and SDS). Content of free thiol group Cys34 decreases upon binding of copper (II) ions to HSA (up to 13 % of starting value). There are no significant differences in fluorescent spectra and there is no difference in electrophoretic mobility, but there is an increase (10 %) in dimer band content shown by native electrophoresis. Based on these finding it can be concluded that binding of copper (II) ions leads to decrease in the content of free thiol group Cys34 without influencing the conformation of HSA and its electrophoretic mobility.

БХ П12

Podobnost odabranih hibrida kukuruza za proizvodnju bioetanola i suve kukuruzne džibre

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Bioetanol se najčešće proizvodi od skrobne komponente kukuruznog zrna čime zaostaju značajne količine vrednih sporednih proizvoda među kojima je i suva kukuruzna džibra sa rastvorenim materijama koja se može koristiti kao zamena tradicionalnoj hrani za životinje. Cilj ovog istraživanja bio je da se odredi podobnost šest hibrida Instituta za kukuruz „Zemun Polje“ za proizvodnju bioetanola i suve kukuruzne džibre. Određena je i korelacija između fizičko-hemijskih karakteristika zrna, prinosa bioetanola i kvaliteta kukuruzne džibre, njenog hemijskog sastava i *in vitro* svarljivosti suve materije. Najveći prinos etanola 94,5 % od teorijske vrednosti i volumetrijska produktivnost od 2,01 g $L^{-1}h^{-1}$ nakon 48 h fermentacije postignuti su sa hibridom ZP 434, a najniži sa hibridom ZP 611k. Prema hemijskom sastavu, svi uzorci kukuruzne džibre su ispoljili potencijalno dobre karakteristike kao komponente hrane za životinje. Svi uzorci kukuruzne džibre imali su visok sadržaj proteina, visoku svarljivost suve materije kao i zadovoljavajuću koncentraciju minerala, naročito Ca i P. Hibrid ZP 434 se pokazao kao najpodobniji za proizvodnju bioetanola zbog najvišeg procenta mekog endosperma koji je podložniji enzimskoj hidrolizi skroba.

Suitability of some selected maize hybrids for the production of bioethanol and dried distillers' grains

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Bioethanol is mostly produced from starchy parts of the corn grain kernel leaving significant amounts of valuable byproducts such as distillers' dried grains with solubles (DDGS) which can be used as a substitute for traditional feedstuff. The suitability of six maize hybrids from Maize Research Institute „Zemun Polje“ was investigated for bioethanol and DDGS production. In addition, the correlation between physical and chemical characteristics of the grain, bioethanol yield and quality of the corresponding DDGS, its chemical composition and *in vitro* dry matter digestibility was assessed for these maize hybrids. The highest ethanol yield of 94.5 % of theoretical and volumetric productivity of 2.01 g $L^{-1}h^{-1}$ after 48 hours of fermentation were obtained with hybrid ZP 434, and the lowest with ZP 611k. Regarding chemical composition, all DDGS samples manifested potentially good properties as feed components. All DDGS samples had high protein levels, showed high digestibility and high mineral content, especially of Ca and P. A hybrid ZP 434 was selected as the most promising ethanol producer due to the highest level of soft endosperm fraction which is more susceptible to starch hydrolyzing enzymes.

БХ П13

Sekundarni metaboliti vrsta *Fagopyrum esculentum* Moench., *Polygonum aviculare* L. i *Rumex patientia* L. kao prirodni inhibitori biosinteze eikozanoida

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Heljda (*Fagopyrum esculentum* Moench.), običan troskot (*Polygonum aviculare* L.) i zelje (*Rumex patientia* L.) su jestive biljke iz familije Polygonaceae. U ovom radu, ispitan je inhibitorni uticaj 80 % etanolnih ekstrakata herbi i rizoma na kalcimicinom indukovanu produkciju metabolita arahidonske kiseline u humanim trombocitima. Nastali metaboliti praćeni su LC-MS/MS tehnikom. Krive inhibicije produkcije PGE_2, $PGF_{2\alpha}$, 12-HHT i TXB_2 korišćene su za studiju inhibicije COX puta, koji ima ulogu u procesima inflamacije, indukciji bola i povišene telesne temperature, dok je 12-HETE korišćen kao indikator aktivnosti 12-LOX puta, koji ima ulogu u proliferaciji tumorskih ćelija, kao i u nastanku alergijskih reakcija i autoimunih oboljenja. Ispitani ekstrakti pokazali su značajnu aktivnost u primenjenom testu (IC_{50} u opsegu 0,60–4,5 mg/ml za produkciju 12-HHT, 0,094–3,4 mg/ml za 12-HETE, 1,4-3,4 mg/ml za PGE_2 i 0,74–2,9 mg/ml za TXB_2), čime je potvrđen njihov potencijal kao komponenata funkcionalne hrane.

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Fagopyrum esculentum Moench., *Polygonum aviculare* L. and *Rumex patientia* L. secondary metabolites as natural inhibitors of eicosanoids biosynthesis

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Buckwheat (*Fagopyrum esculentum* Moench.), common knotgrass (*Polygonum aviculare* L.) and patience dock (*Rumex patientia* L.) are edible plants from the Polygonaceae family. In this paper, inhibitory effects of 80 % ethanolic herb and rhizome extracts on calcimicine-induced eicosanoids biosynthesis in human platelets were investigated. Formed metabolites were detected using LC-MS/MS. Inhibition curves of PGE_2, $PGF_{2\alpha}$, 12-HHT and TXB_2 production were used to investigate the inhibition of the COX pathway, which is involved in inflammatory processes, induction of pain and elevated body temperature, whereas 12-HETE was used as an indicator of the 12-LOX pathway, which has a role in proliferation of tumor cells, as well as in allergic reactions and autoimmune diseases. Investigated extracts exhibited significant activity (IC_{50} in range 0.60–4.5 mg/ml for 12-HHT production, 0.094–3.4 mg/ml for 12-HETE, 1.4–3.4 mg/ml for PGE_2 and 0.74–2.9 mg/ml for TXB_2), thus confirming their potential as functional foods components.

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БХ П14

Proizvodnja, svojstva i korisna jedinjenja suvog ekstrakta biljne vrste *Ocimum basilicum*

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Suvi ekstrakt biljne vrste *Ocimum basilicum* je dobijen postupkom sušenja vodeno-etanolnog ekstrakta pomoću laboratorijskog Anhydro spray dryer uređaja. Ulazna temperatura u toku procesa sušenja je bila u rasponu od 135 °C do 140 °C. Izlazna temperatura je bila u rasponu od 60 °C do 70 °C. U toku procesa dobijanja suvog ekstrakta brzina atomizera se kretala od 20.000 do 21.000 rpm. Za 14 dm^3 tečnog ekstrakta *O. basilicum,* dobijenog ekstrakcijom pomoću 50 % etanola kao rastvarača, ukupno vreme sušenja je 2,5 h. Kao agens za sušenje u suvom ekstraktu *O. basilicum* upotrebljen je maltodekstin. U pripremljenom suvom ekstraktu sadržaj ukupnih fenola iznosio je 58,7 mg GAE/g. Primenom DPPH testa za suvom ekstraktu *O. basilicum* određena je njegova antioksidativna aktivnost sa vrednošću IC_{50} 3,9 μg/ml. Sadržaj vlage u iznosi je 4,17 %. Nasipna zapremina ovako pripremljenog suvog ekstrakta iznosi 155,8 mg/ml. Ispitane su i senzorne karakteristike suvog ekstrakta primenom “Sniffing” testa.

Production, properties and beneficial compounds of *Ocimum basilicum* dry extract

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A dry extract of *Ocimum basilicum* was prepared from an aqueous-ethanol extract by a spray drying process using an Anhydro laboratory spray dryer. During the process, the inlet temperature was in the range from 135 °C to 140 °C. The outlet temperature was in the range from 60 °C to 70 °C. During the production of the dry extract the atomizer speed ranged from 20,000 to 21,000 rpm. For 14 dm^3 of *O. basilicum* liquid extract, obtained using 50 % ethanol, total drying time was 2.5 hours. *Ocimum basilicum* dry extract was prepared using Maltodextrin as the drying agent. The prepared extract contained an amount of total phenols equivalent to 58.7 mg GAE/g. A DPPH test was used to assess the antioxidant activity of *O. basilicum* dry extract and the IC_{50} calculated was 3.9 μg/ml. The moister content of the dry extract was 4.17 %. The bulk density of the extract prepared this way was 155.8 mg/ml. Using a “Sniffing test” sensor an evaluation of the olfactory properties of the *O. basilicum* dry extract was done as well.

БХ П15

Adsorpcija lipaze iz *Candida rugosa* na hidroksiapatitu

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Enzimi imaju brojne prednosti nad klasičnim hemijskim katalizatorima. Lipaze (E.C.3.1.1.3, hidrolaze estara glicerola) su posebno značajni biokatalizatori zbog stabilnosti u ekstremnim reakcionim uslovima, široke suspstratne specifičnosti i podjednako efikasne katalize i u vodenoj i nevodenoj sredini. Usled inhibicije supstratom ili proizvodom, produktivnost rastvornih lipaza može se smanjiti, što je značajan nedostatak kod industrijskih procesa na visokoj skali. Povećanje produktivnosti i poboljšanje ukupnih performansi enzima može se postići njihovom imobilizacijom na nekom od čvrstih nosača, poput hidroksiapatita. Pre imobilizacije lipaze bilo je neophodno ispitati i ustanoviti optimalne uslove za vezivanje enzima za nosač. Utvrdili smo da kapacitet hidroksiapatita iznosi 0,016 mg (proteina)/mg (matriksa) i da je optimalno trajanje inkubacije enzima i matriksa 30 min. Pod navedenim uslovima smo imobilizovali lipazu iz komercijalnog preparata *Candida rugosa* lipaza i ostvarili prinos vezivanja od 99,93 % , odnosno prinos imobilizacije aktivnog enzima od 20 %.

Adsorption of *Candida rugosa* lipase on hydroxyapatite

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Enzymes have numerous advantages over classical chemical catalysts. Lipases (E.C.3.1.1.3, glycerol ester hydrolase) are of great importance, because of their wide substrate specificity, stability in extreme reaction conditions and efficient catalysis in both aqueous and non-aqueous media. Due to substrate or product inhibition, productivity of free lipases can be reduced, which is a great problem in large-scale industrial processes. Productivity increase and improvement of overall enzyme performance can be achieved by enzyme immobilization on some of the solid supports, such as hydroxyapatite. Before the immobilization of lipase, it was necessary to investigate and determine the optimum conditions for the binding of the enzyme to the support. We have determined that the capacity of hydroxyapatite is 0,016 mg (proteins)/mg (matrix) and that the optimal duration of incubation of enzyme and matrix is 30 min. Lipase from commercial preparation of *Candida rugosa* lipase was immolized on hydroxyapatite with immobilization yield of 99,93 % and activity yield of 20 %.

