

**Srpsko hemijsko društvo**  
Serbian Chemical Society



**XLIX SAVETOVANJE  
SRPSKOG HEMIJSKOG  
DRUŠTVA**

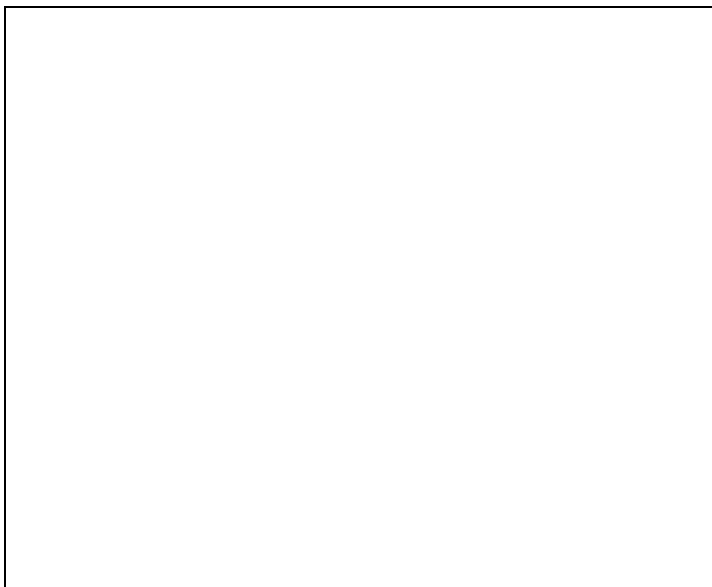
**PROGRAM  
I**

**KRATKI IZVODI RADOVA**

**49<sup>th</sup> Meeting of the Serbian Chemical Society**

**Programme  
&  
Book of Abstracts**

**Kragujevac, 13-14. maj 2011.  
Kragujevac Serbia, May 13-14, 2010**



***XLIX SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA, KRAGUJEVAC, 13-14. MAJ 2011.***  
***PROGRAM I KRATKI IZVODI RADOVA***

*49<sup>TH</sup> MEETING OF THE SERBIAN CHEMICAL SOCIETY, KRAGUJEVAC, SERBIA, MAY 13-14, 2011*  
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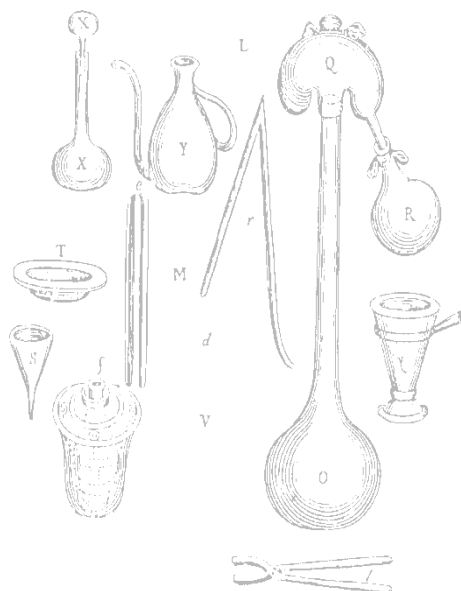
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***Ova knjiga sadrži kratke izvode  
tri plenarna predavanja (PP)  
dva predavanja po pozivu (PPP) i  
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***na desnoj strani iznad naslova rada.***



*This book contains short abstracts of  
3 Plenary Lectures (PP),  
2 Invited Lectures (PPP),  
150 contributions accepted  
for the presentation at the Meeting,*

*The Proceedings of the papers (consisting of four pages)  
are published on compact-disk (CD),  
as an integral part of the Meeting material.  
The papers published on the CD are designed in this book by*



*symbol above the paper title.*

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# PROGRAM / PROGRAMME

## Četvrtak, 12. maj 2011. / Thursday, May 12, 2011

- 18.00 – 19.00** **Registracija učesnika** - hol u prizemlju glavne zgrade  
*Registration - Lobby on the ground floor*
- 19.00 – 20.30** **Hemija između magije i realnosti** (neobični ogledi u hemiji)  
Velika sala u prizemlju glavne zgrade  
*Chemistry between magic and reality (extraordinary experiments in chemistry)*  
*Great hall on the ground floor*

## Petak, 13. maj 2011. / Friday, May 13, 2011

- 09.00 – 13.30** **Registracija učesnika** - hol u prizemlju glavne zgrade  
*Registration - Lobby on the ground floor*
- 09.00 – 09.45** **Postavljanje postera – sesija I / Poster Mounting – session I**  
**Velika sala na prvom spratu / Great hall on the first floor**
- 09.45 – 10.00** **Svečano otvaranje / Opening Ceremony**  
**Plenarno predavanje / Plenary Lecture**  
Predsedavajući / *Chairperson*: Živadin **Bugarčić**
- 10.00 – 10.45** **Prof. Dr. Enzo ALESSIO**, University of Trieste, Italy  
**PP1** **Ruthenium anticancer drugs**  
*Рутенијумски антитуморски лекови*
- 10.45 – 11.15** **Predavanje po pozivu / Invited Lecture**  
**Dr Dragana STANIĆ-VUČINIĆ**  
**PPP1** **Hemijski fakultet Univerziteta u Beogradu, Srbija**  
*Faculty of Chemistry. University of Belgrade, Serbia*  
**Enzimsko procesovanje alergena hrane**  
*Enzymatic processing of food allergens*
- 11.15 – 12.00** **Koktel / Cocktail** – hol na prvom spratu / lobby on the first floor
- 12.00 – 12.15** **Predstavljanje monografije Ljiljane Ristić:**  
**Žene u hemiji krajem XIX i početkom XX veka u Srbiji**  
**Usmena izlaganja / Oral Presentations**  
**Sala A prvi sprat / Room A first floor**  
Predsedavajući / *Chairperson*: Ivan **Gutman**
- 12.15 – 12.30** **Milan Senčanski, Milovan D. Ivanović, Sonja Vučković, Ljiljana Došen-Mićović**  
**TH01-O** **Aktivne konformacije  $\mu$ - i  $\delta$ -opioidnih receptora specifičnih za pojedine ligande**  
*Active Ligand Specific Conformations of  $\mu$ - and  $\delta$ -Opioid Receptors*
- 12.30 – 12.45** **Marko R. Perić, Matija Zlatar, Maja Gruden-Pavlović, Sonja Grubišić**  
**TH02-O** **DFT i MM analiza strukture i magnetnih osobina kompleksa mangana(ii) sa X-fenil-cijanamidnim mostnim ligandom**  
*DFT and MM Description of the Structure and Magnetic Properties of Manganese Complexes with X-phenylcyanamido Bridging Ligand*
- 12.45 – 13.00** **Ljubica D. Andjelković, Matija Zlatar, Maja Gruden-Pavlović**  
**TH03-O** **Multideterminantni DFT pristup analize Jahn-Teller-ovog efekta u malim organskim radikalima**  
*Multideterminantal DFT Approach in Analysis of Jahn-Teller Effect in Small Organic Radicals*



- 13.00 – 13.15**  
TH04-O **V. Mićović, I. Juranić**  
**Ispitivanje interakcija nesteroidnih anti-inflamatornih lekova (NSAID) sa ciklo-oksigenazama, metodama molekulske dinamike**  
*Study of interactions between nonsteroid anti-inflammatory drugs (NSAID) with cyclo-oxygenase, using molecular-dynamics*
- 13.15 – 13.30**  
TH05-O **Dubravka Z. Vojislavljević, Jelena Blagojević, Goran V. Janjić, Dušan Ž. Veljković, Snežana D. Zarić**  
**Teorijsko proučavanje O-H/ $\pi$  interakcija između koordinovanog i nekoordinovanog molekula vode i C<sub>6</sub>-aromatičnog prstena**  
*Theoretical study of O-H/ $\pi$  interactions between coordinated and non-coordinated water molecule with C<sub>6</sub>-aromatic ring*
- 13.30 – 13.45**  
FH01-O **Zorica D. Mojović, Srđan P. Petrović, Ljiljana S. Rožić, Tatjana B. Novaković, Zorica M. Vuković**  
**Sinteza i karakterizacija kiselinski aktiviranog bentonita modifikovanog sa 12-volframfosforom kiselinom i njegova primena u reakciji oksidacije nitrita**  
*Synthesis and characterization of acid activated bentonite with various loading of H<sub>3</sub>PW<sub>12</sub>O<sub>40</sub> modified electrode for the oxidation of nitrite*
- Sala B prvi sprat / Room B first floor**  
Predsedavajući / Chairperson: Tanja Čirković-Veličković
- 12.15 – 12.30**  
BH01-O **Iva A. Vukićević, Tina Kamčeva, Maja Radisavljević, Marijana Petković**  
**Poređenje kolorimetrijskog i masenospektrometrijskog esaja za određivanje aktivnosti pankreasne fosfolipaze A<sub>2</sub>**  
*Comparison of colorimetric and mass spectrometric assays to determine the activity of pancreatic phospholipase A<sub>2</sub>*
- 12.30 – 12.45**  
BH02-O **Vladimir B. Šukalović, Jelena Penjišević, Goran Roglić, Deana Andrić, Vukić Šoškić, Slađana Kostić-Rajačić**  
**Modelovanje druge ekstralcelularne petlje dopaminskog D2 receptora**  
*Modeling Dopamine D2 Receptor Second Extracellular Loop*
- 12.45 – 13.00**  
BH03-O **Uroš Ž. Andjelković, Jurij Lah**  
**Termodinamička analiza razvijanja izoformi eksterne invertaze**  
*Thermodynamic analysis of unfolding of external invertase isoforms*
- 13.00 – 13.15**  
BH04-O **Kevrešan E. Slavko, Popović M. Boris, Dubravka Štajner, Ksenija Kuhajda**  
**Oksidativni status biljaka pšenice nakon tretmana holnom kiselinom**  
*Oxidative status of wheat plants after treatment with cholic acid*
- 13.15 – 13.30**  
BH05-O **Niko S. Radulović, Marija S. Denić, Zorica Z. Stojanović-Radić**  
**Novi antimikrobni fenolni abietanski diterpen iz biljne vrste *Lycopus europaeus* L. (Lamiaceae)**  
*A new antimicrobial phenolic abietane diterpene from *Lycopus europaeus* L. (Lamiaceae)*
- Sala D prvi sprat / Room D first floor**  
Predsedavajući / Chairperson: Branislav Nikolić
- 12.15 – 12.30**  
EH01-O **Ž. Jovanović, J. Stojkowska, A. Krklješ, N. Bibić, B. Obradović, Z. Kačarević-Popović, V. Mišković-Stanković**  
**Uticaj vrste polimera na oblik i veličinu nanočestica srebra dobijenih elektrohemijom sintezom**  
*The effect of polymer type on the size and shape of electrochemically synthesized Ag nanoparticles*
- 12.30 – 12.45**  
EH02-O **Sanja Eraković, Đorđe Veljović, Papa Diouf, Tatjana Stevanović, Miodrag Mitrić, Đorđe Janačković, Vesna Mišković-Stanković**  
**ATR-FTIR i XRD analiza kompozitnih hidroksiapatit/lignin prevlaka dobijene postupkom elektroforetskog taloženja**  
*ATR-FTIR and XRD evaluation of composite hydroxyapatite/lignin coatings obtained by electrophoretic deposition method*
- 12.45 – 13.00**  
EH03-O **Isidora Cekić-Lasković, Dragica M. Minić, Rade Marković, Elena Volanschi**  
**ULj-VID spektroeletrohemijom proučavanje supstituisanih 4-oksothiazolidinskih derivata u nevodenoj sredini**  
*UV-Vis spectroelectrochemical study of substituted 4-oxothiazolidine derivatives in aprotic medium*





- 13.00 – 13.15**  
EH04-O **Danijela M. Jašin**, Andjela-Abu Rabi i Slavko Mentus  
Spontano i elektrohemijsko formiranje kompozita Au/TiO<sub>2</sub> i Au/Ta<sub>2</sub>O<sub>5</sub>  
*Spontaneous and electrochemical formation of the composite Au/TiO<sub>2</sub> and Au/Ta<sub>2</sub>O<sub>5</sub>*
- 13.15 – 13.30**  
EH05-O **Dalibor Stanković**, Dragan Manojlović, Goran Roglić, Ivan Anđelković, Biljana Dojčinović, Jelena Mutić  
Simultano određivanje Pb i Cd u uzorcima vode Anodnom Stripping Voltametrijom korišćenjem modifikovane GC elektrode  
*Simultaneous determination of Pb and Cd traces in water samples by Anodic Stripping Voltammetry using modified GC electrode*
- 13.30 – 13.45**  
TI01-O **Jovana Ž. Milanović**, Mirjana Kostić, Biljana Pejić, Petar Škundrić  
Uticaj selektivne TEMPO-oksidacije na mehanička svojstva vlakana pamuka  
*Influence of selective TEMPO-oxidation on mechanical properties of cotton fibers*
- 13.45 – 14.45** **Posterske prezentacije I / Poster Session I**  
hol na prvom spratu / lobby on the first floor  
**Sekcije / Sections:**  
Biohemija / Biochemistry; Biotehnologija / Biotechnology;  
Hemija i tehnologija hrane / Food Chemistry and Technology;  
Fizička hemija / Physical Chemistry; Elektrohemija / Electrochemistry;  
Spektrohemijska / Spectrochemistry; Tekstilno inženjerstvo / Textile Engineering.
- 13.45 – 16.00** **Pauza za ručak / Pause – Lunch**  
(Uklanjanje postera – sesija I / Posters dismantling – session I)
- 16.00 –** **IZLET / EXCURSION**  
Povratak oko 22.30 h / Return approximately at 10.30 pm

## **Subota, 14. maj 2011. / Saturday, May 14, 2011**

- 08.30 – 13.00** **Registracija učesnika** - hol u prizemlju glavne zgrade  
*Registration - Lobby on the ground floor*
- 08.30 – 09.00** **Postavljanje postera – sesija II / Poster Mounting – session II**  
**Velika sala na prvom spratu / Great hall on the first floor**  
**Plenarna predavanja / Plenary Lectures**  
Predsedavajući / Chairperson: Srećko Trifunović
- 09.00 – 09.45**  
PP2 **Dr Mario MALINCONICO**  
Institute of Chemistry and Technology of Polymers, Napoli, Italia  
**Green chemistry: recent results in the development of sprayable agricultural films from waste polysaccharides**  
*Зелена хемија: нови резултати у развоју распршивих пољопривредних фолија на бази отпадних полисахарида*
- 09.50 – 10.35**  
PP3 **Dr Ljubinka RAJAKOVIĆ**  
Tehnološko-metalurški fakultet Univerziteta u Beogradu, Srbija  
*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*  
**Arsenic Species in Water - Separation, Preconcentration and Determination**  
*Облици (специје) арсена у води – сепарација, предконцентрисање и одређивање*
- 10.35 – 11.00** **Pauza / Pause**  
**Postavljanje postera – sesija II / Poster Mounting – session II**



## Usmena izlaganja / Oral Presentations

### Sala A prvi sprat / Room A first floor

Predsedavajući / Chairperson: Dušanka **Milojković-Opsenica**

- 11.00 – 11.15**  
**AH01-O** **Tatjana Ž. Verbić**, Mire Zloh, Dalibor M. Stanković, Milica N. Sentić, Dragan D. Manojlović, Ivan O. Juranić  
**Proučavanje keto-enolne tautomerije arildiketo kiselina u vodenoj sredini upotrebom NMR spektroskopije i ciklične voltametrije**  
*Keto-enol Tautomerism of Aryldiketo Acids in Aqueous Solution: NMR Spectroscopy and Cyclic Voltammetry Study*
- 11.15 – 11.30**  
**AH02-O** **Tina T. Kamčeva**, Maja Radisavljević, Iva Vukićević, Bojana Damjanović, Milovan Stoiljković, Marijana Petković  
**Izotopski „otisak prsta“ metala upotrebom MALDI TOF MS**  
*Isotopic fingerprinting of metals by MALDI TOF MS*
- 11.30 – 11.45**  
**AH03-O** **D. M. Sejmanović, B. B. Petković**, M. V. Budimir, S. P. Sovilj, V. M. Jovanović  
**Određivanje Ag<sup>+</sup> i Cl<sup>-</sup> jona u uzorcima ekoloških voda primenom jednostavnog poli(vinil hlorid-ko-vinil acetat)/srebro potencimetrijskog senzora**  
*Determination of Silver and Chloride Ions in Environmental Water Samples by Simple PVC/Ag Potentiometric Sensor*
- 11.45 – 12.00**  
**AH04-O** **Ivan Ž. Jakovljević**, Predrag Đurđević, Ljubinka Joksović, Andrija Ćirić, Ivan Lazarević, Ratimir Jelić  
**Ravnoteže kompleksiranja Gd(III)-jona sa nekim fluorohinolonima**  
*Complex formation equilibria between Gd(III)-ion and some fluoroquinolones*
- 12.00 – 12.15**  
**AH05-O** **S. Sunarić**, R. Pavlović, S. Mitić, A. Pavlović, S. Tošić  
**HPLC Determination of Tetracycline in Human Control Serum**  
*HPLC određivanje tetraciklina u humanom kontrolnom serumu*
- 12.15 – 12.30**  
**AH06-O** **Marija M. Vukčević**, Marina Radišić, Ana Kalijadis, Biljana Babić, Biljana Pejić, Zoran Laušević, Mila Laušević  
**Adsorpcija pesticida na karbonizovanim kratkim vlaknima konoplje aktiviranim kalijum hidroksidom**  
*Adsorption of pesticides onto the carbonized short hemp fibers activated with potassium hydroxide*
- 12.30 – 12.45**  
**AH07-O** **Vesna P. Lukić**, Živoslav Lj. Tešić, Mirjana B. Ninković  
**Primena jonske hromatografije u kontroli kvaliteta vode na postrojenju za preradu vode Makiš**  
*Application of Ion Chromatography for water quality control at water treatment plant Makis*
- 12.45 – 13.00**  
**AH08-O** **Mirjana P. Vojić**, Ilija N. Cvijetić, Tatjana Ž. Verbić, Ivan. O. Juranić  
**Efekti supstituenata i rastvarača na UV-Vis apsorpcione spektre p-supstituisanih aroilakrilnih kiselina**  
*Substituent and solvent effect on the UV-Vis absorption spectra of p-substituted aroilacrylic acids*

### Sala B prvi sprat / Room B first floor

Predsedavajući / Chairperson: Miloš Đuran

- 11.00 – 11.15**  
**NH01-O** **Maja Radisavljević**, Tina Kamčeva, Iva Vukićević, Ilija Brčeski, Živadin D. Bugarčić, Marijana Petković  
**Inhibitorski efekat kompleksa platine (II) na fosfolipazu A<sub>2</sub>**  
*Inhibitory effect of platinum(II) complexes on phospholipase A<sub>2</sub>*
- 11.15 – 11.30**  
**NH02-O** **Biljana Đ. Glišić**, Snežana Rajković, Miloš I. Đuran  
**<sup>1</sup>H NMR ispitivanje reakcija [AuCl(dien)]Cl<sub>2</sub> kompleksa sa N-acetilovanim derivatima nekih dipeptida**  
*<sup>1</sup>H NMR study of reactions of the [AuCl(dien)]Cl<sub>2</sub> complex with N-acetyl derivatives of some dipeptides*
- 11.30 – 11.45**  
**NH03-O** **Mirjana M. Lalović**, Ljiljana S. Vojinović-Ješić, Valerija I. Češljević, Vukadin M. Leovac  
**Sinteza i struktura kompleksa bakra(II) sa piridoksalaminogvanidinom**  
*Synthesis and structure of copper(II) complex with pyridoxalaminoguanidine*
- 11.45 – 12.00**  
**NH04-O** **Aleksandar R. Savić**, Ljiljana E. Mihajlović, Marija Dulović, Ivanka Marković, Tibor J. Sabo, Sanja R. Grgurić-Šipka  
**Novi rutenijum(II) kompleksi sa anti-leukemijskom aktivnošću**  
*New ruthenium(II) complexes with anti-leukaemic activity*



- 12.00 – 12.15**  
NH05-O **Snežana M. Jovanović, Tanja V. Soldatović, Živadin D. Bugarčić**  
**Kinetika i mehanizam supstitucionih reakcija dinuklearnih kompleksa platine(II) sa biološki važnim ligandima**  
*Kinetics and mechanism of the substitution reactions of dinuclear complexes platinum(II) with biologically important ligands*
- 12.15 – 12.30**  
NH06-O **Ana S. Đeković, Biljana V. Petrović, Živadin D. Bugarčić**  
**Ispitivanje interakcija nekih monofunkcionalnih Au(III) kompleksa sa S-donorskim ligandima**  
*Study of interactions of some monofunctional Au(III) complexes with S-donor ligands*
- 12.30 – 12.45**  
NH07-O **Mirjana D. Đurović, Jovana V. Bogojeski, Biljana V. Petrović, Živadin D. Bugarčić**  
**Kinetika i mehanizam supstitucionih reakcija monofunkcionalnih Pt(II) kompleksa,  $[(TL^{tBu})PtCl]ClO_4$  i  $[PtCl(tpdm)]^+$**   
*Kinetics and the mechanism of the substitution reactions of monofunctional Pt(II) complexes,  $[(TL^{tBu})PtCl]ClO_4$  and  $[PtCl(tpdm)]^+$*
- 12.45 – 13.00**  
NH08-O **Bojana B. Laban, Vesna Vodnik, Ana Vujačić, Anja B. Jokić, Sofija P. Sovilj**  
**Vesna M. Vasić**  
**Apsorpcioni spektri i kinetika građenja J-agregata kolidnih čestica srebra sa tiocijano bojom u vodenoj sredini**  
*Absorption spectra and kinetics of J-aggregation of TC-coated Ag colloidal nanoparticles in aqueous solutions*
- Sala D prvi sprat / Room D first floor**  
**Predsedavajući / Chairperson: Rastko Vukićević**
- 11.00 – 11.15**  
OH01-O **Jelena Randelović, Slavica Erić, Vladimir Savić,**  
**Kompjuterski dizajn peptidnih inhibitora interakcije proteina CDK9 i ciklina T1**  
*Computational design of peptide inhibitors for CDK9/cyclin T1 protein interaction*
- 11.15 – 11.30**  
OH02-O **Jelena Z. Penjišević, Vladimir V. Šukalović, Deana B. Andrić, Goran M. Roglić**  
**Sladana V. Kostić-Rajačić**  
**1-(2-metoksifenil)-4-((1-(arilmetil)piperidin-4-il)metil) piperazina**  
*Synthesis and biological activity of 1-(2-methoxyphenyl)-4-((1-(arylmethyl)piperidin-4-yl)methyl)piperazines*
- 11.30 – 11.45**  
OH03-O **Ivana Kovačević, Mirjana Popsavin, Goran Benedeković, Vesna Kojić, Gordana Bogdanović, Velimir Popsavin**  
**Nova sinteza i antiproliferativna aktivnost goniobutenolida A i B**  
*Novel synthesis and antiproliferative activity of goniobutenolides A and B*
- 11.45 – 12.00**  
OH04-O **Vera M. Divac, Marina D. Rvović and Zorica M. Bugarčić**  
**Kinetička ispitivanja ciklizacionih reakcija nekih terpenskih alkohola**  
*Kinetic investigation of cyclization reactions of some terpenic alcohols*
- 12.00 – 12.15**  
OH05-O **Dejan M. Opsenica, Igor M. Opsenica, James C. Burnett, Rekha G. Panchal,**  
**Sina Bavari, Bogdan A. Šolaja**  
**1,7-bis(alkilamino)diazahrizeni inhibitori tri različita patogena: botulinum neurotoksin (BoNT/A LC), parazita malarije *P. falciparum* i filovirusa Ebola**  
*1,7-bis(alkylamino)diazachrysene as Inhibitors of Three Unrelated Pathogens: The Botulinum Neurotoxin (BoNT/A LC), *P. falciparum* Malaria, and the Ebola Filovirus*
- 12.15 – 12.30**  
OH06-O **Dragana D. Steanović, Ivan S. Damjanović, Anka Z. Pejović, Danijela S. Ilić-Komatina, Rastko D. Vukićević**  
**Sinteza 3-aminoaryl-1-ferocenilpropan-1-ona**  
*Synthesis of 3-aminoaryl-1-ferrocenyl-propan-1-ones*
- 12.30 – 12.45**  
OH07-O **Aleksandar V. Teodorović, Dalibor M. Badžuk, Nenad Stevanović**  
**Premeštanja alkil-radikala dugog niza**  
*Long-chain alkyl radicals rearrangements*
- 12.45 – 13.00**  
OH08-O **Bojan Đ. Božić, Nemanja Trišović, Milica Rančić, Gordana Ušćumlić**  
**Sinteza novih derivata propionske kiseline iz 5-ariliden-2,4-dioksotetrahidrotiazola**  
*Synthesis of new propionic acid derivatives from 5-arylidene-2,4-dioxotetrahydrothiazol*
- 13.00 – 14.00** **Posterske prezentacije II / Poster Session II**  
hol na prvom spratu / lobby on the first floor  
**Sekcije / Sections:**  
**Analitička hemija / Analytical Chemistry; Organska hemija / Organic Chemistry**



- 14.00 – 15.00 Pauza za ručak / Pause – Lunch**  
(Uklanjanja postera -sesija II / Posters dismantling - session II)  
**Postavljanje postera – sesija III / Poster Mounting – session III**  
**Velika sala na prvom spratu / Great hall on the first floor**  
**Predavanje po pozivu / Invited Lecture**  
Predsedavajući / Chairperson: Živadin **Bugarčić**
- 15.00 – 15.30 Dr Marijana PETKOVIĆ**  
**PPP2**  
INN „Vinča“ Univerziteta u Beogradu, Srbija  
*Institute of Nuclear Science „Vinča“ University of Belgrade, Serbia*  
**Interakcija kompleksa prelaznih metala sa fosfolipidima i enzimima uključenim u metabolizam fosfolipida**  
*The interaction of transition metal complexes with phospholipids and enzymes involved in phospholipid metabolism*  
**Usmena izlaganja / Oral Presentations**  
**Sala A prvi sprat / Room A first floor**  
Predsedavajući / Chairperson: Goran **Roglić**
- 15.35 – 15.50 HŽS01-O**  
**Miljana D. Radović, Jelena Z. Mitrović, Ivana S. Kostić, Danijela V. Bojić, Branislava D. Kocić, Aleksandar Lj. Bojić**  
**Dekolorizacija tekstilne boje Reactive Blue 19 procesom UV/H<sub>2</sub>O<sub>2</sub>**  
*Decolorization of the textile dye Reactive Blue 19 by the UV/H<sub>2</sub>O<sub>2</sub> process*
- 15.50 – 16.05 HŽS02-O**  
**Milica S. Jović, Biljana Dojčinović, Jelena Nešić, Bratislav Obradović, Goran Roglić**  
**Degradacija mezotriona primenom unapređenih oksidacionih postupaka (AOP)**  
*Degradation of mesotrione using advanced oxidation processes (AOP)*
- 16.05 – 16.20 HŽS03-O**  
**Dragana D. Četojević-Simin, Sanja J. Kler, Biljana F. Abramović**  
**Uticaj metoprolola i njegovih fotokatalitičkih degradacionih intermedijera u prisustvu TiO<sub>2</sub> na rast odabranih ćelijskih linija**  
*Effect of metoprolol and products of its photocatalytic degradation in the presence of TiO<sub>2</sub> on the growth of selected cell lines*
- 16.20 – 16.35 HŽS04-O**  
**Mirjana D. Antonijević Nikolić, Jelena Đuričić Milanković, Slavica Ilić, Đorđe V. Nikolić**  
**Teški metali u zemljištu parkova u Šapcu**  
*Heavy metals in soil from parks in Šabac*
- 16.35 – 16.50 HŽS05-O**  
**Marijana D. Marković, Dragan D. Manojlović, Goran Roglić, Bratislav Obradović, Milorad Kuraica, Biljana Dojčinović**  
**Artemia salina test akutne toksičnosti – određivanje toksikološkog efekta tekstilne boje Reactive black 5 posle obezbojavanja primenom koaksijalnog DBD reaktora**  
*Artemia salina acute toxicity test - determining toxicological effect of Reactive Textile Dye (RB 5) after decolorization using coaxial DBD reactor*
- 16.50 – 17.05 HŽS06-O**  
**Bojana, D. Špirović, Milica M. Mojašević, Vesela Ž. Karan, Majda E. Milak, Nenad D. Tamaš**  
**Depozit hlorpirifosa u zasadu višnje i šljive**  
*Chlorpyrifos deposit in a sour cherry and plum orchard*
- Sala B prvi sprat / Room B first floor**  
Predsedavajući / Chairperson: Marijana **Petković**
- 15.35 – 15.50 BH06-O**  
**Niko S. Radulović, Ana B. Miltojević, Michael McDermott, Steve Waldren, John Adrian Parnell, Mariana Martins Gomes Pinheiro, Patricia Dias Fernandes, Fabio de Sousa Menezes**  
**Identifikacija izopropil-N-metilantranilata, novog alkaloida sa analgetskom aktivnošću, u etarskom ulju biljne vrste Choisia ternata Kunth**  
*Identification of a new antinociceptive alkaloid isopropyl N-methyl-anthranilate from the essential oil of Choisya ternata Kunth (Rutaceae)*
- 15.50 – 16.05 BH07-O**  
**Senka Popović, Draginja Peričin, Ljiljana Popović i Žužana Vaštag**  
**Uticaj pH i koncentracije glicerola na karakteristike biorazgradivih filmova od proteinskog izolata uljane tikve golice**  
*Effects of pH and glycerol concentration on the properties of pumpkin oil cake protein isolate biodegradable films*



- 16.05 – 16.20**  
**BT01-O** Omar Ali Saied moftah, Sanja Ž. Grbavčić, Nevena D. Luković, Milena G. Žuža, Dejan I. Bezbradica, Zorica D. Knežević-Jugović  
**Karakterizacija lipaze iz *Candida utilis* dobijene tehnikom gajenja na čvrstoj podlozi korišćenjem uljane pogače maslina kao supstrata**  
*Characterization of Candida utilis lipase produced by solid state fermentation using olive oil cake as a substrate*
- 16.20 – 16.35**  
**BT02-O** Milena G. Rikalović, Miroslav M. Vrvic, Gordana Gojgić-Cvijović, Ivanka Karadžić  
**Ispitivanje tolerancije soja *Pseudomonas aeruginosa* san ai na živu, kadmijum i bakar**  
*Study of tolerance of Pseudomonas aeruginosa san ai to mercury, cadmium and copper*
- 16.35 – 16.50**  
**BT03-O** Žužana Vaštag, Draginja Peričin, Ljiljana Popović, Senka Popović  
**Temperaturna i pH stabilnost biološki aktivnih enzimskih hidrolizata proteinskog izolata pogače uljane tikve golice**  
*Temperature and pH stability of biological active enzymatic hydrolysates of hull-less pumpkin oil cake protein isolate*
- Sala D prvi sprat / Room D first floor**  
**Predsedavajući / Chairperson:** Mirjana Kijevčanin
- 15.50 – 16.05**  
**HI01-O** Mihal M. Đuriš, Željko Grbavčić, Zorana Arsenijević, Radmila Garić-Grulović  
**Segregacija u fluidizovanom sloju voda-polidisperzna smeša čestica**  
*Segregation in fluidization bed water-polydisperse particle mixtures*
- 16.05 – 16.20**  
**HI02-O** Đorđe Vujičić, Dragan Čomić, Sanja Ratković, Radoslav Mičić, Goran Bošković  
**Katalitička aktivnost CaO u sintezi biodizela u funkciji različitih reakcionih parametara**  
*Catalitical activity of CaO in biodiesel synthesis as a function of various reaction parameters*
- 16.20 – 16.35**  
**HTM01-O** M. Lučić, N. Milosavljević, S. Grujić, M. Laušević, M. Kalagasidis Krušić  
**Uticaj sastava hidrogelova na bazi hitozana na kontrolisano otpuštanje diazepama, paracetamola i diklofenaka**  
*Influence of chitosan hydrogel composition on controlled release of diazepam, paracetamol and diclofenac*
- 16.35 – 16.50**  
**HTM02-O** Stojanka M. Petrušić, Bojana Bursać, Svetlana Grujić, Petar Jovančić, Jasna Donlagić  
**Termosetljive mikročestice hidrogela na bazi poli(N-izopropilakrilamida) namenjene kontrolisanom otpuštanju lekova**  
*Thermosensitive hydrogel microbeads based on poly(N-isopropylacrylamide) for controlled drug release*
- 17.05 – 17.15** **Pauza / Pause**  
(Postavljanje postera – sesija III / Poster Mounting – session III)
- 17.15 – 18.15** **Posterske prezentacije III / Poster Session III**  
hol na prvom spratu / lobby on the first floor  
**Sekcije / Sections:**  
Neorganska hemija / Inorganic Chemistry; Keramika / Ceramics;  
Hemijsko inženjerstvo / Chemical Engineering; Metalurgija / Metallurgy;  
Hemija životne sredine / Environmental Chemistry;  
Nauka o materijalima / Materials Science; Nastava hemija / Chemistry Education;  
Hemija i tehnologija makromolekula / Chemistry and Technology of Macromolecules;
- 18.15 – 18.20** **Pauza / Pause**  
(Uklanjanje postera -sesija III / Posters dismounting - session III)
- 18.20 – 19.00** **Velika sala na prvom spratu / Great hall on the first floor**  
**Zatvaranje Savetovanja i dodela nagrada i priznanja**  
*Closing ceremony of the Meeting and the awarding of prizes*
- 20.00 –** **Zajednička večera – restoran Lađa Francuska**  
*Social Dinner – Restaurant Lađa Francuska (French Boat)*





## A collection of vintage scientific glassware and tools, including flasks, retorts, and a large apparatus with a bulb and tube, labeled with letters X, Y, Z, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z. The central text reads "KRATKI IZVODI ABSTRACTS".







### Ruthenium anticancer drugs

Enzo Alessio, Ioannis Bratsos, Teresa Gianferrara

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34127 Trieste, Italy (alessi@units.it)

Cisplatin is one of the most used anticancer agents and is present in a large number (>50%) of chemotherapy regimens. The extraordinary and long-term research activity focused on metal-based anticancer compounds was inspired by the great efficacy of cisplatin in testicular cancer treatment, where cure rates around 80% are obtained. In addition to cisplatin, two other platinum drugs are at present in worldwide clinical use: carboplatin and oxaliplatin, approved by FDA in 1989 and 2002, respectively.

The major limitations of such Pt drugs are a narrow range of activity (they are scarcely active against a number of malignancies with high social incidence), severe toxic side-effects, and intrinsic or acquired tumor resistance observed during treatment.

Soon after the serendipitous discovery of the antitumor activity of cisplatin in 1969, much of the early research effort was carried out on murine tumors, aimed at identifying the structure-activity relationships of platinum compounds. In parallel and subsequently, mechanistic investigations performed in mammalian cells led to the identification of DNA as pharmacological target of cisplatin.

These results induced the hope of repeating that clinical success in other solid tumors, exploiting also compounds of metals different from platinum. In principle, non-platinum compounds may be expected to have anticancer activity and toxic side-effects markedly different from those of Pt drugs for a number of obvious reasons: their different coordination geometries, binding preferences, and ligand-exchange rates are likely to lead to different mechanism(s) of action and, as a consequence, to different biological properties.

Among the several metal compounds that have been investigated for anticancer activity, those of ruthenium occupy a prevalent position.

Indeed, since several years the authors have been involved in the development of Ru-dmso complexes, many of which were shown to possess anticancer activity [1,2]. The most advanced representative in this series is the Ru(III) compound NAMI-A which is selectively active against metastases of solid tumors. NAMI-A has successfully accomplished a phase 1 clinical study on humans and is undergoing a phase 1-2 combination study.

After a general introduction [3], the lecture will give an update of the clinical status of NAMI-A and then will focus on new classes of Ru compounds that were developed more recently in the attempt to find new antitumor active species and establish some general structure-activity relationships [4].

1. E. Alessio, G. Mestroni, A. Bergamo, G. Sava, G. *Curr. Topics Med. Chem.* **4** (2004) 1525–1535.
2. I. Bratsos, T. Gianferrara, E. Alessio, C. G. Hartinger, M. A. Jakupec, B. K. Keppler in *Bioinorganic Medicinal Chemistry*, E. Alessio ed., Wiley-VCH, Weinheim, 2011, pp. 151-174.
3. T. Gianferrara, I. Bratsos, E. Alessio *Dalton Trans.* **37** (2009) 7588-7598.
4. T. Gianferrara, A. Bergamo, I. Bratsos, B. Milani, C. Spagnul, G. Sava, E. Alessio *J. Med. Chem.*, **53** (2010) 4678-4690.





## **Green chemistry: recent results in the development of agricultural films and pots from waste polysaccharides**

Mario Malinconico

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In the last years the use of plastic films for agricultural soils mulching and for low tunnels -in particular based on polyethylene (PE) and ethylene-vinylacetate copolymers (EVA)- has shown an increasing diffusion. In Europe the plastics employed for these purposes cover an area of more than 1.100.000 hectares with an annual consumption of about 800.000 tons that, for the vast majority (about 80%) are abandoned on the soil or burnt without control by the farmers, with a consequent emission of severe pollutants in the atmosphere and in the soil. Another field of great concerns is the use of nursery pots, normally made of foamed polystyrene. At same time, the agro-food sector produces every year hundred of thousand tons of wastes potentially useful for recovery and reuse of valuable soluble carbohydrates and cellulosic fibers. The authors have developed a sustainable approach in which a waterborne solution of natural polymers (polysaccharides of marine and terrestrial origin) is obtained and sprayed on an agricultural soil to form a film resistant for the time required for the mulching application. Also, biodegradable nursery pots can be obtained by thermoforming or wet forming technologies, which are then left in the soil, with reduced stress for the plants and positive effects on the soils structure. The selected polysaccharides come from renewable sources, like seaweeds in the case of alginates, and crustaceous shells in the case of chitosan. The fibers used to reinforce the coatings and the pots also comes from waste materials, such as seeds and peels from tomatoes processing, olives processing, hemp processing. Mechanical properties, degradation behaviour, agronomic tests all demonstrate the suitability of the new materials for sustainable agriculture application.

### References

1. R. Russo, M. Malinconico, G. Santagata, Effect of cross-linking with calcium ions on the physical properties of Alginate films, *Biomacromolecules*, **8** (2007) 3193-3197.
2. G. Scarascia-Mugnozza, E. Schettini, G. Vox, B. Immirzi, M. Malinconico, S. Pagliata, "Mechanical properties decay and morphological behaviour of biodegradable films for agricultural mulching in real scale experiment". *Polymer Degradation and Stability*, **91** (2006) 2801



## PP 3

**Oblici (specije) arsena u vodi - razdvajanje, pretkoncentrovanje i određivanje**

Ljubinka V. Rajaković

*Tehnološko-metalurški fakultet, Univerzitet u Beogradu, Karnegijeva 4, 11 Beograd, Srbija*

U radu je razvijen jednostavan postupak za razdvajanje i određivanje neorganskog (iAs) i organskog arsena (oAs) kao i njihovih oblika u prirodnim vodama. Za razdvajanje As(III) od As(V), koji reprezentuju iAs oblike arsena u prirodnim vodama, ispitana je i primenjena hromatografska kolona sa jako baznom anjonskom smolom (JBAS) za koju se, ukoliko je pH vrednost vode podešena na vrednosti niže od 8, vezuju samo jonski oblici As(V). Molekulski oblici As(III) ostaju u propuštenom rastvoru u kome se može odrediti njihova koncentracija. Za pripremu uzoraka vode u cilju pretkoncentrisanja i određivanja tragova arsena u vodi, ispitane su hibridne smole, HY, u kojima je integrisana aktivna komponenta (hidratisan gvožđe(III)-oksid, tip-HY-Fe, i srebro-hlorid, tip-HY-AgCl) kojom se favorizuje pored jonske izmene adsorpcija i hemisorpcija, a time i vezivanje svih oblika arsena u vodi. Hibridne smole su efikasne u širokom opsegu pH vrednosti od 5,00 do 11,00. U radu su ispitani uticaji svih parametara koji utiču na vezivanja arsenovih vrsta u šaržnom i protočnom sistemu. Primenom standardnih analitičkih postupaka, definisani su postupci za razdvajanje, koncentrisanje i određivanje neorganskih i organskih oblika arsena u vodi. Za određivanje koncentracije arsena u vodi ( $\mu\text{g L}^{-1}$ ) primenjene su ICP-MS i AAS-GH metode.

**Arsenic Species in Water - Separation, Preconcentration and Determination**

Ljubinka V. Rajaković

*Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11 Belgrade, Serbia*

A simple method for separation and determination of inorganic arsenic (iAs) species in natural and drinking water was developed in this work. Procedures for sample preparation, separation of As(III) and As(V) species and preconcentration of total iAs on fixed bed columns were defined. A strong base anion exchange (SBAE) resin and two hybrid (HY) resins (HY-Fe and HY-AgCl) were utilized. The governing factors for ion exchange/sorption of arsenic on resins in a batch and a fixed bed flow system were analyzed and compared. Acidity of water, which plays an important role in control of the ionic or molecular forms of arsenic species was beneficial for separation: by adjusting pH values less than 8.00, SBAE resin separates As(V) and As(III) in water, by retaining As(V) and allowing As(III) to pass through. Sorption activity of hydrated iron oxides particles integrated in HY resin was beneficial for bonding of all arsenic species in a wide range of pH values from 5.00 to 11.00. Validation of methods was established through basic analytical properties. ICP-MS and AAS-HG techniques were applied as analytical methods for the determination of arsenic concentration in water.



## Predavanja po pozivu / Invited Lectures

PPP 1



### Enzimsko procesovanje alergena hrane

Dragana J. Stanić-Vučinić  
*Hemijski fakultet, Beograd*

Danas više od 4% humane populacije u razvijenim zemljama pati od alergije na hranu. Premda je striktno izbegavanje uzročnika alergije najbolji način sprečavanja alergijske reakcije, sveprisutna upotreba hrane, kao što su mleko, kikiriki i soja, u prehrambenoj industriji aleričnim osobama znatno otežava izbegavanje slučajnog unosa alergena hrane. Ova činjenica nameće potrebu za iznalaženjem procesujućih metoda koje imaju za cilj da smanjenje alergenog potencijala hrane i kreiranje hipoalergenih prehrambenih proizvoda. Enzimске modifikacije molekula alergena mogu promeniti njihovu strukturu i onemogućiti vezivanje IgE antitela za konformacione ili linearne epitope. Najčešće korišćeni enzimi za smanjenje alergenosti prehrambenih proizvoda su proteaze, koje fragmentacijom alergena daju hipoalergene hidrolizate. Promena strukture alergena može se postići i njegovom polimerizacijom primenom enzima koji katalizuju unakrsno povezivanje proteina. Trenutno se u prehrambenoj industriji u cilju usavršavanja različitih funkcionalnih atributa hrane koriste transglutaminaze, za koje je pokazano da su efikasane i u smanjenju imunoreaktivnosti alergena hrane. Veliki potencijal imaju i okidaze, kao što su peroksidaze i polifenol okidaze koje, pored polimerizacije, mogu katalizovati i uvođenje malih molekula u strukturu polimernog alergena i tako maskirati vezujuća mesta IgE antitela. U budućnosti enzimске metode za modifikaciju prehrambenih alergena moći će da se primene i u razvoju bezbednih, a efikasnih, preparata za imunoterapiju alergija na hranu.

### Enzymatic processing of food allergens

Dragana J. Stanić-Vučinić  
*Faculty of Chemistry, Belgrade, Serbia*

Today more than 4 % of human population in industrialized countries suffers of food allergy. While strict avoidance is the best way to prevent allergic reaction, the ubiquitous use of food such as milk, peanuts and soy in the food industry makes it very hard for allergic individuals to avoid accidental ingestion. Therefore there is growing demand for methods aimed to reduce allergenic potential of food products and create hypoallergenic food. Enzymatic modification of allergen molecule may alter its structure and obstruct binding of IgE antibodies to conformational or linear epitopes. The most frequent used enzymes for reducing food allergenicity are proteases leading to allergen fragmentation resulting in hypoallergenic hydrolysates. Altering the structure of proteins can be attained by polymerization of allergens by usage of enzymes catalyzing protein cross-linking. Presently, microbial transglutaminase, utilized in the food industry to modify various functional attributes of food, was shown to be efficient in reducing immunoreactivity of food allergens. High potential have also oxidases, like peroxidase and polyphenol oxidases, beside cross-linking able to introduce small molecule into polymerized allergen structure and mask IgE antibody binding sites. In the future enzymatic methods for modification of food allergen have potential in development of safe, but efficient, preparations for immunotherapy of food allergies as well.



PPP 2



**Interakcija kompleksa prelaznih metala sa fosfolipidima i enzimima uključenim u metabolizam fosfolipida**

Tina Kamčeva\*, Bojana Damjanović\*\*\*, Maja Radisavljević\*, Živadin Bugarčić\*\*\*

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*\*\*\*\*Institut za medicinsku fiziku i biofiziku, Medicinski fakultet, Univerzitet u Lajpcig  
Lajpcig, Nemačka*

U ovom izlaganju će biti dat pregled rezultata koji govore o interakciji lekova na bazi metalnih kompleksa sa fosfolipidima, osnovnim sastojcima ćelijskih membrana, kao i sa enzimima koji su uključeni u metabolizam fosfolipida i produkciju važnih signalnih molekula. Pokazano je da čak i najmanje modifikacije u lipofilnosti liganda koji je u sastavu kompleksa dovode do značajnih izmena u unosu metalnog kompleksa u ćeliju. Pored interakcije kompleksa prelaznih metala, uglavnom sa negativno naelektrisanim fosfolipidima, uticaj kompleksa na osobine membrane je takođe pokazan: prisustvo kompleksa u membrani menja njene osobine i povećava njenu permeabilnost. Pored inhibicije raznih enzima, kompleksi prelaznih metala inhibiraju i enzime koji su uključeni u metabolizam fosfolipida, kao što je fosfolipaza A<sub>2</sub>. Pored pregleda dobijenih rezultata, u toku izlaganje će se diskutovati o prirodi navedenih interakcija, kao i o mogućim fiziološkim efektima i uticaju na progresiju tumora.

**The interaction of transition metal complexes with phospholipids and enzymes involved in phospholipid metabolism**

Tina Kamčeva\*, Bojana Damjanović\*\*\*, Maja Radisavljević\*, Živadin Bugarčić\*\*\*

Jürgen Arnhold\*\*\*\* and Marijana Petković\*

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Overview on the results obtained on the interaction of the transition metal complexes with phospholipids, main constituents of the cell membrane, as well as with enzymes involved in the phospholipid metabolism will be given in this presentation. It has been demonstrated that even slight modifications in the ligand lipophilicity significantly affect the drug uptake by a cell and its interaction with cellular targets. Cisplatin and several other transition metal complexes, potential anti-tumor agents interact with negatively-charged phospholipids in the membrane, but several authors indicate that the presence of transition metal complexes in the phospholipid bilayer affects also the properties of the bilayer/membrane. Furthermore, the membrane permeability increases after interaction with transition metal complexes, as demonstrated on the model systems and some cells. Inhibitory effect of transition metal complexes on the activity of several enzymes including phospholipase A<sub>2</sub> was also shown. Potential consequences of these interactions for the tumor cell progression and in host defense are discussed.



## Saopštenja / Contributions

### Analitička hemija / Analytical Chemistry Usmena saopštenja / Oral Presentations

AH01-O



#### Proučavanje keto-enolne tautomerije arildiketo kiselina u vodenj sredini upotrebom NMR spektroskopije i ciklične voltametrij

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$\beta$ -Diketo kiseline selektivno inhibiraju proces integracije HIV-1 provirusne DNK u DNK ćelije domaćina. U rastvoru podležu reakciji tautomerizacije, a afinitet ka kompleksiranju sa  $Mg^{2+}$  jonom (u aktivnom centru HIV-1 integraze), kao i reakcija hidrolitičkog raskidanja C–C veze u diketo delu molekula  $\beta$ -ketolazama zavise od oblika u kom se ova jedinjenja nalaze na mestu dejstva. NMR spektroskopijom i cikličnom voltametrijom, proučavana je keto-enolna tautomerija četiri jedinjenja iz grupe aril diketo kiselina u vodenom rastvoru u pH oblasti 1–10. Rezultati dobijeni NMR spektroskopijom pokazuju da se, nesupstituisana ADK (H-) nalazi u obliku enola **I**, enolni oblik **III** je prisutan u tragovima. Prema cikličnim voltamogramima izveden je zaključak da se, 4-Me i 3,4-di-Me- ADK u rastvoru nalaze takođe u obliku enola **I**, dok je 2,5-di-Me ADK prisutna kao smeša enola **I** i **III**. Izračunavanja dobijena semiempirijskim molekulsko-orbitalnim PM6 metodom nude moguće objašnjenje: veći torzioni ugao između aril grupe i ostatka molekula kod 2,5-di-Me ADK može biti razlog višeg potencijala na kome se ova ADK oksiduje, u poređenju sa ostalima.

#### Keto-enol Tautomerism of Aryldiketo Acids in Aqueous Solution. NMR Spectroscopy and Cyclic Voltammetry Study.

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Aryldiketo acids (ADK) complexation ability with  $Mg^{2+}$  ion (present in HIV-1 IN) and the hydrolytic C–C bond cleavage by  $\beta$ -ketolases depend on predominant tautomeric form in which they are present at the reaction site. Thus, the keto-enol tautomerism of H-, 4-Me-, 2,5-di-Me-, and 3,4-di-Me- ADK in the aqueous solution within pH range 1–10 was studied by NMR spectroscopy and cyclic voltammetry. The NMR results for H- ADK showed that the predominant tautomeric form in the studied pH range is the enolate **I**. The cyclic voltammetry data in acidic media (pH 1) suggest that the ratio of possible tautomeric forms for 4-Me- and 3,4-di-Me- ADK is similar to H-ADK, *i.e.* that enolate **I** is the dominant form in the solution, whilst two tautomeric forms of 2,5-di-Me- ADK (enolates **I** and **III**) may be present in solution. The higher oxidation potential observed for  $H_2A$  form of 2,5-di-Me- ADK at pH 1 may be due to non-planarity of molecule and steric hindrance imposed by *ortho* substituents.





### **Izotopski „otisak prsta“ metala upotrebom MALDI TOF MS**

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U ovom radu predočene su mogućnosti primene MALDI TOF masene spektrometrije u analizi metala i molekula koji sadrže metale. Akcenat je stavljen na mogućnost identifikacije i kvantitativnog određivanja izotopskog sastava elemenata u uzorku na osnovu MALDI-TOF masenih spektara. Pokazano je da je ova meka jonizaciona tehnika dovoljno osetljiva za detekciju sva četiri izotopa olova i određivanje njihove relativne zastupljenosti, što omogućava njenu široku primenu, na primer, u arheologiji za utvrđivanje starosti i porekla predmeta od olova, u forenzici i balistici kao i u ekologiji za određivanje izvora zagađenja olovom u biljkama, sedimentima i vodenim organizmima. Granica detekcije za izotopski „otisak prsta“ olova u celini omogućava ograničenu primenu u analizi hrane. Posebna pogodnost MALDI TOF masene spektrometrije je što omogućava analizu bioloških materijala bez dodatne fragmentacije, pa se njom mogu analizirati ne samo pojedinačni metalni joni, već i elementi koji ulaze u sastav biomolekula ili metalnih kompleksa. Pored olova, izotopski sastav rutenijuma i platine se takođe može odrediti MALDI-TOF masenom spektrometrijom, a može se pretpostaviti da je moguća i analiza drugih metala.

### **Isotopic fingerprinting of metals by MALDI TOF MS**

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In this work potentials of MALDI TOF mass spectrometry in analysis of metals and metals containing molecules are described. The accent is on the possibility of metal identification and quantitative determination of isotope composition based on the MALDI-TOF mass spectra. It has been shown that this soft ionisation technique is sufficiently sensitive for detection of all four isotopes of lead and determination of their relative abundances, what enables its widely application in archaeology for determination of origin and date of lead samples, in forensic sciences and ballistics and in ecology for searching the source of pollution by lead in plants, sediments and aquatic organisms. Detection limit for „isotopic fingerprint“ of lead at whole allows limited usage of this technique in food safety. Study of platinum and ruthenium complexes, as potential chemotherapeutics, showed preserved isotopic distribution of these transition metals. Possibility of analysis of other metals by this approach can be assumed.





### **Određivanje $\text{Ag}^+$ i $\text{Cl}^-$ jona u uzorcima ekoloških voda primenom jednostavnog poli(vinil hlorid-ko-vinil acetat)/srebro potenciometrijskog senzora**

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Cilj ovog rada je bio ispitivanje mogućnosti primene novog Ag-selektivnog potenciometrijskog senzora napravljenog samo od poli(vinil hlorid-ko-vinil acetata), plastifikatora i lipofilne soli i nanešenog direktno na štapić staklastog ugljenika. Predloženi senzor može da funkcioniše u jako kiseljoj sredini, jer je njegov radni pH opseg < 1 do 7. Pored jednostavnosti izrade i širokog pH opsega, prednost ove elektrode je i veoma dobra selektivnost. PVCAc/Ag elektroda je uspešno primenjena kao indikatorska elektroda u potenciometrijskim titracijama. Praktična primena predloženog senzora je testirana određivanjem srebrnih i hloridnih jona u uzorcima ekoloških voda i koloidnoj srebrnoj vodi. Povratni prinos srebra iz različitih uzoraka voda je bio skoro kvantitativan. Hloridni joni su uspešno određivani potenciometrijskom titracijom u uzorcima česmenske, rečne i morske vode. Takođe, rezultati dobijeni za hloridne jone u ekološkim vodama, kao i za jone srebra u koloidnoj srebrnoj vodi, se dobro slažu sa vrednostima dobijenim uporednim metodama.

