

Srpsko hemijsko društvo
Serbian Chemical Society



53. SAVETOVANJE
SRPSKOG HEMIJSKOG
DRUŠTVA

PROGRAM
i
KRATKI IZVODI RADOVA

**53nd Meeting of
the Serbian Chemical Society**

**Program
&
Book of Abstracts**

Prirodno-matematički fakultet, Kragujevac 10. i 11. jun 2016.
Faculty of Science, Kragujevac, Serbia, June 10 and 11, 2016

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*Ova knjiga sadrži kratke izvode
tri plenarna predavanja (PP),
tri predavanja po pozivu (PPP) i
111 saopštenja prihvaćenih
za prezentovanje na Savetovanju,
od čega 4 sekcijaska (S) predavanja,
24 usmena (O) i 83 posterska (P) saopštenja.*

*Zbornik radova (radovi obima od najmanje četiri stranice)
publikovan je na kompakt disku (CD),
kao sastavni deo materijala Savetovanja.
Radovi koji su publikovani na disku
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na desnoj strani iznad naslova rada.

*This book contains short abstracts of
3 Plenary Lectures (PP),
3 Invited Lectures (PPP),
111 contributions accepted
for the presentation at the Meeting,
of which 4 sectional (S) lectures,
24 oral (O) and 83 poster (P) presentations*

*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 on the right side above the paper title.

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PROGRAM

Petak, 10. jun 2016. / Friday, June 10, 2016

08.30 – 12.30 Registracija – Hol u prizemlju glavne zgrade
Registration – Lobby on the ground floor

Velika sala u prizemlju / Great hall on the ground floor

09.00– 09.30 Postavljanje postera / Poster Mounting (Sesija 1 / Session 1)

Velika sala na prvom spratu / Great hall on the first floor

09.30 – 09.45 Svečano otvaranje / Opening Ceremony

Plenarna predavanja / Plenary Lectures

Predsedavajuća / Chairperson: Ivan Gutman

09.45 – 10.30 Tanja Parac-Vogt, KU Leuven, Department of Chemistry, Leuven, Belgium

PP 1 Poliokosmetalati kao veštački enzimi / Polyoxometalates as artificial enzyme

10.30 – 11.15 Marcel Swart* Adrià Romero-Rivera**, Kallol Ray***, Aidan McDonald******

PP 2 *Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

****Inst. Química Computacional i Catàlisi, Dept. Química, Univ. Girona, Spain**

*****Dept. Chemistry, Humboldt-Universität zu Berlin, Germany**

******School of Chemistry, Trinity College Dublin, Ireland**

Spinning around in transition-metal chemistry

Hol na prvom spratu / Lobby of the first floor

11.15 – 11.45 Koktel / Cocktail

Velika sala na prvom spratu / Great hall on the first floor

Predavanja po pozivu / Invited Lectures

Predsedavajući / Chairperson: Velimir Popsavin

11.45 – 12.10 Ivana Drvenica, Olgica Nedić*, Aleksandar Dekanski**

PPP 1

Inovacioni centar TMF, *INEP, **IHTM - CEH, Univerzitet u Beogradu, Srbija

***Institut za hemiju, tehnologiju i metalurgiju, CEH, Univerzitet u Beogradu, Srbija**

Proces recenziranja radova u časopisima iz hemije i srodnih oblasti koji se izdaju u Srbiji / Peer-review process in journals dealing with chemistry and related subjects published in Serbia

Velika sala u prizemlju / Great hall on the ground floor

12.15 – 13.30 Posterska sesija 1 / Poster Session 1
(OH P1 – OH P22; NH P01 – NH P04; EH P01 – EH P04;
HŽS P01 – HŽS P05; HTM P01 – HTM P06)

13.30 – 14.30 Ручак / Lunch

Uklanjanje postera / Poster Dismounting (Sesija 1 / Session 1)

Sale Instituta za hemiju, prvi sprat / Halls of the Department of Chemistry, first floor

Sala A / Hall A

Sekcijsko predavanje / Keynote Lecture

Predsedavajući / Chairperson: Maja Gruden-Pavlović

14.30 – 14.50 Snežana Rajković, PMF, Univerzitet u Kragujevcu, Srbija

NH S

Dinuklearni platina(II) kompleksi kao katalitički reagensi za selektivnu hidrolizu peptide / Dinuclear platinum(II) complexes as catalytic reagents for the selective hydrolysis of peptides

Usmena izlaganja / Oral presentations

- 14.50 – 15.05** Snežana M. Jovanović, Biljana V. Petrović, Živadin D. Bugarčić
NH 01 **Sinteza i karakterizacija novih bimetalnih kompleksa platine(II) i paladijuma(II) i ispitivanje njihovih interakcija sa važnim biomolekulima**
Synthesis and characterisation of the new bimetallic complexes of platinum(II) and palladium(II) and study of their interactions with important biomolecules
- 15.05 – 15.20** Jovana V. Bogojeski, Milan M. Milutinović, Olivera R. Klisurić, Sofi K.C.
NH 02 **Elmroth, Živadin D. Bugarčić**
Sinteza i struktura Rh(III) kompleksa sa pincer-tipom liganda; Interakcije sa biomolekulima
Synthesis and structures of pincer-type rhodium(III) complex; Interactions with biomolecules
- 15.20 – 15.35** Milan M. Milutinović, Ana Rilak, Ioannis Bratsos, Olivera R. Klisurić,
NH 03 **Živadin D. Bugarčić**
Novi 4'-(4-hlorofenil)-2,2':6',2''-terpiridin rutenijum(II) kompleksi: Sinteza, karakterizacija i interakcije sa biomolekulima
New 4'-(4-chlorophenyl)-2,2':6',2''-terpyridine ruthenium(II) complexes: Synthesis, characterization and interaction with biomolecules
- 15.35 – 15.50** Nada D. Savić, Beata Warżajtis, Biljana Đ. Glišić, Marija Antić,
NH 04 **Slavko Radenković, Urszula Rychlewska, Miloš I. Djuran**
Sinteza i karakterizacija kompleksa zlata(III) sa tricikličnim aromatičnim jedinjenjima koja sadrže azot
Synthesis and characterization of gold(III) complexes with tricyclic aromatic nitrogen-containing heterocycles
- 15.50 – 16.05** Maja D. Nešić, Jelena Žakula, Lela Korićanac, Milutin Stepić, Iva Popović,
NH 05 **Boris Rajčić, Marijana Petković**
Sistem za fotoaktivnu terapiju kancera na bazi nanočestica TiO₂ i kompleksa rutenijuma
Sistem za fotoaktivnu terapiju kancera na bazi nanočestica TiO₂ i kompleksa rutenijuma
- 16.05 – 16.20** Marko G. Pavlović, Vanessa Prevot, Elodie Bourgeat-Lami, Istvan Szilagyi
NM 01 **Uticaj adsorpcije polimera na koloidnu stabilnost Dvostrukih Slojevitih Hidroksida**
Tuning colloidal stability of Layered Double Hydroxides by polymer adsorption

Sala B / Hall B

Sekcijsko predavanje / Keynote Lecture

Predsedavajući / Chairperson: Igor Opsenica

- 14.30 – 14.50** Mario Zlatović, Hemijski fakultet, Univerzitet u Beogradu, Beograd, Srbija
OH S **Potruga za mehanizmom dejstva inhibitora botulinum neurotoksina ili Kako pokvariti molekulska mašinu**
In a search of a mechanism of action of botulinum neurotoxin inhibitors or How to sabotage the molecular machine

Usmena izlaganja / Oral presentations

- 14.50 – 15.05** Violeta R. Marković, Katarina Jakovljević, Milan D. Joksović, Ivana Matić
OH 01 **Sinteza i biološko ispitivanje novih triazolskih Mannich-ovih baza**
Synthesis and biological screening of novel triazole Mannich bases
- 15.05 – 15.20** Ivana Kovačević, Mirjana Popsavin, Jovana Francuz, Goran Benedeković,
OH 02 **Vesna Kojić, Gordana Bogdanović, Milka Jadranin, Velimir Popsavin**
Sinteza i antitumorska aktivnost defenilovanih analoga goniofufurona
Synthesis and antitumour activity of dephenylated goniofufurone analogues

- 15.20 – 15.35 **Jovana Jovanović, Danijela Ilić-Komatina, Ivan Damljanović,**
OH 03 **Rastko D. Vukičević**
Sinteza 6-acil-5-feniltetrahidropirazolo[1,2-a]pirazol-1(5H)-ona
Synthesis of 6-acyl-5-phenyltetrahydropyrazolo[1,2-a]pyrazol-1(5H)-ones
- 15.35 – 15.50 **Života Selaković, Sandra B. Šegan, Rekha G. Panchal, Bogdan A. Šolaja**
OH 04 **Nova farmakofora aktivna na Ebola virus**
A novel anti-Ebola pharmacophore
- 15.50 – 16.05 **Milica Videnović, Tatjana Srdić-Rajić, Igor Opsenica, Siniša Radulović,**
OH 05 **Bogdan Šolaja**
Ispitivanje antiproliferativne aktivnosti novih derivata benzotiazolamina prema MCF-7 ćelijskoj liniji humanog kancera dojke
Investigation of antiproliferative activity of new benzothiazolamine derivatives against MCF-7 human breast cancer cell line
- 16.05 – 16.20 **Slavko Radenković, Marija Antić, Nada D. Savić, Biljana Đ. Glišić,**
TH 01 **Miloš I. Djuran**
Priroda Au-N veze i aromatičnost N-heterocikličnih liganada koordinovanih za zlato(III) jon
The nature of Au-N bond and aromaticity of N-heterocycles coordinated to Au(III) ion
- 15.45-16.30 **IZLET / EXCURSION**
Polazak autobusa sa parkinga ispred glavnog ulaza Prirodno-matematičkog fakulteta (ulica Radoja Domanovića 12)
Bus departure from the parking lot in front of the main entrance of Faculty of Science (Radoja Domanovića street, 12)
- 20.00 **Večera u tradicionalnom šumadijskom restoranu ORANICA (Šumarice)**
Dinner in the traditional Šumadia restaurant ORANICA

Subota, 11. jun 2016. / Saturday, June 11, 2016

- 08.30 – 12.30 **Registracija – Hol u prizemlju glavne zgrade**
Registration – Lobby on the ground floor

Velika sala u prizemlju / Great hall on the ground floor

- 09.00– 09.30 **Postavljanje postera / Poster Mounting (Sesija 2 / Session 2)**

Velika sala na prvom spratu / Great hall on the first floor

- Plenarno predavanje / Plenary Lecture**
Predsedavajuća / Chairperson: Živadin Bugarčić
- 09.30 – 10.15 **Iztok Turel, Faculty of Chemistry and Chemical Technology, University of Ljubljana,**
PP 3 **Slovenia**
Interactions of metal ions with old drugs
- Predavanja po pozivu / Invited Lectures**
- 10.15 – 10.45 **Jakob Kljun, Izток Turel**
PPP 2 **Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia**
 β -Diketonate scaffolds in medicinal chemistry:
The case of organoruthenium anticancer compound

Hol na prvom spratu / Lobby of the first floor

- 10.45 – 11.15 **Koktel / Cocktail**

Velika sala na prvom spratu / Great hall on the first floor

- Predavanja po pozivu / Invited Lectures**
Predsedavajući / Chairperson: Mirjana Popsavin
 11.15 – 11.45 **Janoš Čanadi, Jacquelyn Gervay-Hague***
 Prirodno-matematički fakultet, Univerzitet u Novom Sadu, Srbija
 *Department of Chemistry, University of California, Davis, USA
 PPP 3 **Sinteza sulfonskih C-glikozida kao potencijalnih inhibitora glikozil transferaza**
 Synthesis of C-glycoside sulfones as potential glycosyltransferase inhibitors

Sale Instituta za hemiju, prvi sprat / Halls of the Department of Chemistry, first floor

- Sala A / Hall A**
Sekcijsko predavanje / Keynote Lecture
Predsedavajući / Chairperson: Slavica Ražić
 12.00 – 12.20 **Zsanett Dorkó,*** Miloš P. Pešić,*** Anett Szokolczai,***
 AH S **Miljana D. Todorov***, Tatjana Ž. Verbić***, George Horvai***,**
 *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Budapest, Hungary; **MTA-BME Research Group of Technical Analytical Chemistry, Budapest, Hungary; *** Faculty of Chemistry, University of Belgrade, Serbia
Molekulski obeleženi polimeri
 Molecularly imprinted polymers
Usmena izlaganja / Oral presentations
 12.20 – 12.35 **Marko Z. Krstić, Svetlana R. Ibrić, Slavica S. Ražić**
 AH O1 **Karakterizacija čvrstih samo-mikroemulgujućih sistema sa karbamazepinom izrađenim sa poroznim adsorbenisima**
 Characterization of solid self-microemulsifying drug delivery systems of carbamazepine with porous adsorbents
 12.35 – 12.50 **Iva A. Popović, Maja Nešić, Zoran Šaponjić, Marijana Petković**
 AH O2 **Kvalitativno i kvantitativno poređenje masenih spektara vitamina E i A dobijenih MALDI, SALDI i LDI TOF MS tehnikama**
 Quantitative and qualitative comparison of mass spectra of vitamin E and A acquired with MALDI, SALDI and LDI TOF MS techniques
 12.50 – 13.05 **Miloš P. Pešić, Vesna S. Živanović, Elisabet Fuguet, Clara Ràfols,**
 AH O3 **Ilija N. Cvijetić, Alex Avdeef, Tatjana Ž. Verbić**
Terfenadine solubility – MS studies of pH dependent aggregation
 Rastvorljivost terfenadina – MS proučavanje pH zavisne agregacije
 13.05 – 13.20 **Maja M. Sremački, Jovana Lj. Simić, Jelena R. Radonić, Maja M. Turk**
 HŽS O1 **Sekulić, Mirjana B. Vojinović Miloradov**
Otpadna voda mesne industrije – skrining analiza
 Meat processing industry wastewater – screening analysis
 13.20 – 13.35 **Aleksandra M. Dramićanin, Filip Lj. Andrić, Nebojša M. Momirović,**
 HTH O1 **Sandra B. Šegan, Dušanka M. Milojković-Opsenica**
Šećerni profil kore i jezgra krompira kao indikator botaničkog porekla i sistema gajenja
 Sugar composition of potato peel and core as an indicator of its botanical origin and system of agriculture
 13.35 – 13.50 **J. Lović, N. Prlainović, D. Mijin, S. Stevanović, B. Andjelković, S. Petrović,**
 EH O1 **M. Avramov Ivić**
Detekcija glukoze korišćenjem glukoze okidaza-glutaraldehyd-cistein modifikovane elektrode od zlata primenom ciklične voltametrije
 Glucose sensing using glucose oxidase-glutaraldehyde-cysteine modified gold electrode using cycling voltammetry

Sala B / Hall B**Sekcijsko predavanje / Keynote Lecture****Predsedavajući / Chairperson: Tanja Ćirković Veličković**

12.00 – 12.20 **BH S** **Danijela Apostolović**, Hemijski fakultet, Univerzitet u Beogradu, Beograd, Srbija

Razotkrivanje alergena Proteomikom: struktura, funkcija i epitopi
Revealing the allergens by Proteomics: structure, function and epitopes

Usmena izlaganja / Oral presentations

12.20 – 12.35 **BH O1** **Jelena Ćimović, Ana Penezić, Ivan Pavićević, Vesna Jovanović,**

Marija Takić, Tamara Uzelac, Ljuba Mandić

Vezivanje slobodnih masnih kiselina i bakar(II)-jona za HSA dovodi do promena u karbonilaciji i reaktivnosti Cys34 tiolne grupe sa metilgliksalom

Binding of FAs and Cu(II)-ions to HSA changes its carbonylation pattern and Cys34 thiol group reactivity with methylglyoxal

12.35 – 12.50 **BH O2** **Suzana S. Jovanović-Šanta, Dimitar S. Jakimov, Vesna V. Kojić,**

Lidija D. Aleksić, Evgenija A. Đurendić, Jovana J. Ajduković

Efekat odabranih 17-supstituisanih androstanskih derivata na ćelije kancera

The effect of selected 17-substituted androstane derivatives on cancer cells

12.50 – 13.05 **BH O3** **Katarina T. Smiljanić, Danijela Lj. Apostolović, Marija B. Peruško, Sara V.**

Trifunović, Luka D. Mihajlović, Lidija Burazer, Tanja D. Ćirković Veličković

Sub-polenske čestice kao potencijalno najopasniji alergenski nosioci u poređenju proteoma različitih polenskih frakcija ambrozije (*Ambrosia artemisiifolia* L.)

Proteomic comparison reveals sub-pollen particles as potentially the most dangerous allergenic carriers among different pollen fractions of short ragweed (*Ambrosia artemisiifolia* L.)

13.05 – 13.20 **BH O4** **Milan P. Mladenović, Rino Ragno**

Racionalni dizajn novih inhibitora MAO B kao terapeutika u lečenju Parkinsonove bolesti baziran na 3-D QSAR studijama

The 3-D QSAR studies based rational design of novel MAO B inhibitors as therapeutics in Parkinson's disease treatment

13.20 – 13.35 **BH O5** **Simeon Minić, Dragana Stanić-Vučinić, Maja Krstić, Jelena Mihailović,**

Milan Nikolić, Tanja Ćirković Veličković

Određivanje strukture hromopeptida dobijenih pepsinskom digestijom C-fikocijanina iz mikroalge *Spirulina platensis*

Determination of chromopeptides structure obtained by pepsin digestion of C-phycoyanin from microalga *Spirulina platensis*

13.35 – 13.50 **HTM O1** **Marijana M. Ponjavić, Marija S. Nikolić, Jasmina Nikodinović-Runić,**

Sanja Jeremić, Sanja Stevanović, Jasna Đonlagić

Poređenje hidrolitičke, enzimske i degradacije u kompostu PCL/PEO diblok kopolimera

Comparative analysis of hydrolytic, enzymatic and degradation in compost of PCL/PEO diblock copolymers

14.00 – 15.30 **Ručak / Lunch**

Velika sala u prizemlju / Great hall on the ground floor

15.30 – 16.45 **Posterska sesija 2 / Poster Session 2**

(AH P01 – AH P15; BH P01 – BH P04; FH P01 – FH P05;
HTH P01 – HTH P08; HI P01 – HI P08; NM P01)

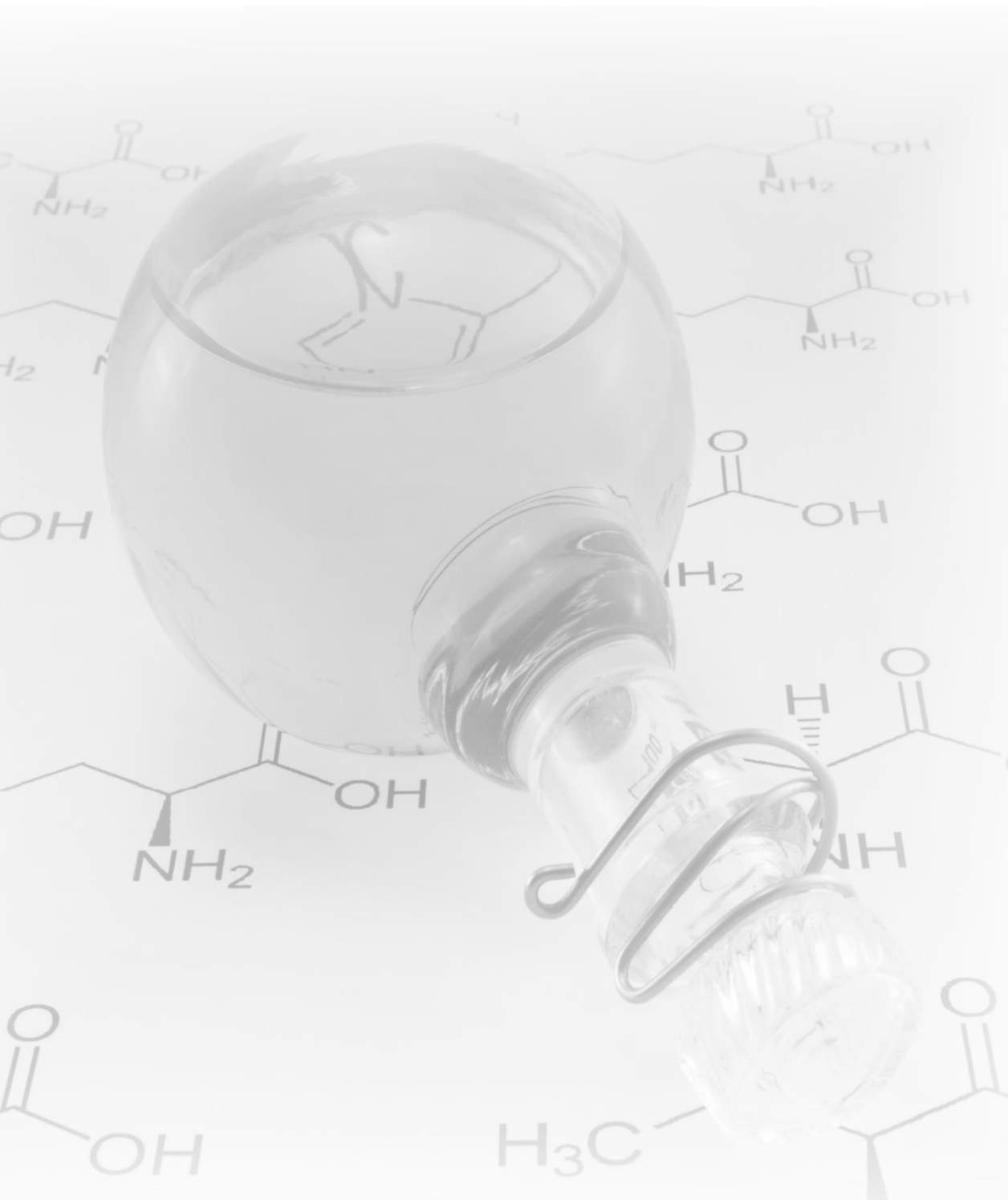
16.45 – 17.00 **Uklanjanje postera / Poster Dismounting**

Velika sala na prvom spratu / Great hall on the first floor

17.30 **Dodela IUPAC poster nagrada i zatvaranje Savetovanja**

IUPAC poster prize award and Closing Ceremony

KRATKI IZVODI
ABSTRACTS



Plenarna predavanja / Plenary Lectures

PP 1

Polyxometalates as artificial enzymes

Tatjana N. Parac-Vogt

Department of Chemistry, KU Leuven, 3001 Leuven, Belgium

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Selective hydrolysis of proteins is an important procedure in numerous biochemical applications. Based on the non-covalent, electrostatic interaction between negatively charged polyoxometalates (POMs) and positive surface domains of proteins¹, we recently introduced a conceptually new approach in the development of artificial proteases by using POMs as ligands for Lewis acid metal ions. In our approach the POM acts as a ligand for the Zr ion, and due to its three-dimensional shape and negative charge it also induces the selectivity that is necessary for a controlled fragmentation of the polyamide backbone. Zr(IV)-substituted POMs were proven to be catalytically active towards the hydrolysis of the highly inert amide bond in dipeptides and oligopeptides.² More importantly, these POMs were shown to display unprecedented hydrolytic activity towards insulin chain B, lysozyme, myoglobin and albumin proteins.³ The hydrolysis occurs at peptide bonds which are located either at clearly defined positive patches that are able to accommodate the POM ligand, or on the interface of positive surface zones containing negatively charged Asp or Glu residues that allow for additional anchoring of Zr(IV).

1. Goovaerts V., Stroobants K., Absillis G., Parac-Vogt T.N., *Phys. Chem. Chem. Phys.*, **2013**, *15*, 18378.
2. a) Absillis G., Parac-Vogt T. N., *Inorg. Chem.*, **2012**, *51*, 9902. b) Ly H.G.T., Absillis G., Parac-Vogt T.N., *Dalton Trans.*, **2013**, *42*, 10929.
3. a) Stroobants K., Moelants E., Ly H.G.T., Proost P., Bartik K., Parac-Vogt T.N., *Chem. Eur. J.*, **2013**, *19*, 2848. b) Stroobants K., Goovaerts V., Absillis G., Moelants E., Proost P., Parac-Vogt T.N., *Chem. Eur. J.*, **2014**, *20*, 9567. c) Stroobants K., Absillis G., Moelants E., Proost P., Parac-Vogt T.N., *Chem. Eur. J.* **2014**, *20*, 3894. d) Sap A, Absillis G., Parac-Vogt T.N, *Dalton Trans.* 2015, *44*, 1539. e) Ly, H. G. T.; Absillis, G.; Janssens, R.; Proost, P.; Parac-Vogt, T. N. *Angew. Chem. Int. Ed.* **2015**, *54*, 7391.

Spinning around in transition-metal chemistry

Marcel Swart*,** Adrià Romero-Rivera**, Kallol Ray***, Aidan McDonald****

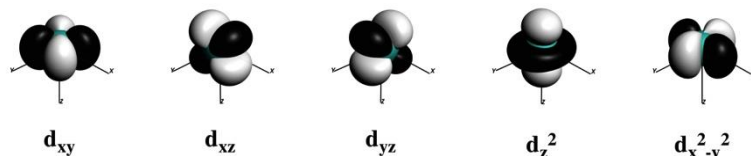
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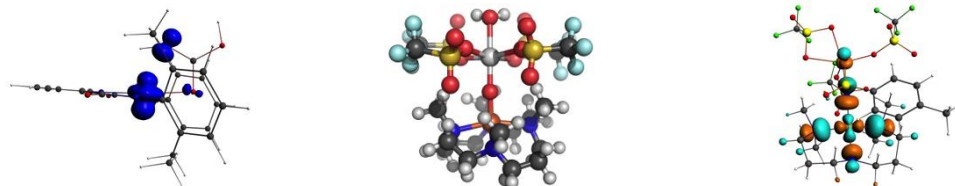
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The chemistry of the first-row transition-metals is highly diverse with a multitude of different reactivity and property patterns. This richness results principally from the partial occupation of the shell of d-orbitals, which leads to different oxidation and spin states.



Especially the spin states remain an enigmatic property that has triggered many studies, and recently the first text-book devoted entirely to it has appeared.^[1] Of course, having a different number of unpaired electrons has a direct effect on the structure, magnetism, and reactivity of molecules. Insights into spin states of transition-metal complexes can be obtained from synthesis, spectroscopy, computational studies, and in some cases from catalysis. However, the assignment of spin states, and the role it plays in e.g. reactivity, is not unambiguous. The combination of a variety of techniques therefore is needed, which has led to the formation of an European collaborative network (COST Action CM1305),



Here I will present recent computational studies on iron(III/IV)-(hydro)(per)oxo species,^[2,3] Mössbauer spectroscopy,^[4] Sc³⁺-capped iron-oxygen^[2,3] and copper-nitrene^[5,6] complexes, and terminal Ni(III)-oxygen adducts.^[7]

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References

1. M. Swart, M. Costas (Eds.), Spin states in Biochemistry and inorganic chemistry: Influence on Structure and Reactivity, Wiley, Chichester UK, 2015
2. M. Swart, *Chem. Commun.* **2013**, 49, 6650-6652
3. J. Prakash, G.T. Rohde, K.K. Meier, A.J. Jasniewski, K.M. Van Heuvelen, E. Münck, L. Que Jr., *J. Am. Chem. Soc.* **2015**, 137, 3478-3481
4. A. Romero-Rivera, M. Swart, *in preparation*, 2016
5. S. Kundu, E. Miceli, E. Farquhar, F.F. Pfaff, U. Kuhlmann, P. Hildebrandt, B. Braun, C. Greco, K. Ray, *J. Am. Chem. Soc.* **2012**, 134, 14710-14713
6. M. Swart, K. Ray, and co-workers, *in preparation*, 2016
7. P. Pirovano, E. Farquhar, M. Swart, A.J. Fitzpatrick, G.G. Morgan, A.R. McDonald, *Chem. Eur. J.* **2015**, 21, 3785-3790



Interactions of metal ions with old drugs

Interakcije jona metala i jedinjenja sa poznatim farmakološkim svojstvima

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One of important fields that bioinorganic chemistry deals with are interactions of metal ions with biologically important compounds. Without any doubt it was Rosenberg's discovery of cisplatin's cytotoxic properties¹ that was the most important cause for great interest and development in this field of chemistry.

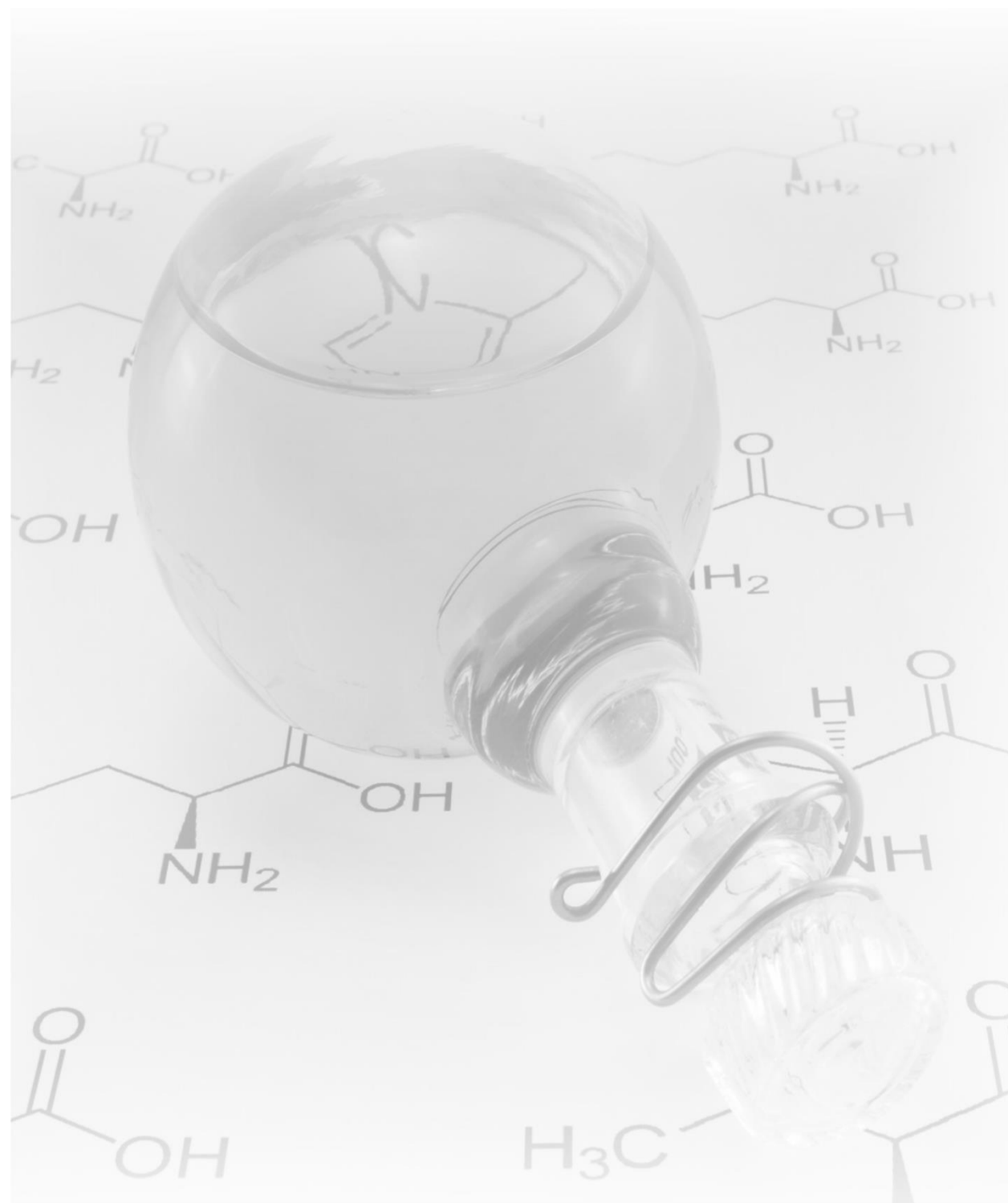
Nowadays, it is well established that many drugs used in clinical practice require the presence of metal ions for their activity. On the other hand, metal ions can also react with drugs and decrease their activity (e.g. due to formation of sparingly soluble compounds). Moreover, it became evident that metal complexes of clinical drugs (that frequently contain electron donor atoms or groups) might exert increased or changed biological activity. With other words – a so called synergistic activity can occur.²

The design of a novel drug is a long-lasting and extremely expensive process.³ Therefore the repurposing of old drugs is very attractive topic nowadays. The quote of Sir James Whyte Black (winner of the 1988 Nobel Prize in medicine) that 'The most fruitful basis for the discovery of a new drug is to start with an old drug', is thus very stimulating.⁴

In the last two decades my lab was and still is involved in studies of metal ions interactions with drugs used in clinical practice. In this review I will shortly present our efforts in the most representative systems. Quinolone antibacterial agents act most commonly as O,O-ligands. Bidentate bonding of oxygen atoms to the metal center is also typical for some ligands from non-steroidal anti-inflammatory drugs (NSAID) family and also pyrithione analogues (in some of these also O,S- coordination is possible). We have also studied interactions with molecules that contain nitrogen atoms which coordinate to the metal. Among these I will present the cases of antiviral drug acyclovir (N or N,O- binding) which is a representative of nucleobase molecules, antibacterial agent clioquinol and its derivatives (N,O- binding) and antifungal azoles (N- binding).

References:

1. B. Rosenberg, L. Vancamp, J. E. Trosko, V. H. Mansour, *Nature*, **222** (1969), 385-386.
2. I. Turel, J. Kljun, *Curr. Top. Med. Chem.*, **11** (2011), 2661-2687 and the references therein.
3. D. J. Payne, M. N. Gwynn, D. J. Holmes, D. L. Pompliano, *Nat. Rev. Drug Disc.*, **6** (2007), 29-40.
4. T. N. K. Raju, *Lancet*, **355** (2000), 1022.