Наука о материјалима

HM O9

Površinska modifikacija tankih slojeva jednoslojnih ugljeničnih nanotuba pod dejstvom mikrotalasa

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U ovom radu su predstavljeni rezultati ispitivanja tankih slojeva jednoslojnih ugljeničnih nanotuba tretiranih mikrotalasnim zračenjem. Tanki slojevi jednoslojnih ugljeničnih nanotuba su deponovani vakuumskom filtracijom na keramičke pločice. Slojevi su izloženi mikrotalasnom zračenju snage 25 i 250 W i frekvencije 2,45 GHz. Uzorci su ispitani ramanskom spektroskopijom i mikroskopijom atomske sile. Ramanska spektroskopija je pokazala da ne dolazi do selektivnog uništavanja ni metalnih ni poluprovodnih nanotuba. Zapaženo je da su se pod dejstvom mikrotalasa uzorci zagrevali samo tokom ozračivanja pri snazi od 250 W. Glavni efekat mikrotalasa na tanke slojeve jednoslojnih ugljeničnih nanotuba je smanjenje prosečnog prečnika snopova nanotuba.

Surface modification of single wall carbon nanotube thin films by microwaves

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In this work we present the results of Raman spectroscopy study of single wall carbon nanotube thin films treated by microwave irradiation. Single wall carbon nanotube thin films were deposited by vacuum filtration method and transferred onto alumina substrate. These thin films were exposed to microwave irradiation of 25 and 250 W at 2.45 GHz. All samples were characterized by Raman spectroscopy study and atomic force microscopy. Raman spectroscopy analysis showed that there were neither selective destruction of metallic nor semiconducting nanotubes. It was noticed that samples were heated only during microwave irradiation at 250 W. Major effect of microwave irradiation on single wall carbon nanotubes was their debundling.

НМ П01

Električna i morfološka karakterizacija višeslojnih ugljeničnih nanocevi funkcionalizovanih Bingelovom reakcijom

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U ovom radu, višeslojne ugljenične nanocevi (MWCNT) su kovalentno funkcionalizovane primenom dva prostupka modifikacije. U prvom postupku, 1,3-dikarbonilna jedinjenja (dietilmalonat, 2,2-dimetil-1,3-dioksan-4,6-dion, dimedon i barbiturna kiselina) direktno su uvedena na površinu nanocevi Bingelovom reakcijom. U drugom postupku, površina MWCNT-a najpre je modifikovana dietilmalonatom, a potom su izvedene reakcije sinteze barbiturne i tiobarbiturne kiseline sa ureom, odnosno tioureom. Uspešnost funkcionalizacije potvrđena je FTIR spektroskopijom i elementarnom analizom. Utvrđeno je da prisustvo 1,3-dikarbonilnih jedinjenja čini površinu nanomaterijala hidrofobnijom. Ispitivanje morfoloških i električnih svojstava izvršeno je skenirajućom elektronskom mikroskopijom, mikroskopijom atomskih sila, merenjem površinske otpornosti i određivanjem električne provodnosti dispergovanih nanocevi tokom isparavanja *N*-metil-2-pirolidona.

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Electrical and morphological characterization of multiwalled carbon nanotubes functionalized *via* the Bingel reaction

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Covalent sidewall functionalization of multiwalled carbon nanotubes (MWCNTs) was performed using two approaches. In the first approach, a 1,3-dicarbonyl compound (diethyl malonate, 2,2-dimethyl-1,3-dioxane-4,6-dione, dimedone and barbituric acid) was directly attached to the surface of carbon nanotubes under the Bingel reaction conditions. In the second approach, the surface of MWCNTs was firstly modified by diethyl malonate and the subsequent cyclization to barbituric and thiobarbituric acid was accomplished with urea and thiourea, respectively. The success of covalent functionalization was confirmed by FTIR spectroscopy and elemental analysis. The wettability of functionalized MWCNTs was investigated and it was observed that the presence of 1,3-dicarbonyl compounds caused the surface of nanotubes to be more hydrophobic. The surface morphology has been examined by atomic force microscopy and scanning electron microscopy. Surface resistance and electrical conductivity of the functionalized MWCNTs have been measured during the evaporization of *N*-methyl-2-pyrrolidinone in which nanotubes were initially dispersed.

НМ П02

Elektrodepozicija Zn-Mn legura sa visokim procentom Mn iz hloridnog elektrolita

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Dodatak Mn može značajno poboljšati otpornost prema koroziji prevlakama Zn na čeliku. Najbolje osobine Zn-Mn legura se postižu kad je sadržaj Mn između 30 i 40 at. %. Cilj ovog rada je bio da se, po prvi put, upotrebi elektrolit koji sadrži hloride Zn i Mn za elektrodepoziciju Zn-Mn legura, koje će imati visok sadržaj Mn sa jedne strane i kvalitetnu morfologiju površine sa druge strane. Izučavan je uticaj dva parametra elektrodepozicije, i to gustine struje depozicije i koncentracije Mn u elektrolitu. Elektrohemijske reakcije su ispitivane primenom ciklične voltametrije i hronoamperometrije. Dobijeni uzorci su karakterisani primenom sledećih tehnika: SEM, EDS i XRD.

Electrodeposition of Zn-Mn alloys with high Mn percentage from chloride electrolyte

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The manganese addition can significantly improve the corrosion resistance of sacrificial Zn coatings on steel. The best properties are obtained in the Zn-Mn alloys where Mn content is in the range of 30 – 40 at %. The scope of this work was to, for the first time according to our knowledge, employ the electrolyte containing Zn and Mn chlorides in electrodeposition of Zn-Mn alloys which would have high Mn content on one side and satisfactory surface appearance and morphology on another side. The alternation of two deposition parameters, namely, deposition current density and manganese ion concentration in the electrolyte, was investigated. The electrochemical reactions of interest were studied by cyclic voltammetry and chronoamperometry. The samples obtained were characterized by scanning electron microscopy, energy dispersive X-ray spectrometry and X-ray diffraction.

НМ П03

Kinetika osmotskog sušenja alginatnih kuglica

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Bioaerogelovi predstavljaju novu klasu materijala sa veoma atraktivnim i specifičnim fizičko-hemijskim osobinama. U cilju razvoja novih načina proizvodnje bioaerogelova, ispitivana je kinetika osmotskog sušenja aginatinh kuglica. Natrijum alginat je rastvoren u destilovanoj vodi u koncentraciji 2 % i ovaj rastvor je dodavan u kapima u rastvor $CaCl_2$ uz konstantno mešanje. Alginatne kuglice su raspršene u rastvoru saharoze u temperaturskom opsegu između 298 i 318 K. Refratometrijska metoda je korišćena za određivanje koncentraciju saharoze. Sve krive zavisnosti procenta izgubljene vode iz alginatnih kuglica u rastvoru su istog oblika sa karakterističnim platoom. Korišćenjem model fitting metoda, određeno je da se kinetički procesi mogu opisati Janderovim 3D difuzionim modelom, a da su vrednosti kinetičkih parametara: Ea=10.6kJ/mol, ln(A/s)=-4.0. Kinetika sušenja je određena difuzijom vode iz alginatnih kuglica u rastvor saharoze. Zaključeno je da je osmotsko sušenje veoma efikasan metod za uklanjanje vode iz alginatnih kuglica. Ovo istraživanje je podržano od strane Ministarstva prosvete i nauke Republike Srbije, u okviru projekta 172015OI.

Kinetics of osmotic drying of alginate beads

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Bioaerogels present novel class of materials with very attractive and specific physicochemical properties. In order to develop new pathways of bioaerogels production, the kinetics of osmotic drying of alginate beads was examined. Sodium alginate was dissolved in distilled water at a concentration of 2 % (w/w) and alginate solution was added dropwise to a stirred $CaCl_2$ solution. Alginate beads were suspended in sucrose solution in the range of temperatures from 298 to 318 K. The refractory method was used to determine the sucrose concentration. All of the kinetic curves of water loss from alginate beads in osmotic solution are of the same shape, and have the characteristic saturation plateau. Using the model fitting method, it was determined that the kinetics of this process can be described by the Jander's 3-D diffusion model with the values of kinetic parameters: Ea=10.6 kJ/mol, ln(A/s) = -4.0. The drying kinetics is predetermined by the water diffusion from alginate beads to osmotic solution. It was concluded that the osmotic drying is a very effective method for water removing from alginate beads. This paper was supported by Ministry of Education and Science, under a project number 172015OI.

НМ П04

Pasivacija mekog čelika u rastvoru *p*-toluensulfonske kiseline

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U ovom radu ispitivano je anodno ponašanje mekog čelika u vodenom rastvoru *p*-toluensulfonske kiseline, primenom potenciodinamičke i galvanostatske tehnike. Cilj rada je pronalaženje optimalnih uslova za pasivaciju mekog čelika u rastvoru *p*-toluensulfonske kiseline u pogledu koncentracije i gustine struje pasivacije. Utvrđeno je da parametri pasivacije zavise od koncentracije rastvora, pa je na osnovu njihovih vrednosti izabrana koncentracija od 0,5 mol dm^{-3} *p*-toluensulfonske kiseline. Uticaj gustine struje i vremena trajanja pulsa konstantne struje na kvalitet pseudopasivnog filma je potvrđen i na osnovu vizuelne procene uzoraka je utvrđeno da su optimalni uslovi za formiranje pseudopasivnog filma na mekom čeliku iz rastvora *p*-toluensulfonske kiseline, gustina struje 50 mA cm^{-2} i vreme trajanja 800 s. Pseudopasivni film, verovatno na bazi *p*-toluensulfonata, poseduje kratkotrajna zaštitna svojstva.

Passivation of mild steel in aqueous solution of *p*-toluenesulfonic acid

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In this paper we studied the anodic behavior of mild steel in aqueous solution of *p*-toluenesulfonic acid, using potentiodynamic and galvanostatic techniques. The goal of this paper is to determine the optimal conditions for the passivation of mild steel in aqueous solution of *p*-toluenesulfonic acid, regarding concentration and passivation current density. It was determined that the passivation parameters depend on the concentration of the solution, and on the basis of their values selected concentration was 0,5 mol dm^{-3} *p*-toluenesulfonic acid. The influence of current density and constant current pulse duration on the quality of pseudo-passive film is confirmed, and on the basis of visual estimation of the samples was determined that the optimal conditions for the formation of pseudo-passive film on mild steel in aqueous solution of *p*-toluenesulfonic acid are current density of 50 mA cm^{-2} and the time duration of 800 s. Pseudo-passive film, probably on the basis of *p*-toluenesulfonate, has a short-term protective properties.