### **Determination of Silver and Chloride Ions in Environmental Water Samples by Simple PVCAc/Ag Potentiometric Sensor**

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The aim of this work was to investigate possibility of application of new Ag-selective potentiometric sensor made only from PVCAc, plasticizer and lipophilic salt and coated directly on GC rod. Since working pH range of proposed sensor is < 1 to 7, it can operate in very acidic media. Besides simplicity of sensor construction and wide pH range, the excellent selectivity can be also advantage of this electrode. The proposed electrode was successfully applied as an indicator electrode for the potentiometric titrations. The practical utility of the proposed PVCAc/Ag sensor was tested by determination of silver and chloride ions in environmental water samples and silver in colloidal silver water. The recovery of silver from different water samples is almost quantitative. The chloride ions were successfully determined by potentiometric titrations in tap, river and sea water samples. Also, the results obtained for chloride ions in environmental water samples and silver ions in colloidal water samples by the proposed sensor were in satisfactory agreement with data obtained with comparative methods.







### Ravnoteže kompleksiranja Gd(III)-jona sa nekim fluorohinolonima

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Kompleksiranje Gd(III)-jona sa fluorohinolonima ciprofloksacinom (II generacija), ofloksacinom (II generacija) i moksifloksacinom (IV generacija) proučavano je metodom potencijometrijskih titracija na 298 K u jonskoj sredini NaCl (0,1mol/L). U koncentracijom opsegu 0,6mmol/L  $\leq$  [Gd(III)]  $\leq$  3mmol/L i fluorohinolona 1mmol/L  $\leq$  [fluorohinolon]  $\leq$  3mmol/L pri koncentracijom odnosu M:L 1:1 do 1:5 nađeni su binarni kompleksi ML, ML<sub>2</sub> i ML<sub>3</sub> u celokupnoj ispitivanoj pH oblasti (2,0  $\leq$  pH  $\leq$  9,5). Osim ovih kompleksa koji su i dominantni nađeni su i mešoviti kompleksi tipa MH<sub>q</sub>L<sub>p</sub> gde su p i q kod ciprofloksacina (1,1), (1,-1), (2,2), (2,1), (2,-2), (3,3); kod ofloksacina (1,1), (1,-1), (2,2), (2,1), (2,-1), (2,-2), (3,3), (3,2), (3,1), (3,-1) i kod moksifloksacina (1,1), (2,2), (2,1), (3,3), (3,2), (3,1). Negativne vrednosti q označavaju hidrolitičke komplekse. Polinuklearni kompleksi nisu nađeni u ispitivanim sistemima. Na osnovu dobijenih rezultata ispitivan je uticaj navedenih fluorohinolona na biodistribuciju Gd(III)-jona u humanoj plazmi prilikom upotrebe Gd-helata (Gd-DTPA) kao dijagnostičkih agenasa u magnetno-rezonantnim snimanjima.

### Complex formation equilibria between Gd(III)-ion and some fluoroquinolones

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Complex formation between Gd(III)-ion and fluoroquinolones, ciprofloxacin (II generation), ofloxacin (II generation) and moxifloxacin (IV generation) were studied by potentiometric titrations at 298 K in ionic medium NaCl (0.1mol/L). In the concentration range 0.6mmol/L  $\leq$  [Gd(III)]  $\leq$  3mmol/L and 1mmol/L  $\leq$  [fluoroquinolone]  $\leq$  3mmol/L at concentration ratio M:L = 1:1 to 1:5, binary complexes ML, ML<sub>2</sub> and ML<sub>3</sub> were found in the entire pH region (2-9.5). In addition to the dominant binary complexes the following mixed complexes of the MH<sub>q</sub>L<sub>p</sub> type were found: ciprofloxacin, (p,q)= (1,1), (1,-1), (2,2), (2,1), (2,-2), (3,3); ofloxacin, (p,q)= (1,1), (1,-1), (2,2), (2,1), (2,-1), (2,-2), (3,3), (3,2), (3,1), (3,-1) and moxifloxacin, (p,q)= (1,1), (2,2), (2,1), (3,3), (3,2), (3,1). Negative values of q denote hydrolytic complexes. Polynuclear complexes were not found in the systems examined. On the basis of the acquired results the effect of fluoroquinolones on biodistribution of Gd ion in human plasma, during the application of Gd-helates (Gd-DTPA) as diagnostic agents in MR imaging was studied.



### HPLC Determination of Tetracycline in Human Control Serum

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A reversed-phase HPLC with diode-array detection was optimized and validated for the determination of tetracycline in human control serum. The separation was achieved on Zorbax Extend-C18 analytical column at 40°C. The mobile phase, a mixture of *tert*-butyl alcohol, Na<sub>2</sub>HPO<sub>4</sub>, triethylammonium acetate and Na-EDTA, was injected isocratically. UV detection was performed at 375 nm. In human control serum tetracycline was determined by using calibration graph in the range of 1 µg/cm<sup>3</sup>-10 µg/cm<sup>3</sup>. Serum sample was pretreated with 8.0% HClO<sub>4</sub>. The limit of detection and limit of quantification were 4.0 ng and 13.0 ng, respectively. The precision results showed that the relative standard deviation is up 6.3%. The proposed method enables separation and determination of tetracycline with the total time of the analysis not more than 5 min.

### HPLC određivanje tetraciklina u humanom kontrolnom serumu

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U radu je optimizovana i validovana reverzno-fazna HPLC metoda za određivanje tetraciklina u humanom kontrolnom serumu. Razdvajanje je izvršeno na Zorbax Extend-C18 analitičkoj koloni i temperaturi od 40°C. Mobilna faza se sastojala od terc-butil alkohola, Na<sub>2</sub>HPO<sub>4</sub>, trietilamonijum-acetata i Na-EDTA, a u aparat je ubrizgavana izokratno. UV detekcija je izvedena na 254 nm, 275 nm i 375 nm. U kontrolnom serumu tetraciklin je određivan primenom kalibracione prave u intervalu 1 µg/cm<sup>3</sup>-10 µg/cm<sup>3</sup>. Radi uklanjanja proteina uzorak seruma je tretiran 8.0% HClO<sub>4</sub>. Limit detekcije i limit kvantifikacije iznose 4.0 ng i 13.0 ng. Relativna standardna devijacija određivanja kreće se do 6.3%. Predložena metoda omogućava razdvajanje i određivanje tetraciklina u navedenim uzorcima, pri čemu je ukupno vreme trajanja analize kraće od 5 minuta.





### **Adsorpcija pesticida na karbonizovanim kratkim vlaknima konoplje aktiviranim kalijum hidroksidom**

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U ovom radu je predstavljeno dobijanje karbonizovanih otpadnih kratkih vlakana konoplje i njihova aktivacija kalijum hidroksidom uz korišćenje različitih odnosa kalijum hidroksida i karbonizovanog materijala. Površinske karakteristike dobijenih uzoraka predstavljene su specifičnom površinom dobijenom BET metodom i sadržajem površinskih funkcionalnih grupa dobijenih temperaturno-programiranom desorpcijom. Adsorpcija pesticida (actamiprid, dimetoat, nikosulfuron, karbofuran i atrazin) na uzorcima karbonizovanih kratkih vlakana konoplje iz vodenih rasvora ispitivana je u šaržnom sistemu uz neprekidno mešanje. Dobijeni rezultati pokazuju da se aktivacijom sa kalijum hidroksidom može dobiti materijal visoke vrednosti specifične površine ( $S_{BET} = 2192 \text{ m}^2/\text{g}$ ). Specifična površina i količina površinskih funkcionalnih grupa zavise od količine aktivirajućeg agensa. Adsorpcioni kapacitet uzoraka takođe prati ovaj trend. Svi ispitivani uzorci imaju dobre adsorpcione karakteristike, neaktiviran uzorak konoplje snižava koncentraciju pesticida za više od 50 %, dok svi aktivirani uzorci uklanjaju više od 90 % pesticida iz vodenog rastvora.

### **Adsorption of pesticides onto the carbonized short hemp fibers activated with potassium hydroxide**

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This study presents the production of carbonized waste short hemp fibers followed by potassium hydroxide activation using different ratios of potassium hydroxide and carbonized material. The surface properties of the carbonized samples were investigated by BET method (surface area) and temperature-programmed desorption. Adsorption of pesticides (acetamiprid, dimethoate, nicosulfuron, carbofuran and atrazine), from aqueous solution onto carbonized short hemp fibers was studied in batch system, with constant shaking. It was shown that materials with high specific surface area ( $S_{BET} = 2192 \text{ m}^2/\text{g}$ ) can be obtained by activation with potassium hydroxide. Specific surface area and amount of surface oxygen groups depend of the amount of KOH. Pesticide adsorption capacity follows the same trend. All tested samples have good adsorption properties, inactivated sample decreases pesticide concentration for more than 50 %, while activated samples remove more than 90 % of pesticides.



### **Primena jonske hromatografije u kontroli kvaliteta vode na postrojenju za preradu vode Makiš**

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Jedan od glavnih zadataka postrojenja Makiš za preradu vode reke Save je snabdevanje stanovništva higijenski ispravnom vodom za piće koja ispunjava standarde propisane Pravilnikom o higijenskoj ispravnosti vode za piće (Sl. list SRJ br. 42/98). Sve veći zahtevi u pogledu kvaliteta vode uslovljavaju razvijanje novih metoda analize u analitičkoj hemiji. Analiza uobičajenih neorganskih anjona spada u obavezne parametre. Predmet ovog rada je ispitivanje mogućnosti primene supresorske jonske hromatografije sa konduktometrijskim detektorom za svakodnevnu kontrolu anjona u vodama beogradskog vodovodnog sistema. Ovom tehnikom izvršena je kvalitativna i kvantitativna analiza uzoraka vode iz različitih faza proizvodnje na sledeće anjone:  $\text{Cl}^-$ ,  $\text{F}^-$ ,  $\text{Br}^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ,  $\text{PO}_4^{3-}$  i  $\text{SO}_4^{2-}$ . Prerada vode reke Save na PP Makiš obuhvata sledeće faze proizvodnje: predozonizaciju, bistrenje, glavnu ozonizaciju, filtraciju kroz peščane i filtere sa granulisanim aktivnim ugljem i dezinfekciju. Na osnovu rezultata analize zaključeno je da je u svim fazama prerade sirove vode sadržaj anjona nizak, a u uzorku pijaće vode je ispod maksimalno dozvoljene koncentracije propisane Pravilnikom. Ova savremena instrumentalna tehnika se pokazala kao jednostavnija, selektivnija i osetljivija u odnosu na konvencionalne tehnike kao što su titracija, gravimetrija i kolorimetrija. Takođe, ona omogućava brzu analizu sa sposobnošću simultanog određivanja velikog broja komponenti značajnih za kvalitet vode.

### **Application of Ion Chromatography for water quality control at water treatment plant Makis**

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One of the main tasks of water plant Makis for water treatment from the river Sava is supplying the population with hygienic correct drinking water which meets the rules of standards listed in Regulation for drinking water hygiene (Official paper 42/98). The increasing demands in water quality requests developing of new methods of analysis in analytical chemistry. Analysis of common inorganic anions belongs to required parameters. The subject of this paper was to investigate the possibilities of applying ion chromatography with suppressed conductivity detection for daily anion control in Belgrade water distribution system. Qualitative and quantitative analysis of water samples were performed with this technique in different stages of production on the following list of anion:  $\text{Cl}^-$ ,  $\text{F}^-$ ,  $\text{Br}^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ,  $\text{PO}_4^{3-}$  and  $\text{SO}_4^{2-}$ . The water treatment from the river Sava in the water plant Makis includes the following phases of production: preozonisation, clarification, main ozonisation, filtration through sand and granulated activated carbon and disinfection. Based on the results of analysis it was concluded that in all stages of raw water treatment content of anions were low, and in drinking water sample was under the maximum permitted concentration listed by the Regulation. This modern instrumental technique proved to be simpler, more selective, and more sensitive than the conventional techniques such as titration, gravimetry and colorimetry. Also, it allows rapid analysis with capability of simultaneous determination of many important components for water quality.

AH08-O

### **Efekti supstituenata i rastvarača na UV-Vis apsorpcione spektre *p*-supstituisanih aroilakrilnih kiselina**

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U ovom radu proučavani su uticaji supstituenata, polarnosti rastvarača i interakcije vodoničnog vezivanja između rastvarača i rastvorene supstance na UV-Vis apsorpcione spektre *p*-supstituisanih aroilakrilnih kiselina (AAK), jedinjenja koja pokazuju antibakterijsko i antiproliferativno dejstvo. Ispitivano je deset jedinjenja iz grupe AAK: nesupstituisana i devet *p*-supstituisanih (Me-, Et-, *i*-Pr-, *t*-Bu-, *n*-Bu-, F-, Cl-, Br-, MeO-). Apsorpcioni spektri snimljeni su u deset rastvarača različite polarnosti, u opsegu talasnih dužina 220-400 nm. Talasna dužina apsorpcionog maksimuma korelisana je sa literaturnim vrednostima konstanti supstituenata ( $\sigma_p$ ) primenom jednostavne Hammett-ove jednačine. Uticaj polarnosti rastvarača i interakcija vodoničnog vezivanja između rastvorene supstance i rastvarača proučavani su pomoću koncepta linearne korelacije solvatacionih energija (LSER) koji su uveli Kamlet i Taft.

### **Substituent and solvent effect on the UV-Vis absorption spectra of *p*-substituted aroylacrylic acids**

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In this work, the effect of substituent, solvent polarity and solvent/solute hydrogen bonding interactions on UV-Vis absorption spectra of *p*-substituted aroylacrylic acids (AAK), compounds that show antibacterial and antiproliferative activity, were investigated. Ten compounds from the class of AAK: unsubstituted and nine *p*-substituted (Me-, Et-, *i*-Pr-, *t*-Bu-, *n*-Bu-, F-, Cl-, Br-, MeO-) were investigated. UV-Vis absorption spectra were recorded in ten solvents of different polarity in the range 220-400 nm. Wavelength of the observed absorption maximum was correlated with literature substituent constants ( $\sigma_p$ ) by simple Hammett equation. The effect of solvent polarity and solvent/solute hydrogen bonding interactions was analyzed by means of linear solvation energy relationships (LSER) concept proposed by Kamlet and Taft.



Posterska saopštenja / Poster Presentations

AH09-P



**Termohromno ponašanje i termodinamika hlora kompleksa kobalta(II)  
u smeši amonijum-nitrat - formamid**

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Apsorpcioni spektri rastvora kobalta(II) u rastvaraču  $\text{NH}_4\text{NO}_3 \cdot 4\text{HCONH}_2$  snimljeni su u intervalu talasnih dužina od 400-800 nm na temperaturama 308,15, 318,15, 328,15, 338,15 i 348,15 K. Dodatak amonijum-hlorida u rastope koji sadrže određenu koncentraciju kobalta(II) uzrokuje pomeranje osnovnih apsorpcionih traka ka nižim energijama i nagli porast molarnog apsorpcionog koeficijenta što ukazuje na promenu geometrije kompleksa kobalta(II). Ovakvo ponašanje se može objasniti prisustvom nižih oktaedarskih kompleksa kobalta(II) sa nitratnim jonima ili organskim molekulima ili je tetraedarska struktura veoma deformisana. Dobijeni rezultati potvrđuju da se formiraju sledeći kompleksi:  $[\text{CoF}_2(\text{NO}_3)_4]^{2-}$ ,  $[\text{CoF}_2\text{Cl}_2(\text{NO}_3)_2]^{2-}$  i  $[\text{CoCl}_4]^{2-}$ . Bruto konstante stabilnosti izračunate su na 308,15, 318,15, 328,15, 338,15 i 348,15 K. Na osnovu konstanti stabilnosti dobijenih na različitim temperaturama izračunati su termodinamički parametri i zaključeno je da proces građenja svih kompleksa u ispitivanom sistemu je endoterman proces, a građenje ovih kompleksa ide na račun povećanja entropije.

**Termochromic Behaviour and Thermodynamic of Cobalt(II) Chloro Complexes  
in Ammonium Nitrate – Formamide Mixture**

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Absorption spectra of cobalt(II) chloride in  $\text{NH}_4\text{NO}_3 \cdot 4\text{HCONH}_2$  system have been investigated in the wavelength range 400-800 nm at temperatures 308,15, 318,15, 328,15, 338,15 and 348,15 K. Addition of chloride ions to cobalt(II) chloride solution caused a pronounced shift of the absorption maximum toward lower energies and a significant increase of absorption intensity, indicating a change in co-ordination geometry. The increase of the overall molar absorption coefficient in the chloride containing melts with temperature was attributed to mixed complex formation with solvent molecules (or ions) ions and structural changes in the cobalt(II) complexes. From an analysis of the spectra it was concluded that the following complexes were formed:  $[\text{CoF}_2(\text{NO}_3)_4]^{2-}$ ,  $[\text{CoF}_2\text{Cl}_2(\text{NO}_3)_2]^{2-}$  and  $[\text{CoCl}_4]^{2-}$ . The overall stability constants of these complexes and the corresponding resolved species spectra were calculated at 308,15, 318,15, 328,15, 338,15 and 348,15 K. Thermodynamic parameters were calculated using the temperature dependence of stability constants we determined. Complex formation in all systems is endothermic process followed with higher entropy values.





### **Računarsko modelovanje humane krvne plazme**

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Računarsko modelovanje krvne plazme izvršeno je upotrebom kompjuterskog programa za specijacije HySS i publikovanih podataka o konstantama stabilnosti kompleksa esencijalnih jona metala i najzastupljenijih bioliganada niske molekulske mase u humanoj plazmi. Model uključuje 11 jona metala i 42 bioliganda sa oko 3000 kompleksa. U cilju dobijanja pouzdanih rezultata uzete su vrednosti konstanti stabilnosti koje su bliske fiziološkim uslovima, ili je vršena njihova korekcija na fiziološke uslove. Izračunata distribucija metala između bioliganada pod fiziološkim uslovima je u skladu sa do sada publikovanim literaturnim podacima i ukazuje na značajan uticaj malih promena vrednosti pH na specijaciju.

### **Computer modeling of human blood plasma**

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The computer model of human blood plasma has been developed using speciation program HySS and published stability constant data of complexes between essential metal ions and blood bioligands of low molecular mass. Eleven metal ions and 42 ligands forming around 3000 complexes were included in speciation calculations. To obtain reliable results, stability constants data close to physiological conditions were taken, or their correction is made to physiological conditions. The calculated metal distribution between bioligands under physiological conditions is in agreement with so far published data and indicates considerable influence of small pH changes on speciation.



AH11-P

**Određivanje karbonilnih jedinjenja (acetaldehida i formaldehida) u ambalaži od polietilentereftalata namenjenoj za čuvanje vode**

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Poletilen-tereftalat (PET) je u poslednjih nekoliko godina postao glavni materijal za pakovanje mnogih prehrambenih proizvoda, naročito za gazirana pića i flaširane vode, kao i za proizvode hemijske industrije (za pakovanje raznih sredstava za održavanje higijene, pesticida, rastvarača i dr.). Acetaldehid i formaldehid nastaju u toku termoformiranja PET ambalaže. Posle hlađenja acetaldehid i formaldehid ostaju zarobljeni u zidu PET boce i mogu migrirati u vodu posle punjenja i skladištenja. S obzirom da kod nas nisu propisani migracioni testovi za određivanje acetaldehida i formaldehida, cilj ovog rada je bio da se ispita kvantitativni sadržaj karbonilnih jedinjenja (acetaldehida i formaldehida) u PET ambalaži različitih zapremina, od različitih proizvođača flaširane mineralne i izvorske vode, izloženih različitim temperaturama. Sadržaj karbonilnih jedinjenja određivan je metodom obrnuto-fazne tečne hromatografije pod visokim pritiskom (RP-HPLC). S obzirom da formaldehid i acetaldehid nemaju UV aktivnu ili fluorescentnu grupu, hromatografskim određivanjima prethodi derivatizacija u zatvorenom sistemu (zbog niskih tački ključanja formaldehida i acetaldehida), čime se karbonilna jedinjenja prevode u UV aktivna jedinjenja.

**Determination of carbonyl compounds (acetaldehyde and formaldehyde) in polyethylene terephthalate containers designated for water conservation**

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Polyethylene terephthalate (PET) has in the last several years become the main packaging material for many food products, particularly carbonated beverages and bottled water, as well as for products of chemical industry (packaging of various hygiene maintenance agents, pesticides, solvents, etc.). Acetaldehyde and formaldehyde are formed during the thermoforming of PET containers. After cooling, acetaldehyde and formaldehyde remain trapped in the walls of a PET bottle and may migrate into the water after filling and storage. Since there are no migration tests in Serbia prescribed for the determination of acetaldehyde and formaldehyde, the purpose of the paper is to test the quantitative contents of carbonyl compounds (acetaldehyde and formaldehyde) in PET containers of different volumes, made by various manufacturers of bottled mineral and spring water, and exposed to different temperatures. The method used for determining carbonyl compounds is a reversed phase high performance liquid chromatography (RP-HPLC). Taking into consideration that formaldehyde and acetaldehyde have no UV active or fluorescent group, the chromatography was preceded by derivatization in a closed system (due to a low boiling point of acetaldehyde and formaldehyde) in order to transform carbonyl compounds into UV active compounds.





AH12-P

**Primena sulfidnog minerala pirita kao elektrohemijskog senzora  
u nevodenoj sredini: potenciometrijska titracija slabih kiselina u  
*N,N*-dimetilformamidu i piridinu**

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Prirodni monokristal pirita je primenjen kao senzorski materijal za potenciometrijske titracije benzojeve, antranilne, malonske, salicilne kiseline i  $\alpha$ -nitrozo- $\beta$ -naftola u *N,N*-dimetilformamidu i piridinu. Ispitana elektroda pokazuje linearnu zavisnost potencijala od logaritma koncentracije *p*-toluensulfonske kiseline (u opsegu koncentracija od 0,100 do 0,001 M). Potencijal elektrode pokazuje sub-Nernstovsku zavisnost, sa nagibom od 39,0 mV po dekadi u *N,N*-dimetilformamidu. Dobijeni skokovi potencijala u toku titracije slabih kiselina su veći nego skokovi dobijeni primenom staklene indikatorske elektrode. Stabilan potencijal tokom titracije i na tački ekvivalencije veoma brzo se uspostavlja. Potvrđeno je da su natrijum metilat, kalijum hidroksid i tetrabutilamonijum hidroksid veoma pogodna titraciona sredstva za ova ispitivanja. Standardna devijacija određivanja ispitivanih kiselina je 0,10–0,35% u odnosu na rezultate dobijene primenom staklene elektrode. Uzimajući u obzir jednostavnu konstrukciju, nisku cenu proizvodnje, dugotrajnost i veliku reproduktivnost ove elektrode, možemo zaključiti da se pirit može koristiti kao pogodna indikatorska elektroda u potenciometrijskim acido-baznim titracijama u *N,N*-dimetilformamidu i piridinu.

**Use of the sulfide mineral pyrite as electrochemical sensor in non-aqueous solutions:  
potentiometric titration of weak acids in *N,N*-dimethylformamide and pyridine**

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The possibility of applying natural monocrystalline pyrite as a sensor for the potentiometric titration of benzoic acid, anthranilic acid,  $\alpha$ -nitroso- $\beta$ -naphthol, malonic acid and salicylic acids in *N,N*-dimethylformamide and pyridine was investigated. The investigated electrode showed a linear dynamic response for *p*-toluensulfonic acid concentrations in the range from 0.100 to 0.001 M. The potential of the electrode in *N,N*-dimethylformamide and pyridine exhibits a sub-Nernst dependence, with the slope of 39.0 mV per decade in *N,N*-dimethylformamide. The potential jumps at the titration end-point obtained in the titration of weak acids are higher than those obtained by the application of a glass electrode as the indicator electrode. The potential in the course of the titration and at the titration end-point are rapidly established. Sodium methylate, potassium hydroxide and tetrabutylammonium hydroxide proved to be very suitable titrating agents for these titrations. The results obtained in the determination of the investigated weak acids deviate by 0.1–0.35% with respect to those obtained by using a glass electrode as the indicator electrode. The advantages of the electrode are long-term stability, fast response, and reproducibility, while the sensor is easy to prepare and of low cost.

## AH13-P

**Komparativna kinetička i ICP-OES analiza tragova Cu(II) u uzorcima voća**

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U ovom radu je predstavljena komparativna analiza tragova Cu(II) primenom jednostavne, brze i reproduktivne kinetičke metode za određivanje tragova Cu(II) i ICP-OES metode u uzorcima voća. Dinamički opseg primenjene kinetičke metode je u oblasti 13-318 ng/ml. Priprema uzoraka, je kao kritičan korak u svakoj analizi pažljivo izvršena suvim spaljivanjem, uz dodatak HNO<sub>3</sub>, s obzirom na veliku količinu organske materije. Sadržaj Cu(II) varira u različitim uzorcima voća (*breskva* - 0.123 mg/100g; *jagoda* - 0.168 mg/100g ; *jabuka* - 0.128 mg/100g, sa relativnom standardnom devijacijom 1.6, 1.7, 1.5 % respektivno (Tabela I). Rezultati dobijeni primenom kinetičko-spektrofotometrijske i ICP-OES metode su u dobroj saglasnosti. Utvrđeno je da ne postoji statistički značajna razlika među rezultatima dobijenim primenom ove dve metode.

**A comparison of kinetic and ICP-OES analysis of traces of Cu(II) in fruit samples**

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In this work comparative analysis of traces of Cu(II) by simple, fast, reproducible kinetic method and ICP-OES method in fruit samples. Dynamic range of applied kinetic method is in interval of Cu(II) concentration 13-318 ng/ml. Preparation of samples is a critical stage in trace elements analysis. Contents of Cu(II) varies in different kind of fruit samples (peach - 0.123 mg/100g; strawberry - 0.168 mg/100g ; apple - 0.128 mg/100g) with relative standard deviation of 1.6, 1.7, 1.5 %, respectively (Table I). Results obtained using both methods are in good agreement. Statistical comparison of the results showed no significant difference in accuracy and precision between the applied kinetic method and the ICP-OES measurements.

Table I. Kinetic Determination of Copper(II) in Fruit

Samples	Kinetic method <sup>a</sup> , x±S.D., mg/100g	RSD <sup>b</sup> %	R <sup>c</sup> %	ICP-OES method x±S.D.	F-test <sup>d</sup>
<i>Strawberry</i>	0.125 ± 0.002	1.6	101.6	0.123 ± 0.001	4.00
<i>Peach</i>	0.172 ± 0.003	1.7	102.4	0.168 ± 0.002	2.25
<i>Apple</i>	0.134 ± 0.002	1.5	104.7	0.128 ± 0.001	4.00

<sup>a</sup>Mean value ± standard deviation (n = 5); <sup>b</sup>Relative standard deviation; <sup>c</sup>Recovery.

<sup>d</sup>Tabulated F-value for (v<sub>1</sub> = 4, v<sub>2</sub> = 4) degrees of freedom at P(0.05) is 6.39.



АН14-Р

### Одређивање ваздух-вода партиционих коефицијената малих органских молекула реверзно-фазном танкослојном хроматографијом

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Ваздух-вода партициони коефицијент,  $K_{AW}$ , представља један од параметара који одређују судбину супстанце у животној средини. Обично се експериментално одређује мерењем појединачних фракција супстанце у свакој од испитиваних фаза. Међутим, вода, ваздух и гранична површина коју одликује висок површински напон, представљају добар модел за процену липофилности молекула. У оквиру овог рада реверзно-фазна танкослојна хроматографија, као поуздана метода за одређивање липофилности молекула, употребљена је за процену ваздух-вода партиционог коефицијента. Деветнаест стандардних једињења са експериментално одређеним вредностима  $\log K_{AW}$  је употребљено за калибрацију. Октадецил-модификовани силика-гел као стационарна и смеше ацетонитрила и воде, односно диоксана и воде (1:1, v/v), као мобилне фазе коришћене су у хроматографским експериментима. Добијене су калибрационе криве задовољавајућег квалитета са вредностима параметра  $R$  од 0,8219 и 0,8179 на основу којих су одређене  $\log K_{AW}$  непознатим једињењима. Исте вредности су даље поређене са вредностима израчунатим помоћу EPI Suite софтверског пакета (U.S. Environmental Protection Agency, EPA). Добијена је добра корелација за супстанце хемијски сличне испитиваним стандардима.

### Determination of the air-water partition coefficient of the small organic molecules by the means of the reversed phase thin layer chromatography

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The air-water partition coefficient,  $K_{AW}$  is one of the most important constants determining fate of a substance in the environment. It is usually experimentally determined by measuring the fraction of the substance in each of the two phases. On the other hand, water, air, and the border between them made by the water surface characterized with high surface tension, can be used as a good model for the lipophilicity assessment. In the present work reversed-phase thin-layer chromatography which is known to be efficient way of measuring lipophilicity was employed to assess the  $\log K_{AW}$  constants. Nineteen standard compounds with experimentally determined  $\log K_{AW}$  partition coefficients were used to establish calibration curves. Octadecyl-modified silica as a stationary phase combined with acetonitrile-water or dioxane-water mixtures (1:1, v/v), was used in chromatographic experiments. Obtained calibration curves were of good statistical quality with  $R$  values of 0.8219 and 0.8179, respectively and further were used to assess  $\log K_{AW}$  of unknowns. Obtained  $\log K_{AW}$  values were compared with those calculated by the means of EPI Suite software package, freely available from the U.S. Environmental Protection Agency (EPA). A good correlation was established with substances chemically similar to the studied standard compounds.



AH15-P

**Derivativno spektrofotometrijsko određivanje aktivne komponente komercijalne formulacije Mospilan 20 SL u prisustvu 6-hlornikotinske kiseline**

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Predložena je jednostavna i brza spektrofotometrijska metoda na bazi prvog izvoda za istovremeno određivanje acetamiprida i 6-hlornikotinske kiseline (6-HNK) pri pH 7,0. Primenjujući pristup nultog preseka acetamiprid je određivan u model sistemu na 269 nm a 6-HNK na 216 nm, sa granicama detekcije od  $7,19 \times 10^{-7}$  i  $8,25 \times 10^{-7}$  mol dm<sup>-3</sup>, respektivno i standardnom devijacijom manjom od 1,2%. Predložena metoda je primenjena za određivanje ciljnih jedinjenja u 6-HNK-om obogaćenoj komercijalnoj formulaciji acetamiprida Mospilan 20 SP.

Komparativna tečnohromatografska analiza sa detektorom od niza dioda je rađena uz primenu mobilne faze pripremljene od 0,2% fosforne kiseline i acetonitrila u odnosu 7:3, v/v.

Rezultati predložene spektrofotometrijske metode su u dobroj saglasnosti sa rezultatima komparativne metode.

**Derivative spectrophotometric determination of the active compound of the commercial formulation Mospilan 20 SP in the presence of 6-chloronicotinic acid**

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A simple and fast first-order derivative spectrophotometric method was developed for the simultaneous determination of acetmiprid and 6-chloronicotinic acid (6-CNA) at pH 7.0. By using the zero-crossing approach, acetamiprid was determined at 269.0 nm and 6-CNA at 216.0 nm with the detection limits of  $7.19 \times 10^{-7}$  and  $8.25 \times 10^{-7}$  mol dm<sup>-3</sup>, respectively and relative standard deviations not exceeding 1.2% in the case of model systems. The proposed method was applied for the determination of the target compounds in commercial formulation of acetamiprid Mospilan 20 SP spiked with 6-CNA.

The comparative high-performace liquid chromatographic analysis with diode array detection was performed using a mobile phase made from 0.2% phosphoric acid and acetonitrile in ratio 7:3, v/v. The results of the developed spectrophotometric method are in good agreement with those obtained by the comparative method.

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AH16-P

### **Upoređivanje odabranih metoda ekstrakcije za određivanje insekticida klotianidina u medu primenom tečne hromatografije visoke efikasnosti sa detektorom od niza dioda**

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Ispitana je primenljivost tečnohromatografske metode sa detektorom od niza dioda (HPLC-DAD) za određivanje klotianidina, insekticida iz grupe neoinikotinoida, u medu. HPLC-DAD merenja su rađena na reversno-faznoj koloni, pri izokratskim uslovima eluiranja uz mobilnu fazu pripremljenu od vode (sa 0,2% fosforne kiseline) i acetonitrila u odnosu 7:3, v/v, pri čemu je radna talasna dužina detektora bila 266 nm, a retenciono vreme klotianidina 3,2 min. Ispitivana su tri postupka prečišćavanja uzoraka meda obogaćena klotianidinom (0,5 i 2,0 mg/kg), tečno-tečna dihlormetanska ekstrakcija, ekstrakcija na čvrstoj fazi (kolona Discovery-18) i njihova kombinacija. Nađeno je da ni tečno-tečna ekstrakcija, ni kolona za prečišćavanje same nisu obezbedile uzorak zadovoljavajućeg kvaliteta za dalju HPLC-DAD analizu. Zbog složenosti matriksa, kombinacija tečno-tečne ekstrakcije i prečišćavanja na čvrstoj fazi obezbeđuje uzorke zadovoljavajućeg kvaliteta za dalju HPLC-DAD analizu pri čemu prinosi su bili veći od 83%.

### **Comparison of selected extraction methods for determination of clothianidin insecticides in honey samples using liquid chromatography equipped with diode array detector**

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The aim of this work was an investigation of method for liquid chromatographic determination of clothianidin, neonicotinoid insecticide, in honey samples by diode array detector (HPLC-DAD). The chromatographic separation was carried out using reverse phase column with isocratic conditions of mobile phase consist of water (with 0.2% phosphoric acid) and acetonitrile (7:3, v/v). The DAD was set at 266 nm and retention time of clothianidin was 3.2 min. Due to the complexity of the sample matrix three effective sample pretreatment procedures were investigated including dichloromethane extraction, extraction based on solid-phase (with Discovery-18 column) and their combination. From the obtained results it can be concluded that neither one separated step of extraction is providing sample with satisfactory pureness for further HPLC/DAD analysis. For this reason this method proposes a procedure of sample purification based on combination of two clean-up steps: dichloromethane extraction for the first step and purification using solid phase column for the second one providing extraction recovery yield higher than 83%.

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AH 17

**Kvantitativno određivanje antioksidativne aktivnosti Šifovih baza i njihovih bakar(II) kompleksa RP TLC-DPPH metodom na TLC skeneru**

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Cilj ovog rada je određivanje antioksidativne aktivnosti jedinjenja nezavisno od primenjenih rastvarača. Ispitivane su Šifove baze, dobijene kondenzacijom etan-1,2-diamina ili propan-1,2-diamina, kao aaminskog dela, i pentan-2,4-diona i/ili 1-fenilbutan-1,3-diona kao  $\beta$ -diketona, kao i njihovi bakar(II) kompleksi. Antioksidativna aktivnost je ispitivana *in vitro* i određena je RP TLC metodom koja se zasniva na reakciji između DPPH (2,2-difenil-1-pikrilhidrazil) i Šifovih baza, kao i njihovih kompleksa. Rastvori ispitivanih jedinjenja, u odgovarajućem rastvaraču, su nanošeni automatski. Metanolni rastvor DPPH je zatim nanošen na iste zone. Antioksidativne aktivnosti, izražene u ekvivalentima Troloksa (*TEAC*, *Trolox Equivalent Antioxidant Capacity*) su određene na osnovu standardne serije, denzitometrijski, na 515 nm primenom TLC skenera. Ispitivani kompleksi Šifovih baza pokazuju značajno veću antioksidativnu aktivnost u odnosu na odgovarajuće ligande.

**Quantitative evaluation of antioxidant activity of Schiff bases and their Copper(II) complexes by RP TLC-DPPH method by using TLC-Scanner**

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The aim of this work was determination of antioxidative activity of compounds independent of applied solvents. Ligands which obtained by condensation of ethane-1,2-diamine or propane-1,2-diamine as the amine part and pentane-2,4-dione and/or 1-phenylbutane-1,3-dione as a  $\beta$ -diketone and corresponding copper(II) complexes were used for this investigation. Antioxidant activity was determined *in vitro* and has been evaluated using a RP TLC method that involves reaction between DPPH (2,2-diphenyl-1-picrylhydrazyl) and Schiff bases as well as their complexes. The solution of investigated compounds (in appropriate solvent) was applied by auto sampler followed by application of methanolic solution of DPPH on the same spots. The antioxidant activities, expressed in *Trolox Equivalent Antioxidant Capacity (TEAC)*, were determined on the basis of a calibration plot. Their antioxidant capacities were quantitatively evaluated using densitometry with detection at 515 nm by using TLC Scanner. Schiff base complexes showed significantly higher antioxidant activity than the corresponding ligands.



**Fizička hemija / Physical Chemistry**  
**Usmena saopštenja / Oral Presentations**

**FH01-O**

**Sinteza i karakterizacija kiselinski aktiviranog bentonita modifikovanog sa 12-volframfosfornom kiselinom i njegoa primena u reakciji oksidacije nitrita**

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Ispitivano je elektrohemijsko ponašanje elektroda sintetisanih nanošenjem različitog sadržaja 12-volframfosforne kiseline na kiselinski aktivirani bentonit. Uzorci su okarakterisani rendgenostrukturnom analizom, IC spektroskopijom, adsorpciono-desorpcionom BET metodom i ciklovoltametrijski. Svi uzorci poseduju izoterme tipa IV, sa histerezisnom petljom H3, što ukazuje na mezoporozni materijal sa porama tipa prskotina. S obzirom da vrednosti  $S_{BET}$  i  $V_p$  opadaju sa porastom sadržaja heteropolikiseline, zaključeno je da elektrokatalitička aktivnost ispitivanih elektroda ne potiče od difuzije nitrita kroz bentonitne slojeve. Pokazano je da elektroda od kiselinski aktiviranog bentonita sa različitim sadržajem 12-volframfosforne kiseline ima niži radni potencijal od drugih elektroda u ispitivanoj reakciji. Elektrode sa višim sadržajem kiseline poseduju nižu granicu detekcije i bolju osetljivost.

**Synthesis and characterization of acid activated bentonite with various loading of  $H_3PW_{12}O_{40}$  modified electrode for the oxidation of nitrite**

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The effect of 12-tungstophosphoric acid (HPW) immobilization on the electrocatalytic behavior of HPW/acid-activated bentonite electrodes was investigated. The samples were characterized by XRD, IC, BET and CV, and the activity of acid-activated bentonite electrodes with various loadings of HPW were studied in the oxidation of  $NO_2^-$  ions. All of the samples yielded type IV nitrogen isotherms with H3 hysteresis loop, which are indicative of mesoporous materials with slit-shaped pores. Since both,  $S_{BET}$  and  $V_p$  of the investigated samples decrease with HPW content, it can be concluded that electrocatalytic activity of samples toward nitrite ions does not arise from nitrite diffusion through the clay channels. The direct oxidation of nitrite ions on bare glassy carbon electrode requires a large overpotential. HPW/AAB samples successfully decreased the overpotential of nitrite in comparison to carbon glass electrode and increased the catalytic current. With increase of the HPW content on electrodes, lower detection limit and better sensitivity were obtained.





Posterska saopštenja / Poster Presentations

FH02-P



**Određivanje prividnih i parcijalnih molarnih zapremina u sistemu amonijum-nitrat – N,N-dimetilformamid**

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Proučavanje i precizno merenje volumetrijskih svojstava rastvora (gustina, prividne i parcijalne molarne zapremine) je od izuzetne važnosti za razumevanje mnogih industrijskih i prirodnih procesa. Izračunavanje i ispitivanje prividnih i parcijalnih molarnih zapremina u rastvoru elektrolita uglavnom mogu da posluže za razumevanje prirode i različitih interakcija između molekula rastvarača i rastvorka (jon-jon; jon-dipol i dipol-dipol interakcije). Ove elektrostatičke interakcije određuju termodinamičke i transportne osobine rastvora elektrolita. U beskonačno razblaženim rastvorima, gde su jon-jon interakcije zbog međusobne velike udaljenosti jona odsutne, glavni faktor koji ukazuje na osobine rastvora biće isključivo interakcije između jona i molekula rastvarača. Kako *Debye-Hückel*-ov zakon ne važi u oblastima većih koncentracija, gde su od najvećeg značaja upravo jon-jon interakcije, pokazalo se opravdanim dalje teoretsko proučavanje volumetrijskih osobina koncentrovanih rastvora elektrolita. U ovom radu su predstavljeni rezultati proučavanja volumetrijskih osobina sistema amonijum-nitrat – N,N-dimetilformamid (DMF). Određene su gustine smeša  $\text{NH}_4\text{NO}_3 \cdot n\text{DMF}$ , gde je  $n = 2-10, 15, 20, 30, 40$  i  $80$  u temperaturskom intervalu od  $308,15$  do  $348,15$  K. Koristeći podatke za gustine, izračunate su prividne i parcijalne molarne zapremine smeše  $\text{NH}_4\text{NO}_3 \cdot n\text{DMF}$  i čistih komponenti.

**Apparent and Partial Molar Volumes in Ammonium Nitrate – N,N-Dimethylformamide Mixture**

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Accurate volumetric (density, apparent and partial molar volumes) data of different solutions is crucial for understanding many industrial and natural processes. Studies of the apparent and partial molar volumes of the electrolyte solutions are used to examine ion-solvent, ion-ion, and solvent-solvent (structural) interactions, i.e. provide useful information on the nature of the interaction between dissolved ions and molecules of a solvent. Electrostatic interactions govern thermodynamic and transport properties of ionic electrolyte solutions. The ion-solvent interactions are a controlling factor in infinitely dilute solutions where ion-ion interactions are absent. Since the Debye-Hückel theory failed to represent experimental volumetric data at high concentrations where ion-ion interactions become increasingly important, extension of the existing theories to high concentrations and the accurate volumetric data for electrolyte solutions at high concentration are required. In this work, volumetric properties of ammonium nitrate – N,N-dimethylformamide (DMF) mixtures are presented. Density measurements were performed in the temperature range  $308.15-348.15$  K for  $\text{NH}_4\text{NO}_3 \cdot n\text{DMF}$  mixtures, where  $n = 2-10, 15, 20, 30, 40$  and  $80$ . Using these density values apparent and partial molar volumes of ammonium nitrate – DMF mixtures and pure components were calculated.





FH03-P



### **Membranska pertrakcija lutecijuma u kontaktoru sa jednom kapilarnom membranom - uticaj zapremine akceptora na efikasnost procesa**

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U ovom radu ispitivan je uticaj zapremine akceptora na efikasnost pertrakcije Lu(III) u diskontinualnom i kontinualnom sistemu sa jednom kapilarnom membranom, kako bi se povećala efikasnost reekstrakcije Lu(III) iz organske faze u akceptor. Lutecijum je ekstrahovan primenom ekstrakcionog sistema sa imobilisanom tečnom membranom pri uslovima za koje je efikasnost uklanjanja Lu(III) iz donora u organsku fazu najveća. Rezultati su pokazali da zapremina akceptora značajno utiče na efikasnost prenosa Lu(III) iz organske faze u akceptor tj. pertrakciju. Taj uticaj je manje očigledan kod diskontinualnog membranskog sistema jer se i zapremina neznatno povećava sa povećanjem dužine membrane, ali je veoma izražen u kontinualnom membranskom sistemu u kojem se deo ekstrahovanog Lu(III) koji ostaje u organskoj fazi permanentno smanjuje sa vremenom ekstrakcije. Kontinualna membranska pertrakcija sa recirkulacijom akceptora omogućava gotovo potpunu reekstrakciju Lu(III) u vodeni rastvor akceptora.

### **Membrane pertraction of lutetium with a single hollow fibre membrane - influence of the acceptor volume on the process efficiency**

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In order to improve the efficiency of re-extraction of Lu(III) from the organic to the acceptor phase, the influence of the acceptor volume on the pertraction efficiency of Lu(III) in a single hollow fibre pertraction system operated in a batch and continuous mode, was investigated in this study. Lutetium was extracted using the extraction system with immobilised liquid membrane, under the optimal extraction conditions. Results showed that the acceptor volume considerably influences the transport of Lu(III) from the organic to the acceptor phase, and thus the pertraction. This dependency is less pronounced in the case of the batch system, because the volume itself slightly increases with the membrane length, but is very pronounced in the case of the continuous extraction system in which a part of the extracted Lu(III) that is left in the organic phase is continuously decreasing with the extraction time. The continuous extraction system with the acceptor recirculation enables almost complete re-extraction of Lu(III) into the acceptor.



FH04-P

### **Konduktometrijsko ispitivanje mešovityh micela Na-dodecilsulfata i nejonskih surfaktanata (Triton X-100, Tween 20, Tween 60, Tween 85)**

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Određivanje kritične micelarne koncentracije (KMK) mešovityh micela je neophodno kako bi se dobile željene osobine micelarnih sistema koji imaju veliku primenu u industriji. U skladu sa tim, u ovom radu su konduktometrijski određene KMK mešovityh micela Na-laurilsulfata (SDS) sa četiri nejonska surfaktanta (Triton X-100, Tween 20, Tween 60, Tween 85), sa ciljem da se izračunaju parametri interakcije ( $\beta$ ) između surfaktanata u mešovitim micelama. Na osnovu izračunatih  $\beta$  parametara može se zaključiti da kod mešovityh micela SDS-a i Triton-a X-100 dolazi do pojave antagonističkog efekta. Za razliku od smeša sa Triton-om X-100, u mešovitim micelama SDS-Tween pojavljuje se blagi sinergistički efekat čija jačina zavisi od vrste Tween-a. Ova pojava je najverovatnije posledica razlike u dužini hidrofobnog dela molekula nejonskih surfaktanata. Veći sinergistički efekat se javlja kod mešovityh micela SDS-Tween 60 nego kod SDS-Tween 20, usled dužeg hidrofobnog dela Tween-a 60 (C18) od Tween-a 20 (C12). Paradoksalno, SDS-Tween 85 micelarni sistem pokazuje slabiji sinergistički efekat od prethodna dva, najverovatnije zbog prisustva dvostruke veze u hidrofobnim nizovima (tri C18 niza), koje ga čine sterno krutim.

### **Conductometric study of sodium dodecyl sulfate – nonionic surfactant (Triton X-100, Tween 20, Tween 60, Tween 85) mixed micelles in aqueous solution**

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Determination of critical micellar concentration (CMC) is important in order to achieve the desired qualities of micellar systems which have a significant industrial application. In view of this, the present study is concerned with the determination of CMC's of mixed micelles of sodium dodecyl sulfate with four nonionic surfactants (Triton X-100, Tween 20, Tween 60, and Tween 85) from conductance measurements. The aim is to calculate the interaction parameters ( $\beta$ ) of the mixed micelles. Based on the calculated values of the  $\beta$  parameters it was noticed that SDS-Triton X-100 mixed micelles showed antagonistic effect. Contrary to mixtures with Triton X-100, SDS-Tween mixed systems showed weak synergistic effect, depending on type of Tween in the mixed micelles. This behaviour is probably consequence of the different length of the hydrophobic tails in the nonionic surfactants. Stronger synergistic effect was found in SDS-Tween 60 than in SDS-Tween 20 mixed micelles because of the longer hydrophobic tail in Tween 60 (C18) than in Tween 20 (C12). Paradoxically, SDS-Tween 85 micellar system showed weaker synergistic effect than the previous two, most probably because of the presence of double bond in the hydrophobic tails (three C18 tails) which make it sterically rigid.



**Spektrohemijska / Spectrochemistry  
Posterska saopštenja / Poster Presentations**

**SH01-P**

**FTIC ispitivanja efekata trovanja teškim metalima na mineralnim tkivima**

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Kalcijum (Ca) je biogeni element koji se u organizmu nalazi u različitim oblicima. Najveći deo se nalazi u kostima i zubima u obliku hidroksiapatita i karbonapatita. U krvi se nalazi slobodan, jonizovani Ca, kao i Ca vezan za proteine. Dnevna dinamika razmene Ca između ekstracelularne tečnosti i koštanog tkiva je oko 500 mg.

U radu je ispitivan uticaj hroničnog trovanja teškim metalima (Pb, Cd, Cu) na koštanom tkivu eksperimentalnih životinja (pacovi Wisstar soja, ženskog roda, starosti 6 nedelja, prosečne mase 200 g).

AAS merenja su pokazala promene u sadržaju Ca u kostima. FTIC proučavanja kostiju pokazala su da dolazi do pomeranja karakterističnih apsorpcionih traka (od 600-400  $\text{cm}^{-1}$ , asimetrične deformacione vibracije,  $\text{PO}_4^{3-}$  grupe) u spektrima kostiju eksperimentalnih životinja koje su intoksicirane solima Pb, Cd ili Cu. Promena je bilo i na uzorcima kostiju životinja koje su tokom trovanja dobijale kao splete glutation i liponsku kiselinu, supstance koje sadrže reaktivne -SH grupe sa kojima joni teških metala relativno lako stupaju u interakcije i grade stabilne asocijate.

**FTIR analysis of the effect of heavy metals poisoning on mineral tissues**

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Calcium (Ca) is a biogenic element that is presenting in the body in different forms. It is mostly found in bones and teeth in the form of hydroxyapatite and carbonapatite. In the blood it exists as free, ionized Ca and as Ca bound to protein. The daily dynamics of Ca exchange between extracellular fluid and bone tissue is about 500 mg.

This study examines the impact of chronic heavy metals (Pb, Cd, Cu) poisoning on bone tissue of experimental animals (female Wisstar rats, 6 weeks old, average weight 200 g).

AAS analysis showed changes in the content of Ca in the bone tissue. FTIR studies of the bones showed displacement of the characteristic absorption band (from 600-400  $\text{cm}^{-1}$  asymmetric banding vibration of  $\text{PO}_4^{3-}$  group) in the spectra of the experimental animals bones which were intoxicated with Pb, Cd or Cu salts. The change occurred also on bone samples of animals that were treated with supplement glutathione and lipoic acid, which contained the reactive-SH groups, during poisoning. The heavy metal ions relatively easily react with this functional groups and form stable associates.



**Elektrohemija / Electrochemistry**  
**Usmena saopštenja / Oral Presentations**

EH01-O



**Uticaj vrste polimera na oblik i veličinu nanočestica srebra dobijenih elektrohemijском sintezom**

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Elektrohemijска sinteza omogućava brzo i efikasno dobijanje nanočestica metala visoke čistoće, sa mogućnošću precizne kontrole veličine i oblika nanočestica. Ovako dobijene nanočestice se potencijalno mogu primeniti u biomedicini, katalizi, optici.

U ovom radu ispitivan je uticaj vrste biokompatibilnog polimera, korišćenog za stabilizaciju rasta nanočestica, na oblik i veličinu nanočestica srebra dobijenih iz vodenog rastvora koji je sadržao 3,9 mM AgNO<sub>3</sub>, 0,1 M KNO<sub>3</sub> i alginat, odnosno poli(*N*-vinil-2-pirolidon), PVP. Sinteza je vršena galvanostatski, u ćeliji koja je sadržala Pt pločice kao radnu i pomoćnu elektrodu, a kao referentna korišćena je zasićena kalomelova elektroda. Prisustvo nanočestica srebra je potvrđeno UV-Vis spektroskopijom. TEM analiza je pokazala da se u prisustvu alginata dobijaju manje nanočestice (~ 30 nm) sfernog oblika, dok PVP omogućava formiranje nanočestica heksagonalnog oblika, veličine oko 75 nm. FTIR spektroskopija ukazuje na postojanje hemijskih veza između nanočestica srebra i PVP, kao i odsustvo hemijske veze između nanočestica srebra i alginata.

**The effect of polymer type on the size and shape of electrochemically synthesized Ag nanoparticles**

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Electrochemical synthesis is a fast and efficient method for the synthesis of metal nanoparticles of high purity, with the possibility of a precise control of metal nanoparticle size and shape. Electrochemically synthesized metal nanoparticles have a potential applications in biomedicine, catalysis, optics.

In this work, the influence of the type of a biocompatible polymer used as a capping agent, on the size and shape of silver nanoparticles (AgNPs) from the aqueous solution containing 3.9 mM AgNO<sub>3</sub>, 0.1 M KNO<sub>3</sub> and alginate or poly(*N*-vinyl-2-pyrrolidone), PVP, was investigated. The presence of silver nanoparticles was confirmed by UV-Vis spectroscopy. TEM analysis shown that the use of alginate as a capping agent provided smaler (~ 30 nm) round shaped AgNPs, while PVP enabled formation of hexagonal AgNPs, of aproximatelly 75 nm. FTIR spectroscopy pointed to chemical bonding between AgNP surfaces and PVP, but the chemical bonding between AgNP surfaces and alginate was not confirmed.





### ATR-FTIR i XRD analiza kompozitnih hidroksiapatit/lignin prevlaka dobijene postupkom elektroforetskog taloženja

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Kalcijum hidroksiapatit (HAP,  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ) je biokeramički kalcijum-fosfatni materijal, koji se zbog hemijskog i strukturnog sastava sličnog kostima široko klinički primenjuje. Hidroksiapatit se, usled slabih mehaničkih osobina, uglavnom koristi u formi prevlaka na titanu ili kompozita. Stoga, da bi se poboljšale mehaničke karakteristike, adhezija i sprečila krtost HAP prevlaka ispituju se kompozitne HAP prevlake sa biopolimerima. Lignin (Lig), amorfni polifenolni prirodni polimer, koji je korišćen u ovom radu je dobijen postupkom *organosolv* pulpovanjem iz različitih četinara. Cilj ovog rada je dobijanje kompozitnih HAP/Lig prevlaka na titanu postupkom elektroforetskog taloženja i ispitivanje uticaja koncentracije lignina na mikrostrukturu i fazni sastav kompozitnih prevlaka. HAP/Lig prevlake su taložene iz etanolske suspenzije  $10 \text{ g l}^{-1}$  HAP praha i 0,5 – 10 wt. % Lig praha različite na konstantnom naponu od 60 V tokom 45 s. Rezultati ATR-FTIR i XRD merenja potvrđuju integrisanje lignina u HAP rešetku, kao i da njegovo prisustvo ne menja strukturu hidroksiapatita, a da koncentracija veća od 0,5 wt. % sprečava HAP dekompoziciju tokom sinterovanja.

### ATR-FTIR and XRD evaluation of composite hydroxyapatite/lignin coatings obtained by electrophoretic deposition method

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Calcium hydroxyapatite (HAP,  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ) is one of the calcium phosphate based bioceramic material and clinically widely used due to its structural and chemical similarity to the natural bone. Owing to its inferior mechanical properties the main application of HAP is in a form of composites or coatings. In order to improve the mechanical properties, adhesion and overcome brittleness of the HAP coating, the HAP composite coatings containing biopolymers have become of great interest. Lignin (Lig), amorphous poliphenolic natural polymer, used in this study was obtained from *organosolv* pulping of mixed hardwoods. The aim of this work was to produce electrodeposited HAP/Lig biocomposite coatings on titanium and to investigate the effect of lignin concentration on microstructure and phase composition of composite coatings. HAP/Lig coatings were obtained from ethanol suspension of  $10 \text{ g l}^{-1}$  HAP and 0.5 – 10 wt. % Lig powders on titanium at constant voltage of 60 V for 45 s. Obtained ATR-FTIR and XRD results proved that lignin is well incorporated into HAP lattice and does not influence the structure of HAP, but protects HAP decomposition during sintering at concentrations higher than 0.5 wt. %.