Predavanja po pozivu / Invited Lectures

PPP 1

Proces recenziranja radova u časopisima iz hemije i srodnih oblasti koji se izdaju u Srbiji

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Kroz anketu sprovedenu među urednicima naučnih časopisa iz oblasti hemije, hemijske tehnologije i srodnih oblasti, koji se publikuju u Srbiji, prikupljene su informacije o iskustvima, problemima i teškoćama sa kojima se urednici sreću tokom procesa recenziranja radova. Od 27 časopisa koji su u Srbiji izlazili u toku 2015. godine, na anketu su odgovorili urednici iz 22 časopisa. Na osnovu odgovora glavnih i odgovornih urednika, prikupljeni su osnovni podaci o časopisima, dok su svi urednici koji učestvuju u procesu recenziranja (područni, sekcijski) odgovarali na pitanja koja su se odnosila na način sprovođenja procesa recenziranja. Pored toga, oni su ocenjivali kvalitet recenzija i odgovornost recenzenata, davali primedbe na trenutno stanje i sugestije za poboljšanje procesa recenziranja. Pokazano je da su najveći problemi sa kojima se urednici sreću u procesu recenziranja slab odziv recenzenata, recenzije lošeg kvaliteta, nekad uz predrasude recenzenata i njihovo nesnalaženje i/ili nerazumevanje procesa recenziranja. Pored toga, način traženja i pozivanja recenzenata nema suštinskog uticaja na kvalitet recenzija. Značajan broj urednika često sam recenzira radove. Pozivanje recenzenata na predlog autora, barem u anketiranim časopisima, relativno često je uzrok neadekvatnih recenzija.

Peer-review process in journals dealing with chemistry and related subjects published in Serbia

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A survey was conducted among editors of journals publishing in the field of chemistry, chemical technology and related topics in Serbia, aiming to collect information on their experiences, problems and difficulties during peer-review process. Editors from 22 journals out of 27 which regularly published during 2015 replied. Principle data on journals were collected from responses obtained from editors-in-chief, whereas all editors (including sub-editors and section editors) participated in a questionnaire concerning peer-review procedure. Additionally, they were asked to evaluate quality of reports and attitude of reviewers, discuss present situation and suggest measures to improve peer-review process. The greatest problems encountered by editors in peer-review proces can be summarized as follows: low rate of acceptance to review, low quality of reports, sometimes due to reviewer's bias or his/her inability to properly understand review process. A method used to search for reviewers does not substantially influence quality of reports. Significant number of editors often perform peer-review by him/herself. Invitation of reviewers suggested by authors, at least in the surveyed journals, also relatively often results in inadequate reports.

β -Diketone Scaffolds in Medicinal Chemistry: The Case of Organoruthenium Anticancer Compounds

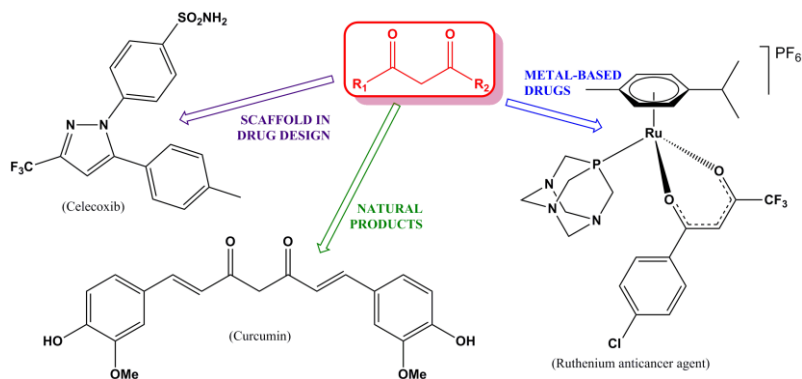
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1,3-Dicarbonyl compounds are of the most important scaffolds in the synthesis of nitrogen heterocycles. The β -diketone subset of this wide range of compounds is a key intermediate in the synthesis non-steroidal anti-inflammatory agents of the coxib family which exert their activity through inhibition of enzyme cyclooxygenase-2 (COX-2).¹ These compounds were recently proven to have excellent anticancer potential at the preclinical stage of research. The anticancer activity is however unrelated to COX inhibition.^{1b}

Moreover the β -diketone scaffold is present in the family of curcuminoids. Both natural products and their synthetic analogs possess interesting antibacterial, neuroprotective and anticancer properties.² Coordination compounds of curcuminoids with platinum-group metals as potential anticancer agents are a hot topic of current research as to our knowledge most scientific articles on this topic were published from 2011 on.³

Structurally simpler diketones e.g. acetylacetonone derivatives are also employed in the design of novel metal-based agents. Most notably, the first non-platinum metal-based anticancer compound to enter clinical trials was budotitane, *cis*-diethoxy(1-phenylbutane-1,3-dionato)titanium(IV).⁴ Recently several papers by the groups of Lippard, Dyson, McGowan and ourselves presenting the synthesis of platinum-group coordination and organometallic compounds with biological evaluation and with mode-of-action studies were published in high impact journals in the field of medicinal chemistry.⁵



1. a) Penning T. D. *et al.*, *J. Med. Chem.* **40** (1997) 1347-1365; b) Half, E.; Arber, N. *Exp. Op. Pharmacother.* **10** (2009) 211-219,
2. Esatbeyoglu, T. *et al.*, *Angew. Chem. Int. Ed.* **51** (2012) 5308-5332
3. a) Caruso, F. *et al.*, *J. Med. Chem.* **55** (2011) 1072-1081; b) Pettinari, R. *et al.*, *Organometallics* **33** (2014) 3709-3715
4. Keppler, B. K. *et al.* (2005) in *Bioinorganic Chemistry*, vol. 78, pp 97-127
5. a) Wilson, J. J.; Lippard, S. J., *J. Med. Chem.* **55** (2012) 5326-5336; b) Lord, R. M. *et al.*, *J. Med. Chem.* **58** (2015) 4940-4953; c) Vock, C. A. *et al.*, *Eur. J. Inorg. Chem.* (2008) 1661-1671; d) Seršen, S. *et al.*, *J. Med. Chem.* **58** (2015) 3984-3996

Sinteza sulfonskih C-glikozida kao potencijalnih inhibitora glikozil transferaza

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U ovom radu prikazane su hemijske sinteze analoga **GDP** i **UDP** fukoze. Naša istraživanja se zasnivaju na očekivanjima da će sulfonski analozi šećernih nukleotida pokazati izuzetnu stabilnost prema glikozidaznoj aktivnosti prouzrokujući superiornu inhibiciju glikozil transferaza.^{1,2} Ključna faza sinteze uključuje Horner-Emmons-Wadsworth-ovu kondenzaciju u kojoj je primenjen jedan nedavno sintetizovan geminalni disulfonski reagens.³ Na taj način, prikazali smo jednu racionalnu višefaznu hemijsku sintezu sulfonskih analoga C-glikozidnih-difosfatnih nukleozida, jedinjenja koja predstavljaju potencijalne supstrate za glikozil transferaze.

Synthesis of C-glycoside sulfones as potential glycosyltransferase inhibitors

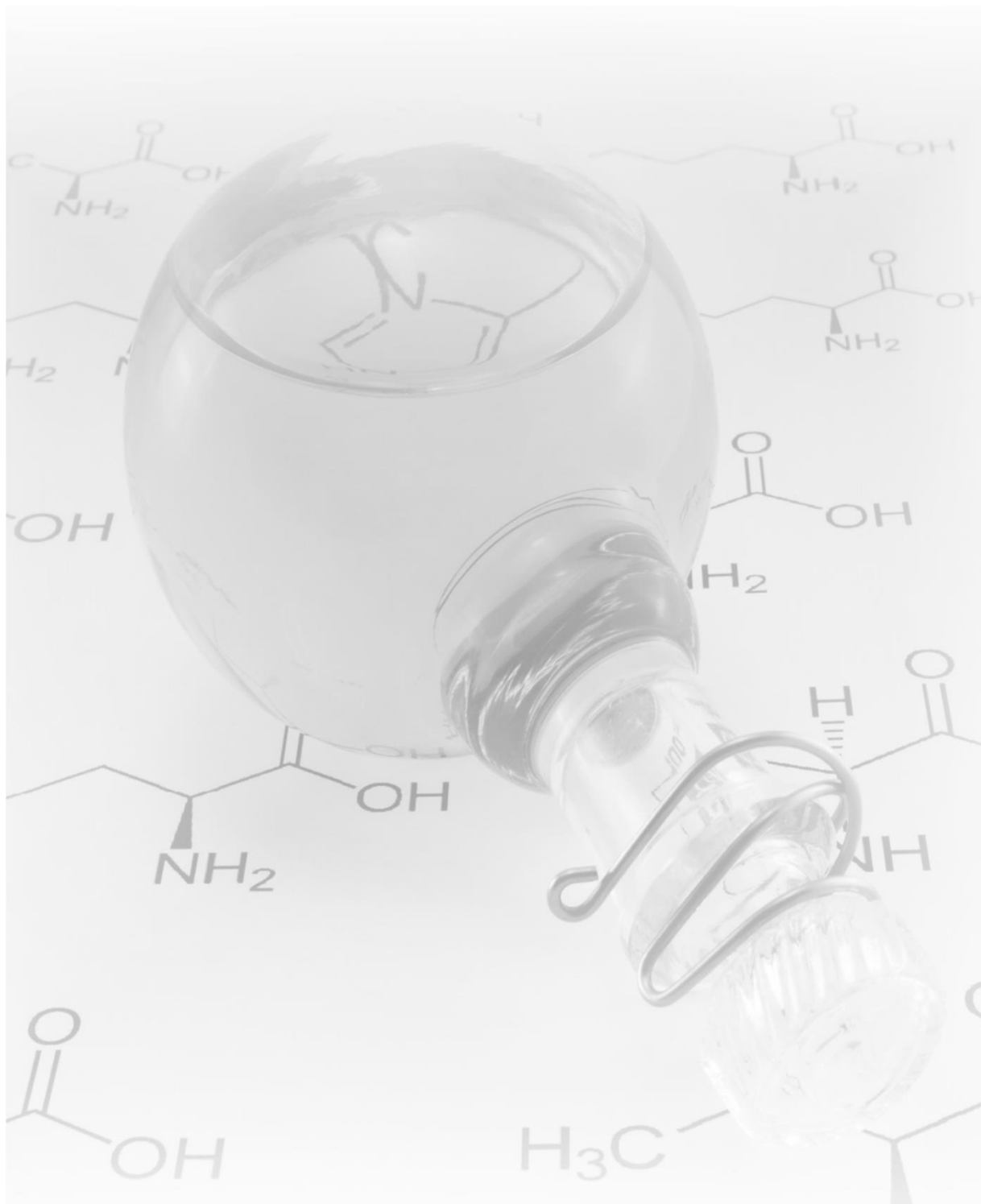
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The synthesis of new **GDP**- and **UDP**-fucose analogs is reported. Our interest in this area is fueled with expectation that sulfone analogs of sugar nucleotides will be exceptionally stable toward glycosidase activity thereby effecting superior glycosyl transferase inhibition^{1,2}. In the key step Horner-Emmons-Wadsworth condensation reaction was explored with a gem-disulfone reagent³. We have demonstrated a rational multistep chemical synthesis of C-glycoside disulfone analogs of sugar-diphosphate-nucleosides compounds which could represent potential substrate for glycosyltransferase enzymes.

1. K. Descroix, G. K. Wagner, *Org. Biomol. Chem.*, **2011**, 9, 1855
2. M. J. Hadd, M. A. Smith, J. Gervay-Hague, *Tetrahedron Lett.*, **2001**, 42, 5137
3. Andrew L. Lovering, Liza H. de Castro, Daniel Lim and Natalie C. J. Strynadka, *Science*, New Series, **2007**, Vol. 315, No. 5817, 1402



Saopštenja / Contributions**Analitička hemija / Analytical Chemistry**

AH S

Molecularly imprinted polymers – preparation and characterization of selective sorbentsZsanett Dorkó^{***}, Miloš P. Pešić^{***}, Anett Szakolczai^{*}, Miljana D. Todorov^{***},
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Molecular imprinting is a technology for creating selective binding sites in a polymeric matrix by polymerization in the presence of the target compound - the template[1]. The template can be washed out from the polymer and the resulting molecularly imprinted polymer (MIP) is capable of selectively rebinding the target compound from a sample matrix. MIPs are mimicking natural receptors (e.g. antibodies) in their selectivity and affinity. At the same time, imprinting is a simple and efficient synthetic method and MIPs have high physical and chemical stability which makes them superior to their biological counterparts. These polymers have versatile applications ranging from chromatographic and SPE sorbents, sensors and catalysts to drug delivery systems. Our research is focused on preparation of new MIP particles with higher selectivity and sorptive power, as well as to the development of chiral MIP particles for separation of enantiomers.

Molekulski obeleženi polimeri – dobijanje i karakterizacija selektivnih sorbenataZsanett Dorkó^{***}, Miloš P. Pešić^{***}, Anett Szakolczai^{*}, Miljana D. Todorov^{***},
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Molekulsko obeležavanje predstavlja tehnologiju usmerenu ka stvaranju selektivnih vezivnih mesta u polimernom matriksu polimerizacijom u prisustvu željenog molekula - templata. Nakon polimerizacije i uklanjanja templata, u polimeru ostaju vezivna mesta po veličini i naelektrisanju komplementarna templatu. Molekulski obeleženi polimeri (MOP) imaju univerzalnu primenu u analitici, koriste se kao sorbenti za hromatografiju, ekstrakciju, ali i kao senzori, katalizatori, za kontrolisano oslobađanje lekova itd. Cilj naših istraživanja je priprema novih MOP, selektivnijih i sa većom sorptivnom moći, kao i razvoj hiralnih MOP čestica za razdvajanje enantiomera.

Acknowledgements: OTKA, Hungary (Grant No. K104724) and the Ministry of Education, Science, and Technological Development of Serbia (Grant No. 172035) support this work.

References:

1. B. Sellergren, Molecularly Imprinted Polymer: Man Made Mimics of Antibodies and Their Application in Analytical Chemistry; Techniques and instrumentation in Analytical Chemistry, Elsevier Science, Amsterdam, 2001.
2. Zs. Dorkó, A. Szakolczai, T. Verbić, G. Horvai, *J. Sep. Sci.* **38** (2015) 4240-4247

AH O1

Rastvorljivost terfenadina – MS proučavanje pH zavisne agregacije

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Terfenadin, ranije korišćeni antihistaminik, je supstanca teško rastvorna u vodi i kao takav dobar model molekula za proučavanje rastvorljivosti. Koristeći različite tehnike i program p-DISOL-XTM određena je osnovna rastvorljivost ($S_0=(1,60\pm 0,11)\times 10^{-9}$ M) i prepostavljene su moguće ravnoteže u vodenoj sredini u pH intervalu pH 1,00-10,90.^[1] Pretpostavljeno je formiranje trimera u kiselim rastvorima, ali ne u neutralnim i baznim; potvrda ove pretpostavke tražena je na osnovu MS eksperimenta. Četiri rastvora Tf u etilendiamin-mlečna kiselina puferu (pH 4,54; 6,02; 7,62; 10,57) su ispitana na DP 70 i 200 V. Na pH 4,54 na obe DP vrednosti utvrđeno je prisustvo monomera, dimera i trimera. MS/MS eksperiment potvrđuje prisustvo dimera i trimera. Na pH 6,02 i 7,62 mogu se zapaziti monomeri i dimeri, ali je na pH 7,62 prisustvo dimera veoma malo. Na najvišoj pH prisutni su samo monomeri. Na osnovu eksperimentalnih podataka potvrđene su početne pretpostavke.

Terfenadine solubility – MS studies of pH dependent aggregation

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Terfenadine (Tf), a practically insoluble drug, has shown to be a very challenging molecule in solubility studies. Thorough study of Tf solubility with number of methods involved (powder XRD, FT-IR, elemental analysis, SEM, HPLC-MS/MS) and the use of computer program p-DISOL-XTM for data processing and refinement of equilibrium constants resulted in the determination of Tf intrinsic solubility ($S_0=(1.60\pm 0.11)\times 10^{-9}$ M) and an assumption of all the equilibrium reactions within the pH range 1.00-10.90.^[1] In this previous studies, formation of trimers in an acidic solution, but not in neutral and alkaline ones, was assumed. In this present work MS experiment were conducted to confirm it. Four solutions of Tf in 10 mM ethylenediamine + 10 mM lactic acid buffer have been investigated by MS (pH 4.54; 6.02; 7.62; 10.57) at two declustering potentials (DP) 70 and 200 V. At pH 4.54, at both DP, monomers, dimers and trimers can be observed. MS/MS experiments confirmed presence of dimers and trimers. At pH 6.02 and 7.62 monomers and dimers were found, but sample pH 7.62 at DP 200 V showed very low intensity of the dimers. At highest pH, only monomers were present. This is in agreement with calculations that suggested presence of aggregates in acidic solutions.

Acknowledgements: The Ministry of Education, Science, and Technological Development of Republic of Serbia supports this work (Grant No. 172008).

Reference:

1. T. Verbić et al, Fourth World Conference on PCMDDD, Red Island, Croatia, Sept. 21-24, 2015

Kvalitativno i kvantitativno poređenje masenih spektara vitamina E i A dobijenih MALDI, SALDI i LDI TOF MS tehnikama

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U ovom radu, uporedili smo masene spektre vitamina E i A dobijene laserskom jonizacijom i desorpcijom (LDI), sa organskim matricama (DHB, 9AA, CHCA i THAP) i pomoću supstrata na bazi titan dioksid (TiO_2) nanokristala različitih oblika i dimenzija (koloidne nanočestice, prolatni nanosferoidi i nanotube) jer ovi faktori utiču na procese desorpcije i jonizacije. Za procenu ponovljivosti merenja unutar jednog dana i između dana LDI, MALDI i SALDI TOF tehnika korišćena je Excel alatka (ANOVA). Homogenost distribucije ko-kristala (smeše) uzorka/matrice (supstrata) na M(S)ALDI pločici je izražena kao srednja vrednost koeficijenta varijacije serije merenja.

Rezultati su pokazali da je homogenost distribucije vitamina E i A na pločici povećana ukoliko se koristi bilo koji od nanokristala TiO_2 u odnosu na homogenost samog uzorka i bilo koje kombinacije uzorak/matrica. Za ponovljivost rezultata u toku jednog dana pokazano je da se vrednosti varijacija sa određenim matricama smanju u odnosu na LDI. Međutim, sa supstratima je slika drugačija, vrednosti varijacija unutar jednog dana neuporedivo su niže nego što su vrednosti dobijene LDI i MALDI metodom. Isti trend kao za varijacije unutar jednog dana, zapaža se i za vrednosti varijacija između dana, ponovo su se supstrati pokazali kao znatno bolji izbor. Sumarno, pokazan je veliki potencijal koji imaju supstrati na bazi TiO_2 za detekciju i kvantitativnu analizu vitamina E i A.

Quantitative and qualitative comparison of mass spectra of vitamin E and A acquired with MALDI, SALDI and LDI TOF MS techniques

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In this work, we have compared mass spectra of vitamin E and A acquired with LDI TOF MS, MALDI TOF MS with organic matrices (DHB, 9-AA, CHCA and THAP) and SALDI TOF MS analysis with substrates based on TiO_2 nanocrystals i.e. colloidal nanoparticles, prolate nanospheroids and nano tubes. Different size and shape of nanocrystals were used because of the already known fact that these factors have impact on desorption and ionization processes. The within-day and day-to-day precision LDI, SALDI and MALDI TOF MS was analysed using Excel tool (ANOVA). For calculation of homogeneity, we used the mean value of coefficient of variation of eight S/N values with nine repetition within three days for each analyte/substrate combination.

The results showed that homogeneity of vitamin E and A was significantly improved when either of nanocrystals were used compared to LDI and MALDI approach. Within day precision with some matrices were slightly higher, but with some matrices precision were even lower comparing to LDI. The same pattern was observed with values of day-to-day variations, again nanocrystals were much better choice. In summary, it is shown that substrates based on TiO_2 nanocrystals have the great potential for qualitative and quantitative analysis of vitamin E and A.

AH O3

Karakterizacija čvrstih samo-mikroemulgujućih sistema sa karbamazepinom izrađenim sa poroznim adsorbenima

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Jedan od načina za povećanje brzine rastvaranja/rastvorljivosti karbamazepina jeste formulacija čvrstih samo-mikroemulgujućih sistema (SSMEDDS). Cilj rada je fizičko-hemijska karakterizacija izrađenih formulacija SSMEDDS sa karbamazepinom. SSMEDDS se sastoji od karbamazepina, tečnog samo-mikroemulgujućeg sistema i različitih adsorpcionih nosača. Prilikom izrade SSMEDDS-a kao adsorpcioni nosači korišćeni su: Neusilin[®] FL2, Neusilin[®] UFL2, Sylysia[®] 320 i dijatomiti, pri čemu odnos adsorpcioni nosač/tečni SMEDDS je varirao (1:1 ili 3:1), dok je sadržaj karbamazepina stalan u svim izrađenim formulacijama i iznosi 20%. Za izradu SSMEDDS-a korišćene su dve metode: metoda direktne adsorpcije i metoda uparavanja pomoću etanola (99,5%, v/v). Detaljnom fizičko-hemijskom karakterizacijom (TGA, DSC, HSM, PXR, FT-IR, SEM) utvrđeno je da udeo i vrsta adsorpcionog nosača nemaju uticaj na polimorfni oblik karbamazepina. Međutim, utvrđeno je da u formulacijama izrađenim metodom direktne adsorpcije karbamazepin ostaje u farmakološki aktivnom polimorfnom obliku III, dok u formulacijama izrađenim metodom rastvaranja karbamazepin prelazi u polimorfni oblik II. Ovom polimorfnim prelazom se može objasniti razlika u brzini rastvaranja karbamazepina iz SSMEDDS izrađenim različitim metodama. Tromesečna stabilnost odabrane optimalne formulacije, čuvanjem na sobnoj temperaturi, potvrđena je primenom Ramanske spektroskopijom.

Characterization of solid self-microemulsifying drug delivery systems of carbamazepine with porous adsorbents

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Formulation of solid self-microemulsifying drug delivery systems (SSMEDDS) is one of many approaches to increase the dissolution rate/solubility of carbamazepine. The aim of this study is characterization of SSMEDDS. SSMEDDS consists of carbamazepine, liquid SMEDDS and different adsorption carriers. Different adsorption carriers that were used are: Neusilin[®] FL2, Neusilin[®] UFL2, Sylysia[®] 320 and diatomite. The ratio adsorption carrier/liquid SMEDDS varied (1:1 or 3:1), but the share of carbamazepine was constant (20%). SSMEDDS were formed by using two different methods: direct adsorption and evaporation with ethanol (99,5%, v/v). A detailed physicochemical characterization (TGA, DSC, HSM, PXR, FT-IR, SEM) has shown that the ratio and type of adsorbent carrier have no effect to the polymorphous form of carbamazepine. However, it was determined that in formulations created by the direct adsorption method carbamazepine remains in the pharmacologically active polymorphous form III, while in formulations made by dissolution methods carbamazepine turns into polymorphous form II. This polymorphous transfer can explain the difference in dissolution rates of carbamazepine from SSMEDDS created by different methods. A three month stability of the selected optimal formulation, kept at room temperature, has been confirmed by application of Raman spectroscopy.



AH P01

Primena plazme indukovane TEA CO₂ laserskim zračenjem za određivanje koncentracije magnezijuma u aluminijumskim legurama

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Ispitivana je mogućnost analitičke primene plazme indukovane nanosekundnim infracrvenim TEA CO₂ laserskim zračenjem za određivanje koncentracije Mg u aluminijumskim legurama, pri sniženom pritisku vazduha. Oštre i dobro razložene spektralne linije Mg, uz nisku emisiju pozadine, dobijene su posmatranjem plazme na rastojanju 3 mm od površine mete. Kalibraciona kriva za Mg konstruisana je korišćenjem sertifikovanih uzoraka aluminijumskih legura. Dobijena je linearna zavisnost između LIBS signala i koncentracije analita ($r^2=0,9957$) u opsegu od 0,26-1,10 % m/m i korišćena je za određivanje koncentracije Mg u kontrolnom uzorku. Kao referentna metoda za kvantifikovanje Mg u kontrolnom uzorku korišćena je induktivno spregnuta plazma - optičko emisiona spektroskopija (ICP-OES). Dobijeno je odlično slaganje između LIBS i ICP-OES rezultata. Rezultati potvrđuju da je TEA CO₂ LIBS efikasna tehnika za kvantitativnu analizu Mg u uzorcima aluminijumskih legura.

Zahvalnica: *Ova istraživanja su podržana od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat br. 172019).*

Application of plasma induced by TEA CO₂ laser for determining the concentration of magnesium in the aluminum alloys

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The analytical capability of plasma induced by nanosecond infrared TEA CO₂ laser radiation under reduced air pressure for determination of Mg in aluminum alloys was investigated. Sharp and well resolved spectral lines of Mg, with negligibly low background emission, were obtained from a plasma region 3 mm above the target surface. A calibration curve for Mg was constructed using certified aluminium alloy samples. A linear relationship between LIBS signal and analyte concentration was obtained ($r^2 = 0.9957$) in the range from 0,26 - 1,10 % w/w, and used for determination of Mg in a control sample. As a reference method for quantification of Mg in the control sample inductively coupled plasma - optical emission spectroscopy (ICP-OES) was used. Good agreement between LIBS and ICP-OES results was obtained. The results confirm that TEA CO₂ LIBS is an effective technique for quantitative analysis of Mg in aluminum alloy samples.

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AH P02

Isparljiva jedinjenja cvasti i listova biljne vrste *Cephalaria ambrosioides* (Sibth. & Sm.) Roem. & Schult. (Caprifoliaceae): hemotaksonomski aspekti

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U ovom radu je prikazan hemijski sastav i hemotaksonomski značaj etarskih ulja dobijenih hidrodestilacijom iz cvasti (*inf*) i listova (*lf*) biljne vrste *Cephalaria ambrosioides* (Sibth. & Sm.) Roem. & Schult. (Caprifoliaceae). GC i GC-MS analizom je utvrđeno da su ova etarska ulja (dobijena u niskim prinosima - 0,008%, odnosno 0,004%, w/w) kompleksne smeše jedinjenja, od kojih je identifikovano 284 (88,6% sastojaka *inf* ulja, odnosno 96,1% *lf* ulja). Nađeno je da su glavni sastojci palmitinska kiselina (24,3% (*lf*); 32,5% (*inf*)), heksahidrofarnesilacetone (1,4% (*lf*); 10,8% (*inf*)), (3Z)-heksen-1-ol (7,0% (*lf*); <0,1% (*inf*)) i linolna kiselina (1,9% (*lf*); 6,5% (*inf*)). Derivati karotenoida su činili najraznovrsniju klasu jedinjenja oba etarska ulja, a zastupljeni su sa 15,9% (*lf*) i 12,5% (*inf*). Ostatak predstavljaju "green leaf" alkoholi (*lf* -10,7%, *inf* - 1,2%) i derivati masnih kiselina (*lf* - 38,3%, *inf* - 48,7%). Multivarijanta analiza je pokazala da je metabolizam isparljivih jedinjenja iz porodice Dipsacaceae i rodno-specifičan i u saglasnosti sa njihovom morfološkom evolucijom. Takođe je pokazala tesnu povezanost rodova *Cephalaria* i *Scabiosa* i pružila dokaze za potencijano isključivanje *Morina* spp. iz te biljne podfamilije.

Inflorescence and leaf volatiles of *Cephalaria ambrosioides* (Sibth. & Sm.)**Roem. & Schult. (Caprifoliaceae): chemotaxonomical aspects**

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In this work, the chemical composition of the hydrodistilled essential oils of *Cephalaria ambrosioides* (Sibth. & Sm.) Roem. & Schult. (Caprifoliaceae), obtained in low yields from air-dried inflorescence (*inf*, 0.008%, w/w) and leaves (*lf*, 0.004%, w/w), and its use in chemotaxonomic purposes was presented. GC and GC-MS analyses revealed a complex mixture of compounds constituting both essential oils. Among them 284 components, accounting for 88.6% and 96.1% of the total peak areas detected, were successfully identified. The main components were found to be palmitic acid (24.3% (*lf*); 32.5% (*inf*)), hexahydrofarnesyl acetone (1.4% (*lf*); 10.8% (*inf*)), (3Z)-hexen-1-ol (7.0% (*lf*); <0.1% (*inf*)) and linoleic acid (1.9% (*lf*); 6.5% (*inf*)). Carotenoid-derived compounds represented one of the most diverse and abundant compound classes in the leaves and inflorescence oils, representing 15.9% (*lf*) and 12.5% (*inf*) of the essential oils. The remaining parts of the oils were comprised of "green leaf" volatiles and fatty acid-derived compounds, 10.7% (*lf*), 1.2% (*inf*) and 38.3% (*lf*), 48.7% (*inf*) respectively. Multivariate statistical analyses demonstrated that the evolution of the volatiles' metabolism of Dipsacaceae taxa was both genera-specific and was in agreement with their morphological evolution. These analyses showed a close relationship between the genera *Cephalaria* and *Scabiosa*, and provided evidence for the potential exclusion of *Morina* spp. from this plant subfamily.

Uticaj vrste filtera na kvalitet određivanja rastvorljivosti "shake-flask" metodom

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Određivanje rastvorljivosti je važno u svim fazama razvoja leka. Dobijeni podaci se koriste za nalaženje potencijalnih lekova-kandidata, biofarmaceutsku klasifikaciju i optimizaciju formulacije leka. Na merenje rastvorljivosti utiču različiti faktori: vreme mešanja, vreme sedimentacije, sastav pufera, temperatura, višak čvrste faze i tehnika odvajanja faza.[1] Cilj ovog rada je ispitivanje uticaja vrste membrane filtera u procesu odvajanja faza pri određivanju rastvorljivosti „shake-flask“ metodom. Izabrani su polietar-sulfon (hidrofobni) i poliviniliden-fluorid (hidrofilni) filteri. Koncentracija je merena pomoću UV/Vis spektrofotometrije. Kao model supstance korišćeni su karvedilol (baza) i ibuprofen (kiselina). Minijaturizovanom „shake-flask“ metodom i optimizovanom metodom potenciometrijske titracije određene su i logP vrednosti. Pokazano je da rezultat određivanja rastvorljivosti može zavisiti od vrste membrane filtera koji se koristi za odvajanje filtrata nakon uspostavljanja ravnoteže u rastvoru tokom rastvaranja. Jačina uticaja zavisi od lipofilnosti i pK_a vrednosti ispitivanog molekula kao i od pH vrednosti rastvora u kom se izvodi određivanje.

The effect of the filter type on the quality of "shake-flask" solubility determinations

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Solubility determination is important in both early and development phase of drug research. This data is used to screen out drug-like candidates, biopharmaceutical classification and formulation optimization. Solubility measurements are influenced by several experimental factors: stirring and sedimentation time, composition of the aqueous buffer, temperature, amount of solid excess and the technique of phase-separation.¹ The aim of the present study was to examine the influence of the filter type during phase separation on solubility determination. Polyether sulfone (hydrophobic) and polyvinylidene fluoride (hydrophilic) filters were chosen. The concentration was measured by UV/Vis spectrophotometry. Carvedilol (base) and ibuprofen (acid) are used as a model compounds. LogP values were determined by miniaturized shake-flask method and by optimized potentiometric titration. It is shown that solubility data can be influenced by membrane filter type which is used for filtration, after the equilibrium is established during dissolution. Magnitude of this influence depends of lipophilicity and pK_a value of molecule and a solution pH value.

Acknowledgement: Ministry of Education, Science, and Technological Development of Serbia (Grant No. 172008) supported this work.

References:

1. E. Baka, J. E. A. Comer, K. Takács-Novák, *J. Pharm. Biomed. Anal.*, **2008**, *46*, 335-341

Primena odabranih molekulskih osobina u proceni eliminacije inhibitora enzima koji konvertuje angiotenzin

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Inhibitori enzima koji konvertuje angiotenzin (ACE) predstavljaju često propisivane lekove za sniženje pritiska. U ovom radu, za osam odabranih ACE inhibitora (enalapril, kvinapril, fosinopril, ramipril, benazepril, perindopril, moeksipril, trandolapril) ispitan je odnos eliminacije i osobina njihovih molekula. Za ispitivane ACE inhibitore, korišćenjem softverskih paketa izračunate su vrednosti molekulskih deskriptora: rastvorljivost u vodi (logS), polarna površina molekula (PSA), molekulska masa (Mw), volumen molekula (Vol) kao i deskriptor lipofilnosti (logP vrednosti). Primenom proste linearne regresione analize najbolja zavisnost ($R^2 = 0,5742$) dobijena je između podataka o eliminaciji inhibitora ACE i deskriptora lipofilnosti, AClogP vrednosti. U nastavku istraživanja primenjena je metoda višestruke regresione analize (MLR) kako bi se dobila bolja zavisnost između podataka o eliminaciji i lipofilnosti (AClogP) ACE inhibitora uz primenu dodatnog molekuskog deskriptora kao nezavisno promenljive. Dobre korelacije dobijene su između podataka o eliminaciji i lipofilnosti (AClogP vrednosti) ACE inhibitora uz primenu molekulske mase ($R^2 = 0,7425$) ili zapremine molekula ($R^2 = 0,7224$) kao nezavisno promenljive. Mogućnost primene izračunatih molekulskih deskriptora u proceni eliminacije lekova je može biti velikog značaja u njihovom istraživanju.

The application of selected molecular properties in estimation of angiotensin-converting enzyme inhibitor's elimination

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Angiotensin-converting enzyme (ACE) inhibitors are commonly prescribed antihypertensive drugs. In this study, for eight selected ACE inhibitors (enalapril, quinapril, fosinopril, ramipril, benazepril, perindopril, moexipril, trandolapril) relationship between literature available elimination data and several molecular properties were investigated. The ACE inhibitors molecular descriptors: aqueous solubility data (logS), polar surface area (PSA), molecular mass (Mw), volume value (Vol) and lipophilicity descriptors (logP values) were calculated using software packages. Simple linear regression analysis showed the best correlation ($R^2 = 0.5742$) between ACE inhibitor's elimination data and lipophilicity descriptor AClogP values. Following, multiple linear regression analysis was applied to assess better correlations between ACE inhibitor's elimination data and lipophilicity, AClogP, using additional descriptor as independent variable. The good correlations were established between literature available elimination data and AClogP lipophilicity descriptor, using molecular mass or volume as independent variables (with $R^2 = 0.7425$ and $R^2 = 0.7224$ respectively). Application of computed molecular descriptors in evaluating drugs elimination can be of great importance in drugs research.