НМ П05

Primena organskog inhibitora za sprečavanje pojave korozije niskougljeničnog čelika u CO_2 sredini

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Cilj ovog istraživanja je ispitivanje efikasnosti TOFA/DETA imidazolina kao inhibitora korozije niskougljeničnog čelika pod dejstvom CO_2. Inhibitorska svojstva TOFA/DETA imidazolina su ispitana u 3 mas. % vodenom rastvoru NaCl zasićenom sa CO_2 na temperaturi od 20°C i 70°C primenom sledećih tehnika: spektroskopija elektrohemijske impedancije, metoda polarizacije linearno promenljivim potencijalom, gravimetrijska metoda određivanja gubitka mase, metoda merenja električne otpornosti, skenirajuća elektronska mikroskopija kao i metoda mikroskopije atomskih sila. Rezultati merenja brzine korzije pokazuju da dodati inhibitor u koncentraciji od 70 ppm značajno smanjuje stepen korozije u odnosu na sistem bez inhibitora. Mikrofotografije površine čelika pokazuju da TOFA/DETA imidazolin smanjuje oštećenja površine čelika svojom sposobnošću da se adsorbuje na metalnoj površini, dok je primenom metode mikroskopije atomskih sila potvrđeno da TOFA/DETA imidazolin smanjuje prosečnu hrapavost površine niskougljeničnog čelika.

Zahvalnica: Ministarstvo prosvete i nauke Republike Srbije, III 45019

Evaluation of organic inhibitor for corrosion of mild steel in CO_2 environment

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In this study talloil diethylenetriamine imidazoline (TOFA/DETA imidazoline) was evaluated as corrosion inhibitor for mild steel in CO_2 environment. The inhibition behavior of TOFA/DETA imidazoline on mild steel in 3 wt. % aqueous NaCl solution at 20°C and 70°C was studied using the following techniques: the electrochemical impedance spectroscopy, linear polarization resistance, the electrical resistance measurements and weight loss measurements. In order to define surface morphological characteristics scanning electron microscopy was applied. Atomic force microscopy was used to identify the surface roughness of the mild steel sample with and without inhibitor. All the measurements performed indicated that TOFA/DETA imidazoline significantly decreased the corrosion rate when 70 ppm of corrosion inhibitor was added. Scanning electron micrographs of the carbon steel surface revealed that TOFA/DETA imidazoline inhibits the corrosion process, due to his ability to adsorb on the metal surface, while the atomic force microscopy confirmed that in the presence of TOFA/DETA imidazoline the average roughness of the mild steel surface was reduced.

Acknowledgments: Ministry of Education and Science, Republic of Serbia, III 45019

НМ П06

Elektrohemijska sinteza nanočestica srebra u rastvoru natrijum-alginata

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Brzo i efikasno dobijanje nanočestica metala visoke čistoće, precizno definisane veličine i oblika, značajno je za potencijalne primene naročito u biomedicini. Jednostavnom i čistom procedurom, elektrohemijska sinteza omogućava ostvarenje navedenih zahteva.

U ovom radu ispitivani su optimalni uslovi elektrohemijske sinteze nanočestica srebra u rastvoru Na-alginata. Variranjem koncentracije $AgNO_3$, gustine struje i vremena, različiti koloidni rastvori nanočestica srebra u Na-alginatu dobijeni su iz vodenih rastvora koji su sadržali 0,1 M KNO_3, 2 % Na-alginat i $AgNO_3$. Galvanostatska sinteza je vršena u ćeliji sa tri elektrode: dve Pt pločice u funkciji radne i pomoćne elektrode, i referentna zasićena kalomelova elektroda. UV-vis spektroskopijom je potvrđeno prisustvo nanočestica srebra, kao i porast koncentracije dobijenih nanočestica srebra sa porastom vrednosti parametara sinteze (koncentracija $AgNO_3$, gustina struje, vreme). TEM analizom je pokazano da su dobijene nanočestice sfernog oblika, prečnika 10-30 nm, nezavisno od vrednosti gustine struje. Potvrda izbora Na-alginata kao odgovarajućeg agensa stabilizacije pri sintezi nanočestica srebra je dobijena FTIR spektroskopijom i cikličnom voltametrijom, koje su ukazale na postojanje interakcija između nanočestica srebra i molekula Na-alginata, preko hidroksilnih i etarskih grupa, kao i atoma kiseonika iz prstena ostataka uronskih kiselina.

Electrochemical synthesis of silver nanoparticles in sodium alginate solution

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Fast and efficient synthesis of metal nanoparticles of high purity, with the precisely defined size and shape, is important for potential applications especially in biomedicine. With simple and clean procedure, the electrochemical synthesis makes these requests achievable.

Here, the investigation of the optimal conditions for the electrochemical synthesis of silver nanoparticles (AgNPs) in Na-alginate solutions is presented. By varying the concentration of the $AgNO_3$ solution, current density and time, different colloid solutions of AgNPs in Na-alginate solutions were obtained, from the aqueous solution containing 0.1 M KNO_3, 2 % Na-alginate and $AgNO_3$. Galvanostatic synthesis was performed in the three-electrode cell, having two Pt plates as a working and a counter electrode, and a saturated calomel electrode as a reference. UV-vis spectroscopy confirmed the presence of AgNPs, as well as the increase of AgNPs concentration with the increase of the parameters of synthesis ($AgNO_3$ solution concentration, current density and time). TEM analysis showed that the obtained AgNPs were spherical in shape, with the diameter size of 10-30 nm, regardless the current density. The choice of Na-alginate as the appropriate stabilizing agent for the AgNPs synthesis is confirmed by FTIR spectroscopy and cyclic voltammetry, indicating the interactions between AgNPs and Na-alginate molecule, through the hydroxyl and ether groups, as well as ring oxygen atoms in uronic acid residues.

НМ П07

Adhezija ćelija mišjih fibroblasta na površinu novog hidroksiapatit/fulerenol nanokompozita

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U ovom radu su predstavljeni rezultati bioloških testova u kojima je ispitivana razlika u sposobnosti mišjih fibroblasta (L929) da adheriraju na površinu sterilnih tableta hidroksiapatita (HAp) i hidroksiapatit/fulerenol nanokompozita (HAp/FNP). Pored dobrih površinskih osobina bitnih za adheziju fibroblasta, nanokompozit HAp/FNP čestice poseduju hidrofilne polianjonske nanočestice fulerenola, koje se odlikuju anti-inflamatornim, antioksidativnim i proliferativnim osobinama, što sve ukazuje na potencijalnu upotrebu HAp/FNP nanokompozita kao osnovne komponente za sintezu praškastih nanokompozita i prevlaka.

Ovaj rad je urađen kao deo projekta Ministarstva prosvete i nauke Republike Srbije, br. III 45005.

Cell adhesion of mouse fibroblasts to the surface of a novel hydroxyapatite/fullerenol nanocomposite

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This paper reports the results of biological tests in which we examined the difference in the ability of mouse fibroblasts (L929) to adhere to the sterile tablets of hydroxyapatite (HAp) and hydroxyapatite/fullerenol nanocomposite (HAp/FNP). Beside good surface properties suitable for adhesion of fibroblasts, nanocomposite HAp/FNP particles possess hydrophilic polyanion of fullerenol nano particles, which have anti-inflammatory, antioxidant and proliferative properties, which altogether can suggest that HAp/FNP nanocomposite has a great potential to be used as an initial powder source for the production of the array of nanocomposites and coatings.

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НМ П08

Adsorpcija azo boje Reactive Orange 16 na filmu hitozan/zeolit A

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U ovom radu je ispitivana adsorpcija anjonske azo boje Reactive Orange 16 na novi materijal, kompozit hitozana i zeolita A. Ispitivan je uticaj početne koncentracije i pH rastvora boje na kapacitet adsorpcije. Ispitivana su 2 različita kinetička modela radi određivanja kinetike i mehanizma adsorpcije Reactive Orange 16 na kompozit hitozan/zeolit A. Analizom rezultata ustanovljeno je da se kinetika adsorpcije Reactive Orange 16 boje na hitozan/zeolit odigrava po modelu pseudo-drugog reda. Maksimalni kapacitet adsorpcije jena pH 6 i iznosi 228 mg/g.

Adsorption of azo dye Reactive Orange 16 onto chitosan/zeolite film

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The adsorption of anionic azo dye Reactive Orange 16 onto new material – a composite ofchitosan and zeolite A was the object of this investigation. The influence of the inital concentration and pH of dye solution on the adsorption capacity was investigated. In order to determine kinetics of adsorption of Reactive orange 16 dye onto chitosan/zeolite A, two kinetic models were used. The results showed that the adsorption of Reactive Orange 16 dye onto chitosan/zeolite A was followed by pseudo-second order model. The maximum adsorption capacity was obtained at pH 6 and reached 228 mg/g.

НМ П09

Adsorpcione karakteristike geopolimera baziranog na metakaolinu

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Porozni materijali često imaju funkciju adsorbera pa se ovo istraživanje usmerilo ka ispitivanju adsorpcije dva metala na geopolimeru. Geopolimer je sintetički materijal koji je napravljen alkalnom aktivacijom metakaolina. Metakaolin je aluminosilikatni materijal generisan termalnom aktivacijom kaolinita. Mikrostrukturna karakterizacija dobijenog geopolimera je izvršena XRD i SEM analizom. Sadržaj Al i Si je određen uz pomoć ICP-OES. U ovom radu ispitana je i adsorpciona efikasnost geopolimera za različite hemijske elemente (Cu(II) i Cs(I)) u vodenom rastvoru. Sadržaj ovih elemenata je određen uz pomoć AAS. Rezultati su veoma zadovoljavajući, pogotovo za adsorpcionu efikasnost bakra. Ovo otkriće moglo bi da omogući razvoj optimizovanih procedura za prečišcavanje otpadnih voda, čime bi se obezbedilo alternativno rešenje za sprečavanje zagađenja životne sredine.

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Adsorption characteristics of metakaolin-based geopolymers

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Since porous materials often function as adsorbers, this study chose to investigate the adsorption of two metals by geopolymers. The geopolymer is synthetic material wich was made of the alkali activation of metakaolin. Metakaolin is an aluminosilicate material generated by thermal activation of kaolinite clay. The microstructure of obtained geopolymer has been characterized by X-ray diffraction and scanning electron microscopy. The content of Al and Si was determined using ICP-OES (ICP-AES/Perkin-Elmer). This paper examined the adsorption efficiency of the geopolymer for different elements (Cu(II) and Cs(I)) in aqueous solutions. Content of Cu(II) was determined using flame atomic absorption spectroscopy, while content of Cs(I) was determined using flame atomic emission. The results are very satisfactory, expecialy for copper adsorption efficiency. This discovery may facilitate the development of optimized procedures for wastewater trearment, thus providing an alternative solution to environmental damages caused by pollutants.