### **ULj -VID spektroeletrohemijsko proučavanje supstituisanih 4–oksotiazolidinskih derivata u nevodenoj sredini**

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U cilju predlaganja reakcionog mehanizma i identifikacije reakcionih intermedijera (5-eto-ksikarbonilmetiliden-4-oksotiazolidin-2-iliden)-1-feniletanon je proučavan u DMSO spregnutim ciklovoltametrijskim i ULJ-V spektroeletrohemijskim metodama. Upoređivanjem eksperimentalnih podataka sa teorijskim krivama dobijenim primenom softvera DigiSim, ukazano je na ECECE mehanizam kao glavnu reakcionu sekvencu. Hemijski stupanj koji sledi prvi prenos elektrona je deprotonacija početnog jedinjenja pod uticajem elektrogenerisane baze, anjon radikala. Uzimajući u obzir uticaj rastvarača, izvršeni su semiempirijski MO proračuni kako bi se objasnile redoks osobine ispitivanog jedinjenja u pogledu elektronske strukture i reaktivnosti.

### **UV-Vis spectroelectrochemical study of substituted 4–oxothiazolidine derivatives in aprotic medium**

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Coupled cyclovoltametric and UV-Vis spectroelectrochemical study has been used to elucidate the mechanism and to determine the reaction intermediates of the electrochemical reduction of (5-ethoxycarbonylmethylidene-4-oxothiazolidine-2-ilydene)-1-phenylethanone in DMSO. The comparison between experimental data and theoretical curves, calculated by means of the DigiSim software, indicates an ECECE reaction sequence as a major reaction pathway. The chemical step, following the first ET, is the deprotonation of the starting compound, under the action of the electrogenerated base (EGB) anion radical. Semiempirical MO calculations were performed with consideration of the solvent effect in order to explain the redox properties of the investigated compound in terms of the electronic structure and reactivity.



EH04-O

### Spontano i elektrohemijsko formiranje kompozita Au/TiO<sub>2</sub> i Au/Ta<sub>2</sub>O<sub>5</sub>

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Ispitivana je mogućnost povećanja elektrokatalitičke aktivnosti zlatne elektrode dispergovanjem zlata u vidu nanočestica na neistorodnoj podlozi, kao i efektom interakcije metal-podloga, koji prema literaturnim podacima može takođe da dovede do povećanja efikasnosti katalitički aktivnog metala. Formiranje kompozitnih nanosa Au/oksid izvršeno je spontano - cementacijom, ili elektrodeponovanjem potenciodinamičkom polarizacijom. Kompozitni nanosi zlata su dalje ispitivani u cilju definisanja njihove morfologije i raspodele veličine čestica pomoću skenirajuće elektronske mikroskopije (SEM). Dobijeni rezultati ukazuju na činjenicu da je morfologija metalnih čestica direktno povezana sa uslovima pod kojima se deponovanje odigrava. Ventilni metali, titan i tantal, zbog formiranja površinskih oksida, pokazuju templatno dejstvo - određuju položaj i broj nukleusa zlata, tako da depoziti poprimaju formu nizova mikroelektroda.

### Spontaneous and electrochemical formation of the composite Au/TiO<sub>2</sub> and Au/Ta<sub>2</sub>O<sub>5</sub>

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The possibility of increasing the electrocatalytic activity of gold electrodes was investigated by dispersing gold in the form of nanoparticles on different support, as well as by the effect of metal-surface interaction, which according to the literature may also improve the efficiency of catalytically active metals. Formation of composite layers of Au/oxide was carried out either spontaneously – by cementation, or by electrodeposition by potentiodynamic polarization. Composite deposits of gold were further investigated in order to define their morphology and particle size distribution using scanning electron microscopy (SEM). The results indicate that the morphology of metal particles is directly related to the conditions under which the deposition occurs. Valve metals, titanium and tantalum, because of the formation of surface oxide, show a template effect by defining the position and number of nuclei of gold, so that deposits take the form of microelectrode arrays.



EH05-O

### **Simultano određivanje Pb i Cd u uzorcima vode Anodnom Stripping Voltametrijom korišćenjem modifikovane GC elektrode**

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U radu je opisano određivanje olova i kadmijuma koristeći Nafion-modifikovanu elektrodu sa Cu-kompleksom (Cu-DPABA-NA/GCE; DPABA je Methyl 3,5-bis{bis-[(pyridin-2-yl)methyl]amino}methyl-benzoate) kao alternativnu elektrodu za anodnu stripping voltametriju. Pb i Cd su akumulirani 120 s, u acetatnom puferu pH 4, na potencijalu -1.4 V (vs Ag/AgCl elektrodi) i sniman je DP ASV u intervalu od -1.2 do -0.2 V. Pod optimalnim uslovima određivanja kalibracione krive one su bile linearne u opsegu od  $4.8 \times 10^{-9}$  –  $5.0 \times 10^{-5}$  za Pb i  $5.0 \times 10^{-9}$  –  $5 \times 10^{-5}$  molL<sup>-1</sup> za Cd. Optimizovani su različiti parametri i uslovi, kao što su sastav membrane, vreme akumuliranja, potencijal i pH vrednost. Ispitivani su i ometajući metali. Značajan porast u struji je primećen sa modifikovanim elektrodom u odnosu na čistu glassy carbon elektrodu. Potvrda predložene metode je uradjena za određivanje olova i kadmijuma u sertifikovanom referentnom materijalu Groundwater CRM 610 (BCR, Community Bureau of Reference, Brussels, Belgium). Elektroda je uspešno primenjena za određivanje Pb i Cd u rečnoj vodi sa visokim sadržajem organske materije bez ikakve prethodne pripreme.

### **Simultaneous determination of Pb and Cd traces in water samples by Anodic Stripping Voltammetry using modified GC electrode**

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The determination of Pb and Cd with a Nafion-modified glassy carbon electrode and Cu-DPABA complex (Cu-DPABA-NA/GCE; DPABA is Methyl 3,5-bis{bis-[(pyridin-2-yl)methyl]amino}methyl-benzoate) as an alternative electrode for anodic stripping voltammetry was described. Pb and Cd were accumulated in acetate buffer pH 4 at potential of -1.4 V (vs. Ag/AgCl electrode) for 120 s followed by a DP ASV scan from -1.2 to -0.2 V. Under the optimum conditions the calibration curves were linear in the range  $4.8 \times 10^{-9}$  –  $5.0 \times 10^{-5}$  and  $5.0 \times 10^{-9}$  –  $5 \times 10^{-5}$  molL<sup>-1</sup> for Pb and Cd, respectively. Detection limits were  $1.8 \times 10^{-9}$  and  $1.2 \times 10^{-9}$  molL<sup>-1</sup> for Pb and Cd, respectively. Different parameters and conditions, such as membrane ingredients, accumulation time, potential and pH value were optimized. A study of the interfering substances was also performed. A significant increase in current was achieved at the modified electrode in comparison with the bare glassy carbon electrode. The validation of the proposed method was made by Pb and Cd determination in the certified reference material Groundwater CRM 610 (BCR, Community Bureau of Reference, Brussels, Belgium). The electrode was successfully applied for determination of Pb and Cd in river water with a high content of organic contaminants without any pretreatment.







### **Volfram-karbid kao nosač nanočestica Pt u elektrohemijskoj oksidaciji metanola**

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Volfram-karbid razvijene površine je sintetizovan metodom sol-gel polikondenzacije i zatim je korišćen kao nosač nanočestica Pt, koje su deponovane borhidridnom metodom. Određivanje faznog sastava nosača je pokazalo da se sastoji od WC i  $W_2C$ . Pokazano je da je elektrohemijška stabilnost nosača zadovoljavajuća u oblasti potencijala relevantnoj za oksidaciju metanola. Ispitane su reakcije oksidacije adsorbovanog CO i metanola na Pt/WC u kiselom rastvoru. Poređenjem dobijenih rezultata sa komercijalnim katalizatorom Pt/C zaključeno je da prisustvo WC ubrzava oksidaciju CO. Oksidacija metanola počinje na istim potencijalima na Pt/WC i na Pt/C katalizatorima, ali se na Pt/WC postižu veće struje na pozitivnijim potencijalima. Pretpostavljeno je da veće gustine struja oksidacije metanola na Pt/WC-T2 u odnosu na Pt/C na pozitivnijim potencijalima potiču od brže oksidacije adsorbovanog CO na Pt/WC-T2, dok činjenica da WC nema efekta na potencijal na kojem počinje reakcija, ukazuje da ne dolazi do elektronske modifikacije platine volframom. Takođe je pokazano da je smanjenje aktivnosti Pt/WC za oksidaciju metanola tokom vremena manje u poređenju sa Pt/C.

### **Tungsten carbide as support of Pt nanoparticles in electrochemical methanol oxidation**

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High surface area tungsten carbide was synthesized by sol-gel polycondensation and used as Pt support. Pt nanoparticles were deposited by borohydride reduction method. Phase composition of the support was found to be a mixture of WC and  $W_2C$ . The material is electrochemically stable within the potential window relevant for methanol oxidation. Electrochemical oxidation of pre-adsorbed CO and methanol were investigated in acid solution. Contrasting the results with those on the commercial Pt/C catalyst, it was concluded that CO oxidation on Pt is promoted by the presence of WC. Methanol oxidation onset potential was found to be the same on Pt/WC and Pt/C catalysts, but at higher potentials Pt/WC exhibited larger current densities. It was assumed that larger current densities at higher potentials originate in the facilitated oxidation of adsorbed CO, while the same onset potentials on both catalysts indicate that electronic modification of Pt by W is not significant. The loss of the activity for methanol oxidation over time exhibited by Pt/WC was found to be lower comparing to the Pt/C catalyst.

EH07-P

### **Elektrohemijsko određivanje linurona primenom elektroda od staklastog ugljenika**

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U ovom radu prikazano je elektrohemijsko određivanje linurona, 3-(3,4-dihlorofenil)-1-metoksi-1-metilurea, u vodenim rastvorima primenom tri elektrode na bazi staklastog ugljenika. U našoj laboratoriji su sintetisane dve elektrode: čist staklasti ugljenik (GC) i staklasti ugljenik hemijski dopiran borom (GCB), a komercijalnu elektrodu od staklastog ugljenika (Metrohm) smo koristili za poređenje rezultata. Odredili smo polutalasni potencijal oksidovanja linurona na ovim elektrodama, uticaj pH elektrolita, opseg linearnosti i granicu detekcije. Porastom pH elektrolita od 0.7 do 7, površina maksimuma koji odgovara oksidaciji linurona se smanjuje, a potencijal oksidacije se pomera prema negativnijim vrednostima. Poređenjem rezultata dobijenih primenom sintetisanih elektroda i komercijalne elektrode, može se zaključiti da je najširi opseg linearnosti dobijen za elektrodu od staklastog ugljenika dopiranog borom ( $2.3 - 31.7 \mu\text{g mL}^{-1}$ ) dok je za komercijalnu elektrodu opseg od  $0.6 - 9.5 \mu\text{g mL}^{-1}$ . Određene granice detekcije su, 1,8; 2,6 i 3,7  $\mu\text{g mL}^{-1}$  za komercijalnu, GCB i GC elektrodu, redom.

### **Electrochemical determination of linuron using electrodes based on glassy carbon**

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Zoran V. Laušević, Milovan M. Purenović\*, Tatjana M. Trtić-Petrović  
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This paper presents the electrochemical determination of linuron 3-(3,4-dichlorophenyl)-1-methoxy-1-methylureum, in aqueous solutions using three electrodes based on glassy carbon. Two electrodes were synthesized in our laboratory: glassy carbon (GC) and boron doped glassy carbon (GCB), while a commercial glassy carbon electrode (Metrohm) was used for comparison of results. We determined an oxidation peak potential of linuron on these electrodes, the influence of the electrolyte pH, the linear range and limit of detection. With the increase of the electrolyte pH from 0.7 to 7, the peak area that corresponds to the oxidation of linuron was reduced and the oxidation potential shifted towards more negative values. Comparing the results which were obtained using our electrodes with commercial one, it can be concluded that the broadest linear range was obtained using GCB electrode ( $2.3 - 31.7 \mu\text{g mL}^{-1}$ ), the linear range of the commercial electrode was between  $0.6 - 9.5 \mu\text{g mL}^{-1}$ . The determined limits of detection were 1.8, 2.6 and 3.7  $\mu\text{g mL}^{-1}$  for commercial, GCB and GC electrodes, respectively.





### **Koroziona stabilnost prevlaka viniltrietskoksilana na aluminijumu u rastvorima NaCl**

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U ovom radu je ispitivana koroziona stabilnost prevlaka viniltrietskoksilana (VTES) na aluminijumu. Prevlake silana su dobijene hemijskim putem, potapanjem u rastvor 2 i 5vol.% VTES, a potom su pečene na 100 °C tokom 10 ili 30 min. Koroziona stabilnost prevlaka silana je karakterisana elektrohemijom analizama: spektroskopijom elektrohemijske impedancije (SEI), kao i praćenjem promene potencijala otvorenog kola u 0.03mas.% NaCl. Dobijeni rezultati su poređeni sa standardizovanim ispitivanjima u slanoj komori. Udeo površine uzorka koji je prekriven korozionim produktima je određen snimanjem uzoraka optičkim mikroskopom i kompjuterskim programom ImageProPlus. Pokazan je uticaj i koncentracije rastvora VTES kao i vremena pečenja na korozionu stabilnost ispitivanih uzoraka. Najveću korozionu stabilnost su imale prevlake silana dobijene taloženjem iz 5% rastvora i pečenjem 30 min, a najlošija svojstva su imale prevlake dobijene taloženjem iz 2% VTES i pečene 10 min.

### **Corrosion stability of Vinyltriethoxysilane Coatings on Aluminium in Sodium Chloride Solutions**

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In this work the corrosion stability of vinyltriethoxysilane (VTES) coatings on aluminium was investigated. The silane coatings were deposited chemically, by immersion in 2 and 5vol.% VTES, and then cured at 100 °C during 10 or 30 min. The corrosion stability of the silane coatings was determined by electrochemical methods: electrochemical impedance spectroscopy (EIS) and by tracking the change of the open circuit potential in 0.03wt.% NaCl. The results obtained were compared with the standardized analysis in the salt spray chamber. The corroded area on each sample was determined by analysis of microphotographs, obtained by optical microscopy and analyzed with ImageProPlus computer programme. The influence of both VTES concentration and curing time on the corrosion stability of silane films on aluminium was shown. The highest corrosion stability was obtained by silane films deposited from 5% VTES solution with 30 min curing, while the lowest stability was determined for silane films deposited from 2% VTES solution with 10 min curing.

**Nauka o materijalima / Materials Science**  
**Posterska saopštenja / Poster Presentations**

NM01-P



**Mehanička i optička svojstva kompozitnog materijala  
poli (metilmetakrilat)- bizmut- silicijum-oksidi**

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U radu su predstavljeni i diskutovani rezultati dobijeni pri procesiranju i karakterisanju kompozitnog materijala PMMA-Bi<sub>12</sub>SiO<sub>20</sub>. Uzorci čistog PMMA i kompozita sa udelom čestica monokristalnog Bi<sub>12</sub>SiO<sub>20</sub> (BSO) od 0,5 mas% i 1,0 mas%, dobijeni su na laboratorijskom uređaju za umešavanje kompozita sa termoplastičnom matricom. Karakterizacija polaznih komponenti kao i kompozita izvedena je metodama FTIR i spektroskopskom elipsometrijom. Rezultati merenja indeksa refrakcije metodom spektroskopske elipsometrije pokazuju da vrednost indeksa refrakcije kompozita u odnosu na čist PMMA raste sa porastom udela BSO. Ispitivanjem na zatezanje utvrđeno je da modul elastičnosti raste sa povećanjem udela BSO.

**Mechanical and optical properties of composite material  
poly (methymethacrylate)-bismuth-silicon-oxide**

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The results obtained through processing and characterization of composite material PMMA-Bi<sub>12</sub>SiO<sub>20</sub> are presented and discussed. Samples of pure PMMA and composite with 0.5 mas% and 1.0 mas% of powder were made using laboratory mixing molder. Characterization of starting components as well as composite was performed using FTIR and spectroscopic ellipsometry methods. Measurements of refraction indices using spectroscopic ellipsometry method have shown that refraction index of composite material has increased with increasing of BSO content. Results of tensile testing have shown increase of Young's modulus with the BSO content.



NM02-P

### Ugljenične nanotube poboljšane mezoporozne strukture

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Ugljenične nanotube (UNT) sintetisane su metodom katalitičke hemijske dekompozicije etilena na 700°C, tokom 1h u prisustvu Fe-Co/SiO<sub>2</sub> katalizatora. U cilju uklanjanja prisutnih nečistoća, kao i drugih ugljeničnih struktura, UNT su prečišćene tretiranjem bazom i kiselinom. Morfološke i strukturne karakteristike neprečišćenog i prečišćenog uzorka ispitane su metodama TEM, HR-TEM, XRD i Raman spektroskopije, dok su njihove teksturalne osobine ispitane metodom nisko-temperaturne adsorpcije azota. Rezultati ukazuju na višezidne izvijane UNT, gusto konfigurisane po jedinici površine katalizatora, sa srednjim spoljašnjim prečnikom u opsegu od 10-30 nm. Nanotube rastu mehanizmom izdizanja čestica aktivnog metala na vrhu rastuće UNT, što ukazuje na slabu interakciju metal-nosač u katalizatoru. Primenjena metoda prečišćavanja je izuzetno efikasna jer su iz sintetisanog uzorka uklonjene sve prisutne nečistoće bez narušavanja strukture nanotuba. Takođe, na ovaj način dobijene UNT karakterišu se poboljšanom mezoporoznošću što je od izuzetnog značaja za njihovu dalju primenu.

### Carbon nanotubes with improved mesoporous structure

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Carbon nanotubes (CNTs) were synthesized by the catalytic chemical vapor decomposition of ethylene at 700°C for 1h over Fe-Co/SiO<sub>2</sub> catalyst. In order to remove the catalyst remains and carbon structures other than CNTs, the as-synthesized sample was purified by basic and acid treatments. The morphological and structural characteristics of raw and purified samples were investigated by TEM, HR-TEM, XRD and Raman spectroscopy, while low temperature nitrogen adsorption was employed to characterize their textural properties. According to the obtained results, the as-synthesized CNTs are multi-walled highly interwoven structures densely populated over the catalyst surface, having mean outer diameter in the range 10-30 nm. They grow by “tip-mode” mechanism indicating weak metal-support interaction in the applied catalyst. The applied purification procedure was proven to be very efficient in terms of removing impurities while preserving CNTs structure. The accomplished enhanced mesoporosity of the purified sample might be beneficial with regard to further applications of the CNTs.

**Hemijsko inženjerstvo / Chemical Engineering**  
**Usmena saopštenja / Oral Presentations**

HI01-O



**Segregacija u fluidizovanom sloju voda-polidisperzna smeša čestica**

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Prilikom fluidizacije polidisperznih smeša istih gustina, fluidizovani slojevi tečnost čestice imaju osobinu da će se fluidizovani materijal jasno razdvojiti po veličini zrna. Najkrupnije čestice će fluidizirati na dnu sloja, a najsitnije na vrhu. U ovom radu su izvršeni fluidizacioni eksperimenti u koloni prečnika  $D=144$  mm sa jednom frakcijom filtracionog (kvarcnog) peska granulacije  $d_p=0.75-1.25$  mm visine 1030 mm, čiji je srednji prečnik dobijen prosejavanjem  $d_m=1.0$  mm, a karakterističan odnos prečnika najkrupnijih prema najsitnijim česticama u populaciji  $d_R=1.25/0.75=1.67$ . U cilju određivanja raspodele veličine čestica unutar ovog intervala izorak od 1230 nasumično izabranih čestica je skeniran i analiziran pomoću softvera SigmaScan u cilju određivanja projektovanog prečnika i faktora oblika. Izvršena je i klasifikacija, tako što se sloj čestica peska posle fluidizacije hidrauličkim isisavanjem podelio na deset frakcija po visini, svaka od ovih frakcija je osušena i izmerena a potom su za svaku od ovih frakcija u koloni prečnika  $D_c=64$  mm su određeni fluidizacioni parametri ( $U_{mFi}$ ,  $\epsilon_{mFi}$ ) i parametri ekspanzije prema relaciji Richardson-Zaki-a. Experimentalno dobijene vrednosti ekspanzije polidisperznog sloja upoređene su sa Epstein modelom.

**Segregation in fluidization bed water-polydisperse particle mixtures**

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During a fluidization of polydisperse particle mixtures of same density, fluidization of water-particle layer have the property that will clearly separate material by grain size. The largest particles will fluidized at bottom layer, and smallest will fluidized at top layer. In this study experimental investigations were conducted in the cylindrical column of 144 mm in diameter with one filtering fraction of sand, grain size of the sand was  $d_p=0.75-1.25$  mm, with an average diameter obtained by sieving  $d_m = 1.0$  mm, and a characteristic ratio of the diameter of the largest against the smallest particles in the population is  $d_R=1.25/0.75=1.67$ . In order to determined the size distribution of particles within this interval, the samples of 1230 randomly selected particles is scanned and analyzed using the SigmaScan software to determine the projected diameter and shape factor. To analysis clasification of sand particles in fluidized column, the layer of sand is divide into ten equal fractions by height, each of this fraction was dried and than measured. For each of this fraction, fluidization parameter ( $U_{mFi}$ ,  $\epsilon_{mFi}$ ) and the parameters of the expansion according the Richardson-Zaki equation has been determined in column  $D_c=64$  mm in diameter. The experimentally obtained values of expansion of polydisperse sand layer were correlated according to Epstein model.



HI02-O

### **Katalitička aktivnost CaO u sintezi biodizela u funkciji različitih reakcionih parametara**

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Većina komercijalnih tehnologija za proizvodnju biodizela se bazira na homogenoj katalizi koju odlikuje čitav niz relativno skupih i ekološki nepovoljnih koraka. Upotreba odgovarajućeg heterogenog katalizatora bi donela poboljšanje kako sa aspekta tehnologije tako i sa aspekta zaštite životne sredine. U ovom radu ispitivana je aktivnost i stabilnost različito aktiviranog CaO katalizatora u reakciji transesterifikacije suncokretovog ulja i metanola kao funkcija različitih reakcionih parametara: temperature (60-120 °C), pritiska (0-20 bar), odnosa ulje-metanol (1:6 – 1:12) i sadržaja vode kao nečistoće. Reakcije su izvođene u komercijalnom šaržnom laboratorijskom reaktoru sa mogućnošću rada pod pritiskom. Na atmosferskom pritisku maksimalna konverzija od 92.4% je ostvarena na temperatura 80 °C nakon 5.5h. Povećanje pritiska je imalo pozitivan uticaj do 10 bar-a ali samo u smislu skraćivanja potrebnog vremena do postizanja maksimalne konverzije (2.5h). Viši molarni odnos ulje-metanol je rezultovao višim prinosom biodizela dostižući 95.1% pri odnosu 1:12 na 80 °C i 10 bar-a. Kalcinacija u struji vazduha na 900 °C ima presudan uticaj na performanse katalizatora što može biti povezano sa čistoćom CaO, stvaranjem povoljne porozne strukture i formiranja snažnijih baznih centara na površini u poređenju sa katalizatorom kalcinisanim na nižim temperaturama. Povećana koncentracija vode u reakciji dovodi do deaktivacije katalizatora i snižava konverziju.

### **Catalitical activity of CaO in biodiesel synthesis as a function of various reaction parameters**

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Most commercial technologies for biodiesel production are based on homogenous catalysis characterized by numerous relatively expensive and ecologically unfavorable steps. Application of a suitable heterogeneous catalyst would bring improvements to both technology and environmental protection. In this paper activity and stability of variously activated CaO catalyst were studied in transesterification reaction of sunflower oil and methanol as a function of various reaction parameters: temperature (60-120 °C), pressure (0-20 bar), oil-to-methanol ratio (1:6 – 1:12) and content of water as impurity. The reaction was carried in a high pressure semi-batch commercial laboratory reactor. At atmospheric pressure temperature of 80 °C was found to give maximum conversion to methyl esters of 92.4%, requiring, however, the maximum reaction time of 5.5h. Pressure had a positive impact up to 10 bar, but only in terms of shortening the reaction time (2.5 h) to reach the same maximal ester fraction. Higher the oil-to-methanol molar ratio resulted in higher biodiesel yield, reaching the maximal of 95.1% at 1:12 oil-to-methanol ratio, 80 °C and 10 bar. Pretreatment at 900 °C in air was found to have crucial consequences on catalyst performances, which might be related to CaO purity, beneficial pores structure and higher surface basicity relative to samples treated at lower temperatures. Increased water concentration in reaction mixture leads to catalyst deactivation and lower conversion.







### Modelovanje kinetike sorpcije olova na prirodnom i sintetičkom apatitu

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Zagađenje zemljišta usled prisustva toksičnih metala dovodi do brojnih negativnih uticaja na prirodnu sredinu, kao što su uništenje ekosistema, zagađenje izvora vode i negativni uticaj na zdravlje ljudi. Olovo predstavlja jednu od najrasprostranjenijih zagađujućih materija. Ispiranjem iz zagađenih zemljišta, olovo dospeva u podzemne i površinske vode. *In situ* imobilizacija teških metala korišćenjem jeftinih mineralnih sirovina predstavlja pogodnu tehniku remedijacije zagađenog zemljišta. U ovom radu su korišćene dve vrste apatita: sintetički hidroksiapatit (HAP) i prirodni apatit iz ležišta Lisina (LA). Na eksperimentalne podatke kinetike sorpcije olova iz vodenog rastvora korišćenjem HAP i LA, primenjena su dva kinetička modela: model pseudo prvog reda i model pseudo drugog reda. Na osnovu dobijenih rezultata može se zaključiti da vrednosti  $q_e$  dobijene primenom modela pseudo drugog reda pokazuju dobro slaganje sa eksperimentalnim rezultatima. Na osnovu izračunatih vrednosti  $q_e$  i  $R^2$ , za oba sistema je odabran kinetički model pseudo drugog reda. Uticaj temperature na ova dva sistema je različit. Konstanta brzine reakcije u sistemu Pb-HAP opada sa porastom temperature. U sistemu Pb-LA, konstante brzine reakcije imaju slične vrednosti na temperaturama 37 °C i 50 °C, dok je vrednost na temperaturi 25 °C značajno veća. Ovi rezultati ukazuju na različite mehanizme reakcije sorpcije prisutne u ova dva sistema.

### Modeling of the kinetics of aqueous Pb sorption on synthetic and natural apatite

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The contamination of soils due to the presence of toxic metals can result in serious negative consequences, such as loss of ecosystems, damaged water resources and human health problems. Lead is one of the most wide-spread heavy metals present in the environment.<sup>1</sup> Pb leaching from contaminated soils is a constant source of surface and ground water contamination. The *in situ* immobilization of metals in soils using inexpensive amendments is considered a promising technique for the remediation of contaminated sites. In this work, two types of apatites were used for Pb contamination remediation: synthetic hydroxyapatite and natural mineral apatite from Lisina. Experimental data of the kinetics of aqueous Pb sorption by HAP and LA were fitted with two kinetic models: pseudo-first order model and pseudo-second order model. Based on the results obtained it can be concluded that calculated  $q_e$  values, obtained using the pseudo-second order equation, agree well with experimental values. Based on  $q_e$  and  $R^2$  the pseudo-second order model was chosen as more appropriate for both systems at all the temperatures investigated. The influence of temperature on these two systems is different. The rate constant of sorption reaction in Pb-HAP system gradually decreases with increase of temperature. In the case of Pb-LA system  $k_2$  (25 °C) >  $k_2$  (37 °C)  $\approx$   $k_2$  (50 °C).







### Prenos toplote zid-pseudofluid u vertikalnom toku tečnost krupne čestice

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Ispitivan je prenos toplote u vertikalnom jednofaznom i dvofaznom toku fluid inertne sferične čestice prečnika 1.20, 1.94 i 2.98 mm, u bakarnoj transportnoj cevi prečnika 25.4 mm, snabdevenoj omotačem za zagrevanje zasićenom vodenom parom.

Vertikalni dvofaznom tok tretiran je kao pseudofluid i uveden je modifikovani koeficijent trenja smeše fluid-čestice sa zidom cevi ( $f_w$ ) i modifikovani Reynoldsov broj za smešu fluid-čestice ( $Re_m$ ). Takođe, prikazana je zavisnost promene bezdimenzionog faktora prenosa mase ( $j_H$ ) i modifikovanog koeficijenta trenja ( $f_w$ ) od Reynoldsovog broja za smešu.

Eksperimentalni podaci pokazuju da je koeficijent prelaza toplote zid-pseudofluid u vertikalnom dvofaznom toku, znatno viši u odnosu na jednofazni tok za niže vrednosti Reynoldsovog broja ( $Re_m < 15000$ ), dok za više vrednosti Reynoldsovog broja ( $Re_m > 15000$ ), između podataka nema značajnije razlike.

Eksperimentalna ispitivanja prenosa toplote u vertikalnom dvofaznom toku čestica, tj. hidrauličkom transportu, ukazuju da postoje dva karakteristična režima strujanja: turbulentni fluid-čestice tok i paralelni fluid-čestice tok. Eksperimentalni podaci, takođe, pokazuju da je koeficijent prenosa toplote dosta viši u turbulentnom od koeficijenta prenosa toplote u paralelnom toku.

### Wall-to-pseudofluid heat transfer in vertical flow of liquid coarse particles

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Heat transfer in single-phase and vertical two phase flow of inert spherical particles 1.20, 1.94 and 2.98 mm in diameter in a 25.4 mm I.D. copper tube equipped with a steam jacket, was studied.

The vertical two-phase flow is treating as the pseudofluid, and is introduced modified mixture-wall friction coefficient ( $f_w$ ) and modified mixture Reynolds number ( $Re_m$ ). Also, there is represent the dependence of changes for the heat transfer factor and modified mixture-wall friction coefficient ( $f_w$ ) of modified mixture Reynolds number ( $Re_m$ ).

Wall-to-pseudofluid heat transfer in hydraulic transport of particles is much higher then in single-phase flow for lower Reynolds numbers ( $Re_m < 15000$ ), while for high Reynolds numbers ( $Re_m > 15000$ ), there is no significant difference.

In our hydraulic transport experiments the two characteristic flow regimes were observed: turbulent fluid-particle flow and parallel fluid-particle flow. Our experimental data show that the heat transfer coefficients in turbulent fluid-particle regime are much higher then in parallel fluid-particle flow.



### **Ravnoteža tečnost-tečnost u vodenim rastvorima tečnih polietilen glikola sa toluenom**

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Toluen je važan organski rastvarač, koji rastvara i brojne neorganske supstance i značajan je kako sa industrijskog i ekološkog aspekta. Toluen je manje toksičan od benzena pa se često koristi umesto njega kao rastvarač u industrijskim procesima.

S druge strane, polietilen glikol (PEG) ima izuzetno nisku toksičnost, tako da ulazi u sastav lekova kao i kozmetičkih preparata. S obzirom na velike mogućnosti upotrebe PEG, značajno je ispitati njegovo ponašanje u različitim rastvorima, na primer mogućnost da polarni PEG menja svoju polarnost (prilagođava je) prema okolini (solventu).

U ovom radu su eksperimentalnim određivanjem ravnoteže tečnost-tečnost, ispitivane mogućnosti korišćenja tečnih polietilen glikola (PEG 200 i PEG 400) i njihovih vodenih rastvora kao "zelenih" rastvarača za prečišćavanje i izdvajanje štetnih supstanci.

### **Liquid-Liquid Equilibria in Aqueous Solution of Liquid Polyethylene Glycol and Toluene**

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Toluene is an important organic solvent, but is also capable of dissolving a number of inorganic chemicals and it represents a substance of diverse importance – industrial and ecological. Toluene is less toxic than benzene, and has consequently largely replaced it as an aromatic solvent in process industry.

On the other hand, polyethylene glycol (PEG) has an extremely low toxicity and is used in a variety of products, for example as a constituent of medicaments and beauty products etc. Bearing in mind very wide industrial application of PEGs, studying their behavior is very important especially examination the possibility of the polar PEGs to change their polarity according to the solvent behavior.

In this work, the possibility of using liquid polyethylene glycol (PEG 200 and PEG 400) and its aqueous solutions as "green" solvents for toxic substances have been investigated by measurement of liquid-liquid equilibria.



HI06-P



### **Uticaj temperature na promenu termodinamičkih i transportnih osobina binarnih smeša dimetilftalata (ili dimetiladipata) i alkohola**

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Eksperimentalno su određene gustine, indeksi refrakcije i viskoznosti četiri binarna sistema: dimetilftalat (ili dimetiladipat) + 1-butanol i dimetilftalat (ili dimetiladipat) + 2-butanol, na osam temperatura (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15 i 323.15) K i na atmosferskom pritisku. Merenja gustina, indeksa refrakcije i viskoznosti su izvršena pomoću Anton Paar DMA 5000 digitalnog gustinomera, odnosno Anton Paar RXA 156 refraktometra i Anton Paar SVM 3000/G2 digitalnog viskozimetra. Iz podataka za gustine, indekse refrakcije i viskoznosti smeša izračunate su dopunske molarne zapremine ( $V^E$ ), promene indeksa refrakcije ( $\Delta n_D$ ) i promene viskoznosti ( $\Delta \eta$ ), koje su zatim korelisane Redlich-Kisterovim polinomom.

### **Temperature influence on change of thermodynamic and transport properties of the binary systems containing dimethylphthalate (or dimethyladipate) and alcohols**

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Density, refractive index and viscosity data of the four binary systems of dimethylphthalate (or dimethyladipate) + 1-butanol and dimethylphthalate (or dimethyladipate) + 2-butanol have been measured at eight temperatures (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15 and 323.15) K and atmospheric pressure. Densities, refractive indices and viscosities were measured with an Anton Paar DMA 5000 digital vibrating tube densimeter, Anton Paar RXA 156 refractometer and Anton Paar SVM 3000/G2 digital viscometer, respectively. Excess molar volumes ( $V^E$ ), deviations of refractive indices ( $\Delta n_D$ ) and viscosity deviations ( $\Delta \eta$ ) were determined from these densities, refractive indices and viscosities data, respectively and were fitted by the Redlich-Kister polynomial.



HI07-P

**Karakterizacija emulzija voda/ulje sa različitim odnosom tikvinog i suncokretovog ulja u kontinualnoj fazi**

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Cilj ovog rada je ispitivanje uticaja sastava kontinualne faze dobijene mešanjem ulja različitih fizičko-hemijskih osobina, odnosno suncokretovog i tikvinog ulja, na dobijanje stabilnih i monodisperznih emulzija voda/ulje, sa malim prečnicima kapljica. Takođe, istovremeno je ispitan uticaj sadržaja površinski aktivne materije i sadržaja disperzne faze na veličinu i raspodelu veličina kapi vode. Pri planiranju eksperimenata primenjen je centralno kompozitni plan koji uključuje variranje parametara u sledećim opsezima: sadržaj poliglicerol poliricinoleata (PGPR) od 1-5% (m/m), vodene faze od 10-32% (v/v) i sadržaja tikvinog ulja u smeši sa suncokretovim uljem od 0 do 100% (m/m). Srednji prečnik kapi u emulzijama dobijenim na homogenizeru velike brzine je bio u opsegu od 350 do 800 nm, sa odgovarajućim vrednostima širine pika od 100 do 220 nm. Metodom odzivne površine procenjen je i potvrđen uticaj sva tri ispitivana faktora na veličinu prečnika kapi. Takođe su određeni optimalni uslovi za formiranje emulzija.

**Characterization of w/o emulsions with different ratio of pumpkin seed and sunflower oil in continuous phase**

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This work was aimed to determine an influence of the presence of pumpkin seed oil in continuous phase comprising of pumpkin seed oil and sunflower oil on the formation of stable, monodispersed emulsions water/oil. Namely, these two oils are of different physical-chemical properties that influence emulsification process. Moreover, an influence of surfactant content as well as dispersed phase content were a subject of investigation. Centrally composite rotatable experimental design was implemented and the contents of polyglycerol polyricinoleat, dispersed phase, and pumpkin seed oil were 1-5% (w/w), 10-32% (v/v) and 0-100% (w/w), respectively. Mean size diameter of water droplets was in a range of 350 to 800 nm, with mean peak width of 100 to 220 nm, respectively. Response surface methodology confirmed and determined the influence of all three investigated factors on emulsification. These results are used for optimization of operational parameters.



**Metalurgija / Metallurgy**  
**Posterska saopštenja / Poster Presentations**

M 01



**Ispitivanje arheometalurških nalaza sa lokaliteta  
Šetaće i Paulešti u okolini Bora**

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U okolini Bora se nalazi značajan broj arheometalurških lokaliteta imajući u vidu kontinuiran razvoj rudarstva i metalurgije na ovom području od praistorije, pa do današnjih dana. U ovom radu su predstavljeni rezultati ispitivanja arheometalurških nalaza šljake metodama hemijske analize i DTA, kao i XRD i EDXRF metodama, u cilju potvrđivanja ranih metalurških aktivnosti na dva manje poznata lokaliteta – Šetaće i Paulešti.

**Investigation of archaeometallurgical findings  
from Šetaće and Paulešti localities near Bor**

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Surroundings of Bor is typical for numerous archaeometallurgical localities, having in mind continuous development of mining and metallurgy in this area from prehistory up to nowadays. The results of investigation of archaeometallurgical slag findings by using chemical analysis, DTA, XRD and EDXRF methods, in order to determine early metallurgical activities at two mentioned less known localities - Šetaće i Paulešti.





### **Fazne promene tokom oksidacije halkopiritnog i polimetalichnog koncentrata ležišta “Rudnik”**

Miroslav Sokić, Nada Štrbac\*, Branislav Marković, Vladislav Matković, Dragana Živković\*

Ivan Mihajlović\*, Ljubiša Balanović\*, Aleksandra Mitovski\*

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U radu su prikazani rezultati ispitivanja procesa oksidacije halkopiritnog i polimetalichnog koncentrata ležišta „Rudnik“. U cilju određivanja mehanizma procesa vršena su DTA-TG ispitivanja koncentrata u atmosferi vazduha i temperaturnom opsegu 298–1173 K, kao i XRD ispitivanja produkata oksidacije halkopiritnog koncentrata na 723, 873 i 1173 K. Na osnovu dobijenih rezultata predložen je mehanizam oksidacije halkopiritnog koncentrata uključujući i hemijske reakcije koje prate stvaranje odgovarajućih međuproizvoda.

Oksidacija sulfidnih minerala u polimetalichnom koncentratu protiče uz njihovu oksidaciju do sulfata na nižim temperaturama, a potom sledi dosocijacija sulfata do oksida na višim temperaturama.

### **Phase changes during oxidation of chalcopyrite and polymetallic concentrate from the ore body “Rudnik”**

Miroslav Sokić, Nada Štrbac\*, Branislav Marković, Vladislav Matković, Dragana Živković\*

Ivan Mihajlović\*, Ljubiša Balanović\*, Aleksandra Mitovski\*

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This paper presents the results of investigation of the chalcopyrite and polymetallic concentrate from the ore body „Rudnik” oxidation process. Aiming to determination of the investigated process mechanism, DTA-TG analyses in the air atmosphere and temperature ranges 298–1173 K were performed. Products of chalcopyrite concentrate oxidation at 723, 873 and 1173 K were analysed using the XRD investigations. According to the results obtained this way, the mechanism of chalcopyrite concentrate oxidation, including the chemical reactions of certain by-products development, was proposed. Oxidation of sulphide minerals from the polymetallic concentrates is resulting with sulphate generation at low and followed with their dissociation at higher temperatures.



**Neorganska hemija / Inorganic Chemistry**  
**Usmena saopštenja / Oral Presentations**

NH01-O



**Inhibitorski efekat kompleksa platine (II) na fosfolipazu A<sub>2</sub>**

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Proizvodi aktivnosti fosfolipaze A<sub>2</sub> (PLA<sub>2</sub>) utiču na veliki broj fizioloških funkcija u čovečijem organizmu, tako da su inhibitori ovog lipolitičkog enzima veoma korisni za određivanje biološke uloge PLA<sub>2</sub> u složenim ćelijskim procesima. Pored toga, inhibitori PLA<sub>2</sub> mogu imati i terapijski potencijal. Izučavanja interakcija između kompleksa metala i PLA<sub>2</sub>, kao i njihovog uticaja na aktivnost ovog enzima su veoma bitna u ispitivanjima antitumorskih lekova. Istraživanja upućuju na to da se inhibicijom ovog enzima može sprečiti rast i razvoj tumorskih ćelija tako da PLA<sub>2</sub> predstavlja potencijalnu metu za razvoj novih citostatika.

S obzirom na nedostatak podataka koji govore o dejstvu kompleksa metala na pankreasnu PLA<sub>2</sub>, cilj ovog istraživanja bio je da se ispituju interakcije između *cis*-[PtCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub>] (citostatika koji se tradicionalno koristi u hemoterapiji), [PtCl<sub>2</sub>(dach)] (potencijalnog citostatika) i pankreasne PLA<sub>2</sub> pomoću UV/VIS spektrofotometrijskih titracija; zatim da se ispita uticaj ovih kompleksa platine na aktivnost PLA<sub>2</sub>, kao i da se uporedi dejstvo tradicionalno korišćenog citostatika sa dejstvom koje ima potencijalni citostatik na ovaj enzim. Dobijeni rezultati pokazuju da oba navedena kompleksa interaguju sa pankreasnom PLA<sub>2</sub> što za posledicu ima smanjenje njene aktivnosti. Fiziološke posledice ispitivanog dejstva su razmotrene u ovom radu.

**Inhibitory effect of platinum(II) complexes on phospholipase A<sub>2</sub>**

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Action of phospholipases A<sub>2</sub> (PLA<sub>2</sub>) affects a wide range of human physiological functions. Inhibitors of these lipolytic enzymes are useful in determining the biological roles of PLA<sub>2</sub> in complex cellular processes. In addition, they may have therapeutic potential. The study of the interaction of metal complexes with PLA<sub>2</sub> and their effect on PLA<sub>2</sub> activity is especially important in antitumor drugs research. It has been demonstrated that inhibition of this enzyme might alter cancer cell growth and death, therefore PLA<sub>2</sub> represents potential target for anticancer drug development.

Due to lack of information about the effect of metal complexes on pancreatic PLA<sub>2</sub> the aim of this study was to investigate interaction of *cis*-[PtCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub>] (traditional cytostatic) and [PtCl<sub>2</sub>(dach)] (potential cytostatic) with pancreatic PLA<sub>2</sub> using UV/VIS spectral titration, to detect influence of these platinum complexes on PLA<sub>2</sub> activity and to compare the action of traditionally used cytostatic with potential cytostatic. Our results show that both platinum complexes interact with enzyme, resulting in decrease of the activity of pancreatic PLA<sub>2</sub>. Physiological consequences of this action are discussed in this work.



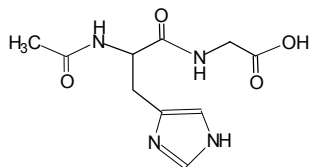
NH02-O

**$^1\text{H}$  NMR испитивање реакција  $[\text{AuCl}(\text{dien})]\text{Cl}_2$  комплекса са  $N$ -ацетилованим дериватима неких дипептида**

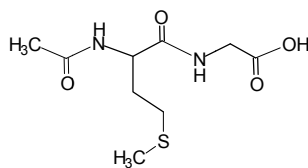
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Монофункционални  $[\text{MCl}(\text{dien})]^{n+}$  комплекси ( $\text{M} = \text{Pd}(\text{II}), \text{Pt}(\text{II}), \text{Au}(\text{III})$ ;  $\text{dien}$  = диетилен-триамин) се често користе као модели за испитивање кинетике и механизма реакција комплекса различитих јона метала са биомолекулима.<sup>1</sup> У овом раду, испитиване су реакције  $[\text{AuCl}(\text{dien})]\text{Cl}_2$  комплекса са дипептидима,  $N$ -ацетил- $S$ -хистидил-глицином (Ac- $S$ -His-Gly-OH) и  $N$ -ацетил- $S$ -метионил-глицином (Ac- $S$ -Met-Gly-OH) у pH области 2,0-7,0 на собној температури. Применом  $^1\text{H}$  NMR спектроскопије окарактерисани су производи ових реакција на различитим pH вредностима. Добијени резултати су поређени са одговарајућим литературним подацима за реакције  $[\text{PtCl}(\text{dien})]\text{Cl}$  комплекса са пептидима који у бочном низу садрже аминокиселине  $S$ -хистидин и  $S$ -метионин.<sup>2</sup>



Ac- $S$ -His-Gly-OH



Ac- $S$ -Met-Gly-OH

**$^1\text{H}$  NMR study of reactions of the  $[\text{AuCl}(\text{dien})]\text{Cl}_2$  complex with  $N$ -acetyl derivatives of some dipeptides**

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The monofunctional  $[\text{MCl}(\text{dien})]^{n+}$  complexes ( $\text{M} = \text{Pd}(\text{II}), \text{Pt}(\text{II}), \text{Au}(\text{III})$ ;  $\text{dien}$  = diethylenetriamine) have proved to be very useful model for the study of the kinetics and mechanism of the metal-biomolecules interactions.<sup>1</sup> In the present study, we used the  $[\text{AuCl}(\text{dien})]\text{Cl}_2$  complex to investigate its interactions with  $N$ -acetyl- $S$ -histidyl-glycine (Ac- $S$ -His-Gly-OH) and  $N$ -acetyl- $S$ -methionyl-glycine (Ac- $S$ -Met-Gly-OH) in the pH range 2.0-7.0 at ambient temperature. The characterization of the final products in these reactions at different pH values was done by applying  $^1\text{H}$  NMR spectroscopy. The obtained data from these investigations were compared with those previously reported in literature for interactions of the  $[\text{PtCl}(\text{dien})]\text{Cl}$  complex with  $S$ -histidine and  $S$ -methionine side chains.<sup>2</sup>

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





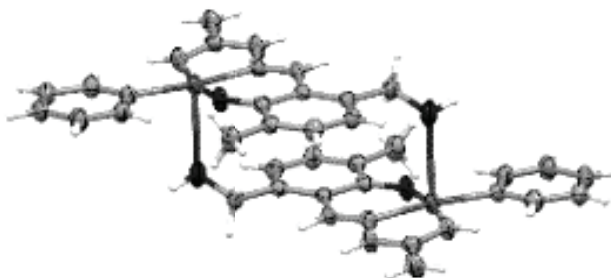
NH03-O

**Sinteza i struktura kompleksa bakra(II) sa piridoksalaminogvanidinom**

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Šifove baze piridoksala, kao jedne od formi vitamina B<sub>6</sub>, zbog dobrih kompleksirajućih osobina i biološke aktivnosti u novije vreme su postale predmet interesovanja ne samo koordinacionih hemičara, već i farmakologa. Među ovim jedinjenjima značajno mesto zauzima Šifova baza piridoksala sa aminogvanidinom (PLAG), čija je koordinaciona hemija počela radovima Leovca i saradnika. Do sada je sintetisan i strukturno okarakterisan ograničen broj njegovih kompleksa, u kojima je nađen očekivani tridentatni ONN način koordinacije ovog liganda.

U ovom radu opisana je sinteza i stuktura prvog dimernog kompleksa i to Cu(II) sa PLAG koordinacione formule  $[\{Cu(PLAG)py\}_2](NO_3)_4$ , u kome je po prvi put nađena tetradentatna koordinacija PLAG. Naime, nađeno je da u koordinaciji, pored atoma kiseonika fenolnog hidroksila i atoma azota azometinske i gvanido grupe, učestvuje i atom kiseonika hidroksimetil grupe piridoksalnog ostatka, kao mostovni ligator, koji gradi vezu sa atomom bakra susedne podjedinice. U dobijenom kompleksu Cu(II) se nalazi u blago deformisanom kvadratno-piramidalnom okruženju sa mostovnim atomom kiseonika u apikalnom položaju.

**Synthesis and structure of copper(II) complex with pyridoxalaminoguanidine**

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Recently, Schiff bases of pyridoxal, as one of the forms of vitamin B<sub>6</sub>, have become the subject of studies not only for coordination chemistry reasons, but for pharmacological as well, due to their good complexing properties and significant biological activity. Among them, Schiff base of pyridoxal and aminoguanidine (PLAG) occupies a special place and the examination of its coordination chemistry have been initiated by Leovac et al. So far, only a few metal complexes with PLAG have been synthesized and structurally characterized.

In this work the synthesis and structure of the first dimer Cu(II) complex with PLAG, of the coordination formula  $[\{Cu(PLAG)py\}_2](NO_3)_4$ , are given. This is the first complex involving the tetradentate coordination mode of the ligand. Beside the usual ligands, *i.e.* oxygen atom of phenolic hydroxyl and nitrogen atoms of azomethine and guanido group, oxygen atom of hydroxymethyl group of the pyridoxal moiety is involved in coordination as the bridging ligand, connecting the subunits. In this complex, Cu(II) is in a deformed square-pyramidal environment with the bridging oxygen in the apical position.



NH04-O

**Novi rutenijum(II) kompleksi sa anti-leukemijskom aktivnošću**

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Tibor J. Sabo, Sanja R. Grgurić-Šipka  
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Poslednjih decenija organorutenijum(II) kompleksi dobili su na značaju kao antikancerogeni agensi.

U ovom radu opisana je sinteza, karakterizacija i biološka aktivnost četiri nova rutenijum(II) kompleksa, opšte formule  $[(\eta^6\text{-}p\text{-cymene})\text{RuClL}]\text{PF}_6$ , gde su L metil, etil, *n*-propil i *n*-butil estri (*S,S*)-etilendiamin-*N,N'*-di-2-(3-cikloheksil)-propanske kiseline. Karakterizacija jedinjenja na osnovu spektroskopskih podataka ukazuje da je estarski ligand koordinovan preko azotovih atoma, sa "piano stool" geometrijom.

Vijabilitet humanih leukemičnih ćelija HL-60, K562 i REH, kao i C6 glioma pacova, L929 fibrosarkom miša i B16 melanom miša je dobijen merenjem aktivnosti citosolne kisele fosfataze. Povećanje antitumorske aktivnosti novih rutenijumskih kompleksa prati povećanje dužine alkil niza estra ( $\text{IC}_{50}$  min.-max. 2.3 - 32.2  $\mu\text{M}$ ).

Način delovanja novih Ru kompleksa verovatno uključuje uvođenje u apoptozu preko unutrašnjeg mitohondrijalnog puta, ali mehanizmom koji se razlikuje od mehanizma platinskih lekova.

**New ruthenium(II) complexes with anti-leukaemic activity**

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*\*Institute of Medicinal and Clinical Biochemistry, Faculty of Medicine,*  
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In the last decades organoruthenium(II)-complexes have reached major interest as anticancer agents.

In the present study, the preparation, characterization and biological activity of four new ruthenium(II) complexes, general formula  $[(\eta^6\text{-}p\text{-cymene})\text{RuClL}]\text{PF}_6$  where L are methyl, ethyl, *n*-propyl and *n*-buthyl esters of (*S,S*)-ethylenediamine-*N,N'*-di-2-(3-cyclohexyl)-propanoic acid are described. Spectroscopic data indicate that the coordination of the ligands occurs via nitrogen donor atoms of the ester ligands, with "piano stool" geometry.

The viability of human leukaemic cell lines HL-60, K562 and REH, as well as C6 rat glioma, L929 mouse fibrosarcoma and B16 mouse melanoma cell lines was assessed by measuring cytosolic acid phosphatase activity. The increase in antitumor activity of novel ruthenium complexes follows the increase in the alkyl side chain length of esters ( $\text{IC}_{50}$  min.-max. 2.3 - 32.2  $\mu\text{M}$ ).

The mode of action of novel Ru complexes seems to involve induction of apoptosis via the intrinsic mitochondrial pathway, but through mechanisms different from that of the platinum drugs.



NH05-O

### Kinetika i mehanizam supstitucionih reakcija dinuklearnih kompleksa platine(II) sa biološki važnim ligandima

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Multinuklearni kompleksi platine(II) predstavljaju novu generaciju antitumorskih lekova.<sup>1</sup> S obzirom da su neki tumori otporni na dejstvo cisplatine istraživanja idu u smeru sinteze novih antitumorskih kompleksa čije strukturne karakteristike omogućavaju alternativni mehanizam antitumorskog dejstva, koji se razlikuje od mehanizma dejstva cisplatine i njenih analoga.<sup>2</sup> Ispitivane su supstitucione reakcije dinuklearnih kompleksa platine(II) kao što su: [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-pyrazine)](ClO<sub>4</sub>)<sub>2</sub>, [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-4,4'-bipyridyl)](ClO<sub>4</sub>)<sub>2</sub> · DMF i [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-1,2-bis(4-pyridyl)ethane)](ClO<sub>4</sub>)<sub>2</sub> sa biološki značajnim nukleofilima tiouream, glutationom i guanozin-5'-monofosfatom na pH = 2.5 (0.01M NaClO<sub>4</sub>) i pH = 7.2 (25mM Hepes pufer i 20 mM NaCl) pri temperaturi od 37°C. Spektrofotometrijskom pH titracijom rastvora akva kompleksa određene su dve pKa vrednosti. Sve reakcije su izučavane kao reakcije *pseudo*-prvog reda, veliki višak nukleofila, a korišćene su stop-flow i UV-VIS spektrofotometrijske metode. Red reaktivnosti kompleksa je: TS3 > PTTS > PTTS1, a red reaktivnosti ispitivanih liganada je Tu > GSH > 5'-GMP.