AH P05

Brza selekcija prekursor i produkt jona sintetskog kanabinoida JWH-018 za njegovo određivanje metodom GC-EI/MS/MS

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Cilj ovog rada je bio razvoj visoko specifične metode za određivanje JWH-018 (1-pentil-3-(1-naftoil)indol) u biljnom materijalu metodom gasne hromatografije sa tandem masenom spektromerijom (GC-MS/MS). U radu je prikazan postupak odabira prekursor, produkt jona i odgovarajućih kolizionih energija (CE) za specifične reakcije fragmentacije određenog kanabinoida. Najpre je snimljen EI Full scan spektar JWH-018 na osnovu koga su odabrani najintenzivniji m/z joni 341, 324, 284 i 270, koji su selektovani u prvom kvadrupolu (Q1), fragmentisani u kolizionoj ćeliji (q) na 5, 10, 15, 20, 25 i 30 eV, a nastali specifični joni (produkt joni) praćeni u drugom kvadrupolu (Q2). Na osnovu prinosa jonskih masa m/z izvršen je odabir prekursor jona, produkt jona i CE za odgovarajući prekursor. Tri specifične reakcije prelaza jona 341>324, 341>284 i 324>254 (CE 10, 10 i 23 eV) u MRM modu su korišćene za kvantitativnu analizu. Metoda je primenjena za određivanje sadržaja JWH-018, sintetskog kanabinoida iz grupe naftoilindola, u biljnom materijalu čija primena izaziva psihoaktivno delovanje. **Zahvalnica.** Ovaj rad je podržan od strane Ministarstva prosvete i nauke, Republike Srbije, Pr. Br. TR37016.

Quick selection of precursor and product ion of synthetic cannabinoids JWH-018 for its determination by GC-EI/MS/MS

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The aim of this study was the development of highly specific measurement of JWH-018 (1-pentyl-3-(1-naphthoyl)indole) in plant material by gas chromatography with tandem mass Spectrometry (GC-MS/MS). The paper describes the process of selecting a precursor and product ions and the corresponding collision energy (CE) for specific reactions fragmentation of determined cannabinoids. First, recorded EI Full scan spectrum of JWH-018 on the basis of which the most intense selected m/z ions 341, 324, 284 and 270, which were selected in the first quadrupole (Q1), fragmented in a collisional cell (q) at 5, 10, 15, 20, 25, and 30 eV, and the resulting specific ions (product ions) were followed in the second quadrupole (Q 2). Based on the yield of ion mass m/z procedure of the selection precursor ions, product ions and CE for the corresponding precursor was performed. Three specific reactions of ions crossing 341> 324 341> 284 and 324> 254 (CE 10, 10 and 23 eV) in MRM mode were used for quantitative analysis. The method was applied for the determination of JWH-018, synthetic cannabinoids from the group naphthoindols, in plant material whose application may causes psychoactive effect. **Acknowledgements.** This paper was supported by the Ministry of Education and Science, Republic of Serbia, Project No. TR37016.

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AH P06

Sadržaj polifenola u košticama šljive različitog porekla i perioda zrenja

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Šljiva je komercijalno najznačajnija vrsta voća u Srbiji čije se seme može dobiti kao sporedni proizvod tokom proizvodnje alkoholnih pića, sokova i konzervirane hrane. Međutim, velike količine semena se odbacuju zbog nepostojanja programa za organizovano sakupljanje i korišćenje. Cilj ovog istraživanja je karakterizacija semena šljive različitog porekla i perioda zrenja određivanjem sadržaja fenolnih jedinjenja. Fenolne kiseline i flavonoidi, kao potencijalni antioksidansi, određeni su ultraefikasnom tečnom hromatografijom spregnutom sa masenom spektrometrijom visoke rezolucije uz primenu različitih hemometrijskih tehnika za obradu rezultata. Primenjenom tehnikom pouzdano su detektovane fenolne kiseline, njihovi derivati i flavonoidi na osnovu molekulskih masa i fragmenata. Fenolne kiseline, kao što su protokatehinska, *p*-hidroksibenzoeva, ferulna i hlorogenska kiselina, su u ispitivanim uzorcima zastupljenije od flavonoida. Među flavonoidima, izomeri, katehin i epikatehin i glikozid rutin, su prisutni u najvećoj količini.

Zahvalnica: Ova istraživanja su podržana od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat br. 172017).

Phenolic composition of plum kernels differing in origin and ripening time

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Plum is commercially the most important type of fruit in Serbia whose seeds could be obtained as a byproduct from alcoholic beverage processing and juice and commercial canning industry. However, enormous amounts of seeds are discarded with no organized collection and utilization. This study emphasizes the importance of plum seeds of different origin and ripening time by characterization of their phenolic composition. Phenolic acids and flavonoids, as a potential antioxidants, were determined by ultra-high-performance liquid chromatography (UHPLC) coupled with hybrid mass spectrometry, which combines the Linear Trap Quadrupole (LTQ) and Orbitrap MS/MS mass analyzer together with several chemometric techniques. The UHPLC–LTQ Orbitrap MS technique was proven to be reliable for the unambiguous detection of phenolic acids, their derivatives, and flavonoids based on their molecular masses and fragmentation pattern. The phenolic acids prevail over the flavonoids, with protocatechuic, *p*-hydroxybenzoic, ferulic and chlorogenic acid as the most abundant ones. Among flavonoids, isomers, catechin and epicatechin, and glycoside rutin were the most abundant.

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AH P07

Ispitivanje primenljivosti obnovljive srebro-amalgam film elektrode za voltametrijsko određivanje makrolidnog antibiotika azitromicin-2-hidrata

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Karakterizacija azitromicin-2-hidrata (AZI) izvršena je primenom obnovljive srebro-amalgam film elektrode i voltametrije sa pravougaonim talasima (SWV) u Briton-Robinson puferu (pH 4,0-11,9). U ispitivanoj oblasti potencijala pri $\text{pH} \geq 6,0$ uočava se prisustvo jednog ili dva redukciona signala AZI u zavisnosti od pH vrednosti sredine. Kao optimalna pH vrednost za analizu AZI odabrana je pH 7,2. Određivanje ciljnog analita vršeno je u model sistemu primenom SWV i adsorptivne voltametrije sa pravougaonim talasima. Linearnosti kalibracionih krivi postignute su u opsegu $3,9\text{-}23,3 \mu\text{g mL}^{-1}$ odnosno $1,0\text{-}2,5 \mu\text{g mL}^{-1}$. Relativna standardna devijacija primenom obe razvijene metode nije prelazila 4,0%.

Zahvalnica: Za finansijsku podršku Ministarstvu nauke i tehnološkog razvoja Republike Srbije (Projekat broj 172059, 172012 i CEEPUSIII (CZ-0212-09-1516) mreži).

Investigation of the applicability of renewable silver-amalgam film electrode for voltammetric determination of macrolide antibiotic azithromycin-2-hydrate

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Characterization of azithromycin-2-hydrate (AZI) was performed by renewable silver-amalgam film electrode and square wave voltammetry (SWV) in the presence of aqueous Britton-Robinson buffer (pH 4.0-11.9). In the investigation potential range, at $\text{pH} \geq 6.0$ one or two reduction peaks of AZI were obtained depending on pH. As the optimal pH for analysis of AZI pH 7.2 was chosen. Determination of target analyte in model system was performed by SWV and adsorptive stripping square wave voltammetry. The linearity of calibration curves were obtained in ranges $3.9\text{-}23.3 \mu\text{g mL}^{-1}$ and $1.0\text{-}2.5 \mu\text{g mL}^{-1}$, respectively. Relative standard deviation in both optimized method did not exceed 4.0%.

AH P08

Ispitivanje mogućnosti uklanjanja tiametoksama primenom native forme višezidnih ugljeničnih nanocevi iz vodenih suspenzija metodom visoko efikasne tečne hromatografije

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Ispitivana je mogućnost uklanjanja tiametoksama (TMX) iz vodene suspenzije primenom native forme višezidnih ugljeničnih nanocevi različitih odvaga. Proučavani su standard i odabrana komercijalna formulacija ciljnog analita. Za praćenje koncentracije TMX primenjena je HPLC-DAD metoda, pri čemu uzorci su filtrirani neposredno posle uzorkovanja. Efikasnost uklanjanja komercijalne formulacije iz suspenzije u prisustvu 0,7 mg cm⁻³ nanocevi i početnoj koncentraciji TMX od 2,4 µg cm⁻³ iznosi 90%. Rezultati ispitivanja ukazuju na to da je uklanjanje TMX-a bolje sa većom masom native forme nanocevi. U slučaju standarda i komercijalne formulacije postiže se slična efikasnost uklanjanja.

Zahvalnica: Autori se zahvaljuju za podršku CEEPUSIII mreže (CZ-0212-09-1516).

Investigation of thiamethoxam removal with native form multiwalled carbon nanotubes from water suspensions by high-performance liquid chromatography

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The possibility of thiamethoxam (TMX) removal was investigated from the water suspension of the native form of multiwalled carbon nanotubes with different masses. As for the analyte, the TMX standard and a selected commercial formulation were investigated. For the monitoring the TMX concentration the HPLC-DAD method was applied, while the samples were filtered immediately after sampling. The efficiency of the TMX removal in the presence of 0.7 mg cm⁻³ carbon nanotubes and 2.4 µg cm⁻³ TMX is 90%. The results showed that at higher concentration of the nanotubes the removal of the TMX is with higher efficiency. In the case of standard and commercial formulation the similar removal efficiency was obtained.

AH P09

Optimizacija protočno injektione (FI) metode sa amperometrijskom detekcijom za određivanje diazepama u pićima

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Diazepam pripada grupi benzodiazepina. Konzumiranjem diazepama uz alkohol pojačava se smirujuće dejstvo leka i povećava apsorpcija. Zbog toga se diazepam može koristiti kao droga za silovanje. U našem ispitivanju primenili smo protočno injekcioni sistem za određivanje diazepama na elektrodi od staklastog ugljenika. Redukcija azometinske grupe diazepama se dešava na negativnom potencijalu (-0,75V vs. Ag/AgCl), a da bi se sprečila redukcija rastvorenog kiseonika na primenjenom potencijalu radni rastvori su držani pod azotom. Sva ispitivanja su urađena u KCl/HCl puferu na pH 1. Injekcioni ventil je opremljen petljom za uzorak zapremine 0,5 ml. Linearni opseg metode je od 10 do 1000 $\mu\text{mol}/\text{dm}^3$, granica detekcije 5 $\mu\text{mol}/\text{dm}^3$, a granica kvantifikacije 15 $\mu\text{mol}/\text{dm}^3$ diazepama. Metoda je primenjena na određivanje diazepama u uzorcima komercijalno dostupnih napitaka, dva bezalkoholna (energetski i gazirani napitak) i u uzorku piva. Rezultati pokazuju da je ovom metodom moguće određivanje niskih koncentracija diazepama u uzorcima pića.

Optimisation of flow injection (FI) method with amperometric detection for diazepam determination in beverages

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Diazepam belongs to the group of benzodiazepine. Its consumption with alcohol enhances its sedative effect and absorption rate. That is why it is often used as "date rape drug". In our experiments we applied the flow injection system on diazepam determination on glassy carbon electrode. The azomethine group of diazepam is reduced at negative potential (-0,75V vs. Ag/AgCl), to avoid the reduction of dissolved oxygen working solutions were kept under nitrogen. All experiments were performed in KCl/HCl buffer at pH 1. The injection valve was equipped with 0,5 ml sample coil. Linear range of the method was 10 to 1000 $\mu\text{mol}/\text{dm}^3$, limit of detection was 5 $\mu\text{mol}/\text{dm}^3$ and limit of quantification was 15 $\mu\text{mol}/\text{dm}^3$. The method was applied on diazepam determination in commercially available beverages, two non-alcoholic (energetic and carbonated) and a beer sample. The results show that it is possible to determine low levels of diazepam in beverage samples.

AH P10

Primena Boemovih titracija za određivanje kiseoničnih površinskih grupa različitih biougljeva

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Biougalj je nusproizvod dobijen pirolizom organskog otpada i biomase. Boemove titracije koriste se za kvantifikaciju organskih kiselih grupa na površini biougljeva. Sadržaj kiselih funkcionalnih grupa je određen titracijom po Boemu na dva načina: uvođenje N_2 tokom titracije i predtretman sa $BaCl_2$ [1]. Pripremljena su tri Boemova rastvora ($NaOH$, Na_2CO_3 i $NaHCO_3$, približnih koncentracija $0,05 \text{ mol/dm}^3$). Koncentracija $NaOH$ je određena potencimetrijskom titracijom sa kalijum-hidrogenftalatom, a koncentracija HCl koja se koristi za titraciju kod barijumove metode je određena potencimetrijski sa $NaOH$. Korišćeni su sledeći uzorci biougljeva: aktivni ugalj kao referentni, biougalj celuloznog, kukuruznog porekla i od biljke slonove trave (poznata i kao kineska trska). Da bi se proverila efikasnost ovih metoda, ekstrakti su snimani spektrofotometrijski na talasnoj dužini 250 nm. Urađena je i karakterizacija biougljeva pomoću skenirajuće elektronske mikroskopije (SEM).

Application of Boehm titration on determination of oxygen surface groups on different biochars

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Biochars are byproduct of pyrolysis of the organic waste and biomass. Boehm titrations are used for quantification of oxygen surface groups of the biochars. The content of functional groups is determined by Boehm titration in optimised for two procedures: spargin with N_2 during titration and pretreatment with $BaCl_2$ [1]. Three Boehm solutions were prepared ($NaOH$, Na_2CO_3 i $NaHCO_3$, approximate concentrations $0,05 \text{ mol/dm}^3$ each). Hydroxide concentration was determined potentiometrically with potassium-hydrogenphthalate, whereas concentration of HCl , used as titrant in Barium method, was also potentiometrically determined with $NaOH$. Following biochar samples were used: active coal as a referent sample, biochar of cellulose and corn origin and biochar from the miscanthus plant. In order to check the efficiency of this methods, spectrofotometry was used at a wavelenght of 250 nm. Characterisation of biochars with SEM was also performed.

Reference:

1. Rivka B. Fidel, David A. Laird, Michael L. Thompson, *Journal of Environmental Quality* **42** (2013) 1771-1778

Optimizacija uslova ciklične voltametrije za ispitivanje trifluorometilovanih Šifovih baza

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Šifove baze se zbog svojih karakteristika bi se mogle primeniti kao medijatori kod biosenzora druge generacije. U cilju odabira pogodnog medijatora ispitivano je elektrohemijsko ponašanje seta tetradentatnih trifluorometilovanih Šifovih baza. Primenom eksperimentalnog dizajna definisani su uslovi i tok eksperimenata. Definisani faktori i podnivoi svakog faktora su: radna elektroda (elektroda od staklastog ugljenika i platinska elektroda), osnovni elektrolit (acetonitril i dimetilsulfoksid), supstituenti (metil-, trifluorometil- i fenil grupa), brzina skeniranja (50 i 200 mV/s) i osetljivost skeniranja ($1 \cdot 10^{-4}$ i $1 \cdot 10^{-5}$ A/V). Odabrani su faktori i njihovi podnivoi sa najvećim uticajem na potencijale oksidacije i redukcije elektroaktivnih grupa ispitivanih Šifovih baza i određena je njihova statistička značajnost. Brzina i osetljivost skeniranja nemaju značajnog uticaja, dok najveći uticaj ima faktor suspituenata. Pored značajnosti faktora, utvrđene su i njihove optimalne vrednosti. Optimalni uslovi su primenjeni na dalja istraživanja.

Optimisation of cyclic voltammetry conditions for investigations of the trifluoromethylated Schiff bases

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Schiff bases could be applied as mediators for the second generation of biosensors because of their characteristics. In order to select appropriate mediator we investigated electrochemical behavior of some tetradentate trifluoromethylated Schiff bases. Experimental design was applied to determine the optimal conditions for experiments. Defined factors and sublevels of each factor were: working electrode (glassy carbon and platinum electrode), electrolyte (ACN and DMSO), substituents (methyl-, trifluoromethyl-, phenyl groups), scan rate (50 and 200 mV/s) and scanning sensitivity ($1 \cdot 10^{-4}$ and $1 \cdot 10^{-5}$ A/V). Factors and their sublevels, with strongest influence on oxidation and reduction potentials on electro-active groups of Schiff bases, were chosen and their statistical significance was determined. Scan rate and sensitivity have no significant effect; while substituents have the strongest influence. Beside factor significance, their optimal values were determined. Optimal conditions were applied on further investigations.

AH P12

Ispitivanje elektroanalitičkih karakteristika i primene magnetitne elektrode za određivanje pirogroždane kiseline

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Netoksičan i veoma rasprostranjen prirodni mineral magnetit, Fe_3O_4 , upotrebljen je kao senzorski materijal za laboratorijsku izradu jon-selektivne elektrode.¹ Elektroanalitička karakterizacija elektrode urađena je primenom voltametrijske i potenciometrijske metode. Voltametrijskim merenjima je objašnjeno elektrohemijsko ponašanje i reaktivnost površine elektrode. Na površini minerala formiran hidroksid/oksidni sloj se ponaša kao sensor osetljiv na H_3O^+ jone. Magnetitna elektroda, upotrebljena kao indikatorska elektroda za kvantitativna merenja u acetonitrilu, pokazuje dobru osetljivost i reproduktivnost, kratko vreme odgovora (manje od 15 s), sub-Nernstovsku zavisnost sa nagibom od 41 mV po dekadi u intervalu koncentracija *p*-toulensulfonske kiseline 0,1 – 0,001 M. Jedna od najmanjih i najjednostavnijih α -keto kiselina, pirogroždana kiselina, kao esencijalni biomolekul u ljudskom organizmu, uspešno je određena u acetonitrilu, primenom opisanog senzora i direktne/indirektne potenciometrijske analitičke tehnike.

Investigation of the electroanalytical characteristics and applicability of magnetite electrode for the pyruvic acid determination

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Voltammetric and potentiometric electrochemical methods have been used for determination of the analytical performance characteristics of the handmade magnetite electrode. Natural magnetite mineral, Fe_3O_4 , has been widely investigated as an electrode material due to its ease of preparation, non-toxicity and availability in natural environment.¹ Cyclic voltammetric measurements have been performed to explain the electrochemical behavior and reactivity of the magnetite surface in acetonitrile. Iron ions are susceptible to hydrolysis and form a hydroxyde/oxide layer on the surface of the electrode, which acts as a sensor for the hydronium ions. This electrode, applied as a sensor for quantitative measurements in acetonitrile, exhibits a good sensitivity and reproducibility, stable potential with respect to time, short response time (less than 15 s), the sub-Nernstian response, with a slope of 41.0 mV per decade over the concentration range 0.1 – 0.001 M of *p*-toluenesulphonic acid, as well as a possibility of application without a time limit. One of the smallest and the simplest α -keto acid, pyruvic acid, as an essential and physiological biomolecule in a human body, has been successfully determined by using the both potentiometric acid-base titration and proposed sensor.

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1. Z. Stanic, J. Stepanovic, Z. Simic, *Polyhedron* **45** (2012) 43.

Određivanje sadržaja metala i izotopskog odnosa olova u zubima ICP-QMS metodom

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Podaci o bioakumulaciji metala u zubima omogućavaju identifikaciju dugotrajne izloženosti nekom metalu i u određenim slučajevima mogu da pruže više informacija od tradicionalnog uzimanja uzoraka krvi. Cilj ovog rada je određivanje sadržaja metala (Sr, Ni, Mn, Fe and Pb) i izotopskog odnosa olova ($^{208}\text{Pb}/^{206}\text{Pb}$ i $^{207}\text{Pb}/^{206}\text{Pb}$) u ljudskim zubima u cilju dobijanja informacija o stepenu izloženosti čoveka olovu tokom određenog vremenskog perioda i mogućnost određivanja lokacije stanovanja pojedinca. Za analiziranje, zubi su podeljeni na koren, srž i gleđ. Sadržaj metala i izotopski odnos olova su određeni metodom indukovano spregnute plazme masene spektrometrije (ICP-QMS). Na osnovu dobijenih rezultata u korenu su uočene veće koncentracije Sr, Ni i Mn, dok su u gleđi dominantniji Zn, Fe i Pb. Za određivanje izotopskog odnosa olova na ICP-QMS optimizovani su eksperimentalni parametri (integraciono vreme, mrtvo vreme detektora i *mass-bias*). Kao standard je korišćen NIST SRM 981 koji ima tačno definisan izotopski odnos olova. Vrednosti izotopskog odnosa olova pokazuju grupisanje uzoraka, na osnovu kojih se može doneti zaključak da ispitanici potiču sa iste lokacije, kao i da nisu bili izloženi izrazitom antropogenom zagađenju.

Determination of metal content and lead isotope ratios in human teeth by ICP-QMS

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Data of bioaccumulation of elements in teeth allow identification of long-term trace metal exposure and, in certain cases, may provide more information than traditional blood sampling. In this study, metal content (Sr, Ni, Mn, Fe and Pb) and isotope lead ratios ($^{208}\text{Pb}/^{206}\text{Pb}$ i $^{207}\text{Pb}/^{206}\text{Pb}$) in teeth were determined in order to provide information of metal exposure in the past. Tooth samples were divided on three parts: roots, marrow and enamel. Metal content and isotope lead ratios were determined by inductively coupled plasma mass spectrometry (ICP QMS). The obtained results showed higher concentrations of Sr, Ni and Mn in the roots, while Zn, Fe and Pb were dominant in enamel. For determination of lead isotope ratios by ICP-QMS, experimental parameters (integration time, dead time of the detector and mass-bias) were optimized. As a standard, NIST SRM, 981, which has a defined isotopic ratio of lead, was used. The values of the lead isotope ratios showed clustering of samples and indicated that the volunteers come from the same location, without being exposed to any extreme anthropogenic pollution.

Uticaj neorganskog i organskog ugljenika na određivanje selena Indukovano Sprengnutom Plazmom – Optički Emisionom Spektrometrijom (ICP-OES)

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Primećeno je da određivanje selena u pečurkama ICP-OES metodom daje netačne i neprecizne rezultate, jer se javljaju spektralne i nespektralne smetnje koje potiču od ugljenika. Smetnje nastaju kao posledica jako bliske energije jonizacije ova dva elementa (Se 1098 kJ/mol; C 1086 kJ/mol), ali i bliske talasne dužine emitovanog zračenja (Se 196,090 nm; C 193,091 nm). Ovaj matriks efekat dovodi do povećanja intenziteta linije Se 196,090 nm, ali i drugih linija selena (Se 203,985 nm i Se 206,279 nm). Spektralne smetnje potiču od prisustva CN (196,084 nm) i CO (206,76 nm) trake, dok nespektralne smetnje potiču od same jonizacije ugljenika. Kao izvor organskog ugljenika korišćen je 1% etanol (čist ili u smeši sa 1% i 5% HNO₃), kao i 1% sirćetna kiselina. Na osnovu dobijenih rezultata uočeno je da 1% etanol dovodi do povećanja intenziteta Se 196,090 za 60 - 80%, ali i do povećanja intenziteta Se 203,985 i Se 206,279 za 10 - 20%, u zavisnosti od koncentracije selena. Etanol sa 5% HNO₃ dovodi do povećanja intenziteta Se 196,090 do čak 140% u odnosu na etanol, verovatno zbog stvaranja CN trake. Sirćetna kiselina (1%) dovodi do povećanja intenziteta Se 196,090 do 30%, dok na ostale linije selena nema uticaja. Kao izvor neorganskog ugljenika upotrebljen je 1% i 5% kalijum-karbonat, pri čemu je uočeno da ova vrsta ugljenika nema uticaja na intenzitet Se 196,090, ali dovodi do povećanja Se 206,279 za 10 do 20% najverovatnije zbog stvaranja CO trake.

The influence of inorganic and organic carbon on the determination of selenium by Inductively Coupled Plasma - Optical Emission Spectrometry (ICP-OES)

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It is noted that the determination of selenium in mushrooms by ICP-OES provides inaccurate or imprecise results, because of spectral and non-spectral interference originating from carbon. Interferences arise as a result of very close ionization energies of these two elements (Se 1098 kJ / mol; C 1086 kJ / mol), but also because of close wavelength of the emitted radiation (Se 196.090 nm; C 193.091 nm). The observed matrix effect leads to an increase of intensity of Se 196.090 nm line, and other lines of this element (Se 203.985 nm and Se 206.279 nm). Spectral interferences could be explained with appearance of CN (196.084 nm) and CO (206,76 nm) bands, while non-spectral interference originate from the ionization of of carbon. As a source of organic carbon 1% ethanol (pure or in a mixture with 1% and 5% HNO₃) and 1% acetic acid were used. It was observed that 1% ethanol caused increased intensity of Se 196.090 for 60 - 80%, or an increase in the intensity Se 203.985 and Se 206.279 for 10 - 20%, depending on the concentration of selenium. Ethanol with 5% HNO₃ leads to an increase in the intensity of Se 196.090 to 140% compared to pure ethanol, probably due to formation CN band. Acetic acid (1%) leads to an increase in the intensity of Se 196.090 to 30%, while the other lines of selenium has no influence. As a source of inorganic carbon used is 1% and 5% potassium-carbonate, whereby it was noted that this type of carbon has no influence on the intensity of Se 196.090, or lead to an increase of Se 206.279 for 10 to 20% most likely due to the formation of CO band.

AH P15

Status tokoferola i karotenoida u koricama

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Konsumiranje kukuruza specifičnih svojstava kao što je kukuruz kokičar, veoma je popularno u ishrani. Prilikom termičke obrade postoji mogućnost gubljenja ili degradiranja nutritivno važnih supstanci kao što su vitamini, antioksidansi i dr. Glavni cilj istraživanja bio je ispitivanje sadržaja tokoferola (α -, $\beta+\gamma$ -, δ -) i karotenoida (lutein, zeaksantin i β -karoten) u zrnu kukuruza kokičara pre i posle kokanja (u mikrotalasnoj rerni), primenom visoko efikasne tečne hromatografije (HPLC). Tokoferoli i karotenoidi su veoma snažni antioksidansi. Od testiranih tokoferola, najveću biološku aktivnost poseduje α - tokoferol dok je β - karoten prekursor vitamina A. Koncentracije α -, $\beta+\gamma$ -i δ - tokoferola u koricama približno su smanjene za 23.16%, 17.74% i 6.14 %, respektivno, u odnosu na zrno kukuruza kokičara. Sadržaj luteina, zeaksantina i β - karotena nakon kokanja smanjen je za 78.17%, 79.65% i 21.53%, respektivno. Dobijeni rezultati pokazuju da se sadržaj α - tokoferola i β -karotena, nakon kokanja, najmanje promenio. Ovo ukazuje da se jedinjenja sa najvećom biološkom aktivnošću, tj. sa najvećim značajem u ljudskoj ishrani uglavnom zadržavaju u koricama nakon termičke obrade.

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The status of tocopherols and carotenoids in popcorn

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Consuming maize with specific traits, such as popping maize, is very popular in diet. There is a possibility of losing or degradation of nutritionally important substances, such as vitamins, antioxidants, etc., during popcorn making, i.e. heat treatment. The aim of this study was to investigate content of tocopherols (α -, $\beta+\gamma$ -, δ -) and carotenoids (lutein zeaxanthin and β - carotene) in popcorn kernel before and after popping (in microwave oven), using high performance liquid chromatography (HPLC). Tocopherols and carotenoids are very powerful antioxidants. From analyzed tocopherols, the highest biological activity has α - tocopherol, whilst β - carotene is a precursor for vitamin A. Concentration of δ -, $\beta+\gamma$ - and α - tocopherols in the tested samples approximately decreased for 23.16%, 17.74% and 6.14 %, respectively in popcorns flakes, in relation to popcorn kernel. The amounts of lutein, zeaxanthin and β - carotene, after popping have been roughly reduced for 78.17%, 79.65% and 21.53% respectively. Obtained results indicate that α -tocopherol and β - carotene shows the slightest changes in content after popping. This indicates that compounds with the highest biological activity, i.e. with the highest importance for human nutrition are mainly retained in the popcorn after heat treatment.

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Fizička hemija / Physical Chemistry

FH P01

Fizičko-hemijska karakterizacija i primena binarnih smeša jonskih tečnosti i laktona kao elektrolita za litijum-jonske baterije

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Jedan od najboljih načina za poboljšanje sigurnosti i pouzdanosti elektrolita u litijum-jonskim baterijama je upotreba elektrolita na bazi elektrohemijski i termički stabilnih jonskih tečnosti. Budući da je limitirajući faktor za praktičnu primenu jonskih tečnosti njihova velika viskoznost, binarne smeše jonskih tečnosti sa odabranim laktonom, γ -butirolaktonom (GBL) biće istražene u cilju prevazilaženja visoke viskoznosti. Volumetrijske i transportne osobine binarnih smeša 1,3-dialkilimidazolijum i 1,2,3-trialkilimidazolijumovih jonskih tečnosti na bazi *bis*(trifluorometilsulfonyl)imida, sa GBL, merene su u intervalu $T = 293,15 - 323,15$ K. Ispitivaće se uticaj dužine alkil niza di- i tri-supstituisanih jonskih tečnosti na fizičko-hemijska svojstva binarnih smeša u cilju pronalazjenja odgovarajućeg optimalnog medijuma za buduću primenu kao elektrolita za litijum-jonske baterije. Ispitivaće se fizička, elektrohemijaska i termalna svojstva elektrolita nakon dodatka odgovarajuće litijumove soli u optimizovanu smešu jonska tečnost+GBL. Sveobuhvatna studija karakterizacije i optimizacije binarnih smeša i elektrolita je potrebna radi ispitivanja interakcija koje mogu poboljšati performanse elektrolita.

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Physico-chemical characterization and application binary mixtures of ionic liquids with lactones as electrolytes for lithium-ion batteries

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One of the best ways to improve safety and reliability of the lithium-ion battery electrolytes is the use of an emerging class of electrolytes based on ionic liquids (ILs) with high electrochemical and thermic stability. Since the limiting factor for the ILs application is their high viscosity, their binary liquid mixtures with selected lactone, γ -butyrolactone (GBL) will be investigated in order to overcome high viscosity. Volumetric and transport properties of binary mixtures of 1,3-dialkylimidazolium and 1,2,3-trialkylimidazolium based ILs *bis*(trifluoromethyl-sulfonyl) imide with GBL were examined in the temperature range from (293.15 to 323.15) K. Investigating the side alkyl chain length influence of dialkyl- and trialkyl-substituted imidazolium ILs on physicochemical properties of binary mixtures was examined in order to obtain suitable medium for future application as electrolyte for lithium-ion batteries. After that, lithium salt was added at the appropriate IL+GBL mixture and physicochemical, electrochemical and thermal properties were investigated. A comprehensive study of characterization and optimization of binary mixtures and electrolytes is necessary to investigate the interactions that can improve the performance of electrolyte.

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Molekulsko modelovanje novosintetisanih hidroksi i etarski funkcionalizovanih jonskih tečnosti

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Poslednjih godina, mogućnost dizajniranja željenih jonskih tečnosti je značajno proširila mogućnost njihove upotrebe u raznim granama fizičkih i hemijskih nauka. Posebna pažnja se posvećuje funkcionalizovanim („task - specific“) jonskim tečnostima (TSIL), koje u bočnom nizu katjona sadrže različite funkcionalne grupe sa ciljem poboljšanja fizičkih, hemijskih i bioloških svojstava. Glavni cilj njihove sinteze jesu poboljšanja ekstrakcionih karakteristika, veći kapacitet za apsorpciju CO₂ i značajno niža toksičnost u odnosu na nefunkcionalizovane analoge. U ovom radu teorijski su ispitane novosintetisane hidroksi i/ili etarsko funkcionalizovane jonske tečnosti upotrebom računarskih simulacija (DFT proračuna i molekulske dinamike) sa ciljem pronalaženja optimalne geometrije, teorijskih vrednosti različitih fizičko-hemijskih parametara, kao i boljeg razumevanja interakcija unutar samih jonskih tečnosti.

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Molecular modeling of newly synthesized hydroxyl and ether functionalized ionic liquids

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In recent years the designer nature of ILs has driven their exploration and exploitation in countless fields among the physical and chemical sciences. The special attention of scientific community is focused to so-called task-specific ionic liquids (TSIL), which are obtained by the introduction of specific functional groups in the side chains of cations in order to improve their physical, chemical and biological properties. The main objective of their synthesis is to improve extraction characteristics, increasing capacity of CO₂ absorption and reducing toxicity in relation to non-functionalized ILs. In this work computational analysis (DFT calculations and molecular dynamics) of newly synthesized oxygen functionalized ILs was performed, in order to obtain optimal geometry and theoretical values of different physicochemical parameters (density, dipole moment, diffusion coefficient, binding energy) and to better understand interactions in pure ionic liquids.

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Dizajn-eksperiment matematička metoda primenjena u MALDI-TOF-MS analizi

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U ovom radu, matematička metoda Dizajn eksperimenta (eng. Design of Experiment, DoE) korišćena je za optimizaciju instrumentalnih parametara masenog spektrometra sa laserskom desorpcijom i jonizacijom pomoću „matriksa“ i sa analizatorom na bazi vremena preleta (MALDI TOF MS), a za analizu metalnih kompleksa. Ulazni parametri DoE metodologije bili su intenzitet lasera, napon na „gridu“ i broj impulsa lasera, dok su kao izlazni parametri od interesa bili odnos signal/šum i rezolucija. Različite vrednosti ulaznih parametara (njihovi nivoi) definisane su na osnovu dobijenih preliminarnih eksperimenata. Nakon utvrđivanja ulaznih i izlaznih parametara DoE eksperiment je izveden primenom Box-Behnken-ove metode. Teorijski predviđene vrednosti za dobijanje kvalitetnog masenog spektra metalnog kompleksa (snaga lasera-1220 W, napon „grida“-79 V i broj impulsa lasera-360) su eksperimentalno potvrđeni.

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Design of Experiments mathematical methodology applied in MALDI-TOF-MS analysis

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In this work Design of Experiment mathematical methodology (DoE) was used for optimization the instrumental parameters of matrix-assisted laser desorption/ionization (MALDI) time-of-flight (TOF) mass spectrometer (MS) for the analysis of metal complex. The input factors in DoE methodology were laser intensity, grid voltage and number of laser shots, while the output response of interest were signal-to-noise ratio and resolution. The different values of input factors (their level) are defined according to the results obtained in preliminary experiments. After the identification of input factors and responses of interest the DoE experimental plan is created using Box-Behnken metode. Theoretically predicted values for obtaining high-quality mass spectra of metal complex (laser power – 1220 W, grid voltage – 79 V and number of laser shots – 360) are experimentally confirmed.