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НМ П10

Malodimne usporačke pirotehničke smeše na bazi mangana kao goriva

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U radu su prikazani rezultati ispitivanja trokomponentnih, malodimnih usporačkih pirotehničkih smeša na bazi mangana kao goriva, srednjeg prečnika čestice, d_{sr} = 4,5 µm i 23 µm, barijum-hromata d_{sr} = 4,5 µm i olovo-hromata d_{sr} = 1,08 µm kao oksidanasa i nitroceluloze u svojstvu veziva. Definisano je su sastavi, tehnološki parametri izrade i laboracije i izvršen je izbor pirotehničkog lanca pripaljivanja. Ispitane su funkcionalne karakteristike izrađenih sastava (linearna brzina sagorevanja, energetski potencijal, temperatura samozapaljenja). Ispitan je uticaj masenog udela goriva i masenog odnosa gorivo-oksidans na osnovne kakteristike sagorevanja. Promenom masenog odnosa oksidanasa i variranjem sadržaja mangana, dobijene su brzine sagorevanja u širokom opsegu od 1,69 mm/s do 10,86 mm/s.

Smokeless delay pyrotechnic mixtures based on manganese as a fuel

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This paper presents the investigation results of ternary, smokeless delay pyrotechnic mixtures based on manganese as a fuel, of middle particle diametert d_{mid} = 4,5 µm and 23 µm, barium chromate d_{mid} = 4.5 µm and lead chromate d_{mid} = 1.08 µm as oxidants and nitrocellulose as a binder. Various delay compositions, technological production, laboration parameters and pyrotechnical ignition chains were defined. The influence of the mass fraction of fuel mass and fuel to oxidant ratio on combustion characteristics. Changes in the oxidants mass ratio and manganese content resulted generation of a wide scale of linear burning rates going from 1.69 mm/s up to 10.86 mm/s.

НМ П11

Modifikacija površine nano-SiO_2 čestica za imobilizaciju lipaze iz *Candida rugosa*

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Zbog brojnih nedostataka koji postoje pri upotrebi nativnih enzima različiti pristupi i materijali korišćeni su u cilju razvoja efikasnog imobilisanog sistema. Među nosačima koji se koriste za imobilizaciju enzima neorganski materijali imaju prednost u odnosu na, nestabilnije, organske nosače, ali je zbog male gustine funkcionalnih grupa njihovu površinu najčešće potrebno prethodno modifikovati.

Kao nosač za imobilizaciju lipaze iz *Candida rugosa* u ovom radu su korišćene nano-SiO_2 čestice. Njihova površina je najpre, u cilju uvođenja amino grupa, modifikovana pomoću 3-aminopropiltrimetoksisilana (APTMS), a zatim je ovako dobijeni aminopropil silika nosač (SiO_2-APTMS) pre vezivanja lipaze aktiviran pomoću trihlortriazina (TCT). Uspešnost modifikacije i prisustvo uvedenih grupa potvrđena je FT-IR spektroskopijom. Takođe, ispitan je uticaj koncentracije lipaze na aktivnost imobilisanog preparata i u tom cilju je koncentracija lipaze varirana u opsegu od 7,4 do 108 IU cm^{-3}, a dobijeni imobilizati su pokazali visoku aktivnost od 128 IU g^{-1} nosača.

Rad je proistekao iz istraživanja u okviru projekata koje finansira Ministarstvo prosvete i nauke Republike Srbije (projekti 172013 i III 46010)

Surface modification of silica nanoparticles for immobilization of lipase from *Candida rugosa*

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Due to many limitations that exists when enzymes are used in the native form, numerous approaches and materials have been explored in order to develop an efficient immobilized system. Among present carriers used for immobilization, inorganic materials have advantage compared to less stable organic ones, but due to small amount of active functional groups their surface usually needs to be chemicaly modified.

The present study is focused on the immobilization of lipase from *Candida rugosa* on nano-SiO_2 particles. In order to introduce amino groups on the surface, nano particles were treated with 3-aminopropyltrimethoxysilane (APTMS), and then, before the immobilization of lipase, obtained aminopropyl silica carrier (SiO_2-APTMS) was activated with trichlorotriazine (TCT). Modification of the surface and the presence of introduced groups was confirmed with FT-IR spectroscopy. Also, the influence of the initial enzyme concentration on the activity of immobilized preparation was examined. The lipase concentartion was varied in the range from 7.4 to 108 IU cm^{-3}, and preparations showed a great activity of 128 IU g^{-1} carrier.

The authors are grateful for financial support to the Ministry of Education and Science of the Republic of Serbia (projects: 172013, III 46010).

НМ П12

Complexes of pectin and poly(ethylene glycol)

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The aim of this study was to synthesize complexes of pectin and poly (ethylene glycol), in order to improve the characteristics of pectin-based films and investigated the possibility of interaction of these polymers. Poly (ethylene glycol) has properties that make it very interesting for a variety of biomedical applications - a biocompatible, non-toxic, soluble in water, it does not interfere with the immune system and can easily be removed from the organism. Pectin, because of its extraordinary gelling ability has been applied in systems for controlled release of therapeutics and transport through the gastrointestinal tract.

Samples were prepared with different amounts of poly (ethylene glycol) (PEG-400, PEG-9000), while the type and concentration of pectin (4 mass %) were constant. Changing the temperature and pH of the reaction mixture resulted in products with different structural characteristics.

FTIR spectroscopy confirmed the establishment of hydrogen bonds between pectin and polyethylene glycol, and their intensities depend on the molecular weight of PEG used. SEM microscopy showed the difference in the structure of the complex pectin-PEG 9000 and pectin-PEG 400 as a function of temperature and pH of the reaction mixture.

Kompleks pektina i poli(etilen glikola)

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Cilj ovog rada bila je sinteza kompleksa pektina i poli(etilen glikola), kako bi se poboljšale karakteristike filmova na bazi pektina i ispitala mogućnost interakcije ovih polimera. Poli(etilen glikol) ima svojstva koja ga čine vrlo interesantnim za različite biomedicinske primene – biokompatibilan je, nije toksičan, dobro se rastvara u vodi, ne ometa imuni sistem i lako se odstranjuje iz organizma. Pektin, zbog svojih izvanrednih gelirajućih sposobnosti, našao je primenu kod sistema za kontrolisano otpuštanje i transport terapeutika kroz gastrointestinalni trakt.

Sintetisani su uzorci sa različitim količinama poli(etilen glikola) (PEG-400, PEG-9000), dok su tip i koncentracija pektina (4 mas%) bili konstantni. Promenom temperature i pH reakcione smeše dobijeni su proizvodi različitih strukturnih karakteristika. FTIR spektroskopijom potvrđeno je uspostavljanje vodoničnih veza između pektina i poli(etilen glikola) i njihov intenzitet zavisi od molarne mase poli(etilen glikola). Razlike u strukturi pektin-PEG 9000 i pektin-PEG 400 kompleksa potvrđene su SEM mikroskopijom.

НМ П13

Uticaj sastava na procesibilnost livenih kompozitnih eksploziva

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U radu je ispitan uticaj sastava na procesibilnost livenog kompozitnog eksploziva. Prema planu eksperimenta, tehnološkim postupkom livenja izrađeno je 14 različitih eksplozivnih sastava kod kojih je variran maseni udeo tri komponente: termoumrežavajućeg polimernog veziva - HTPB od 15 do 20 %, amonijum-perhlorata – AP od 0 do 20 %, i udeo magnezijuma u ukupnoj količini od 30 % metala, tj. 0 % do 30 % aluminijuma je zamenjeno pirolitičkim magnezijumom.

Kompatibilnost komponenata je potvrđena mikrokalorimetrijskom metodom na uređaju LKB Bioactivity Monitor 2277. Ispitana je zavisnost viskoziteta od sastava i od vremena. Viskozitet je meren na 50 °C na Brookfield-ovom viskozimetru tipa RVT, po završetku homogenizacije smeše i dodavanja umreživača na svakih 15 min u toku 90 min. Gustine uzoraka određene su prema metodi MIL 286B, na 25 ºC.

Pokazalo se da na reološko ponašanje ispitanih sastava najveći uticaj ima udeo HTPB, a potom udeo AP. Veća količina Mg kod sastava sa istim udelima ostalih komponenata uzrokuje brži porast i više vrednosti viskoziteta, što uzrokuje smanjenje vremena procesibilnosti (livljivosti) ovih sastava, dok veći udeo HTPB i AP imaju povoljan uticaj.

Cast composite explosives composition influence on processability

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Influence of cast composite explosives composition on their psocessability is investigated. According to a plan of experiment, 14 different explosive compositions were made by technology of casting. Three components content was varied: thermosetting polymer binder – HTPB from 15 to 20 %, ammoniumperchlorate – AP from 0 to 20 %, and magnesium participation in total metal content of 30 %, that is 0 – 30 % of aluminium was replaced by pyrolitic magnesium.

Compatibility of components was confirmed by the microcalorimeter LKB Bioactivity Monitor 2277. Viscosity dependance of composition and time is determined. Viscosity was measured at 50 °C in the Brookfield viscometer's type RVT, after homogenization of the mixture and curing agents added, every 15 min during 90 min. Densities of the samples were determined by the method of MIL 286B at 25 º C.

It turned out that HTPB share had the largest effect on the rheological behavior of the examined compositions, then the share of AP. The higher amount of Mg in compositions with the same share of other components caused faster growth and higher values of viscosity, thus reducing the time of processability (casting) of the composition. Greater content of HTPB and AP have favorable influence.

НМ П14

Elektrohemijsko generisanje katalizatota za Ferijeovo premeštanje i tia-Majklovu adiciju sa rastvorne cirkonijumove elektrode

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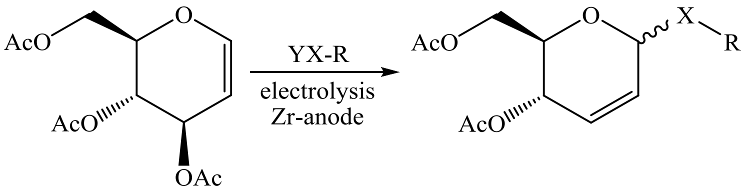
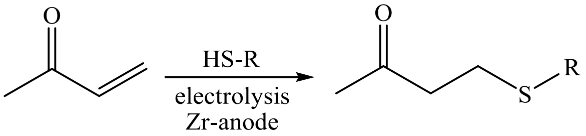
Elektrohemijski generisani katalizator sa rastvorne cirkonijumove elektrode uspešno je primenjen za alilno premeštanje peracetilovanog D-glukala u prisustvu S-nukleofila (Ferijeva reakcija) i adiciju S-nukleofila na dvostruku vezu ugljenik-ugljenik metil vinil ketona (tia-Majklova reakcija). Prva reakcija daje 2,3-nezasićene derivate D-glukopiranoze (pseudoglikale), a druga odgovarajuće 5-tia-2-alkanone.