### Kinetics and mechanism of the substitution reactions of dinuclear complexes platinum(II) with biologically important ligands

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Multinuclear complexes of platinum(II) represent a novel generation of antitumor drugs.<sup>1</sup> Considering the fact that some tumors are resistant to the effects of cisplatin, the investigations are going to direction of synthesis of new antitumour complexes which their structural characteristics provide an alternative mechanism of action that is different from cisplatin mechanism of action and its analogues.<sup>2</sup>

The substitution reactions of dinuclear complexes platinum(II) such as: [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-pyrazine)](ClO<sub>4</sub>)<sub>2</sub>, [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-4,4'-bipyridyl)](ClO<sub>4</sub>)<sub>2</sub> · DMF, i [*trans*-Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>(μ-1,2-bis(4-pyridyl)ethane)](ClO<sub>4</sub>)<sub>2</sub> were investigated with biologically relevant nucleophiles thiourea, glutathione and guanosine 5'-monophosphate at pH = 2.5 (0.01M NaClO<sub>4</sub>) and pH = 7.2 (25mM Hepes buffer i 20 mM NaCl) at 37°C. Spectrophotometric pH titration of aqua solutions was used to determinate two pKa values. All reactions were followed as pseudo-first order rate by stopped-flow and UV-VIS spectrophotometric methods. The order of reactivity complexes is: TS3 > PTTS > PTTS1, while order of reactivity investigated ligands is Tu > GSH > 5'-GMP.

1. Kasparkova J, Novakova O, Vrana O, Farrell N, Brabec V, *Biochemistry*, **38(34)** (1999) 10997-11005.
2. Kelland LR, *Drugs* **59** (2000) 1-8.



### Ispitivanje interakcija nekih monofunkcionalnih Au(III) kompleksa sa S-donorskim ligandima

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Jedinjenja zlata su korišćena u lečenju plućne tuberkuloze, a neki tiolato kompleksi zlata su efikasni u procesu lečenja reumatskog artritisa. S obzirom da su Au(III) kompleksi izoelektronski i izostrukturalni sa Pt(II) kompleksima, ispitivanja ponašanja kompleksa Au(III) kao potencijalnih antitumorskih agenasa su od velikog značaja za biološka istraživanja<sup>1,2</sup>.

U nastavku naših istraživanja<sup>3</sup> proučavali smo kinetiku i mehanizam reakcija substitucije  $[\text{AuCl}(\text{dien})]^{2+}$ ,  $[\text{AuCl}(\text{bpma})]^{2+}$  i  $[\text{AuCl}(\text{terpy})]^{2+}$  kompleksa sa glutationom, metioninom i cisteinom u 0.1M HCl (pH = 1.0) pomoću stopped-flow UV-VIS spektrofotometrije. Da bi se zadovoljili uslovi reakcije pseudo-prvog reda korišćen je veliki višak liganda. Reakcije su ispitivane na tri različite temperature što je omogućilo određivanje konstanti brzina, aktivacionih parametara  $\Delta H^\ddagger$  i  $\Delta S^\ddagger$ . Terpy kompleks je najreaktivniji, a red reaktivnosti korišćenih liganada je: Met > GSH > Cis. Negativne vrednosti za  $\Delta S^\ddagger$  potvrđuju asocijativni mehanizam substitucije.

### Study of interactions of some monofunctional Au(III) complexes with S-donor ligands

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Gold compounds are used in the treatment of pulmonary tuberculosis, but some of tholato complexes of gold gave good results as a drug for rheumatoid arthritis. Since Au(III) is isoelectronic and isostructural with Pt(II) metal ion, square planar gold(III) complexes could be suitable candidates for biological testing<sup>1,2</sup>.

To continue our previous studies<sup>3</sup> we followed the kinetic of the reactions between  $[\text{AuCl}(\text{dien})]^{2+}$ ,  $[\text{AuCl}(\text{bpma})]^{2+}$  and  $[\text{AuCl}(\text{terpy})]^{2+}$  complexes with Methionine, glutathione and cysteine in 0.1M HCl (pH = 1.0) using stopped-flow UV-VIS spectrophotometry. The excess of ligand concentration was used to observed pseudo-first order conditions. Kinetic traces for all substitution reactions at three different temperatures gave us a possibility to calculate the rate constant,  $\Delta H^\ddagger$  i  $\Delta S^\ddagger$ . Obtained results shown that the terpy complex is more reactive than bpma and dien. The order of reactivity of used ligands is: Met > GSH > Cis. Negative values for  $\Delta S^\ddagger$  confirm associative mechanism of substitution.

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NH07-O

### Kinetika i mehanizam supstitucionih reakcija monofunkcionalnih Pt(II) kompleksa, $[(\text{TL}^{\text{tBu}})\text{PtCl}]\text{ClO}_4$ i $[\text{PtCl}(\text{tpdm})]^+$

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Platina(II), koja pripada grupi metala sa  $d^8$  elektronskom konfiguracijom, tipični je predstavnik kvadratno-planarnih kompleksa. Supstitucione reakcije kompleksa platine(II) odvijaju se po A ili Ia mehanizmu, čiji tok zavisi od osobina reagujućih supstanci kao i od uslova pod kojima se proces odigrava (rastvarač, jonaska sila, pH, temperatura i pritisak).<sup>1</sup>

Kao nastavak novijih istraživanja,<sup>2</sup> ispitivanja smo vršili na monofunkcionalnim kompleksima platine(II), i to  $[(\text{TL}^{\text{tBu}})\text{PtCl}]\text{ClO}_4$  i  $[\text{PtCl}(\text{tpdm})]^+$ , gde je  $\text{TL}^{\text{tBu}}$ =2,6-bis[(1,3-di-*tert*-butilimidazolin-2-imino)metil]piridin i tpdm=terpiridindimetan, sa nukleofilima: tiourea, NaI, KBr,  $\text{NaNO}_2$ , piridin i dimetilsulfoksid (DMSO). Sve reakcije su izučavane u 0,1 M  $\text{NaClO}_4$ , u prisustvu 10 mM NaCl, na tri temperature (288, 298 i 308 K). Reakcije su praćene UV-VIS spektrofotometrijski, zadovoljavajući uslove reakcije *pseudo*-prvog reda. Dobijeni red reaktivnosti nukleofila: tiourea >  $\text{I}^- > \text{Br}^- > \text{NO}_2^- > \text{DMSO} > \text{py}$ , je u saglasnosti sa sternim i elektronskim efektima. Takođe, ovim ispitivanjem je potvrđena očekivana veća reaktivnost kompleksa  $[\text{PtCl}(\text{tpdm})]^+$ .

### Kinetics and the mechanism of the substitution reactions of monofunctional Pt(II) complexes, $[(\text{TL}^{\text{tBu}})\text{PtCl}]\text{ClO}_4$ and $[\text{PtCl}(\text{tpdm})]^+$

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Platinum(II), as metal with a  $d^8$  electronic configuration, is a typical representative of the square-planar complexes. The substitution reactions of the platinum(II) complexes proceed *via* A or Ia mechanism. Mentioned reactions depend on the nature of reacting substances and of the conditions under which the process proceed (solvent, ionic strength, pH, temperature, pressure, *trans*-effect...).<sup>1</sup>

As a continuation of recent research,<sup>2</sup> we investigated monofunctional complexes of platinum(II):  $[(\text{TL}^{\text{tBu}})\text{PtCl}]\text{ClO}_4$  and  $[\text{PtCl}(\text{tpdm})]^+$ , where  $\text{TL}^{\text{tBu}}$ =2,6-bis[(1,3-di-*tert*-butylimidazolin-2-imino)methyl]pyridine and tpdm=terpyridinedimethane, with nucleophiles: thiourea, NaI, KBr,  $\text{NaNO}_2$ , pyridine and dimethylsulfoxide (DMSO). All reactions were studied in aqueous 0.1 M  $\text{NaClO}_4$ , in the presence of 10 mM NaCl, at three different temperatures (288, 298 and 308 K). The reactions were followed by using Uv-Vis spectrophotometry under the *pseudo*-first-order conditions. The order of reactivity of the nucleophiles: thiourea >  $\text{I}^- > \text{Br}^- > \text{NO}_2^- > \text{DMSO} > \text{py}$ , is consistent with steric and electronic effects. Also, in this research, the expected higher reactivity of  $[\text{PtCl}(\text{tpdm})]^+$  complex was confirmed.

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NH08-O

**Apsorpcioni spektri i kinetika građenja J-agregata koloidnih čestica srebra sa tiocijano bojom u vodenoj sredini**

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U ovom radu izučavani su apsorpcioni spektri i kinetika građenja J-agregata tiocijano boje (TC, 5,5'-disulfopropil 3,3'-dihlorotiocianin natrijumova so) u prisustvu koloidnih čestica srebra. Sintetizovane Ag koloidne čestice okarakterisane su UV-Vis spektrofotometrijskim i fluorescentnim merenjima. Građenje J-agregata TC-boje na površini nanočestica praćeno je apsorpcionom i fluorescentnom spektroskopijom. Za izučavanje mehanizma J-agregata vršena su kinetička merenja metodom zaustavnog toka. Formiranje J-agregata opisano je sigmoidalnom krivom. Kinetika i mehanizam J-agregata racionalizovani su u smislu autokatalize i određeni su odgovarajući parametri.

**Absorption spectra and kinetics of J-aggregation of TC-coated Ag colloidal nanoparticles in aqueous solutions**

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The optical absorption spectra and kinetics of J-aggregation of thiocyanine dye (TC, 5,5'-disulfopropyl 3,3'-dichlorothiacyanine sodium salt) was studied in the presence of silver colloid. The synthesized Ag colloidal dispersions were characterized by UV-Vis spectrophotometry and fluorescence measurements. Formation of TC dye J-aggregates on the surface of nanoparticles was monitored by absorbance and fluorescence spectra. Kinetic measurements were carried out using a stopped-flow method to study the mechanism of J-aggregation. The formation of J-aggregates is described by a sigmoidal time course. The kinetics and mechanism of J-aggregation are rationalized in terms of autocatalysis and the relevant parameters were determined by fitting procedures.



Posterska saopštenja / Poster Presentations

NH09-P

**Начини везивања новог динуклеарног комплекса Со(III) са кондензационим производом 2-ацетилпиридина и дихидразида малонске киселине за ДНК**

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Неки од комплекса метала се користе у клиничкој пракси као антитуморни агенси. Мета већини ових агенаса су молекули ДНК. Комплекси полидентантних дихидразонских лиганата са суседним координационим активним местима, углавном кондензациони деривати 2-ацетилпиридина и дихидразида малонске киселине, у фокусу су интереса наше истраживачке групе. Со(III) је одабран због високог позитивног наелектрисања и редокс својства. Динуклеарни комплекс Со(III) са кондензационим производом 2-ацетилпиридина и дихидразида малонске киселине, *N',N''*-бис[(1*E*)-1-(2-пиридил)етилиден]пропандихидразид, синтетисан је и окарактерисан елементарном, спектроскопском (NMR и IC) и рендгенском структурном анализом. Интеракције комплекса са високо полимеризованом ДНК тимуса телета, праћене су у UV-Vis спектру померањем ка нижим таласним дужинама и хиперхромизмом. Унутрашња константа везивања ( $K_b = 4.2 \times 10^5 \text{ M}^{-1}$ ) заједно са структурном анализом комплекса указује на везивање у малој бразди. Детектовано је и кидање суперувичене циркуларне ДНК плазмида pUC18 комплексом, за шта није било потребно UV зрачење.

**DNA binding properties of the novel dinuclear Co(III) complex with the condensation product of 2-acetylpyridine and malonic acid dihydrazide**

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Some metal complexes have entered the clinical praxis as antitumor agents. Most of these agents target DNA molecules. The complexes of polydentate dihydrazone ligands with adjacent coordination pockets, predominantly condensation derivatives of 2-acetylpyridine and malonic acid dihydrazide are in focus of interest of our research group. Co(III) was selected for its high positive charge and redox properties. A dinuclear Co(III) complex with the condensation product of 2-acetylpyridine and malonic acid dihydrazide, *N',N''*-bis[(1*E*)-1-(2-pyridyl)ethylidene]propanedihydrazide was synthesized and characterized by elemental analysis, spectroscopy (NMR and infrared), and X-ray crystal analysis. The interaction of the complex with highly polymerized calf thymus DNA was monitored by blue shift and hyperchromism in the UV-Vis spectra. The observed intrinsic binding constant ( $K_b = 4.2 \times 10^5 \text{ M}^{-1}$ ) together with structural analysis of the complex indicate the minor groove binding. The cleavage of supercoiled circular DNA from plasmid pUC18 by the complex was detected, for which no UV irradiation was necessary.





NH10-P

**Синтеза и карактеризација никал(II) комплекса са  
1,3-пентандиамин-*N,N,N',N'*-тетраацетато лигандом**

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У реакцији између  $\text{Ba}_2(1,3\text{-pndta})\cdot 3\text{H}_2\text{O}$  и  $\text{NiSO}_4\cdot 6\text{H}_2\text{O}$  у 1 : 1 молском односу синтетисан је нови комплекс никла(II),  $[\text{Mg}(\text{H}_2\text{O})_6][\text{Ni}(1,3\text{-pndta})]\cdot 4\text{H}_2\text{O}$  (1,3-pndta = 1,3-пентандиамин-*N,N,N',N'*-тетраацетат). За карактеризацију овог комплекса употребљена је инфра-црвена и електронска апсорпциона спектроскопија. Структура комплекса је одређена на основу рендгенске структурне анализе. Добивени спектроскопски и рендгеноструктурни подаци овог комплекса су поређени са одговарајућим подацима за раније описане никал(II) комплексе који садрже 1,3-pdta (1,3-pdta = 1,3-пропандиамин-*N,N,N',N'*-тетраацетат) и 1,3-pddadp (1,3-pddadp = 1,3-пропандиамин-*N,N'*-диацетат-*N,N'*-ди-3-пропионат) лиганде.<sup>1,2</sup>

**Synthesis and characterization of the nickel(II) complex with  
1,3-pentanediamine-*N,N,N',N'*-tetraacetate ligand**

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In the reaction between  $\text{Ba}_2(1,3\text{-pndta})\cdot 3\text{H}_2\text{O}$  and  $\text{NiSO}_4\cdot 6\text{H}_2\text{O}$  in 1:1 molar ratio, new Ni(II) complex,  $[\text{Mg}(\text{H}_2\text{O})_6][\text{Ni}(1,3\text{-pndta})]\cdot 4\text{H}_2\text{O}$  (1,3-pndta = 1,3-pentanediamine-*N,N,N',N'*-tetraacetate), was synthesized and characterized by applying infrared and electronic absorption spectroscopy. The structure of the complex was determined by X-ray analysis. The spectroscopic and X-ray data of this complex were compared with those for the corresponding Ni(II) complexes with 1,3-pdta (1,3-pdta = 1,3-pentanediamine-*N,N,N',N'*-tetraacetate) and 1,3-pddadp (1,3-pddadp = 1,3-propandiamine-*N,N'*-diacetate--*N,N'*-di-3-propionate) ligands.<sup>1,2</sup>

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NH11-P

**Prvi tetranuklearni kompleks Co(II) sa  $N,N',N'',N'''$ -tetrakis(2-piridilmetil)-1,4,8,11-tetraazaciklotetradekanom (tpmc-om) i polikarboksilatnim koligandom**

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U ranije opisanim dinuklearnim kompleksima Co(II) sa oktaazamakrocikličnim ligandom  $N,N',N'',N'''$ -tetrakis(2-piridilmetil)-1,4,8,11-tetraazaciklotetradekanom (tpmc-om) i alifatičnim ili aromatičnim amino-/mono-, odnosno dikarboksilatnim koligandima predložen je mostovni, helatni, ili kombinovani način koordinacije karboksilatata. U ovom radu opisan je prvi tetranuklearni Co(II)tpmc kompleks sa tetraanjonom 1,2,4,5-benzen-tetrakarbonske (piromelitin) kiseline ( $\text{pmkH}_4$ ). Rezultati elementarne analize, molarne električne provodljivosti, UV-VIS i FTIR spektroskopije, kao i magnetnog momenta na sobnoj temperaturi u skladu su sa formulom  $[\text{Co}_4(\text{pma})(\text{tpmc})_2](\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  i visoko-spinskim stanjem Co(II). Pretpostavljeno je da su tpmc ligandi u konformaciji *lađe*, a po 2 Co(II) jona premošćena sa 2 -N-(CH<sub>2</sub>)<sub>3</sub>-N- fragmenta ciklamovog prstena unutar svake  $[\text{Co}_2(\text{tpmc})]^{4+}$  subjedinice, dodatno povezane ko-ligandom kombinovano preko -OCO<sup>-</sup>. Preliminarni *in vitro* test na citotoksičnu aktivnost ovog kompleksa prema ćelijama kancera grudi (MCF-7) bio je pozitivan.

**First tetranuclear Co(II) complex with  $N,N',N'',N'''$ -tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane (tpmc) and polycarboxylate co-ligand**

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In previously reported binuclear Co(II) complexes with octaazamacrocyclic ligand  $N,N',N'',N'''$ -tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane and aliphatic or aromatic amino-/mono-, or dicarboxylate coligands the bridged, chelate or combined coordination of carboxylate is proposed. In this work the first tetranuclear Co(II)tpmc complex with tetraanion of 1,2,4,5-benzen-tetracarboxylic (pyromelitic) acid ( $\text{pmkH}_4$ ) is described. Results of elemental analysis, molar electrical conductivity, UV-Vis and FTIR spectroscopy, as well as magnetic moment at room temperature are in accordance with the formula  $[\text{Co}_4(\text{pma})(\text{tpmc})_2](\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  and high-spin Co(II) state. It is assumed that tpmc ligands are in *boat* conformation, while 2 Co(II) ions are bridged with 2 -N-(CH<sub>2</sub>)<sub>3</sub>-N- portions of cyclam ring within each  $[\text{Co}_2(\text{tpmc})]^{4+}$  sub-units, connecting additionally with co-ligand through each -OCO<sup>-</sup> in a combined manner. Preliminary *in vitro* test against cytotoxic activity of this complex toward breast cancer cells (MCF-7) was positive.



NH12-P

**Kompleks Co(II) sa amonijum N,N-diacetato-N-ditiokarbamatom**

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Ditiokarbamato ligandi (dtc) grade stabilne komplekse sa velikim brojem prelaznih metala. Ovi ligandi imaju sposobnost da stabilizuju komplekse u neobičnim oksidacionim stanjima centralnog metalnog jona stvarajući na taj način mogućnost sinteze ditiokarbamato kompleksa Cu(III), Fe(IV), Ni(IV) i Mn(IV). Osim sa teorijskog ovi ligandi su značajni sa praktičnog aspekta jer imaju široku primjenu u poljoprivredi (kao fungicidi) i industriji (kao akceleratori u vulkanizaciji i dodaci mazivima). Kobalt je esencijalni metal za žive organizme.  $(\text{NH}_4)_3\text{idatdc}$  je ditiokarbamato-ligand sa više potencijalnih donorskih atoma (dva atoma sumpora, četiri atoma kiseonika i jednim atomom azota). Reakcijom  $\text{CoCl}_2$  sa  $(\text{NH}_4)_3\text{idatdc}$ , dobijen je novi kompleks koji je okarakterisan mikroanalizom, IR i UV/VIS spektrima, molarnom provodljivosti i magnetnim mjerenjem. Na osnovu dobijenih rezultata pretpostavljena je dinuklearna stuktura kompleksa, amonijum penta (N,N-diacetato-N-ditiokarbamato)dikobaltat(II),  $(\text{NH}_4)[\text{Co}_2(\text{H}_2\text{idatdc})_5]$ . Uprkos činjenici da su tri dtc-liganda bila dodata Co(II) jonu, dobijen je dinuklearni kompleks Co(II) sa dvije dtc-grupe na svakom Co(II) jonu i jednom dtc-grupom koja povezuje dva Co(II) jona.  $\text{H}_2\text{idatdc}$  ligand se koordinovao preko atoma sumpora za Co(II) a nespareni elektroni svakog atoma Co korišteni za Co – Co vezu slično kompleksu  $\text{K}_6[\text{Co}_2(\text{CN})_{10}]^1$ .

**Complex of Co(II) with ammonium N,N-diacetato-N-dithiocarbamate**

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Dithiocarbamate ligands (dtc) form stable complexes with many transition metals. These ligands have the ability to stabilize complexes in unusual oxidation states of the central metal ion thus creating the possibility of synthesis of dithiocarbamate complexes of Cu(III), Fe(IV), Ni(IV) and Mn(IV). Dithiocarbamate ligands are significant not only from theoretical but also from practical point of view because they have wide application in agriculture (as fungicides) and industry (as vulcanization accelerators and additives to lubricants). Cobalt is an essential metal for living organisms.  $(\text{NH}_4)_3\text{idatdc}$  is dithiocarbamate ligand with several potential donor atoms (two sulfur atoms, four oxygen atoms and one nitrogen atom). New dithiocarbamate complex was prepared by reaction of  $\text{CoCl}_2$  with  $(\text{NH}_4)_3\text{idatdc}$ . This complex was characterized by microanalysis, IR and UV/ VIS spectra, molar conductivity and magnetic measurements. Based on these results, a binuclear structure of the complex, ammonium penta(N,N-diacetato-N-dithiocarbamate)dikobaltate(II),  $(\text{NH}_4)[\text{Co}_2(\text{H}_2\text{idatdc})_5]$ , was assumed. Despite the fact that the three dtc-ligand was added to Co (II) ion, the binuclear complex of Co (II) with two dtc groups at each Co (II) ion was obtained. These two Co(II) ions are bridged by one dtc-ligand. In the complex, dtc-ligand coordinated via sulfur atoms with Co (II) and unpaired electrons of each atom Co used for the Co - Co link, analogous compound  $\text{K}_6[\text{Co}_2(\text{CN})_{10}]^1$ .

1. E. Wiberg, N. Wiberg, A. F. Holleman *Inorganic Chemistry* by Academic Press (2001) p. 1484



**Hemija životne sredine / Environmental Chemistry**  
**Usmena saopštenja / Oral Presentations**

ŽS01-O



**Dekolorizacija tekstilne boje Reactive Blue 19 procesom UV/H<sub>2</sub>O<sub>2</sub>**

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Predmet ovog rada je ispitivanje uticaja pH, inicijalne koncentracije boje i koncentracije peroksida na razgradnju tekstilne boje Reactive Blue 19 (RB19) UV zračenjem u prisustvu vodonik-peroksida, u vodenoj sredini. Tretman je vršen u UV reaktoru sa živinim lampama niskog pritiska čiji je maksimum energije zračenja na talasnoj dužini 254 nm. Rezultati pokazuju da sa povećanjem inicijalnog pH, raste efikasnost procesa dekolorizacije boje RB19. Sa porastom inicijalne koncentracije boje od 10 do 100 mg dm<sup>-3</sup> smanjuje se brzina njenog razlaganja u prisustvu H<sub>2</sub>O<sub>2</sub>. Uticaj inicijalne koncentracije peroksida na dekolorizaciju tekstilne boje RB19 UV/H<sub>2</sub>O<sub>2</sub> procesom proučavan je u opsegu od 10 do 100 mmol dm<sup>-3</sup> H<sub>2</sub>O<sub>2</sub>. Pokazalo se da sa povećanjem koncentracije peroksida najpre raste efikasnost procesa, do koncentracije od oko 30 mM, dok iznad ove koncentracije brzina procesa opada.

**Decolorization of the textile dye Reactive Blue 19 by the UV/H<sub>2</sub>O<sub>2</sub> process**

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This work deals with effects of pH, concentration of dye and concentration of hydrogen peroxide on photodegradation of textile dye Reactive Blue 19 (RB19) by ultraviolet radiation in presence of hydrogen peroxide, in water environment. The UV treatment was done in the UV reactor with low-pressure mercury lamps, with maximum energy output at the wavelength 254 nm. The results show that by increasing of initial pH, the efficiency of decolorization of dye increases. Photodegradation efficiency decreases with the increase of dye concentration from 10 to 100 mg dm<sup>-3</sup>. The influence of initial concentration of H<sub>2</sub>O<sub>2</sub> on degradation of textile dye RB19 by UV/H<sub>2</sub>O<sub>2</sub> system has been studied at initial concentrations of H<sub>2</sub>O<sub>2</sub> from 10 to 100 mmol dm<sup>-3</sup>. It is shown that the increase of concentration of H<sub>2</sub>O<sub>2</sub> brings to an increase of degradation process efficacy until the concentration of peroxide reaches approximately 30 mM, while above this concentration process rate decreases.



HŽS02-O

**Degradacija mezotriona primenom unapređenih oksidacionih postupaka (AOP)**

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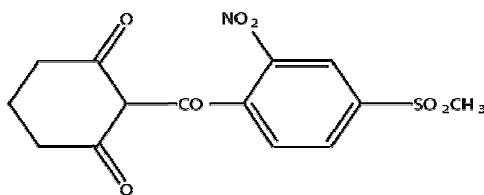
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Danas je zagađenje površinskih i podzemnih voda pesticidima jedan od vodećih problema u velikom broju zemalja, zbog perzistentnosti pesticida i potencijalnih negativnih efekata na zdravlje ljudi. Otpadne vode mogu sadržati visoke koncentracije pesticida (mg/l), dok površinske i podzemne vode sadrže tragove pesticida (μg/l).

Mezotrion, predstavlja nov herbicid koji spada u kategoriju triketona. On je selektivan herbicid koji se koristi protiv jednogodišnjih trava i širokolisnih korova u ykukuruzu. Primenjuje se u periodu razvoja biljke od pojave prvih izdanaka pa do V8 stepena razvoja (kada biljka sadrži osam listova). Deluje inhibicijom 4-hidroksifenilpiruvat dioksigenaze (HPPD) kod biljaka.

U radu su prikazani rezultati degradacije mezotriona primenom unapređenih oksidacionih postupaka: DBD (dielektrično barijerno pražnjenje) -O<sub>3</sub>, O<sub>3</sub>-DBD, ozonizacija, Fenton, foto-Fenton. Stepen degradacije mezotriona je praćen preko HPK vrednosti, i primenom HPLC tehnike.



**Degradation of mesotrione using advanced oxidation processes (AOP)**

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Today, the pollution of surface and groundwater with pesticides is one of the major problems in many countries, due to persistence of pesticides and the potencial adverse effects on human health. Waste water can contain high concentrations of pesticides (mg/l). Surface and groundwater contain traces of pesticides (μg/l).

Mesotrione, is a new herbicide that belongs to the category of triketons. It is a selective herbicide used against annual grasses and broadleaf weeds in corn. It is used during plant development from the first shoot to the V8 stage of development (when the plant contains eight leaves). It works by inhibition of 4-hydroxyfenilpiruvate dioxigenaze in plants (HPPD).

In this paper the results of mesotrione degradation will be presented. Degradation was carried out using advanced oxidation processes (AOP): DBD (Dielectric Barrier Discharge)-O<sub>3</sub>, O<sub>3</sub>-DBD, ozonization, Fenton, photo-Fenton. The degradation of mesotrione was monitored using COD values, and using HPLC technique.

HŽS03-O

### Uticaj metoprolola i njegovih fotokatalitičkih degradacionih intermedijera u prisustvu TiO<sub>2</sub> na rast odabranih ćelijskih linija

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Ispitana je *in vitro* aktivnost metoprolola, kao i smeše metoprolola i njegovih intermedijera nastalih tokom fotokatalitičke razgradnje (u prisustvu TiO<sub>2</sub> katalizatora Wackherr ili Degusa P25 i UV zračenja u prisustvu O<sub>2</sub>) na rast tri histološki različite ćelijske linije: hepatoma pacova (H-4-II-E), humani adenokarcinom debelog creva (HT-29) i humana fetalna pluća (MRC-5), u opsegu masenih koncentracija od 13,4-214 µg/cm<sup>3</sup> upotrebom sulforodamin B (SRB) kolorimetrijske analize. Neozračen metoprolol i aspirin su korišćeni kao negativna kontrola, dok su citotoksični lekovi i HgCl<sub>2</sub> korišćeni kao pozitivna kontrola. Uticaj ispitivanih uzoraka zavisio je od vrste primenjenog katalizatora, koncentracije metoprolola, odnosno intermedijera i vrste ćelijske linije. U svakoj ćelijskoj liniji toksičnost analiziranih uzoraka dobijena nakon različitog vremena ozračivanja je veća u slučaju primene TiO<sub>2</sub> Degussa P25 kao katalizatora nego Wackherr-a, tj. isti nivo toksičnosti je dobijen pri nižoj koncentraciji intermedijera primenom katalizatora Degussa P25. Kao najosetljivija se pokazala ćelijska linija hepatoma pacova, a najmanje osetljiva ćelijska linija humanog adenokarcinoma debelog creva.

### Effect of metoprolol and products of its photocatalytic degradation in the presence of TiO<sub>2</sub> on the growth of selected cell lines

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The growth activity of metoprolol, as well as mixture of metoprolol and its photocatalytic degradation intermediates (obtained by applying TiO<sub>2</sub> catalyst Wackherr and Degussa P25, and UV irradiation in the presence of O<sub>2</sub>) was evaluated *in vitro* in a panel of three histologically different cell lines: rat hepatoma (H-4-II-E), human colon adenocarcinoma (HT-29) and human fetal lung (MRC-5), in the mass concentration range of 13.4-214 µg/cm<sup>3</sup> using colorimetric Sulforhodamine B (SRB) assay. Nonirradiated metoprolol and aspirin were used as negative controls, while cytotoxic drugs and HgCl<sub>2</sub> were used as positive controls. Effects of examined samples were dependent on the type of used catalyst, concentration of metoprolol and intermediates, and the type of cell line. With all cell lines, the toxicity of samples obtained after different irradiation times was higher when using Degussa P25 than Wackherr catalyst, i.e. the same level of toxicity was observed at lower concentrations using Degussa P25. The most sensitive cell line was rat hepatoma and the least sensitive was human colon adenocarcinoma cell line.

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### Teški metali u zemljištu parkova u Šapcu

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Aktuelna oblast istraživanja koja se odnosi na zemljišta u gradovima je monitoring opterećenosti teškim metalima. U prethodnom periodu praćen je kvalitet urbanog zemljišta u većim gradovima Srbije gde su analizirani parkovi, dečja igrališta i ostale zelene površine. Cilj ovog rada bio je određivanje sadržaja odabranih teških metala (Pb, Cd i Cu) u zemljištu parkova u Šapcu, upoređivanje rezultata sa podacima za urbano zemljište u Beogradu i Novom Sadu kao i sa nekim gradovima u svetu i uticaj saobraćaja na zagađenost zemljišta na ispitivanim lokacijama. Zemljište je uzorkovano tokom avgusta i septembra 2010. godine. Analizirano je 32 uzorka sa tri lokacije. Uzorci su pripremljeni digestijom zemljišta u smeši HCl:HNO<sub>3</sub> (3:1, v/v). Pseudo-totalna koncentracija teških metala određena je atomskom apsorpcionom spektroskopijom. Upoređivanjem dobijenih rezultata sa maksimalno dozvoljenim koncentracijama u zemljištu (MDK) definisanim u Pravilniku Republike Srbije zaključeno je da se koncentracija Cd i Cu nalazi ispod vrednosti MDK u uzorcima sa sve tri lokacije. Koncentracija Pb u uzorcima jednog parka je ispod MDK vrednosti, što se može pripisati znatno manjoj frekventnosti saobraćaja u tom delu grada u odnosu na druge ispitivane lokacije, dok je u preostala dva parka u pojedinim uzorcima njegov sadržaj povećan, što se može pripisati blizini tačaka uzorkovanja prometnim ulicama u gradu.

### Heavy metals in soil from parks in Sabac

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Actual field of research referring to the soil in urban areas is monitoring of heavy metal contents. In the previous period the quality of the soil in urban areas was monitored in bigger Serbian cities, where the parks, children playgrounds and other green areas were analyzed. The aim of this paper was to determine the concentration of selected heavy metals (Pb, Cd and Cu) in the soil of parks in Sabac, comparison of the results with those obtained for the urban soils in Belgrade and Novi Sad, as well as for some cities in the world and the traffic influence to the pollution of soil on tested locations. The soil was sampled during August and September in 2010. 32 samples from three locations were analyzed. They were prepared by the soil digestion in the mixture HCl:HNO<sub>3</sub> (3:1, v/v). Pseudo total heavy metal contents was determined by atomic absorption spectroscopy. By comparing the obtained results with maximum allowed quantity in soil (MAQ) defined in Book of regulations of Republic of Serbia it was concluded that concentration of Cd and Cu is below the MAQ values in the samples from all three locations. Concentration of Pb in the samples from one park is below MAQ values, which could be due to the less frequent traffic in that part of the town compared with the other two tested locations, whereas in the same samples from other two parks its concentration is higher, which may be ascribed to the closeness of tested points to the busy town streets.



HŽS05-O

***Artemia salina* test akutne toksičnosti – određivanje toksikološkog efekta tekstilne boje Reactive black 5 posle obezbojavanja primenom koaksijalnog DBD reaktora**

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Tekstilna industrija danas predstavlja veliki problem za održivo upravljanje vodnim resursima. Otpadne vode tekstilne industrije sadrže visok sadržaj boje. Između 10 i 20% upotrebljene boje ostaje u efluentu. Obojenost vode umanjuje prodiranje sunčeve svetlosti, utiče na intenzitet primarne produkcije u vodenoj sredini, kao i biološku aktivnost vodenih organizama. Boje mogu biti uzrok akutne i hronične toksičnosti u životnoj sredini. Efluent osim boje odlikuju visok salinitet i provodljivost, a to su kritični parametri za slatkovodne organizme. Zato je u ovom radu primenjen *Artemia salina* test za ispitivanje akutne toksičnosti. Cilj rada je bio poređenje mortaliteta (%) bioindikatora *Artemia salina* pri koncentraciji tekstilne boje Reactive black 5 od 40, 80, 200, 500 i 1000 ppm, odnosno određivanje LC<sub>50</sub> za ovu boju. Procenat mortaliteta je određen i posle obezbojavanja ovih rastvora boje primenom unapređenog oksidacionog postupka, AOP-a. Za obezbojavanje je korišćen koaksijalni plazma reaktor koji radi na principu dielektričnog barijernog pražnjenja (DBD) i to pri unetoj gustini energije u rastvore boje od 135 i 495 kJ/L. Toksikološki test je urađen u triplicatima.

***Artemia salina* acute toxicity test - determining toxicological effect of Reactive Textile Dye (RB 5) after decolorization using coaxial DBD reactor**

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Textile industry presents a major concern today, as it stands in the way of sustainable management of water resource. Waste waters from this industry carry about 10 to 20 % of textile day used in the dying process (residual liquors). Color affects the adsorption of solar radiation, thus reducing intensity of primary production, causing changes in behavior of organisms and the aquatic environment. It can cause acute and hronic toxicity in the environment. Since the effluent has high salinity and therefore high conductivity we used *Artemia salina* as bioindicator instead of freshwater organisama. Aim was to determine relation between mortality (%) of bioindicator *Artemia salina* and concentration of color during the treatment 40, 80, 200, 500, 1000 ppm. That is to establish LC<sub>50</sub> for textile color reactive black 5 (RB 5). Percentage of mortality has been determine also after degradation of color that was carried out using advanced oxidation processes (AOP). Coaxial plasma reactor, which works on a principle of dielectric barrier discharge was used for process of decoloration (DBD). We introduced energy density of 135 i 495 kJ/L in staining solutions. Toxicology test was carried out in triplicates.







### Depozit hlorthirifosa u zasadu višnje i šljive

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U zaštiti bilja pesticidi se najčešće primenjuju prskanjem listova čime nastaje inicijalni depozit. Inicijalni depozit na površini biljaka predstavlja osnovu za sve efekte koje pesticidi izazivaju (biološka efikasnost, delovanje na ne ciljane organizme, ostaci u hrani i životnoj sredini, itd). Ispitivanje depozita je od velikog značaja za podešavanje prskalica, unapređenje kvaliteta primene, utvrđivanje odnosa doze i efekta kod ispitivanja efikasnosti pesticida, kao i za pitanja vezana za životnu sredinu.

U radu su prikazani nivoi depozita hlorthirifosa u zasadu višnje i šljive. Posle primene jedne komercijalne formulacije (Radar 300EW), depozit je praćen na filter papirima (prečnik 9 cm) postavljenim u krošnju stabala tako da simuliraju listove, i na zemljište neposredno ispod stabala. Tretmani su se sastojali od po četiri ponavljanja. Za ekstrakciju a.s. sa filter papira korišćen je etil-acetat i GC/FPD.

Prosečni depozit hlorthirifosa na filter papirima koji su se nalazili u krošnji bio je  $1.49 \mu\text{g}/\text{cm}^2$  (višnja) i  $2.07 \mu\text{g}/\text{cm}^2$  (šljiva) uz CV od ~ 36 % za višnju i ~ 82 % za šljivu. Prosečan depozit na filter papirima postavljenim, ispod stabala bio je znatno manji  $0.63 \mu\text{g}/\text{cm}^2$  (višnja) i  $0.56 \mu\text{g}/\text{cm}^2$  (šljiva).

### Chlorpyrifos deposit in a sour cherry and plum orchard

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Foliar application of pesticides is the predominant procedure in plant protection and results in the initial spray deposit on the plant surface. The initial deposit on plants is the starting point of any effect of pesticides like biological efficacy, side effects on non-target-organisms, residues, etc. The investigation of such deposits is of major interest with respect to the evaluation of sprayer function, improvement of application quality, investigation of dose response and efficacy as well as environmental issues.

Our study presents deposit levels ( $\mu\text{g}/\text{cm}^2$ ) obtained after the application of a commercial formulation of chlorpyrifos (Radar 300EW) in a sour cherry and a plum orchard. Treatments consisted of four replicates with 5 trees/replicate. Filter paper (diameter 9 cm) was used as the sampling surface and placed in the tree canopy (to simulate leaves) and on the soil below. For each replicate 20 „leaf“ and „soil“ samples were collected. Prior to GC/FPD analysis samples were extracted with ethyl acetate. Recovery for 3 spiking levels was > 90% .

Obtained results indicated that the average chlorpyrifos deposit measured on the „leaves“ was of the same order of magnitude in both experiments:  $1.49 \mu\text{g}/\text{cm}^2$  (cherries) and  $2.07 \mu\text{g}/\text{cm}^2$  (plums). Variability (CV%) was higher for plums. Average deposits on filter papers placed under the trees was considerably lower:  $0.63 \mu\text{g}/\text{cm}^2$  and  $0.56 \mu\text{g}/\text{cm}^2$ .



Posterska saopštenja / Poster Presentations

HŽS07-P



**Kvalitet vode Dunava, Donjeg Podunavlja, u periodu od 1999. do 2009. godine**

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Vode Dunava se zagađuju iz gornjeg sliva, ali i iz Srbije, Rumunije i Bugarske što se odražava na kvalitet voda Đerdapskog jezera, pa je u tom smislu neophodno uspostaviti prekograničnu saradnju sa Rumunijom. Za Dunav se po ključnim planskim dokumentima zahteva da bude u II klasi. Kvalitet vode Dunava u Donjem Podunavlju je najvećim delom II-III klase, uglavnom zahvaljujući velikom kapacitetu razblaživanja, što omogućava njegovo korišćenje za rekreaciju, ribolov, sportove na vodi i kampovanje. Na bazi sistematskih merenja koje obavlja RHMZS mogu se izvući zaključci u pogledu promena parametara kvaliteta vode Dunava Donjeg Podunavlja. Srbija je jedna od retkih podunavskih zemalja koja se može pohvaliti da se na njenoj teritoriji kvalitet vode Dunava poslednjih godina poboljšava.

**Water quality of the Danube, the Lower Danube, in the period since 1999 by 2009**

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Water in the Danube River is polluted from the different point and non point sources in upper and lower part of the river basin which influence also the quality of water in the Đerdap lake. In order to improve the current situation regarding water quality in the Đerdap lake it is necessary to enhance cross border cooperation between Serbia and Romania. According to the required standards the Danube water should be in II class. At present, quality of water in lower Danube is II-III class thanks to the high capacity of dilution which make it suitable for recreation, angling, water sports and camping. Based on results of permanent monitoring that has been conducted by Republic Hydrometeorological Bureau of Serbia changes of water quality in the lower Danube could be observed. Serbia is one of the rare country in the Danube basin where quality of water in the Danube River increases.





## A proper evaluation of interaction between solvent and thiophene from the middle distillation fraction of oil through extraction

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**Withdrawn**





### **Primena unapređenih oksidacionih postupaka, AOP-a, za uklanjanje boje Ractive black 5 iz vode**

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Boje su našle primenu u mnogim industrijskim granama, kao što su tekstilna industrija, industrija kože, proizvodnja plastičnih masa, zbog čega u procesu bojenja nastaju zabrinjavajuće velike količine obojenih otpadnih voda. Obojenost sprečava prodiranje sunčeve svetlosti zbog čega je onemogućen proces fotosinteze u vodenoj sredini, što u velikoj meri utiče na biološku aktivnost vodenih organizama. Azo boje, u koje spada ispitivana Reactive black 5, su najtoksičniji tip tekstilnih boja. Obrada otpadnih voda predstavlja postupke pomoću kojih se vrši smanjenje prisutnog zagađenja do onih količina s kojima prečišćene otpadne vode ispuštene u prirodne vodene sisteme ne predstavljaju opasnost za žive organizme i ne uzrokuju neželjene promene u životnoj sredini. Oksidacione metode su visoko efikasne i u velikoj meri se primenjuju unapređeni oksidacioni postupci (eng. *Advanced Oxidation Process - AOPs*) za prečišćavanje otpadnih voda, u kojima nastaju visoko reaktivni, hidroksilni radikali ( $\text{OH}\cdot$ ), koji predstavljaju oksidacionu vrstu odgovornu za degradaciju zagađivača. U okviru ovog rada ispitana je efikasnost dekolorizacije Reactive black 5 pomoću različitih oksidacionih sistema:  $\text{O}_3$ ,  $\text{H}_2\text{O}_2/\text{UV}$ ,  $\text{O}_3/\text{H}_2\text{O}_2/\text{UV}$ , Fentonov reagens i foto-Fentonov reagens.

### **The application of advanced oxidation processes, AOPs, for removing Reactive black 5 dye from the water**

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Decolorization of solution of Reactive black 5 was examined using following oxidation systems: oxidation by ozone ( $\text{O}_3$ ), where the effect of initial pH of dye solutions determined the degree of decolorization, the system  $\text{H}_2\text{O}_2 / \text{UV}$ , where the influence of dosage of  $\text{H}_2\text{O}_2$  on the decolorization rate was examined, the system  $\text{O}_3/\text{H}_2\text{O}_2/\text{UV}$ , Fenton reagent ( $\text{Fe}^{2+}/\text{H}_2\text{O}_2$ ) and photo-Fenton reagent ( $\text{Fe}^{2+}/\text{H}_2\text{O}_2/\text{UV}$ ). According to the results, we can conclude that the optimal pH value is 9,00 in the systems with  $\text{O}_3$  and the optimal concentration of  $\text{H}_2\text{O}_2$  is 20 mmol/L. All measurements were performed immediately (after 5 min), and 24 h after the treatment of dye solutions. Based on the results, it could be concluded that photo-Fenton and  $\text{O}_3/\text{H}_2\text{O}_2/\text{UV}$  systems are very efficient methods for removal of Reactive black 5 dye from the water. The most effective decolorization of 100 % was obtained by photo-Fenton during the period of 25 minutes. The second most efficient process of the examined oxidative processes was the combination of  $\text{O}_3/\text{H}_2\text{O}_2/\text{UV}$ , with 97 % decolorization rate for a reaction time of 40 minutes. Our results indicate that studied Advanced Oxidation Processes may be effectively used for decolorization of dye wastewater.

### Моделовање емисије одабраних параметара животне средине у оквиру одрживог развоја применом неуронских мрежа

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Увођење концепта одрживог развоја, који подразумева рационално коришћење природних ресурса, економичну употребу енергије и очување животне средине за будуће генерације, је данас приоритет на националном и глобалном нивоу. У овом раду приказано је моделовање емисије оксида азота и сумпора, честица (Particulate Matter -  $PM_{10}$ ) и прекурсора формирања озона, који се прате као параметри одрживог развоја, путем неуронских мрежа. Тестиране су три различите архитектуре, при чему су истовремено моделовани сви параметри. За развој мрежа коришћени су подаци о економском и индустријском развоју земаља Европске уније, као и земаља кандидата. Адекватном селекцијом улазних параметара, приликом тренирања мреже, постигнуто је задовољавајуће слагање измерених вредности са вредностима добијеним моделовањем. Провером сва три модела, са подацима који нису коришћени за тренинг, закључено је да се најбољи резултати постижу применом архитектуре са општом регресијом (*General Regression Neural Network-GRNN*). Добијени модел је веома значајан са аспекта предвиђања параметара одрживог развоја, а посебно за земље у којима се не врши мониторинг загађујућих материја анализираних у овом раду.

### ANN emission modelling of some sustainable development parameters

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Sustainable development ensures a harmonious relationship between social, economic and environmental factors, provides a rational use of natural resources, energy and economical use of space, and preserves the environment for future generations. This paper presents an innovative application of artificial neural networks (ANN) for the modelling of selected sustainable development parameters: emissions of acid oxides, ozone precursors and particulate matter ( $PM_{10}$ ). Three different ANN architectures have been tested for the simultaneous modelling of all three selected parameters. For the training of neural networks, industrial and economic development data of the EU and the candidate countries have been used. It has been shown that, with a good selection of input parameters, a satisfactory agreement of measured values with the values given by models was obtained for the training dataset. All three models were also tested with a validation dataset consisting of the data which was not used for the training of the models. The best results were achieved by the general regression neural network (GRNN) model. The obtained GRNN model is very important both for sustainable development modelling and for countries where monitoring of the parameters of sustainable development is not being performed sufficiently.

HŽS11-P

### Optimizacija HPLC metode za praćenje fotostabilnosti vodenog rastvora mezotriona

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Mezotrion (2-(4-metil-2-nitrobenzoi)cikloheksan-1,3-dion,  $M_r = 339,3$ ), CAS No 104206-82-8,  $C_{14}H_{13}NO_7S$  je selektivni herbicid iz klase triketona. Registrovan je 2001. godine od strane EPA za kontrolu širokog spektra korovskih vrsta, posebno širokolisnih korova i nekih trava na kukuruznim poljima. Budući da prema dostupnim literaturnim podacima razgradnja mezotriona primenom heterogene fotokatalize nije ispitivana do sada, cilj ovoga rada je bio pre svega utvrđivanje optimalnih uslova rada HPLC–DAD za proučavanje stabilnosti vodenog rastvora mezotriona. Nakon snimanja UV spektara i utvrđivanja odgovarajuće talasne dužine koja će poslužiti za praćenje kinetike razgradnje aromatičnog jezgra, ispitana je uticaj sastava mobilne faze ACN : voda, kao i protoka na efikasnost razdvajanja mezotriona od intermedijara koji nastaju tokom njegove razgradnje. Nakon toga, ispitana je i stabilnost pomenutog supstrata na svetlu i u mraku u prisustvu/odsustvu  $TiO_2$  Degussa P25. Ustanovljeno je da se mezotrion razlaže na svetlu u prisustvu katalizatora i da je u svim drugim slučajevima stabilan.

### Optimization of HPLC method for monitoring the stability of aqueous solution of mesotrione

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Mesotrione (2-(4-mesyl-2-nitrobenzoyl)cyclohexane-1,3-dione,  $M_r = 339.3$ ), CAS No 104206-82-8,  $C_{14}H_{13}NO_7S$  is a selective herbicide from the chemical class of triketone. It has been registered in 2001 by EPA for controlling a wide range of weed species, especially broadleaf weeds and some grass on corn fields. Since there are no data in the available literature on the degradation of mesotrione by applying heterogeneous photocatalysis, the aim of this work was to find out optimum working conditions of a HPLC–DAD method for studying stability of aqueous solutions of mesotrione. After recording UV spectra and establishing the appropriate wavelength that will be used for monitoring the degradation kinetics of the aromatic ring it was necessary to study the effect of the composition of the mobile phase ACN: water, as well as of the flow rate on the efficiency of separation of mesotrione from its intermediates formed during the degradation. After that the stability of the mentioned substrate was studied in the presence of light and in the dark in the presence/absence of  $TiO_2$  Degussa P25. It was found that mesotrione decomposes in the presence of the catalyst, while in all other cases is stable.

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HŽS12-P

**Fotokatalitička razgradnja kvinmeraka u vodenoj suspenziji TiO<sub>2</sub>**

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Derivati hinolinkarboksilne kiseline su relativno nova klasa herbicida velike selektivnosti od kojih se kvinmerak (7-hlor-3-metilhinolin-8-karboksilna kiselina) komercijalno primenjuje u poslednjih desetak godina. Za razliku od drugih sintetičkih auksina kvinmerak ispoljava selektivno dejstvo prema dikotiledonim korovima, kao što je prilip (*Galium aparine*), u usevima, kao što su šećerna trska i uljana repica. Cilj ovoga rada je ispitivanje fotokatalitičke razgradnje kvinmeraka (0,05 mmol dm<sup>-3</sup>) primenom UV zračenja u prisustvu TiO<sub>2</sub> Degussa P25. Kinetika razgradnje je proučavana praćenjem promene koncentracije kvinmeraka primenom LC–DAD. Na osnovu dobijenih rezultata može se zaključiti, da direktnom fotolizom dolazi do razgradnje kvinmeraka, s tim da je fotokatalitička razgradnja mnogo efikasnija. Ispitan je uticaj količine katalizatora TiO<sub>2</sub> Degussa P25 (0,1–2 mg cm<sup>-3</sup>), prisustva elektron-akceptora (H<sub>2</sub>O<sub>2</sub>, S<sub>2</sub>O<sub>8</sub><sup>2-</sup> i BrO<sub>3</sub><sup>-</sup>), kao i pH (2,0–10,5) na kinetiku fotorazgradnje.

**Photocatalytic degradation of quinmerac in water suspensions of TiO<sub>2</sub>**

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Substituted quinolinecarboxylic acids are a new class of highly selective auxin herbicide, of which quinmerac (7-chloro-3-methylquinoline-8-carboxylic acid) has been introduced commercially in the past ten years. Unlike other synthetic auxins quinmerac effectively controls important dicotyledonous weeds, such as cleavers (*Galium aparine*), in crops, such as sugarbeet and oilseed rape. The aim of this work was to investigate the photocatalytic degradation of quinmerac (0.05 mmol dm<sup>-3</sup>) by applying UV radiation in the presence of TiO<sub>2</sub> Degussa P25. The degradation kinetics was studied by following the changes of quinmerac concentration using HPLC–DAD technique. On the basis of the obtained results it is possible to conclude that direct photolysis causes quinmerac degradation, the process of photocatalytic degradation being much more efficient. The effects of the amount of the catalyst TiO<sub>2</sub> Degussa P25 (0.1–2.0 mg cm<sup>-3</sup>), electron-acceptors (H<sub>2</sub>O<sub>2</sub>, S<sub>2</sub>O<sub>8</sub><sup>2-</sup> and BrO<sub>3</sub><sup>-</sup>), and pH (2.0–10.5) on the photodegradation kinetics were investigated.

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HŽS13-P

### Heterogena foto-Fentonska razgradnja tiakloprida

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Proučavana je kinetika heterogene foto-Fentonske razgradnje insekticida tiakloprida primenom Fe/TiO<sub>2</sub> fotokatalizatora u kombinaciji sa UV/H<sub>2</sub>O<sub>2</sub>. Fotokatalitička razgradnja tiakloprida je praćena primenom HPLC–DAD, kao i TOC. U svim eksperimentima je primenjeno UV zračenje (živina lamp, 125 W, emisioni maksimumi u UV oblasti na 304, 314, 335 i 366 nm, sa najintenzivnijim emisionim maksimumom na 366 nm). Pre svega je određen optimalni maseni odnos Fe prema TiO<sub>2</sub>, a zatim je za ovaj heterogeni sistem proučavana kinetika razgradnje tiakloprida u širokom opsegu koncentracija tiakloprida i fotokatalizatora, kao i pH. Takođe je ispitana i brzina taloženja fotokatalizatora, kao i mogućnost ponovne upotrebe fotokatalizatora. Primenom heterogenog foto-Fentonskog procesa koji uključuje 7,2Fe/TiO<sub>2</sub>/UV/H<sub>2</sub>O<sub>2</sub> uz kontinualno dodavanje H<sub>2</sub>O<sub>2</sub> mineralizacija tiakloprida je dva puta efikasnija u poređenju sa najčešće primenjivanim TiO<sub>2</sub> Degussa P25.

### Heterogeneous photo-Fenton degradation of thiacloprid

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The kinetics of heterogeneous photo-Fenton degradation of thiacloprid was studied using the Fe/TiO<sub>2</sub> photocatalyst in combination with UV/H<sub>2</sub>O<sub>2</sub>. The process of photocatalytic degradation of the substrate was monitored by HPLC–DAD and TOC. In all experiments use was made of UV radiation (mercury lamp, 125 W, emission maxima in the UV region at 304, 314, 335 and 366 nm, with the most intensive maximum at 366 nm). As first, the optimum mass ratio of Fe and TiO<sub>2</sub> was determined, and then for that heterogeneous system the kinetics of thiacloprid degradation was examined in a wide range of concentrations of thiacloprid and photocatalyst, as well as of pH. Also, the study encompassed the investigation of the rate of the photocatalyst sedimentation, as well as the possibility of reusing the photocatalyst. The application of the photo-Fenton process involving 7.2Fe/TiO<sub>2</sub>/UV/H<sub>2</sub>O<sub>2</sub> with continuous addition of H<sub>2</sub>O<sub>2</sub>, resulted in the thiacloprid mineralization that was two times more efficient compared to the process involving the most often used TiO<sub>2</sub> Degussa P25 photocatalyst.