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Efekat izoljavanja i uticaj temperature na bifazne vodene sisteme na bazi dicianamidnih jonskih tečnosti

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Pod jonskim tečnostima (JT) se podrazumevaju jonska jedinjenja koja su tečna na temperaturama ispod 100°C. Među brojnim zanimljivim svojstvima koje poseduju hidrofilne jonske tečnosti je i njihova sposobnost da grade dvofazne vodene sisteme u kombinaciji sa neorganskim ili organskim solima. U ovom radu su određeni i okarakterisani fazni dijagrami (binodalne krive) za ispitivane bifazne vodene sisteme {JT + neorganska so + H₂O} za dve novosintetisane jonske tečnosti: 1-etil-3-etilimidazolijum-dicianamid [1-C₂3-C₂im][DCA] i 1-butil-3-etilimidazolijum-dicianamid [1-C₄3-C₂im][DCA] u kombinaciji sa neorganskim solima: K₃PO₄ i K₂CO₃. Eksperimentalni rezultati su fitovani na osnovu Merchuk-ove jednačine i pokazuju da priroda jonske tečnosti kao i neorganske soli utiču u velikoj meri na formiranje bifaznih vodenih sistema. Pokazano je da K₃PO₄ ima veću sposobnost za građenje bifaznih sistema od K₂CO₃, što je posledica veće entropije hidratacije anjona. Povećanje bočnog niza na imidazolijum jonu dovodi do lakšeg indukovanja bifaznih sistema tj. potrebna je manja količina neorganske soli da bi se nagradile dve faze. Uticaj temperature na formiranje bifaznih vodenih sistema postoji i dvofazna oblast se povećava sa snižavanjem temperature.

The salting-out effect and impact of temperature on phase diagrams of aqueous biphasic systems based on novel synthesized dicyanamide ionic liquids

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Ionic liquids (IL) are ionic compounds which are liquid below 100 °C. One of many interesting features of ionic liquids miscible with water near room temperature is that they can induce ionic-liquid-based aqueous biphasic system (ABS) in combination with inorganic/organic salts. In this work, phase diagrams for aqueous solutions of 1-ethyl-3-ethylimidazolium-dicyanamide [1-C₂3-C₂im][DCA] and 1-butyl-3-ethylimidazolium-dicyanamide [1-C₄3-C₂im][DCA] based ILs combined with phosphate and carbonate-based salts, K₃PO₄ and K₂CO₃, are reported and discussed. Merchuk equation was applied in order to correlate the experimental binodal data. It was found that K₃PO₄ has better salting-out ability to induce aqueous biphasic system than K₂CO₃ because of higher hydration entropy. The cation influence on the ability to form ABS is investigated for the IL with the same anion, dicyanamide [DCA]⁻ and various alkyl chain lengths. It was found that ability to form ABS increases with the increase of the alkyl chain length on the imidazolium ion because of increasing ionic liquid hydrophobicity and poorer affinity for water. The experimental results also show that biphasic region expands with reduction of temperature.

Hemometrijska analiza parametara lipofilnosti novosintetisanih spirohidantoina koji su određeni primenom RP-TLC sa protičnim rastvaračima

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Predmet ovog rada je ispitivanje lipofilnosti novosintetisanih derivata cikloalkilspiro-5-hidantoina. Parametri lipofilnosti (R_M^0) za ispitivana jedinjenja dobijeni su primenom reversno fazne hromatografije na tankom sloju C-18 modifikovanog slikagela. Kao pokretne faze korišćene su dvokomponentne smeše vode i protičnih organskih rastvarača (metanola, etanola, *n*-propanola, *i*-propanola i *t*-butanola). Linearna zavisnost između R_M vrednosti i zapreminskog udela organskog modifikatora u pokretnoj fazi, φ , omogućava izračunavanje R_M^0 ispitivanih jedinjenja. Uticaj supstituenata, kao modifikatora pokretne faze na R_M^0 vrednosti procenjen je primenom hemometrijskih metoda, hijerarhijske kalster analize (HCA) i analize glavnih komponenata (PCA). Ove metode omogućavaju grupisanje ispitivanih derivata spirohidantoina, kao i primenjenih pokretnih faza prema njihovoj polarnosti.

Chemometric analysis of lipophilicity parameters of newly synthesized spirohydantoin derivatives determined by RP-TLC and protic solvents

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The subjects of this paper are newly synthesized derivatives of cycloalkylspiro-5-hydantoin and the analysis of their lipophilicity. The parameters of lipophilicity (R_M^0) were determined by reverse phase thin layer chromatography on C-18 modified silica gel. Mobile phases were two-component mixtures of water and protic organic solvents (i.e. methanol, ethanol, *n*-propanol, *i*-propanol and *t*-butanol). Linear relationship between R_M values and volume fraction of organic solvent, φ , allows calculation of R_M^0 for investigated compounds. The effect of the substituents in the molecule as well as mobile phase modifier on R_M^0 value was assessed using chemometric methods, hierarchical cluster analysis (HCA) and principal component analysis (PCA). This allows clustering of spiro hydantoin derivatives as well as applied mobile phases according to their polarity.



Detekcija glukoze korišćenjem glukozo okidaza-glutaraldehyd-cistein modifikovane elektrode od zlata primenom ciklične voltametrije

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Zbog povećanog interesovanja intenzivno se razvijaju elektrohemijski biosenzori za glukozu imobilizacijom redoks enzima na površinu elektrode.

U ovom radu biosenzor za glukozu je dobijen nanošenjem cisteina, glutaraldehyda i glukoze-oksidadaza na površinu elektrode od zlata. Dobijeni biosenzor testiran je pomoću ciklične voltametrije pokazujući da je oksidacije glukoze difuziono kontrolisan proces. Dobijeni biosenzor pokazuje brz transfer elektrona ($k^0 = 20.4 \text{ s}^{-1}$), veliki afinitet prema glukozu ($K_M^{app} = 1.15 \text{ mM}$), nisku granicu detekcije od 0.94 mM i linearnu zavisnost u oblasti 1.5-7 mM. Pokazana je dobra stabilnost i reproduktivnost ispitivanog biosenzora.

Glucose sensing by glucose oxidase-glutaraldehyde-cysteine modified gold electrode using cycling voltammetry

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There is an increasing interest and need to develop an electrochemical glucose biosensor by immobilizing enzyme on an electrode surface.

In this work glucose biosensor is performed with successive attachment of cysteine, glutaraldehyde and glucose oxidase onto gold electrode. It is tested for glucose sensing using cyclic voltammetry suggesting the diffusion controll of the glucose oxidation. The obtained biosensor shows a fast electron transfer ($k^0 = 20.4 \text{ s}^{-1}$), high affinity for glucose ($K_M^{app} = 1.15 \text{ mM}$), a low detection limit of 0.94 mM and a linear response between 1.5-7 mM. This biosensor exhibits good stability and reproducibility.



Nanocrystalline ruthenium oxide coating on titanium, prepared by the sol-gel procedure from colloidal oxide dispersions synthesized in the microwave reactor

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Ruthenium oxide coating on titanium was prepared by the sol-gel procedure from well-defined colloidal oxide dispersions synthesized by the microwave (MW)-assisted hydrothermal route under defined temperature and pressure heating conditions. The dispersions were characterized by dynamic light scattering (DLS) measurements and scanning electron microscopy (SEM). The electrochemical properties were analyzed as capacitive performances gained by cyclic voltammetry and electrochemical impedance spectroscopy, and as the electrocatalytic activity for oxygen evolution from acid solution. The obtained dispersions were polydisperse and contained single particles and agglomerates of increasing surface energy and decreasing particle size as the MW-assisted heating conditions were intensified. Owing to these features of the precursor dispersions, the obtained coatings had considerably improved capacitive performances and good electrocatalytic activity for oxygen evolution at high overpotentials.

Превлаке нанокристалног Ru оксида на титану, добијене сол-гел поступком из колоидне оксидне дисперзије синтетисане у микроталасном ректору

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На титанској основи формирана је превлака нанокристалног рутенијум оксида сол-гел поступком, полазећи од дефинисане колоидне дисперзије оксида синтетисаног хидротермалном реакцијом у микроталасном реактору у условима контролисаног притиска и температуре током загревања. Дистрибуција величине честица у суспензији одређена је методом динамичког расипења светлости (Dynamic Light Scattering - DLS), а површинска морфологија скенирајућом електронском микроскопијом. Електрохемијска карактеризација превлаке је укључивала одређивање капацитивних особине путем цикличне волтаметрије и спектроскопије електрохемијске импеданције и одређивање електрокаталитичке активности за реакцију издвајања кисеоника у киселом раствору. Добијене честице су полидисперзне и садрже како појединачне честице тако и агломерате. Са интензивирањем услова микроталасног загревања површинска енергија честица расте, а њихова величина се смањује. Захваљујући оваквим особинама прекурсора (дисперзије), добијене превлаке имају побољшане капацитивне особине и добру електрокаталитичку активност за реакцију издвајања кисеоника при високим пренапетостима.

Koroziona stabilnost i mehanička svojstva nanokompozita epoksidna smola/glina

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Dodatak malih količina (1–5 mas%) nanoglina u polimere dovodi do značajnih poboljšanja zaštitnih svojstava premaza zahvaljujući velikoj specifičnoj površini i čvrstoći glina. Stepem dispergovanja glina u polimer/glina nanokompozitima (NC) određuje njihovu korozionu stabilnost, barijerna, mehanička i adhezivna svojstva. U ovom radu, pripremljena je serija epoksidnih NC na bazi diglicidil-etra bisfenola A, poli(amidoamina) kao umreživača i 1 mas% nanoglina. Komercijalne organogline (Cloisite 30B; Cloisite 15A) i glina modifikovana heksadecilaminom (CHDA) su direktno umešavane sa epoksidnom smolom (DM) ili prethodno dispergovane u smeši organskih rastvarača (SM). XRD analizom dokazano je postojanje interkalarne strukture nanokompozita, uz izraženu difuziju epoksidne smole u prostor između slojeva C30B i CHDA glina. Optička mikroskopija je pokazala da SM metoda pripreme dovodi do smanjenja veličine i broja aglomerata gline u NC. Ogledi istezanja su pokazali da se modul elastičnosti epoksidnih filmova povećava dodatkom nanoglina, naročito koristeći SM metodu. Spektroskopija elektrohemijske impendancije (SEI) je pokazala da poboljšanje korozione stabilnosti epoksidne smole u prisustvu nanoglina zavisi od metode pripreme NC i tipa organogline. NC na bazi CHDA gline, pripreman SM metodom, je imao najbolja mehanička svojstva i korozionu stabilnost.

Corrosion stability and mechanical properties of epoxy/clay nanocomposites

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The incorporation of nanoclays into polymers in small quantities (1–5 wt%) leads to significant improvements in the protective performances of coatings due to large surface area and high stiffness of clays. Dispersion degree of nanoclays in polymer/clay nanocomposites (NC) determinates their corrosion stability, barrier, mechanical and adhesion properties. In this work, the series of epoxy NC, based on diglycidyl ether of bisphenol A, poly(amidoamine) curing agent and 1 wt% of nanoclays, was prepared. Commercial organoclays (Cloisite 30B; Cloisite 15A) and synthesized hexadecylamine-clay (CHDA) were directly mixed with epoxy resin (DM) or previously swelled in a thinner (SM). Based on XRD analyses, NC had intercalated structure, with pronounced diffusion of epoxy resin between layers of C30B and CHDA clays. Optical microscopy showed that the size and number of agglomerates in NC were reduced when SM method was used. Tensile tests confirmed that the Young modulus of epoxy films increased when nanoclays were added, especially by using SM method. The electrochemical impedance spectroscopy (EIS) showed that improvement in corrosion stability of NCs was dependent on the preparation method and type of organoclay. The incorporation of CHDA in epoxy matrix with SM method led to the highest improvement in mechanical properties and corrosion stability.

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Uticaj leucina na anodno rastvaranje halkopirita u sumpornoj kiselinu

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U radu je ispitivano anodno rastvaranje halkopirita u sumpornoj kiselinu u prisustvu leucina. Snimani su ciklični voltamogrami u rastvorima 10^{-2} mol L⁻¹ H₂SO₄ i 10^{-2} mol L⁻¹ Leu pri brzinama od 1 mVs⁻¹, 5 mVs⁻¹, 10 mVs⁻¹ i 20 mVs⁻¹, a nakon toga je izvršena analiza rastvora. Rezultati su pokazali da pri svim brzinama prisustvo leucina pospešuje rastvaranje bakra, a smanjuje rastvaranje gvožđa iz halkopirita u odnosu na sumpornu kiselinu bez leucina. Najveće količine bakra i gvožđa se u oba rastvora oslobađaju pri brzini od 1 mVs⁻¹.

The effect of leucin on the anodic dissolution of chalcopyrite in sulfuric acid

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In this paper, the effect of leucine on the anodic dissolution of chalcopyrite in sulfuric acid is investigated. The cyclic voltammograms in solution of 10^{-2} mol L⁻¹ H₂SO₄ and 10^{-2} mol L⁻¹ Leu at the scan rates of 1 mVs⁻¹, 5 mVs⁻¹, 10 mVs⁻¹ and 20 mVs⁻¹, were recorded. After that the analysis of the solutions were done. The results have shown that the presence of leucine increases the Cu dissolution and decreases the Fe dissolution from chalcopyrite with respect to corresponding dissolutions in the sulfuric acid without leucin. The most large Cu and Fe quantities are obtained at the scan rate of 1 mVs⁻¹.

EH P04

Corrosion stability of composite Gr-based coatings in simulated body fluid

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The general idea of using Gr as nanofiller is to minimize the brittleness of HAP and gain an improved composite. Any reinforcement material for HAP should not only significantly effect the mechanical properties, but also must retain HAP's original biocompatibility. Biomimetic mineralization of Ag/HAP/Gr composite coatings was proved by newly formed apatite in SBF that enhance its corrosion stability. The antibacterial activity against *Staphylococcus aureus* and non-cytotoxicity against healthy peripheral blood mononuclear cells (PBMC) showed that these coatings have potential as bone-tissue implants.

Koroziona stabilnost kompozitnih prevlaka na bazi grafena u simuliranoj telesnoj tečnosti

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Generalna ideja korišćenja Gr kao nanofilera je da se umanjuje krtoća HAP u svrhu dobijanja poboljšanog kompozitnog materijala. Svaki ojačavajući materijal za HAP ne treba samo značajno da utiče na mehaničke karakteristike, već i da zadrži originalnu bioaktivnost HAP-a. Biomimetička mineralizacija Ag/HAP/Gr kompozitnih prevlaka je potvrđena formiranjem novog apatita u SBF-u što unapređuje korozionu stabilnost. Antibakterijska aktivnost protiv *Staphylococcus aureus* i ne citotoksičnost prema zdravim mononuklearnim perifernim ćelijama krvi su pokazali da ove prevlake imaju potencijala kao implantirani koštani tkiva.



Uklanjanje fosfata iz otpadne vode procesom elektrokoagulacije primjenom aluminijumske elektrode

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U radu je vršeno ispitivanje efikasnosti aluminijumske (Al) elektrode pri elektrokoagulaciji otpadnih voda koje sadrže fosfate ($P-PO_4$). Istraživanja su sprovedena na sintetski pripremljenoj otpadnoj vodi u laboratorijskom elektrohemijskom šaržnom reaktoru. Tokom istraživanja praćen je uticaj vremena trajanja elektrolize, gustine struje, različite koncentracije pomoćnog elektrolita i fosfata, primjene nerđajućeg čelika kao katode i uticaj režima reversne struje. Rezultati su prikazani preko efikasnosti uklanjanja fosfata. Za 40 minuta tretmana postignuta je efikasnost uklanjanja od 98,9%, pri $pH=3$, $j=1 \text{ mA/cm}^2$ i $\gamma_0=50 \text{ mg/L } P-PO_4$, a dodatkom NaCl kao pomoćnog elektrolita ($\gamma=0,25 \text{ g/L}$), postiže se efikasnost uklanjanja 93,6% za 20 minuta tretmana.

Phosphate removal from wastewater by electrocoagulation process using aluminium electrode

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This study focused on testing the efficacy of aluminium (Al) electrode in an electrocoagulation treatment of wastewater containing phosphates ($P-PO_4$). The research was conducted on a prepared synthetic wastewater in a laboratory batch electrochemical reactor. Research has followed the effect of the electrolysis duration, current density, different concentration of supporting electrolyte and phosphate in wastewater, application of stainless steel as the cathode, effect of *pulsed current regime*. The results are shown through phosphates removal efficacy. For 40 minutes of treatment is achieved removal efficiency of 98,9%, at the initial pH value 3, $j=1 \text{ mA/cm}^2$ and $\gamma_0=50 \text{ mg/L } P-PO_4$. Addition of NaCl as a supporting electrolyte ($\gamma=0.25 \text{ g/L}$), is achieved 93.6% removal efficiency for 20 minutes of treatment ($pH=3$, $j= 1\text{mA/cm}^2$).



Experimental measurement of volumetric, transport, ultrasonic and refractive index properties of binary mixtures (ethyl oleate + *n*-hexadecane) at different temperatures and atmospheric pressure

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Some of the most important properties in diesel engine design and operation are density and viscosity of a fuel under different conditions. Thanks to increasing awareness of global warming and environmental pollution, the interest in renewable energy sources and, particularly, non-toxic fuel supplements grows progressively. One of the best solutions for transport sector is the use of biodiesel and its mixtures with petro diesel which requires knowledge of the fundamental thermodynamic properties of their blends. Pure ethyl oleate, that is one of the main components of most of biodiesel fuels, and *n*-hexadecane, which serves as a reference for diesel fuels, were examined here, as well as their mixtures. Density, viscosity, sound velocity and refractive index data for the binary system (ethyl oleate + *n*-hexadecane) were measured in the whole concentration range and within a wide range of temperature (with temperature step 5 K) at atmospheric pressure. The measurements were performed on DMA 5000 densimeter, Stabinger SVM 3000 viscometer, DSA 5000 M density and sound velocity meter and RXA 156 refractometer, all produced by Anton Paar. Based on the corresponding experimental data, the isentropic bulk modulus was computed and presented.

Eksperimentalno određivanje volumetrijskih, transportnih, ultrazvučnih svojstava i indeksa refrakcije binarnih smeša (etil oleat + *n*-heksadekan) na različitim temperaturama i atmosferskom pritisku

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Neka od najbitnijih svojstava za dizajn i rad dizel motora su gustina i viskoznost goriva pri različitim uslovima. Zahvaljujući rastu svesti o globalnom zagrevanju i zagađenju životne sredine, progresivno raste interesovanje za obnovljive izvore energije i, posebno, netoksične dodatke gorivima. Jedno od najboljih rešenja u oblasti transporta jeste upotreba biodizela i njegovih smeša sa petro dizelom, što zahteva poznavanje osnovnih termodinamičkih svojstava njihovih smeša.

Čist etil oleat, koji je jedna od osnovnih komponenata većine biodizel goriva, i *n*-heksadekan, koji se koristi kao reper za dizel goriva, su ispitivani u ovom radu, kao i njihove smeše. Gustina, viskoznost, brzina prostiranja zvuka i indeks refrakcije za binarne sisteme (etil oleat + *n*-heksadekan) su merene u čitavom opsegu koncentracija i širokom opsegu temperatura (sa korakom 5 K) na atmosferskom pritisku. Merenja su vršena na gustinomeru DMA 5000, viskometru Stabinger SVM 3000, uređaju za merenje gustine i brzine prostiranja zvuka u uzorku DSA 5000 M i refraktometru RXA 156, proizvođača Anton Paar. Na osnovu odgovarajućih eksperimentalnih podataka izračunat je i predstavljen i izentropski modul stišljivosti.



Influence of resolution in digital characterization of sand particles size and shape

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This paper investigated the influence of resolution and two image analysis softwares for image analysis (SigmaScan Pro and ImageJ) on parameters and shape factors commonly used in the characterization of particles. In our previous paper characterization of polydisperse sand particles was investigated at two scanning resolutions, and arisen a need to examine in more detail the impact of different scanning resolutions on shape factors. The analyzed particles were the polydisperse fractions of quartz filtration sand with sieve diameters in the intervals of 0.85-1.030 mm, 1.406-1.600 mm and 2.00-2.83 mm. The scanned image of particles was used for analysis. In addition, the images of circles as reference were generated. The scanning resolutions used in this study were 75 to 4800 dpi, and grayscale thresholds were optimized for discrimination of particle background. The results indicate that the resolution (pixel size) and algorithms used in image analysis softwares have influences on obtained shape factors, and most significant effect was observed in the calculated particle perimeters.

Утицај резолуције на дигиталну карактеризацију величине и облика честица песка

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У овом раду је испитиван утицај резолуције и два софтвера за анализу слике, "SigmaScan Pro" и "ImageJ", на величину и факторе облика који се обично користе у карактеризацији честица. У нашем претходном раду карактеризација честица полудисперзне смеше песка је вршена на две резолуције и појавила се потреба да се испита детаљније утицај скенирања при различитим резолуцијама на факторе облика. Анализиране честице су различите фракције кварцног филтрационог песка пречника просејавања у интервалима од 0.85-1.030 мм, 1.406-1.600 мм и 2.00-2.83 мм. Поред тога, анализиране су слике кругова ради поређења. Резолуција скенирања коришћена у овом раду је била од 75 до 4800 dpi и подешавањем "grayscale thresholds", тј. интензитета сивих тонова, на оптималну вредност одређена је граница честице у односу на позадину. Резултати указују да резолуција (величина пиксела) и алгоритми који се користе у софтверима за анализу слике имају утицаја на добијене факторе облика, а најзначајнији утицај је запажен при одређивању обима честица.



Koeficijent trenja pri strujanju vode kroz pakovani sloj sferičnih čestica

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Cilj ovog rada je eksperimentalna procena različitih korelacionih modela za određivanje koeficijenta trenja f_p pri strujanju vode kroz pakovani sloj sferičnih čestica. Eksperimenti su izvedeni merenjem pada pritiska u pakovanom sloju. U eksperimentima su korišćeni 7 različitih pakovanih sloja sačinjenih od staklenih sferičnih čestica različitih prečnika. Opseg poroznosti sloja se kretao 0.359 – 0.486, dok je Rejnoldsov broj čestica bio u opsegu od 0.3 do 286. Dobijeni rezultati upoređeni su sa dostupnim literaturnim korelacijama. U cilju poboljšanja rezultata korelacija predložena je nova jednačina u formi Ergunove korelacije sa modifikovanim koeficijentima. Srednja apsolutna greška odstupanja između eksperimentalnih vrednosti pada pritiska u sloju i vrednosti dobijenih korišćenjem nove predložene jednačine je 9.04 %.

Friction factor for water flow through packed beds of spherical and non-spherical particles

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The aim of this work was the experimental evaluation of different friction factor correlations for water flow through packed beds of spherical. The experiments were performed by measuring the pressure drop across the bed. Packed beds made of monosized glass spherical particles of seven different diameters were used. The range of bed voidages was 0.359 – 0.486, while the range of bed particle Reynolds numbers was from 0.3 to 286. The obtained results were compared using a number of available literature correlations. In order to improve the correlation results for spherical particles, a new simple equation was proposed in the form of Ergun's equation, with modified coefficients. The new correlation had mean absolute deviation between experimental and calculated values of pressure drop of 9.04%.



HI P05

Pressure drop in packed beds of spherical particles at ambient and elevated air temperatures

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The aim of this work was the experimental investigation of the particle friction factor for air flow through packed bed of particles at ambient and elevated temperatures. The experiments were performed by measuring the pressure drop across the packed bed, heated to the desired temperature by hot air. Glass spherical particles of seven different diameters were used. The temperature range of the air flowing through the packed bed was from 20°C to 350°C and the bed voidages were from 0.3574 to 0.4303. The obtained results were correlated using a number of available literature correlations. The overall best fit of all of the experimental data was obtained using Ergun¹ equation, with mean absolute deviation of 10.90%. Ergun`s equation gave somewhat better results in correlating the data at ambient temperature with mean absolute deviation of 9.77%, while correlation of the data at elevated temperatures gave mean absolute deviation of 12.38%. The vast majority of the correlations used gave better results when applied to ambient temperature data than to the data at elevated temperatures.

Pad pritiska u pakovanom sloju sferičnih čestica na sobnoj i povišenim temperaturama

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Cilj ovog rada je bio eksperimentalno ispitivanje koeficijenta trenja fluid-čestice prilikom strujanja vazduha kroz pakovani sloj čestica, na sobnoj i povišenim temperaturama. Izvršeno je eksperimentalno merenje pada pritiska u pakovanim slojevima različitih temperatura zagrejanih korišćenjem vreloug vazduha. Kao materijal za pakovanje korišćene su sferične staklene kuglice 7 različitih prečnika. Temperaturni interval u kom su vršeni eksperimenti bio je od 20°C do 350°C, dok su poroznosti sloja iznosile od 0,3574 do 0,4303. Dobijeni rezultati korelisani su korišćenjem većeg broja literaturnih korelacija. Najbolje slaganje sa eksperimentalnim podacima pokazala je Ergunova jednačina¹, sa srednjim procentnim odstupanjem od 10,90%. Ergunova jednačina je dala bolje rezultate prilikom korelisanja podataka na sobnoj temperaturi (srednja procentna greška 9,77%), dok je korelisanje podataka na povišenim temperaturama izvršeno sa greškom od 12,38%. Većina testiranih literaturnih korelacija je dala bolje rezultate pri korelisanju podataka dobijenih na sobnoj temperaturi u odnosu na podatke dobijene na povišenim temperaturama.



**Densities, viscosities and refractive indices of binary system
N, N-dimethylaniline + 1-butyl-3-methylimidazolium triflate at
288.15 to 333.15 K and at atmospheric pressure**

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In this study densities, viscosities and refractive indices of binary system N, N-dimethylaniline + 1-butyl-3-methylimidazolium triflate ([bmim][OTf]), were measured at atmospheric pressure and in temperature range $T = (288.15 \text{ to } 333.15) \text{ K}$. Excess molar volumes, deviations in refractive indices, viscosity deviations and excess molar Gibbs free energies of activation of viscous flow were calculated and the results were fitted to a Redlich-Kister polynomial equation. Considering the calculated thermodynamic properties, molecular interactions in the investigated binary system were analyzed and discussed.

**Gustina, viskoznost i indeks refrakcije binarnog sistema
N, N-dimetilanilin + 1-butil-3-metilimidazolium triflat na
temperaturama od 288.15 do 333.15 K i na atmosferskom pritisku**

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U ovom radu merene su gustine, viskoznosti i indeksi refrakcije binarnog sistema N, N-dimetilanilin + 1-butyl-3-methylimidazolium triflate ([bmim][OTf]) na atmosferskom pritisku i u temperaturnom opsegu $T = (288.15 \text{ do } 333.15) \text{ K}$. Na osnovu eksperimentalnih podataka vršeno je izračunavanje dopunske molarne zapremine, promene indeksa prelamanja, promene viskoznosti, promene dopunske molarne Gibsove energije. Rezultati su fitovani Redlich-Kister-ovim polinomom. Na osnovu izračunatih termodinamičkih veličina analizirane su i diskutovane molekulske interakcije u pomenutom binarnom sistemu.

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HI P07

Izolovanje i optimizacija sterola, vitamina E i vitamina D iz semena *Trigonella foenum-graceum* L. natkritičnom ekstrakcijom

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Grčko seme je poznato po nizu povoljnih dejstava u vidu hipoholesterolemijske, hipoglikemijske i antioksidativne aktivnosti. Shodno ovim i ostalim pozitivnim učincima, grčko seme je dobilo na značaju proizvodnjom i primenom za očuvanje ljudskog zdravlja. Primenjena je natkritična CO₂ ekstrakcija (NK-CO₂) sterola, vitamina E i vitamina D iz grčkog semena (*Trigonella foenum-graecum* L., Fabaceae) u cilju dobijanja ekstrakata sa bogatim farmakološkim dejstvom. Prinosi ekstrakata, kao i njihovi sastavi su bili determinisani i analizirani pri različitim procesnim uslovima pritiska, temperature i količine utrošenog CO₂ po masi grčkog semena tokom ekstrakcionog procesa. Centralno kompozitni dizajn i metodologija odzivnih površina (CCD/RSM) su primenjeni u definisanju uticaja procesnih parametara ekstrakcije i optimizaciji izolovanja totalnog ekstrakta, bogatog fitosterolima, vitaminom E i vitaminom D.

Optimization and isolation of sterols, vitamin E and vitamin D from *Trigonella foenum-graecum* seeds L.

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Fenugreek seeds have been known for benefit properties of hypocholesterolemic, hypoglycaemic and antioxidative activity. On the basis of these and other benefits, the fenugreek seeds have reached a growing interest in increased production and implementation of different products for human health. Supercritical CO₂ extraction (SC-CO₂) of sterols, vitamin E and vitamin D from fenugreek seeds (*Trigonella foenum-graecum* L., Fabaceae) was applied using SC-CO₂. The yields of extract as well as its composition were determined and analyzed at different process conditions of pressure, temperature, which correspond to appropriate SC-CO₂ density and for different solvent consumption defined as mass of used CO₂ for extraction per mass of dry fenugreek seeds. A central composite design (CCD) combined with response surface methodology (RSM) was applied to study extraction conditions and to determine the optimal conditions for isolation of total extract, rich in phytosterols, vitamin E and vitamin D.



Molecular interactions in the binary system diethyl succinate + 1-hexanol according to mixing deviation properties and FT-IR analysis

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Density, viscosity and refractive index data for the binary system diethyl succinate + 1-hexanol have been measured in temperature range 288.15–323.15 K with temperature step 5K, and at atmospheric pressure. The measurements were performed on Anton Paar DMA 5000 digital vibrating tube densimeter, Anton Paar SVM 3000 digital viscometer and Anton Paar RXA 156 refractometer. Based on the corresponding experimental data, excess molar volumes (V^E), viscosity deviations ($\Delta\eta$) and refractive index deviations (Δn_D) were determined and fitted by the Redlich-Kister polynomial equation. Molar excess Gibbs free energies of activation of viscous flow (ΔG^E) were additionally calculated from measured density and viscosity data. Excess and deviation functions, with FT-IR study, were further used in the analysis of molecular interactions present in the mixture.

Molekulske interakcije prisutne u binarnom sistemu dietil sukcinat + 1-heksanol prema izvedenim veličinama mešanja i FT-IR analizi

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Eksperimentalno su određene gustine, viskoznosti i indeksi refrakcije binarnog sistema dietil sukcinat + 1-heksanol u temperaturnom intervalu 288.15–323.15 K sa korakom 5 K, i na atmosferskom pritisku. Eksperimentalna merenja su izvršena na digitalnom gustinomeru Anton Paar 5000, digitalnom viskozimetru Anton Paar SVM 3000 i refraktometru Anton Paar RXA 156. Na osnovu odgovarajućih eksperimentalnih podataka, izračunate su dopunske molarne zapremine (V^E), promene viskoznosti ($\Delta\eta$) i promene indeksa refrakcije (Δn_D), i korelisane Redlich-Kister polinomom. Dodatno je izračunata molarna dopunska Gibsova energija aktivacije viskoznog toka (ΔG^E) iz izmerenih podataka za gustinu i viskoznost. Pomoću izvedenih veličina, kao i FT-IR merenja, urađena je analiza molekulskih interakcija prisutnih u smeši.

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Uticaj adsorpcije polimera na koloidnu stabilnost dvostrukih slojevitih hidroksida

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Razvijanje novih polimer-neorganskih nanomaterijala zasnovanih na dvostrukim slojevitim hidroksidima (LDH) predstavlja veoma uspešnu oblast istraživanja kao posledica izuzetnih mehaničkih i termalnih osobina novosintetisanih materijala. Uprkos tome, poznavnje koloidne stabilnosti novog materijala zasnovanog na LDH česticama, kao i adekvatne doze polimera koja se može adsorbovati, i time čak povećati stabilnost koloidne suspensije, je od izuzetnog značaja. Prvenstveno su LDH čestice sintetisane metodom koprecipitacije. Uticaj četiri macroRAFT (reverzibilni-adiciono-fragmentacioni transfer lanca) kopolimera, sačinjenih od akrilne kiseline (AA) i butil-akrilata (BA), na koloidnu stabilnost Mg^{2+} - Al^{3+} LDH čestica je bila ispitivana. Čestice su umereno stabilne pri niskoj dozi kopolimera, dostižući brzu, difuzijom ograničenu, agragaciju na izoelektričnoj tački (IEP). Nakon IEP disperzija nanočestica je ponovo stabilna usled inverzije naelektrisanja čestica. Zapažen je i značajan efekat odnosa AA prema BB, kao i molekulske mase samog polielektrolita. Nakon analiziranja uzoraka mikroskopom atomskih sila i transmisijom elektronskim mikroskopom jasno je da čestice agreguju preferirajući lice-lice orijentaciju.

Tuning colloidal stability of layered double hydroxides by polymer adsorption

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Development of novel polymer-inorganic nanomaterials based on layered double hydroxides (LDHs) is a thriving research area due to enhanced mechanical and thermal properties. However, understanding colloidal stability of the LDH based materials and determining proper amount of polymer that can adsorb on the surface of the nanoparticles, and furthermore, improve colloidal stability are of crucial importance. Firstly, LDH were synthesized by coprecipitation. Secondly, the effect of four macroRAFT (reversible addition fragmentation chain transfer) copolymers of acrylic acid (AA) and butyl acrylate (BA) on colloidal behavior of Mg^{2+} - Al^{3+} LDH was investigated. Particles are moderately stable at low copolymer dose, reaching fast, diffusion limited, aggregation close to isoelectric point (IEP). After IEP, LDH nanoparticles become stable due to substantial charge reversal. Significant effects of AA-to-BA ratio and molecular mass of polyelectrolytes were observed. Images taken by atomic force and transmission electron microscopes revealed that the nanoplatelets prefer face-to-face orientation in the aggregates.

Modifikovana nanoceluloza kao nosač za imobilizaciju lipaze iz *Candida rugosa*

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Sa ubrzanim razvojem nanotehnologije, celuloza kao najrasprostranjeniji i najvažniji prirodni polimer na zemlji privlači sve veću pažnju u formi nanoceluloze. Zbog svoje biodegradabilnosti, biokompatibilnosti i velike specifične površine nanoceluloza je veoma pogodan materijal za imobilizaciju enzima. U cilju ostvarivanja stabilnije veze između nosača i enzima i dobijanja biokatalizatora sa što većom katalitičkom aktivnosti, u ovom radu su različitim metodima funkcionalizacije na površinu nanoceluloze uvedene amino i karboksilne grupe. Određen je broj uvedenih grupa, svi materijali okarakterisani su FT-IR spektroskopijom i TG analizom, a određen je i zeta potencijal površina. Ispitan je uticaj jonske jačine rastvora i adsorpcija lipaze iz *Candida rugosa* testirana je u 0,1 i 1 M fosfatnom puferu, a rezultati ispitivanja aktivnosti pokazali su da je enzim nakon imobilizacije zadržao čak 54,5 % od početne aktivnosti.