X=S, Y=H, R=alkyl, aryl, carbalkoxyalkyl
X=CH_2, Y=Si$(CH_3)_3$, R=-CH=CH_2



R=alkyl, aryl, carbalkoxyalkyl

Electrochemical generation of a catalyst for Ferrier rearrangement and thia Michael addition from a sacrificial zirconium anode

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The electrochemically generated catalyst from a sucrificial zirconium anode successfully promoted the allylic rearrangement of peracetylated D-glucal in the presence of S-nucleophiles (Ferrier reaction) and conjugate addition of S-nucleophiles to carbon-carbon double bond of methyl vinyl ketone (thia-Michael reaction). The first reaction afforded the corresponding 2,3-unsaturated D-glucopyranose (pseudoglycal), whereas the second one gave the corresponding 5-thia-2-alkanones.

НМ П15

Elektrohemijska sinteza i karakterizacija samo-dopovanog polianilina

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Iako atraktivan za praktičnu primenu, PANI ima određena ograničenja zbog pojave degradacionih proizvoda prilikom sinteze i ciklizacije kao i gubitka električne provodljivosti na pH vrednostima većim od 3. Otkriveno je da samo-dopovani PANI ima proširen rang pH vrednosti u kojima pokazuje električnu provodljivost i elektrohemijsku aktivnost. U ovom radu uspešno je, elektrohemijskim putem, formirana elektroda na bazi polianilina pri konstantnoj gustini struje od 2,0 mA cm^{-2} tokom 600 s iz sledećih rastvora: 1) 1,0 M HCl + 0,2 M anilin, 2) 1,0 M HCl + 0,17 M anilin + 0,03 M MABA, 3) 1,0 M HCl + 0,15 M anilin + 0,05 M MABA, 4) 1,0 M HCl + 0,1 M anilin + 0,1 M MABA. Pokazano je da sadržaj provodnog oblika zavisi od izbora rastvora za sintezu i da zavisi od udela MABA. Najznačajniji ograničavajući faktor u primeni PANI elektrode jeste sklonost ka pojavi degradacionih proizvoda, pa je zbog toga vršena karakterizacija PANI elektrode. U rastvoru HCl svi uzorci su bili relativno stabilne aktivnosti i na vrednostima 0,4 V - 0,5 V nalaze se pikovi koji su karakteristični za pojavu degradacionih proizvoda. U rastvorima soli, pokazano je da samo-dopovani uzorci pokazuju manji pad aktivnosti.

Electrochemical synthesis and characterization of self-doped polyanilines

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Although attractive for practical use, PANI has certain limits due to the appearance of degradation products during the synthesis and cyclization and loss of electrical conductivity at pH values above 3. It has been found that self-doped PANI has an extended pH range of electric conductivity and electrochemical activity. In this essey, in an electrochemical way, an electrode has been successfuly made based on polianiline, with constant current density of 2,0 mA cm^{-2} during 600 s from the following solutions : 1) 1,0 M HCl + 0,2 M aniline, 2) 1,0 M HCl + 0,17 M aniline + 0,03 M MABA, 3) 1,0 M HCl + 0,15 M aniline + 0,05 M MABA, 4) 1,0 M HCl + 0,1 M aniline + 0,1 M MABA. It has been shown that the content of conductive form depends on the choise of the solution for synthesis and depends on share of MABA. The most important limiting factor in the usage of PANI electrode is a tendency to appearance of degradation products, therefore we have executed caracterisation of PANI electrode. In the solution of HCl all the samples had a relatively stable activity and on the values 0,4 V - 0,5 V peeks are shown, which are caracteristic for the appirance of degradation products. In the solution of salts, it is shown that the self-doped samples show a lesser fall in activity.

НМ П16

Uticaj nafiona na elektrokatalitčku aktivnost platine – poređenje Pt/C katalizatora i polikristalne platine

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Razvoj novih katodnih materijala za PEM gorivne ćelije uključuje fundamentalno ispitivanje njihovih elektrokatalitičkih svojstava kao i ispitivanje ponašanja u MEA konfiguraciji. Rezultate ova dva načina analize performansi katalizatora često je teško direktno korelisati. Uticaj Nafiona na elektrokatalitičku aktivnost Pt/C katalizatora i polikristalne platine za reakciju redukcije kiseonika analiziran je korišćenjem ciklične voltametrije sa rotirajućom disk elektrodom. Održavajući konstantnu količinu Pt/C katalizatora nanetu na rotirajući disk, uočeno je da povećanje sadržaja nafiona u katalitičkom sloju do određenog procenta dovodi do povećanja elektroaktivne površine i masene aktivnosti katalizatora za reakciju redukcije kiseonika. S druge strane, povećanje debljine nafionskog sloja na polikristalnom platinskom disku dovodi do smanjenja elektroaktivne površine i elektrokatalitičke aktivnosti za redukciju kisoenika. Uočene razlike u ponašanju Pt/C elektrokatalizatora i polikristalne Pt su iskorišene za objašnjene uticaja nafiona na performanse PEM gorivne ćelije.

The effects of Nafion on electrocatalytic activity of platinum – comparison of Pt/C catalyst and Pt-poly

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Development of new cathode material for PEM fuel cell includes investigation of their fundamental electrochemistry as well as behavior in MEA configuration. Rather often the correlation of these two sets of results is hard to be done. The effects of nafion on electrocatalytic activity of Pt/C catalyst and Pt-poly electrode have been analyzed using rotating disk electrode technique coupled with cyclic voltammetry. By keeping the amont of Pt/C catalyst loaded at rotating disk constant, it was observed that increase of nafion content in catalyst layer up to a certain amount increases electroactive surface area and mass activity of Pt/C catalyst towards oxygen reduction. On the other hand, increase of nafion layer thickness on rotating Pt-poly disk decreases electroactive surface area, as well as electrocatalytic activity towards oxygen reduction. Observed differences in electrochemical behavior of Pt/C catalyst and Pt-poly served as a basis for the explanation of the effects of nafion on the PEM fuel cell performance.

НМ П17

Optimizacija uslova elektrohemijske sinteze nanočestica srebra u rastvoru poli(vinil alkohola)

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Uočeno je da nanokristalno srebro pokazuje efikasnu antimikrobnu aktivnost u odnosu na širok spektar mikroorganizama. Efikasnost dejstva je uslovljena čistoćom metala, kao i veličinom i oblikom nanočestica. Elektrohemijska sinteza se pokazala pogodnom za dobijanje nanočestica srebra željenih karakteristika.

U ovom radu ispitivani su optimalni uslovi za elektrohemijsku sintezu nanočestica srebra u rastvoru poli(vinil alkohola), PVA, variranjem vrednosti gustine struje, u opsegu od 5 do 50 mA cm^{-2}. Za sintezu su korišćeni 10 % vodeni rastvori PVA, sa 0,1 mol dm^{-3} KNO_3 i 3,9 10^{-3} mol dm^{-3} $AgNO_3$. Galvanostatska sinteza je vršena u ćeliji koja je sadržala tri elektrode, dve Pt pločice kao radnu i pomoćnu elektrodu, i zasićenu kalomelovu elektrodu kao referentnu. Prisustvo nanočestica srebra je potvrđeno UV-vis spektroskopijom. Takođe, utvrđen je i trend rasta koncentracije dobijenih nanočestica srebra sa porastom vrednosti gustine struje. TEM analizom je pokazano da su dobijene nanočestice sfernog oblika, prečnika od 10 do 30 nm. Uočeno je da se na nižim vrednostima gustine struje dobija veći broj manjih nanočestica srebra. FTIR spektroskopijom je pokazano postojanje interakcija između nanočestica srebra i molekula PVA, preko hidroksilnih grupa.

The optimization of the electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol) solution

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It is shown that nanocrystalline silver exhibits efficient antimicrobial activity against wide spectrum of microorganisms. The effects are influenced by the metal purity, as well as by the size and shape of nanoparticles. The electrochemical synthesis is quite suitable for obtaining the silver nanoparticles of the desired characteristics.

In this work, the optimal conditions for the electrochemical synthesis of silver nanoparticles in the solution of poly(vinyl alcohol), PVA, were investigated, by varying the value of the applied current density, ranging from 5 to 50 mA cm^{-2}. The galvanostatic synthesis is performed using aqueous solutions of 10 % PVA, containing 0.1 mol dm^{-3} KNO_3 and 3.9·10^{-3} mol dm^{-3} $AgNO_3$, in three-electrode electrochemical cell, consisting of two Pt plates as a working and a counter electrode, and a saturated calomel electrode as a reference. The presence of silver nanoparticles was confirmed by UV-vis spectroscopy. Also, the increase in silver nanoparticle concentration, as a consequence of the increase in the value of the applied current density, is observed. TEM analysis shown that the obtained silver nanoparticles were spherically shaped, with the diameter between 10 and 30 nm. It is also observed that the synthesis at lower values of the applied current density lead to the higher number of smaller nanoparticles. FTIR spectroscopy indicates the interactions between silver nanoparticles and PVA molecules, through hydroxyl groups.

НМ П18

Uticaj gustine struje na kapacitet punjenja/pražnjenja elektrode na bazi polianilina

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Jedna od mnogobrojnih potencijalnih primena elektroprovodnih polimera je izrada materijala elektroda primarnih i sekundarnih elektrohemijskih izvora električne energije. Imajući u vidu prednosti i jednostavnost elektrohemijske sinteze, u ovom radu je elektrohemijski formirana elektroda na bazi polianilin-*para*-toluensulfonata, polimerizacijom anilina u rastvoru *para*-toluensulfonske kiseline. Određena je aktivna masa dobijenog polimera na bazi polianilna i ona iznosi 1,31 mg kao i količina naelektrisanja raspoloživa za razmenu i ona iznosi 14 % od ukupne količine naelektrisanja potrebne za sintezu polianilina. Na osnovu eksperimenata ciklične voltametrije procenjene su anodne i katodne granice potencijala koje će biti primenjivane tokom ciklizacije (punjenje/pražnjenje). Utvrđena je pojava degradacionih proizvoda na vrednostima većim od 0,5 V. Elektroda na bazi polianilina je pokazala najbolje elektroprovodne osobine pri gustini struje od 0,5 mA cm^{-2}.