### **Uklanjanje arsenata iz vode za piće primenom modifikovanih višeslojnih ugljeničnih nanocevi**

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Prema preporukama Svetske zdravstvene organizacije, maksimalno dozvoljena koncentracija arsena u vodi za piće smanjena je sa 50 na 10  $\mu\text{g L}^{-1}$ . Ovako niska granična vrednost nameće potrebu za razvojem novih sorbenata za uklanjanje arsena iz vode. U ovom radu su, kao potencijalni sorbenti, ispitane različito tretirane višeslojne ugljenične nanocevi (Multi-Walled Carbon Nanotubes - MWCNTs). MWCNTs su modifikovane postupcima oksidacije (o-MWCNTs) i aminofunkcionalizacije (e-MWCNTs). Sorpcione karakteristike netretiranih i modifikovanih MWCNTs analizirane su u šaržnim uslovima. Ispitan je uticaj pH vrednosti rastvora (pH opseg 3 - 7) kao i početne koncentracije As(V), od 47 do 3600  $\mu\text{g L}^{-1}$ . Koncentracija As(V) merena je primenom ICP-MS tehnike (Agilent Technologies 7500ce). Sorpcioni kapaciteti ispitivanih materijala određeni su primenom Langmuir-ovog i Freundlich-ovog modela izoterma. Utvrđeno je da dobijenim rezultatima najbolje odgovara Langmuir-ov model. Najveći sorpcioni kapacitet za As(V) jone imale su e-MWCNTs. Primenom ovako modifikovanih MWCNTs, koncentracija As(V) u vodi je smanjena sa 94 na 8  $\mu\text{g L}^{-1}$ , čime su zadovoljeni i najnoviji propisi vezani za maksimalno dozvoljenu koncentraciju arsena u vodi za piće.

### **Arsenate separation from drinking water by modified multi-walled carbon nanotubes**

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In accordance with the World Health Organization recommendations, maximal allowed concentration of arsenic in drinking water is reduced from 50 to 10  $\mu\text{g L}^{-1}$ . The low restrictive limit for arsenic implies the development of new sorbents for its separation from water. In this work, differently treated multiwalled carbon nanotubes (MWCNTs) were tested as potential sorbents. MWCNTs were modified by oxidation (o-MWCNTs) and by aminofunctionalization (e-MWCNTs). Sorption characteristics of raw and modified MWCNTs were investigated in batch sorption experiments. The influence of solution pH (pH range 3 – 7) and As(V) initial concentration (from 47 to 3600  $\mu\text{g L}^{-1}$ ), was studied. The concentration of As(V) has been measured using an ICP-MS system (Agilent Technologies 7500ce). Sorption capacities of examined materials were determined by Langmuir and Freundlich isotherm model. The obtained results for both raw and modified MWCNTs fitted better to the Langmuir model. The best sorption capacity for As(V) ions was achieved by e-MWCNTs. The application of thus modified material has led to the reduction of As(V) concentration from 94 to 8  $\mu\text{g L}^{-1}$ , in accordance with the new regulation value for arsenic concentration in drinking water.



### **Concentration levels of POPs in the biotic material in Novi Sad, Serbia**

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In the frame of the FP5 project APOPSBAL and Project funded by the Secretariat for Science and Technological Development of the Autonomous Province of Vojvodina (Determination of Persistent Organic Pollutants in Abiotic and Biotic Matrix of South Bačka) the residual quantities of persistent organic pollutants (POPs) were monitored in human milk. Human milk is a subtle eco-indicator of contamination of the female population and the newborn as well as valuable indirect indicator of environmental pollution. Determination of 7 EPA polychlorinated biphenyl (PCB) congeners and 11 organochlorine pesticides (OCPs) was performed to 22 human milk samples and 5 infant formulas (one manufactured in Serbia and four imported). Average concentrations of PCBs and OCPs (n=22) in human milk samples were in ranges 0.094 - 0.565 ng/g and 0.15-4.74 ng/g, respectively. Concentration levels of target POPs in milk formulas were about ten times lower. Only one compound from the group of OCPs (aldrin) was found in infant formula manufactured in Serbia. Results within this study pointed out that long year environmental presence of POPs caused bioaccumulation and biomagnifications in human organisms and also mother-child transfer by human milk. These determinations in Serbia are very scarce and till now, performed only by this group of authors.

### **Koncentracioni nivoi perzistentnih organskih polutanata u biotskom materijalu u Novom Sadu, Srbija**

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U okviru Projekta FP5 APOPSBAL i Projekta koji je finansirao Sekretarijat za nauku i tehnološki razvoj Autonomne Pokrajine Vojvodine (Određivanje perzistentnih organskih polutanata u abiotskom i biotskom matriksu Južne Bačke) praćene su rezidualne količine perzistentnih organskih polutanata u humanom mleku. Humano mleko je suptilni pokazatelj kontaminacije ženske populacije i novorođenčeta kao i veoma značajan indirektni pokazatelj zagađenja životne sredine. Određivanje 7 EPA kongenera polihlorovanih bifenila (PCB) i 11 organohlorornih pesticida (OCP) je izvršeno u 22 uzorka humanog mleka i 5 uzoraka preparata mleka (jednog proizvedenog u Srbiji i 4 uvezene). Srednje vrednosti PCB-a i OCP-a (n=22) u uzorcima humanog mleka su analitički detektovane u opsezima 0.094 - 0.565 ng/g i 0.15-4.74 ng/g, redom. Koncentracioni nivoi ispitivanih perzistentnih organskih polutanata u uzorcima preparata „veštačkog“ mleka bili su oko deset puta niži od vrednosti u uzorcima humanog mleka. Samo jednasupstancija iz grupe organohlorornih pesticida (aldrin) je detektovana u preparatu mleka za odojčad proizvedenom u Srbiji. Rezultati u okviru ovog istraživanja ukazuju na dugogodišnje prisustvo POP-a u životnoj sredini koje je izazvalo bioakumulaciju i biomagnifikaciju u ljudskim organizmima kao i transfer ispitivanih jedinjenja sa majke na novorođenče preko mleka. Ovakva istraživanja su veoma osetljiva i retka i do sada sprovedena jedino od strane ove grupe autora u Srbiji.



HŽS16-P

### Određivanje odabranih pesticida u površinskim vodama

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Pesticidi su hemijska jedinjenja koja se koriste za suzbijanje štetnih insekata i bolesti biljaka, kao i za uništavanje korova u cilju očuvanja kvaliteta poljoprivrednih proizvoda i povećanja prinosa, kontrole parazita i vektora opasnih bolesti čoveka i životinja. Međutim, neselektivna, nestručna i prekomerna upotreba pesticida, nosi sa sobom potencijalne opasnosti zagađivanja životne sredine i može izazvati rizike po ljudsko zdravlje. Ova jedinjenja dospevaju u vodu spiranjem sa površine zemljišta i biljaka, direktnim putem prilikom aerotretmana, pri nepravilnoj tehnologiji prskanja i zaprašivanja, itd. Pesticidi se vremenom transportuju i transformišu fizičkim, hemijskim i biološkim procesima. Naročito često pesticidi se nagomilavaju na neprotočnim ili slabo protočnim mestima - na nereguliranim delovima reka, plitkim i močvarnim mestima, u manjim veštačkim i prirodnim jezerima.

Cilj eksperimenta bio je određivanje pesticida u površinskoj vodi iz Orašca, mesta nadomak Arandelovca, podno planine Bukulje. Uzorci su uzeti na terenu i ispitivani u laboratoriji na gasnom hromatografu. Upoređivanjem dobijenih eksperimentalnih rezultata sa Pravilnikom o opasnim materijama u vodama, došlo se do zaključka da se u uzorcima ispitivane vode ostaci pesticida nalaze u tragovima, tj. ispod maksimalno dozvoljenih koncentracija.

### Determination of selected pesticides in surface waters

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Pesticides are chemical compounds that are used to control insect pests and plant diseases and weed killers in order to preserve the quality of agricultural products and increase yields, control of parasites and vectors of infectious diseases in humans and animals. However, non-selective, improper and excessive use of pesticides, carries potential risks of environmental pollution and can cause risks to human health. These additive compounds can reach the water by erosion from the ground surface and the plants, by direct way through air treatment, under the missappropriate sprinkling/splattering and dusting technology, etc. The pesticides are being transported and transformed in the run by physical, chemical and biological processes. Especially often, the pesticides are being accumulated in places with no throughout or where throughout is very small, i.e. at unregulated river parts, shallow and mossy places, in smaller-size artificial and natural lakes. The main purpose of the experiment was pesticide specification at the surface water level from village Orasac, near Arandelovac, beneath mountain Bukulja. Samples have been collected at the territory and researched in the laboratory with gas chromatography. Comparing the received experimental data with the Rule Book on dangerous substances in waters, it has been concluded that the samples of researched water contain traces of debris of pesticides, in other words, bellow the approved maximum concentration level.



**Teorijska hemija / Theoretical Chemistry**  
**Usmena saopštenja / Oral Presentations**

TH01-O

**Aktivne konformacije  $\mu$ - i  $\delta$ -opioidnih receptora specifičnih za pojedine ligande**

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Opisano je modelovanje aktivnih konformacija  $\mu$ - i  $\delta$ -opioidnih receptora specifičnih za pojedine ligande. Polazne strukture su bile ranije publikovani modeli ovih receptora, modelovani prema kristalnoj strukturi adrenoreceptora (2RH1). Dokovanjem serije liganada u polazne modele receptora dobijene vrednosti vezivne energije nisu bile u dobroj korelaciji sa eksperimentalnim vrednostima. Optimizacijom specifičnih protein-ligand kompleksa metodom molekulske mehanike, a potom kratkom molekulsko dinamičkom simulacijom i ponovnim dokovanjem serija liganada dobijene su bolje korelacije sa eksperimentalnim vrednostima. Kvalitet korelacije je zavisio od zapremine liganada izabranog za optimizaciju. Korišćeni ligandi za  $\mu$ - receptor su bili morfijum i njegovi analozi, uključujući i neke 3-estre morfijuma, dok su za  $\delta$ - receptor korišćeni neki poznati agonisti. Primenjeno polje sila je bilo CHARMM.

**Active Ligand Specific Conformations of  $\mu$ - and  $\delta$ -Opioid Receptors**

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Modeling of active conformations of  $\mu$ - and  $\delta$ - opioid receptors will be described. Initial receptor structures, used in this work, were published earlier and were modeled based on crystal structure of adrenoreceptor (2RH1). The binding energies obtained by docking series of ligands to the initial receptor models were not in a good correlation with experimental values. After optimization of specific protein-ligand complexes using molecular mechanics, followed by short molecular dynamics simulation, and redocking the ligands, better correlations with experimental values were obtained. The quality of correlation was dependent on a volume of a ligand chosen for optimization. The ligands used for  $\mu$ - receptor were morphine, its analogues including some morphine 3-esters, while for  $\delta$ - receptor some known agonists were used. The force field applied was CHARMM.

1. D. N. Sredojević, G. A. Bogdanović, Z. D. Tomić, S. D. Zarić, *Cryst. Eng. Comm.* **9** (2007) 793-798.



TH02-O

**DFT i MM Analiza Strukture i Magnetnih Osobina Kompleksa Mangana(II) sa X-fenilcijanamidnim Mostnim Ligandom**

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Magnetne osobine kompleksa  $[\text{Mn}(3\text{-Clpcyd})(\text{H}_2\text{O})-(\text{phen})_2]^+$  (gde je Xpcyd = halogeno-fenilcijanamid; phen = 1, 10- fenantrolin),  $[\{\text{Mn}(3\text{-Fpcyd})(\text{EtOH})(\text{phen})\}_2(\mu\text{-}3\text{-Fpcyd})_2]$ ,  $[\{\text{Mn}(3\text{-Clpcyd})(\text{MeOH})(\text{phen})\}_2(\mu\text{-}3\text{-Clpcyd})_2]$ ,  $[\{\text{Mn}(4\text{-lpcyd})(\text{EtOH})(\text{phen})\}_2(\mu\text{-}4\text{-Clpcyd})_2]$ , analizirane su DFT metodom. Konstante magnetnog sprezanja ( $J$ ) izračunate su iz razlike u energijama između stanja visokog spina i broken symmetry stanja. Postignuta je dobra saglasnost između izračunatih parametara i eksperimentalno dobijenih vrednosti, opisanih u literaturi. Za geometrijsku optimizaciju mononuklearnog i četiri binuklearnih kompleksa korišćena je metoda molekulske mehanike (MM), CFF konformacioni program, sa novo razvijenim setom parametara. Verodostojnost MM rezultata potvrđena je poređenjem magnetnih osobina računatih na MM optimizovanim strukturama sa eksperimentalnim vrednostima.

**DFT and MM Description of the Structure and Magnetic Properties of Manganese Complexes with X-phenylcyanamido Bridging Ligand**

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Magnetic properties of the complexes  $[\text{Mn}(3\text{-Clpcyd})(\text{H}_2\text{O})-(\text{phen})_2]^+$  (where Xpcyd = halogeno-phenylcyanamido; phen = 1, 10- phenantrolin),  $[\{\text{Mn}(3\text{-Fpcyd})(\text{EtOH})(\text{phen})\}_2(\mu\text{-}3\text{-Fpcyd})_2]$ ,  $[\{\text{Mn}(3\text{-Clpcyd})(\text{MeOH})(\text{phen})\}_2(\mu\text{-}3\text{-Clpcyd})_2]$ ,  $[\{\text{Mn}(4\text{-lpcyd})(\text{EtOH})(\text{phen})\}_2(\mu\text{-}4\text{-Clpcyd})_2]$ , have been explored by means of DFT. Exchange coupling constants ( $J$ ) were calculated from the energy differences between the high spin and broken symmetry states. Very good agreement between theoretical and experimental data was achieved. Molecular mechanics (MM) calculations with new developed force-field have been performed to elucidate structural features in mononuclear and four binuclear complexes. Finally, the reliability of the MM results was confirmed by comparing the magnetic couplings calculated on MM optimized structures with experimental data.



TH03-O

### **Multideterminantni DFT pristup analize Jahn-Teller-ovog efekta u malim organskim radikalima**

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Po Jahn-Teller-ovoj (JT) teoremi svi nelinearni molekuli sa degenerisanim elektronskim stanjem spontano se distorguju duž vibracija koje nisu totalno simetrične, pri čemu dolazi do uklanjanja degeneracije uz sniženje energije. Korišćenjem multideterminantnog DFT pristupa, analiziran je niz JT aktivnih ugljovodoničnih prstenova,  $C_nH_n$  ( $n= 5-7$ ) i izračunati su JT parametri. Problem uticaja većeg broja JT aktivnih vibracija rešen je pomoću Intrinsic Distortion Path (IDP) metoda, gde JT distorzija može biti izražena kao linearna kombinacija svih totalno simetričnih normalnih vibracija u strukturi niže simetrije. Rezultati dobijeni na osnovu oba metoda su konzistentni, komplementarni, i u dobroj saglasnosti sa eksperimentalnim i teorijskim vrednostima, objavljenim u literaturi. Ovo je značajno jer je eksperimentalno određivanje JT parametara teško i često neprecizno, a detaljniji uvid u vibronsku spregu daje i metod dekompozicije energije.

### **Multideterminantal DFT Approach in Analysis of Jahn-Teller Effect in Small Organic Radicals**

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The Jahn-Teller (JT) theorem states that a molecule with a degenerate electronic state spontaneously distorts along a non-totally symmetric vibrational coordinates. This removes the degeneracy and lowers the energy. Family of the Jahn-Teller active hydrocarbon rings,  $C_nH_n$  ( $n= 5-7$ ), was analysed by the means of multideterminantal DFT, which can be applied for the calculation of the JT parameters. The multimode problem was solved with the Intrinsic Distortion Path (IDP) method, in which the JT distortion can be expressed as a linear combination of all totally symmetric normal modes in the low symmetry minimum energy conformation. The results obtained by both methods are consistent, complement each other, and are in a good agreement with experimental and theoretical values reported in the literature. This is of interest because experimental determination of JT parameters is often very difficult, and there is uncertainty in the values. Partitioning of the energy has been performed in order to get further chemical insight into the coupling of the nuclear movements and the electron distribution.





TH04-O

**Ispitivanje interakcija nesteroidnih anti-inflamatornih lekova (NSAID) sa ciklooksigenazama, metodama molekulske dinamike**

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Ciklooksigenaze su jedan od najvažnijih enzima u organizmu, i igraju bitnu ulogu u metabolizmu prostaglandina. Od otkrića nesteroidnih anti-inflamatornih lekova, kao što su aspirin i ibuprofen, do danas se pokazalo da skoro svi deluju putem inhibicije ciklooksigenaza. Isti ti lekovi su pokazali i mnoge toksične efekte koji su takođe vezani za inhibiciju ciklooksigenaza. Cilj ovog rada je da se molekulsko-dinamičkim modelovanjem interakcija nesteroidnih anti-inflamatornih lekova sa modelom ciklooksigenaze objasne njihovi poželjni i toksički efekti.

**Study of interactions between nonsteroid anti-inflammatory drugs (NSAID) with cyclooxygenase, using molecular-dynamics**

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Cyclooxygenases are one of the most important enzymes in our bodies, and they play a vital roll in the metabolism of prostaglandin. Since the discovery of nonsteroid anti-inflammatory drugs (NSAID), such as aspirin and ibuprofen it has been shown that their effects rest on the inhibition of the cyclooxygenases. Those same drugs have shown toxic effects that have also been linked to the inhibition of the cyclooxygenases. The goal of this research is to shed light on the causes of those beneficial and toxic effects by studying the interactions between nonsteroid anti-inflammatory drugs (NSAID) with cyclooxygenase, using molecular-dynamics.



TH05-O

### Teorijsko proučavanje O-H/ $\pi$ interakcija između koordinovanog i nekoordinovanog molekula vode i C<sub>6</sub>-aromatičnog prstena

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U ovom radu proučavane su intermolekulske interakcije između molekula vode, nekoordinovanog (OH/ $\pi$  interakcije) i koordinovanog (MLOH/ $\pi$  interakcije) i C<sub>6</sub>-aromatičnog prstena. Statistička analiza interakcija temelji se na kristalnim strukturama pohranjenim u Kembričkoj banci podataka. Rezultati ukazuju da su interakcije koordinovanog molekula vode jače od interakcija nekoordinovanog molekula. Ovi podaci pokazuju da se koordinovana voda nalazi na kraćim H $\cdots$  $\Omega$  rastojanjima, gde je  $\Omega$  centar C<sub>6</sub>-aromatičnog prstena. Primećeno je da su kod MLOH/ $\pi$  interakcija H $\cdots$  $\Omega$  rastojanja kraća za pozitivno naelektrisane akva komplekse. DFT proračuni su urađeni na model sistemima. Proračuni su dali dobro slaganje sa geometrijskom analizom i pokazuju da je energija veća za koordinovan molekul vode. Prema rezultatima DFT proračuna, energije najstabilnijih MLOH/ $\pi$  orijentacija između koordinovanog molekula vode i aromatičnog prstena imaju vrednosti od -4.9 kcal/mol za neutralne komplekse, do -12.5 kcal/mol za pozitivno naelektrisane akva komplekse. Izračunata energija OH/ $\pi$  interakcija između nekoordinovanog molekula vode i aromatičnog prstena iznosi -1.5 kcal/mol.

### Theoretical study of O-H/ $\pi$ interactions between coordinated and non-coordinated water molecule with C<sub>6</sub>-aromatic ring

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In this study, intermolecular interactions of coordinated (OH/ $\pi$  interactions) and non-coordinated (MLOH/ $\pi$  interactions) water molecule, with C<sub>6</sub>-aromatic rings were studied. Statistical analysis of interactions was based on crystal structures archived in Cambridge Structural Database. Results indicated that interactions of coordinated water molecule are stronger than interactions of non-coordinated molecule. These data shows that coordinated water molecule have a tendency to make shorter H $\cdots$  $\Omega$  distances, where  $\Omega$  is centre of C<sub>6</sub>-aromatic ring. It was observed that for the MLOH/ $\pi$  interactions, the H $\cdots$  $\Omega$  distances are shorter with positive charged aqua complexes. DFT calculations were performed on model system. DFT calculations were in very good agreement with geometrical analysis of crystallographic data and shows that energy is higher for coordinated water molecule. Based on the results of the DFT calculations, the energy of the most stable MLOH/ $\pi$  orientation between the aqua ligand and the aromatic ring can be estimated to be -4.9 kcal/mol, for neutral complex, and -12.5 kcal/mol, for positive aqua complex. The energy of the OH/ $\pi$  interaction calculated for a non-coordinated water molecule and the aromatic ring is -1.5 kcal/mol.



**Biohemija / Biochemistry**  
**Usmena saopštenja / Oral Presentations**

**BH01-O**



**Poređenje kolorimetrijskog i masenospektrometrijskog eseja za određivanje aktivnosti pankreasne fosfolipaze A<sub>2</sub>**

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Fosfolipaza A<sub>2</sub> pripada velikoj grupi enzima koji igraju važnu ulogu u procesima vezanim za ćelijski membranski sistem i transdukciju signala u ćeliji. Postoji nekoliko eseja za određivanje aktivnosti fosfolipaze A<sub>2</sub>, koji se razlikuju po osetljivosti, jednostavnosti i vremenu potrebnom za izvođenje. Glavni nedostatak većine eseja je što podrazumevaju hromogeno ili radioaktivno obeležavanje supstrata, što utiče na enzimsku aktivnost i skupo je. S druge strane, masena spektrometrija je interesantan metod za određivanje aktivnosti fosfolipaze A<sub>2</sub>, jer ne zahteva obeležavanje supstrata, omogućava brzu i jednostavnu analizu i određivanje kinetičkih parametara upotrebom odgovarajućeg unutrašnjeg standarda. U ovom radu, predstavljene su prednosti MALDI TOF MS eseja u odnosu na kolorimetrijski esej fosfolipaze A<sub>2</sub>.

**Comparison of colorimetric and mass spectrometric assays to determine the activity of pancreatic phospholipase A<sub>2</sub>**

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Phospholipase A<sub>2</sub> belongs to very large class of enzymes with the important role in cell membrane systems. Several activity assays are established, differing in sensitivity, simplicity and duration of experiment. The main problem is that most assays require chromogenic or radioactive labelling of substrate which can affect the enzyme activity and is not cost-effective. On the other hand, mass spectrometry is rather attractive method for determining phospholipase A<sub>2</sub> activity, since it does not require substrate labelling, it is not time consuming, it is easy to perform and enables determination of kinetic parameters, using suitable internal standard. In this work, advantages of MALDI TOF MS assay in comparison to colorimetric assay of phospholipase A<sub>2</sub> are described.





### Modelovanje druge ekstracelularne petlje dopaminskog D2 receptora

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Druga ekstracelularna petlja dopaminskog D2 receptora je esencijalni deo vezivnog mesta receptora. Da bi sa gornje strane ograničila vezivno mesto receptora, ona mora da se savije nadole, i orijentiše ka transmembranskom domenu dopaminskog receptora. U ovom radu opisan je proces modelovanja druge ekstracelularne petlje dopaminskog D2 receptora i njene interakcije sa arilpiperazinskim ligandima. Model receptora je modelovan uz pomoć Accelrys Discovery Studio paketa programa. Predloženi model je testiran doking analizom, literaturno dostupnih liganada, i poređenjem dobijenih rezultata sa njihovim afinitetom vezivanja za D2 receptor. Određeni su amino-kiselinski ostaci, koji stupaju u interakcije sa ligandima. Ključne interakcije su definisane i upoređene sa afinitetima liganada ka receptoru, kako bi se predloženim modelom objasnile razlike u eksperimentalnim rezultatima. Naša istraživanja su pokazala da druga ekstracelularna petlja dopaminskog D2 receptora, može stupati u različite interakcije sa arilpiperazinskim ligandima koje između ostalih uključuju hidrofobne, aromatične interakcije, ali i vodnonične veze. Ova saznanja, u kombinaciji sa predloženim modelom D2 receptora, koji uključuje ekstracelularne petlje, može biti od velike koristi prilikom budućeg dizajna novih dopaminergičkih liganada.

### Modeling Dopamine D2 Receptor Second Extracellular Loop

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Second extracellular loop (ecl2) of dopamine (DA) D2 receptor is an essential part of the dopaminergic ligands' binding pocket. In order to be a part of the ligand binding surface it has to fold down into the transmembrane domain of the DA receptor. The current study describes modeling of the D2 DA receptor ecl2 and its interactions with arylpiperazine ligands.

In order to model the D2 DA receptor ecl2, a number of arylpiperazine ligands were used to propose the pharmacophore model. The D2 DA receptor ecl2 model was built using Accelrys Discovery Studio. To test the proposed model, docking analysis was performed and key amino acid residues determined. Proposed receptor-ligand interactions were rationalized and compared with measured binding affinity. Our findings show that the D2 DA receptor ecl2 can form a number of interactions - aromatic, hydrophobic and polar. The ligand D2 DA ecl2 interactions are essential for G protein-coupled receptors (GPCRs) molecular modeling and put forward new data that could facilitate the design of novel drugs.





### Termodinamička analiza razvijanja izoformi eksterne invertaze

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Termodinamički parametri ( $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $T\Delta S^\circ$ ,  $\Delta C_p^\circ$ ) razvijanja nedavno izolovanih izoformi eksterne invertaze izračunati su simultanom (globalnom) termodinamičkom analizom kriva razvijanja izoformi indukovanog gvanidinium-hloridom. Krive razvijanja merene za svaku izoformu na različitim temperaturama opisane su reverzibilnim modelom dva stanja. Rezultati pokazuju da izoforme imaju različite termodinamičke parametre razvijanja. Pokazali smo da su termodinamički parametri u korelaciji sa gustinom negativnog naelektrisanja na površini nativnih izoformi, koja raste redom  $\text{EINV1} < \text{EINV2} < \text{EINV3} < \text{EINV4}$ . Termodinamička stabilnost izoformi na fiziološkim temperaturama prati isti redosled, dok na temperaturama iznad 50 °C ovaj redosled je suprotan  $\text{EINV1} > \text{EINV2} > \text{EINV3} \approx \text{EINV4}$ . Kvasac *S. cerevisiae* sintetizuje smešu izoformi eksterne invertaze, u cilju poboljšanja efikasnosti industrijskih procesa potrebno je izolovati najstabilniju izoformu EINV1 za primenu na temperaturama iznad 50 °C.

### Thermodynamic analysis of unfolding of external invertase isoforms

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Thermodynamic parameters ( $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $T\Delta S^\circ$ ,  $\Delta C_p^\circ$ ) were calculated by simultaneous (global) thermodynamic analysis of guanidinium chloride induced unfolding of four, recently isolated, external invertase isoforms. The resulting unfolding curves measured for each isoform at different temperatures were described by a reversible two-state model. Obtained thermodynamic parameters are different for different isoforms. We demonstrate that they correlate with surface charge density of the native isoforms which follows the order  $\text{EINV1} < \text{EINV2} < \text{EINV3} < \text{EINV4}$ . Thermodynamic stability of the isoforms at physiological temperatures follows the same order while above 50 °C the order is the opposite  $\text{EINV1} > \text{EINV2} > \text{EINV3} \approx \text{EINV4}$ . Yeast *S. cerevisiae* synthesizes mixture of external invertase isoforms, improving efficiency of industry processes would require isolation of most stable isoform EINV1 for application at temperatures above 50 °C.



BH04-O

### Oksidativni status biljaka pšenice nakon tretmana holnom kiselinom

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Cilj ovog rada je bio ispitivanje efekta tretmana različitim koncentracijama holne kiseline na oksidativni status mladih biljaka pšenice. Mlade biljke pšenice su uzgajane hidroponski dve nedelje a zatim tretirane dodavanjem holne kiseline u hranjivi rastvor u koncentracijama 20, 40, 60 i 80 mg/dm<sup>3</sup>. Kontrola je bila bez dodatka holne kiseline. Folijarno tretiranje je izvršeno rastvorima holne kiseline koncentracije 40 i 80 mg/dm<sup>3</sup>. Nedelju dana nakon tretmana određeni su sledeći parametri oksidativnog statusa u listovima i korenu biljaka: količina hidroksil radikala (OH) i glutationa (GSH), sadržaj rastvorljivih proteina, lipidna peroksidacija (LP) kao i aktivnost enzima glutation peroksidaze (GSH-Px). Tretman holnom kiselinom doveo je do smanjenja intenziteta LP kao i količine OH radikala i GSH. Prilikom tretmana holnom kiselinom dolazi do smanjenja aktivnosti GSH-Px, sem u listu pšenice kod većih koncentracija holata (60 i 80 mg/dm<sup>3</sup>). Utvrđeno je takodje i blago povećanje sadržaja rastvorljivih proteina, a naročito pri većim koncentracijama i kod folijarnog tretmana. Na osnovu svih dobijenih rezultata može se zaključiti da tretmani holnom kiselinom imaju antioksidantni efekat na pšenicu što se manifestuje smanjenjem količine HO• radikala i intenziteta LP.

### Oxidative status of wheat plants after treatment with cholic acid

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The aim of this work was to study the effect of treatments with different concentrations of cholic acid on oxidative status of young wheat plants. Young wheat plants grown hydroponically for two weeks were treated by adding cholic acid in nutrient solution at concentrations 20, 40, 60 and 80 mg/L. Foliar treatments were carried out by spraying plants with solutions of cholic acid with concentrations of 40 and 80 mg/dm<sup>3</sup>. Control was without addition of cholic acid. After one week several parameters of oxidative status were determined in leaves and roots of plants: quantities of hydroxyl radicals (OH) and glutathione (GSH), soluble protein content, lipid peroxidation (LP) and glutathione-peroxidase activity (GSH-Px) activity. Cholic acid treatments decreased LP intensity, OH and GSH quantities. The treatment with cholic acid also decreased GSH-Px activity, except in leafs of plants treated by higher cholate concentrations (60 and 80 mg/dm<sup>3</sup>). Mild increase of soluble protein content, especially by higher cholate concentrations and by foliar treatments, was established. On the basis of the obtained results, it can be concluded that treatments with cholic acid had antioxidant effects on wheat, which is manifested by reducing the amount of HO• radicals and the intensity of LP.



BH05-O

**Novi antimikrobni fenolni abietanski diterpen iz biljne vrste  
*Lycopus europaeus* L. (Lamiaceae)**

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Novi diacilovani, polioksigenovani diterpen abietanskog skeleta je izolovan iz semena biljne vrste *Lycopus europaeus* L. (Lamiaceae). Struktura ovog diterpena, koji je nazvan euroabienol, je određena na osnovu detaljne spektralne i hemijske analize. Prisustvo fenolnog prstena C, sa veoma retkim šablonom oksigenacije u strukturi euroabienola, kao i njegov relativno visok sadržaj u semenu (oko 1%, u odnosu na masu semena), naveli su nas da pokušamo da odredimo njegovu moguću biološku ulogu. Stoga je ispitana *in vitro* mikrobiološka aktivnost euroabienola protiv petnaest sojeva bakterija i šest sojeva gljivica. Euroabienol je pokazao veoma širok spektar antimikrobnog dejstva, pa bi se mogao smatrati sekundarnim metabolitom koji učestvuje u primarnoj odbrambenoj reakciji biljke na napad patogena. Hemotaksonomski gledano, važno je istaći da je euroabienol prvi diterpen abietanskog skeleta nađen u rodu *Lycopus*.

**A new antimicrobial phenolic abietane diterpene from  
*Lycopus europaeus* L. (Lamiaceae)**

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A new acetylated highly oxygenated abietane-type diterpenoid named euroabienol was isolated in pure state from *Lycopus europaeus* L. (Lamiaceae) fruits and its structure elucidated through both extensive spectral and chemical means. The presence of a phenolic C ring with a rare substitution pattern in euroabienol and its high relative amount in the fruits (1%, based on the weight of the fruits) urged us to try to establish its possible biological role. Thus, it was screened for its *in vitro* antimicrobial activity against fifteen strains of bacteria and six fungal strains. Euroabienol showed a broad spectrum of activity and probably is a first line defense plant metabolite against pathogen attack. This is the first report on the occurrence of abietanes in the genus *Lycopus*.





BH06-O

**Identifikacija izopropil-*N*-metilantranilata, novog alkaloida sa analgetskom aktivnošću, u etarskom ulju biljne vrste *Choisia ternata* Kunth**

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Detaljnou analizom hemijskog sastava etarskog ulja biljne vrste *Choisia ternata* Kunth (Rutaceae) metodama GC i GC-MS identifikovano je ukupno 157 komponenata i utvrđeno prisustvo jedinjenja (u tragovima) za koje je pretpostavljeno da je izopropil-*N*-metilantranilat (**1**). Izopropil-*N*-metilantranilat je sintetisan (ukupan prinos 43%) u cilju potvrde identiteta navedenog biljnog sastojka i dobijanja gramskih količina radi testiranja biološke aktivnosti (centralne i periferne analgetske aktivnosti). GC koinjektiranjem sintetisanog jedinjenja sa etarskim uljem biljne vrste *C. ternata* dokazano je njegovo prisustvo u ulju. Metil-*N*-metilantranilat (**2**, prinos 76%), koji je, takođe, detektovan u etarskom ulju *C. ternata*, kao i propil-*N*-metilantranilat (**3**, prinos 43%) sintetisani su na analogan način. Svi sintetisani estri *N*-metilantranilne kiseline su spektralno okarakterisani (MS, IR, 1D i 2D – NMR) čime su potvrđene njihove strukture. Rezultati testiranja analgetske aktivnosti ovih estara (**1-3**) je ukazalo na postojanje značajne doza-zavisne aktivnosti (čak i pri dozi 0,3 mg/kg) ovih jedinjenja. Izopropil-*N*-metilantranilat je pokazao najveću, a metil-*N*-metilantranilat najmanju aktivnost.

**Identification of a new antinociceptive alkaloid isopropyl *N*-methyl-anthranilate from the essential oil of *Choisia ternata* Kunth (Rutaceae)**

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Detailed GC and GC-MS analyses of the essential oil of *Choisia ternata* Kunth (Rutaceae) revealed, among 157 other volatiles, the presence of a minor constituent tentatively identified as isopropyl *N*-methylantranilate (**1**). A synthesis of **1** (total yield 43%) was undertaken in order to corroborate this assumption and obtain gram quantities that would allow the testing of its biological activity (peripheral and central antinociceptive activity). Co-injection of the obtained synthetic compound with the essential oil sample of *C. ternata* confirmed the compound's identity. Methyl *N*-methylantranilate (**2**, yield 76%), that was also detected in the oil of *C. ternata*, as well as propyl *N*-methylantranilate (**3**, total yield 50%) were likewise synthesized. All of the synthesized compounds were spectrally characterized (MS, IR, 1D and 2D – NMR, <sup>1</sup>H and <sup>13</sup>C), which provided conclusive proof of their structures. Compounds **1-3**, were assayed for peripheral and central analgesic activities. The results clearly demonstrate a very high (even significant at 0.3 mg/kg) dose dependent activity for the anthranilates. Isopropyl *N*-methylantranilate showed the highest, while methyl *N*-methylantranilate showed the lowest activity.



BH 07

**Uticaj pH i koncentracije glicerola na karakteristike biorazgradivih filmova od proteinskog izolata uljane tikve golice**

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U ovom radu praćen je uticaj pH i koncentracije glicerola na osobine biorazgradivih filmova dobijenih od proteinskog izolata (PI) uljane tikve golice (*Cucurbita pepo*). Efekat pH i koncentracije glicerola ocenjen je merenjem mehaničkih (zatezna jačina – ZJ i izduženje pri kidanju – IK), hemijskih (sadržaj vlage, rastvorljivost, antioksidativna aktivnost) i barijernih osobina (propustljivost gasova). Praćeno je formiranje filmova na pH=2-12, pri koncentraciji glicerola od 0,4 i 0,5g/g PI. Rezultati pokazuju da se filmovi formiraju na svim pH, sem u opsegu pH=4-8. PI Dobijeni rezultati ukazuju da pH značajno utiče na osobine dobijenih filmova, a koncentracija glicerola značajno utiče ( $p<0.05$ ) na ZJ, IK i rastvorljivost. Film sa najvećom ZJ (6.56 MPa) dobijen je pri pH=11, kada je dodato 0.4g glicerola/g PI. Povećanjem količine glicerola, smanjila se ZJ. Izduženje pri kidanju je bilo najbolje (196,61%) kod filma dobijenog pri pH=12, a sa povećanjem količine glicerola, povećava se vrednost IK. Najveća rastvorljivost bila je kod filmova pripremanih u kiseloj sredini (>79%), pri količini glicerola od 0,5g/g PI. Filmovi sa najvećim sadržajem vlage i najvećom antioksidantnom aktivnošću su dobijeni kada je pH>10. Propustljivost gasova dobijenih filmova ukazuje na odlična barijerna svojstva prema O<sub>2</sub>, N<sub>2</sub> i CO<sub>2</sub>.

**Effects of pH and glycerol concentration on the properties of pumpkin oil cake protein isolate biodegradable films**

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Pumpkin oil cake protein isolate (PI) biodegradable films were prepared and pH and glycerol concentration effect on these films were studied by measuring mechanical (tensile strength - TS, and elongation at break – EB), chemical (moisture content, solubility and antioxidant activity) and barrier characteristics (gas permeability) of obtained films. The PI film-forming ability was evaluated at pH=2-12, while glycerol concentration was 0.4 and 0.5g/g PI. Results showed that films could not be formed at pH=4-8, while showed film-forming ability at other examined pH. Obtained results indicate that pH affected all tested characteristics, while glycerol concentration had significant effect ( $p<0.05$ ) only on TS, EB and solubility. The best TS (6.56 MPa) has film made at pH=11, and when 0.4g glycerol/g PI was used. Increasing glycerol amount, TS decreased. Elongation at break was the best (196.61%) for film prepared at pH=12, and EB values increased with increase of glycerol concentration. The highest solubility have film made at acidic pH, and it was over 79%, when glycerol concentration was 0.5g/g PI, while moisture content, and antioxidant activity was the best for film prepared at pH>10. Gas permeability of obtained films showed that PI films present excellent barrier for O<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>.



Postarska saopštenja / Poster Presentations

BH08-P

**Karakterizacija glavnih proteina mleka različitog porekla elektroforezom korišćenjem Tris pufera visokog molariteta**

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Upotreba natrijum-dodecil-sulfat-poliakrilamidne gel elektroforeze (SDS-PAGE) za karakterizaciju proteina mleka različitog porekla je dobro poznata laboratorijska procedura. Najcitiranija SDS-PAGE procedura je po Laemmli-u. Korišćenjem ovog postupka ne uočavaju se razlike u proteinskim profilima različitih vrsta mleka. Primenom modifikovanog protokola, koju su predložili Fling i Gregerson (1984), razlike u proteinskim profilima kozjeg, kravljeg i ovčijeg mleka postaju uočljive. Dvostrukim povećanjem molariteta Tris-a u elektrodnom puferu i gelu za odvajanje, postignuta je bolja definisanost proteinskih traka, njihova rezolucija i detekcija glavnih proteina mleka.

U ovom radu primenili smo modifikovanu tehniku i pokazali značajne razlike u elektroforetskom ponašanju  $\kappa$ -kazeina i parak-kazeina analiziranih mleka. Redosled  $\kappa$ -kazeina prema rastućoj pokretljivosti u gelu bio je: kravljji  $\kappa$ -kazein, kozji  $\kappa$ -kazein i ovčiji  $\kappa$ -kazein. U slučaju para  $\kappa$ -kazeina redosled je bio: kozji parak-kazein, ovčiji parak-kazein i kravljji parak-kazein. Poznato je da je parak-kazein protein koji ne pokazuje proteolitičke promene tokom zrenja sireva. Zato upotreba ove procedure može biti vrlo efikasna za utvrđivanje autentičnosti mleka upotrebljenog za njihovu proizvodnju.

**Characterisation of major milk proteins from different species by electrophoresis using a high-molarity Tris buffer**

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The use of sodium dodecyl sulfate-polyacrilamide gel electrophoresis (SDS-PAGE) for the characterisation of milk proteins has become a firmly established laboratory procedure. The most widely cited SDS-PAGE procedure is Laemmli procedure. Using this procedure no differences among protein profiles of different milk species was observed. Using the modified protocol, proposed by Fling and Gregerson (1984), the differences among protein profiles of bovine, caprine and ovine milk, could be detected. Increasing the molarity of Tris in the resolving gel and running buffer twofold over the Laemmli concentrations, yielded superior banding, resolution and detection of major milk proteins.

In this study we applied the modified technique and approved significant differences among electrophoretic properties of  $\kappa$ -caseins and parak-caseins of different species. The order of  $\kappa$ -caseins in electrophoretic gel according to increasing mobility was: bovine  $\kappa$ -casein, caprine  $\kappa$ -casein and ovine  $\kappa$ -casein. In the case of parak-caseins, the order was: caprine parak-casein, ovine parak-casein and bovine parak-casein. It is known that parak-casein is protein which does not show proteolytic changes during the cheeses ripening. Thus, the application of this procedure could be very effective in estimating the authenticity of milk species used for their production.



BH09-P

### Ispitivanje mikrobiološke aktivnosti cinamil derivata arilpiperazina

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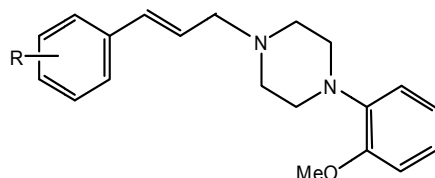
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S obzirom na to da i derivati cimetine kiseline i *N*-aril derivati piperazina pokazuju antibakterijsku aktivnost<sup>1,2</sup>, cilj ovog rada bio je proučavanje potencijalne aktivnosti cinamil derivata arilpiperazina na izabrane sojeve bakterija.

Dobijenim derivatima **1-9**, sintetisanim po ranije objavljenoj proceduri<sup>3</sup>, određene su: minimalne inhibitorne koncentracije na Gram pozitivne bakterije *Bacillus subtilis*, *Clostridium sporogenes*, *Enterococcus* sp., *Micrococcus flavus*, *Sarcina lutea* i *Staphylococcus aureus* i Gram negativne bakterije *Proteus vulgaris*, *Pseudomonas aeruginosa*, *Salmonella enteritidis* i *Escherichia coli* kao i toksičnost na račice *Artemia salina*.



R: **1**=H, **2**=2-OCH<sub>3</sub>, **3**=3-OCH<sub>3</sub>,

**4**=4-OCH<sub>3</sub>, **5**=2-NO<sub>2</sub>, **6**=3-NO<sub>2</sub>,

**7**=4-NO<sub>2</sub>, **8**=2-Cl, **9**=3-Cl

### Antibacterial activity of *N*-cinnamyl-aryl piperazines

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Since both the derivatives of cinnamic acid and *N*-aryl piperazine show antibacterial activity<sup>1,2</sup>, the objective of this study was to examine the potential activity of cinnamyl derivatives of arylpiperazine against selected bacteria.

For a chosen set of derivatives **1-9**, synthesized by a previously published method<sup>3</sup>, we determined: the minimum inhibitory concentration for Gram positive: *Bacillus subtilis*, *Clostridium sporogenes*, *Enterococcus* sp., *Micrococcus flavus*, *Sarcina lutea* and *Staphylococcus aureus* and Gram negative bacteria: *Proteus vulgaris*, *Pseudomonas aeruginosa*, *Salmonella enteritidis* and *Escherichia coli* and the toxicity against the nauplii of *Artemia salina*.

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BH10-P

### Uticaj varijeteta i proizvodnog procesa na sadržaj proteina u sojinom mleku

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Prinos i kvalitet sojinog mleka zavisi od nekoliko faktora: način proizvodnje, uslovi gajenja sojinog zrna i sorte soje. Tradicionalno pripremljeno sojino mleko ima tzv. leguminozni miris i ukus. Kada se u pripremi sojinog mleka primenjuje kuvanje sojinog zrna uz ubacivanje vodene pare pod pritiskom, poznato kao hidrotermičko kuvanje (HTC), mleko ima manje izraženu nepovoljnu aromu. Sojino mleko je pripremljeno od 6 domaćih sorti soje HTC-postupkom. Sagledani su efekti varijeteta i primenjenih uslova proizvodnje na sadržaj i sastav glavnih rezervnih proteina sojinog mleka. Različiti varijeteti soje imaju različite sastave proteinskih frakcija u zrnu i mleku. Pomoću SDS-PAGE (sodium dodecyl sulfate polyacrylamide gel electrophoresis) je utvrđeno prisustvo  $\beta$ -konglicinina, glicinina i njihovih podjedinica u sojinom mleku ( $\alpha' + \alpha = 8,11-10,24\%$ ;  $\beta + \beta' = 2,56-3,85\%$  - podjedinice  $\beta$ -konglicinina; kiseli =  $35,21-43,52\%$  i bazni =  $8,52-10,97\%$  glicininski polipeptidi). Kod svih ispitivanih sorti vrednost iskoristivosti proteina u toku pripreme sojinog mleka bila je oko 80-96%, što je pokazatelj efikasnosti ekstrakcije proteina u primenjenom postupku proizvodnje. Primenjena istraživanja mogu biti korisna u budućem radu na poboljšanju kvaliteta hrane biljnog porekla.

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### Varietal and processing method effects on soymilk proteins content

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Yield and quality of soymilk are affected by several factors, such as soymilk-processing methods, soybean growth environment and variety. Traditionally prepared soymilk has painty and beany flavor. Soymilk produced by a steam-infusion cooking process, known as hydrothermal cooking (HTC), has a less beany flavor. In this work, soymilk samples were made from six Serbian soybean genotypes by HTC-process. This was undertaken to estimate the effects of soybean genotype and processing conditions on the composition of major soymilk proteins. Soybean varieties had different storage protein compositions in beans and milk. SDS-PAGE separated  $\beta$ -conglycinin and glycinin in soymilk ( $\alpha' + \alpha = 8.11-10.24\%$ ;  $\beta + \beta' = 2.56-3.85\%$   $\beta$ -conglycinin subunits; acidic =  $35.21-43.52\%$  and basic =  $8.52-10.97\%$  glycinin polypeptides). The examined genotypes are characterized by relatively high total protein content in beans and respective milks. For all soybean varieties, there was approximately a 80-96% recovery in protein content during the preparation of soymilk. This would be an indication of the processing method efficiency of the protein extraction. The results of this study may improve the quality of processed vegetarian foods. The study was financed by the Serbian ministry of Science and Technological Development (Project TR 31022).



BH11-P

**Termalna stabilnost konjugata polienskog antibiotika sa polisaharidom**

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Polienski makrolidni antibiotici su veoma efikasni u medicinskom tretmanu mikoza koje izazivaju patogene gljive, kao što su vrste rodova *Candida* i *Aspergillus*. U cilju smanjenja toksičnosti ovih antibiotika i povećavanja njihove rastvorljivosti na fiziološkim pH-vrednostima, sintetizovani su konjugati sa oksidovanim polisaharidima rastvornim u vodi. Imino polimeri polienskog makrolidnog antibiotika nistatina i oksidovane gumiarabike dobijeni su formiranjem struktura Schiff-ovih baza, posle čega su redukovani u stabilnije alkilamine reakcijom sa natrijum-borhidridom. Sintetizovana jedinjenja su ispitana termogravimetrijskom analizom u odnosu na polienski antibiotik, nativni polisaharid i uzorke oksidovane gumiarabike.

Utvrđeno je da sintetizovani konjugati pokazuju bolju termalnu stabilnost u odnosu na polazna jedinjenja kao i na oksidovani polisaharid. Ove razlike se mogu objasniti otvaranjem pojedinih heksopiranoznih prstenova šećera u toku oksidacije, čime je omogućena slobodnija rotacija oko  $\beta$ -glikozidnih veza polisaharidnog niza.

**Conjugates of Polyene Antibiotic with Polysaccharide - Thermal Stability**

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Polyene macrolide antibiotics are very efficient agents in medical treatment of mycoses caused by pathogenic fungi, such as *Candida* and *Aspergillus*. With the aim of reducing toxicity of these antibiotics and increasing their solubility at the physiological pH-values, conjugates with oxydized polysaccharides soluble in water were synthesized. Imino polymers of the polyene macrolid antibiotic nystatine and oxidized gum arabic were obtained by forming of the Schiff bases structures, after which they were reduced in stable alkylamines by reaction with sodium borohydride. Synthesized compounds were examined by thermogravimetric analysis, in regards to pure polyene antibiotic, native polysaccharide and samples of the oxidized gum arabic.

It was found that synthesized conjugates showed better thermal stability compared to starting compounds and oxidized polysaccharide. These differences could be explained by the opening of some of the polysaccharide hexopyranose rings during the oxidation, which enabled free rotation around  $\beta$ -glycosidic linkages of the polysaccharide chain.



BH12-P

### **Najčešći isparljivi kontaminanti etarskih ulja i biljnih ekstrakata uvedeni u toku izolovanja: brzo i lako profilisanje**

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Kako bi se utvrdio identitet i skrenula pažnja na neke od najčešćih isparljivih kontaminantata etarskih ulja (EO) i biljnih ekstrakata (PE), uvedenih u toku izolovanja, vršene su GC i GC-MS analize ostataka nakon isparavanja šest komercijalnih dietil-etara (rutinski korišćeni rastvarač u hemiji prirodnih proizvoda) i hidrodestilata plastične mase. Skoro 200 jedinjenja, koja se mogu podeliti u dve grupe, je identifikovano u 7 tipova analiziranih uzoraka. Prvu grupu su sačinjavala široko upotrebljavana sintetička jedinjenja (npr. butilovani hidroksitoluen, estri ftalne kiseline, neki uobičajeni plastifikatori i sl.). Ova jedinjenja treba ili izostaviti iz konačnih lista EO/PE sastojaka, ili ih treba jasno označiti kao kontaminante. U drugu grupu su svrstana jedinjenja koja mogu biti sintetskog i/ili prirodnog (biljnog) porekla: jedinjenja izvedena iz metabolizma masnih kiselina, proizvodi anaerobne intracelularne/mikrobne fermentacije (npr. izomerni 2,3-butandiol), i sl. Pri navođenju nekog od ovih jedinjenja kao EO/PE sastojaka treba biti posebno obazriv, a najbolje bi bilo utvrditi da li je dati sastojak prisutan u rastvaraču(ima) korišćenom(im) za izolovanje EO/PE smeše. Brzo i jednostavno profilisanje rastvarača se može izvršiti pomoću odgovarajućeg usrednjenog masenog skena ukupnog joskog hromatograma.

### **The most frequently encountered volatile contaminants of essential oils and plant extracts introduced during the isolation procedure: fast and easy profiling**

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In order to explore and point out to some of the most common volatile anthropogenic contaminants of essential oils (EO) and plant extracts (PE), detailed GC and GC-MS analyses of the evaporation residues of six commercially available diethyl ethers (routinely used solvent in natural product chemistry) and of a plastic bag hydrodistillate were performed. Almost 200 different compounds were identified in the seven types of analyzed samples. These compounds could be generally divided into two groups. The first group was comprised of those constituents that could only be of a synthetic/artificial origin (e.g. butylated hydroxytoluene, phthalic acid esters and some other usual plasticizers, etc.). Such compounds should be omitted from the final list of EO/PE constituents, or should be clearly designated as potential contaminants. Members of the second group were constituents that could be of both synthetic and/or natural (plant) origin: compounds derived from the fatty acid metabolism or products of anaerobic intracellular (or microbial) fermentation (e.g. the isomeric 2,3-butandiol). Identification of some of these compounds as EO/PE constituents should be taken with caution. In such cases, solvent(s) used for the EO/PE isolation should be screened for the presence of certain EO/PE constituents. A fast and easy way for such screening of solvents could be done using their average mass scans of the total ion chromatograms (AMS profiles).





BH13-P

**Antioksidantne osobine ekstrakata *Marrubium peregrinum* L. (Lamiaceae)**

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Antioksidantna aktivnost metanolnog ekstrakta biljke *Marrubium peregrinum*, akupljene sa tri različite lokacije (Backo Gradiste - Rimski Sanac, Novi Kneževac i Senta) je ispitana određivanjem slobodno-radikalnog kapaciteta (RSC), kao i efekta na lipidnu peroksidaciju (LP). RSC je određen merenjem „scavenging“ aktivnosti metanolnog ekstrakta na 2,2-difenil-1-pikrilhidrazil (DPPH<sup>•</sup>), super oksid anjon (O<sub>2</sub><sup>•-</sup>), NO<sup>•</sup> i OH<sup>•</sup> radikala. Efekat na LP je procenjen praćenjem aktivnosti etarskih ulja u Fe<sup>2+</sup>/askorbat sistemu indukcije. Biljni materijal je osušen na vazduhu i samleven u mikseru. Radi dobijanja biljnih ekstrakata izvršena je maceracija (ekstrakcija na hladno) na sledeći način: 200 g biljnog materijala je potopljeno u 70%-ni metanol. Posle 24h macerat je filtriran i postupak je ponovljen još dva puta. MeOH ekstrakt je uparen na rotacionom vakuum uparivaču i ostatak je vodeni ekstrakt. Taj ostatak je rastvoren u 50%-nom etanolu da bi se napravili 10%-ni rastvori. I 10%-ni, i razblaženi rastvori su korišćeni u daljem ispitivanju. Eksperimentalni rezultati ukazuju da je metanolni ekstrakt *M. peregrinum* sakupljene sa lokaliteta Senta ispoljio najjači inhibitorski efekat, s obzirom da je IC<sub>50</sub> vrednost postignuta sa najnižom koncentracijom. Isti rezultati su dobijeni prilikom ispitivanja uticaja metanolnog ekstrakta na LP. Razlike uočene u delovanju pojedinih ekstrakata su verovatno posledica različitog sadržaja flavonoida i drugih antioksidantnih komponenata.

**Antioxidant properties of *Marrubium peregrinum* L. (Lamiaceae) extracts**

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The antioxidant activity of *Marrubium peregrinum* methanol extracts, collected from three different locations (Backo Gradiste - Rimski Sanac, Novi Knezevac and Senta) was evaluated as a free radical scavenging capacity (RSC), together with effects on lipid peroxidation (LP). RSC was assessed measuring the scavenging activity of the MeOH extracts on 2,2-diphenyl-1-picrylhydrazil (DPPH<sup>•</sup>), super oxide anion (O<sub>2</sub><sup>•-</sup>), NO<sup>•</sup> and OH<sup>•</sup> radicals. Effects on LP was evaluated following the activities of MeOH extracts in Fe<sup>2+</sup>/ascorbate system of induction. The plant leaves were dried in air and ground in a mixer. 200 g of finely powdered material was macerated three times in 70% methanol (MeOH) during a 24-h period. The macerates were collected, filtered, and evaporated to dryness under vacuum. The residues were dissolved in 50% ethanol to make 10% (w=v) solutions. Both, these and the diluted solutions, were further used for examination. The results obtained show that the methanol extract of *M. peregrinum* collected from Senta locality exhibited the strongest inhibitory effect, as the IC<sub>50</sub> value was achieved with the lowest concentration. The same result was obtained in investigation of extracts impact on LP. The differences observed in the action of particular extracts are probably due to the different contents of flavonoids and some other antioxidant compounds.