Modified nanocellulose as a support for adsorption of lipase from *Candida rugosa*

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With the rapid development of nanotechnology, cellulose as the most abundant and important natural polymer on earth, is attracting increasing attention in its form of nanocellulose. Due to its biodegradability, biocompatibility and large specific surface nanocellulose is a very suitable material for the immobilization of enzymes. In order to accomplish more stable bond with the enzyme and obtain biocatalyst with high catalytic activity, in this paper nanocellulose surface was functionalized with different methods, and amino and carboxyl groups were introduced. All materials were characterized by FT-IR spectroscopy and TG analysis, and in addition, zeta potential of all surfaces was determined. The effect of the ionic strength of the solution on the adsorption of the lipase from *Candida rugosa* was tested in 0.1 and 1 M phosphate buffer, and the activity results showed that after immobilization lipase retained 54.5% of the initial activity.



Dinuklearni Pt(II) kompleksi kao efikasni katalitički reagensi za selektivnu hidrolizu peptida

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Poslednjih godina intenzivno se izučavaju reakcije Pt(II) kompleksa sa peptidima i proteinima, koji u bočnom nizu sadrže aminokiseline L-metionin i L-histidin, jer ovi kompleksi predstavljaju veoma efikasne katalizatore hidrolize peptidne veze u ovim peptidima. Poznato je da nakon koordinovanja akva-platina(II) kompleksa za heteroatom u bočnom nizu aminokiselina L-metionina i L-histidina, dolazi do hidrolize peptidne veze koja sadrži karboksilnu grupu koordinovane aminokiseline. U ovom radu prikazan je pregled rezultata postignutih u oblasti ispitivanja reakcija hidrolize peptidne veze u peptidima koji sadrže aminokiseline L-metionin i L-histidin u prisustvu dinuklearnih $[\{Pt(L)(H_2O)\}_2(\mu-X)]^{4+}$ kompleksa (L je etilendiamin, en; (\pm) -1,2-propilendiamin, 1,2-pn; izobutilendiamin, ibn; *trans*- (\pm) -1,2-diaminocikloheksan, dach; 1,3-propilendiamin, 1,3-pd; 2,2-dimetil-1,3-propilendiamin, 2,2-diMe-1,3-pd; (\pm) -1,3-pentandiamin, 1,3-pnd i X je mostni diazinski ligand pirazin, pz ili piridazin, pydz).¹ Nađeno je da brzina hidrolize peptidne veze zavisi od sternog efekta bidentatno koordinovanog diaminskog (L) i mostnog liganda (X) u $[\{Pt(L)(H_2O)\}_2(\mu-X)]^{4+}$ kompleksu.

Dinuclear Pt(II) complexes as effective catalytic reagents for the selective hydrolysis of peptides

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Recent years have witnessed an increasing interest in the study of the interactions of Pt(II) complexes with methionine- and histidine-containing peptides and proteins as effective catalyst for the hydrolytic cleavage of the above mentioned peptides. In general, it was shown that platinum(II) aqua complexes spontaneously bind to the heteroatom in the side chain of L-methionine or L-histidine and promote cleavage of the amide bond involving the carboxylic group of the anchoring amino acid. The present work provides overview of the results achieved in the studies of the hydrolytic reactions of the amide bond in L-methionine- and L-histidine containing peptides in the presence of dinuclear $[\{Pt(L)(H_2O)\}_2(\mu-X)]^{4+}$ complexes (L is ethylenediamine, en; (\pm) -1,2-propylenediamine, 1,2-pn; isobutylenediamine, ibn; *trans*- (\pm) -1,2-diaminocyclohexane, dach; 1,3-propylenediamine, 1,3-pd; 2,2-dimethyl-1,3-propylenediamine, 2,2-diMe-1,3-pd; (\pm) -1,3-pentanediamine, 1,3-pnd and X is bridging diazine ligand pyrazine, pz or pyridazine, pydz).¹ It was found that the amount of hydrolyzed peptide bound strongly depends from the steric bulk of bidentate coordinated diamine ligand (L) and pyrazine- or pyridazine-bridged ligand (X) in $[\{Pt(L)(H_2O)\}_2(\mu-X)]^{4+}$ complex.

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1. S. Rajković, M. D. Živković, M. I. Djuran, *Current Protein & Peptide Science*, **17** (2015) 95-105.

NH PO1

**Novi 4'-(4-hlorofenil)-2,2':6',2''-terpiridin rutenijum(II) kompleksi:
Sinteza, karakterizacija i interakcije sa biomolekulima.**

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U ovom istraživanju sintetisana je serija novih monofunkcionalnih Ru(II) kompleksa opšte formule mer-[Ru(Cl-Ph-tpy)(N-N)Cl]Cl gde je Cl-Ph-tpy 4'-(4-hlorofenil)-2,2':6',2''-terpiridin, N-N helatni bidentatni ligand (1,2-diaminoetan (en, **1**), 1,2-diaminocikloheksan (dach, **2**) i 2,2'-bipiridin (bpy, **3**)). Svi kompleksi su u potpunosti okarakterisani elementalnom analizom i spektroskopskim tehnikama (IR, UV-Vis, 1D i 2D NMR). DNK vezivanje je ispitivano pomoću UV-Vis spektroskopije i merenjem fluorescencije. U konkurentnoj reakciji sa etidijum bromidom (EB) pokazano je da kompleksi mogu zameniti EB vezan za DNK ukazujući na jaku konkurenciju sa EB ($K_{sv} = 3.7 - 9.6 \times 10^4 \text{ M}^{-1}$). Ova ispitivanja pokazuju da rutenijum kompleksi interaguju sa DNK kovalentno i preko interkalacije. Ovi kompleksi vezuju se za albumin serum protein pokazujući relativno visoku konstantu vezivanja ($K_{sv} = 10^4 - 10^5 \text{ M}^{-1}$).

**New 4'-(4-chlorophenyl)-2,2':6',2''-terpyridine ruthenium(II) complexes:
Synthesis, characterization and interaction with biomolecules.**

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In this study, we have developed a series of new monofunctional Ru(II) complexes of the general formula mer-[Ru(Cl-Ph-tpy)(N-N)Cl]Cl in which Cl-Ph-tpy is 4'-(4-chlorophenyl)-2,2':6',2''-terpyridine, N-N is a bidentate chelating ligand (1,2-diaminoethane (en, **1**), 1,2-diaminocyclohexane (dach, **2**) or 2,2'-bipyridine (bpy, **3**)). All complexes were fully characterized by elemental analysis and spectroscopic techniques (IR, UV-Vis, 1D and 2D NMR). DNA binding was studied using UV-Vis spectroscopy and fluorescence quenching measurements. Competitive studies with ethidium bromide (EB) showed that the complexes can displace DNA-bound EB, suggesting strong competition with EB ($K_{sv} = 3.7 - 9.6 \times 10^4 \text{ M}^{-1}$). These experiments show that the ruthenium complexes interact with DNA covalently and via intercalation. The complexes bind to serum protein albumin displaying relatively high binding constants ($K_{sv} = 10^4 - 10^5 \text{ M}^{-1}$).

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References:

1. A. Rilak, I. Bratsos, E. Zangrando, J. Kljun, I. Turel, Ž. D. Bugarčić and E. Alessio, *Inorg. Chem.*, 2014, **53**, 6113-6126.

Sinteza i karakterizacija novih bimetaljskih kompleksa platine(II) i paladijuma(II) i ispitivanje njihovih interakcija sa važnim biomolekulima

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Polinuklearni kompleksi platine(II) i paladijuma(II) predstavljaju novu generaciju antitumorskih lekova.¹ S obzirom da su neki tumori otporni na dejstvo cisplatine istraživanja idu u smeru sinteze novih antitumorskih kompleksa čije strukturne karakteristike omogućavaju alternativni mehanizam dejstva, koji se razlikuje od mehanizma dejstva cisplatine i njenih analoga.²

Sintetisana su tri nova bimetaljska dinuklearna kompleksa platine(II) i paladijuma(II), $[\{\text{PdCl}(\text{bipy})\}\{\mu\text{-(pyrazine)}\}\{\text{PtCl}(\text{bipy})\}]\text{Cl}(\text{ClO}_4)$ (**1**), $[\{\text{PdCl}(\text{en})\}\{\mu\text{-(pyrazine)}\}\{\text{PtCl}(\text{en})\}]\text{Cl}(\text{ClO}_4)$ (**2**) i $[\{\text{PdCl}(\text{bipy})\}\{\mu\text{-(NH}_2(\text{CH}_2)_6\text{H}_2\text{N})\}\{\text{PtCl}(\text{bipy})\}]\text{Cl}(\text{ClO}_4)$ (**3**). Izvršena je detaljna karakterizacija njihove strukture primenom različitih eksperimentalnih metoda. Rezultati ispitivanja interakcija kompleksa sa molekulom DNA i etidium bromidom (EB) pokazuju da se sva tri kompleksa mogu vezati za DNA ispoljavajući visoke vrednosti konstanti vezivanja. Ispitivanje interakcije sa goveđim serum albuminom takođe ukazuje na veliki afinitet kompleksa, ispoljavajući vrednosti konstanti vezivanja koje opadaju u nizu: (**2**) > (**1**) > (**3**).

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Synthesis and characterisation of the new bimetallic complexes of platinum(II) and palladium(II) and study of their interactions with important biomolecules

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

The three new bimetallic dinuclear complexes of platinum(II) and palladium(II), $[\{\text{PdCl}(\text{bipy})\}\{\mu\text{-(pyrazine)}\}\{\text{PtCl}(\text{bipy})\}]\text{Cl}(\text{ClO}_4)$ (**1**), $[\{\text{PdCl}(\text{en})\}\{\mu\text{-(pyrazine)}\}\{\text{PtCl}(\text{en})\}]\text{Cl}(\text{ClO}_4)$ (**2**) and $[\{\text{PdCl}(\text{bipy})\}\{\mu\text{-(NH}_2(\text{CH}_2)_6\text{H}_2\text{N})\}\{\text{PtCl}(\text{bipy})\}]\text{Cl}(\text{ClO}_4)$ (**3**) were synthesized. Additionally, a detailed characterization of their structure was carried out using different experimental methods. Study of the interactions of complexes with DNA molecule and ethidium bromide (EB) showed that all three complexes can bind to a DNA exhibiting high binding constants. Interactions of complexes with bovine serum albumin indicate a high binding affinity of complexes, displaying the values of the binding constants in the following order: (**2**) > (**1**) > (**3**).

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1. P. E. N. Barry, J. P. Sadler, *Chem. Commun.* **49** (2013) 5106.

2. T. Soldatović, S. Jovanović, Ž. D. Bugarčić, R. van Eldik, *Dalton Trans.* **41** (2012) 876.

**Sinteza i struktura Rh(III) kompleksa sa Pincer-tipom liganda:
Inetrakcije sa biomolekulima**

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Poslednjih par godina intezivno se ispituje antitumorska aktivnost kompleksa Rh(III).[1] Shodno tome sintetisali smo i okarakterisali novi kompleks Rh(III) sa 2,6-bis(5-terc-butyl-1H-pirazol-3-il)piridinom (LH₂). Zatim smo ispitivali supsticione reakcije sintetisanog kompleksa sa malim biomolekulima i sa fragmentima DNK i RNK Uv-Vis spektrofotometrijski. Ispitivane su i interakcije sintetisanog kompleksa sa CT-DNK i albumin serum proteinom spektrofotometrijski i spekstrofluorimetrijski. Na osnovu dobijenih rezultata možemo da zaključimo da sintetisani kompleks Rh(III) pokazuje zadovoljavajući afinitet kako prema malim biomolekulima tako i prema DNK i albuminu.

**Synthesis and Structures of Pincer-Type Rhodium(III) complex:
Interactions with Biomolecules**

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In the last few years there has been much attempts to examined the anti-tumor activity of the Rh(III) complexes.[1] Accordingly, we have synthesized and characterized a new complex of the Rh(III) with 2,6-bis (5 -tert-butyl-1H-pyrazol-3-yl)pyridine (LH₂). Afterwards the substitution reaction of the synthesized complexes with small biomolecules and with fragments of DNA and RNA were examined by UV-Vis spectrophotometry. We have investigated the interaction of the synthesized complexes with CT-DNA and serum protein albumin by spectrophotometry and spectrofluorimetry. Based on these results we can conclude that the synthesized complex Rh(III) shows good affinity towards small biomolecules and also to the DNA and albumin.

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1. C-H. Leunga, H-J. Zhonga, D. S-H. Chanb, D-L. Mab, *Coord. Chem. Rev.*, **257** (2013) 1764– 1776.

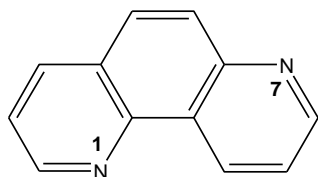
NIH PO4

Sinteza i karakterizacija kompleksa zlata(III) sa tricikličnim aromatičnim jedinjenjima koja sadrže azot

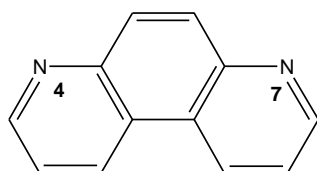
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1,7-fenantrolin



4,7-fenantrolin

U ovom radu, sintetisana su dva nova mononuklearna kompleksa zlata(III) opšte formule $[AuCl_3L]$, L je x,7-fenantrolin ($x = 1$ i 4), u reakciji između $K[AuCl_4]$ i odgovarajućeg N-heterocikličnog liganda u 1 : 1 molskom odnosu. Dobijeni zlato(III) kompleksi su okarakterisani primenom elementarne mikroanalize, NMR (1H i ^{13}C) i IR spektroskopije, UV-vis spektrofotometrije i rendgenske strukturne analize. Dobijeni podaci za ove komplekse su upoređeni sa odgovarajućim podacima za ranije sintetisane $[AuCl_3(N\text{-heterocikl})]$ komplekse.¹ Primenom teorije funkcionala gustine (DFT) optimizovane su geometrije zlato(III) kompleksa sa x,7-fenantrolinom u vakuumu i etanolu i ispitivan je mehanizam njihovog formiranja.

Synthesis and characterization of gold(III) complexes with tricyclic aromatic nitrogen-containing heterocycles

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In the present study, we have synthesized two new mononuclear gold(III) complexes of the general formula $[AuCl_3L]$, L is x,7-phenanthroline ($x = 1$ and 4), in the reactions between $K[AuCl_4]$ and the corresponding N-heterocycle in 1 : 1 molar ratio. The obtained gold(III) complexes were characterized by elemental microanalysis, NMR (1H and ^{13}C), UV-vis and IR spectroscopy and single-crystal X-ray diffraction analysis. Spectroscopic and crystallographic data for these complexes were compared with those for the previously reported $[AuCl_3(N\text{-heterocycle})]$ complexes.¹ Density functional theory (DFT) calculations were performed in order to optimize geometry of the newly synthesized gold(III) complexes with x,7-phenanthroline and to gain more insight into the coordination mode of these N-heterocycles toward $AuCl_3$ fragment.

Acknowledgements: This work was funded in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project Nos. 172036 and 174033).

1. B. Warzajtis, B. Đ. Glišić, N. S. Radulović, U. Rychlewska, M. I. Djuran, *Polyhedron* **79** (2014) 221
B. Đ. Glišić, B. Warzajtis, N. S. Radulović, U. Rychlewska, M. I. Djuran, *Polyhedron* **87** (2015) 208.

NH PO5

Sistem za fotoaktivnu terapiju kancera na bazi nanočestica TiO₂ i kompleksa rutenijuma

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Lečenje kancera u današnje vreme uključuje primenu različitih terapija koje se uglavnom zasnivaju na primeni kompleksa prelaznih metala. Kada se razmatraju nove strategije u lečenju kancera, ističe se fotodinamička terapija. Ovaj vid terapije koristi svetlo kao aktivator leka ili nosača leka na mestu obolelog tkiva. Uzimajući u obzir navedeno, testirali smo potencijal prethodno sintetisanog fotoaktivnog nanokompozitnog sistema i njegovih komponenti za primenu u fotodinamičkoj terapiji. Pomenuti sistem se sastoji od nanočestica TiO₂ kao nosača leka i kompleksa [Ru(II)(dcbpy)₂Cl₂], kao potencijalnog citostatika, vezanog za površinu nanočestica. Rutenijumov kompleks iskazuje svoje citotoksično delovanje vezivanjem za ciljane biomolekule, dok došač, TiO₂, vezujući kompleks može smanjiti njegovu reaktivnost sa zdravim ćelijama dok ne dođe do tumorskog tkiva. Pomenuti nanokompozitni sistem i njegove komponente su testirane na ćelijama melanoma. Rezultati ukazuju na to da dejstvom UV svetla, nakon tretmana sa obe komponente sistema (kompleksom i TiO₂) dolazi do značajnog smanjenja u broju tumorskih ćelija, dok je nanokompozitni sistem pokazao sinergistički efekat i dovodio do smanjenja broja tumorskih ćelija ispod 50%. Stoga, ovaj sistem ostavlja mesta za dalja izučavanja jer pruža mogućnost razvoja efikasnije terapije u kojoj bi doziranje leka bilo kontrolisano svetlom.

System for photodynamic cancer therapy based on TiO₂ and Ru-complex

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The treatment of cancer involves different therapies mainly based on transition metal complexes. When exploring new strategies for the treatment of cancer, one possibility is the use of photodynamic therapy. Photodynamic therapy utilizes light to activate a drug or a drug/carrier system when they are localized in the tumor tissue. Therefore, we have tested the potential of previously synthesized photoactive nanocomposite system and its components as a candidate for photodynamic therapy. The nanocomposite system consists of TiO₂ nanoparticles as drug/carrier and ruthenium complex [Ru(II)(dcbpy)₂Cl₂] bound to its surface as a potential antitumor drug. This Ru complex have been shown to exert cytotoxic effect through binding to target biomolecules, while TiO₂ carrier can serve to minimize side reactivity in the bloodstream and healthy cells until it reaches tumor cells. The nanocomposite system and its components are successfully applied on melanoma tumor cell lines. It was demonstrated that the illumination by UV light, after treatment either with Ru-complex or TiO₂ nanoparticles significantly decreases melanoma cell survival rate, while NCS shown synergistic effect and have reduced the number of melanoma cells under 50%. Hence, this system might be of interest from the standpoint of development of more efficient, light controllable drug delivery approaches.

Sinteza i karakterizacija kadmijum(II) kompleksa sa 1,4-butandiamin-*N,N,N',N'*-tetraacetato ligandom

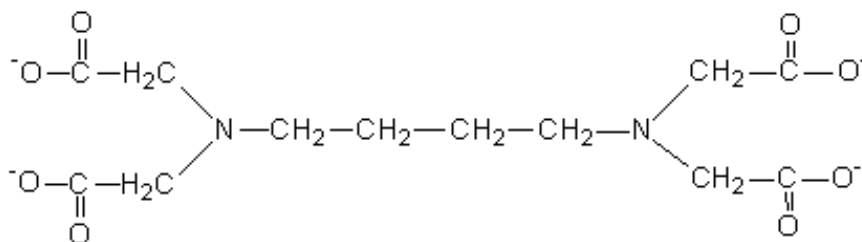
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U reakciji između $\text{Ba}[\text{Ba}(1,4\text{-bdta})] \cdot 2\text{H}_2\text{O}$ i $\text{CdSO}_4 \cdot 7\text{H}_2\text{O}$ u 1:1 molskom odnosu sintetisan je novi 1,4-bdta-Cd(II) kompleks (1,4-bdta = 1,4-butandiamin-*N,N,N',N'*-tetraacetat). Za karakterizaciju ovog kompleksa upotrebljena je infra-crvena (IR) i nuklearno-magnetno-rezonantna (^1H i ^{13}C NMR) spektroskopija. Dobijeni IR spektroskopski podaci ovog kompleksa su poređeni sa odgovarajućim podacima za ranije sintetisane 1,4-bdta- i 1,3-pdta-Co(II) komplekse (1,3-pdta = 1,3-propandiamin-*N,N,N',N'*-tetraacetat).^{1,2} Pored toga, ^1H i ^{13}C NMR spektroskopski podaci za 1,4-bdta-Cd(II) kompleks su poređeni sa odgovarajućim NMR podacima za nekoordinovan H_4 -1,4-bdta ligand.



1,4-bdta

Synthesis and characterization of the cadmium(II) complex with 1,4-butanediamine-*N,N,N',N'*-tetraacetate ligand

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In the reaction between $\text{Ba}[\text{Ba}(1,4\text{-bdta})] \cdot 2\text{H}_2\text{O}$ and $\text{CdSO}_4 \cdot 7\text{H}_2\text{O}$ in 1:1 molar ratio, new 1,4-bdta-Cd(II) complex (1,4-bdta = 1,4-butanediamine-*N,N,N',N'*-tetraacetate) was synthesized and characterized by IR and NMR (^1H and ^{13}C) spectroscopy. The IR spectroscopic data of this complex were compared with those for the corresponding Co(II) complex with 1,4-bdta and 1,3-pdta ligands (1,3-pdta = 1,3-propanediamine-*N,N,N',N'*-tetraacetate).^{1,2} Furthermore, ^1H and ^{13}C NMR spectroscopic data for 1,4-bdta-Cd(II) complex were compared with those for the uncoordinated H_4 -1,4-bdta ligand.

Acknowledgements: This work was funded in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172036).

1. D.D. Radanović, U. Rychlewska, B. Warzajtis, M.S. Cvijović, M.Dj. Dimitrijević, M. I. Djuran, *Polyhedron* **29** (2007) 4799.
2. D.D. Radanović, U. Rychlewska, M. I. Djuran, N. S. Drašković, M.M. Vasojević, I.M. Hodžić, D.J. Radanović, *Polyhedron* **22** (2003) 2745.



Adsorpcija bakarnih jona na modifikovanom i nemodifikovanom zeolitu 5A

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Joni mnogih metala, kao i nemetala, često su prisutni u zagađenim prirodnim vodama. Bakarni joni su, takođe, jedni od tih toksičnih metala, koji se u vodenoj sredini mogu naći u tri osnovna oblika: suspendovanom, koloidnom i rastvornom. Kako adsorpcija predstavlja jedan od postupaka prečišćavanja otpadnih voda, ova studija je pokušaj u pronalaženja ekonomičnijeg, a boljeg adsorbensa za prečišćavanje vode zagađene jonima bakra. Kao adsorbens korišten je sintetički zeolit 5A, te njegove kiselinsko i bazno aktivirane forme. Polazni uzorak 5A je kiselinski tretiran sa 20% - tnim rastvorom H_2SO_4 . Bazna aktivacija je češći način poboljšanja kvaliteta zeolita, a u ovoj studiji polazni uzorak je tretiran sa 20 % - tnim rastvorom Na_2CO_3 . Ispitivanje adsorpcionog ponašanja polaznog, kiselinski i bazno aktiviranog uzorka zeolita 5A u kontaktu sa Cu (II) sulfat penta hidratom vršeno je u laboratorijskim uslovima. Adsorpcija $CuSO_4 \cdot 5H_2O$ na polaznim i modifikovanim uzorcima 5A, praćena je spektrofotometrijski. Praćenjem adsorpcije, zaključeno je da je adsorpcija fizička i višeslojna. Ispitivana je prema Freundlichovoj adsorpcionoj izotermi.

Adsorption of copper ions on modified and unmodified 5A zeolite

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Ions of many metals, as well as of nonmetals, are often present in polluted natural waters. Copper ions are also some of those toxic metals, which may be found in water environment in three basic forms: suspended, colloidal and solution one. Since adsorption represents one of the procedures for purification of waste waters, this study is an attempt to find a more economical and, at the same time, better adsorbent for purification of water polluted with copper ions. The adsorbent used is synthetic 5A zeolite and its acid and base activated forms. The original sample 5A has been acid treated with 20% H_2SO_4 solution. Base activation is a more frequent manner of improving quality of zeolite, and in this study the original sample has been treated with 20% Na_2CO_3 solution. Examination of adsorption behavior of the original, acid and base activated 5A zeolite sample, in contact with Cu (II) sulfate pentahydrate, has been conducted in laboratory conditions. Adsorption of $CuSO_4 \cdot 5H_2O$ on original and modified 5A samples has been observed spectrophotometrically. By observing adsorption, it has been concluded that adsorption is physical and multilayer. It has been examined according to Freundlich adsorption isotherm.

Oksido-redukциони procesi u SW-480 kancerogenim ćelijama u prisustvu rutenijuma(II) kompleksa

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Kompleksi rutenijuma su interesantna jedinjenja koja imaju različitu primenu u hemiji, industriji i medicini. Jedna od najvažnijih njihovih osobina je antioksidativna aktivnost i citotoksičnost. Efekat dva kompleksa Ru(II), opšte formule $TF.2H[RuCl_3(DMSO)_3]$ (**1**) i $TF.2H[RuCl_3(\eta^6\text{-p-cymen})]$ (**2**) ($TF.2H$ je protonovani trifluoperazin), u dve različite koncentracije (5 i 15 μM) ispitan je na oksido-redukcione procese u SW-480 kancerogenim ćelijama (sadržaj sulfhidrilnih (SH) i karbonilnih (CO) grupa proteina, sadržaj nitrita, aktivnost superoksidne-dismutaze (SOD), katalaze (CAT) i laktat-dehidrogenaze (LDH)). Primenom kompleksa zabeležena je povećana aktivnost SOD, a smanjena aktivnost CAT, dok kompleks **1** inhibira 45% aktivnosti CAT. Kompleksi indukuju produkciju reaktivnih azotovih vrsta preko sadržaja nitrita, a veća koncentracija kompleksa **2** izaziva veću produkciju nitrita. Slobodne SH grupe proteina su oksidovane 74% nižom koncentracijom kompleksa **1**, dok je primenom kompleksa **2** utvrđeno veće oštećenje proteina praćenjem sadržaja CO grupa. Inhibicija aktivnosti LDH primenom Ru kompleksa u SW 480 ćelijama rezultat je povećanja reaktivnih kiseoničnih i azotovih vrsta i oksidativnog stresa, što dovodi do nekroze odnosno kasnije ćelijske smrti.

Oxidation-reduction processes in SW-480 cancer cells in the presence of ruthenium(II) complexes

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Ruthenium complexes are very interesting compounds with multiple different applications in fields of chemistry, as well as in industry and medicine. Today, the most attractive biological properties are their antioxidant activity and cytotoxicity. The effects of two Ru(II) complexes of the general formulae, $TF.2H[RuCl_3(DMSO)_3]$ (**1**) and $TF.2H[RuCl_3(\eta^6\text{-p-cymen})]$ (**2**) ($TF.2H$ is protonated trifluoperazine), applied in two different concentrations (5 and 15 μM) are investigated on the oxidation-reduction processes in SW-480 cancer cells (sulfhydryl (SH) and carbonyl (CO) group of proteins, nitrite content, superoxide dismutase (SOD), catalase (CAT) and lactate-dehydrogenase (LDH) activity). The highest value of SOD and the lowest value of CAT activity is observed using the complexes, while complex **1** inhibited 45% of the CAT. The complexes induced the production reactive nitrogen species *via* nitrite content, while complex **2** showed greater production application in higher concentration. The free SH groups of proteins are oxidized 74% of a lower concentration of complex **1**, while complex **2** shows high damage on CO groups of proteins. Inhibition of LDH activity by Ru complexes in SW 480 cells resulted in an increase of reactive oxygen and nitrogen species and oxidative stress, leading to increased necrosis or late cell death.

NH P04

**Zlato(III) kompleks sa (O,O')-dietil estrom (S,S)-etilendiamin-
N,N'-2-(4-metil)pentanske kiseline: Sinteza i karakterizacija**

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Zlato(III) kompleksi sa *N,N'* bidentatnim ligandima su već pokazali značajnu *in vitro* antiproliferativnu aktivnost [1,2]. Novi zlato(III) kompleks sa (O,O')-dietil estrom (S,S)-etilendiamin-*N,N'*-2-(4-metil)pentanske kiseline, $[\text{AuCl}_2\{(\text{S,S})\text{-Et}_2\text{eddl}\}]\text{PF}_6$, je sintetisan i okarakterisan elementalnom analizom, IC, ^1H i ^{13}C NMR spektroskopijom i masenom spektrometrijom. Rezultati elementalne analize odgovaraju pretpostavljenoj stehiometrijskoj formuli. IC spektar pokazuje karakteristične apsorpcione trake: $\nu(\text{C}=\text{O})$ na 1736, $\nu(\text{C}-\text{O})$ na 1241 i $\nu(\text{N}-\text{C})$ na 863 cm^{-1} . U ^1H NMR spektru, vodonikovi atomi koji pripadaju sekundarnoj amino grupi se nalaze na 4,6 ppm, dok etilenski protoni iz etilendiaminskog dela molekula na 3,75 ppm, što ukazuje na koordinaciju azotovih atoma. U ^{13}C NMR spektru karbonilni ugljenikovi atomi se nalaze na očekivanoj vrednosti hemijskog pomeranja za ovu klasu jedinjenja kod kojih kiseonik ne učestvuje u koordinaciji (169 ppm).

**Gold(III) complex with (O,O')-diethyl ester of ethylenediamine-
N,N'-2-(4-methyl)pentanoic acid: Synthesis and characterization**

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Gold(III) complexes with *N,N'* bidentate ligands have already shown significant *in vitro* antiproliferative activity [1,2]. A novel gold(III) complex with (O,O')-diethyl ester of ethylenediamine-*N,N'*-2-(4-methyl)pentanoic acid, $[\text{AuCl}_2\{(\text{S,S})\text{-Et}_2\text{eddl}\}]\text{PF}_6$, was synthesized and characterized by elemental analysis, IR, ^1H and ^{13}C NMR spectroscopy and mass spectrometry. Results of elemental analysis are in agreement with proposed stoichiometric formula. IR spectrum shows specific absorption bands: $\nu(\text{C}=\text{O})$ at 1736, $\nu(\text{C}-\text{O})$ at 1241 and $\nu(\text{N}-\text{C})$ at 863 cm^{-1} . In ^1H NMR spectrum, hydrogen atoms belonging to secondary amino groups appeared at 4.6 ppm, while protons from ethylenediamine moiety are found at 3.75 ppm, indicating nitrogen coordination. In ^{13}C NMR spectrum, carbonyl atoms show resonances at expected chemical shifts for this class of compounds where oxygen is not participating in coordination (169 ppm).

1. N. Pantelić, T. Stanojković, B. B. Zmejkovski, T. J. Sabo, G. N. Kaluđerović, *Eur. J. Med. Chem.* **90** (2015) 766.
2. N. Pantelić, B. B. Zmejkovski, J. Trifunović-Macedoljan, A. Savić, D. Stanković, A. Damjanović, Z. Juranić, G. N. Kaluđerović, T. J. Sabo, *J. Inorg. Biochem.* **128** (2013) 146.

Hemija životne sredine / Environmental Chemistry

HŽS 01

**Meat processing industry wastewater – screening analysis**

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Wastewater from meat processing industries is a complex mixture of different compounds with a high load of organic matter. The meat processing industry wastewater represents a serious threat to the river ecosystem, which has to be continuously monitored. The main problem with this type of wastewater in Serbia is lack of treatment and direct discharge into sewer and natural recipient. Very often, none of the analysed samples meet the legal set of physicochemical and microbiological criteria. Since meat industry produces large amounts of wastewater, it would be of great significance if the treated wastewater could be reused for various agricultural activities. The newly recognised pollutant emerging substances (EmS) occur at very low concentration levels (ppb, ppt and lower) and are not included in the routine monitoring programs at EU level. The aim of this study was to perform a screening analysis of 8 wastewater samples taken from the discharges near meat processing industries and abattoir facilities, obtained in 3 different sampling campaigns, during the period of 2012-2014. During screening analysis, 1133 compounds were detected, and 314 identified with high certainty. The results of screening analysis for 3 samples will be presented in this paper. The three selected samples represent the wastewater before and after treatment.

Otpande vode iz mesne industrije – skrining analiza

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Otpadna voda mesne industrije je kompleksna mešavina jedinjenja sa visokim sadržajem organske materije. Otpadna voda mesne industrije predstavlja ozbiljnu pretnju za ekosistem, koji mora da se kontinuirano prati. Glavni problem ove vrste otpadnih voda u Srbiji je nedostatak njihovog tretmana i direktno ispuštanje u kanalizaciju ili prirodni recipient. Vrlo često, analizirani uzorci ne ispunjavaju zakonski minimum fizičko-hemijski i mikrobioloških graničnih vrednosti. Pošto mesna industrija proizvodi velike količine otpadnih voda, bilo bi od velikog značaja ako se može ponovo koristiti u različite svrhe u poljoprivrednim aktivnostima. Emergentne supstance (EMS), koje se učestalo koriste u različitim antropogenim sferama (od industrije i privrede do proizvoda koji se koriste u domovima) se u prirodi nalaze u vrlo niskim koncentracijama (ppb, ppt i niže) i nisu uključene u rutinskim programima za monitoring ni nivou EU. Cilj istraživanja je da se izvrši skrining analiza 8 uzoraka otpadne vode mesa industrije i klanica, koji su dobijeni u 3 različite kampanje uzorkovanja, u periodu od 2012. do 2014. Tokom semi-kvantitativne skrining analize otkriveno je 1133 jedinjenja, a 314 jedinjenja je identifikovano sa visokom sigurnošću. Rezultati skrining analize za 3 uzoraka će biti prikazani u ovom radu. Tri odabrana uzorka predstavljaju uzorke pre i posle tretiranja otpadne vode.

HŽS P01

Linearno modelovanje podeonog koeficijenta vazduh-voda ($\log K_{AW}$) Senzor boje sa optičkim vlaknima za praćenje kvaliteta površinskih voda

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Potreba za uređajima i opremom sa poboljšanim performansama za monitoring različitih vodnih tela je omogućila intenzivni razvoj senzora sa optičkim vlaknima koji se upotrebljavaju za različite medijume u životnoj sredini. Senzori boje sa optičkim vlaknima (SOV) predstavljaju novu i inovativnu tehnologiju za monitoring kvaliteta površinskih voda. SOV na osnovu HSV modela boja (H- nijansa, S-zasićenost, V-vrednost) i intenziteta boje uzorka određuje koncentraciju i talasne dužine posmatranih parametara u ispitivanom vodnom telu. Hemijski parametri posmatrani sa SOV su: ortofosfati, sulfati, nitriti, hrom (VI) i ukupni hlor. Sprovedena je komparacija rezultata dobijenih sa SOV i standardnom laboratorijskom opremom (UV-vis spektrofotometra) da bi se dokazala efikasnost i primenljivost nove metode. Odstupanje upoređenih rezultata su manje od 5%, čime se dokazala mogućnost upotrebe SOV u laboratoriji kao zamena za skupu standardnu opremu.