The influence of current density at capacity of charging/discharging polyaniline-based electrode

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One of many potential applications of the electroconducting polymers is the development of electrode material in primary and secondary electrochemical power sources. Given the advantages of simplicity and electrochemical synthesis, in this work electrode based on polyaniline-*p*-toluenesulfonate was electrochemically formed, with polymerization of aniline in the solution of *para*-toluenesulfonic acid. Active mass of the obtained polyanilne-based polymer is determined and it is 1,31 mg. The amount of charge available for exchange is also determined and it is 14 % of the total amount of charge needed for the synthesis of polyaniline. On the basis of cyclic voltammetry experiments, anodic and cathodic potential limit was evaluated, which will be applied during the cyclization (charging/discharging). There was the appearance of degradation products at values greater than 0,5 V. The polyaniline-based electrode showed the best electrically conductive properties at current density of 0,5 mA cm^{-2}.

This work was funded by the Ministry of Education and Science of Serbia (Project 172061) and UNESCO-L'OREAL National Fellowships Programme for Young Women in Life Sciences.

Теоријска хемија

TX O6

Trimeri benzena u kristalnim strukturama malih i srednjih molekula i njihova energetska kvantifikacija

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Nekovalentne interakcije u kojima učestvuju aromatični prstenovi igraju važnu ulogu u procesima hemijskog i biološkog prepoznavanja, supramolekulskoj hemiji i kristal-inženjeringu. U ovoj studiji ispitivani su trimeri benzena u kristalnim strukturama smeštenim u Kembričkoj bazi strukturnih podataka. Trimerom benzena smatran je svaki klaster od tri molekula benzena u kome su bar dva rastojanja između centroida prstenova kraća od 6,0 Å. Na osnovu geometrijskih parametara izdvojenih kontakata, pronađeno je 15 tipova trimera benzena. Tri najzastupljenija trimera sadrže po dva benzen-benzen kontakta T-tipa, dok su najudaljeniji molekuli paralelni. Optimizacijom trimera DFT-D2 metodama utvrđeno je da su sve zastupljenije strukture lokalni minimumi na potencijalnoj površini trimera benzena. Globalni minimum ima energiju od -9,09 kcal/mol i u njemu svi molekuli međusobno interaguju, gradeći strukturu nalik na trougao. Najzastupljeniji trimeri u kristalnim strukturama imaju više energije (oko -6 kcal/mol), ali su zastupljeniji u kristalnim strukturama od globalnog minimuma jer njihove geometrije omogućavaju građenje više simultanih interakcija, kao i dalje agregiranje na isti način.

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Benzene trimers in crystal structures of small and medium-sized molecules and their energy quantification

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Noncovalent interactions involving aromatic rings play important role in chemical and biological recognition processes, supramolecular chemistry, and crystal-engineering. Here we present the study of benzene trimers in crystal structures archived in Cambridge Structural Database (CSD). Benzene trimers were described as clusters containing three benzene molecules with at least two centroid-centroid distances shorter than 6.0 Å. Based on geometrical parameters of the contacts, 15 types of benzene trimers were found. The three predominant benzene trimers each contain two T-shaped benzene-benzene contacts, while the farthest molecules are parallel. By optimizing the trimers using DFT-D2 methods, it was shown that all predominant structures are minima on potential energy surface of benzene trimer. The energy of triangle-like global minimum is -9.09 kcal/mol, with all molecules interacting with each other. Predominant trimers have higher energies (about -6 kcal/mol), but they dominate crystal structures because their geometries are suitable for more simultaneous interactions and further aggregation in a similar fashion.

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TX O7

Volfram karbid kao podloga za elektrokatalizatore – teorijska studija

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Tanki metalni slojevi platine (Pt) i paladijuma (Pd) na W- i C-terminiranoj površini WC(0001) su analizirani primenom teorije funkcionala gustine kao model-sistemi elektrokatalizatora za izdvajanje/oksidaciju vodonika. Pt i Pd se snažno vežu za površinu WC(0001), a formiranje monoatomskog sloja metala je praćeno značajnim promenama elektronske strukture u odnosu na površine Pt(111) i Pd(111). U slučaju formiranja dvoatomskog sloja elektronska struktura je određena skoro isključivo razlikom konstanti rešetki Pt i Pd u odnosu na WC. Uočena je veza energije adsopcije vodonika na analiziranim površinama sa elektronskom strukturom, što je dalje povezano sa njihovom elektrokatalitičkom aktivnošću za reakciju izdvajanja vodonika. Ni za jedan od analiziranih sistema nije očekivano da po elektrokatalitičkim osobinama prevaziđe Pt(111). Na osnovu dobijenih rezultata zaključeno je da WC može da zameni platinu u slučaju nanočestičnih katalizatora u formi jezgro-omotač, ali da, imajući u vidu inherentnu elektrokatalitičku aktivnost Pt, nema značaj, osim u smislu smanjenja količine platine i cene elektrokatalizatora.

Tungsten carbide as an electrocatalyst support – theoretical study

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Platinum (Pt) and palladium (Pd) overlayers on W- and C-terminated WC(0001) surface have been studied using density functional theory approach as a model systems for hydrogen oxidation/evolution reaction (HOR/HER) electrocatalysts. While strong adhesion of metal monolayers to the support was evidenced, monolayer formation is followed by significant modification of the electronic structure with respect to clean Pt(111) and Pd(111). When Pt or Pd bilayer is formed electronic structure is predominantly determined by strain effect due to lattice mismatch between Pt(Pd) and WC support. Hydrogen adsorption energies at studied overlayers have been correlated to electronic structure and further related to the differences in their electrocatalytic activity towards HER. None of the investigated systems are expected to surpass Pt(111) surface in terms of HER electrocatalytic activity. Based on the obtained results it was proposed that WC might be good candidate for the substitution of bulk Pt in the core-shell arrangement of nanosized Pt electrocatalysts, but no benefits from WC support in terms of HER/HOR intrinsic activity other than reduction of Pt loading and the price of the catalyst should be expected.

ТХ П01

Da li su CH/O interakcije linearne? Piridin-voda interakcije

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CH/O interakcije su veoma važne za mnoge hemijske sisteme i supramolekulsku hemiju, pri čemu se energija ovih interakcija uglavnom kreće od -0,3kcal/mol do -3,8 kcal/mol.[1] CH/O interakcije su ispitivane analizom kristalnih struktura koje sadrže nekoordinovane monosupstituisane molekule piridina i molekule vode iz Kembričke kristalografske banke (CSD). Kontakt je smatran CH/O interakcijom ukoliko je rastojanje između vodonikovog atoma piridina i atoma kiseonika iz molekula vode manje od 2.9 Å i ugao $\alpha \geq 110°$.[2] U CSD-u pronađeno je 747 CH/O interakcija od kojih 545 imaju simultane vodoninčne veze sa atomom azota iz piridina. Daljom analizom ovih struktura pokazano je da najstabilnije geometrije imaju molekul vode između C-H veza piridina. Ab-initio proračuni, urađeni na MP2/cc-pVQZ nivou, pokazali su da je najjača interakcija bifurkovana sa energijom $\Delta E_{CCSD(T)limit}$ = -2.30kcal/mol za sistem piridin/voda i $\Delta E_{CCSD(T)limit}$ = -2.69kcal/mol kada je uključena i vodonična veza sa azotom.

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Are CH/O interactions linear? Pyridine-water interaction

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The CH/O interactions are very important in many chemical systems and supramolecular chemistry, with the interaction energy usually between -0.3 kcal/mol and -3.8 kcal/mol.[1] Study of CH/O interactions is based on analysis of crystal structures archived in the Cambridge Structural Database (CSD) involving non-coordinated monosubstituted pyridine molecules and water. A contact was considered as a CH/O interaction if the distance between a hydrogen atom of pyridine molecule and a water oxygen atom was less than 2.9 Å and angle $\alpha \geq 110°$.[2] In CSD, we found 747 CH/O interactions, of which 545 interacions were simul-atanous with additional hydrogen bond with nitrogen atom of pyridine molecule. Further analysis of these structures showed that CH/O interactions favor geometries with oxygen atoms between adjacent C-H bonds of pyridine molecule. Ab-initio calcuations, performed on MP2/cc-pVQZ level, showed that the strongest interaction is bifurcated with energy of $\Delta E_{CCSD(T)limit}$ = -2.30kcal/mol for pyridine and water system and $\Delta E_{CCSD(T)limit}$ = -2.69kcal/mol for interaction with hydrogen bond.

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1. R. K. Castellano, *Curr. Org. Chem.*, **8.** (2004) 845-865.
2. D. Ž. Veljković, G. V. Janjić, S. D. Zarić, *CrystEngComm*, **13.** (2011) 5005.

ТХ П02

Uticaj prirode susednih atoma vezanih za Cl na jačinu Cl...π interakcija

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Cl···π interakcije su ispitivane analizom kristalnih struktura iz Kembričke kristalografske banke (CSD). Izolovane su strukture sa Cl..π kontaktima koje smatramo interakcijama ukoliko je rastojanje između centroida benzenovog prstena i Cl atoma od 3.0 Å do 3.5 Å i ugao δ (ugao vektora X-Cl veze i ravni normalne na prsten benzena) od 0° do 90°. U CSD-u je pronađeno 4203 struktura sa 6020 Cl···π kontakata.

Cl···π kontakte podelili smo prema vrsti atoma (X) za koji je Cl vezan u 4 grupe (X = metal, nemetali osim C, aromatični i nearomaticni C atomi). Najviše kontakata pronađeno je sa nearomatičnim C atomima, 4215 kontakata. Sa aromatičnim C atomima je pronađeno 709 kontakata, sa metalnim atomima 974 i nemetalnim osim C atoma 116 kontakata.

The influence nature of neighboring atoms bonded to Cl to the strength of Cl ... π interactions

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Study of Cl···π interactions is based on analysis of crystal structures archived in the Cambridge Structural Database (CSD). Isolated Cl .. π contacts considered as interactions are those with the distance between the centroid of benzene ring and Cl atom between 3.0 Å and 3.5 Å and angle δ (angle of vector X-Cl bond and to the plane normal of benzene ring) is between 0° do 90°. In The CSD it was found 4203 structures and 6020 Cl···π contacts.

Cl···π contacts are distributed by atoms (X), which is bonded to Cl, in 4 groups (X = metal, all non-metals except C, aromatic and aliphatic C atoms). It was found that the most of the contacts are with aliphatic C atoms, 4215 contacts. With aromatic C atoms 709 contacts were found, with metal atoms 974 and with non-metal except C atom 116 contacts.

This work was supported by Ministry of Education, Science and Technological Development of Republic of Serbia (grant No. 172065).