ВН14-Р

### Стероиди из кукуте (*Conium maculatum* L.) — ГХ-МС анализа

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У овом раду су изнети резултати испитивања стероида биљне врсте *Conium maculatum* L. (кукута), из породице Апицеае, добро познате отровне коровске биљке. Урађене су детаљне ГХ-МС анализе двадесет и два узорка (дихлорметански екстракти биљних органа врсте *C. maculatum*; материјал је сакупљан са три локације, у току три или четири фенофазе). Двадесет и четири стероида су идентификована, од којих шест има ергостанско језгро, док остали поседују стигмастански скелет. Идентификација ових једињења је вршена на основу њихове МС фрагментације, као и ГХ коинјекцијом чистих једињења и хемијском трансформацијом (силиловањем). Уочено је да су стероиди главни састојци екстракта корена (до 70%) ове биљне врсте у последњој фази фенолошког развића. Најзаступљенији су били стигмаста-5,22-диен-3 $\beta$ -ол (стигмастерол) и стигмаста-5-ен-3 $\beta$ -ол ( $\beta$ -ситостерол). Да би покушали да класификујемо наше узорке, урађена је статистичка обрада добијених резултата коришћењем методе анализе главне компоненте (РСА) и агломеративне хијерархијске кластер анализе (АНС), са релативним садржајем стероида као варијаблама.

### Steroids from Poison Hemlock (*Conium maculatum* L.): a GC-MS analysis

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The steroid content of *Conium maculatum* L. (Poison Hemlock), Apiaceae, a well known weed plant species, has been studied herein for the first time. This was achieved by detailed GC-MS analyses of twenty two samples (dichloromethane extracts of different plant organs of *C. maculatum* at three or four different stages of phenological development, collected from three locations). In total, twenty four different steroids were identified. Six steroids had an ergostane nucleus while the other ones possessed a stigmasterane carbon framework. The identity of these compounds was determined by spectral means (MS fragmentation), GC co-injections with authentic standards and chemical transformations (silylation). Steroid compounds were noted to be the main chemical constituents of root extracts (up to 70%) of this plant species in the last phase of development. The predominant were stigmasterol and  $\beta$ -sitosterol. In an attempt to classify our samples, we performed principal component analysis (PCA) and agglomerative hierarchical clustering (AHC) using steroid percentages as variables.



BH15-P

### **Sinteza estara metoksi-(propenil)fenola u cilju identifikacije sastojaka etarskog ulja biljne vrste *Anthemis segetalis* Ten. (Asteraceae)**

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Detaljnou analizom hemijskog sastava etarskog ulja biljne vrste *Anthemis segetalis* Ten. (Asteraceae), korišćenjem GC i GC-MS, identifikovano je ukupno 155 sastojaka. Analiza je ukazala i na prisustvo još 3 jedinjenja (u količinama manjim od 0,5%), a za koje je, na osnovu njihovih masenih spektara, pretpostavljeno da su neki od izomernih metoksi-(propenil)fenil-pentanoata, odnosno -pentenoata. U cilju identifikacije nepoznatih jedinjenja, a i dobijanja dovoljnih količina za testiranja biološke aktivnosti, izvršena je sinteza 36 estara regioizomera eugenola sa angelika- ((Z)-2-metil-2-butenskom), tiglinskom ((E)-2-metil-2-butenskom), senecio (3-metil-2-butenskom), valerijanskom (pentanskom), izovalerijanskom (3-metilbutanskom) i 2-metilbutanskom kiselinom. Svi sintetisani estri (od kojih 31 predstavlja nova jedinjenja) su, ponaosob, GC ko-injektirani sa etarskim uljem ove biljne vrste. Zaključeno je da su jedinjenja, prisutna u ulju, estri angelika, izovalerijanske i 2-metilbutanske kiseline, međutim identitet fenola ((estri šest alilmetoksifenola (od ukupno mogućih deset izomernih eugenola), koji su u ovom radu sintetisani, nisu odgovarali prirodnim estrima iz ulja *A. segetalis*) nije utvrđen.

### **Synthesis of methoxy-(propenyl)phenyl esters from the essential oil of *Anthemis segetalis* Ten. (Asteraceae)**

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A detailed GC and GC-MS analysis of the essential oil of *Anthemis segetalis* Ten. (Asteraceae) resulted in the identification of 155 components. The analysis also pointed to the presence of 3 interesting compounds (in amounts of less than 0.5%), that were, according to their mass spectral fragmentation, tentatively identified as the isomeric methoxy-(propenyl)phenyl pentanoates and pentenoate. In order to identify the unknown volatile compounds, and obtain sufficient quantities for biological activity assays, a synthesis was undertaken of 36 esters of regioisomers of eugenol with angelic ((Z)-2-methyl-2-butenic), tiglic ((E)-2-methyl-2-butenic), senecioic (3-methyl-2-butenic), valeric (pentanoic), isovaleric (3-methylbutanoic) and 2-methylbutanoic acids. All synthesized esters (of which 31 represent new compounds) were separately GC co-injected with the essential oil of this plant species. It was concluded that the compounds present in the oil are esters of angelic, isovaleric and 2-methylbutanoic acids, but the phenol ((esters of six allylmethoxyphenols (out of ten possible isomeric eugenols), which were synthesized in the course of this work, did not correspond to any of the natural esters from the essential oil of *A. segetalis*) remained unidentified.



BH16-P

### **Kloniranje i optimizacija ekspresije rekombinantnog cistatina iz kivija**

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Cistatin, inhibitor cistein proteaza, predstavlja jedan od manje zastupljenih proteina kivija (*Actinidia deliciosa*), ali i jedan od važnih alergena ovog alergenskog izvora. Nalazi se pretežno u kori kivija, a njegova fiziološka uloga nije sasvim razjašnjena. Ovaj protein bi mogao imati primenu u dijagnostifikovanju alergije na kivi zbog njegove interakcije sa IgE.

Svrha ovog rada je optimizacija dobijanja rekombinantnog cistatina iz kivija u cilju dobijanja veće količine proteina i utvrđivanja njegovih strukturnih osobina, prvenstveno IgE reaktivnosti u poređenju sa prirodnim cistatinom.

U ovom radu gen za cistatin je ukloniran iz pUC57 u ekspresioni vektor pQE60 i optimizovana je ekspresija cistatina u *Escherichia coli*. Laboratorijska proizvodnja proteina je indukovana u ćelijama soja BL21 pomoću IPTG-a. Ćelije su gajene u LB medijumu uz selektivne markere (ampicilin, hloramfenikol i kanamicin). Varirani su temperatura i dužina trajanja ekspersije. Proizvodnja proteina je detektovana anti-His i anti-cistatin antitelima u Western blotu.

### **Cloning and optimizing of protein expression of recombinant cystatin from kiwifruit**

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Cistatin, a cystein protease inhibitor, represents one of the less abundant proteins of kiwifruit (*Actinidia deliciosa*), however it is an important allergen from kiwi. It is found mostly in the peel of kiwifruit but its physiological role is unknown. Due to its IgE reactivity and capability to induce allergic symptoms this protein could find application in the diagnosis of kiwifruit allergies.

The main goal of this work was to optimize the expression of recombinant cistatin from kiwifruit in order to obtain larger amounts of the protein and to be able to elucidate its structural features, primarily IgE reactivity in comparison to the natural counterpart.

The gene for cistatin was cloned from pUC57 vector into pQE60 expression vector and the protein expression was done in *Escherichia coli*. The protein production was optimized on a small scale in BL21 cells by using isopropyl- $\beta$ -D-thio-galactoside (IPTG), by varying the temperature and duration of protein expression. The recombinant protein was detected with anti-His and anti-cistatin antibodies in the Western blot.



**Biotehnologija / Biotechnology**  
**Usmena saopštenja / Oral Presentations**

BT01-O



**Karakterizacija lipaze iz *Candida utilis* dobijene tehnikom gajenja na čvrstoj podlozi korišćenjem uljane pogače maslina kao supstrata**

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U radu je ispitana kinetika rasta i produkcije lipaze tokom kultivacije *Candida utilis* na uljanoj pogači maslina poreklom iz Libije. Na optimizovanoj podlozi, obogaćenoj maltozom i ekstraktom kvasca, maksimalni prinos lipaze ostvaren je nakon 5 dana fermentacije, u kasnoj stacionarnoj fazi rasta ćelija. Ova lipaza je delimično prečišćena metodom frakcionog taloženja amonijum-sulfatom (12 puta sa prinosom 85%). Ispitani su uticaji temperature i pH na aktivnost/stabilnost dobijene lipaze. Proizvedena lipaza pokazuje optimum delovanja na 45 °C u kiselim uslovima, na pH 5,0. Molekulska masa određena je SDS-PAGE elektroforezom i iznosi 64,9 kDa. Joni  $\text{Sn}^{2+}$ ,  $\text{Zn}^{2+}$  i nejonski detergentsi Tween 80, Tween 20 i Triton X-100 inhibiraju proizvedenu lipazu, dok joni  $\text{K}^+$ ,  $\text{Cu}^{2+}$ ,  $\text{Ca}^{2+}$  i natrijum-deoksiholat deluju kao aktivatori dobijene lipaze.

**Characterization of *Candida utilis* lipase produced by solid state fermentation using olive oil cake as a substrate**

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In this work kinetics of *Candida utilis* growth and lipase production on Libyan olive oil cake was studied. Maximum of produced lipases occurred after 5 days, in late stationary phase of cell growth, on medium supplemented with maltose and yeast extract. Lipase was partially purified by fractional ammonium sulphate technique (12 fold with 85% yield). The effects of temperature and pH on lipase activity/stability were studied. The produced lipase showed highest activity at 45 °C in acidic conditions (pH=5.0). The molecular weight of produced enzyme determined by SDS-PAGE was 64.9 kDa. Tween 80, Tween 20, Triton X-100 and  $\text{Sn}^{2+}$ ,  $\text{Zn}^{2+}$  had inhibitory effect on lipase activity, whereas  $\text{K}^+$ ,  $\text{Cu}^{2+}$  and  $\text{Ca}^{2+}$  salts and sodium deoxycholate had effect as activators.



BT02-O

### **Ispitivanje tolerancije soja *Pseudomonas aeruginosa* san ai na živu, kadmijum i bakar**

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Zagađenje životne okoline teškim metalima je ozbiljan problem savremenog sveta. Među metalima koji su česti zagađivači su: bakar, kadmijum i živa. Cilj ovog rada je bilo ispitivanje osetljivosti soja *Pseudomonas aeruginosa* san ai na pomenute teške metale. Minimale inhibitorne koncentracije kadmijuma i bakra od 2 i 4 mM, redom, pokazale su da je soj otporan na ova dva metala. MIK za živu je bila najniža testirana koncentracija metala od 0,5 mM. Dobijene vrednosti MIK-a za kadmijum i bakar stavljaju soj *P. aeruginosa* san ai u grupu bakterija koje ispoljavaju visoku toleranciju prema ovim teškim metalima. Utvrđeno je da je živa toksična za soj. Ispitivanja mehanizama detoksikacije soja *P. aeruginosa* san ai u cilju potencijalne primene u procesima bioremedijacije su u toku.

### **Study of tolerance of *Pseudomonas aeruginosa* san ai to mercury, cadmium and copper**

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The pollution of the environment with toxic heavy metals is spreading throughout the world along with industrial progress. Among the common heavy metals used and the more widespread contaminants of the environment are mercury, cadmium and copper. Present research was performed in order to screen tolerance of strain *Pseudomonas aeruginosa* san ai to these heavy metals. Study showed that *P. aeruginosa* san ai is tolerant to cadmium and copper with MIC's of 2 and 4 mM, respectively. MIC for mercury was the lowest tested concentration of 0.5 mM. This suggests that *P. aeruginosa* san ai has large potential for bioremediation of environments contaminated with cadmium and copper and that mercury is toxic for the strain. In order to improve possible application of strain *P. aeruginosa* san ai in processes of bioremediation the study of mechanisms of metal uptake are underway.

**BT03-O**

**Temperaturna i pH stabilnost biološki aktivnih enzimskih hidrolizata proteinskog izolata pogače uljane tikve golice**

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Proteinski hidrolizati sa biološki aktivnim svojstvima imaju veliku perspektivu primene kao funkcionalni i bioaktivni ingredijenti široke lepeze prehrambenih proizvoda. Zbog velikog interesovanja da se biološki aktivni proteinski hidrolizati koriste u pripremi hrane, od praktičnog je značaja ispitati njihovu stabilnost pod uticajem povišenih temperatura, kao i promena pH. U radu je ispitana temperaturna i pH stabilnost biološki aktivnih hidrolizata proteinskog izolata (PI) pogače uljane tikve golice. U prethodnim istraživanjima, u hidrolizatu sa alkalazom sa stepenom hidrolize (DH)  $53,23 \pm 0,7\%$  utvrđena je antiradikalska aktivnost od  $7,59 \pm 0,081 \text{ mTEAC/mg}$  i inhibitorna aktivnost prema enzimu konvertazi angiotenzina (ACE) od  $71,05 \pm 7,5\%$  ( $\text{EC}_{50} = 0,422 \text{ mg/ml}$ ). Hidrolizati nakon termičkih tretmana na temperaturama od  $50^\circ\text{C}$  do  $100^\circ\text{C}$  nisu pokazali promenu antiradikalne aktivnosti ( $p < 0.05$ ), sa prosečnom aktivnosti od  $7,63 \pm 0,5 \text{ mTEAC/mg}$ . Ispitivanja stabilnosti pH u opsegu pH od 2,00 do 9,00 pokazala su i da se antiradikalska aktivnost hidrolizata ne menja ni pod uticajem promene pH ( $p < 0.05$ ). Pod uticajem temperature od 50 da  $80^\circ\text{C}$  ACE inhibitorne aktivnosti hidrolizata nisu izmenjene ( $p < 0.05$ ), dok je nakon tretmana na  $100^\circ\text{C}$ , utvrđena povećana aktivnost na  $86,56 \pm 5,68\%$ . Slični rezultati dobijeni su i kod drugih ispitanih hidrolizata, ukazujući da biološki aktivni enzimski hidrolizati PI pogače uljane tikve pokazuju zadovoljavajuću temperaturnu i pH stabilnost.

**Temperature and pH stability of biological active enzymatic hydrolysates of hull-less pumpkin oil cake protein isolate**

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Biological active protein hydrolysates have great potential of use as functional and bioactive ingredients in various food. With the great interest in preparing foods with these functional ingredients, it is important to test their processing stability. In this study, the temperature and pH stability of biological active hydrolysates of hull-less pumpkin oil cake protein isolate were investigated. In previous study, it was shown that alcalase hydrolysates with degree of hydrolysis (DH) at 53.23%, had antiradical and Angiotensin Converting Enzyme (ACE) inhibitory activity of  $7.59 \pm 0.081 \text{ mTEAC/mg}$  and  $71.05 \pm 7.5\%$  ( $\text{EC}_{50} = 0.422 \text{ mg/ml}$ ), respectively. The hydrolysates showed temperature stability in temperature range from  $50^\circ\text{C}$  to  $100^\circ\text{C}$  for 1h, with average antiradical activity being at  $7.63 \pm 0.5 \text{ mTEAC/mg}$ . The antiradical activity of hydrolysates was not affected by pH ( $p < 0.05$ ) in range from 2.00 to 9.00. The ACE inhibitory activity of hydrolysate was not affected ( $p < 0.05$ ) after heat treatments at temperatures from 50 to  $80^\circ\text{C}$ , while after treatment at  $100^\circ\text{C}$  ACE inhibitory activity increased to  $86.56 \pm 5.68\%$ . Similar results were obtained in testing of stability of other hydrolysates, indicating that biological active hydrolysates derived from pumpkin oil cake PI have satisfactory heat and pH resistance/stability.



Posterska saopštenja / Poster Presentations

BT04-P



**Delimično prečišćavanje prirodnih koagulanata iz zrna pasulja primenom hromatografije sa izmenom jona na IRA 900**

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Iz ekstrakta belog pasulja su izdvojeni proteini isoljavanjem sa  $(\text{NH}_4)_2\text{SO}_4$  i zatim oslobođeni viška soli dijalizom. Ovako dobijeni proteini su prečišćavani hromatografijom sa izmenom jona na anjonskoj jonoizmenjivačkoj smoli Amberlit IRA 900Cl.

Praćeno je vezivanje proteina za jonoizmenjivačku smolu sa vremenom, iz rastvora u kome je pH bio podešen na 5, 7 i 9. Vezivanje je rađeno pri odnosu rastvora proteina i smole 20 : 1, 10 : 1 i 5 : 1. Ustanovljeno je da se najefikasnije i najstabilnije vezivanje proteina, izdvojenih iz ekstrakta pasulja, za jonoizmenjivačku smolu dešava pri pH 9, kada je odnos razblaženog dijalizata i smole 5 : 1. Dovoljno vreme za vezivanje proteina za smolu IRA 900Cl je 30 minuta. Proteini vezani za smolu pod datim uslovima su nakon toga eluirani sa smole pomoću 0,5 mol/l, 1 mol/l, 1,5 mol/l i 2 mol/l NaCl. Eluati sa 1 i 1,5 mol/l NaCl su sadržali oko dva puta više proteina od druga dva eluata. Sa tako dobijenim eluatima je izveden ogled koagulacije u model vodi sa kaolinom mutnoće 35 NTU, pri pH 9 i sa različitim dozama eluata (0,67, 1, 1,66 i 3,33 ml/l). Ustanovljeno da svi eluati pokazuju dobru koagulacionu aktivnost pri najmanjoj dozi. Frakcija proteina eluirana sa 0,5 mol/l rastvorom NaCl pokazuje najbolju, a frakcija eluirana sa 2 mol/l NaCl nešto slabiju koagulacionu aktivnost u odnosu druge dve frakcije proteina.

**Partial purification of natural coagulants obtained from common bean seeds by ion exchange chromatography on IRA 900**

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The proteins were isolated from common bean extract by precipitation with  $(\text{NH}_4)_2\text{SO}_4$  and obtained precipitate was dialysed. Resolved proteins were partially purified by ion exchange chromatography on anion ion exchange resin Amberlit IRA 900Cl.

The protein binding on ion exchange resin in time was measured, from solutions with pH 5, 7 and 9. Protein solution : resin ratios were 20 : 1, 10 : 1 i 5 : 1. It was established that the most effective and the most stable protein binding on ion exchange resin occurred at pH 9, with protein solution: resin ratio = 5 : 1. Enough contact time for this process was 30 minutes. Proteins that were bond on resin at those conditions were eluted from resin by 0.5 mol/L, 1 mol/L, 1.5 mol/L and 2 mol/L NaCl solutions. Eluates with 1 and 1.5 mol/L NaCl were contained about two times more protein than the others. Coagulation tests were performed with obtained eluates on model water with kaolin which turbidity was 35 NTU and at pH 9. Different doses of eluates (0.67, 1, 1.66 and 3.33 ml/L) were applied. It was established that eluates showed good coagulation activity with the lowest applied dose. Fraction of protein eluated with 0.5 mol/L NaCl had the highest coagulation activity followed by other fraction, and eluate with 2 mol/L NaCl had somewhat lower activity.



BT05-P

**Bakterijsko luženje metala iz elektronskog otpada pomoću *At. ferrooxidans***

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Reciklaža elektronskog otpada je pirometalurški ili hidrometalurški proces koji izaziva zagađenje vazduha emisijom toksičnih jedinjenja u atmosferu.

U ovom radu su prikazani rezultati bakterijskog luženja metala (Cu, Sn, Ni, Zn i Ag) iz matičnih ploča personalnih računara pomoću soja *Acidithiobacillus ferrooxidans* izolovanog iz odlagališta jalovine rudnika bakra Bor. Eksperimenti su urađeni u podlozi 9K (9 gFe<sup>2+</sup>/L) inokulisanoj sa *At. ferrooxidans* u poredjenju sa abiotičkom kontrolom. Odnos podloge i supstrata (isečeni elektronski otpad) bio je 1:100 (m/v). Eksperiment je trajao 14 dana na temperaturi 28 °C uz mešanje na rotacionoj mešalici. Koncentracija metala u rastvoru je određivana pomoću ICP.

Po isteku eksperimenta, u uzoraku u kome je bakterijski generisani Fe(III)-jon visoka koncentracija metala u rastvoru ukazuje na snažno oksidaciono dejstvo Fe(III)-jona u kiseljoj sredini. To potvrđuju i koncentracije metala određene u kontrolnoj probi koji su za 10 puta manje u odnosu na biotički uzorak. Dobijeni rezultati pokazali su veliki potencijal čistih mezofilnih kultura *At. ferrooxidans* za rastvaranje/luženje metala iz elektronskog otpada.

**Bacterial leaching of metals from electronic waste by *At. Ferrooxidans***

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Re-cycling of electronic waste is either pyrometallurgical or hydrometallurgical which generate atmospheric pollution by releasing toxic compounds into the atmosphere.

This paper presented results of bacterial leaching of metals (Cu, Sn, Ni, Zn and Ag) from printed circuit boards using *Acidithiobacillus ferrooxidans* isolated from copper mine dump Bor. Experimental flasks contained 9K medium (9 gFe<sup>2+</sup>/L) inoculated with *At. ferrooxidans*, and compared with abiotic control medium. In all solutions shredded electronic waste were added with pulpe density 1:100 (m:v). The experiments were run in rotary shaker, for 14 days at 28°C. The amounts of released metals were determined by ICP.

At the end of experiment, in test solution in which Fe(III)-ion has been produced microbiologically, high concentrations of metals in solutions indicated the oxidation role of Fe(III)-ions in acid environment, which is confirmed by 10 fold lower metals concentration in abiotic control. The presented results showed great potential of pure mesophile bacteria culture *At. ferrooxidans* to bring metals into solution from electronic waste.



BT06-P

### **Optimizacija i karakterizacija enzimске sinteze $\alpha$ -izosalicina i ispitivanje njegovih antioksidativnih osobina**

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Salicin i njegovi strukturni izomeri pokazuju izraženu antikoagulatornu aktivnost i inhibitorni efekat na tirozinazu, a koriste se i kao anti-inflamatorni, antipiretički i analgetički agensi. Koristeći metodologiju odyivnih površina (RSM), našli smo optimalne parametre za sintezu  $\alpha$ -izosalicina, u reakciji maltoze i salicil alkohola, katalizovanoj  $\alpha$ -1,4-glukozidazom iz pekarskog kvasca. Nađeno je da je optimalna temperatura za ovu transglukozilacionu reakciju  $36,5^{\circ}\text{C}$ , koncentracija maltoze 40% (w/v), a pH 6,5. Koristeći 10 U/mL enzima maksimalni prinos od 75% (mol/mol) se dobija za samo 16h. Odredili smo i glavne kinetičke parametre za sintezu  $\alpha$ -izosalicina:  $K_m=6,62\text{mM}$  za salicil alkohol i  $V_{\text{max}}=0,616\text{ }\mu\text{mol/min/mg}$ . Nakon prečišćavanja  $\alpha$ -izosalicina od ostalih molekula u reakcionoj smeši, pokazali smo da ovaj izomer salicina ima izuzetno jaku antioksidativnu aktivnost: I.C.50 vrednost prema TBARS eseju iznosi 178mM a prema DPPH eseju 51mM.

### **Optimisation and characterization of enzymathic synthesis of $\alpha$ -isosalicin and examination of it antioxidant properties**

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Salicin and its structural isomers exhibit pronounced anticoagulant activity, tyrosinase inhibitory activity, and are also used as anti-inflammatory, analgesic and antipyretic prodrugs. Using responce surface methodology (RSM) we found optimal parameters for synthesis of  $\alpha$ -isosalicin, in reaction of maltose and salicyl alcohol, catalyzed by  $\alpha$ -1,4-glucosidase from baker's yeast. It was found that optimal temperature for this transglucosylation reaction was  $36.5^{\circ}\text{C}$ , maltose concentration 40% (w/v) and pH 6.5. With concentration of enzyme of 10 U/mL, maximal yield of 75% (mol/mol) is achieved for only 16h. We also determined key kinetic parameters for synthesis of  $\alpha$ -isosalicin and these are  $K_m=6.62\text{mM}$  of salicyl alcohol and  $V_{\text{max}}=0.616\text{ }\mu\text{mol/min/mg}$ . After purification  $\alpha$ -isosalicin from reaction mixture, we have shoven that this salicin isomer is very potent antioxidant molecule: I.C. 50 value according to TBARS assay is 178mM and according to DPPH assay is 51mM.



**Ispitivanje potencijala lipaze *Pseudomonas aeruginosa* san-ai  
za sintezu estara u nevodenoj sredini**

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Poslednjih godina povećano je interesovanje za enzimsko dobijanje estara kao alternativa hemijskom postupku. Enzimski kataliza se odvija pod umerenim reakcionim uslovima i omogućava transformacije supstrata koji su osetljivi na ekstremne uslove. Ispitan je biokatalitički potencijal lipaze izolovane iz fermentacione tečnosti *Pseudomonas aeruginosa* san-ai NCAIM (P) B 001380 za sintezu estara. Sve reakcije su izvođene na 30 °C uz mešanje (200 rpm). U sistemu bez rastvarača potvrđena je sinteza metil-estara. Relativni prinosi u reakcijama esterifikacije benzojeve i salicilne kiseline su 90% i 92%, redom, a za sirćetnu, propionsku, kaprilnu i oleinsku kiselinu nakon 24h su 77%, 47%, 33% i 25%, redom. Relativni prinosi za sintezu estara sirćetne kiseline u n-heksanu sa metanolom, etanolom, izopropanolom, holesterolom i mentolom nakon 24h iznose 77%, 73%, 54%, 46%, 79%, 50%, redom. Može se zaključiti da je lipaza efikasan katalizator u reakcijama sinteze estara u nevodenoj sredini. Dalja optimizacija uslova esterifikacije je u toku.

**Screening of *Pseudomonas aeruginosa* san ai lipase for ester synthesis potential**

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In the last decade interest for enzyme-catalyzed production of esters has increased. One of the advantages of enzyme-catalyzed process (besides the energy saving) are mild conditions which allow transformations of sensitive substrates. Potential of lipase produced by *Pseudomonas aeruginosa* san ai NCAIM (P) B 001380, as biocatalyst for ester synthesis was investigated. All reactions were performed at 30 °C with rotational shaking (200 rpm). Synthesis of methyl esters in solvent free system was confirmed. Relative yields of esterification for benzoic and salicylic acid after 2h were 90% and 92%, respectively; and for: acetic, propanoic, capric and oleic acid after 24h were 77%, 47%, 33% and 25% , respectively. Relative yields for esterification of acetic acid in n-hexane with methanol, ethanol, isopropanol, cholesterol and menthol after 24h were: 77%, 73%, 54%, 46%, 79% and 50%, respectively. It could be concluded that the lipase is efficient biocatalyst for ester synthesis. Further optimization for esterification process is underway.

BT08-P

### **Adsorpcija lipaze iz *Candida rugosa* na višeslojne ugljenične nanocevi**

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Imobilizacija enzima je jedan od najefikasnijih načina za njihovu upotrebu kao katalizatora u industriji. Praktična primena imobilisanog enzima u najvećoj meri zavisi od fizičkih i hemijskih karakteristika upotrebljenog nosača. Potrebno je da ima veliki kapacitet vezivanja enzima, da bude hemijski i mikrobiološki stabilan, da omogući lako izdvajanje imobilizata iz reakcione smeše i td. Svojstva, kao što su maksimalna površina po jedinici mase, minimalna difuziona ograničenja, maksimalna količina vezanog enzima i visoka mehanička stabilnost čine ugljenične nanocevi idealnim nosačima.

U ovom radu ispitivana je adsorpcija lipaze iz *Candida rugosa* na višeslojne ugljenične nanocevi (MWCNT). U tom cilju praćen je tok imobilizacije pri različitim koncentracijama enzima. Ispitivan je uticaj vremena imobilizacije i koncentracije lipaze na masu vezanog enzima i aktivnost imobilisanog preparata. Koncentracija lipaze varirana je u opsegu  $0,8 - 2,0 \text{ mg cm}^{-3}$ , a vreme imobilizacije u opsegu  $0,25 - 2 \text{ h}$ . Postignuti su visoki prinosi imobilizacije, a maksimalna količina enzima veže se već nakon jednog sata.

### **Adsorption of lipase from *Candida rugosa* onto multi-walled carbon nanotubes**

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For efficient use and potential industrial application, enzymes usually need to be immobilized. The success of an immobilized enzyme for practical application largely depends on the physical and chemical properties of the used carrier. The carrier should have ability to bind a large amount of enzyme, to be chemically stable, inert toward microbiological contamination, and to allow easy separation from the reaction mixture. High surface area, minimal diffusional limitations, maximal enzyme loadings and high mechanical stability makes carbon nanotubes an ideal carrier for enzyme immobilization.

In this study the adsorption of lipase from *Candida rugosa* onto multi-walled carbon nanotubes (MWCNTs) was investigated. Therefore, the influence of the enzyme concentration and the immobilization time on enzyme loading and enzyme activity was examined. Concentration of lipase was varied between  $0.8 - 2.0 \text{ mg cm}^{-3}$ , and the time of immobilization was between  $0.25 - 2 \text{ h}$ . High enzyme loading values were achieved and it can be considered that the immobilization was complete after one hour.



BT09-P

**$\beta$ -D-glukan iz pekarskog kvasca: antioksidativne i bifidogene osobine**

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Ćelijski zid pekarskog kvasca je glavni izvor nesvarljivog polisaharida  $\beta$ -D-glukana ((1 $\rightarrow$ 3),(1 $\rightarrow$ 6)- $\beta$ -D-glukan).  $\beta$ -D-glukan je fiziološki aktivno jedinjenje (opšte poznato kao modulator biološkog odgovora), koji aktivira imuni odgovor domaćina protiv bakterijske, virusne, gljivične i parazitske infekcije, kao i neoplazija. Cilj našeg istraživanja je ispitivanje bifidogenog i antioksidativnog potencijala (1 $\rightarrow$ 3),(1 $\rightarrow$ 6)- $\beta$ -D-glukana izolovanog iz pekarskog kvasca, kao novog prebiotskog dodatka infant formulama. Ukupan broj bifidobakterija nakon 48 h inkubacije u infant formuli sa dodatkom 0,1% (m /V)  $\beta$ -D-glukana (čistoće 99,54%) bio je značajno viši u odnosu na zrelo majčino mleko, infant formulu sa dodatkom inulina ili infant formulu bez prebiotika, kao referentne supstrate. Promene broja bifidobakterija praćene su promenama suve biomase, ukupnih bakterijski generisanih kiselina i pH.  $\beta$ -D-glukan najveće čistoće nema antioksidativnu aktivnost, dok prečišćeni ekstrakti glukana (93,15%, 75,54% i 49,30%) uklanjaju hidroksil radikale. Na osnovu bifidogenog efekta možemo da zaključimo da je  $\beta$ -D-glukan iz kvasca dobar kandidat kao novi prebiotik za dopunu infant formula.

**Antioxidative and bifidogenic properties of baker's yeast  $\beta$ -D-glucan**

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The cell wall of baker's yeast is a major source of nondigestible polysaccharide  $\beta$ -glucan ((1 $\rightarrow$ 3),(1 $\rightarrow$ 6)- $\beta$ -D-glucan). Baker's yeast  $\beta$ -glucan is a physiologically active compound (generally named "biological response modifier") and is a broad-spectrum enhancer of host defense against bacterial, viral, fungal and parasitic infections, as well as neoplasia. The aim of our study was to investigate the bifidogenic and antioxidative potential of (1 $\rightarrow$ 3),(1 $\rightarrow$ 6)- $\beta$ -D-glucan isolated from the baker's yeast (*Saccharomyces cerevisiae*) in relation to digestibility and purity, as a new infant formula prebiotic supplement. The total number of bifidobacteria after 48 h of incubation in the substrate composed of infant formula supplemented with 0.1 % (m/v)  $\beta$ -D-glucan (purity 99.54 %) was significantly higher than in mature breast milk, infant formula supplemented with inuline or infant formula without added prebiotic, which were used as reference substrates. Changes in the number of bifidobacteria were followed by the changes in dry biomass, total bacteria-generated organic acids and pH. In contrast, the purest  $\beta$ -D-glucan did not show any antioxidative activity, while partially purified glucan extracts (93.15%, 75.54% and 49.30%) scavenged hydroxyl radicals. Regarding to digestibility and bifidogenic efficacy *Saccharomyces cerevisiae*  $\beta$ -D-glucan could be a candidate as a new infant formula prebiotic supplement.





BT10-P

### **Etarsko ulje i ekstrakti bosiljka (*Ocimum basilicum*)**

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Ispitana je ekstrakcija bosiljka (*Ocimum basilicum*) u cilju dobijanja različitih proizvoda, odnosno etarskog ulja dobijenog destilacijom pomoću vodene pare i ekstrakata dobijenih primenom različitih rastvarača. Droga (*Basilici herba*) je usitnjena (srednji prečnik čestica  $d=0,385$  mm), određen je sadržaj vlage u drogi (1,73%; m/m) i sadržaj etarskog ulja (1,05%; V/m). Primenom hromatografije na tankom sloju (TLC) identifikovana su dominantna jedinjenja dobijenog etarskog ulja, metil-havikol i linalool. Ekstrakcijom po Soxhlet-u primenom metilen-hlorida kao ekstragensa dobijen je prinos ekstrakcije, odnosno prinos suvog ekstrakta 18,03% (m/m). Iz ovog ekstrakta je, destilacijom pomoću vodene pare, izolovano etarsko ulje i određen je udeo etarskog ulja u ekstraktu (4,15%; V/m). I u ovom uzorku etarskog ulja su primenom TLC detektovani metil-havikol i linalool kao dominantna jedinjenja. Ekstrakcija bosiljka je izvršena i etanolom različitih koncentracija (od 0 do 70%). Sa porastom koncentracije etanola u ekstragensu smanjuje se prinos ekstrakcije od 26,42 do 13,60% (m/m). Proizvodi na bazi bosiljka (etarska ulja i tečni i/ili suvi ekstrakti dobijeni različitim rastvaračima i metodama ekstrakcije) su različitog kvalitativnog i kvantitativnog sastava, pa samim tim i različitog potencijalnog farmakološkog delovanja, odnosno različite potencijalne primene u farmaciji.

### **Essential oil and extracts of basil (*Ocimum basikicum*)**

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Extraction of common basil (*Ocimum basilicum*) for obtaining different products, i.e. essential oils by steam distillation and extracts using different solvents, was investigated. Drug (*Basilici herba*), first of all, was milled (mean diameter particle size,  $d$ , of 0.385 mm), and, after that, the moisture content (1.73%; w/w) and essential oil content (1.05%; v/w) were determined. Identification of predominant essential oil compounds (methyl-chavicol and linalool) were done by thin layer chromatography (TLC). By Soxhlet extraction, using methylene-chloride as an extragent, the yield of extraction, i.e. yield of dry extract of 18.03% (w/w) was obtained. The essential oil was separated from this extract by steam distillation and content of essential oil in dry extract was determined (4.15%; v/w). In this sample of essential oil both methyl-chavicol and linalool as dominant compounds were detected by TLC method. Extraction of common basil was done by different concentration of ethanol (from 0 to 70%) as solvent. The yield of extraction decreased from 26.42 to 13.60% (w/w) by increasing the ethanol concentration. The products on common basil basis (essential oils and liquid and/or dry extracts) have a different qualitative and quantitative composition, i.e. posses a different potentialy pharmacological activities and use in pharmacy.





BT11-P

### **Optimizacija rastvorljivosti proteina pogače uljane tikve enzimskim umrežavanjem sa transglutaminazom**

Peričin Draginja, Popović Ljiljana, Vaštag Žužana i Popović Senka  
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Uljana tikva (*Cucurbita pepo*) se na prostorima Austrije, Mađarske, Slovenije i Vojvodine uzgaja, prvenstveno, zbog dobijanja ulja. Uljana pogača, koja zaostaje kao nus-proizvod, nakon procesa ceđenja ulja iz semena predstavlja pogodan izvor za valorizaciju proteina. Kukurbitin je glavni rezervni protein u semenu i pogači uljane tikve. Primena ovog proteina kao ingradijenta hrane, još uvek, nije dovoljno istražena. Glavni nedostatak ovog proteina je njegova slaba rastvorljivost u uslovima za formulaciju hrane. Primena enzimskih metoda modifikacije proteina se pokazala kao veoma uspešna za unapređenje funkcionalnih karakteristika proteina i time za povećanje mogućnosti njihove primene u hrani. Cilj ovog rada je enzimska modifikacija kukurbitina transglutaminazom, procesom umrežavanja, radi povećanja rastvorljivosti proteina. Optimizacija enzimskog procesa umrežavanja kukurbitina izvedena je primenom metodologije odzivnih površina. Ispitan je uticaj procesnih parametara: vrednosti pH, koncentracije enzima i vremena reakcije na rastvorljivost proteina, kao izlaznu veličinu. Vrednost pH = 7,0, reakciono vreme od 59 minuta i enzim/ supstrat odnos 1/7,5 (w/w) su određeni kao optimalni uslovi za dobijanje maksimalne rastvorljivosti modifikovanog kukurbitina (2,89 mg/ml). Adekvatnost modela je potvrđena poređenjem sa eksperimentalno dobijenom vrednošću pri optimalnim uslovima.

### **Optimization of solubility of protein from pumpkin oil cake by enzymatic cross-linking with transglutaminase**

Peričin Draginja, Popović Ljiljana, Vaštag Žužana i Popović Senka  
*Faculty of Technology, Novi Sad, Serbia*

Cultivation of pumpkin (*Cucurbita pepo*) in the middle-south Europe region (Austria, Hungary, Slovenia and Serbia-province of Vojvodina) is wide-spread, primarily for oil production from seed. Oil extraction from pumpkin seeds yields a large amount of defatted pumpkin oil cake which contains a significant amount of protein, and represent good source for valorization of proteins. Cucurbitin is the major storage protein in pumpkin seed. There is no much information about cucurbitins applications in different food formulations. The major limitation to the extensive utilization of cucurbitin is its low solubility. Applications of enzymatic methods for improving solubility and thus functional properties of protein are an attractive mean. The objective of this study was optimization of solubility of cucurbitin by enzymatic cross-linking with transglutaminase. The response surface methodology was employed for investigation of effect of enzyme/substrate ratio, pH and reaction time on solubility of cucurbitin, as response. A pH value of 7.0, reaction time of 59 min and E/S ratio of 1/7.5 (w/w) were found to be optimal conditions to achieve the highest solubility (2.89 mg/ml). By means of additional experiments, the adequacy of the suggested model was confirmed.



BT12-P

### **Unapređenje funkcionalnih osobina globulina pogače uljane tikve: Enzimске modifikacije**

Popović Ljiljana, Peričin Draginja, Popović Senka i Vaštag Žužana  
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U prehrambenoj industriji konstantno postoji potražnja za novim proteinskim proizvodima koji moraju da zadovolje sve više kriterijume i potrebe potrošača. Sa druge strane, značajne količine, proteinski bogatih materijala zaostaju kao nusprodukti uljane industrije i predstavljaju problem i sa ekološkog i ekonomskog aspekta. Primena enzimskih procesa za modifikaciju proteina predstavlja veoma atraktivan način za dobijanje produkata, sa novim, poboljšanim funkcionalnim svojstvima. Takođe, enzimski procesi predstavljaju pogodan način za valorizaciju proteinski bogatih nusprodukata.

U ovom radu izvedene su enzimske modifikacije globulina (kukurbitina) iz pogače uljane tikve (*Cucurbita pepo*) i to: (i) enzimsko umrežavanje transglutaminazom i (ii) enzimска hidroliza primenom alkalaze. Funkcionalne osobine proteinskih modifikata, kao što su: rastvorljivost, sposobnost formiranja emulzija i pene ispitane su i poređene sa osobinama nemodifikovanог globulina. Rastvorljivost proteina se značajno povećava (i do 50%) primenom oba enzimska tretmana. Hidroliza dovodi do formiranja hidrolizata sa znatno unapređenim sposobnostima formiranja pene i emulzije ( $FC=242\pm3.21$ ,  $EA=0.452\pm0.02$  A500nm i  $ES=45.3\pm0.62$ min). Ovi rezultati dokazuju da se enzimskim modifikacijama mogu dobiti proteini sa znatno unapređenim funkcionalnim karakteristikama i omogućiti njihova priomena u različitim formulacijama hrane.

### **Improving of functional properties of globulin from pumpkin oil cake: Enzymatic modifications**

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The demand for high-quality food proteins, which should regarding consumers' acceptance and preferences, has always increased. On the other hand, significant quantities of protein rich products which remained as by products from oil industry represent problem from economical, as well as, environmental reasons. Application of enzymatic processes for protein modification represents an attractive mean for obtaining new products with improved functional properties. Also, valorization of protein rich by-products it could be done with enzymatic processes.

Enzymatic modifications of globulin, named cucurbitin, from pumpkin oil cake were carried in this study: (i) enzymatic cross-linking by transglutaminase and (ii) enzymatic hydrolysis by alcalase. Functional properties of proteins modification, such as: solubility, foam and emulsion properties were determined and compared with those of unmodified globulin. Both studied enzymatic treatment indicated in significant increased (to 50%) of protein solubility. Enzymatic hydrolysis produced hydrolysates with improved foaming and emulsion properties ( $FC=242\pm3.21$ ,  $EA=0.452\pm0.02$  A500nm and  $ES=45.3\pm0.62$ min). These results demonstrate that enzymatic modification is suitable for production of proteins with improved functional properties indicating their possible use in different food systems.



**Hemija i tehnologija hrane / Chemistry and Technology of Food**  
**Posterska saopštenja / Poster Presentations**

HTH01-P

**Pro-nutritivna svojstva katehina zelenog čaja pri gastričnoj digestiji alergena kikirikija**

Danijela Apostolović, Bojana Kravić, Luka Mihajlović, Dragana Stanić-Vucinić  
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Ekstrakti katehina zelenog čaja (GTC), posebno njihova glavna komponenta, epigalokatehin 3-galat, imaju znatan uticaj na zdravlje ljudi. U ovoj studiji, mi smo ispitivali simuliranu želudačnu digestiju sirovog ekstrakta proteina kikirikija u prisustvu katehinima bogatog ekstrakta zelenog čaja, oksidovanih katehina i smeša alergena hrane i katehina zelenog čaja procesovanih polifenol oksidazom. Proteini rezistentni na pepsin se brže degradiraju u prisustvu katehina is zelenog čaja. Korišćenjem specifičnih antitela, u imonoblotu je pokazano da u prisustvu GTC dolazi do kompletne digestije Ara h 1 i Ara h 2 pepsinom, u poređenju sa kontrolnom reakcijom. Aktivirajući efekat GTC je zavistan od njegove koncentracije. Polimerizacijom GTC dolazi do suprotnog efekta GTC na digestiju pepsinom. U prisustvu polimerizovanih GTC alergeni kikirikija, Ara h 2 i Ara h, postaju nešto manje rastvorni u simuliranom želudačnom soku.

Katehini zelenog čaja imaju pro-nutritivna svojstva i mogu uticati na sudbinu proteina u procesu digestije, a time i na količinu proteina koja je izložena imunom sistemu. Polimerizacija i procesovanje GTC polifenol oksidazama smanjuju aktivirajući uticaj GTC-a na aktivaciju pepsina.

**Green tea catechins have pro-nutritive properties in peanut allergens gastric digestion**

Danijela Apostolovic, Bojana Kravic, Luka Mihajlovic, Dragana Stanic-Vucinic  
Tanja Cirkovic Velickovic

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Extracts of green tea catechins (GTC), especially their major component, epigallocatechin 3-gallate, have profound effect on human health. In this study, we have examined simulated gastric digestion of crude peanut proteins in the presence of catechin-enriched extract of green tea, oxidized catechins and a polyphenol-oxidase processed mixtures of food allergens and green tea catechins. A pepsin-resistant protein degrades faster in the presence of green tea catechins. GTC completes Ara h 1 and Ara h 2 digestion by pepsin comparing to the control reaction as observed in immunoblot using specific antibodies. The activating effect of GTC is concentration dependent. Polymerization of GTC reversed the activating effect of GTC on pepsin digestion. In the presence of polymerized GTC, peanut allergens Ara h 2 and Ara h 3 become slightly less soluble in simulated gastric fluid.

Green tea catechins have pro-nutritive properties and may influence the fate of protein in the digestion process, and thus the dosage of the protein exposed to the immune system. Polymerization and processing of GTC by polyphenol oxidase diminish pepsin-activating effect of GTC.



HTH02-P

### **Citotoksična aktivnost napitaka uobičajenih u ljudskoj ishrani na kancerskim ćelijama karcinoma grlića materice**

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Kafa, zeleni čaj i kakao su popularni napitci bogati antioksidansima, pogotovu fenolnim kiselinama i derivatima katehina, poznatim po svojim blagotvornim svojstvima. Zeleni čaj je posebno bogat izvor katehina, polihidroksi flavan-3-ol derivata, sa poznatim antikancerskim, antiinflamatornim i antialergijskim efektima.

Etanolni ekstrakti kafe, zelenog čaja i kakaa su okarakterisani HPLC-ESI-MS metodom. Koncentracija ukupnih fenola u ekstraktima je određivana metodom po Folin-Ciocalteu, a antioksidativna aktivnost ABTS esejem. Citotoksična aktivnost na ćelijama karcinoma grlića materice (HeLa ćelijska linija) je određivana MTT esejem. Intraćelijske reaktivne kiseonične vrste (ROS) su određivane protočnom citometrijom, nakon inkubacije ćelija sa fenolnim ekstraktima i ROS-reaktivnom fluorescentnom probom. Ekstrakt zelenog čaja je pokazao najveću citotoksičnu aktivnost sa vrednošću IC<sub>50</sub> od 0,027 mg ekvivalenata galne kiseline/ml ekstrakta, dok je ekstrakt kafe pokazao IC<sub>50</sub> od 0,123 mg/ml, a ekstrakt kakaa IC<sub>50</sub> od 311,66861 mg/ml. Sadržaj intraćelijskih ROS-a raste u ćelijama inkubiranim sa ekstraktom zelenog čaja, dok umereno raste u ćelijama tretiranim ekstraktima kafe i kakaa. Različit način delovanja testiranih napitaka na ćelije ukazuje na prisustvo dodatnih aktivnih komponenti u ekstraktima kafe i kakaa.

### **Cytotoxic activity of common food beverages in human cervical carcinoma cell line**

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Coffee, green tea and cocoa are popular beverages rich in antioxidants, especially phenolic acids and derivatives of catechins, known for their health promoting properties. Green tea is a particularly rich source of catechins, polyhydroxy flavan-3-ol derivatives, known to exert anti-cancer, anti-inflammatory and anti-allergic effects.

Ethanol extracts of coffee, green tea and cocoa were characterized by HPLC-ESI-MS. Total phenolics of extracts were determined by Folin-Ciocalteu's method and antioxidative activity by ABTS assay. Cytotoxic activity in human cervical carcinoma cell lines (HeLa) was assayed by viability testing using MTT. Intracellular reactive oxygen species (ROS) were determined by flow cytometry following incubation of cells with phenolic extracts and ROS reactive fluorescent probe 2,7-dichlorofluorescein diacetate. All the tested extracts exhibited cytotoxic activity in HeLa cell lines, while green tea has the strongest activity with IC<sub>50</sub> of 0.027 mg of gallic acid equivalents/mL of extract, followed by coffee extract with IC<sub>50</sub> of 0.123 mg/mL and cocoa extract with IC<sub>50</sub> of 311.669 mg/mL. Intracellular ROS content increased in cells incubated with green tea phenolics, and moderately in cells treated with coffee and cocoa extracts. Different mode of action of the tested beverages suggests presence of additional active components in coffee and cocoa extracts.



HTH03-P

### **Hemijski sastav i antimikrobno dejstvo etarskog ulja samoniklog origana (*Origanum vulgare* L.)**

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Origano (*Origanum vulgare* L.), Lamiaceae, se često koristi u narodnoj medicini jer ima terapeutsko dejstvo (karminativno, antispazmolitičko, antiseptično, tonično).

U ovom istraživanjima, korišćena je svježa herba origana, sakupljena u junu 2010. godine u Bokokotorskom zalivu (južni dio Crne Gore), koja je ekstrahovana vodenom parom u aparatu po Klevendžer-u u toku 2 h.

Prinos etarskog ulja origana je bio 1.12% (w/w) dok je GC/MS analiza pokazala prisustvo 22 komponente. Kao glavne komponente identifikovani su karvakrol (22.79%) i timol (18.15%). Dobijeni rezultati ispitivanja antimikrobnog dejstva su pokazali da etarsko ulje *O. vulgare* ima značajnu antimikrobnu aktivnost posebno na *Staphylococcus aureus* i *Klebsiella pneumoniae*.

Ovi rezultati potvrđuju potencijalno korišćenje etarskog ulja origana u farmaceutskoj industriji, a može biti korisno i kao alternativa u liječenju nekih infektivnih bolesti.

### **Chemical composition and antimicrobial activity of essential oil of wild-growing oregano (*Origanum vulgare* L.)**

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Oregano (*Origanum vulgare* L.), Lamiaceae family, is widely known as possessing therapeutic properties (carminative, antispasmodic, antiseptic, tonic) while it is widely used in traditional medicine in many countries.

In this study, fresh *O. vulgare* herba collected in June 2010 from the southern part of Montenegro (Boka Kotorska Bay), were extracted by hydrodistillation in a Clevenger-type apparatus for 2 h. *O. vulgare* essential oil yield was 1.12% (w/w) based on a fresh weight basis whereas GC/MS analysis resulted in the identification of a total of 22 constituents. The major components in the essential oil were carvacrol (22.79%) and thymol (18.15%).

The gained results revealed that essential oil of *O. vulgare* has rather strong antimicrobial activity, especially against *Staphylococcus aureus* and *Klebsiella pneumoniae*.

Obtained results confirm the potential use of oregano essential oil in the pharmaceutical industry, and may be useful as an alternative antimicrobial agent in medicine for treatment of some infectious diseases.



**Hemija i tehnologija makromolekula**  
Chemistry and Technology of Macromolecules  
**Usmena saopštenja / Oral Presentations**

HTM01-O



**Uticaj sastava hidrogelova na bazi hitozana na kontrolisano otpuštanje diazepama, paracetamola i diklofenaka**

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Poslednjih godina sve više pažnje se poklanja kontrolisanom otpuštanju lekova iz polimernih matrica. Kao polimerne matrice za lekove vrlo često se koriste hidrogelovi, a među njima su posebno interesantni hidrogelovi na bazi prirodnih polimera. Hitozan je prirodni polimer koji se dobija procesom deacetilovanja hitina. Njegove prednosti su biokompatibilnost, biodegradabilnost, bioadhezivnost i netoksičnost. Hidrogelovi hitozana imaju loša mehanička svojstva, tako da se prilikom sinteze često dodaju sintetski polimeri u cilju poboljšanja istih.

Tema rada je ispitivanje uticaja sastava hidrogelova hitozana, itakonske i metakrilne kiseline na kontrolisano otpuštanje diazepama, paracetamola i diklofenaka. Otpuštanje je izvedeno u puferskom rastvoru pH-vrednosti 6,8, koja odgovara srednjoj vrednosti pH u donjem delu gastrointestinalnog trakta. Utvrđeno je da se najviše leka otpušta iz gela koji sadrži najviše metakrilne kiseline i koji najviše bubri. Takođe je utvrđeno da sa porastom stepenja umreženja opada stepen bubrenja, kao i otpuštanje lekova.

**Influence of chitosan hydrogel composition on controlled release of diazepam, paracetamol and diclofenac**

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In the recent years, polymer-based drug delivery systems have been considered for controlled drug release. As a polymer matrix for drugs, hydrogels are frequently used, and among them hydrogels based on natural polymers are particularly interesting. Chitosan, the deacetylated product of chitin, is a natural polymer. Its advantages include biocompatibility, biodegradability, bioadhesion and non-toxicity. Chitosan hydrogels have poor mechanical properties, and for the improvement, synthetic polymers are added during synthesis.

The paper is examining the influence of the chitosan/itaconic acid/methacrylic acid hydrogels on the controlled release of diazepam, paracetamol and diclofenac. The release was performed in a buffer solution (pH 6.8), which corresponds to the average pH values in the lower part of the gastrointestinal tract. It was found that the most drug was released from the gel which contains the most methacrylic acid and which swells the most. It was also determined that with the increase of crosslinking agent content, swelling degree and drug release are decreasing.

Autori se zahvaljuju Ministarstvu nauke i prosvete Republike Srbije za finansijsku podršku ovom radu u okviru projekata br. 172062 i 172007.



HTM02-O

**Termoosetljive mikročestice hidrogela na bazi poli(*N*-izopropilakrilamida) namenjene kontrolisanom otpuštanju lekova**

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Cilj ovog rada je bila optimizacija strukture i svojstava termoosetljivih mikročestica hidrogela na bazi umreženog poli(*N*-izopropilakrilamida) (PNIPA) sintetisanih inverznom suspenzionom polimerizacijom, variranjem reakcionih parametara. Pored variranja odnosa uljane i vodene faze, koncentracije emulgatora i stepena umreženja, PNIPA mikročestice su funkcionalizovane uvođenjem maleinske kiseline (MA) kao komonomera u vodenu fazu. Pravilnost oblika mikročestica hidrogela procenjivana je optičkom mikroskopijom. Veličina i raspodela veličina mikročestica određivana je metodom rasipanja svetlosti. Ravnotežni stepen bubrenja je određivan gravimetrijski, dok je morfologija mikročestica ispitivana skenirajućom elektronskom mikroskopijom. Temperatura zapreminske pseudo-fazne transformacije analizirana je diferencijalnom skenirajućom kalorimetrijom. Pokazano je da srednji prečnik, kao i ravnotežni stepen bubrenja mikročestica, zavise od udela emulgatora u uljanoj fazi, stepena umreženja PNIPA i koncentracije MA. Uočeno je da mikročestice u ravnotežnom stanju na sobnoj temperaturi imaju poroznu, sačastu strukturu. Da bi se ispitalo ponašanje ovih mikročestica hidrogela pri otpuštanju leka (lokalni anestetik – prokain-hidrohlorid) transdermalnim putem, korišćena je Francova difuziona ćelija. Dobijene mikročestice namenjene su dizajnu tekstil-hidrogel sistema za transdermalno kontrolisano otpuštanje leka promenom temperature.