The color sensor with optical fiber for monitoring surface water quality

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The need for devices and equipment with improved performance for the monitoring of different water bodies has enabled intensive development of sensors with optical fibers that are used for different media in the environment. Fiber optic colour sensor (FOCS) is a new and innovative technology for monitoring the quality of surface water. FOCS based on the HSV color model (H- hue, saturation, S, V-value) and the color intensity of the sample determines the concentration and wavelength parameters observed in the examined water body. Chemical parameters observed with the FOCS are: orthophosphates, sulfates, nitrates, chromium (VI) and total chlorine. Results obtained with the FOCS were compared with standard laboratory equipment (UV-vis spectrophotometer) to demonstrate the effectiveness and applicability of new methods. Deviations of obtained results are less than 5%, which demonstrated the ability to use the FOCS in laboratory as a substitute for expensive standard equipment.

Uticaj organskih i neorganskih jedinjenja na fotokatalitičku degradaciju nicosulfurona u vodenoj suspenziji TiO₂

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Problem zagađenja vode pesticidima je stalno prisutan zahvaljujući njihovoj postojanosti u zemljištu, visokoj rastvorljivosti u vodi i fotohemijskoj stabilnosti.

Nicosulfuron se razlikuje od ostalih pesticida zbog svoje selektivnosti, minimalne doze primene i povoljnih ekoloških svojstava.

Fotokatalitička degradacija nicosulfurona, sulfonilurea herbicida, proučavana je u prisustvu TiO₂ Degussa P25 kao fotokatalizatora i pri UV osvetljenju. Ispitivan je uticaj različitih vrsta soli (NaF, NaCl, NaNO₃, NaHCO₃, Na₂SO₄, CaSO₄, Al₂(SO₄)₃), a posebno uticaj katjona (Na⁺, Ca²⁺, Al³⁺) i anjona (F⁻, Cl⁻, NO₃⁻, HCO₃⁻, SO₄²⁻). Takođe, je ispitivan i uticaj H₂O₂. Uticaj organskih jedinjenja na brzinu degradacije nicosulfurona u vodenoj suspenziji TiO₂ ispitivan korišćenjem acetona i 2-propanola. Brzina razgradnje praćena je HPLC metodom.

The effect of organic and inorganic compounds on the photocatalytic degradation of sulfonylurea herbicide nicosulfuron in TiO₂ aqueous solution

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Pollution of water by pesticides is a subject of environmental concern due to their persistence in soil, high water solubility and photochemical stability.

Among other pesticides, nicosulfurons have gained attention due to their good crop selectivity, low application rates and favorable environmental properties.

The photocatalytic degradation of nicosulfuron, a sulfonylurea herbicide, has been studied in the presence of TiO₂ Degussa P25 as photocatalyst under UV irradiation.

The influence of inorganic salts was investigated (NaF, NaCl, NaNO₃, NaHCO₃, Na₂SO₄, CaSO₄, Al₂(SO₄)₃). Effect of cations (Na⁺, Ca²⁺, Al³⁺) and anions (F⁻, Cl⁻, NO₃⁻, HCO₃⁻, SO₄²⁻) on the degradation rate of nicosulfuron in water suspension with TiO₂ was established. Also, the effect of H₂O₂, acetone and 2-propanol was investigated. The rate of photodecomposition was monitored using HPLC measurements.

HŽS P03

Fungicidne aktivnosti Ni(II) i Cu(II)-dtc kompleksa na fitopatogenu gljivu *Phomopsis viticola*

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Ditiokarbamati (dtc) pokazuju različite biološke efekte uključujući antibakterijsku aktivnost, antifungalnu aktivnost i antioksidantnu aktivnost. Kompleksi $\text{Ni}(\text{H}_2\text{idadc})_2$ i $\text{Cu}(\text{H}_2\text{idadc})_2$ kao i sami ligand, $(\text{NH}_4)_3\text{idadc}$, su sintetisani po ranije objavljenim procedurama. Sinteza kompleksa je vršena sa ciljem ispitivanja njihovih fungicidnih aktivnosti na fitopatogenu gljivu *Phomopsis viticola* (Sacc.) Sacc. uzročnika crne pjegavosti vinove loze, čestog oboljenja u crnogorskim vinogradima. Vršeno je upoređivanje inhibicionog efekta sintetisanih kompleksa na rast micelije *Ph. viticola* sa inhibitorni efektom komercijalnog fungicida na bazi mankozeba, koji je najefikasniji dtc fungicid prema *Ph. viticola*. Rezultati su statistički obrađeni analizom varijanse i testirani pomoću LSD testa (test najmanje značajne razlike); sintetisani kompleksi su pokazali određeni fitotoksični efekat, naročito Cu(II)-dtc kompleks, ali značajno manji efekat u odnosu na mankozeb.

Fungicidal activity of the Ni(II) and Cu(II)-dtc complexes on phytopathogenic fungus *Phomopsis viticola*

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Dithiocarbamates (dtc) show the different biological effects, including antibacterial activity, antifungal activity and antioxidant activity. $\text{Ni}(\text{H}_2\text{idadc})_2$ and $\text{Cu}(\text{H}_2\text{idadc})_2$ complexes, as well as $(\text{NH}_4)_3\text{idadc}$ ligand were synthesized according to previously published procedures. Synthesis of the complexes is carried out with the aim of researching their fungicidal activities on the phytopathogenic fungus *Phomopsis viticola* (Sacc.) Sacc. *Ph. viticola* causes Phomopsis cane and leaf spot of grapevine, a common disease in the Montenegrin vineyards. We compared the inhibition effects of synthesized complexes on the growth of mycelium *Ph. viticola* with the inhibitory effect of commercial fungicide based on mancozeb, which is the most effective dtc fungicide on the *Ph. viticola*. The results were statistically analyzed by variance analysis and tested using LSD test (least squares difference) test; the synthesized complexes showed a certain phytotoxic effect, especially DTC complex with Cu(II) as metal ion, but significantly less than mancozeb fungicide.



Proučavanje adsorpcije pertehnetata iz vodenog rastvora primenom površinski modifikovanog klinoptilolita

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Prirodni zeolit klinoptilolit, modifikovan dugolančanim organskim stearyl-dimetil benzil amonijum- hlorid (SDBAC) jonom, korišćen je kao adsorbens za uklanjanje pertehnetata (TcO_4^-) iz vodenih sistema. Ispitivanja su urađena u šaržnom sistemu, praćenjem uticaja različitih parametara (količina organskog katjona, vreme kontakta, pH vrednost polaznog rastvora) na efikasnost uklanjanja TcO_4^- iz vode. Rezultati su pokazali da je prirodni klinoptilolit neefikasan za uklanjanje TcO_4^- ($E < 20\%$). Klinoptilolit, modifikovan SDBAC katjonom, pokazao je mnogo veću efikasnost za uklanjanje TcO_4^- u odnosu na prirodni, nemodifikovani klinoptilolit. Potvrđeno je da pokrivenost površine zeolita organskim katjonom ima važnu ulogu u poboljšanju efikasnosti uklanjanja TcO_4^- , zahvaljujući formiranju dvosloja SDBAC katjona. Klinoptilolit, na čijoj površini je formiran organski dvosloj, uspešno je primenjen za uklanjanje TcO_4^- iz vode u opsegu pH vrednosti 5.0-8.0 ($E > 98\%$). Ravnoteža je uspostavljena nakon kontakta faza u trajanju od 15 minuta. Dobijeni rezultati pokazuju da klinoptilolit, modifikovan dvoslojem SDBAC katjona, ima potencijal da prečišćava otpadne vode od ekološkog zagađivača pertehnetata.

Study of pertechnetate adsorption from aqueous solution by surfactant-modified clinoptilolite

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Natural clinoptilolite, modified with a stearyl-dimethylbenzylammonium chloride, SDBAC, was used as an adsorbent for the removal of pertechnetate (TcO_4^-) from aqueous solutions. Adsorption studies were performed in a batch system, and the effects of various experimental parameters, such as the amount of surfactant loading, contact time and pH solution, on the removal efficiency of TcO_4^- were investigated. The obtained results showed that natural clinoptilolite was inefficient for the removal of TcO_4^- from aqueous solution ($E < 20\%$). Surfactant-modified clinoptilolite showed much higher removal efficiency of TcO_4^- than natural, unmodified clinoptilolite. It was confirmed that the surface coverage of zeolite plays an important role in improving the efficiency of removing TcO_4^- . SDBAC-modified clinoptilolite with organo-bilayer was successfully applied for the removal of TcO_4^- from aqueous solutions in the pH range of 5.0-8.0 ($E > 98\%$). These results showed that surfactant-modified clinoptilolite with bilayer SDBAC coverage have potential to remove pertechnetate from contaminated groundwaters.

Esterifikacija stearinske kiseline sa alkoholima C1-C4

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Estri masnih kiselina sa nižim alkoholima se koriste kao biodizel goriva. Stearinska kiselina i njeni estri imaju i značajnu upotrebu u kozmetici. U ovom radu je ispitivan uticaj strukture alkohola na reakciju esterifikacije stearinske kiseline. Reakcije esterifikacije su vršene u nepolarnim rastvaračima na temperaturi ključanja rastvarača uz sumpornu kiselinu kao katalizator (1:0,5 w/w) i uz višak alkohola (1:10). Opadajući redosled alkohola u odnosu na količinu i vrijeme dostizanja maksimalnog prinosa estera je bio: 1-butanol > 2-metil-1-propanol > 1-propanol > etanol > 2-propanol > metanol > 2-butanol > 2-metil-2-propanol. Najmanja konverzija stearinske kiseline (15,75%) u estar je postignuta u reakciji sa *tert*-butanolom nakon 240 min trajanja procesa. Najveći sadržaj stearinske kiseline je preveden u estar sa 1-butanolom (99%) nakon 60 min. Sa primarnim alkoholima se postižu najveći prinosi pri čemu se brzina reakcije povećava sa povećanjem broja C-atoma. Sekundarni i tercijarni alkoholi i alkoholi sa razgranatim nizom, zbog sternih smetnji, reaguju sporije i daju manje prinose.

Esterification of stearic acid with C1-C4-alcohols

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Esters of fatty acids and lower alcohols are used as biodiesel fuel. Stearic acid and its esters have significant use in cosmetics. In this paper, we examined the impact of the alcohol structure to esterification reaction of stearic acid. Esterifications were carried out in non-polar solvents, at the boiling point of the solvent, with sulfuric acid as catalyst (1:0.5 w/w) and with an excess of alcohol (1:10). Decreasing order of the alcohol relative to the amount and the time to reach a maximum yield of the ester was: 1-butanol > 2-methyl-1-propanol > 1-propanol > ethanol > 2-propanol > methanol > 2-butanol > 2-methyl-2-propanol. The minimum conversion of stearic acid (15.75%) of the ester is achieved by reaction with *tert*-butanol - 240 min after the length of the reaction. The highest content of stearic acid was converted to ester with 1-butanol (99%) after 60 min. The highest yields were achieved with a primary alcohols and the rate of reaction increases with increasing number of C-atoms. Secondary and tertiary alcohols and alcohols with branched chain, react more slowly and give lower yields, due to steric hindrance.

Teorijska hemija / Theoretical Chemistry

TH 01

**Priroda Au-N veze i aromatičnost N-heterocikličnih liganada koordinovanih za zlato(III) jon**

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U ovom radu ispitivana je priroda Au-N veze u kompleksima zlata(III) sa aromatičnim heterocikličnim ligandima koji sadrže jedan atom azota u prstenu. Analiza Au-N veze u ispitivanim kompleksima vršena je pomoću B3LYP/cc-pVTZ+LanL2TZ(f) teorijskog modela u kombinaciji sa NBO i AIM metodama. Za ispitivanje aromatičnosti korišćeni su sledeći kriterijumi: elektronski (multicentrični delokalizacioni indeks, MCI i elektronska gustina, ρ), geometrijski (HOMA indeks) i magnetni kriterijum (NICS indeksi). Dobijene vrednosti za pomenute indekse ukazuju da prisustvo zlato(III) jona smanjuje aromatičnost prstena koji se preko atoma azota koordinuje za zlato(III) jon.

The nature of Au-N bond and aromaticity of N-heterocycles coordinated to Au(III) ion

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In this work, the nature of Au-N bond and aromaticity of different N-containing heterocycles coordinated to Au(III) ion have been studied. The nature of Au-N bond in the gold(III) complexes was investigated by means of the B3LYP/cc-pVTZ+LanL2TZ(f) method in combination with NBO and AIM approaches. The local aromatic distribution in the investigated systems was quantified through the following indices: the multicenter delocalization index (MCI), electron density at ring critical points (ρ), harmonic oscillator model of aromaticity (HOMA) index and nucleus-independent chemical shifts (NICS). It was found that the aromatic character of the nitrogen-containing ring in gold(III) complexes is decreased in comparison with the same ring of uncoordinated ligands.

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Biohemija / Biochemistry

BH S

Razotkrivanje alergena Proteomikom: struktura, funkcija i epitopi

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Proteomika je napravila „veliki prasak“ u mnogom istraživanjima pomažući u razotkrivanju „duše“ proteina. Alergija predstavlja ozbiljnu bolest modernog doba sa povećanom učestalošću. Glavni fokus u molekularnoj alergologiji, zarad poboljšanja dijagnoze i razvoja terapije, su alergeni (proteini, hapteni, itd.), koji suprezentovani humanom imunom sistemu u formi epitopa. Ovde proteomika predstavlja moćan alat zbog nedostatka kvalitativnih i kvantitativnih izvrsnosti u analizi alergena i tako su se otvorila nova polja proteomike kao npr: alergenomika, foodomika, digestomika, itd. Postoje nekoliko pristupa proteomike koji se koriste u molekularnoj alergologiji. Komparativna dvodimenzionalna elektroforeza i maseno spektrometrijski pristup povezan sa imunoblot tehnikom može da se koristi kod identifikacije novih alergena, izoformi alergena i karakterizaciji posttranslacionih modifikacija. Sa druge strane „shotgun“ podrazumeva „bottom-up“ pristup u proteomici koji se može koristiti u identifikovanju alergena u kompleksnim smešama, ili pak otkrivanju modifikovanih epitopa. Ovo je jedan od najboljih pristupa za kvantifikaciju alergena. „Top-down“ proteomika u molekularnoj alergologiji pak pomaže pri detaljnoj karakterizaciji alergena i razotkrivanju funkcije njegovih epitopa. Nedavno, računarska proteomika – molekularno modelovanje i dinamiku proteina zajedno sa proteomikom vodi do boljeg razumevanja glavnih uzročnika alergije. Ova dostignuća vode do razvoja novih formi imunoterapija koje imaju benefit za pacijente.

*Zahvalnica: Ministarstvo Prosvete Nauke i Tehnološkog Razvoja, projekat 172024***Revealing the allergens by Proteomics: structure, function and epitopes**

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Proteomics made a “big bang” in many research fields helping for revealing “the soul” of proteins. Allergy represent the severe and common disease of modern era with increases in prevalence. The major focus in molecular allergology for improvement of allergy diagnosis and therapy are allergens (proteins, haptens, etc.), presented to human immune system in form of epitopes. Here the proteomics represent a powerful tool due to its proven excellent quantitative and qualitative drawbacks in allergen analysis which opened new fields in proteomics for example: allergenomics, foodomics, digestomics, etc. There are several proteomics approaches used in molecular allergology. Comparative two dimensional electrophoresis and mass spectrometry approach coupled with immunoblotting can be used for identification of new allergens, allergen isoforms and characterisation of posttranslational modifications. On the other hand, shotgun refers to use bottom-up proteomics identifying the allergen in complex mixture, or revealing the modified epitopes. This is one of the best approaches for quantification of allergens. The top-down proteomics in molecular allergology is useful for deep structure characterisation of allergen and revealing the function of its epitopes. Recently, computational proteomics – molecular modelling and dynamics of proteins together with proteomics lead to better understanding of major allergy causatives. These findings lead for development of novel forms of immunotherapies for benefits of patients.

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Sub-polenske čestice kao potencijalno najopasniji alergenski nosioci na osnovu poređenja proteoma različitih polenskih frakcija ambrozije (*Ambrosia artemisiifolia* L.)

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Sub-polenske čestice izazivaju teže i ozbiljnije simptome astme nego celo polenovo zrno. Sem njihove manje veličine, dodatni razlozi tome rasvetljeni su poređenjem proteoma različitih frakcija polena ambrozije: celog, sub-polenskog i vodenog ekstrakta celog zrna pomoću visko razdvajajuće 2D-elektroforeze, kvantitativne „shotgun“ proteomike i gel-podržane proteomike. Sub-polenska frakcija sadrži najviše različitih izoformi konzervativnih alergenskih grupa polena ambrozije. Takođe ona poseduje jedinstvene proteine sa važnom ulogom u alergiji kao što je NADH dehidrogenaza i najviši udeo alergoma u proteomu, sa vodećim količinama Amb a 4 (sporedni alergen) i Amb a 1 (glavni alergen) u poređenju sa drugim polenskim frakcijama ambrozije.

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Proteomic comparison reveals sub-pollen particles as potentially the most dangerous allergenic carriers among different pollen fractions of short ragweed (*Ambrosia artemisiifolia* L.)

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Sub-pollen particles are causing more severe asthma symptoms than the whole pollen grains. Beside its smaller size, more light was shed on other reasons for more severe asthma symptoms induced by *Ambrosia artemisiifolia* sub-pollen particles (SPP) than its whole pollen grains by comparing 3 different fractions of the short ragweed pollen: total, SPP and water-extractable, with high resolution 2D-PAGE, quantitative shotgun and gel based-proteomics. SPP fraction contains the most diversified Amb a major and minor conservative allergen groups. In addition, SPP possesses unique protein with important role in allergy such as NADH dehydrogenase and the highest total abundance of potential allergome, leading in Amb a 4 (minor allergen) and Amb a 1 (major allergen) quantities compared to other two pollen fractions.

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Racionalni dizajn novih inhibitora MAO B kao terapeutika u lečenju Parkinsonove bolesti baziran na 3-D QSAR studijama

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Disfunkcija monoamino oksidaze B (MAO B) indukuje oksidativni stres u mitohondrijalnoj DNK što dovodi do razvoja Parkinsonove bolesti. Koristeći 3-D QSAutogrid/R procedure razvijen je 3-D QSAR model ($q^2_{\text{LOO}} = 0.576$; $q^2_{\text{K5FCV}} = 0.497$, PC=3), pomoću 23 ko-kristalizovanih MAO B inhibitora i amidnog azota kao probe. Dobijeni PLS-koeficijenti i polja doprinosa aktivnosti svakog od inhibitora sumirani su u univerzalni SAR model pomoću koga je optimizovana struktura najaktivnijeg kumarinskog inhibitora (PDB ID: 2V61) uvođenjem izobutiramida na poziciji C3 kumarinskog jezgra da bi se aktivirao Gln206, zatim grupa koje sadrže akceptor vodonične veze i hidrofobni ostatak na poziciji C4 da intereaguje sa Tyr435 i akceptora vodonične veze na C5 u blizini Cys172. Model je predvideo aktivnost 267 kumarina iz literature, nakon čega je pomoću virtuelnog skeniranja izvršen dizajn 12 novih potencijalnih farmaceutika za lečenje Parkinsonove bolesti.

Rad podržava Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije (Projekat III43004).

The 3-D QSAR studies based rational design of novel MAO B inhibitors as therapeutics in Parkinson's disease treatment

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Monoamine oxidase B (MAO B) malfunction induces oxidative damage to mitochondrial DNA and mediates the development of Parkinson's disease. Applying the 3-D QSAutogrid/R protocol, structure-based (SB) N probe anti MAO B 3-D QSAR model ($q^2_{\text{LOO}} = 0.576$; $q^2_{\text{K5FCV}} = 0.497$, PC=3) was generated using 23 co-crystalized inhibitors to derive PLS-coefficients and Actual Activity Contribution Fields, summarized in universal SAR model. Accordingly, the structure of highest active coumarin-based inhibitor (PDB ID: 2V61) was optimized introducing the isobytiramide at position C3 of coumarin core to activate Gln206, hydrogen-bond accepting/hydrophobic groups at C4 to mimic Tyr435, and hydrogen-bond accepting group at C5 towards Cys172. The model was structure-based (SB) or ligand-based (LB) validated by the activity prediction of 267 coumarin compounds from literature, after which 12 novel potential anti-Parkinson's pharmaceuticals were designed, utilizing the virtual screening (VS) protocol.

Ministry of Education, Science and Technological Development, Government of Republic of Serbia (Grant No. III43004) supports this work.

Određivanje strukture hromopeptida dobijenih pepsinskom digestijom C-fikocijanina iz mikroalge *Arthrospira platensis*

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Plavi C-fikocijanin (C-PC), glavni protein mikoalge *Arthrospira platensis*, poseduje značajnu antioksidativnu, antikancersku, anti-inflamatornu i imunomodulatornu aktivnost, koje se pre svega pripisuju fikocijanobilinu (PCB), kovalentno (tioetarskom vezom) vezanoj tetrapirolnoj hromofori. Jedan PCB molekul je vezan za α -subjedinicu preko Cys84, dok β -subjedinica vezuje dva molekula PCB-a preko Cys82 i Cys153. Oralno unet C-PC je podložan proteolizi, pri čemu se mogu dobiti biološki aktivni hromopeptidi (peptidi sa kovalentno vezanom hromoforom). Cilj ove studije je bio da se strukturno okarakterišu fiziološki relevantni hromopeptidi dobijeni nakon pepsinske digestije C-PC-a. SDS-PAGE je pokazala da se C-PC brzo digestuje pepsinom u simuliranoj želudačnoj tečnosti. Pet dominantnih frakcija je izolovano uz pomoć reverzno-fazne HPLC. Manuelni *de novo* pristup, u visoko rezolutivnoj tandemskoj masenoj spektrometriji, upotrebljen je u cilju određivanja strukture izolovanih hromopeptida. Sekvence hromopeptida su određene iz MS spektara, dok su za potvrđivanje sekvenci iskorišćeni MS2 i MS3 spektri roditeljskih jona, kao i MS i MS2 spektri čistog PCB-a. Šest hromopeptida je identifikovano, veličine 2-13 aminokiselinskih ostatka. Opisan pristup može biti od koristi za određivanje strukture hromopeptida i kovalentnih adukata proteina i tetrapirolnih hromofora.

Structure determination of chromopeptides obtained by pepsin digestion of C-phycoyanin from microalga *Arthrospira platensis*

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Blue C-phycoyanin (C-PC), the major protein of microalga *Spirulina*, possesses significant antioxidant, anticancer, antiinflammatory and immunomodulatory effects, mostly ascribed to the covalently bonded (*via* tioether bond) linear tetrapyrrole chromophore phycocyanobilin (PCB). One PCB molecule is attached to α -subunit *via* Cys84, while β -subunit binds two molecules of PCB *via* Cys82 and Cys153. Orally administrated C-PC is susceptible to proteolysis, wherein biologically active chromopeptides could be obtained. The aim of this study was the structural characterization of physiologically relevant chromopeptides obtained after the pepsin digestion of C-PC. SDS-PAGE revealed that C-phycoyanin is rapidly digested by pepsin in simulated gastric fluid. Five dominant chromopeptide fractions were isolated from pepsin digest by reversed phase HPLC. Manual *de novo* high resolution tandem mass spectrometry approach was applied to the determine structure of the isolated chromopeptides. Chromopeptide sequences were resolved from MS spectra. Confirmation of sequences was done by the analysis of MS2 and MS3 spectra of parent ions, and MS and MS2 spectra of the pure PCB. Six chromopeptides were identified, varying in size from 2 to 13 amino acid residues. The approach described here can be used for the identification of the structure of both chromopeptides and protein-tetrapyrrole covalent adducts.

Veživanje slobodnih masnih kiselina i bakar(II)-jona za HSA dovodi do promena u karbonilaciji i reaktivnosti Cys34 tiolne grupe sa metilglioksalom

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Ljudski serumski albumin (Human serum albumin, HSA) predstavlja glavni antioksidant plazme zahvaljujući redukovanom Cys34. Veživanje masnih kiselina (FAs) za HSA može dovesti do promene u dostupnosti i reaktivnosti Cys34 tiolne grupe, njenog kapaciteta kao hvatača/antioksidanta. Cilj ovog rada je bio da se ispita efekat izabranih FAs (stearinska, miristinska, oleinska, ekstrakt ribljev ulja-FO i smeša-MixFAs) na veživanje Cu(II) jona za HSA, kao i sinergistički uticaj na reaktivnost HSA-SH i modifikaciju HSA metilglioksalom (MG). Veživanje FAs povećava reaktivnost HSA-Cys34-SH, k' vrednost (konstanta brzine pseudo prvog reda reakcije tiola sa Elmanovim reagensom) je bila povećana u nizu: MixFAs, oleinska, stearinska, FO i miristinska. Veživanje Cu(II) jona (0,1 mol/mol HSA) dovelo je do povećanja k' vrednosti ako je bio prisutan FO, ali je bila smanjena kada su ostale FAs bile prisutne. Sadržaj slobodne HSA Cys34-SH je bio smanjen za 10% posle veživanja Cu(II) jona, a dalje tokom inkubacije 24 h na 37 °C, bio je dodatno smanjen za 10% (stearinska, MixFAs) i 20% (miristinska, FO, oleinska). Karbonilovanje FA-HSA-Cu(II) kompleksa sa MG (20 mol/mol HSA) u toku 24 h, dovelo je do smanjenja sadržaja Cys34-SH 30-40% zavisno od prisutne FA. Karbonilovanje FA-HSA-Cu kompleksa može doprineti povećanju karbonilnog i oksidativnog stresa u dijabetesu i drugim bolestima.

Binding of FAs and Cu(II)-ions to HSA changes its carbonylation pattern and Cys34 thiol group reactivity with methylglyoxal

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Human serum albumin (HSA) represents a major plasma antioxidant due to its Cys34 reduced/sulfhydryl form. FAs binding to HSA could lead to changes of Cys34 thiol group accessibility and reactivity, i.e. its scavenger capacity/antioxidant properties. The aim of this work was to investigate the effects of selected FAs (stearic, myristic, oleic, fish oil extract-FO, FAs mixture-MixFAs), on Cu(II) ion binding to HSA, and the synergistic influence on the reactivity of HSA-SH and HSA modified with methylglyoxal (MG). Binding of FAs increased HSACys34-SH reactivity, k' values (pseudo first order rate constant for thiol reaction with Ellman's reagent) increased in the order: MixFAs, oleic, stearic, FO and myristic. Binding of Cu(II) (0.1 mol/mol HSA) led to an increase of k' value if FO was present, but for other bound FAs k' value decreased. The content of free HSACys34-SH decreased 10% after Cu(II) ion binding, and during 24 h incubation at 37 °C, it further decreased for another 10% (stearic acid, MixFAs) or 20% (myristic, FO, oleic). Carbonylation of FA-HSA-Cu(II) complexes with MG (20 mol/mol HSA) for 24 h, lead to a decrease in Cys34-SH content depending on FA present: 30-40%. Carbonylation of FA-HSA-Cu complexes could contribute to a further enhancement of the oxidative and carbonyl stress in diabetes, as well as other diseases.

BH 05

Efekat odabranih 17-supstituisanih androstanskih derivata na ćelije kancera

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Modifikovani steroidi najčešće ispoljavaju biološka i fiziološka svojstva različita u odnosu na prirodne, nemodifikovane steroide. Stoga se neka jedinjenja iz ove klase koriste za terapiju različitih steroidni hormon-zavisnih bolesti. U ovom radu je ispitivan antiproliferativni i pro-apoptotski potencijal 17α -pikolil i $17(E)$ -pikolinilidenskih derivata androstana, kao i uticaj ovih jedinjenja na ćelijski ciklus najsenzitivnijih ćelijskih linija. Svi modifikovani steroidi su značajno smanjili proliferaciju MCF-7 i HT-29 ćelija. Rezultati protočno-citometrijske analize su pokazali da neka od jedinjenja menjaju ćelijski ciklus tretiranih ćelija kancera. Neka od jedinjenja su indukovala apoptozu u izvesnoj meri, što se moglo kvantifikovati na osnovu morfoloških promena tretiranih ćelija. Dobijeni rezultati bi mogli da ukažu na nove pravce u sintezi potencijalno bioaktivnih modifikovanih steroida za terapiju kancera.

The effect of selected 17-substituted androstane derivatives on cancer cells

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Modified steroids usually exhibit biological and physiological properties different from the natural, unmodified steroids. Therefore, certain compounds of this class are used for the therapy of various steroid hormone-dependent diseases. In this study the antiproliferative and pro-apoptotic potential of 17α -picolyl and $17(E)$ -picolinylidene androstane derivatives were studied, as well as the effect of these compounds on the cell cycle of the most sensitive cell lines. All modified steroids significantly reduced the proliferation of MCF-7 and HT-29 cells. The results of flow-cytometric analysis revealed that some of the compounds altered the cell cycle of the treated cancer cells. Some of the compounds induced apoptosis to some extent, quantifiable on the basis of the morphological changes of the treated cells. The results could indicate new directions in the synthesis of potentially bioactive modified steroids in the treatment of cancer.

BH P01

Efekti Majlardove reakcije na imunogenost β -laktoglobulina

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Majlardova reakcija se odvija tokom obrade hrane i dolazi do formiranja naprednih glikacionih krajnjih produkata (Advanced Glycation Endproducts - AGE) proteina hrane. AGE imaju značajan uticaj na alergene hrane. Mi smo izveli Majlardovu reakciju između model alergena hrane, β -laktoglobulina (BLG), i glukoze. Glikovanje BLG-a ne utiče na sekundarnu strukturu proteina, ali smanjuje njegov transport kroz jednoslojne Caco-2 ćelije. Nezrele dendritične ćelije (Dendritic Cells - DCs) preuzimaju glikovani BLG u značajno većoj meri nego nativni BLG. Unutar endolizozomalnih odeljaka DCs glikovani BLG podleže bržoj degradaciji. $CD4^+$ T ćelije specifične na BLG pokazuju smanjenu produkciju citokina (IL-5, IL-13, $INF\gamma$) kada se uzgajaju zajedno sa DCs koje su prethodno preuzele glikovani BLG, u odnosu na nativni BLG. Naši rezultati ukazuju da Majlardova reakcija ima značajan uticaj na imunogenost BLG-a, jer menja njegovu gastrointestinalnu biodostupnost, interakcije sa ključnim ćelijama imunskog sistema – DCs, i utiče na njegovu sposobnost da stimuliše $CD4^+$ T ćelije.

Ovo istraživanje je podržano od strane Ministarstva za prosvetu, nauku i tehnološki razvoj Republike Srbije, projekat br. 172024.

Effects of Maillard reaction on immunogenicity of β -lactoglobulin

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Maillard reaction occurs during food processing and results in formation of Advanced Glycation Endproducts (AGE) of proteins. AGE of food allergens are of particular importance. We performed an extensive Maillard reaction with a model food allergen, β -lactoglobulin (BLG), and glucose. Glycation of BLG did not influence protein secondary structure but reduced its transport through Caco-2 monolayer. Uptake of glycated BLG by immature dendritic cells (DCs) significantly increased when compared to native BLG. Inside endolysosomal compartments of DCs, glycated BLG undergoes faster degradation. Compared to the native BLG, glycated BLG diminished cytokine production (IL-5, IL-13, $INF\gamma$) by BLG-specific $CD4^+$ T cells co-cultured with DCs. Our data indicate that the Maillard reaction plays a significant role in immunogenicity of BLG, influencing its gastrointestinal bioavailability, interactions with crucial cells of immune system, DCs, and its ability to stimulate $CD4^+$ T cells.

This study was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Grant No. 172024.

**Optimizacija visoko specifičnog fluorescentnog testa kod kvasca
Saccharomyces cerevisiae za identifikaciju liganada androgenog receptora i
kvantifikaciju njihovog afiniteta vezivanja**

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Poznato je da signalni put androgenih receptora (AR) ima važnu ulogu u razvoju i progresiji kancera prostate. Supresija njihove aktivnosti antagonistima AR može inhibirati rast kancera prostate. Stoga, AR predstavljaju obećavajuću metu u lečenju ove bolesti. Naš cilj je bio da razvijemo i optimizujemo neradioaktivni i visoko specifičan fluorescentni test kod kvasca za identifikaciju liganada androgenog receptora i kvantifikaciju njihovog afiniteta vezivanja. Ekspimirali smo ligand vezujući domen (LBD) AR spojen sa žutim fluorescentnim proteinom (YFP) kod *Saccharomyces cerevisiae*. Test se zasniva na fluorescentnom rezonantnom transferu energije (FRET) između dva molekula YFP nakon vezivanja liganda za AR i dimerizacije receptora. Testirano je vezivanje AR liganda, dihidrotestosterona, u različitim koncentracijama i kreirana je standardna kriva. Naš ćelijski fluorescentni test se može primeniti za skrining jedinjenja koja se vezuju za AR, kao što su potencijalni antikancerski lekovi.

Ovaj rad je finansiralo Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije (ON 172021).

**Optimization of highly specific fluorescent assay in *Saccharomyces cerevisiae*
for the identification of androgen receptor ligands and quantification of their
binding affinity**

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It is known that the androgen receptor (AR) signaling pathway plays a major role in prostate cancer development and progression. Suppression of AR activity by antagonists could inhibit prostate cancer growth. Hence, ARs represent a promising target in the treatment of this disease. Our aim was to develop and optimize a nonradioactive and highly specific fluorescent assay in yeast for the identification of androgen receptor ligands and quantification of their binding affinity. We expressed the ligand binding domain (LBD) of AR fused with yellow fluorescent protein (YFP) in *Saccharomyces cerevisiae*. Our assay is based on the fluorescence resonance energy transfer (FRET) between two YFPs after ligand binding to the AR and receptor dimerization. Binding of the AR ligand, dihydrotestosterone, at various concentrations was tested and a standard curve was set up. Our cellular fluorescent assay could be applied for the screening of compounds that bind to ARs, such as potential anticancer drugs. This work was funded by the Ministry of Education, Science and Technological Development, Republic of Serbia (Project 172021).