ТХ П03

Теоријско испитивање CH/O интеракција између нуклеинских база и молекула воде

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CH/O интеракције спадају у најзначајније нековалентне интеракциеа у природи. У нашем претходном раду испитивали смо CH/O интеракције између C-H група ароматичних молекула и различитих типова акцептора.[1] Резултати су показали да ароматични C-H донори не показују јасну тежњу ка грађењу линеарних контаката и да та тежња зависи од типа атома или групе у *o*-положају у односу на интерагујућу C-H групу.
У овом раду урађено је кристалографско испитивање геометрије CH/O интеракција између C-H група нуклеинских база и атома кисеоника из молекула воде. Урађена је анализа података добијених из Кембричке банке кристалографских података (CSD). Резултати анализе кристалографских података су показали да C-H фрагменти из нуклеинских база немају јасну тежњу ка грађењу линеарних контаката са кисеоником из молекула воде. Ово је у складу са нашим претходним резултатима за геометрију CH/O интеракција ароматичних CH група. Изведени закључци могу бити од великог значаја за препознавање CH/O интеракција у биолошким молекулима који садрже нуклеинске базе.

Овај рад је подржан средствима Министарства просвете и науке (пројекат бр. 172065).

Theoretical study of f CH/O interactions between nucleic bases and water molecule

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CH/O interactions are one of the most important noncovalent interactions in nature. In our previous work, we performed systematic study of the CH/O interactions between aromatic CH groups and different acceptors.[1] Results showed that the aromatic C-H donors do not show strong preference for linear contacts and that the preference for linear contact depends on the type of the atom or group in *o*-position to the interacting C-H group.
In this work, we performed crystallographic study of geometry of CH/O interactions formed between C-H groups from nucleic bases and oxygen atom from water molecule. Study was performed by analyzing data archived in the Cambridge Structural Database (CSD). The results of crystallographic analysis showed that C-H fragments from nucleic acids do not show clear preference for linear contacts with oxygen atom from water. This is in agreement with our previous results for CH/O interactions of aromatic CH groups. These conclusions could be very important for recognizing CH/O interactions in biomolecules containing nucleic bases.

1. D. Ž. Veljković, G. V. Janjić, S. D. Zarić, *CrystEngComm*, **13.** (2011).

ТХ П04

Modelovanje emisija amonijaka, metana i ne-metanskih isparljivih organskih jedinjenja neuronskim mrežama

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U ovom radu prikazan je razvoj modela zasnovanog na neuronskim mrežama (*Artificial Neural Network* - ANN) za predviđanje emisije ne-metanskih organskih jedinjenja (NMVOC), amonijaka (NH_3) i metana (CH_4), na nacionalnom nivou. Kao ulazni podaci modela korišćeni su dostupni ekonomski podaci i podaci o indikatorima održivog razvoja za evropske zemlje. Korišćenjem nekoliko statističkih indikatora, rezultati dobijeni ANN modelom upoređeni su sa modelom koji se zasniva na višestrukoj linearnoj regresiji (*Multiple Linear Regression* – MLR). ANN model, dao je odlične rezultate kod dvogodišnjeg predviđanja emisije na nacionalnom nivou. Kod dvogodišnjeg predviđanja rezultati ANN modela imaju *index of agreement (IA)* jednak 0,94 za NMVOC, 1,00 za NH_3 i 1,00 za CH_4 (max. 1), što je znatno bolje od rezultata koji su dobijeni MLR modelom *IA*=0,38 pri modelovanju emisije NMVOC, dok su dobijene vrednosti *IA* bile samo za nijansu lošije kod modelovanja emisije NH_3 i CH_4: 0.97, i 0.98, redom. Pomoću ovog modela mogu se predvideti vrednosti emisije NMVOC, NH_3 i CH_4, značajne za sprovođenje nacionalnih strategija održivog razvoja i zaštite životne sredine.

Zahvalnica: Istraživanja su realizovana u okviru naučnog projekta Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, broj 172007.

Modelling of NH_3, CH_4 and NMVOC emissions using Artificial Neural Networks

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This study presents the development of an Artificial Neural Network (ANN) model for the prediction of NH_3, CH_4 and NMVOCs emissions. Available sustainability, economical and industrial parameters for European countries were used as input. The performance of the ANN models were compared with multiple linear regression (MLR) models, using multiple statistical indicators. The ANN model analysis has shown excellent performance and demonstrated that a forecast of NH_3, CH_4 and NMVOCs emission can be made successfully and accurately for up to two years. The forecasts provided by the ANN model, with the index of agreement (*IA*) of 0.94 for NMVOCs, 1.00 for NH_3 and 1.00 for CH_4 (max. 1), was much better than the one obtained from the MLR model (*IA*=0.38) in case of modeling NMVOCs emission, while for modeling NH_3 and CH_4 emission, MLR gave lower but also good *IA* of 0.97 for NH_3 and 0.98 for CH_4. This model can predict NH_3, CH_4 and NMVOCs emission, which are necessary for the implementation of sustainable development strategies and environmental management policies.

TX П05

Uticaj orjentacije akva liganada na stabilnost akva-metalnih kompleksa

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Svojstva kompleksa zavise od orjentacije liganada. Orjentacija koordinovanih molekula ili jona zavisi od efekata stabilizacije kristalnog polja i od intramolekulskih interakcija sa ostalim ligandima[1]. U ovom radu je proučavan uticaj orjentacije akva liganada na stabilizaciju heksaakva kompleksa Zn(II) i Ca(II). U Kembričkoj banci podataka (CSD) pretraživane su kristalne strukture heksaakva kompleksa Zn(II) i Ca(II) jona. Upoređivanje geometrije Zn(II) i Ca(II) kompleksa pokazuje da orjentacija akva liganada nema iste tendencije. Akva ligandi, u heksaakva-Zn(II) kompleksima imaju tendenciju ka tetraedarskoj geometriji u odnosu na metalni jon, dok u heksaakva-Ca(II) kompleksima akva ligandi nastoje da se orjentišu tako da se akva ligand i metalni jon nalaze u istoj ravni. Rezultati *ab initio* proračuna pokazuju da orjentacija akva liganada ima uticaj na stabilizaciju heksaakva-metal kompleksa.

Influence of aqua ligands orientation on stablity of of aqua-metal complexes

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The properties of complexes depend on orientations of ligands. The orientation of coordinated molecules or ions depends on crystal field stabilization effects and intramolecular interactions with other ligands [1].

The influence of aqua lignads orientation on stability of hexaaqua complexes of Zn(II) and Ca(II) ions were studied. The Cambridge Structural Database (CSD) was searched for crystal structures of hexaaqua complexes of Zn(II) and Ca(II) ions. A comparison of geometries of Zn(II) and Ca(II) complexes, shows that orientation of aqua ligands do not have the same tendencies. Aqua ligands, in hexaaqua-Zn(II) complexes, have the tendency to tetrahedral geometry, respect to metal ion, while in hexaaqua-Ca(II) complexes, aqua ligands prefers the orientations where aqua ligan and metal ion share the same plane. The results of *ab initio* calculations show that the orientation of aqua ligands has the influence on stability of hexaaqua-metal complexes.

1. A. A. Rakić, V. B. Medaković, S. D. Zarić, *Journal of Inorganic Biochemistry*, **100** (2006) 133–142.

ТХ П06

Paralelne interakcije porfirinskih liganada

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Steking interakcije između aromatičnih molekula ili fragmenata intenzivno su proučavane.[1] Međutim, publikovano je nekoliko radova u kojima i helatni prstenovi, sa delokalizovanim π-sistemom, formiraju steking interakcije,[2] na način sličan aromatičnim organskim molekulima.[1] Proučavali smo paralelne interakcije između porfirinskih liganada kvadratno-planarnih kompleksa u kristalnim strukturama, analizirajući podatke dobijene pretragom Kembričke banke kristalografskih podata. U cilju pronalaženja intermolekulskih paralelnih interakcija, kao granični kriterijum korišćeno je rastojanje između jona metala, manje od 10 Å. Rezultati statističke analize pokazuju da većina kontakata imaju ofset vrednosti od 3.0 do 4.0 Å, što odgovara steking interakcijama. Međutim, neočekivano veliki broj kontakta sa vrednosti r parametra većom od 7 Å, što odgovara paralelnim inerakcijama sa velikim horizontalnim pomeranjima.

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Parallel interactions of porphyrine ligands

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Stacking interactions between aromatic molecules or fragments are generally studied.[1] However, several studies of chelate rings with delocalized π-bonds, which can be involved in similar stacking interactions [2] to aromatic organic molecules,[1] were published.

We have studied parallel interactions between porphyrine ligands of square-planar complexes in crystal structures by analyzing the data from Cambridge Structural Database. In order to find intermolecular parallel interactions, we used the criterion where the distance between metal ions was below 10.0 Å. The results of statistical analysis show that most of contacts have offset values in the range 3.0-4.0 Å, that corresponds to stacking interactions. However, unexpectedly large number of contacts with r value larger than 7.0 Å, that corresponds to parallel interactions at large offsets.

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1. D. B. Ninković, G. V. Janjić, D. Ž. Veljković, D. N. Sredojević, S. D. Zarić, *ChemPhysChem*, **12.** (2011) 3511-3514.
2. G. Janjić, J. Andrić, A. Kapor, Ž. D. Bugarčić, S. D. Zarić, *CrystEngComm*, **12.** (2010), 3773-3779.

ТХ П07

Model of the complex open thermodynamic System

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ТХ П08

MLXH/π interakcije u kristalnim strukturama

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Intezivna ispitivanja nekovaletnih interakcija, koje uključuju π-sisteme, pokazuju da su ove interakcije veoma bitne u mnogim oblastima hemije, biohemije i molekularne biologije. Vezivne interakcije između X-H grupa (X=O, N, C) i π-sistema se zovu XH/π interakcije, dok se interacije koordinovanih liganada sa aromatičnim prstenovima mogu se posmatrati kao specifičan tip XH/π vodočnih veza, metal-ligand XH/π (MLXH/π) i one su nađene u kristalnim stukturama metaloproteina i u komleksima prelaznih metala.
Rezultati statisticke analize pokazuju da geometrija MLXH/π najviše zavisi od prirode XH grupe. MLXH/π interakcije sa najkraćim d rastojanjem u kristalnim strukturama se javljaju kod MLOH/π kontakata, dok su najduža rastojanja nađena u kristalnim strukturama sa MLCH/π kontaktima. Analiza kristalnih struktura kompleksa metala iz CSD-a pokazuje da se u većini ovih struktura MLXH/π interakcije javljaju između XH grupe i π-sistema fenil grupe. Rezultati geometriske analize MLXH/π interakcija u kristalnim strukturama su u saglasnosti sa izračunatim energijama OH/π, NH/π i CH/π interakcija.