**Thermosensitive hydrogel microbeads based on poly(*N*-isopropylacrylamide) for controlled drug release**

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This study was carried out to optimize the structure and properties of thermosensitive hydrogel microbeads based on crosslinked poly(*N*-isopropylacrylamide) (PNIPA) through variation of the reaction parameters of the inverse suspension polymerization. In addition to variation of the oil-to-water phase ratio, concentration of emulsifier, and the crosslinking degree, PNIPA microbeads were functionalized by using maleic acid (MA) as a comonomer in the water phase. Regularity of the microbeads shape was estimated by optical microscopy. A technique of laser diffraction was used for determination of the microbeads mean size and size distribution. Equilibrium swelling ratio was studied gravimetrically, whereas scanning electron microscopy was a tool for investigation of microbeads morphology. The values of volume pseudo-phase transition temperature were obtained by differential scanning calorimetry. The mean diameter of microbeads and their equilibrium swelling ratio showed dependence on the fraction of emulsifier in oil phase, the crosslinking degree of PNIPA and the content of MA. It was determined that microbeads swollen at room temperature have a porous, honeycomb-like structure. The Franz diffusion cell was employed for the study of the microbeads behavior in the drug release (local anesthetic - procaine hydrochloride) via transdermal route. Prepared thermosensitive hydrogel microbeads are intended for design of a textile-based system for transdermal release of a drug in a controlled manner, via temperature changes.





Posterska saopštenja / Poster Presentations

HTM03-P

**Hiperrazgranate alkidne smole prve i druge generacije na osnovu ricinolne kiseline**

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Hiperrazgranate alkidne smole se mogu dobiti modifikacijom hiperrazgranatih poliestara masnim kiselinama. U poređenju sa klasičnim alkidnim smolama istih molskih masa hiperrazgranati alkidi imaju niže viskoznosti i bolju hemijsku otpornost. U ovom radu sintetisane su prva i druga generacija hiperrazgranatih poliestara na osnovu ditrimetilolpropana i 2,2-di(hidroksimetil)propionske kiseline. Esterifikacijom sintetisanih poliestara sa ricinolnom kiselinom dobijene su hiperrazgranate alkidne smole prve i druge generacije. Smole su karakterisane određivanjem hidroksilnog i kiselinskog broja, viskoznosti, srednjih molskih masa i njihove raspodele. Struktura sintetisanih smola je potvrđena infracrvenom spektroskopijom sa Furijeovom transformacijom (FTIR). Sintetisane hiperrazgranate alkidne smole imaju velik sadržaj OH grupa, a mali kiselinski broj. Prisustvo OH grupa, kao krajnjih funkcionalnih grupa, omogućuje modifikaciju alkida u cilju dobijanja materijala različitih svojstava. Indeks polidisperznosti alkidnih smola raste od 1,59 do 3,84 sa porastom generacije istih. Niske viskoznosti dobijenih alkida omogućuju da proizvodi na osnovu njih sadrže malu količinu organskih rastvarača.

**First and second generations hyperbranched alkyd resins based on ricinoleic acid**

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The hyperbranched alkyd resins are hydroxylated hiperbranched polyesters modified with fatty acids. Highly branched chains have several advantages compared to the conventional alkyd resins with the same molecular weight, such as, a lower viscosity and better chemical resistance. In this work, first and second generations of hyperbranched polyesters have been synthesized from ditrimethylol propane and 2,2-bis(hydroxymethyl) propionic acid via an acid catalyzed reaction. Hyperbranched alkyds were obtained by esterification of synthesized hyperbranched polyesters with ricinoleic acid. The resins were characterized by determination of acid and hydroxyl numbers, viscosity, average molecular masses and molecular masses distribution. The structures of the resins were confirmed by Fourier transform infrared spectroscopy (FTIR). Synthesized alkyd resins have high hydroxyl and low acid numbers. The presence of hydroxyl groups as functional end groups opens up a high potential for further chemical modifications. The index of resin polydispersity increases from 1.59 to 3.84 with increase of alkyd resin generation. Due to low viscosities of synthesized resins, corresponding alkyd products contain less organic solvents.



HTM04-P

**Uticaj sadržaja poli(dimetilsiloksana) na neka fizička svojstva termoplastičnih poliuretana**

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Segmentirani poliuretani predstavljaju važnu klasu termoplastičnih elastomera koji su našli primenu u medicini za izradu dugotrajnih implanata. Jedan od načina da se poboljša biostabilnost i biokompatibilnost termoplastičnih poliuretana je uvođenje poli(dimetilsiloksana) u polimerni lanac. Serija novih termoplastičnih poliuretana (TPUs) sintetisana je dvostepenom poliadicijom u rastvoru polazeći od 4,4'-metilendifenildiizocijanata (MDI), 1,4-butandiola (BD) i  $\alpha,\omega$ -dihidroksipropil-poli(dimetilsiloksana) (PDMS). Sadržaj mekih PDMS segmenata je variran od 34 do 62 mas%. Struktura i sastav kopolimera određeni su  $^1\text{H}$  i  $^{13}\text{C}$  NMR spektroskopijom, dok su vrste vodoničnih interakcija u TPUs analizirane FTIR spektroskopijom. Uticaj sadržaja mekog PDMS segmenta na strukturu, termička i neka fizička svojstva kopolimera, su takođe ispitani. Termička stabilnost kopolimera se povećavala sa povećanjem sadržaja PDMS-a. Pokazano je da stepen kristaliničnosti, a samim tim i temperature topljenja i kristalizacije, kao i temperatura ostakljivanja TPUs rastu sa povećanjem masenog udela tvrdih MDI-BD segmanata. SEM analiza je pokazala da sintetisani kopolimeri imaju fibrilarnu morfologiju, koja potiče od kristalizacije MDI-BD segmenata.

**The influence of poly(dimethylsiloxane) content on some physical properties of thermoplastic polyurethanes**

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Segmented polyurethanes are an important class of thermoplastic elastomers that are used in medicine as long-term implants. Biostability and biocompatibility of polyurethanes can be improved by the introduction of poly(dimethylsiloxane) in the polymer chain. A series of novel thermoplastic polyurethanes (TPUs) was synthesized by two-step polyaddition reaction in solution from 4,4'-methylenediphenyl diisocyanate (MDI), 1,4-butanediol (BD) and  $\alpha,\omega$ -dihydroxypropyl-poly(dimethylsiloxane) (PDMS). The content of soft PDMS segment was varied between 34 and 62 wt.%. The structure and composition of the TPUs were determined by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy, while the hydrogen bonding interaction in the TPUs were analyzed by FTIR spectroscopy. The influence of PDMS content on the structure, thermal and some physical properties of the TPUs were also investigated. Thermal stability of the copolymers increased with increasing PDMS content. It was clearly demonstrated that the degree of crystallinity, the melting and crystallization temperatures as well as glass transition temperatures increased with increasing weight fraction of the hard MDI-BD segment. SEM analysis confirmed the presence of a fibrillar morphology, which arises from the crystallization of the MDI-BD segments.



HTM05-P

### **Sekvencijalna anjonska polimerizacija materijala kome rapidno opada rastvorljivost sa porastom temperature**

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Značaj membrana koje menjaju permeabilnost sa promenom temperature je naglo porasla zbog mogućnosti primene ovih membrana za separaciju proteina. Materijali koji mogu da budu primenjeni u ovu svrhu obuhvataju diblok-kopolimere kod kojih jedan blok daje mehaničku čvrstoću membrani, dok drugi blok menja svoju rastvorljivost sa promenom temperature. Da bi sintetisani diblok-kopolimer imao zahtevana svojstva, neophodno je da indeks polidisperzije bude što je manji mogući (da bi se postigla mikrofazna separacija), a da srednja molarna masa bude veća od 100000 g/mol (da bi se postigla odgovarajuća mehanička čvrstoća membrane). Poli(stiren) (PS) je korišćen kao mehanički stabilna komponenta, a poli(2-(metoksietoksi)etil metakrilat) (PDEEMA), koji ima donju kritičnu temperaturu rastvorljivosti (LCST) na 299 K je korišćen kao aktivna komponenta membrane. Zbog veoma strogih zahteva kada je u pitanju struktura diblok-kopolimera, za sintezu je korišćen postupak sekvencijalne anjonske polimerizacije. Vrednost indeksa polidisperznosti je zadržana na niskom nivou (do 1.1) uz molarni udeo PDEEMA od 15 %, dok je srednja molarna masa po brojnoj vrednosti određena pomoću gelpropusne hromatografije (GPC) iznosila 30000 g/mol.

### **Sequential anionic polymerization of material with rapid decrease in solubility with temperature increase**

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The significance of the membranes that change their permeability with the change of the temperature has rapidly increased as they could be applied for the protein separation. Materials that could be used for this purpose include diblock-copolymers with one block which would act as the mechanical supporter of the membrane, and the other one that rapidly changes its solubility with the temperature. To fulfill the task, the synthesized diblock-copolymer must have polydispersity index as low as possible (in order to obtain microphase separation) and average molar mass exceeding 100000 g/mol (in order to get sufficient mechanical stability). Poly(styrene) (PS) acted as a mechanically stable component, and the poly(2-(methoxyethoxy)ethyl methacrylate) (PDEEMA) which shows the lower critical solution temperature (LCST) at 299 K acted as an active component. Due to the strict conditions for the desired structure of the diblock-copolymer, sequential anionic polymerization was used for the synthesis. The polydispersity index remained low (up to 1.1) with the molar amount of PDEEMA up to 15 %, while the number average molar mass, determined by gel permeation chromatography (GPC) was up to 30000 g/mol.



HTM06-P

### Mehanička svojstva smeša linernog i hiperrazgranatih uretan akrilata umreženih dejstvom UV zračenja

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Ispitivane su smeše uretan akrilata na bazi linearnog poliestra i dva uretan akrilata, sa istim stepenom akrilovanja, na bazi alifatskih hiperrazgranatih poliestara (HRP). Linearni poliestar sintetisan je od neopentil glikola i adipinske kiseline. HRP treće generacije dobijen je od 2,2-bis(hidroksimetil)propionske kiseline i di-trimetilol propana. Modifikacija 60 % završnih OH grupa HRP-a izvedena je masnim kiselinama sojinog ulja ili izononskom kiselinom. Linearni uretan akrilat (LUA) i hiperrazgranati uretan akrilat (HUA) na bazi HRP modifikovanog masnim kiselinama sojinog ulja i HUA na bazi HRP modifikovanog izononskom kiselinom dobijeni su reakcijom određenog poliestra i izocijanatnog adukta, prethodno dobijenog reakcijom ekvimolarnih količina izoforon diizocijanata i 2-hidroksietil akrilata. Procena mešljivosti smeša LUA i HUA izvršena je na osnovu viskozimetrijskih merenja koristeći metodu koju je ustanovio Chee. Ovako pripremljenim smešama dodato je 20 mas. % heksandioldiakrilata i 4 mas. % fotoinicijatora, Irgacure 184, i umrežene su pod dejstvom UV zračenja. Umreženi uzorci ispitivani su u ogledima dinamičkog uvijanja i jednoosnog istezanja. Mehanička svojstva umreženih uzoraka zavise od mešljivosti komponenata smeše i od njenog sastava.

### Mechanical Properties of UV Cured Mixture of Linear and Hyperbranched Urethane Acrylates

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The mixtures of urethane acrylate resin based on linear polyester and two urethane acrylates, with the same degree of acrylation, prepared from partially modified aliphatic hyperbranched polyesters (HBP), were examined. Linear polyester was obtained from neopentil glycol and adipic acid. HBP of the third generation was synthesized from 2,2-bis(hydroxymethyl)propionic acid and di-trimethylol propane. The modification of 60 % OH end-groups of HBP was carried out with soybean fatty acids or isononanoic acid. Linear urethane acrylate (LUA) and hyperbranched urethane acrylate (HUA) based on the HBP modified with soy been faty acid and HUA based on the HBP modified with isononanoic acid were obtained by reaction of appropriate polyester and NCO adduct, previously obtained by reaction of equimolar amount of isophorone diisocyanate and 2-hydroxyethyl acrylate. The miscibility of the prepared mixtures of LUA and HUAs was estimated according to viscosity measurements using the approach developed by Chee. UV curable formulation was obtained by adding hexanediol diacrylate (20 wt. %) and photoinitiator, Irgacure 184, (4 wt. %) to the prepared LUA and HUA mixtures. The UV cured samples were examined by dynamic torsion and uniaxial tension. It was obtained that mechanical properties of the UV cured samples depend on miscibility of mixture's constituents and on its composition.



**Organska hemija / Organic Chemistry**  
**Usmena saopštenja / Oral Presentations**

OH01-O

**Kompjuterski dizajn peptidnih inhibitora interakcije proteina CDK9 i ciklina T1**

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Ciklin zavisna kinaza 9 (CDK9) i ciklin T1 stupaju u interakciju u proteinskom kompleksu PTEF-b koji predstavlja jedan od opštih pozitivnih faktora transkripcije. Studije ukazuju da njegova inhibicija dovodi do apoptoze tumorskih ćelija u ćelijskim linijama neuroblastoma.

Aminokiseline značajne za interakcije proteinskih komponenti utvrđene su proučavanjem kristalne strukture kompleksa koja je u literaturi poznata od 2008. godine. Na osnovu tih saznanja dizajnirano je više peptida kao mogućih liganada CDK9 koji bi potencijalno inhibirali nastanak kompleksa CDK9/ciklin T1. Četiri peptida su zasnovana na vezivnoj sekvenci ciklina T1 (i vezani za aktivno mesto docking-om), a ostali su dizajnirani iz fragmenata (fragment-based design), primenom SEED/GANDI programa. Energije vezivanja potencijalnih inhibitora procenjene su MMPBSA metodologijom.

Peptidi sa najpovoljnijim izračunatim energijama vezivanja su potencijalni kandidati za dizajn inhibitora peptidomimetika.

**Computational design of peptide inhibitors for CDK9/cyclin T1 protein interaction**

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Cyclin-dependent kinase 9 (CDK9) and cyclin T1 interact as parts of the PTEF-b protein complex, which is one of general positive transcription factors. Studies indicate that its inhibition induces apoptotic tumor cell death in neuroblastoma cell lines.

Amino acids important to complex stability were determined by studying the crystal structure of the complex, published in 2008. Based on these findings several peptides were designed as possible ligands of CDK9 that could potentially inhibit the complex formation. Four of the peptides are based on the binding sequence of cyclin T1 and docked virtually to the active site, while the rest have been designed through the methods of fragment based design, using SEED/GANDI software. The binding energies of potential inhibitors have been evaluated through use of MMPBSA methodology.

Peptides with the most favourable calculated binding energies are potential candidates for peptidomimetic inhibitor design.



OH02-O

**Sinteza i biološka aktivnost  
1-(2-metoksifenil)-4-((1-(arilmetil)piperidin-4-il)metil) piperazina**

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U nastavku ispitivanja slabih interakcija između liganada i receptora dopaminskog i serotoniniskog sistema, sintetisana je serija aril-piperazinskih derivata sa elektron akceptorskom nitro grupom. Kod svih novosintetisanih liganada ispitan je afinitet vezivanja za dopaminske ( $D_2$ ), serotoniniske ( $5HT_{1A}$  i  $5HT_{2A}$ ) receptore. Sintetisana jedinjenja su testirana *in vitro* u eksperimentima kompeticije sa odgovarajućim radioaktivnim ligandima. Testovi su rađeni na sinaptosomalnim membranama izolovanim iz mozga pacova.

**R**

**H**

2-NO<sub>2</sub>

3-NO<sub>2</sub>

4-NO<sub>2</sub>

**Synthesis and biological activity of  
1-(2-methoxyphenyl)-4-((1-(arylmethyl)piperidin-4-yl)methyl)piperazines**

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In order to continue our investigation in weak interactions between ligands and dopaminergic and serotonergic receptors we synthesized series of arylpiperazines ligands with electron withdrawing nitro-group.

All newly synthesized compounds were evaluated for the binding affinity towards dopaminergic ( $D_2$ ), serotonergic ( $5HT_{1A}$  and  $5HT_{2A}$ ) receptors by *in vitro* displacement of corresponding specific radioactive ligands from rat striatal or cortical synaptosome.



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D-Glucose  $\xrightarrow{\text{3 Steps}}$  **3**  $\xrightarrow[\text{reflux}]{\text{Imd}_2\text{CO, toluene}}$  **4**  $\xrightarrow[0^\circ\text{C} \rightarrow \text{rt}]{\text{9:1 TFA/H}_2\text{O}}$  **5**  $\xrightarrow[0^\circ\text{C, atm. N}_2]{\text{Ph}_3\text{P:CHCO}_2\text{Me, MeOH, Et}_3\text{N}}$  **1** + **2**

(+)-Goniobutenolide A (**1**)      (–)-Goniobutenolide B (**2**)

Ivana Kovačević, Mirjana Popsavin, Goran Benedeković, Vesna Kojić\*  
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A new and efficient synthetic approach toward naturally occurring styryl lactones (+)-goniobutenolide **1** and (-)-goniobutenolide **2** is described. Benzylic alcohol **3** that was easily available from D-glucose, was converted to the target compounds through a three-step sequence outlined in the reaction scheme. The key step of the synthesis was a new one-pot process that started with a *Z*-selective Wittig olefination of **4** under basic conditions, followed by subsequent lactonisation and final decarboxylation to furnish a mixture of **1** and **2**. Additionally, the results of evaluation of antiproliferative activity of both final products against certain human tumour cell lines, will be presented and discussed in details.



OH04-O

**Kinetička ispitivanja ciklizacionih reakcija nekih terpenskih alkohola**

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Supstituisani tetrahidrofuranski i tetrahidropiranski ciklični sistemi predstavljaju vrlo česte strukturne jedinice koje ulaze u sastav mnogih bioaktivnih prirodnih proizvoda. Intramolekularna heterociklizacija  $\Delta^4$ - i  $\Delta^5$ - alkenola je jedna od nabrzih i najlakših metoda za sintezu cikličnih etara velike strukturne raznovrsnosti i mogućnosti za dalje transformacije.

Predmet istraživanja ovog rada je uticaj nekih Luisovih baza (triethylamin, piridin, hinolin, 2, 2'-bipiridin i piperidin) na brzinu reakcije ciklizacija  $\alpha$ -terpineola, linalola i nerolidola sa PhSeCl i PhSeBr kao reagensima. Reakcije su praćene UV-VIS spektrofotometrijski kao reakcije *pseudo*-prvog reda, u prisustvu i odsustvu pomenutih baza, pri čemu je THF korišćen kao rastvarač. Dobijene vrednosti konstanta brzina su pokazale da su reakcije sa PhSeBr sporije, nego kada se kao reagens koristi PhSeCl. U poređenju sa reakcijama u kojima nije bio prisutan katalizator, brzine katalizovanih reakcija su rasle u zavisnosti od jačine korišćene Lewi-ove baze i njene volumenoznosti. Sterne smetnje koje se javljaju u fazi zatvaranja prstena, koja ujedno i određuje brzinu posmatrane hemijske reakcije, su jedne od glavnih karakteristika koje utiču na vrednost brzine hemijske reakcije.

**Kinetic investigation of cyclization reactions of some terpenic alcohols**

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Substituted tetrahydrofuran and tetrahydropyran ring systems are common structural units found in many bioactive natural products. Intramolecular heterocyclization of  $\Delta^4$ - and  $\Delta^5$ - alkenols is one of the fastest and easiest ways for obtaining cyclic ethers with very high structural diversity and possibility for further functionalization.

In this work we investigated the influence of some Lewis bases (triethylamine, pyridine, quinoline, 2, 2'-bipyridine and piperidine) on rate constants of the electrophile-mediated cyclization of  $\alpha$ -terpineol, linalool and nerolidol with PhSeCl and PhSeBr as reagents. Reactions were performed under the *pseudo*-first order conditions, in the presence and absence of bases, by UV-VIS spectrophotometry in THF as a solvent. The obtained values for rate constants have shown that the reactions with phenylselenenyl bromide are slower than with chloride. Depending on the catalyst basicity and bulkiness, reaction rate is increased with a different degree compared to no catalyzed reaction. Steric hindrance in the rate determining ring closing phase is the one of the main reasons that influence the value of rate constants in these reactions.



OH05-O

### 1,7-bis(alkilamino)diazahrizeni inhibitori tri različita patogena: botulinum neurotoksin (BoNT/A LC), parazita malarije *P. falciparum* i filovirusa Ebole

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Sina Bavari\*\*\*, Bogdan A. Šolaja\*,

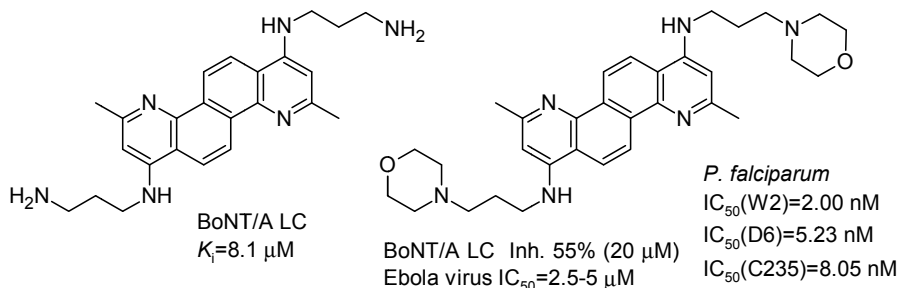
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Opisana je sinteza derivata 1,7-bis(alkilamino)diazahrizena (**1,7-DAAC**) i rezultati detaljnih ispitivanja biološke aktivnosti. Dobijeni rezultati pokazuju da derivati efikasno inhibiraju aktivnost tri različita tipa patogena: botulinum neurotoksin (BoNT/A LC), parazit malarije (*P. falciparum*) i filovirus EBOV). Rezultati inhibicije građenja  $\beta$ -hematina ukazuju da **1,7-DAAC** imaju sličan mehanizam dejstva kao 4-hlor-4-aminohinolinski antimalarici. Dobijeni rezultati biće detaljno prikazani u radu.



### 1,7-bis(alkylamino)diazachrysenes as Inhibitors of Three Unrelated Pathogens: The Botulinum Neurotoxin (BoNT/A LC), *P. falciparum* Malaria, and the Ebola Filovirus

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Herein, we provide results that derivatives of **1,7-DAAC** (1,7-bis(alkylamino)diazachrysenes) possess the ability to inhibit the three unrelated pathogens (described above): a bacterial toxin (the BoNT/A LC), a protozoan (malaria), and a filovirus (EBOV). Several of the 1,7-DAAC derivatives are potent *in vitro* inhibitors of *P. falciparum*, and in general, are more efficacious against CQ-resistant strains than against CQ-susceptible strains. By inhibiting  $\beta$ -hematin formation, the most efficacious 1,7-DAAC-based antimalarials employ a mechanism of action analogous to that of 4,7-ACQ-based antimalarials, and are well tolerated by normal cells. Finally, the 1,7-DAAC-based derivatives exhibited promising activities against Ebola filovirus inhibition. Observed results will be discussed in details.

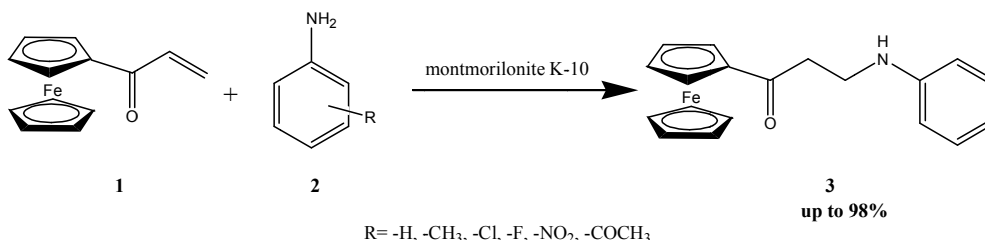
**Acknowledgment:** This research was supported by NATO's Public Diplomacy Division in the framework of "Science for Peace" project SfP983638 and by the Ministry of Science and Technological Development of Serbia (grant no. 172008)



### Синтеза 3-аминоарил-1-фероценилпропан-1-она

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β-Аминокарбонилна једињења (Mannich-ове базе) су цењени синтетички блокови који се могу трансформисати у бројне деривате, као што су 1,3-аминоалкохоли и производи нуклеофилне супституције атома азота. Међу бројним применама Mannich-ових база и њихових деривата најважнија је, свакако, синтеза разноврсних фармацеутских препарата.<sup>1</sup> У овом раду биће описана синтеза серије Mannich-ових база (**3**) аза-Michael-овом адисијом одговарајућих анилина (**2**) на фероценил-винил кетон (**1**), катализованом монтморилонитом K-10 у микроталасној пећи.



### Synthesis of 3-aminoaryl-1-ferrocenyl-propan-1-ones

Dragana D. Stevanović, Ivan S. Damljanović, Anka Z. Pejović  
 Danijela S. Ilić-Komatina\*, Rastko D. Vukićević  
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β-Aminocarbonyls (Mannich bases) are versatile synthetic building blocks, which can easily be converted into a range of useful derivatives, such as 1,3-aminoalcohols and products of the substitution of the amino group with some other nucleophile. Among many applications of Mannich bases and their derivatives, however, the most important ones are surely those applied in synthesis of pharmaceuticals.<sup>1</sup> In this report will be described the synthesis of a series of Mannich bases (**3**) via montmorillonite K-10 catalyzed aza-Michael addition assisted by MW irradiation of the corresponding anilines (**2**) to ferrocenyl-vinyl ketone (**1**).

1. M. Tramontini, L. Angiolini, Mannich-Bases, Chemistry and Uses, CRC, Boca Raton, FL, 1994.

OH07-O

### Premeštanja alkil-radikala dugog niza

Aleksandar V. Teodorović, Dalibor M. Badjuk, Nenad Stevanović  
*Prirodno-matematički fakultet, Kragujevac, Radoja Domanovića 12, Kragujevac, Srbija*

U ovom radu je ispitivano premeštanje 1-oktil, 1-decil i 1-tridecil intermedijera (radikalskog i/ili katjonskog tipa) analizom proizvoda i njihovom distribucijom. Ovi intermedijeri dobiveni su termičkom i fotolitičkom olovo(IV)-tetraacetatnom dekarboksilacijom nonanove, undekanove i tetradekanove kiseline u benzenskom rastvoru. Poređenje distribucije tridecil- i oktil-acetata dovodi do pretpostavke da je 1,7~homolitičko premeštanje vodonika značajno zastupljeno kod 1-oktil-radikala. Odnosi 1,5~, 1,6~ i eventualno postojećeg 1,7~homolitičkog premeštanja vodonika u 1-oktil-radikalu, kao i sukcesivnih 1,2~hidridnih premeštanja u odgovarajućim katjonima simulirani su Monte-Carlo metodom. Izgleda da je ova tehnika korisna za razlikovanje 1,7~H<sup>•</sup> u odnosu na 1,2~H<sup>•</sup> intermedijere (neobeležene). Uzimajući u obzir da su odnosi 1,5~H<sup>•</sup> /1,6~H<sup>•</sup> za 1-oktil- i 1-tridecil sistem (2,74) uporedivi, i koristeći prinose proizvoda (1-feniloktan, oktan, okteni i acetati) takođe kao ulazne podatke za simulaciju, dobili smo da je 1,5~H<sup>•</sup> /1,6~H<sup>•</sup> /1,7~H<sup>•</sup> = 85/31/1 za termičku dekarboksilaciju. Međutim, manje su prihvatljivi rezultati dobiveni za fotolitičku reakciju.

### Long-chain alkyl radicals rearrangements

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In this work the rearrangements of 1-octyl, 1-decyl and 1-tridecyl intermediates (of the radical and/or carbocation type) were investigated on the product analysis and product distribution. These intermediates were obtained by thermal and photolytic lead(IV) tetraacetate decarboxylation of nonanoic, undecanoic and tetradecanoic acid in a benzene solution. Comparison of the distributions of tridecyl and octyl acetates leads to the assumption that 1,7~homolytical rearrangement of hydrogen is notably included in 1-octyl radical. The relationships between 1,5~, 1,6~ and eventual existing 1,7~homolytic transfer of hydrogen in 1-octyl radical, as well as successive 1,2~hydride shifts in corresponding cations have been simulated by Monte-Carlo (MC) method. It seems that this technique is useful for making distinction between 1,7~H<sup>•</sup> toward 1,2~H<sup>•</sup> in 1-octyl intermediates (unlabeled). Input data for MC simulation are (a) product yields (1-phenyloctane, octane, octenes and acetates) and (b) ratio 1,5~H<sup>•</sup> /1,6~H<sup>•</sup> for 1-tridecyl radical (2.74) taken as equal in rearrangement of 1-octyl radical as well. Thus, in the case of thermal decarboxylation we obtained that 1,5~H<sup>•</sup> /1,6~H<sup>•</sup> /1,7~H<sup>•</sup> = 85/31/1. However, the results obtained for the photolytic reaction being less acceptable.



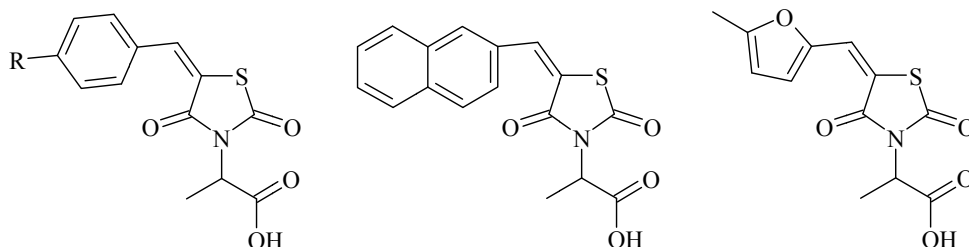
OH08-O

## Sinteza novih derivata propionske kiseline iz 5-ariliden-2,4-dioksotetrahidrotiazola

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Derivati propionske kiseline spadaju u grupu nesteroidnih anti-inflamatornih lekova. Veliki broj nesteroidnih anti-inflamatornih jedinjenja koristi se u kliničkoj praksi za lečenje inflamatornih bolesti, uključujući reumatoidni artritis, osteoartritis, ankilozirajući spondilitis i burzitis, kao i za prevenciju infarkta miokarda i Alchajmerove bolesti.

U cilju pronalaženja novih nesteroidnih anti-inflamatornih agenasa, u ovom radu je sintetizovano šest novih derivata propionske kiseline sa 2,4-dioksotetrahidrotiazolskim jezgrom (Slika 1). Struktura i čistoća novih 2-(5-ariliden-2,4-dioksotetrahidrotiazol-3-il)propionskih kiselina potvrđena je  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR i FT-IR spektrima.



Slika 1. Struktura 2-(5-ariliden-2,4-dioksotetrahidrotiazol-3-il)propionskih kiselina ( $R$ :  $H$ ,  $\text{MeO}$ ,  $N(\text{CH}_3)_2$ ,  $F$ )  
 Figure 1. Structure of 2-(5-arylidene-2-dioxotetrahydrothiazole-3-yl)propionic acids ( $R$ :  $H$ ,  $\text{MeO}$ ,  $N(\text{CH}_3)_2$ ,  $F$ )

## Synthesis of new propionic acid derivatives from 5-arylidene-2,4-dioxotetrahydrothiazol

Bojan Đ. Božić, Nemanja Trišović, Milica Rančić, Gordana Ušćumlić  
 Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

Propionic acid derivatives belong to the group of non-steroidal anti-inflammatory drugs. A great number of non-steroidal anti-inflammatory compounds have been used in clinical practice for the treatment of inflammatory disorders including reumathoid arthritis, osteoarthritis, ankylosing spondylitis and bursitis as well as for prevention of myocardial infarction and Alzheimer's disease. In the search for new non-steroidal anti-inflammatory agents, in this research six new derivatives of propionic acid with 2,4-dioxotetrahydrothiazol core are synthesized (Figure 1). Structure and purity of new 2-(5-arylidene-2-dioxotetrahydrothiazole-3-yl)propionic acids are confirmed by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and FT-IR spectra.

Posterska saopštenja / Poster Presentations

OH09-P



**Кинетика и механизам адисије пиперидина и бензиламина  
на фениламида ароилакрилних киселина**

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Милица Радуловић\*, Бранко Ј. Дракулић\*\*\*  
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\*\*Војно -технички институт, Ратка Ресановића 1, Београд, Србија

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Константе брзине реакције адисије депротонованог пиперидина и бензиламина на конгенерну серију фениламида ароилакрилних киселина у метанолу одређене су помоћу UV-VIS спектрофотометрије, под условима псеудо-првог реда. Утицај супституената на константе брзина реакције квантификован је помоћу Хаметових константи супституената и наелектрисања израчунатих за електрофилни угљеников атом (са и без модела имплицитног растварача), употребом DFT метода. Вредности Хаметових реакционих константи и испитивање реакције у различитим растварачима дају индикације о вероватном механизму ове реакције.

**Kinetic and mechanism of the addition of piperidine and benzylamine  
to the aroylacrilic acid phenylamides**

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Radulović\*, Branko J. Drakulić\*\*\*  
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The rate constants for the addition of deprotonated piperidine and benzylamine to the congeneric series of aroylacrilic acid phenylamines in methanol were determined by UV-VIS spectrophotometry, under the pseudo first-order conditions. The influence of substituents on the rate constants was quantified by Hammett substitution constants, and the charges calculated for the electrophilic carbon atom (with and without implicit solvent), on DFT level of theory. The values of Hammett reaction constants, along with the examination of reaction in different solvents gave indication of reaction mechanism.

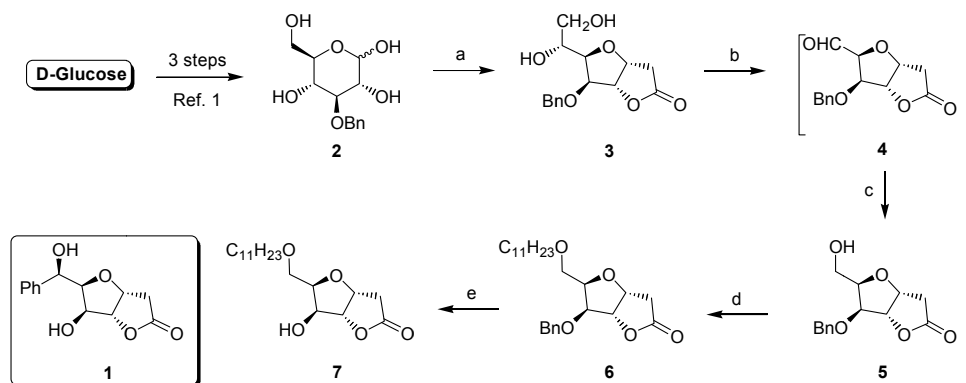


OH10-P

**Sinteza i antiproliferativna aktivnost novog analoga (+)-goniofufurona**

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 Gordana Bogdanović\*, Velimir Popsavin  
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 \*Institut za onkologiju Vojvodine, Institutski put 4, Sremska Kamenica, Srbija

(+)-Goniofufuron (**1**) je prirodni stiril-lakton koji pokazuje *in vitro* antiproliferativnu aktivnost prema izvesnim humanim neoplastičnim ćelijama. U potrazi za novim antitumorskim agensima, planirano je dobijanje odgovarajućeg nestirilnog analoga **7** radi poređenja njegove biološke aktivnosti sa aktivnošću osnovnog molekula **1**. Parcijalno zaštićena piranoza **2**, koja se lako može dobiti iz D-glukoze,<sup>1</sup> poslužila je kao pogodan polazni molekul. Laktol **2** je preveden u analog **7** nizom hemijskih transformacija prikazanih na reakcionoj shemi. Rezultati antiproliferativne aktivnosti molekula **7** prema ćelijama odabranih humanih tumora detaljno će biti prikazani i diskutovani.



Reagents and conditions: (a) Meldrum's acid, Et<sub>3</sub>N, DMF, 46–48 °C, 70 h, 43%;  
 (b) NaIO<sub>4</sub>, 2:1 MeOH/H<sub>2</sub>O, 0 °C → rt, 2 h; (c) NaBH<sub>4</sub>, MeOH, 0 °C → rt, 3 h, 33% (from **3**);  
 (d) C<sub>11</sub>H<sub>23</sub>Br, Ag<sub>2</sub>O, AgOTf, Et<sub>2</sub>O, reflux, 8 h, 56%; (e) H<sub>2</sub>, 10% Pd/C, MeOH, rt, 3.5 h, 83%.

**Synthesis and antiproliferative activity of a novel (+)-goniofufurone analogue**

Bojana M. Srećo, Goran Benedeković, Jovana Francuz, Mirjana Popsavin, Vesna Kojić\*  
 Gordana Bogdanović\*, Velimir Popsavin  
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 \*Oncology Institute of Vojvodina, Institutski put 4, Sremska Kamenica, Serbia

(+)-Goniofufurone (**1**) is naturally occurring styryl lactone that shows *in vitro* antiproliferative activity against some human neoplastic cells. In the search for new antitumour agents, it was of interest to prepare the corresponding non-styryl analogue **7**, in order to compare its biological activity with that observed for the lead compound **1**. Partially protected pyranose **2** that was readily available from D-glycose,<sup>1</sup> served as a convenient starting compound. Lactol **2** was converted to the target **7** through a five-step sequence outlined in the reaction scheme. The results of antiproliferative activity of **7** against a number of human tumour cell lines will be presented and discussed in details.

Reference

1. Bichard, C. J. F.; Wheatley, J. R.; Fleet, W. J. *Tetrahedron: Asymmetry* **5** (1994) 431.





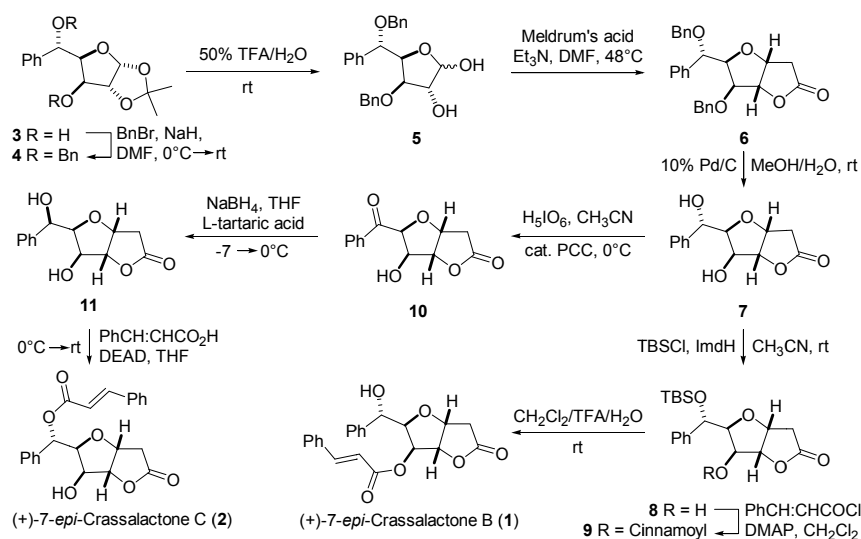
OH11-P

Totalna sinteza 7-*epi*-(+)-krasalaktona B i C iz D-glukoze

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(+)-Krasalaktone B i C su antitumorski stiril-laktone koji su nedavno izolovani iz tropske biljke *Polyalthia crassa*.<sup>1</sup> U ovom radu želimo da saopštimo prvu totalnu sintezu 7-*epi*-(+)-krasalaktone B i C (**1** i **2**). Kao polazno jedinjenje primenjen je diol **3** koji dobijen iz D-glukoze po modifikovanom literaturnom postupku<sup>2</sup>. Molekul **3** je prvo preveden u divergentni intermedijer **7**, koji je zatim transformisan u finalne proizvode **1** i **2** primenom višefazne sintetičke sekvence prikazane na reakcionoj shemi.

Total synthesis of 7-*epi*-(+)-crassalactones B and C from D-glucose

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(+)-Crassalactones B and C are antitumour styryl lactones that were recently isolated from the tropical plant *Polyalthia crassa*.<sup>1</sup> Herein we wish to report on the first total synthesis of 7-*epi*-(+)-crassalactones B and C (**1** and **2**). Diol **3** that was readily available from D-glucose through a slightly modified literature procedure,<sup>2</sup> has served as a convenient starting material in this work. Molecule **3** was first converted to divergent intermediate **7**, which was subsequently transformed to final products **1** and **2**, according to the multi-step sequence shown in the reaction scheme.

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2. T. Gracza, P. Szolcsányi, *Molecules* **5** (2000) 1386.



OH12-P

**Sinteza i citotoksična aktivnost novih heterocikličnih androstanskih derivata**

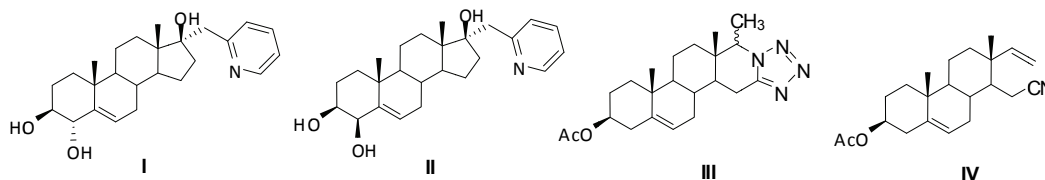
Jovana J. Ajduković, Aleksandar M. Oklješa, Marina P. Savić, Andrea R. Gaković

Evgenija A. Djurendić, Marija N. Sakač, Katarina M. Penov-Gaši

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Poznato je da mnoga steroidna heterociklična jedinjenja koja sadrže atom azota ili sumpora ispoljavaju različitu biološku aktivnost. Polazeći od dehidroepiandrosterona, izvršena je višefazna sinteza u cilju dobijanja novih androstanskih derivata sa heterocikličnim prstenom (jedinjenja **I**, **II**, **III** i **IV**). Jedinjenja **I** i **II** su testirana *in vitro* prema pet različitih tumorskih ćelijskih linija: adenokarcinom dojke estrogen receptor pozitivan, MCF-7, adenokarcinom dojke estrogen receptor negativan, MDA-MB-231, kancer prostate androgen receptor negativan, PC3, karcinom cerviksa, HeLa i karcinom debelog creva, HT-29, kao i prema zdravim ćelijama fetalnih fibroblasta pluća, MRC-5.



**Synthesis and cytotoxic activity of new heterocyclic androstane compounds**

Jovana J. Ajduković, Aleksandar M. Oklješa, Marina P. Savić, Andrea R. Gaković

Evgenija A. Djurendić, Marija N. Sakač, Katarina M. Penov-Gaši

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It is well known that a number of steroidal heterocyclic compounds containing nitrogen or sulphur, exhibited a wide variety of biological activities. Starting from dehydroepiandrosterone, we performed a multistep synthesis in order to obtain a new androstane derivatives with heterocyclic ring (compounds **I**, **II**, **III** and **IV**). The new compounds **I** and **II** were tested *in vitro* against five different tumor cell lines: human breast adenocarcinoma ER+, MCF-7, human breast adenocarcinoma ER-, MDA-MB-231, prostate cancer AR-, PC-3, human cervix carcinoma, HeLa, colon cancer, HT-29 as well as one human non-tumor cell line, MRC-5.

OH13-P

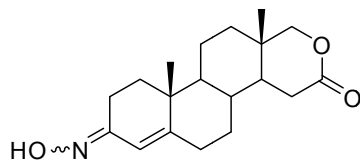
### Sinteza novih A, B i D modifikovanih androstanskih derivata

Andrea R. Gaković, Marina P. Savić, Jovana J. Ajduković, Aleksandar M. Oklješa

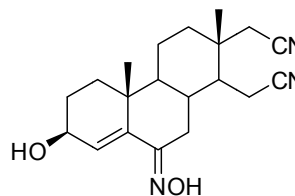
Evgenija A. Djurendić, Marija N. Sakač, Katarina M. Penov-Gaši

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Postoji nekoliko pristupa lečenju kancera dojke, a najefikasniji način za lečenje hormon-zavisnih karcinoma dojke je smanjenje nivoa estrogena u tumorskim ćelijama inhibicijom biosinteze estrogena. Dokazano je da hidroksimino derivati, sa hidroksimino funkcijom u A ili B prstenu pokazuju izuzetnu citotoksičnost na više tipova ćelija raka, što je i opisano u literaturi. Tragajući za novim citotoksičnim jedinjenjima, istraživanja smo usmerili ka sintezi A i/ili B i/ili D modifikovanih androstanskih derivata, koji bi u svojoj strukturi sadržali oksimino funkciju. U tom cilju izvršena je višefazna sinteza oksimino derivata **1**, **2** i **3** polazeći od dehidroepiandrosterona. Odabrani sintetizovani derivati će biti ispitani na odabrane maligne ćelijske linije, kao i na zdrave ćelije fetalnih fibroblasta pluća.



**1,2**



**3**

### Synthesis of some new A, B and D modified androstane derivatives

Andrea R. Gaković, Marina P. Savić, Jovana J. Ajduković, Aleksandar Oklješa

Evgenija A. Djurendić, Marija N. Sakač, Katarina M. Penov-Gaši

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There are several approaches for therapy of breast cancer but the most effective way to treat hormone-dependent breast cancer is to deprive the cancer cells of estrogens by inhibiting their biosynthesis. The hydroximino derivatives with position of hydroximino function on ring A or B displayed remarkable distinct cytotoxicities against a diversity of cancer cell types, which was described in the literature. Searching for new cytotoxic compounds, studies are directed towards the synthesis of A and/or B and/or D modified androstane derivatives with oximino function. With this aim of investigation we have developed some new steroidal cytotoxic agents (**1**, **2**, **3**), with oximino function, in the multistep synthesis starting from dehydroepiandrosterone. Selected synthesized derivatives will be tested on chosen cancer cell lines and normal fetal lung fibroblasts.

OH14-P

**Sinteza 4-(supstituisanih fenil)-6-fenil-3-cijano-2-piridona  
iz etil-2-cijanoakrilata i acetofenona u mikrotalasnom reaktoru**

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U okviru radu ispitivana je sinteza 4-(supstituisanih fenil)-6-fenil-3-cijano-2-piridona reakcijom kondenzacije odgovarajućih etil-2-cijanoakrilata sa acetofenomom u prisustvu amonijum-acetata u mikrotalasnom reaktoru. Reakcije su izvođene u laboratorijskim mikrotalasnim reaktorima na atmosferskom i povišenom pritisku. Polazni etil-2-cijanoakrilati dobijeni su reakcijom etil-cijanoacetata i odgovarajućih arilaldehida. Ispitan je uticaj različitih parametara kao što su odnos reaktanata, reakciono vreme, reakciona temperatura, prisustvo rastvarača. Svi dobijeni proizvodi sinteze okarakterisani su temperaturama topljenja, NMR, IR i UV spektrima. Ostvareni prinosi, i na atmosferskom i na povišenom pritisku, su niski, pri čemu se reakciona vremena kreću od 5 do 15 min.

**Microwave-assisted synthesis of  
4-(substituted phenyl)-6-phenyl-3-cyano-2-pyridones from  
ethyl 2-cyanoacrylates and acetophenone**

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Microwave-assisted synthesis of 4-(substituted phenyl)-6-phenyl-3-cyano-2-pyridones from ethyl 2-cyanoacrylates and acetophenone in the presence of ammonium acetate was studied. Reactions were conducted in open and closed vessels in dedicated microwave reactors. Starting ethyl 2-cyanoacrylates were obtained by the reaction of ethyl cyanoacetate with corresponding aryl aldehydes using conventional methods. Effect of different parameters such as molar ratio of reactants, reaction time, reaction temperature and solvent was studied. All obtained products were characterized by melting points, NMR, IR and UV data. The obtained yields of 4-(substituted phenyl)-6-phenyl-3-cyano-2-pyridones under microwave irradiation were low in both vessels while reaction times were between 5 and 15 min.

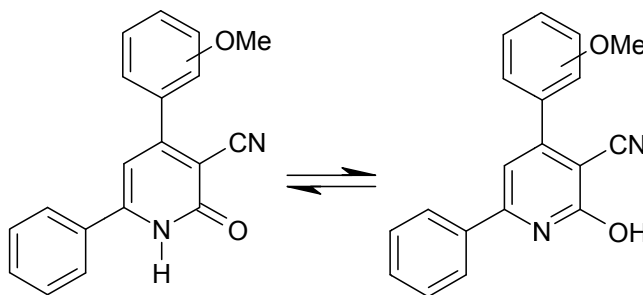


OH15-P

### Proučavanje 2-piridon/2-hidroksipiridin tautomerije na primeru 3-cijano-4-(2-, 3- i 4-metoksifenil)-6-fenil-2(1H)-piridona

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Uticaj supstituenata i rastvarača na ravnotežu tautomernih oblika 2-piridon/2-hidroksipiridin (slika) proučavan je snimanjem UV spektara 3-cijano-4-(2-, 3- i 4 metoksifenil)-6-fenil-2(1H)-piridona. UV apsorpcioni spektri su određeni u sedamnaest rastvarača različitih polarnosti, proton-donorskih i proton-akceptorskih svojstava. Kvantitativne vrednosti doprinosa solvatohromnih parametara  $\pi^*$ ,  $\alpha$ , i  $\beta$  su određene primenom Kamlet-Taftove jednačine. Optimizovane konformacije molekula su izračunate semi-empirijskom metodom MO PM6, a uticaj efekata rastvarača i prisutnih supstituenata je diskutovan u odnosu na definisane strukture.



*Piridon/2-hidroksipiridin tautomerna ravnoteža kod  
3-cijano-4-(2-, 3- i 4-metoksifenil)-6-fenil-2(1H)-piridona  
2-Pyridone/2-hydroxypyridone tautomeric equilibrium of  
3-cyano-4-(2-, 3- and 4-methoxyphenyl)-6-phenyl-2(1H)-pyridones*

### 2-Pyridone/2-hydroxypyridone tautomeric equilibrium of 3-cyano-4-(2-, 3- and 4-methoxyphenyl)-6-phenyl-2(1H)-pyridones

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The effects of substituents and solvents on tautomeric equilibrium of 2-pyridone/2-hydroxypyridone of 3-cyano-4-(2-, 3- and 4-methoxyphenyl)-6-phenyl-2(1H)-pyridones were studied using UV spectroscopy. UV absorption spectra have been recorded in seventeen solvents of different polarity and solvent/solute hydrogen bonding properties. Quantitative contribution of solvatochromic parameters  $\pi^*$ ,  $\alpha$ , and  $\beta$  were analysed by the use of Kamlet and Taft equation. Optimized molecular conformations were calculated on semi-empirical level using of MO PM6 method. Solvents and substituents effects were discussed in relation to such defined structures.

**OH16-P**

**Sinteza i biološka aktivnost nove izostere 7-deoksi-goniofufurona**

Miloš M. Svirčev, Mirjana M. Popsavin, Saša B. Spaić, Vesna V. Kojić\*

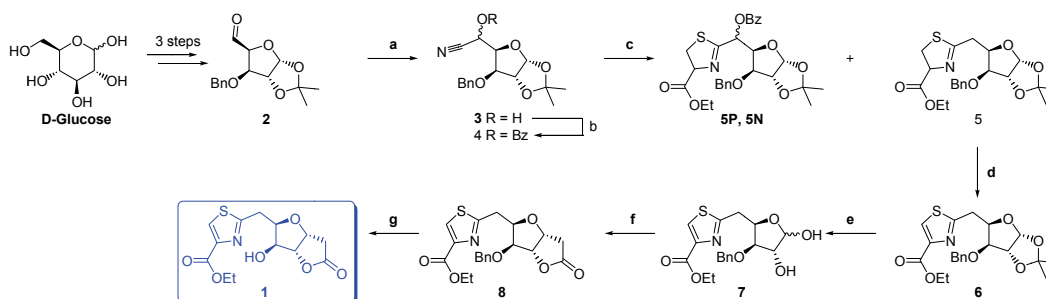
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U radu je ostvarena totalna sinteza nove izostere 7-deoksi-goniofufurona sa etil-estrom 2-tiazolil-4-karboksilne kiseline u položaju 7. Ključni intermedijer (**3**) je dobijen adicijom trimetilsilil-cijanida na poznati aldehid (**2**), koji je dobijen iz D-glukoze po delimično izmenjenom literaturnom postupku. Tiazolni prsten je uveden u dva uzastopna koraka (c i d, u toku kojih je došlo i do deoksigenovanja u položaju C-5), tačnije ciklizacijom i oksidacijom, dok je  $\gamma$ -laktonska funkcija izgrađena u pretposlednjem koraku (f), nakon uklanjanja zaštite u položajima C-1 i C-2 (e). Finalni proizvod **1** se dobija uklanjanjem benzilne zaštite na C-5 (g). U radu će biti prikazani i rezultati antiproliferativne aktivnosti jedinjenja **1** prema nekoliko tumorskih ćelijskih linija.



**Scheme 1.** Reagents and conditions: (a) TMSCN,  $\text{Ph}_3\text{PMel}$ ,  $\text{CH}_2\text{Cl}_2$ , rt; (b)  $\text{BzCl}$ ,  $\text{CH}_2\text{Cl}_2$ , Py,  $0^\circ\text{C} \rightarrow \text{rt}$ ; (c) L-cysteine ethyl ester hydrochloride, MeOH,  $\text{Et}_3\text{N}$ , rt; (d)  $\text{CBrCl}_3$ , DBU,  $\text{CH}_2\text{Cl}_2$ ,  $0^\circ\text{C} \rightarrow +4^\circ\text{C}$ ; (e) 90% aq TFA,  $0^\circ\text{C}$ ; (f) Meldrum's acid, DMF,  $\text{Et}_3\text{N}$ ,  $46-50^\circ\text{C}$ ; (g) Pd/C,  $\text{H}_2$ , rt.

**Synthesis and biological activity of new isostere of 7-deoxy-goniofufurone**

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Herein we report a total synthesis of a novel 7-deoxy-7-thiazolyl isostere of goniofufurone. The key intermediate (**3**) was obtained by addition of trimethylsilyl cyanide to known aldehyde (**2**), which was readily available from D-glucose through a modified literature procedure. Thiazole ring was introduced in two consecutive steps (c and d, during which benzoyloxy group was removed from C-5), which included cyclization and oxidation, respectively, while the  $\gamma$ -lactone function was built in the penultimate step (f), after the deprotection of hydroxyl groups at positions C-1 and C-2 (e). After removal of benzyl protection (g), final product (**1**) was obtained. Results of its antiproliferative activity against a number of tumour cell lines will be presented.