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BH P03

Imunoafinitetno profilisanje molekularnih vrsta specifičnog antigena prostateSanja R. Goč, Miroslava M. Janković*Institut za primenu nuklearne energije, Univerzitet u Beogradu, Banatska 31b, Beograd*

Molekulska vrsta predstavlja najmanju strukturnu i funkcionalnu jedinicu proteoma. Razvoj i primena tehnika masene spektrometrije (MS), otvorili su veliki broj mogućnosti za detekciju i definisanje diskretnih razlika u vrstama, koje su, u najvećoj meri, rezultat post-translacionih modifikacija. Cilj rada je bio imunoafinitetno profilisanje molekularnih vrsta specifičnog antigena prostate (PSA) u serumu. PSA je glikoprotein koji ispoljava izrazitu strukturnu heterogenost polipeptidnog i glikanskog lanca, a uvid u profil njegovih molekularnih vrsta u različitim fiziološkim stanjima, pored proširenja bazičnih znanja može biti od interesa i u laboratorijskoj dijagnostici. Identifikacija i detekcija molekularnih vrsta PSA u serumima osoba sa benignom hiperplazijom (BPH) i kancerom prostate (PCa) je vršena imunoafinitetnom hromatografijom na čipu i MS. Dobijeni rezultati su pokazali da se, bez obzira na fiziološko stanje, PSA-imunoreaktivne vrste u serumu mogu grupisati u četiri glikopeptidne grupe: gp28, gp22, gp18 i gp12 koje odgovaraju zrelom ili „nicked“ PSA. Pored toga, detektovan je i veliki broj vrsta PSA koje bi mogle predstavljati (auto) proteolitičke fragmente. Glavna razlika između BPH i PCa je uočena u broju i učestalosti vrsta u grupi gp18. Imunoafinitetno profilisanje PSA u serumu je ukazalo na moguć biomarkerski potencijal pojedinačnih molekularnih vrsta. Ovaj rad je finansiran od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, br. projekta 173010.

Immunoaffinity profiling of molecular species of prostate-specific antigenSanja R. Goč, Miroslava M. Jankovic*Institute for the Application of Nuclear Energy, University of Belgrade, Banatska 31b Belgrade*

Molecular species is the smallest structural and functional unit of the proteome. The development and application of mass spectrometry (MS) techniques have opened numerous possibilities for detecting and defining discrete differences in species which are mostly a result of post-translational modifications. The aim of this study was to evaluate immunoaffinity profile of molecular species of prostate-specific antigen (PSA) in sera. PSA is a glycoprotein with a pronounced structural heterogeneity of polypeptide and glycan chain. The insight into the profile of PSA species in different physiological conditions, apart from the improvement of basic knowledge, might be of interest for laboratory diagnostics. The identification and detection of PSA species in sera of subjects with benign prostatic hyperplasia (BPH) and prostate cancer (PCa) was performed using immunoaffinity chromatography and MS. Results show that, despite the physiological conditions, PSA-immunoreactive species in sera can be grouped into four glycopeptide groups: gp28, gp22, gp18 and gp12 corresponding to mature PSA or „nicked“ PSA. In addition, species which might represent (auto) proteolytic PSA fragments were detected. The main difference between BPH and PCa was the number and frequency of species in gp18 group. Immunoaffinity profiling of PSA in sera indicated a possible biomarker potential of individual PSA species. This study was supported by The Ministry of Education, Science and Technological Development of the Republic of Serbia, project No 173010.

BH P04

Multivarijantno statističko poređenje hemijskog sastava biljnih ekstrakata: usrednjeni maseni sken ukupnog jonskog hromatograma, UMS-pristup

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Nedavno je pokazano da se relativne zastupljenosti m/z vrednosti usrednjenih masenih skenova ukupnih jonskih hromatograma (UMS) mogu koristiti kao varijable pri multivarijantnoj statističkoj analizi (MVA) etarskih ulja. Ovaj tip varijabli se lakše primenjuje, daje pouzdanije i brže rezultate nego tradicionalne promenljive - procenti (površine ispod pikova) pojedinačnih sastojaka analiziranih ulja. U ovom radu smo ispitivali primenljivost UMS-varijabli za MVA poređenje hemijskog sastava odabranih biljnih ekstrakata. Da bi ovo postigli, usrednjeni maseni skenovi ukupnih jonskih hromatograma i hemijski sastavi (procentualna zastupljenost) 8 dietil-etarskih ekstrakata (6 različitih biljnih vrsta; ekstrakti su analizirani korišćenjem GC-FID i GC-MS) su zasebno upoređivani korišćenjem dve MVA metode: hijerarhijske klaster analize i analize glavne komponente. Dobijeni rezultati ukazuju na to da se MVA analiza složenih smeša isparljivih (pod uslovima GC-MS analize) jedinjenja, zasnovana na primeni UMS varijabli, može koristiti za njihovo lako, brzo i pouzdano poređenje. UMS pristup daje uporedive, ili čak bolje rezultate u odnosu na tradicionalni metod.

Multivariate statistical treatment of plant-extract compositional data: average mass scan of the total ion chromatogram (AMS) approach

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It was recently confirmed that the relative abundances of m/z values of the average mass scan of the total GC chromatograms (AMS) are suitable variables for multivariate statistical comparison (MVA) of essential oils. These were shown to be even more applicable, reliable and faster than the traditionally used variables-percentages (peak areas) of individual oil constituents. Herein, we have explored whether AMS-derived variables are appropriate for MVA-comparison of plant solvent-extract compositional data. To achieve this, average mass scans of the total GC chromatograms and chemical compositions (relative percentages) of eight diethyl ether extracts (six different species; samples were analyzed using GC-FID and GC-MS) were separately compared using two MVA methods: agglomerative hierarchical clustering analysis and principal component analysis. The obtained results strongly suggest that MVA of complex volatile mixtures (GC-MS analyzable fractions of plant solvent extracts), using the corresponding AMS, could be considered as a promising time saving tool for easy and reliable comparison purposes. The AMS approach gives comparable or even better results than the traditional method.

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Hemija i tehnologija hrane / Chemistry and Technology of Food

HTH 01

Šećerni profil kore i jezgra krompira kao indikator botaničkog porekla i sistema gajenja

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Krompir (*Solanum tuberosum* L.) pripada redu vodećih kultura. Na osnovu produktivnosti, hranljive i biološke vrednosti krtola, krompir spada u red najprofitabilnijih ratarskih biljaka. Za ispitivanje ispoljavanja produktivnosti, hranljive i biološke vrednosti krtola krompira odabrane su četiri sorte: dve rane crvene sorte (Fantasy i Laura) i dve žute (Marabel, rana sorta i Jelly, kasna sorta). Sorte su uzgajane u tri različita sistema gajenja: organski, integralni i konvencionalni. Pokazano je da je šećerni profil jezgra i kore krompira dobar indikator botaničkog porekla i sistema gajenja. Kao najzastupljeniji šećeri u krtoli krompira identifikovani su: fruktoza (*Fru*), glukoza (*Glc*) i saharoza (*Sac*), dok se ostali - sorbitol (*Sor*), trehaloza (*Trh*), arabinoza (*Ara*) i turanoza (*Tur*) nalaze u tragovima. Multivarijantnom analizom sadržaja pomenutih šećera utvrđeno je da organski sistem gajenja rezultuje značajno smanjenim sadržajem *Tur* u odnosu na konvencionalne i integralne sisteme koje karakterišu značajno povišeni nivoi *Ara*, *Fru*, *Glc* i *Sor*.

Sugar composition of potato peel and core as an indicator of its botanical origin and system of agriculture

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Potato (*Solanum tuberosum* L.) is one of the most widely produced crops. On the basis of productivity, nutritional and biological values of tubers, it can be considered as one of the most profitable cultivated plants. In order to test the manifestations of productivity, nutritional and biological values of potato tubers, four sorts of potato were selected: two red sorts (Fantasy and Laura), and two yellow sorts (Marabel and Jelly) which were produced using three different growing systems (organic, integrative, and conventional). Sugar profile of core and peel of studied crops have shown to be a good indicator of botanical origin and breeding system. The most abundant sugars in potato tubers are fructose (*Fru*), glucose (*Glc*) and sucrose (*Suc*), while other sugars: sorbitol (*Sor*), trehalose (*Trh*), arabinose (*Ara*), and turanose (*Tur*) can only be found in traces. Multivariate data analysis revealed that organic way of breeding results in significantly lower content of *Tur*, compared to conventional and integrative cultivation systems which yield in increased content of *Ara*, *Fru*, *Glc*, or *Sor*, *Thr* and *Sac*. The most promising chemical indicators of different botanical origin are: *Sah*, *Trh*, and *Glc*, which prominently distinguish yellow form red cultures, *i.e.*, Marabel from the rest of them.

HTH P01

Osobine V/U emulzija stabilizovanih sa polimernim emulgatorom Cithrol DPHS

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Stabilnost emulzija zavisi od niza faktora kao što su osobine emulgatora, osobine vodene i uljne faze i uslova pripreme. Budući da su emulzije V/U vrlo nestabilni sistemi, a da imaju veliku primenu u prehrambenoj i farmaceutskoj industriji, ispitivane su karakteristike 30% (m/m) emulzija vode u parafinskom ulju i ulju koštica grožđa stabilizovanih dodatkom 1% (m/m) nejonskog, polimernog emulgatora Cithrol DPHS. Sprovedena ispitivanja obuhvatila su definisanje međufaznog ponašanja emulgatora primenom tenziometrije, kao i ispitivanje osobina 30% V/U emulzija. Na osnovu rezultata (veličine i raspodele veličina kapi, viskoziteta kontinualne faze i sedimentacione nestabilnosti u toku 30 dana) izvedeni su odgovarajući zaključci.

Rad proistekao iz istraživanja na projektu br. III 46010/3, koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije.

Properties of W/O emulsions stabilized with polymeric emulsifier Cithrol DPHS

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The stability of emulsions depends on many factors such as characteristics of emulsifier, properties of water and the oil phase and on preparation conditions. Since W/O emulsions are very unstable systems that have wide use in food and pharmaceutical industry, characteristics of 30% (w/w) emulsions of water in paraffin oil and grape seed oil, stabilized with 1% (w/w) non-ionic, polymeric emulsifier Cithrol DPHS, were investigated. The behavior of the emulsifier at W/O interface was determined by tensiometry. The characteristics of emulsions (droplet size and size distribution, viscosity of continuous phase and stability during 30 days of storage) were investigated too. On the basis of obtained results appropriate conclusions were made.

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HTH P02

Jonske tečnosti - nove aktivne komponente dijetetskih suplemenata

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U poslednjih nekoliko godina, jonske tečnosti (JT) nalaze se na samom vrhu primenljivosti u nauci i tehnologiji. Predstavljaju novu klasu rastvarača sa jedinstvenim osobinama kao što su zanemarljiv napon pare pri normalnim uslovima, visoka termička, hemijska i elektrohemijska stabilnost, kao i široka mogućnost "podešavanja" njihovih osobina poput polarnosti, hidrofobnosti i rastvorljivosti. Navedena svojstva su posledica mogućnosti neograničenog kombinovanja molekulskih karakteristika njihovih konstitutivnih jona. Ovo daje priliku za sintezu novih aktivnih komponenta dijetetskih suplemenata na bazi jonskih tečnosti sa biološki aktivnim katjonima i anjonima koji su bezbedni za ljudsku upotrebu i odobreni od strane FDA.

Zbog toga smo sintetisali novu jonsku tečnost, holinijum-aurat, i na osnovu rezultata toksikoloških, fizičko-hemijskih i termičkih analiza, razmotrili smo mogućnost njene upotrebe kao dijetetskog suplementa.

Ovaj rad je finansijski podržan od strane Ministarstva za prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat ON 172012) i Pokrajinskog sekretarijata za nauku i tehnološki razvoj AP Vojvodine.

Ionic Liquids - New active ingredients in dietary supplements

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In the past several years, ionic liquids (ILs) have been at the cutting edge of the most promising science and technology. This "neoteric" class of solvents generally presents interesting properties, namely, negligible vapor pressure at relatively ambient conditions; high thermal, chemical, and electrochemical stability; and widely tunable properties with regard to polarity, hydrophobicity, and solvent miscibility. These properties result from a matchless combination of molecular characteristics of their constitutive ions. This provides the ability to synthesize the new active components of dietary supplements based on ionic liquids with the biologically active cations and anions that are safe for human use and approved by FDA as SEDS (Substances Generally Recognized as Safe).

Given these traits, we synthesized a new ionic liquid, cholinium-aurate, and based on the results of toxicity, measurements of physico-chemicals and thermal properties, we considered its potential application as a food additive.

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HTH P03

Određivanje sastava masnih kiselina tokom fermentacije mleka kombuhom i konvencionalnim starter kulturama

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Fermentisani mlečni proizvodi predstavljaju veoma važnu komponentu svakodnevne ishrane pre svega zbog svoje visoke nutritivne vrednosti i pogodnih zdravstvenih efekata. Zdravstveni aspekt fermentisanih mlečnih napitaka u velikoj meri zavisi od sastav masnih kiselina mlečne masti, kao jedne od veoma važnih komponenata ovih proizvoda. U cilju ispitivanja uticaja starter kulture na masno-kiselinski sastav fermentisanih mlečnih napitaka u ovom radu je praćen sastav masnih kiselina tokom fermentacije mleka primenom nekonvencionalne starter kulture, kombuhe, i konvencionalnih starter kultura, jogurtne odnosno probiotske. Za fermentaciju je korišćeno mleko sa 2,8% mlečne masti na temperaturi 42°C. Analiza masnih kiselina izvedena je primenom kapilarne gasne hromatografije u kombinaciji sa kvadrupolnom masenom spektrometrijom nakon prethodne ekstrakcije masti i derivatizacije. Dominantne masne kiseline u fermentisanim mlečnim proizvodima bile su: palmitinska, oleinska, stearinska i miristinska sa prosečnim sadržajem 32,62; 26,59; 11,12 i 10,78%, redom. Najpovoljniji sastav masnih kiselina, sa najnižim sadržajem zasićenih i najvišim sadržajem mononezasićenih i polinezasićenih masnih kiselina, dobijen je u napitcima fermentisanim primenom tradicionalne jogurtne kulture.

Determination of fatty acids during the fermentation of milk by kombucha and conventional starter cultures

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Fermented milk products are a very important component of the daily diet primarily because of their high nutritional value and beneficial health effects. The health aspect of fermented milk beverages depends on the fatty acid composition of milk fat, as one of the most important components of those products. In order to investigate the influence of starter cultures on the fatty acid composition of fermented milk products, in this work the fatty acid composition during the fermentation of milk using non-conventional starter culture, kombucha, and conventional starter cultures or probiotic yoghurt was monitored. For fermentation a milk with 2.8% fat was used, at a temperature of 42 ° C. Fatty acid analysis was performed using capillary gas chromatography in combination with a quadrupole mass spectrometry after previous extraction and derivatization steps. The dominant fatty acids in fermented dairy products were: palmitic, oleic, stearic and myristic acids in content of 32.62; 26.59; 11.12 and 10.78%, respectively. The most favourable fatty acid composition, with the lowest content of saturated and the highest content of monounsaturated and polyunsaturated fatty acids, was derived from the fermented beverage using the traditional yoghurt cultures.

HTH P04

Masno-kiselinski profil polena koji su medonosne pčele sakupile u Srbiji

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Važan deo lipidne frakcije u polenu čine masne kiseline- bilo u obliku estara bilo u slobodnoj formi. Zastupljenost i raznovrsnost masnih kiselina u velikoj meri zavise od palinološkog porekla uzoraka.

U okviru ovog rada ispitano je dvadeset i šest uzoraka polena koji su medonosne pčele sakupile u različitim regionima Srbije. Analiza sadržaja masnih kiselina je izvršena GC metodom.

Ukupno je identifikovano dvadeset masnih kiselina. Od toga, šest kiselina (kaprilna, palmitinska, stearinska, oleinska, linolna i linolenska) je pronađeno u svim uzorcima, šest je bilo prisutno u većini uzoraka a osam masnih kiselina se mogu okarakterisati kao „retke“ jer su identifikovane u svega nekoliko uzoraka (ili u po jednom uzorku). Na pojavu masnih kiselina najveći uticaj je imalo palinološko poreklo uzorka. Po prisustvu „retkih“ masnih kiselina posebno se izdvojio uzorak br. 1 koji je predominantno sadržavao polen jasena. Najzastupljenija zasićena masna kiselina je bila palmitinska, a od nezasićenih oleinska kiselina.

Fatty acids profile of bee pollen collected in Serbia

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An important part of the bee pollen lipid fraction consists of fatty acids- either in the form of esters or as free form. Representation and diversity of fatty acids are largely dependent on palynological origin of samples.

In this work twenty six samples of bee pollen collected in different region of Serbia were examined. Analysis of fatty acids was carried out by GC method. In total, twenty fatty acids were identified. Six acids (caprylic, palmitic, stearic, oleic, linoleic and linolenic) were found in all samples, six acids were present in most of the samples and eight fatty acids can be characterized as "rare" because they were identified only in a few samples (or in one sample). Palynological origin of samples had the greatest impact on the occurrence of fatty acids. According to presence of the "rare" fatty acids sample no. 1 can be pointed as characteristic. It was predominantly consists of pollen of *Fraxinus* genus (ash). The most common saturated and unsaturated fatty acids were palmitic acid and oleic acid, respectively.

Karakterizacija flavan-3-ola u uzorcima šipurka primenom visoko efikasne tankoslojne hromatografije povezane sa masenom spektrometrijom

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Plodovi šipurka se smatraju značajnim izvorom polifenolnih jedinjenja i vitamina. Istraživanja polifenolnog profila plodova šipurka su pokazala visok sadržaj fenolnih kiselina, flavonoid glikozida i proantocijanidina. Cilj ovog istraživanja bio je identifikacija jedinjenja iz grupe flavan-3-ola u četrnaest uzoraka šipurka upotrebom visoko efikasne tankoslojne hromatografije (HPTLC) povezane sa masenim spektrometrom sa elektronsprej jonizacijom (ESI-MS). Ukupno šest flavan-3-ola je identifikovano na osnovu $[M-H]^-$ molekulskog jona i njegove MS/MS fragmentacije (katehin, proantocijanidin dimer, proantocijanidin dimer monoheksozid, proantocijanidin dimer diheksozid, proantocijanidin trimer diheksozid i proantocijanidin trimer triheksozid). Iako je sličan hromatografski profil dobijen za sve uzorke, mogu se uočiti razlike u zastupljenosti pojedinih flavan-3-ola u ispitivanih uzorcima šipurka.

Characterisation of flavan-3-ols from rose hips by high-performance thin-layer chromatography-mass spectrometry

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The rose hip fruits are considered as important source of phenolic compounds and vitamins. Studies on the phenolic composition of rose hip have shown that its fruits are rich in phenolic acids, flavonoid glycosides and proanthocyanidin aglycones. The aim of this study was to investigate flavan-3-ols profile of fourteen rose hip samples using high-performance thin-layer chromatographic (HPTLC) coupled to electrospray ionisation mass spectrometer (ESI-MS). A total of six flavan-3-ols (catechin, proanthocyanidin dimer; proanthocyanidin dimer monohexoside, proanthocyanidin dimer dihexoside, proanthocyanidin trimer dihexoside, and proanthocyanidin trimer trihexoside) were identified based on the search for the $[M-H]^-$ deprotonated molecule and its MS/MS fragmentation. Although similar chromatographic profiles were obtained for all samples, it was observed that there was a significant difference in the presence and zone intensity of some flavan-3-ols.

Detekcija egzogene vode u vinu pomoću masene spektrometrije odnosa izotopa

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Jedna od najvažnijih primena masene spektrometrije odnosa izotopa je merenje odnosa $^{18}\text{O}/^{16}\text{O}$. Određivanje odnosa $^{18}\text{O}/^{16}\text{O}$ iz vode iz vina se primenjuje u više zemalja da bi se definisalo geografsko poreklo vina, i predložena je metoda za detekciju egzogene vode. Cilj ovog rada je da se vidi da li su rezultati razblaženih uzoraka uporedivi i korisni za detekciju dodatka vode u vino. Dva uzorka vina (Rhine Riesling and Cabernet Sauvignon) su razblažena vodom mešanjem česmenske vode i vina u određenom odnosu. Uzorci su analizirani protočnom tehnikom u kojoj je uzorak nošen nosećim gasom. Sve analize su urađene na Finnigan GasBench II periferalu, sa autosemplerom, povezanim sa Delta V Advantage masenim spektrometrom. Dobijena je visoka korelacija između odnosa $^{18}\text{O}/^{16}\text{O}$ i procenta dodate vode za svako vino. Iako eksperiment sa dodatkom vode nema veliku primenljivost zato što voda kojom je razblaženo vino i originalno vino često nisu dostupni, on ipak pokazuje da je ova metoda primenljiva za detekciju dodatka vode u vino.

Zahvalnica: Ova istraživanja su podržana od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat br. 172017).

Detection of exogenous water in wine using isotope ratio mass spectrometry

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One of the most important applications of isotope ratio mass spectrometry (IRMS) is the measurement of the $^{18}\text{O}/^{16}\text{O}$ ratio of water. The determination of oxygen ratio ($^{18}\text{O}/^{16}\text{O}$) from the water content of the wine (wine water), have been used in several countries to define the geographical origin of wine, and it is proposed as a method to detect the addition of exogenous water to wine. The aim of this work was to check the usefulness and the comparability of the results for spiked samples for detection of wine adulteration. To achieve this, two wine samples (Rhine Riesling and Cabernet Sauvignon) were watered-down after mixing specific quantities of tap water with original, unadulterated wine. All samples were analyzed by continuous flow technique in which the sample is entrained in a carrier gas. All analyses were done on Finnigan GasBench II with autosampler-assisted loop injection coupled with Delta V Advantage mass spectrometer. Results show high correlation between $^{18}\text{O}/^{16}\text{O}$ ratio of water and percentage of added water for each wine. Even though this experiment using spiked samples has no great applicability, as the water used to dilute a wine and the original, unadulterated wine are not usually available in the case of suspicious wines, the results prove the workability of the method.

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**Плодови трњине (*Prunus spinosa*) и глога (*Crataegus laevigata*) као
потенцијални антиоксиданти и њихова стабилност у условима
in vitro дигестије**

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У циљу испитивања метанолских екстраката плода биљака *Prunus spinosa* (трњина) и *Crataegus laevigata* (глог) одређена је укупна количина фенолних једињења, флавоноида и антоцијана, као и ниво антиоксидативне активности екстраката. Екстракт плода глога садржи већу количину укупних фенола (541,09 μmol галне киселине/g екстракта) и флавоноида (150,53 μmol кверцетина/g) у односу на екстракт плода трњине (97,52 μmol галне киселине/g, односно 54,89 μmol кверцетина/g), док су количине антоцијана у екстрактима биле приближно исте. Екстракт плода глога показао је знатно бољу антиоксидативну активност у односу на екстракт плода трњине на нивоу DPPH[•] и ABTS⁺ радикала. Такође, испитане су и промене у количини укупних фенолних једињења у екстрактима и нивоу антиоксидативне активности у току процеса симулиране *in vitro* дигестије. Добијени резултати су показали да се количина фенолних једињења у екстрактима и њихов антиоксидативни потенцијал мењају у зависности од времена дигестије.

**Fruits of blackthorn (*Prunus spinosa*) and hawthorn (*Crataegus laevigata*) as
potential antioxidants and their stability during *in vitro* digestion**

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The aim of this study was to determine concentration of total phenolic, flavonoids and anthocyanins in methanol extracts of *Prunus spinosa* (blackthorn) and *Crataegus laevigata* (hawthorn) fruits, as well as the level of antioxidant activity of these extracts. The extract of hawthorn fruit contained higher amounts of total phenolics (541.09 μmol gallic acid/g dry extract) and flavonoids (150.53 μmol quercetin/g) with respect to blackthorn fruit extract (97.52 μmol gallic acid/g and 54.89 μmol quercetin/g, respectively), while the amounts of anthocyanins in the extract were quite similar. The hawthorn fruit extract showed significantly higher antioxidant activity in comparison to blackthorn fruit extract measured by DPPH[•] and ABTS⁺ radical scavenging activity methods. Also, the changes in the amount of the total phenolic compounds in the extracts and the level of antioxidant activity in the process of simulated *in vitro* digestion have been evaluated. The results showed that the amounts of phenolic compounds in the extracts and their antioxidant activity changed depending on the time of digestion.

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Sadržaj sekundarnih metabolita i njihov uticaj na antioksidativnu aktivnost u različitim sortama jagoda

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Određeni su sadržaji sekundarnih metabolita u četiri različite sorte gajenih jagoda (*Fragaria ananassa*): Albion, Senga Sengana, Elsanta i Cleary, u jednoj divljoj jagodi (*Fragaria vesca* L.) i antioksidativne aktivnosti prema stabilnim slobodnim radikalima DPPH i ABTS. Rezultati su pokazali da postoji statistički značajna razlika kako u sadržaju sekundarnih metabolita, tako i u antioksidativnoj aktivnosti među različitim sortama jagoda, te da na ovu aktivnost najviše utiče sadržaj ukupnih fenola i ukupnih flavonola.

The content of secondary metabolites and their impact on the antioxidant activity in different varieties of strawberries

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Contents of secondary metabolites in four different varieties of cultivated strawberries (*Fragaria ananassa*): Albion, Senga Sengana, Elsanta and Cleary, and in a wild strawberry (*Fragaria vesca* L.) were determined. At the same time the antioxidant activities according to the stable free radical DPPH and ABTS were determined. The results showed a statistically significant difference in the content of secondary metabolites and the antioxidant activity among different varieties of strawberries and that this activity is mostly influenced by the content of total phenols and total flavonols.

Hemija i tehnologija makromolekula Chemistry and Technology of Macromolecules

HTM PO1



Poređenje hidrolitičke, enzimске i degradacije u kompostu PCL/PEO diblok kopolimera

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U ovom radu je prikazana hidrolitička i enzimska degradacija poli(ϵ -kaprolaktona) (PCL) i serije diblok kopolimera (PCL/PEO) sa malim sadržajem hidrofilnog poli(etilen-oksidnog) (PEO) segmenta. Ispitivan je uticaj uvođenja lateralnog PEO segmenta u PCL lanac na degradativna svojstva kopolimera. Hidrolitička degradacija je izvođena u fosfatnom puferu tokom 8 nedelja. FTIR analizom je utvrđena bolja degradativna sposobnost diblok kopolimera usled veće hidrofilnosti u poređenju sa PCL-om. Enzimska degradacija, testirana u "cell-free" ekstraktu *Pseudomonas aeruginosa* PAO1, tokom dve nedelje, je praćena na osnovu promena mase, hrapavosti površine polimernih filmova kao i FTIR analizom. Rezultati su potvrdili da svi uzorci podležu enzimskoj degradaciji, koja se odigrava po mehanizmu površinske erozije i uz smanjenje molarne mase. Diblok kopolimeri su pokazali značajno veći gubitak mase i smanjenje molarne mase u odnosu na PCL. AFM analiza je potvrdila intenzivnu površinsku eroziju i povećanje RMS vrednosti. Testirana je i biodegradacija polimernih filmova u kompostu na 37 °C gde je utvrđena izražena degradacija ispitivanih blok kopolimera.

Comparative analysis of hydrolytic, enzymatic and degradation in compost of PCL/PEO diblock copolymers

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In this paper, hydrolytic and enzymatic degradation of poly(ϵ -caprolactone) (PCL) and series of diblock (PCL/PEO) copolymers, with a low content of hydrophilic PEO segments is presented. The effect of the introduction of PEO as lateral segment in the PCL chain on copolymer biodegradation properties was investigated. The hydrolytic degradation was performed in phosphate buffer for up to 8 weeks. FTIR results revealed higher degradation ability of diblock copolymers due to a higher hydrophilicity compared to PCL. Enzymatic degradation was tested using cell-free extracts of *Pseudomonas aeruginosa* PAO1, for two weeks by following the weight loss, changes in surface roughness, and changes in carbonyl and crystallinity index. The results confirmed that all samples underwent enzymatic degradation through surface erosion accompanied with a decrease in molecular weights. Diblock copolymers showed significantly higher weight loss and decrease in molecular weight compared to PCL. AFM analysis confirmed significant surface erosion and increase in RMS values. Biodegradation of polymer films was also tested in compost model system at 37°C, where an effective degradation of block copolymers was observed.

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HTM P01

Sinteza graftovanog kopolimera upotrebom mikrobnog levana i polistirena

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Poslednjih godina se javlja veliki interes za modifikaciju polistirena, kao jednog od najdominantnijih materijala za proizvodnju plastičnih materijala, sa različitim polisaharidima. Publikovane su modifikacije polistirena sa polisaharidima kao što su hitin, celuloza i skrob. Zahvaljujući svojoj antitumornoj, prebiotskoj i imunostimulirajućoj aktivnosti, mikrobn levan privlači mnogo pažnje, kao potencijalni supstrat za primenu u farmaciji, medicini i industriji hrane. Cilj ovog rada je bio izolovanje levana iz soja *Bacillus licheniformis* i sinteza novog levan-polistiren graftovanog kopolimera. Sinteze su rađene slobodnoradikalskom reakcijom i upotrebljavan je kalijum-persulfat kao inicijator reakcije. Ispitivan je uticaj reakcije temperature i atmosfere, a dobijeni kopolimer je karakterisan pomoću skenirajuće elektronske mikroskopije (SEM). Rezultati su pokazali da se najviši procenat graftovanja ($G (\%) = 24,1 (\%)$) postiže na temperaturi od $60\text{ }^{\circ}\text{C}$ i u prisustvu kiseonika. U slučaju atmosfere azota, najpogodnija temperatura bila je $55\text{ }^{\circ}\text{C}$ sa $G (\%) = 50,9 (\%)$. SEM mikrografi levan-polistiren graftovanog kopolimera su pokazali da su u njemu prisutne obe komponente. Zahvalnica: Ovaj rad je podržan od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije kroz stipendije za studente doktorskih studija i projekte III 43004 and OI 172001.

Synthesis of graft copolymer using microbial levan and polystyrene

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In recent years, there has been a great interest in modifications of polystyrene, as one of the most dominant materials for plastic production, with different polysaccharides. Modifications of polystyrene with polysaccharides such as chitin, cellulose and starch have been reported. Due to its antitumor, prebiotic and immune-stimulating activity, microbial levan attracted much attention for potential use in pharmacy, medicine and food industry. The aim of this work was isolation of levan from *Bacillus licheniformis* strain and synthesis novel levan-polystyrene graft copolymer. Syntheses were performed by the free radical reaction using potassium persulfate as initiator. The influence of reaction temperature and atmosphere was investigated and obtained copolymer was characterized by Scanning Electron Microscopy (SEM). Results showed that the highest percent of grafting ($G (\%) = 24.1 (\%)$) was achieved at $60\text{ }^{\circ}\text{C}$ oxygen atmosphere. In case of nitrogen atmosphere, $55\text{ }^{\circ}\text{C}$ was the most suitable temperature for synthesis of levan-polystyrene graft copolymer with $G (\%) = 50.9 (\%)$. SEM micrographs of obtained levan-polystyrene graft copolymer showed presence of both components. Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia through scholarships for PhD students and funding for Projects III 43004 and OI 172001.

Priprema i svojstva nanokompozita biodegradabilnog poli(ϵ -kapolaktona) i organomodifikovanih sepiolita

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Biodegradabilni alifatski poliestri su aktuelno polje istraživanja, jer predstavljaju jedno od rešenja za rastuće ekološke probleme. Mehanička, barijerna i termička svojstva alifatskih poliestara mogu se poboljšati dodavanjem punioca nano-dimenzija, kao što su sepioliti. Tri serije nanokompozita poli(ϵ -kapolaktona) (PCL) i tri vrste sepiolita: nemodifikovani, modifikovani kovalentnim vezivanjem (3-merkaptopropil)trimetoksisilana i modifikovani jonskom izmenom sa heksadecilaminom, su pripremljene iz rastvora u hloroformu. Sadržaj sepiolita u nanokompozitima je iznosio 1, 3 i 5 mas.%, a uzorci su dobijeni u obliku filmova debljine 100 - 220 μm . Morfologija nanokompozita je ispitana optičkom mikroskopijom i uočena je promena sferulitne strukture PCL pri dodatku sepiolita. Ispitivan je efekat dodatka modifikovanog i nemodifikovanog sepiolita na termička, mehanička i reološka svojstva nanokompozita. Temperature topljenja i stepeni kristaliničnosti su određeni DSC analizom, a termička stabilnost nanokompozita je ispitana TG analizom u neizotermnim ogledima. Stepem dispergovanosti nanopunioca je procenjen ispitivanjem reoloških svojstva rastopa u dinamičkim ogledima u temperaturnom opsegu 70 - 140 °C. Mehanička svojstva i termički prelazi u nanokompozitima su ispitani dinamičko-mehaničkom analizom u temperaturnom intervalu od - 120 - 60 °C.

Preparation and properties of nanocomposites of biodegradable poly(ϵ -caprolactone) and organomodified sepiolites

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Biodegradable aliphatic polyesters have become attractive field of research and represent one of the solutions to the growing environmental problems. Mechanical, barrier and thermal properties of aliphatic polyesters can be improved by adding nano-sized fillers, such as sepiolite. Three series of nanocomposites based on poly(ϵ -caprolactone) (PCL), and three types of sepiolite: unmodified, modified by covalent attachment of (3-mercaptopropyl)trimetoxysilane, and modified by ionic exchange with hexadecylamine, were prepared by solution casting from chloroform. The content of sepiolite in the nanocomposites was 1, 3 and 5 wt.%, and the samples were obtained in the form of a film with a thickness of 100 - 220 μm . The morphology of nanocomposites was examined using an optical microscope, and the change in spherulitic structure of the PCL with the addition of sepiolites was observed. The effect of the addition of unmodified and modified sepiolite on thermal, mechanical and rheological properties of nanocomposites was examined. Melting temperatures and degree of crystallinity were determined by DSC analysis, while thermal stability of the nanocomposites was investigated by TG analysis in non-isothermal experiments. The degree of dispersion was estimated by examining rheological properties of the melt in dynamic experiments in a temperature range 70 - 140 °C. Mechanical properties and thermal transitions were investigated by dynamic mechanical analysis in a temperature range from - 120 - 60 °C.

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HTM P03

Uklanjanje tekstilnih boja iz otpadne vode pomoću hidrogelova hitozana

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Porast upotrebe boja u tekstilnoj industriji za posledicu ima povećanje zagađenja otpadnih voda i veliki ekološki problem. Među mnogobrojnim postupcima kojima se obezbeđuje zadovoljavajući stepen obojavanja otpadnih voda, sorpcija se izdvojila kao jednostavan i efikasan način. Kao sorbenti su do sada korišćeni različiti materijali: razne vrste otpada (bademova ljuska, piljevina i dr.), aktivni ugalj, zeoliti, umreženi polimeri, a naročito oni koji se dobijaju iz obnovljivih izvora.