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MLXH/π interactions in the crystal structures

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Intensive investigations of noncovalent interactions, involving π-systems, has shown that these interactions are very important in many fields of chemistry, biochemistry and molecular biology. Bonding interactions between X—H group (X = O, N, C) and a π-system are called XH/π interactions, while the interactions of coordinated ligands with aromatic rings can also be considered as a special type of XH/π hydrogen bonds, metal-ligand XH/π (MLXH/π) and they have been found in crystal structures of metalloproteins and transition-metal complexes. The results of statistical analysis show that geometry of MLXH/π interactions mostly depend on nature of XH group. MLXH/π interactions with the shortest d distances in crystal structures occur in MLOH/π contacts, while the longest distances are found in crystal structures with MLCH/π contacts. The analysis of crystal structures of metal complexes from the CSD show that in most of these structures there are MLXH/π interactions between XH group and π-system of phenyl group. The results of geometric analysis of MLXH/π interactions in crystal structures are in agreement with the calculated energies of the OH/π, NH/π and CH/π.

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Индустријска и примењена хемија

ИХ П01

Difuzija resveratrola iz lipidnih mikročestica dobijenih različitim metodama

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Difuzioni otpori koji se odnose na sisteme za produženo/kontrolisano otpuštanje aktivnih supstanci, poput lipozoma, predstavljaju parametar od ključnog značaja za definisanje same kinetike otpuštanja. U ovom radu, ispitano je nekoliko različitih metoda za dobijanje lipozoma sa inkapsuliranim resveratrolom, sa aspekta raspodele veličina čestica, efikasnosti inkapsulacije i difuzionih otpora. Svi dobijeni uzorci lipozoma pokazali su visok stepen inkapsulacije resveratrola (92-97 %). Iz rezultata kinetike otpuštanja, praćene u Francovoj difuzionoj ćeliji, zaključuje se da je difuzija resveratrola iz lipozoma za ~50 % sporija u odnosu na difuziju resveratrola iz rastvora. Difuzioni otpori koje pružaju membrane lipozoma bili su u opsegu od $5{,}90\cdot10^5$ do $9{,}55\cdot10^5$ s/m u zavisnosti od veličine lipidnih čestica. Difuzioni otpor multilamelarnih lipozoma veći su za ~70-80 %, u poređenju sa manjim lipozomima. Dobijeni rezultati pokazuju opravdanost upotrebe lipozoma kao potencijalnih nosača za produženo oslobađanje resveratrola.

Diffusion of resveratrol from lipid microparticles produced by different methods

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Determination of diffusion resistances is a way of membrane characterisation and it is an important task in estimating the behaviour of the systems for prolonged release. Liposomes are type of membranes commonly used for encapsulation of active compounds. In this work several different methods for production of liposomes incorporating resveratrol were investigated and compared from the aspect of size distribution, entrapment efficiency and diffusion resistances. All obtained samples of liposomes exhibited high resveratrol entrapment efficiency (92-97 %). The release studies performed in Franz diffusion cell showed that liposomes impart slow diffusion of resveratrol, where diffusion resistance derived from liposomal membrane ranged from $5{,}90\cdot10^5$ to $9{,}55\cdot10^5$ s/m, depending on the particle size. Multilamellar liposomes provided an increase of diffusion resistance for ~70-80 %, compared to smaller liposomes. The results in this paper indicate that liposomes could be convenient carriers for resveratrol and insure its prolonged release.

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ИХ П02

Elektrohemijska redukcija Reactive Blue 52 primenom cirkonijumske elektrode

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Tekstilna industrija je jedan od najvećih zagađivača životne sredine. Tekstilne boje značajno utiču na fotosintetičku aktivnost zbog smanjenja količine sunčevih zraka koji prodiru kroz vodu, a takođe mogu biti toksične za vodene organizme. Uobičajene fizičke i hemijske metode koje se koriste za prečišćavanje voda nisu dovoljno efikasne za uklanjanje boja, a zbog male biodegradabilnosti nisu ni konvencionalni biološki tretmani. Zbog toga se poslednjih godina velika pažnja posvećuje elektrohemijskim metodama za degradaciju molekula boja. Kod ovih metoda glavni reagens je elektron, on indukuje redoks reakcije koje dovode do transformacije i destrukcije molekula. Elektrohemijska redukcija je izvedena u elektrohemijskoj ćeliji, kao katoda je primenjena cirkonijumska elektroda, a kao osnovni elektrolit rastvor 0,1M Na_2SO_4. Primenjen je napon razlaganja od 12V. Ispitan je uticaj različitih pH vrednosti početnog rastvora boje na efikasnost elektrolize. Degradacija boje je praćena HPLC tehnikom i preko HPK vrednosti, a stepen dekolorizacije je praćen spektrofotometrijski.

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Study of the Electrochemical Reduction of Reactive Blue 52 using Zirconium electrode

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Textile industry is one of biggest environmental pollutants. Textile dyes significantly affect the photosynthetic activity due to reduction of the amount of sunlight penetrating through the water, and they can be toxic to aquatic organisms. Typical physical and chemical methods used for water purification are not effective enough in dye remediation, and because of the low biodegradability neither are conventional biological treatments. Therefore, in recent years, great attention is given to electrochemical methods for the degradation of the dye molecules. In these methods, the main reagent is the electron, which induces redox reactions that lead to the transformation and destruction of molecules. Electrochemical reduction is carried out in an electrochemical cell, cathode was cirkonium electrode, and supporting electrolyte was 0.1 M Na_2SO_4. Applied voltage during electrolysis was 12V. The effect of different initial pH of dye solution on the efficiency of electrolysis was examined. Color degradation was monitored by HPLC method and COD values, and the degree of decolorization was monitored spectrophotometrically.

ИХ П03

Electrochromism – application in smart window technology

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Electrochromic devices change colour and light transmission properties in response to voltage, thus the amount of heat and light passing through can be controlled. This makes them suitable for application in the so-called smart window technology. The concept is based on electrochromic behavior of certain metal-oxides. This study gives an insight in the phenomena, and presents the properties of a WO_x-$TiVO_x$ electrochromic device, in terms of its optical and electrochemical characteristics.

Elektrohromizam – primena u tehnologiji pametnih prozora

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Elektrohromni uređaji imaju sposobnost da u zavisnosti od primenjenog napona menjaju boju i propustljivost svetlosti. Zahvaljujući tome je moguće kontrolisati količinu svetlosti i toplote koja kroz njih prolazi, što ih čini pogodnim za primenu u tehnologiji takozvanih pametnih prozora. Koncept je zasnovan na elektrohromnom ponašanju određenih oksida nekih metala. Ovaj rad daje fenomenološki uvid u tehnologiju, i prikazuje performanse WO_x-$TiVO_x$ uređaja, u pogledu optičkih i elektrohemijskih karakteristika.

ИХ П04

Ispitivanje ravnoteže faza čvrsto-tečno binarnih smeša sa polietilen glikolom

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Poznavanje ravnoteže faza čvrsto-tečno pojedinih sistema je od izuzetno velikog značaja u različitim industrijskim procesima. U hemijskoj industriji, proizvodi mnogih procesa su izuzetno toksične supstance čiju upotrebu je potrebno regulisati i definisati mere uklanjanja tih supstanci iz otpadnih tokova industrije. Ravnoteža čvrsto-tečno predstavlja osnovu za svaki proces kristalizacije. Takođe, od velike je važnosti i u drugim procesima koji se odvijaju u hemijskoj industriji: separacija termonestabilnih jedinjenja ili izomera, rashladni procesi, projektovanje cevovoda, dobijanje proizvoda visoke čistoće. U ovom radu ispitivana je ravnoteža pojedinih organskih rastvarača sa polietilen glikolom molarne mase 2050, na atmosferskom pritisku. Razmatrani organski rastvarači su piridin, nikotin, benzen, toluen i tetrahidrofuran. Rezultati ove studije ukazuju na mogućnost tretiranja benzena, toluena i piridina polietilen glikolom 2050.

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Investigation of the solid-liquid phase equilibrium of binary mixtures with polyethylene glycol

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The knowledge of the solid-liquid phase equilibrium of certain systems is of great importance for various industrial processes. In the chemical industry, products of numerous processes are highly toxic substances, whose usage is necessary to regulate and define measures to remove these substances from industrial wastewaters. Solid-liquid equilibria are the basis of every crystallization process. Also, it is of great importance for other processes in the chemical industry: separation of thermolabile or isomeric compounds, refrigeration processes, pipeline design, and for obtaining high-purity products. In this study solid-liquid equilibria of certain organic solvents with polyethylene glycol of the molecular mass 2050 was investigated, at the atmospheric pressure. The utilized organic solvents were pyridine, nicotine, benzene, toluene and tetrahydrofuran. The results of this study showed possibilities for sustainable applications of solid polyethylene glycol 2050 for the treatment of benzene, toluene and pyridine.

Хемија у настави

НХ П01

Primena procesa poređenja ontologija u nastavnoj temi ''Ugljeni hidrati''

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Tokom poslednjih decenija, nastavnici i njihovi učenici susreću se sa naglim porastom kvantuma naučnih činjenica i pojmova. Time se povećava potreba za poboljšanjem njihovog predstavljanja, pravilnim izborom ključnih informacija i pronalaženjem odgovarajućih oblika nastavnih instrukcija koje će ispuniti te zahteve.

Sa tim ciljem u ovom radu se navode primeri procesa poređenja ontologija u nastavnoj temi ''Ugljeni hidrati'', prilagođeno učenicima osnovnoškolskog uzrasta. Kao uža specifikacija ontologija, koriste se sistemici kao vid grafičkog predstavljanja znanja, koje su Fahmi i Lagovski definisali kao uređenje koncepata u interaktivni sistem (sistem zatvorenog klastera) u kom su sve veze među konceptima jasno naglašene – posebno za učenika.

Međutim, povezivanjem (poređenjem) dva ili više pojedinačna sistemika učenici ostvaruju i dodatne prednosti: hemijsku pismenost, pravilno razumevanje tekstualnih prikaza, rešavanje raznih problema, sve to zahvaljujući navođenju veza između dve srodne celine.

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The application of ontology matching in teaching “Carbohydrates”

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In recent decades, teachers and their students are faced with sudden increase in quantum of scientific facts and concepts. Because of that, we must improve way of their representation, make proper selection of key information and look at appropriate types of teaching instructions that will fulfill these requirements.

With this aim, in this paper are shown examples of ontology matching for one chemical teaching unit „Carbohydrates“, which are adjusted to primary school students. As a sub ontology specification, this paper presents systemics like graphic form of knowledge representation, which Fahmy and Lagowski defined as arrangement of concepts through interacting system (closed cluster) in which all relationship between concepts are made clear, up front, to the learner.

However, by connecting (comparing, matching) of two or more individual systemics, students can realize additional benefits, such as achieve chemical literacy, proper understanding of textual representation, solving various problems, all those thanks to process of specifying relations between two related units.

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