OH17-P

### Dizajn i sinteza novih antitumorskih stiril-laktona: Strategija otvaranja i zatvaranja prstena

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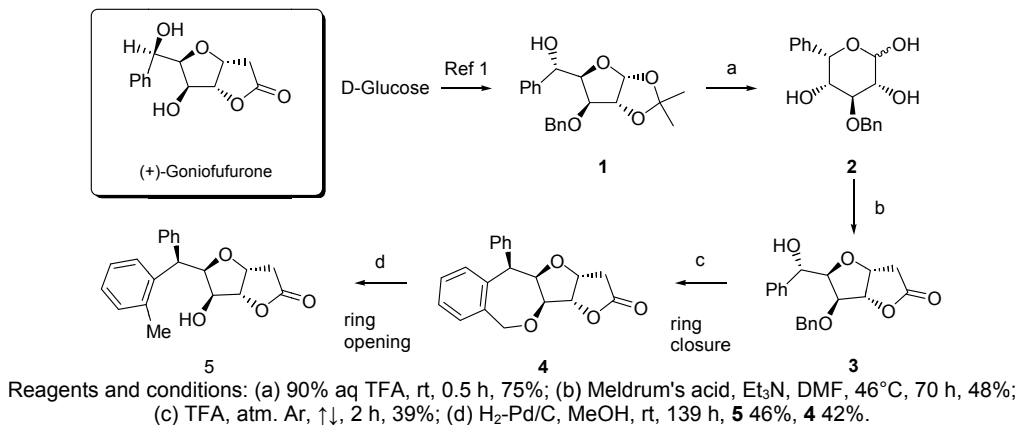
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Jedna od čestih strategija u dizajnu novih lekova jeste formiranje ili otvaranje prstena u strukturi vodećeg molekula. U ovom radu želimo da saopštimo primenu ove strategije u sintezi dva nova antitumorska stiril-laktona (**4** i **5**), kao i preliminarne rezultate bioloških ispitivanja njihove antiproliferativne aktivnosti prema ćelijama odabranih humanih tumora. Benzilni alkohol **1**, koji je lako pristupačan iz D-glukoze, preveden je u analoge **4** i **5** višefaznom sekvencom koja je prikazana na reakcionoj shemi.



### Design and synthesis of new antitumoral styryl lactones: the ring opening and ring closure strategy

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A common strategy in the design of new drugs is the ring closure or ring opening in the structures of lead compound. Herein we want to report the implementation of this strategy in the synthesis of two novel goniofufurone analogues (**4** and **5**), and a preliminary bioassay against selected human tumour cell lines. Benzylic alcohol **1**, which was readily available from D-glucose<sup>1</sup>, was converted to analogues **4** and **5** through multistep sequence outlined in reaction scheme.

1. T. Gracza, P. Szolcsányi, *Molecules*. **5** (2000) 1386-1398.





OH18-P

**Sinteza i *in vitro* antitumorska aktivnost novih mimetika tiazofurina**

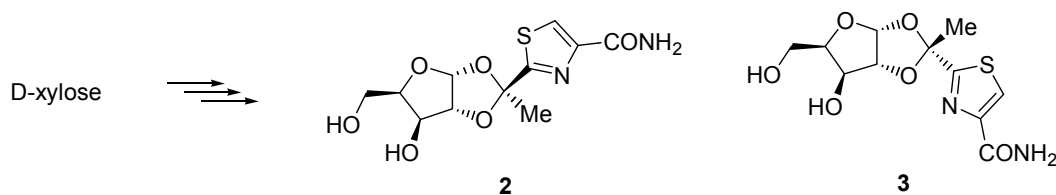
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Tiazofurin je sintetički C-nukleozid koji pokazuje zapaženu citotoksičnost prema izvesnim humanim neoplastičnim ćelijama. Primenom osmo-fazne sintetičke sekvence, dobijena su dva nova triciklična mimetika tiazofurina (**2** i **3**). Sekvenca podrazumeva višefaznu transformaciju D-ksiloze u pogodno zaštićene ksilofuranosil-diacetate, koji nakon reakcije sa trimetilsililecijanidom daju odgovarajuće cijano-ortoestre. Konverzija nitrilne funkcije u tiazolni prsten ostvarena je dejstvom metil-cisteinata, uz naknadnu oksidaciju i finalnu amonolizu, pri čemu se dobijaju finalni proizvodi **2** i **3**. Ispitivana je citotoksična aktivnost mimetika **2** i **3** prema nekoliko malignih i jednoj zdravoj ćelijskoj liniji.



**Synthesis and *in vitro* antitumour activity of novel mimics of tiazofurin**

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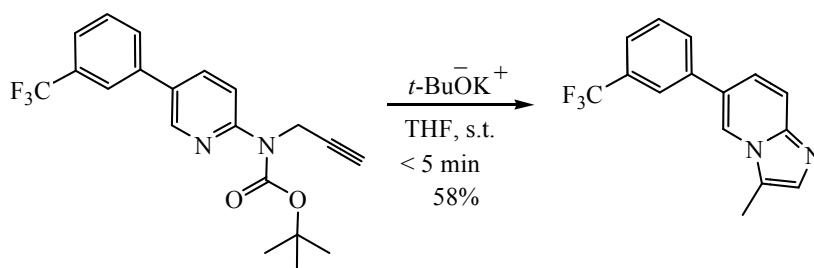
Tiazofurin is a synthetic C-nucleoside that shows remarkable cytotoxicity against certain human neoplastic cells. Two novel tricyclic tiazofurin mimics (**2** and **3**) were prepared through an eight-step sequence starting from D-xylose. The sequence involves a multi-step conversion of D-xylose to suitably protected xylofuranosyl acetates, followed by their subsequent treatment with trimethylsilyl cyanide to give the corresponding cyano-orthoesters. Conversion of the nitrile group into the thiazole ring was carried out by treatment with cysteine methyl ester, followed by oxidation and final ammonolysis to products **2** and **3**. In vitro antiproliferative activities of **2** and **3** against a number of human tumour cells were recorded and compared with those observed for tiazofurin.

OH19-P

**Ciklizacija *N*-propargilaminopiridina u baznoj sredini.  
Sinteza derivata imidazo[1,2-*a*]piridina**

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 \*Farmaceutski fakultet, Institut za organsku hemiju, Beograd, Vojvode Stepe 450,  
 11000 Beograd, Srbija

Ciklizacija zaštićenih *N*-propargilaminopiridina u baznoj sredini se pokazala kao efikasna metoda za sintezu derivata imidazo[1,2-*a*]piridina. Reakcije su izvođene uz mali višak baze na sobnoj ili malo povišenoj temperaturi, pri čemu su dobijeni heterociklični proizvodi u dobrim prinosima. Pokazano je da na proces ciklizacije utiču stereoelektronske osobine supstituenata na piridinskom prstenu.



**A base promoted cyclisation of *N*-propargylaminopyridines.  
Synthesis of imidazo[1,2-*a*]pyridine derivatives**

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 \*Faculty of Pharmacy, Department of Organic Chemistry, Vojvode Stepe 450,  
 11000 Belgrade, Serbia

A base promoted cyclisation of the protected *N*-propargylaminopyridines was shown to be an efficient method for the preparation of imidazo[1,2-*a*]pyridine derivatives. The reactions were carried out with a small excess of base, at room temperature or slightly above producing the heterocyclic products in good yields. The stereoelectronic properties of the substituents on the pyridine ring were shown to influence the cyclisation process.

### Ispitivanje kinetike fenilselenoeterifikacije 2,6-dimetil-hept-5-en-2-ola u prisustvu nekih katalizatora

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*Prirodno-matematički fakultet Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Srbija*

Ciklični etri tetrahidropiranskog- i tetrahidrofuranskog- tipa predstavljaju strukturne fragmente mnogih prirodnih proizvoda i ispoljavaju značajne biološke aktivnosti. Jedna od najefikasnijih metoda za njihovu sintezu jeste ciklofunkcionalizacija nezasićenih alkohola pomoću fenilselenohalogenida kao reagenasa. Upotreba određenih katalizatora u ovim reakcijama vodi do povećanja prinosa, kao i do izražene regio- i stereoselektivnosti. Ispitivanje mehanizma i kinetičkih aspekata ovih reakcija nisu dosad bili zastupljeni u značajnoj meri. U okviru ovog rada su predstavljeni rezultati ispitivanja kinetike fenilselenoeterifikacije 2,6-dimetil-hept-5-en-2-ola sa PhSeX (X=Cl, Br) u prisustvu nekih Lewis-ovih baza kao katalizatora. Sve reakcije su posmatrane kao reakcije *pseudo*-prvog reda gde je tok reakcija praćen merenjem promene absorbance na odgovarajućoj talasnoj dužini u funkciji vremena. Reakcione smeše su termostatirane na 15 °C, a kao rastvarač je korišćen THF. Lewis-ove baze: Et<sub>3</sub>N, piridin i piperidin su korišćene kao katalizatori ovih reakcija. Dobijene vrednosti za  $k_{\text{obsd}}$  su pokazale da upotreba katalizatora utiče na povećanje brzine hemijske reakcije. Reakcije sa PhSeCl su brže od odgovarajućih reakcija sa PhSeBr. Takođe, brzina hemijske reakcije zavisi od baznosti upotrebljenog katalizatora, gde se kao najbrža reakcija pokazala ona sa najjačom bazom-piperidinom.

### Kinetic studie of phenylselenoetherification of 2,6-dimethyl-hept-5-en-2-ol in the presence of some catalysts

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Tetrahydropyran- and tetrahydrofuran types of ethers are structural fragments of many natural products that can exhibit significant biological activity. One of the most effective methods for their synthesis is cyclofunctionalization of unsaturated alcohols with phenylselenylhalides as reagents. Use of certain catalysts in these reactions increases yields and influences very high regio- and stereoselectivity. So far, small accomplishment has been achieved in the area of kinetics and mechanism of these reactions. In this work we presented results of kinetic investigation for phenylselenoetherification of 2,6-dimethyl-hept-5-en-2-ol with PhSeX (X= Cl, Br) in the presence of some Lewis bases as catalysts. All reactions were observed as reactions of *pseudo*-first order, where the reaction flow was monitored by measuring absorbance changes at the appropriate wavelength as a function of time. The reaction mixture was thermostated at 15 °C, and THF was used as solvent. Lewis bases: Et<sub>3</sub>N, pyridine and piperidine were used as catalysts. Obtained values for  $k_{\text{obsd}}$  indicate that use of catalyst increases reaction rate. The reactions with PhSeCl as catalysts are faster than analogue reactions with PhSeBr. In addition, reaction rate depends on catalyst's basicity, therefore the fastest reaction is the one with the strongest base- piperidine.



OH21-P

### **Mikrotalasna sinteza amida iz naftenskih kiselina i uree sa i bez prisustva katalizatora**

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Cilj ovog rada je sinteza primarnih amida iz prirodnih i sintetičkih naftenskih kiselina reakcijom slobodnih kiselina sa ureom bez prisustva rastvarača i bez konvencionalnog zagrevanja izvođenjem u mikrotalasnom reaktoru. Sinteze su rađene na tri načina: u odsustvu hemijskih katalizatora, zatim uz imidazol i uz cirkonil-hlorid kao katalizator. U sva tri slučaja kao ko-katalizator korišćeni su mikrotalasi.

Optimizacija reakcionih uslova amidacije sa ureom uz katalitičko učešće mikrotalasa rađeno je sa prirodnom smešom naftenskih kiselina iz vojvođanske nafte "Velebit" i sa još pet različitih karboksilnih kiselina. Sve sinteze su rađene u laboratorijskoj mikrotalasnoj pećnici, raspon korišćenih snaga mikrotalasa od 20-160W, pritisak do 20 mbara, vreme do 30 min., bez prisustva rastvarača, molski odnos kiselina: urea: imidazol (ili cirkonil-hlorid) 1:2:1. Strukturna analiza proizvoda rađena je IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR- analizom.

### **Microwave assisted synthesis of amides from naphthenic acids and urea in the absence and presence of catalyzator**

Ksenija J. Pavlović, Ljubica M. Grbović, Bojana R. Prekodravac, Slavko E. Kevrešan\*

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The aim of the present work is solvent-free synthesis of primary amids from natural and synthetic naphthenic acids with urea by microwave reactor. Synthesis have been performed in the presence of microwaves like co-catalyzator in three ways: in the absence of catalyzator, with imidazole and zirconyl chloride like catalyst.

Reacton optimization of amidation with urea by catalitic presence of microwaves has been performed on natural naphthenic acids mixture and with fiwe different individual naphthenic acids. All reactions have been performed by solvent-free method in microwave reactor, pressure of 20 mbar, 30 minutes, under power range of 20-160W, optimal reaction conditions are: acid : urea : imidazole (or zirconyl chloride), 1:2:1. Structure analysis of products have been performed by IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR-analysis.



***In vitro* inhibicija sojine lipoksigenaze pomoću novog  
Pd(II)-trietanolaminskog kompleksa i njegovih prekursora**

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*trans*-dihlorbis(trietanolamin-*N*)paladijum(II) kompleks (*trans*-[PdCl<sub>2</sub>(TEA)<sub>2</sub>]) dobijen je u reakciji PdCl<sub>2</sub> i trietanolamonijum acetata [TEA][HOAc] u molarnom odnosu 1:2 na 90 °C (TEA = trietanolamin). Inhibicija sojine lipoksigenaze pomoću kompleksa i njegovih prekursora, PdCl<sub>2</sub> i [TEA][HOAc], praćena je UV spektrofotometrijski<sup>1</sup>. Visoka *in vitro* inhibitorska aktivnost [TEA][HOAc] i Pd(II) kompleksa upućuje na to da ova jedinjenja mogu biti i potencijalni antioksidansi. U cilju objašnjenja značajne inhibitorske sposobnosti ispitivanih jedinjenja analizirane su fizičko-hemijske osobine njihovih aktivnih mesta korišćenjem metode funkcionala gustine (B3LYP).

***In vitro* inhibition of soybean lipoxygenase with new  
Pd(II)-triethanolamine complex and its precursors**

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*trans*-dichlorobis(triethanolamine-*N*)palladium(II) complex (*trans*-[PdCl<sub>2</sub>(TEA)<sub>2</sub>]) was obtained in the reaction of PdCl<sub>2</sub> with triethanolamine acetate [TEA][HOAc] in molar ratio of 1:2 at 90 °C (TEA = triethanolamine). UV absorbance-based enzyme assays were performed with the complex and its precursors, PdCl<sub>2</sub> and [TEA][HOAc], in order to evaluate their inhibitory activity of soybean lipoxygenase (LOX)<sup>1</sup>. High *in vitro* inhibitory activities of [TEA][HOAc] and Pd(II) complex in the investigated reactions show potential antioxidant property of these compounds. Physicochemical properties of active sites of investigated compounds were studied using density functional theory (B3LYP) in order to explain their inhibition of soybean lipoxygenase.

1. Z.D. Petrović, D. Hadjipavlou-Litina, E. Pontiki, D. Simijonović, V.P. Petrović, *Bioorg. Chem.* **37** (2009) 162–166.

OH23-P

### **Mikrotalasna redukcija keto derivata 5 $\beta$ -holanske kiseline**

Bojana R. Prekodravac, Ksenija J. Pavlović, Ljubica M. Grbović, Ksenija N. Kuhajda  
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Cilj ovog rada je primena mikrotalasa kao ko-katalizatora u sintezi 5 $\beta$ -holanske i litholne kiseline redukcijom po Wolff-Kishner-u iz odgovarajućih keto derivata 5 $\beta$ -holanske kiseline. Reakcija redukcije je rađena u maloj skali sa šest različitih keto derivata žučnih kiselina u rastvoru etilen glikola sa hidrazinhidratom u višku.

Modifikacija Wolff-Kishner-ove sinteze ostvarena je izvođenjem u otvorenom sistemu mikrotalasnog reaktora (Discover Bench Mate, CEM). Reakcioni uslovi su : snaga mikrotalasa 200 W, 50 min., 195 °C. Ostvaren je prinos od 70 %, a , vreme trajanja reakcije je redukovano 20 puta u odnosu na konvencionalno zagrevanje. Strukture sintetizovanih žučnih kiselina potvrđene su IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR-spektroskopskim podacima.

### **Microwave-assisted reduction of keto-derivatives 5 $\beta$ -cholanolic acid**

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The aim of these work is in applying microwave technology as co-catalyst in synthesys of 5 $\beta$ -cholanolic and lithocholic acid by Wolff-Kishner reduction from corresponding keto derivatives of 5 $\beta$ -cholanolic acid. Reactions have been performed on small scale of six different keto derivatives of bile acids in solution of ethylene glycol and in excess of hydrazine hydrate.

Modification of Wolff-Kishner synthesis has been achieved under open vessel condition in microwave reactor (Discover Bench Mate, CEM). Reacton conditions were: magnetron power of 200 W, 50 min., 195°C. Noteworthy, in contrast to conventional heating the reaction was completed 20 times faster along with production of 70-80% of pure corresponding products. Structures of synthetised bile acids have been confirmed by IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR-spectroscopic data.



### Mikrotalasna sinteza estara 3-cikloheksilpropanske kiseline

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U našim ranijim radovima estri naftnih kiselina vojvodanske nafte „*Velebit*“ su sintetizovani kiselo-katalizovanom klasičnom metodom esterifikacije, ali takođe i modifikovanom metodom uz ko-katalitičko delovanje mikrotalasa. Cilj ovog rada je modifikacija klasične metode esterifikacije sa odabranom model naftenskom kiselinom, 3-cikloheksilpropanskom kiselinom, u reakciji sa metil-, etil- i *n*-butil-alkoholom u mikrotalasnom reaktoru u kiseloj sredini.

3-Cikloheksilpropanska kiselina spada u monociklične karboksilne kiseline, koja je grupno-strukturnom masenom analizom niske rezolucije identifikovana u naftnim kiselinama zajedno sa alifatičnim, bi-, tri-, tetra- i pentacikličnim karboksilnim kiselinama.

Sinteze izvedene pod dejstvom mikrotalasa snage 150 W, u trajanju od 4 min., dale su metil-, etil- i *n*-butil-estre 3-cikloheksilpropanske kiseline u prinosima od 72.2%, 70.4% i 75.8%, a struktura im je potvrđena IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR-spektroskopskim podacima.

### Microwave Synthesis of Esters of 3-Cyclohexylpropionic acid

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In our previous papers naphthenic acid esters of Vojvodinian oil „*Velebit*“ were synthesised conventionally by acid-catalyzed esterification and by modified method within co-catalytic presence of microwaves. The aim of present work was in modification of conventional acid-catalyzed esterification method on selected model of naphthenic acid, 3-cyclohexylpropionic acid, in reaction with methyl-, ethyl- and *n*-buthyl-alcohol in microwave reactor.

3-Cyclohexylpropionic acid is one of the monocyclic carboxylic acid, which was identified by group-structural mass analysis of low resolution in the mixture of the naphthenic acids along with alyphatic, bi-, tri-, tetra- and pentacyclic carboxylic acids.

Microwave-assisted synthesis of methyl-, ethyl- and *n*-buthyl esters of 3-cyclohexylpropionic acid under 150 W, for 4 min. lead to yield of 72.2%, 70.4% and 75.8%, which structure was confirmed by IR-, <sup>1</sup>H NMR- i <sup>13</sup>C NMR-spectroscopic data.

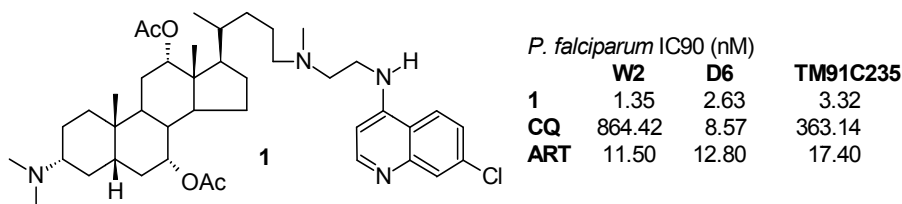


OH25-P

## Nova generacija steroidnih 4-aminohinolina kao potencijalnih antimalarika

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Malaria je infektivna bolest koju izaziva parazit iz roda *Plasmodium*. Od malarije godišnje oboli 250 miliona ljudi, sa smrtnim ishodom kod oko milion pacijenata, usled razvoja rezistencije parazita prema postojećim antimalaricima. U nastavku naših istraživanja u ovoj oblasti<sup>1</sup> sintetisani su novi steroidni 4-amino-7-hlorohinolinski derivati i ispitana je njihova *in vitro* antimalarijska aktivnost prema CQ-rezistentnim (W2 i TM91C235) i CQ-osetljivim (D6) sojevima *P. falciparum*. Kod ispitanih jedinjenja uočena je zavisnost antimalarijske aktivnosti od supstituenata na atomima C3 i C24 steroidnog jezgra i dužine alkil linkera. Biće pokazano da tercijarna amino-grupa značajno povećava antimalarijsku aktivnost.



## New generation of steroidal 4-aminoquinolines as potent antimalarials

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Malaria is an infectious disease caused by parasite *Plasmodia*. It is estimated that malaria causes 250 million cases of fever and approximately one milion deaths annually, because of development of parasite resistance to standard antimalarial drugs. Here we present synthesis of new steroidal 4-amino-7-chloroquinolines and discuss their *in vitro* antimalarial activities against CQ-resistant (W2 i TM91C235) and CQ-susceptible (D6) *P. falciparum* strains. Compounds showed strong dependence of C3 and C24 substitution pattern and length of alkyl linker on antimalarial activity. It will be shown that tertiary amine groups significantly increase the antimalarial activity.

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1. Šolaja, B. A.; Opsenica, D.; Smith, K. S.; Milhous, W. K.; Terzić, N.; Opsenica, I.; Burnett, J. C.; Nuss, J.; Gussio, R.; Bavari, S. *J. Med. Chem.*, **51** (2008) 4388–4391.

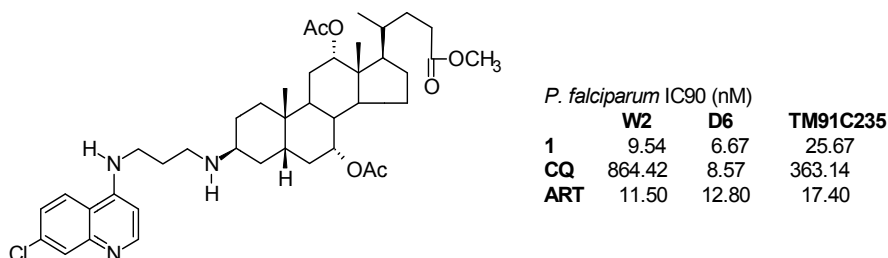


OH26-P

# Sinteza i antimalarijska aktivnost novih 4-aminohinolinskih derivata holne kiseline

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Malarija je parazitska bolest koju kod ljudi izaziva jedna od četiri vrste parazita *Plasmodium*. U 95% smrtnih slučajeva, pacijenti su bili zaraženi *P. falciparum*. Kontrola malarije je otežana razvojem rezistencije parazita prema lekovima kao što je hlorokin. Sintetisana je serija novih<sup>1</sup> steroidnih aminohinolina izvedenih iz holne kiseline i 4-amino-7-hlorhinolina. Proizvodi su dobijeni kao C3 epimeri. Određena je njihova *in vitro* antimalarijska aktivnost prema CQ-rezistentnim (W2 i TM91C235) i CQ-osetljivim (D6) *P. falciparum* sojevima. Pokazano je da antimalarijska aktivnost zavisi od strukture supstituenta na atomu C24 steroida.



## Synthesis and antimalarial activity of novel 4-aminoquinoline derivatives of cholic acid

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Malaria is a vector-borne parasitic infection transmitted by anopheline mosquitoes. *Plasmodium falciparum* is responsible for most of the morbidity and mortality due to malaria worldwide. Widespread drug resistance to chloroquine, the standard antimalarial drug aggravates the burden. Here we report synthesis and antimalarial activity of steroidal aminoquinolines derived from cholic acid and 4-aminoquinolines. Products were obtained as C3 epimers and were screened against CQR (WR and TM91C235) and CQS (D6) *P. falciparum* strains. It was shown that activity depends on C24 substituent structure.

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

- Šolaja, B. A.; Opsenica, D.; Smith, K. S.; Milhous, W. K.; Terzić, N.; Opsenica, I.; Burnett, J. C.; Nuss, J.; Gussio, R.; Bavari, S. *J. Med. Chem.*, **51** (2008) 4388–4391.

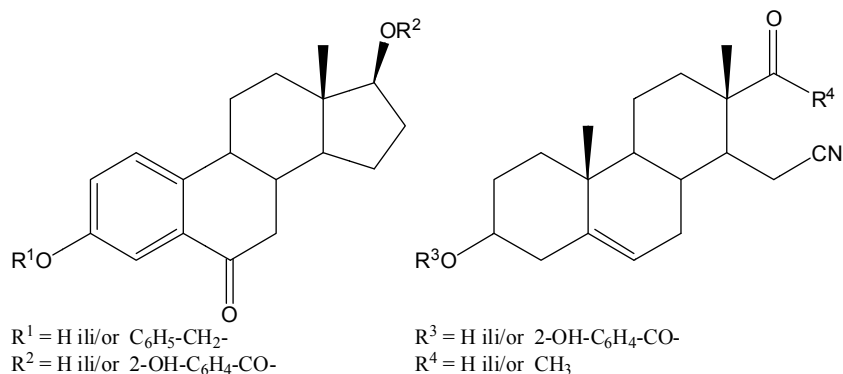


OH27-P

### Sinteza i ispitivanje biološke aktivnosti novih saliciloid derivata estro-1,3,5(10)-triena i androst-5-ena

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Polazeći od estradiol-dipropionata sintetizovani su 17 $\beta$ -saliciloid-6-okso derivati. Beckmann-ovom fragmentacijom 16-oksimino alkohola androst-5-enske serije sa metil-salicilatom, u prisustvu natrijuma kao katalizatora, dobijeni su D-seko derivati. Istovremenom fragmentacijom i acilovanjem 3 $\beta$ ,17 $\beta$ -dihidroksi-16-oksimino derivata androst-5-ena nastao je 3 $\beta$ -saliciloid-D-seko derivat, koji je dobijen i iz odgovarajućeg D-seko-derivata. U *in vitro* testovima neka jedinjenja su se pokazala kao potentni antioksidanti i/ili citotoksični agensi.



### Synthesis and biological evaluation of the new salicyloyl derivatives of estradiol-1,3,5(10)-triene and androst-5-ene

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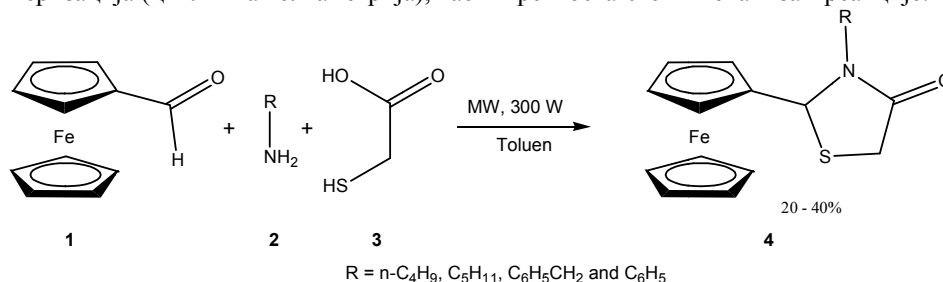
Starting from estradiol dipropionate, 17 $\beta$ -salicyloyl-6-oxo derivatives were prepared. The Beckmann fragmentation of 16-oximino alcohols of androst-5-ene series, with methyl salicylate, in the presence of sodium as catalyst, yielded D-seco derivatives. Simultaneous fragmentation and acylation of 3 $\beta$ ,17 $\beta$ -dihydroxy-16-oximino derivative of androst-5-ene resulted in 3 $\beta$ -salicyloyl-D-seco derivative, which was also obtained from corresponding D-seco-compound. In *in vitro* tests some compounds proved to be potent antioxidants and/or cytotoxic agents.



## 2-Фероценилтиазолидин-4-они: Синтеза, спектроскопска и електрохемијска карактеризација

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Најважније карактеристике тиазолидинонских дериватасу биолошка дејства попут антибиотског, фунгицидног, пестицидног, инсектицидног, антиконвулзивног, антиинфламаторног, анти tiroидалног итд.<sup>1</sup> У овом раду описана је синтеза четири нова N-алкил-2-фероценилтиазо-лидинона (**4**, R = n-C<sub>4</sub>H<sub>9</sub>, n-C<sub>5</sub>H<sub>11</sub>, C<sub>6</sub>H<sub>5</sub> и C<sub>6</sub>H<sub>6</sub>CH<sub>2</sub>), која је остварена озрачивањем толуенског раствора формил фероцена (**1**), тиогликолне киселине (**3**) и одговарајућег примарног амина (**2**) у микроталасној пећи.<sup>2</sup> Поред експерименталних детаља биће дати спектроскопски подаци (IR, <sup>1</sup>H и <sup>13</sup>C NMR), електрохемијска карактеризација (циклична волтаметрија), као и претпостављени механизам реакције.



## 2-Ferrocenylthiazolidin-4-ones: Synthesis and spectral characteristics

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Diverse biological activities such as bactericidal, fungicidal, pesticidal, insecticidal, anticonvulsant, antiinflammatory, antithyroidal have been found to be associated with thiazolidinone derivatives.<sup>1</sup> This report deals with the synthesis of four new ferrocene containing N-alkyl-2-thiazolidinones (**4**, R = n-C<sub>4</sub>H<sub>9</sub>, n-C<sub>5</sub>H<sub>11</sub>, C<sub>6</sub>H<sub>5</sub> и C<sub>6</sub>H<sub>6</sub>CH<sub>2</sub>) achieved by microwave irradiation of the toluene solution of ferrocenecarboxaldehyde (**1**), thioglycolic acid (**3**) and the corresponding amine (**2**).<sup>1</sup> In addition of experimental details, the spectral data (IR, <sup>1</sup>H and <sup>13</sup>C NMR), electrochemical characterization (cyclic voltammetry) and the mechanistic consideration also will be presented.

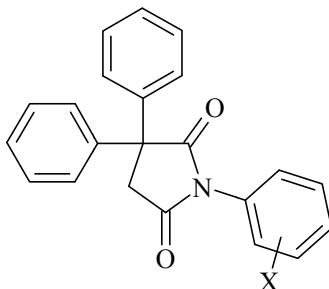
1. S. P. Singh, S. S. Parmar, K. Raman, V. I. Stenberg, *Chem. Rev.* **81** (1981) 175
2. F. C. Brown, *Chem. Rev.*, **61** (1961) 463

OH29-P

### Sinteza, struktura i solvatohromna svojstva novih antikonvulzivnih derivata sukcinimida

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U radu je sintetizovano sedamnaest N-(3- i 4-supstituisanih fenil)-2,2-difenilsukcinimida (Slika 1) i određeni su njihovi apsorpcioni maksimumi u oblasti 200-400 nm u dvanaest rastvarača različite polarnosti. Efekat polarnosti rastvarača i efekat vodoničnog vezivanja rastvarač-rastvorena supstanca su analizirane metodom linearne korelacije energije solvatacije (LSER). Izračunate vrednosti lipofilnosti ( $\log P$ ) su korelisane sa odnosom doprinosa specifičnih i nespecifičnih efekata rastvarača, a na osnovu dobijene linearne zavisnosti je diskutovana farmakološka aktivnost proučavanih derivata sukcinimida. Korelacione jednačine su kombinovane sa odgovarajućim parametrima za elektronske i sterne efekte supstituenata u cilju dobijanja novih izraza koji najpribližnije opisuju postojeću zavisnost između farmakološke aktivnosti ispitivanih jedinjenja i interakcija sa molekulima rastvarača.



**Slika 1.** Struktura N-(3- i 4-supstituisanih fenil)-2,2-difenilsukcinimida  
 (X: H, 4-CH<sub>3</sub>, 4-OCH<sub>3</sub>, 4-Cl, 4-Br, 4-I, 4-F, 4-NO<sub>2</sub>, 4-CN, 4-OH, 4-COCH<sub>3</sub>, 3-CH<sub>3</sub>, 3-Cl, 3-Br, 3-NO<sub>2</sub>, 3-CN, 3-OH)

**Figure 1.** Structure of N-(3- and 4-substituted phenyl)-2,2-diphenylsuccinimides  
 (X: H, 4-CH<sub>3</sub>, 4-OCH<sub>3</sub>, 4-Cl, 4-Br, 4-I, 4-F, 4-NO<sub>2</sub>, 4-CN, 4-OH, 4-COCH<sub>3</sub>, 3-CH<sub>3</sub>, 3-Cl, 3-Br, 3-NO<sub>2</sub>, 3-CN, 3-OH)

### Synthesis, structure and solvatochromic properties of new anticonvulsant succinimide derivatives

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In this work, seventeen N-(3- and 4-substituted phenyl)-2,2-diphenylsuccinimides were synthesized and their UV absorption spectra were recorded in the region 200-400 nm, in twelve solvents of different polarities. The effect of solvent dipolarity/polarizability and solvent/solute hydrogen bonding interactions were analyzed by means of the linear solvation energy relationship (LSER). The calculated values of  $\log P$  were correlated with the ratio of contributions of specific and nonspecific solvent interactions, and by employing the linear dependence thus obtained, the pharmacological activity of the studied succinimide derivatives was discussed. The correlation equations were combined with corresponding equations for electronic and steric parameters of substituents to generate new equations demonstrating the exact relationships between solvent-solute interactions and structure-activity parameters.



**Nastava hemije / Chemistry Education**  
**Posterska saopštenja / Poster Presentations**

**N01-P**



**У свету хемије ученика седмог разреда**

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У овом раду представљена је могућност сагледавања ученичког виђења и знања хемије, посебно субмикросвета, путем цртежа. Дато истраживање реализовано је у две основне школе у Београду, „Краљ Александар I” (А; 71 ученик) и „Веселин Маслеша” (Б; 77 ученика). На часу ликовне културе *Композиција* ученици су добили тему *Свет хемије* на коју је требало да одговоре у року од 45 минута. Сами су бирали и садржај свог цртежа и технику рада. Лабораторијско посуђе и прибор (77% А и 84% Б), атом (49% А и 56% Б) и хемијски елементи (37% А и 56% Б) биле су им најчешће асоцијације на хемију. Увид у менталне представе ученика о структури атома указао је на њихове хемијске заблуде које су одмах биле исправљене. Чињеница да већина ученика (83% А и 91% Б) није истакла примену хемије у свакодневном животу упућује на важан задатак њене савремене наставе у успостављању везе између ове централне природне науке и друштва.

*Захвалница:* Аутори се најлепше захваљују Министарству просвете и науке Републике Србије (пројекат бр. 179048).

**In a chemistry world of seventh-grade primary school students**

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The possibility of considering of students' perceptions and knowledge of chemistry, in particular regarding submicro world, with drawings is presented in this manuscript. The research was conducted in two primary schools in Belgrade, King Aleksandar I (A; 71 students) and Veselin Maslesa (B; 77 students). At the art class *Composition* students were given the topic *A Chemistry World* that was supposed to respond within 45 minutes. Both the content of their drawing and corresponding technique they selected all by themselves. Laboratory ware and accessories (77% A и 84% B), atom (49% A и 56% B) and chemical elements (37% A и 56% B) were the most common associations of chemistry. The insight into students' mental performances of atomic structure pointed out their chemical misconceptions which were immediately corrected. Majority of them did not indicate on the application of chemistry in everyday life. That fact underlines the important task of modern teaching chemistry in establishing a connection between this central natural science and society.

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N02-P



### Осмаци као наставници на првом часу хемије у основној школи

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Пилот студија новог начина праћења исхода двогодишњег учења хемије урађена је у другој половини маја 2008. године у четири основне школе у Србији. У тој активности учествовало је 164 ученика осмог разреда који су се писмено изразили на тему *Ја као наставник хемије* укратко притом изневши садржај и организацију њиховог првог часа хемије у седмом разреду у својству предметног наставника. Резултати овог рада показују да ученици имају различите приступе том школском часу и да су им разговор о хемији (38-54%) и понашање наставника уз атмосферу у учионици (16-48%) од посебне важности, док су огледима дали мањи приоритет (4-37%). У циљу побољшања процеса наставе / учења хемије у основној школи требало би утврдити дата размишљања ученика на већем узорку, а потом их разрадити и каналисати у школску праксу.

Аутори се најлепше захваљују Министарству просвете и науке Републике Србије (пројекат бр. 179048).

### Eighth-grade students as teachers on a first chemistry class in primary school

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A pilot study of new way of monitoring the outcome of a two-year process of learning chemistry is carried out in four primary schools in Serbia in the second half of May, 2008; 164 eighth-grade students are participated in it. They are polled in writing (written task) on the topic *I as a Chemistry Teacher* within which they should briefly present the content and organisation of their first chemistry class in seventh grade as a subject teacher. The results of this paper show different approaches of students to the school class; for majority of them, the talk about chemistry (38-54%) and the behaviour of teacher including the atmosphere in the classroom (16-48%) are of special importance, while a smaller number of students (4-37%) has given priority to performing of chemical experiments. In order to improve teaching / learning process of chemistry in primary school firstly it should be identified the students' thinking on a larger sample, then developed and channeled them into school practice.

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### Открића хемичара у блиској будућности која би одушевила основце

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У овом раду представљени су резултати проистекли из писања есеја које је спроведено на редовном часу хемије у две основне школе у Београду („Краљ Александар I” /А/ и „Веселин Маслеша” /Б/; укупно 173 основаца). У року од 30 минута основци из седам одељења седмог разреда изнели су своје жеље у вези са открићима хемичара у блиској будућности која би их одушевила и укратко су их образложили. Премда је требало да се одреде само за једно откриће, више од половине основаца у обе школе (67% А и 62% Б) навело их је више. Међу открићима за која су се основци првенствено одредили издвајају се она која се односе на нове лекове (55% А и 66% Б), нове сложене супстанце друге намене (10% А и 32% Б) и нове инструменте, машине и превозна средства (42% А и 22% Б), што би наставници хемије требало да имају у виду при обради и систематизацији првих хемијских појмова у основној школи.

*Захвалница:* Аутори се најлепше захваљују Министарству просвете и науке Републике Србије (пројекат бр. 179048).

### The discoveries of chemists in near future which would delight primary school students

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This paper shows the results of an activity which is conducted in two primary schools, King Aleksandar I and Veselin Maslesa, in Belgrade (Serbia). The students from the seventh-grade class (173 students from seven selected sections) were writing an announced essay about the discovery of chemists which would delight them in their regular chemistry class for 30 minutes. The students should choose only one discovery but a great number of them (67% and 62%, respectively) gave more different examples with corresponding explanations. On the basis of this activity it can be concluded that the students are primarily interested in discoveries regarding new drugs (55% and 66%, respectively), novel substances / compounds of other use (10% and 32%, respectively) and development of new instruments, machines and transports (42% and 22%, respectively), which should be taken in consideration by teachers of chemistry in primary schools due to possible reforms in their work.

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N04-P

### Од неорганских супстанци до адитива у храни кроз концептуалне задатке

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У програмима хемије за основну и средњу школу, при изучавању неорганских и органских супстанци не говори се о њиховој примени као адитива у храни. Будући да савремена настава треба да омогући повезивање хемијске науке, технологије и друштва циљ овог рада био да се знања о неорганским супстанцама повежу са адитивима у храни кроз концептуалне задатке и демонстрационе огледе. Припремљен је и испитан тест са пет задатака о синтези једињења, која представљају неорганске адитиве E170, E252, E508, E517 и E529. После теста, ученици су добили домаћи задатак да пронађу податке о ових пет адитива. Прикупљени подаци о својствима и примени адитива основа су за дискусију на наредном часу хемије. Функција одређеног адитива, на пример калијум-нитрата као конзерванса, може се пратити кроз огледе *in vitro*. У истраживању су учествовали ученици (116) другог разреда природног смера из пет београдских гимназија и гимназије у Панчеву. Решавање концептуалних задатака, кроз које су разматране синтезе адитива, доприноси развијању критичког и креативног мишљења ученика и показује у којој мери су знања функционална.

### Conceptual tasks: from inorganic substances to food additives

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In chemistry curriculums for elementary and high school, regarding the study of inorganic and organic substances, there is no mention of their use as food additives. Since modern education should enable the connection of chemical science, technology and society, objective of this study was to link the knowledge about inorganic substances to food additives through conceptual tasks and demonstration experiments. A test with five tasks about synthesis of compounds, which represent inorganic additives E170, E252, E508, E517 and E529, was performed and analyzed. After the test, students were given homework to find information on these five additives. Collected data on the properties and application of additives are the basis for discussion at the next chemistry class. The function of certain additive, e.g. potassium nitrate as preserver, can be followed in *in vitro* experiments. The research has included 116 second-grade students from five Belgrade gymnasiums including a gymnasium in Pancevo.

The resolving of conceptual tasks on additives' synthesis contributes to the development of critical and creative thinking in students and shows in which extent the knowledges are functional.



**Keramika / Ceramics**  
**Posterska saopštenja / Poster Presentations**

K01-P



**Sinterabilnost kordijeritnih prahova sintetizovanih  
koloidnim sol-gel postupkom**

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U ovom radu je ispitana sinterabilnost kordijeritnih prahova koji su sintetizovani koloidnim sol-gel postupkom, polazeći od sola  $\text{SiO}_2$ , bemit sola i vodenog rastvora  $\text{Mg}(\text{NO}_3)_2$ . Na osnovu mikrostrukturnih parametara dobijenih materijala, pokazano je da sinterabilnost kordijeritnih prahova zavisi od temperature kalcinacije gela, dužine trajanja mlevenja kalciniranih gelova i temperature sinterovanja. Najveći uticaj na sinterabilnost ima smanjenje veličine čestica kalciniranih gelova, postignuto dužim mlevenjem. Bolju sinterabilnost ima prah koji sadrži dobro kristalisani  $\alpha$ -kordijerit u odnosu na prah u kome je došlo do viskoznog sinterovanja bez kristalizacije komponente koja sadrži  $\text{SiO}_2$ . Iako je sol-gel postupak omogućio sniženje temperature sinteze  $\alpha$ -kordijerita u odnosu na tradicionalne postupke, optimalna temperatura sinterovanja je visoka i bliska temperaturi inkongruentnog topljenja kordijerita.

**Sinterability of Cordierite Powders Synthesized  
by Colloidal Sol-Gel Method**

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Sinterability of cordierite powders synthesized by colloidal sol-gel method starting from silica sol, boehmite sol and aqueous solution of  $\text{Mg}(\text{NO}_3)_2$  has been studied. According to microstructure of obtained materials, it was shown that sinterability of cordierite powders depends on temperature of gel calcination, time of grinding of calcined gels and sintering temperature. The densification degree was highly improved by decreasing the mean particle size of powders by prolonged grinding. The powder contained well crystallized  $\alpha$ -cordierite had a better sinterability compared to powder obtained by viscous sintering of gel before the onset of crystallization of the  $\text{SiO}_2$ -containing component. Although the sol-gel method enabled decreasing temperature of  $\alpha$ -cordierite synthesis compared to traditional processing, optimal sintering temperature is still high and close to the temperature of incongruent melting of cordierite.



**Tekstilno inženjerstvo / Textile Engineering**  
**Usmena saopštenja / Oral Presentations**

TI01-O



**Uticaj selektivne TEMPO-oksidacije na mehanička svojstva vlakana pamuka**

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Hemijskim modifikovanjem polisaharida, otvaraju se zanimljivi putevi za dobijanje novih biopolimera sa poboljšanim karakteristikama i specifičnom primenom, tzv. "biopolimera za budućnost". Sve aktuelnija istraživanja u oblasti modifikovanja celuloznih vlakana bazirana su na oksidaciji celuloze. U ovom radu je proučavan uticaj selektivne oksidacije katalizovane 2,2,6,6-tetrametilpiperidin-1-oksil radikalom (TEMPO) na mehanička svojstva vlakana pamuka. Takođe, nemodifikovana i modifikovana vlakna pamuka okarakterisana su sa aspekta gubitka mase, promene finoće i stepena kristalnosti. TEMPO-oksidacija vlakana pamuka uticala je na smanjenje mase i promenu finoće modifikovanih vlakana. Za oksidisana vlakna pamuka uočava se minimalno povećanje finoće i dolazi do povećanja indeksa kristalnosti, dok se prekidna jačina vlakana smanjuje. Primena rigoroznih uslova oksidacije dovodi do gubljenja vlaknaste forme, tako da kod takvih uzoraka određivanje prekidne sile i izduženja nije bilo moguće. Stoga, kada je za primenu u tekstilu potrebno da oksidisani uzorci imaju vlaknastu strukturu, oksidaciju je potrebno izvoditi pri blažim uslovima.

*Zahvalnica:* Ovaj rad je proistekao iz rada na Projektu koji finansira Ministarstvo za nauku i tehnološki razvoj Republike Srbije (OI 172029).

**Influence of selective TEMPO-oxidation on mechanical properties of cotton fibers**

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Chemical modifications of polysaccharides are interesting routes for preparing new type of polymers on the basis of cellulose, with advances in performance and application, so-called "biopolymers for the future". The research in the field of cellulose fibers modification, that has been based on cellulose oxidation has become very actual. In this paper, the influence of the selective oxidation catalyzed with 2,2,6,6-tetramethylpiperidine-1-oxy radical (TEMPO) on mechanical properties of cotton fibers was studied. Also, unmodified and modified fibers were characterized in terms of weight loss values, fineness and crystallinity index. The TEMPO-mediated oxidation has influence on weight reduction and changes in fineness of the modified fibers. Oxidized cotton fibers show minimal increase of fineness and higher crystallinity index, while the tensile strength of fiber decreases. Applying severe conditions of TEMPO-mediated oxidation on cotton fibers, results in loosing fibrous structure, and in that case, the determination of tensile strength and elongation was not possible. Therefore, for textile applications only oxidation under mild conditions should be carried out.



Posterska saopštenja / Poster Presentations

TI02-P



**Biosorpcija jona  $\text{Cd}^{2+}$ ,  $\text{Zn}^{2+}$  i  $\text{Pb}^{2+}$  kratkim vlaknima konoplje:  
Matematički model**

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Zagađenje životne sredine teškim metalima utiče kako na kvalitet vode i zemljišta, tako i na zdravlje ljudi. U poslednje vreme za prečišćavanje otpadnih voda, kao biosorbenti sve češće se koriste lignocelulozni materijali. U ovom radu je proces biosorpcije objašnjen sa aspekta različitih fenomena transporta jona teških metala ( $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$  i  $\text{Zn}^{2+}$ ) kroz porozni lignocelulozni materijal (hemijski modifikovana vlakna konoplje). Na samom početku biosorpcioni proces je brz i odnosi se na difuziju jona kroz poroznu strukturu vlakana. Nakon određenog vremena, proces biosorpcije postaje sporiji, a međusobna elektrostatička odbijanja između jona u vlaknu postaju intenzivnija. Matematičkim modelom, baziranim na drugom Fikovom zakonu, za proces biosorpcije jona određeni su: efektivni koeficijent difuzije jona kroz vlakno; profili koncentracija jona u vlaknima i efikasnost biosorpcije.

Ova ispitivanja finansirana su od strane Ministarstva za nauku i tehnološki razvoj Republike Srbije (Projekat OI 172029).

**Biosorption of  $\text{Cd}^{2+}$ ,  $\text{Zn}^{2+}$  i  $\text{Pb}^{2+}$  ions by short hemp fibers:  
Mathematical model**

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The discharge of toxic heavy metals into the environment is a serious pollution problem affecting water and soil quality, hence presenting a direct danger to human health. Recently, lignocellulosic materials are often used as biosorbents for wastewater treatment. In this paper, process of biosorption was explained in the terms of transport phenomena of different ions ( $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$  and  $\text{Zn}^{2+}$ ) through the porous lignocellulosic fiber matrices (chemically modified hemp fibers). At the beginning, biosorption process is very fast and depends on diffusion of heavy metal ions through the porous structure of fibers. After that, biosorption process becomes slower, and mutual electrostatic repulsive interactions between the ions in the fibers become more intensive. Value of effective diffusion coefficient of heavy metal ions through the fibers, effectiveness of sorption and ions concentration profile through the fibers were determined by mathematical model based on the second Fick's law.

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### Uticaj hemijskog modifikovanja na električnu otpornost pamučnih pređa

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U ovom radu ispitivana je električna otpornost pamučne pređe nakon neselektivne oksidacije i sorpcije  $\text{Ag}^+$  jona pomoću novoformiranih karboksilnih grupa. Za proces oksidacije korišćen je vodonik-peroksid koncentracije 3 % i 6 % pri različitim pH vrednostima reakcione sredine i vremenima obrade. Joni srebra su sorbovani iz vodenog rastvora srebro-nitrata tokom četiri sata, pri čemu su korišćeni neoksidisan (polazni) i oksidisani uzorci. Nakon toga, uzorci su osušeni i izmerena je njihova električna otpornost. Sva merenja su vršena na sobnoj temperaturi (25 °C) i pri različitim vrednostima relativne vlažnosti vazduha. Dobijeni rezultati pokazuju da oksidacija, iako pospešuje hemisorpciona svojstva celuloze, dovodi do povećanja njene električne otpornosti. Nadalje, sorpcija jona srebra, kao što je očekivano, smanjuje električnu otpornost i smanjuje uticaj relativne vlažnosti vazduha na električnu otpornost celuloznih pređa.

*Zahvalnica:* Ova ispitivanja finansirana su od strane Ministarstva za nauku i tehnološki razvoj Republike Srbije (Projekat OI 172029).

### Influence of chemical modification on electrical resistance of cotton yarns

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In this paper electrical resistance of cotton yarn after non-selective oxidation and sorption of  $\text{Ag}^+$  ions with newly formed carboxylic groups was studied. Hydrogen peroxide concentration of 3 % and 6 % was used for oxidation, at different pH values of reactive medium and treatment times.  $\text{Ag}^+$  ions were sorbed from aqueous silver nitrate solution by non-oxidized and modified samples during the four hour treatment. Afterwards, samples were dried and their electrical resistance was measured. All measurements were carried out at room temperature (25 °C) at different relative humidities. Obtained results show that oxidation, although improves chemisorption properties of cotton cellulose, leads to an increase of electrical resistance. Further, sorption of silver ions, as expected, decreases electrical resistance, and reduces the influence of relative humidity on electrical resistance of cotton yarns.



### **Adsorpciono ponašanje direktne boje na pamuku u vodi bez drugih dodataka**

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U radu je razmotreno adsorpciono ponašanje direktne boje na pamuku (bojenje) u cilju dobijanja podataka o mehanizmu vezivanja boje i definisanju uslova procesa bojenja prirodnih vlakana bez dodavanja elektrolita i drugih pomoćnih sredstava, kao osnovnog preduslova za njihovu upotrebu. Adsorpcija je vođena pod različitim uslovima. Utvrđeno je da zavisi od vremena kontakta, početne koncentracije boje i količine adsorbenta. Duže vreme kontakta znači i veću količinu boje na predi. Sa trajanjem procesa adsorpcije opada koncentracija boje u rastvoru. Postoji kontinuitet rasta količine uklonjenih boja sa masom adsorbenta. Karakteristični prikazi dobijeni iz Frojndlich-ove izoterme potvrdili su da ovaj model obezbeđuje dovoljno precizan opis eksperimentalnih podataka za direktnu boju u poređenju sa izotermom Langmuir-a.

### **Adsorption behavior of direct dye on cotton in water without other auxiliaries**

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This paper considers the adsorption behavior of direct dye on cotton (dyeing) in order to obtain data on mechanism of dye binding and to define the terms of natural fiber dyeing process without adding electrolytes and other auxiliaries, as basic prerequisites for their use. Adsorption was performed under different conditions. It was found that adsorption depends on the contact time, the dye concentration and amount of adsorbent. The longer the contact time the greater the amount of dye in yarn. The prolongation of the adsorption led to a decrease of dye concentration in solution. There is a continuity of growth amounts exhausted dye with the growth of mass adsorbent. The results indicate that Freundlich's isotherms model provides a sufficiently accurate description of experimental data for direct dye compared to the Langmuir isotherm.







### **Uticaj prisustva nanočestica srebra na antibakterijsku aktivnost i obojenje pamučne tkanine**

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U ovom radu je diskutovan efekat nanočestica srebra na antibakterijsku aktivnost obojenih pamučnih tkanina. Takođe je ispitivan uticaj prisustva nanočestica srebra na promenu obojenja pamučnih tkanina. Pamučne tkanine su bojene direktnim bojama: C.I. Direct Yellow 86, C.I. Direct Red 79 i C. I. Direct Blue 78. Obojene tkanine su modifikovane koloidnim nanočesticama srebra koje su sintetisane bez prisustva stabilizatora. Skenirajućom elektronskom mikroskopijom je potvrđeno da su aglomerati nanočestica srebra približno sfernog obilika i dimenzija između 40-80 nm ravnomerno raspoređeni po površini pamučnih vlakana nezavisno od primenjene boje. Sve ispitivane pamučne tkanine pokazuju odličnu antibakterijsku aktivnost prema G(-) bakteriji *E coli* i G(+) bakteriji *S. aureus*. Međutim, prisustvo nanočestica srebra negativno utiče na obojenje tkanina, što je najočiglednije u slučaju uzorka koji je bio obojen žutom bojom C.I. Direct Yellow 86.

### **The influence of silver nanoparticles on antibacterial activity and color of cotton fabric**

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This study discusses the effect of silver nanoparticles on antibacterial activity of dyed cotton fabrics. Additionally, the influence of silver nanoparticles presence on the color change of cotton fabrics was studied. Cotton fabrics were dyed with direct dyes: C.I. Direct Yellow 86, C.I. Direct Red 79 and C. I. Direct Blue 78. Dyed fabrics were modified with colloidal silver nanoparticles that were synthesized without using any stabilizer. SEM analysis revealed that nearly spherical agglomerates of silver nanoparticles with dimensions between 40-80 nm were evenly deposited onto the surface of cotton fibers independently of applied dye. All cotton fabrics exhibited excellent antibacterial activity against G(-) bacteria *E coli* i G(+) bacteria *S. aureus*. However, the presence of silver nanoparticles negatively affects the color of dyed cotton fabrics. This was particularly pronounced in the case of fabric that was dyed with yellow dye C.I. Direct Yellow 86.



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***Beleške / Notes***



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