Cilj ovog rada je da se ispita mogućnost primene hidrogelova hitozana, itakonske i metakrilne kiseline za prečišćavanje otpadnih voda iz tekstilne industrije. Uklanjanje boja je praćeno u rastvoru koji simulira standardnu otpadnu vodu, a kao model korišćene su boje za bojenje vune, pamuka, najlona (*C.I. Acid Orange 7* i *C.I. Basic Red 1*), kao i bazna boja metilensko plavo (*Methylene Blue*). Praćen je uticaj temperature, pH vrednosti i sadržaja saharoze u simuliranoj otpadnoj vodi na efikasnost uklanjanja boja. Utvrđeno je da na efikasnost uklanjanja boja značajno utiče pH i prisustvo saharoze, dok promena temperature u intervalu od 25 °C do 50 °C nema značajan uticaj.

Removal of textile dyes from wastewater by chitosan hydrogels

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Increased use of dyes in the textile industry has lead to water pollution on a large scale and represents an ecological problem. Among many treatments taken to remove colors from wastewater to a satisfactory level, sorption stands out as simple and efficient process. Up to now, many materials have been used as sorbents: wastes (almond shells, sawdust etc), zeolites, activated carbon, crosslinked polymers, especially those obtained from renewable sources, etc.

The goal of this paper is to investigate possible application of chitosan, methacrylic and itaconic acid based hydrogels for textile wastewater purification. Dye removal was observed in a solution that simulates standard wastewater. Two dyes, which have industrial application in dyeing wool, cotton and nylon (*C.I. Basic Red 1* and *C.I. Acid Orange 7*) were used as model dye, as well as basic dye *Methylene Blue*. The effect of temperature, pH value and sucrose content in wastewater on the removal efficiency was studied. It was found that pH and sucrose affected dye removal, while the removal efficiency was not significantly altered in temperature range from 25 °C to 50 °C.

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Uticaj specifičnih anjona na afinitet sorpcije pektina prema Cu^{2+} jonima

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Cilj ovog rada bilo je ispitivanje specifičnog uticaja anjona Hofmeister-ovog niza (Cl^- , NO_3^- , CH_3COO^- , SO_4^{2-}) na proces umrežavanja pektina jonima bakra, primenom sorpcije kao indirektno metode kvantifikacije. Pektinske čestice dobijene su umrežavanjem u rastvorima četiri bakarne soli (CuSO_4 ; $\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2$; CuCl_2 ; $\text{Cu}(\text{NO}_3)_2$) različite koncentracije ($0,5\text{-}10 \text{ g/dm}^3$). Nađeno je da je uticaj anjona na kapacitet sorpcije pektina u skladu sa specifičnim uticajem jona na makromolekule u vodenim rastvorima koje je predložio Hofmeister: najveći kapacitet sorpcije Cu^{2+} jona postignut je iz rastvora sulfata, dok opada u prisustvu CH_3COO^- , Cl^- i NO_3^- jona, redom. Rezultati sorpcije dobijeni primenom atomske apsorpcione spektroskopije (AAS) opisani su modelima Lengmuir-ove i Freundlich-ove sorpcione izoterme, pri čemu su izračunati parametri potvrdili podsticajnu prirodu sulfatnog jona u procesu vezivanja metala.

The specific anion influence on the sorption affinity of pectin toward Cu^{2+} ions

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The objective of this study was to investigate if there was any (specific) influence of anions from Hofmeister series (Cl^- , NO_3^- , CH_3COO^- , SO_4^{2-}) on the cross-linking process of pectin via Cu^{2+} ions, wherein sorption was implemented as the indirect quantification method. The pectin beads were obtained via cross-linking in four copper salt solutions (CuSO_4 ; $\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2$; CuCl_2 ; $\text{Cu}(\text{NO}_3)_2$) of different initial concentration ($0.5\text{-}10 \text{ g/dm}^3$). It was found that the anions affected the sorption capacity of pectin according to ion-specific influence on macromolecules in aqueous systems proposed by Hofmeister: Cu^{2+} sorption capacity from the sulfate solution was the highest, while it decreased in the presence of CH_3COO^- , Cl^- and NO_3^- ions, respectively. The sorption data obtained from atomic absorption spectroscopy (AAS) were applied to the Langmuir and Freundlich isotherm models and various calculated parameters confirmed the supportive nature of sulfate anion in metal ion binding.

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Termički osetljivi hidrogelovi na bazi poli(*N*-izopropilakrilamida) i hijalorunske kiseline umreženi nanoglinama

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Predmet ovog rada je sinteza semi-interpenetrirajućih polimernih mreža na bazi poli(*N*-izopropilakrilamida) (PNIPA) i vodorastvorne soli hijaluronske kiseline (Na-HI), fizički umreženih sintetskim nanoglinama (Laponit XLG). PNIPA hidrogelovi umreženi glinama pored odličnih mehaničkih svojstva poseduju transparentnost i veliku brzinu absorpcije/otpuštanja vode. Hidrogelovi su sintetisani radikalnom polimerizacijom *N*-izopropilakrilamida u suspenziji nanoglina, čije čestice predstavljaju multifunkcionalna mesta umreženja. Hidrogelovi različite gustine umreženosti su sintetisani variranjem sadržaja gline (1, 3 i 5 mas.%), kao i tri serije semi-IPN sa 0,1; 0,15 i 0,25 mas.% linearnog polimera Na-HI. Izučavan je uticaj sadržaja gline i hijaluronske kiseline na brzinu procesa bubrenja/dehidratacije. Struktura i heterogenost hidrogelova su analizirani pomoću elektronske skenirajuće mikroskopije (SEM) i širokougaone rentgenske difrakcije (WAXS), dok je sadržaj inkorporirane gline određivan pomoću termogravimetrijske analize. Reološka svojstva sintetisanih hidrogelova su analizirana DMA analizom u osnovnom i nabubrelo stanju. Ovi hidrogelovi sa poboljšanim mehaničkim svojstvima su novi nanomaterijali, koji u kombinaciji sa prirodnim polimerom kao što je hijaluronska kiselina mogu da nađu primenu u biomedicini za izradu flastera za brzo zaceljivanje rana i regeneraciju tkiva, kao i u kontrolisanom otpuštanju lekova.

Thermo-sensitive hydrogels based on poly(*N*-isopropylacrylamide) and hyaluronic acid crosslinked with nanoclays

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The subject of this paper is the synthesis of the semi-interpenetrating polymer networks based on poly(*N*-isopropylacrylamide) (PNIPA) and water-soluble sodium salts of hyaluronic acid (Na-HI), physically crosslinked with synthetic nanoclay (Laponite XLG). PNIPA hydrogels crosslinked with nanoclays exhibited excellent mechanical properties, high transparency and fast adsorption/release of water. Hydrogels are synthesized by free radical polymerization of *N*-isopropylacrylamide in nanoclay suspension, whose particles act as multifunctional crosslinker. Hydrogels with different crosslinking densities were prepared by varying the content of clay (1, 3 and 5 wt.%) and three series of semi-IPN with 0.1; 0.15 and 0.25 wt.% of Na-HI. The influence of clay and hyaluronic acid content on the rate of swelling/deswelling was analyzed. The structure and heterogeneity of the semi-IPN hydrogels was examined by SEM and WAXS. The content of clay incorporated in the gel was determined by TGA. Rheological properties of synthesized hydrogels are analyzed by dynamic-mechanical spectroscopy in as-prepared and swollen state. These hydrogels with improved mechanical properties are new nanomaterials, which in combination with a natural polymer, such as hyaluronic acid, may find use in biomedical applications to create patches for fast wound healing and tissue regeneration as well as drug release systems.

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Sinteza i karakterizacija biodegradabilnih triblok kopoliestara na bazi poli(ϵ -kapolaktona), poli(butilen-sukcinata) i poli(butilen-adipata)

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Alifatski poliestri su najznačajnija grupa biodegradabilnih sintetskih polimera, aktuelnih kako za zaštitu životne sredine tako i u biomedicini i farmaciji. Svojstva alifatskih biodegradabilnih poliestara, kao što su termička, mehanička i reološka, kao i podložnost biodegradaciji mogu se podešavati kopolimerizacijom i strukturom kopolimernog lanca. U ovom radu, sintetisane su dve serije biodegradabilnih triblok kopoliestara: poli(ϵ -kapolakton)-poli(butilen-sukcinat)-poli(ϵ -kapolakton), PCL/PBS/PCL, i poli(ϵ -kapolakton)-poli(butilen-adipat)-poli(ϵ -kapolakton), PCL/PBA/PCL, kod kojih je dužina PCL blokova varirana od 10000 do 20000 g/mol. Kopoliestri su sintetisani polimerizacijom otvaranja prstena ϵ -kapolaktona, iniciranom završnim hidroksilnim grupama prepolimera PBS (2810 g/mol) i PBA (2523 g/mol) uz katalizator kalaj(II)-oktoat. Molekulska struktura triblok kopoliestara je potvrđena ^{13}C i ^1H NMR spektroskopijom, dok su vrednosti molarnih masa i polidisperznost određeni GPC analizom, gde je zabeležen očekivani trend. Temperature topljenja i stepeni kristaliničnosti određeni su diferencijalnom skenirajućom kalorimetrijom, a termička stabilnost kopoliestara ispitana je termogravimetrijskom analizom. Uticaj strukture polimernog lanca blok kopoliestara na reološka svojstva njihovih rastopa ispitan je u dinamičkim oscilatornim ogledima na različitim temperaturama.

Synthesis and characterisation of biodegradable triblock copolyesters based on poly(ϵ -caprolactone), poly(butylene succinate) and poly(butylene adipate)

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Aliphatic polyesters are the most important group of synthetic biodegradable polymers, which are relevant materials in environmental protection as well as in biomedicine and pharmacy. Properties of aliphatic polyesters such as thermal, mechanical and rheological as well as susceptibility to biodegradation can be tuned through copolymerization and structure of polymer chain. In this study, two series of block copolyesters are synthesized: poly(ϵ -caprolactone)-poly(butylene succinate)-poly(ϵ -caprolactone), PCL/PBS/PCL, and poly(ϵ -caprolactone)-poly(butylene adipate)-poly(ϵ -caprolactone), PCL/PBA/PCL, where the length of PCL blocks was varied from 10000 to 20000 g/mol. Block copolyesters were synthesized by ring-opening polymerization of ϵ -caprolactone, initiated by the terminal hydroxyl groups of prepolymers PBS (2810 g/mol) and PBA (2523 g/mol) in the presence of catalyst tin(II)-octoate. Molecular structure was confirmed by ^{13}C and ^1H NMR spectroscopy, while the molecular weights and polydispersity indices were determined by GPC analysis, where an expected trend was observed. The melting temperatures and the degrees of crystallinity were determined by differential scanning calorimetry, and thermal stability of copolyesters was investigated by thermogravimetric analysis. The influence of the polymer chain structure of block copolyesters on the rheological properties of their melt was tested in dynamic oscillatory experiments at different temperatures.

Rad je finansiran od strane Ministarstva prosvete i nauke Republike Srbije: Projekat 172062

Organska hemija / Organic Chemistry

OH S

**Potruga za mehanizmom dejstva inhibitora botulinum neurotoksina ili
Kako pokvariti molekulsku mašinu**

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Botulinum neurotoksini (BoNT) su najjači poznati biotoksini, i produkt su anaerobne gram-pozitivne bakterija *Clostridium botulinum*. Postoji sedam serotipova BoNT, koji su sačinjeni od teškog (HC) i lakog lanca (LC). BoNT LC je cink-zavisna metaloproteaza koja fragmetiše specifične proteine u neuronskom citosolu i tako sprečava otpuštanje neurotransmitera u sinaptički prostor i prenos signala. Najjači i najdugotrajniji od svih serotipova BoNT je serotip A. Veliki interes za istraživanja malih molekula koji deluju kao inhibitori njihove protolitičke aktivnosti ne potiče od njihove upotrebe u kozmetici i medicini, već zbog osobina koje ih čine potencijalnim biološkim oružjem i svrstavaju ih u kategoriju A bioloških agenasa.

Da bi razjasnili i istražili inhibitornu aktivnost koje je prema BoNT/A LC u *in vitro* uslovima pokazala serija jedinjenja bazirana na zajedničkom skeletu koristili smo simulirana vezivanja (*molekulski doking*). Male razlike u načinu vezivanja i formiranje različitih interakcija između liganada i aminokiselinskih ostataka u aktivnom centru proteaze su nam dale uvid u različite inhibitorne mogućnosti i podatke za dizajniranje novih struktura, sa potencijalno većim aktivnostima.

**In a search of a mechanism of action of botulinum neurotoxin inhibitors or
How to sabotage the molecular machine**

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Botulinum neurotoxins (BoNT) are the most potent of all biological toxins, and are produced by anaerobic, spore-forming gram-positive bacteria *Clostridium botulinum*. There are seven serotypes of BoNT, consisting of heavy (HC) and light chain (LC). BoNT LC is zinc dependent metalloprotease that fragments specific proteins in neuronal cytosol, eliminating neurotransmitter release in to the synaptic cleft and signal transfer. The most potent and longest acting of the BoNT serotypes is serotype A. The large interest in research of small molecules acting as inhibitors of their proteolytic activity emerged not from their use in cosmetics and medicine, but from the properties that makes them potential biological weapon, classified as category A biothreat agents.

We used docking simulations to rationalize and clarify observed *in vitro* BoNT/A LC inhibitory activities of a series of compounds based on similar scaffold. The small differences in their binding schemes and the formation of different interactions between the ligands and amino acid residues in the protease's catalytic cleft provide the insights into variable inhibitory potencies and data for designing new structures with potentially higher activities.

OH 01

Sinteza i biološko ispitivanje novih triazolskih Mannich-ovih baza

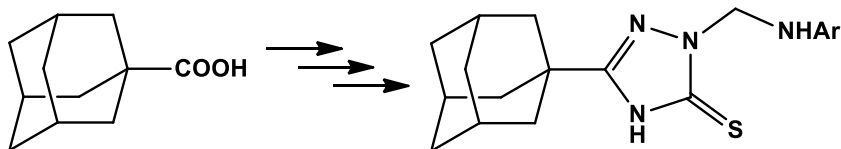
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Sintetizovana je serija od 18 novih *N*-Mannich-ovih baza izvedenih iz 5-adamantil-1,2,4-triazol-3-tiona. Dobijanje finalnih jedinjenja ostvareno je polazeći od 1-adamantanske kiseline koja je prevedena u kiselinski hlorid da bi on dalje bio derivatizovan reakcijom sa tiosemikarbazidom. Nastali 1-adamantoyl tiosemikarbazon u prisustvu baze podleže intramolekularnoj ciklizaciji i daje željeni prekursor, 5-adamantil-1,2,4-triazol-3-tion. U Mannich-ovoj reakciji triazolski prekursor reaguje sa ekvimolarnom količinom formalina i odgovarajućeg primarnog amina u THF-u i nakon 48 h mešanja na sobnoj temperaturi, dobijene su finalne Mannich-ove baze. Tačna struktura dobijenih jedinjenja određena je pomoću rendgenske strukturne analize i NMR spektroskopije. Određena je i citotoksična aktivnost novosintetizovanih jedinjenja, kao i njihov mehanizam delovanja pomoću "western blot" analize ključnih proteina uključenih u apoptozu i ispitivanjem njihove antiangiogene aktivnosti.



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Synthesis and biological screening of novel triazole Mannich bases

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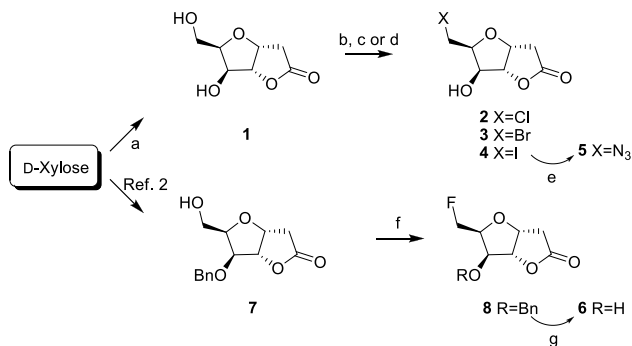
The synthesis of 18 novel 5-adamantyl-1,2,4-triazol-3-thione *N*-Mannich bases was performed. The targeted compounds were obtained starting from 1-adamantanecarboxylic acid, its transformation into corresponding acid chloride and derivatization with thiosemicarbazide. The formed 1-adamantoyl thiosemicarbazone in the presence of a base undergoes intramolecular cyclization giving the desired precursor, 5-adamantyl-1,2,4-triazol-3-thione. Further, in a Mannich reaction, the triazole precursor reacts with equimolar amount of formaline and corresponding primary aromatic amine in THF, giving final Mannich bases after 48 h of stirring at room temperature. The exact structure of newly synthesized compounds was determined by means of X-ray diffraction and NMR spectroscopy. The cytotoxic activity of these compounds was evaluated, as well as their molecular action through western blot analysis of key proteins involved in apoptosis and determination of anti-angiogenic activity.

This work has been funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172016 and 175011).

Sinteza i antitumorska aktivnost defenilovanih analoga goniofufurona

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Goniofufuron, prirodni steryl-lakton izolovan iz kore drveta *Goniothalamus giganteus*, je potentan antitumorski agens.¹ Ovde želimo da saopštimo sintezu defenilovanog analoga goniofufurona (**1**), kao i niza defenilovanih analoga koji na C-7 imaju halogenidnu funkciju (**2–6**). Rezultati ispitivanja *in vitro* antitumorske aktivnosti sintetizovanih jedinjenja prema odabranim tumorskim ćelijskim linijama biće takođe prikazani i detaljno diskutovani.



Scheme 1. (a) Meldum's acid, Et₃N, DMF, 46 °C; (b) CCl₄, Ph₃P, Py, CH₂Cl₂, 0 °C→rt, 38%; (c) CBr₄, Ph₃P, Py, CH₂Cl₂, 0 °C→rt, 28%; (d) I₂, Ph₃P, Im, THF, reflux, 63%; (e) NaN₃, NH₄Cl, DMF, 50 °C, 66%; (f) DAST, CH₂Cl₂, 0 °C→rt, 42% (calc. on reacted **7**); (g) H₂, Pd/C, conc. HCl, EtOAc, rt, 73% (calc. on reacted **8**).

Synthesis and antitumour activity of dephenylated goniofufurone analogues

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Goniofufurone, natural styryl lactone isolated from the stem bark of *Goniothalamus giganteus*, is potent antitumour agent.¹ Herein, we disclose synthesis of dephenylated goniofufurone analogue (**1**) and a series of dephenylated analogues bearing halogen atoms at C-7 (**2–6**). The results of *in vitro* antitumor activities of synthesized compounds against a number of human tumour cell lines were recorded. These results will be presented and discussed in details.

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

- Fang, X. P.; Anderson, J. E.; Chang, C. J.; Fanwick, P. E.; McLaughlin, J. L. *J. Chem. Soc. Perkin Trans. 1* **1990**, 1655.
- Popsavin, V.; Grabež, S.; Popsavin, M.; Krstić, I.; Kojić, V.; Bogdanović, G.; Divjaković, V. *Tetrahedron Lett.* **2004**, 45, 9409.

Nova farmakofora aktivna na Ebola virus

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Ebola virus je veoma virulentan patogen koji uzrokuje smrtonosnu hemoragijsku groznicu kod ljudi i primata. Pokazalo se da imuno terapeutici, kao i druge složene makromolekulske formulacije, predstavljaju obećavajuće kandidate za lek. Ipak, nijedan od njih ne poseduje važne kvalitete malih molekula, kao što su niska cena, relativna jednostavnost pripreme, dug rok trajanja, lakoća skladištenja i mogućnost mehanizma dejstva na koji ne utiču brze mutacije virusa. Raniji rezultati dobijeni sa diazahrizenima¹, naveli su nas da razvijemo novo, manje hidrofobno i rastvorljivije 1,5-naftiridinsko jezgro. Sintetisali smo nekolicinu mono- i di-alkilamino supstituisanih derivata, i ustanovili da najaktivniji (struktura 1) poseduju IC₅₀ vrednosti do 780 nM u *in vitro* testovima baziranim na HeLa ćelijama. Takođe, oni poseduju vreme poluživota duže od 60 minuta u ljudskim mikrozomima, nizak „klirens“ (<23 µL/min/mg) i generalno nisku hepatotoksičnost u *in vitro* testovima na 24 sata sa HepG2 ćelijama (broj ćelija, veličina i intenzitet jedara, zaustavljanje ćelijskog ciklusa, mitohondrijski potencijal i masa, steatoza i aktivnost p53).

A novel anti-Ebola pharmacophore

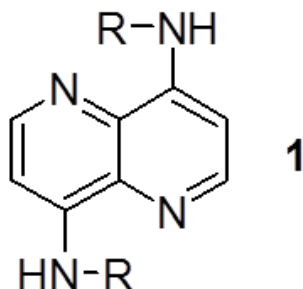
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The Ebola virus is a highly virulent pathogen that causes a deadly hemorrhagic fever in humans and non-human primates. Immuno-based therapeutics, as well as other

intricate macromolecular formulations, have proven to be promising drug candidates. Nevertheless, non of these possess the important attributes associated with small molecules, such as inexpensiveness, ease of preparation, long shelf life, facile storage, and the possibility of mechanisms of action circumventing rapid viral mutations. Earlier results of diazachrysene¹ derivatives led us to develop a novel, less hydrophobic and more water soluble 1,5-naphthyridine core. We synthesized several mono- and di-alkylamino substituted derivatives, and found that the most potent ones (structure 1), poses IC₅₀ values as low as 780 nM in HeLa cell based *in vitro* studies, show a higher than 60 minute half-life in human microsomes, low clearance rates (<23 µL/min/mg) and overall low hepatotoxicity in 24h *in vitro* HepG2 based tests (measuring total cell count, nuclear size and intensity, cell cycle arrest, mitochondrial potential and mass, steatosis and p53 activity).

1. a) Ž. Selaković, D. Opsenica, B. Eaton, C. Retterer, S. Bavari, J. C. Burnett, B. A. Šolaja, R. G. Panchal, *Viruses* **4** (2012) 1279. b) Ž. Selaković, V. Soloveva, D. Gharaibeh, J. Wells, S. Šegan, R. G. Panchal, B. A. Šolaja, *ACS Infectious Diseases* **1** (2015) 264.

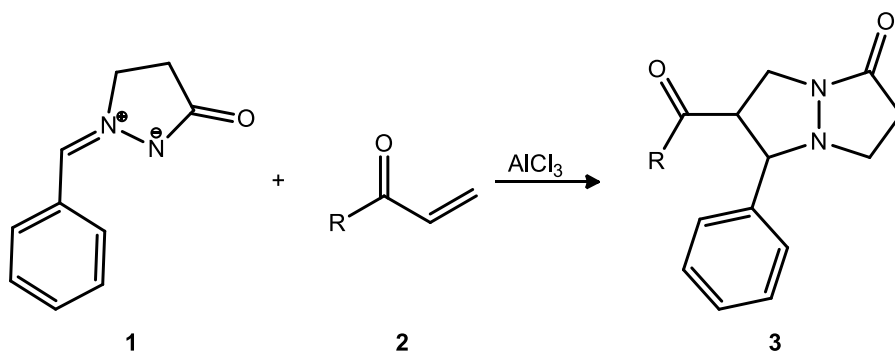
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Sinteza 6-acil-5-feniltetrahidropirazolo[1,2-a]pirazol-1(5H)-ona

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[3+2] Cikloadicije N,N' -cikličnih azometin imina su se ustalile kao pogodan metod za sintezu N,N' -bicikličnih heterocikala.¹ Ovaj strukturni fragment predstavlja čest konstituent brojnih farmaceutskih preparata, agrohemijskih proizvoda i drugih biološki aktivnih jedinjenja. U ovom radu će biti prikazana sinteza serije 6-acil-5-feniltetrahidropirazolo[1,2-a]pirazol-1(5H)-ona (**3**) ostvarena reakcijom između odgovarajućih enona (**2**) i azometin imina **1** u prisustvu AlCl_3 kao katalizatora. Dobijena jedinjenja će biti spektroskopski okarakterisana.



R = Me, Et, Ph, 4-Tol, thienyl, 2-Me-thienyl

Synthesis of 6-acyl-5-phenyltetrahydropyrazolo[1,2-a]pyrazol-1(5H)-ones

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[3+2] Cycloadditions of N,N' -cyclic azomethine imines are established as convenient method for the synthesis of N,N' -bicyclic heterocycles.¹ This structural fragment is the frequent constituent of numerous pharmaceuticals, agrochemicals, and other biologically active compounds. In this report we will describe the synthesis of the series of 6-acyl-5-phenyltetrahydropyrazolo[1,2-a]pyrazol-1(5H)-ones (**3**) achieved by the reaction of corresponding enones (**2**) and N,N' -cyclic azomethine imine **1** in the presence of AlCl_3 as the catalyst. The obtained compounds will be characterized by spectroscopic techniques.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project 172034).

1. C. Nájera, J. M. Sansano and M. Yus, *Org. Biomol. Chem.*, **13** (2015) 8596.

Ispitivanje antiproliferativne aktivnosti novih derivata benzotiazolamina prema MCF-7 ćelijskoj liniji humanog kancera dojke

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Poznato je da se mnogi lekovi, derivati benzotiazola, vrlo uspešno koriste u tretmanu različitih kliničkih stanja.¹ Takođe, značajno mesto zauzimaju u istraživanjima antitumorskih agenasa i veliki broj strukturnih modifikacija jezgra benzotiazola načinjen je s ciljem poboljšanja njihove antitumorske aktivnosti. U okviru naših istraživanja u ovoj oblasti sintetisana je serija novih karbamata i amida 6-alkiltio-supstituisanih benzotiazolamina i ispitana je njihova antiproliferativna aktivnost prema MCF-7 ćelijskoj liniji humanog karcinoma dojke. Pokazano je da derivati benzotiazolamina izazivaju visoko specifičnu programiranu ćelijsku smrt apoptozu u značajnom procentu tretiranih MCF-7 ćelija. Ispitan je i uticaj novih jedinjenja na ćelijski ciklus, mitohondrijski membranski potencijal i nivo unutarćelijskih reaktivnih kiseoničnih vrsta.

Investigation of antiproliferative activity of new benzothiazolamine derivatives against MCF-7 human breast cancer cell line

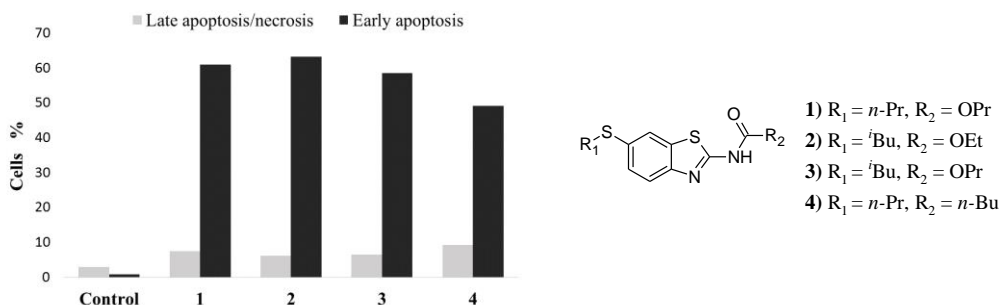
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Numerous benzothiazole-based clinical drugs have been extensively used in practice to treat various type of diseases with high therapeutic efficacy.¹ In addition, benzothiazole derivatives are compounds of an undoubted interest in anticancer research and a lot of structural modifications on their core nuclei have been made to improve their antitumor activity. Therefore, we have synthesized a series of novel 6-alkylthio-substituted benzothiazolamine carbamates and amides. To investigate their anticancer potency, we have used MCF-7 human breast cancer cell line. Benzothiazolamine derivatives show great potency for promoting highly specific programmed cell death apoptosis in MCF-7 cancer cell line. Our research continued towards examination of our compounds influence on cell cycle phase distribution, reactive oxygen species level and mitochondrial membrane potential.



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

1. R. S. Keri, M. R. Patil, S. A. Patil, S. A. Budagumpi, *Eur. J. Med. Chem.* **89** (2015) 207.

OHP 01

Antibakterijska aktivnost arildiketo kiseline prema rezistentnim sojevima bakterija

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****School of Life and Medical Sciences, University of Herfordshire

Sojevi bakterija otporni na dejstvo poznatih antibiotika predstavljaju veliki zdravstveni problem za ljudsku zajednicu. Arildiketo kiseline (ADK) su aktivne prema nekoliko rezistentnih sojeva Gram-pozitivnih *S. aureus* bakterija [1]. Jedinjenja sa voluminoznim supstituentima u *ortho*-položaju fenilnog jezgra su najaktivnija. Strukturnim modifikacijama ove klase molekula pokazano je da je diketo deo molekula esencijalan za antibakterijsku aktivnost ADK. Ovi rezultati, zajedno sa podacima iz literature [2], ukazuju na to da su prenil-transferaze (enzimi uključeni u biosintezu ćelijskog zida bakterije) moguće biološke mete dejstva ADK u bakterijskoj ćeliji. 3D QSAR modelom zasnovanim na poljima molekulskih interakcija izdvojene su važne strukturne karakteristike za antibakterijsku aktivnost ADK. Dobijeni model može se iskoristiti za dizajn aktivnijih derivata ADK kao i za virtuelni skrining.

Antibacterial activity of aryldiketo acids toward multidrug resistant bacterial strains

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Multidrug resistant (MDR) bacterial strains represent major health problem for the community, because of their rapidly growing resistance and pandemic potential. Aryldiketo acids (ADK) exerted antimicrobial activity against several resistant strains of Gram-positive *S. aureus* bacteria. Compounds having bulky alkyl group in *ortho*-position of phenyl ring were the most potent. Structural modifications of this class of molecules confirmed the importance of diketo moiety for antibacterial activity. These results, in combination with literature data, suggest that the enzymes prenyl-transferases (involved in cell wall biosynthesis) could be a possible biological target for ADK in bacterial cells. Using alignment independent 3D QSAR model based on molecular interaction fields, structural features important for antibacterial activity of ADK were found. Obtained model was statistically significant and could be used to guide the design of more potent derivatives as well as in virtual screening of novel antibacterial agents.

Acknowledgement: Ministry of Education, Science, and Technological Development of Serbia (Grant No. 172035) supported this work.

References:

1. B.J. Drakulić, M. Stavri, S. Gibbons, Ž.S. Žižak, T.Ž. Verbić, I.O. Juranić, M. Zloh, *ChemMedChem* 4 (2009) 1971. [2] Y. Zhang, Fu-Yang Lin, K. Li, W. Zhu, Y. Liu, R. Cao, R. Pang, E. Lee, J. Axelson, M. Hensler, K. Wang, K.J. Molohon, Y. Wang, D.A. Mitchell, V. Nizet, E. Oldfield, *ACS Med. Chem. Lett.* 3 (2012) 402.

OH P02

**Kvantitativni odnos strukture i retencionih vremena arilamida
4-aril-4-okso-2-butenskih kiselina zasnovanih na GRIND-2 deskriptorima**

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Arilamidi 4-aril-4-okso-2-butenskih kiselina ispoljavaju antiproliferativnu aktivnost *in vitro* prema ćelijskim linijama humanih tumora u mikromolarnim i submikromolarnim koncentracijama [1]. Tokom rutinske karakterizacije jedinjenja, zapažen je kvalitativan odnos između retencionih vremena određenih HPLC metodom i strukture jedinjenja. Retenciona vremena određena su na RP-C18 koloni i korelisana sa 3D strukturom jedinjenja, optimizovanom na MP2 nivou. Upotrebom GRIND-2 deskriptora, izvedenih iz polja molekulskih interakcija, dobijeni su jasni kvantitativni odnosi između 3D strukture jedinjenja i retencionih vremena. Strukturna svojstva 30 kongenera koja utiču na retenciona vremena su detaljno opisana.

**Quantitative structure-retention relationships of 4-aryl-4-oxo-2-butenic acid
arylamides based on GRIND-2 descriptors**

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4-Aryl-4-oxo-2-butenic acid arylamides exert antiproliferative activity toward human tumor cells *in vitro* in low micromolar to submicromolar concentrations [1]. During routine characterization of compounds, we observed qualitative relationship between HPLC retention times and structure of the compounds. Liquid chromatography (LC) was performed using RP-C18 column, and in this way obtained retention times correlated with the 3D structure of the compounds, optimized on MP2 level of theory. Using GRIND-2 descriptors, derived from molecular interaction fields, robust 3D quantitative structure-retention relationships were obtained. Structural features that differentiate 30 studied congeners in relation to LC retention times are described in details.

Acknowledgements: *This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Grant OI172035.*

References:

1. M. D. Vitorović-Todorović *et al.*, *Eur. J. Med. Chem.* 62 (2013) 40-50.

Ekperimentalno i kvantno-hemijsko proučavanja azo-hidrazon tautomerije kod hinolonskih azo boja

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Veliki broj heterocikličnih jedinjenja koristi se pri sintezi različitih boja i pigmentata. Među njima, najveću pažnju privukli su 2-piridoni i 2-hinoloni. U ovom radu, ispitivana su spektralna svojstva i tautomerija sintetisanih 4-supstituisanih fenilazo-4-hidroksi-2-hinolona (Slika 1), kao i kvantno-hemijski podaci mogućih tautomera. Eksperimentalni podaci su korelisani DFT teorijskim podacima i na osnovu dobijenih rezultata izvedeni su novi zaključci u vezi tautomerije kod ispitivanih hinolonskih azo boja.

Experimental and quantum-chemical study of azo-hydrazone tautomerism in certain quinolone azo dyes

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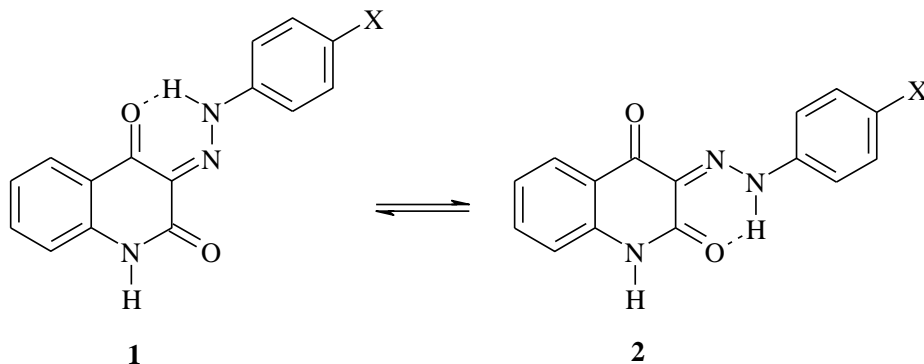
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A number of heterocyclic compounds have been used in the preparation of dyes and pigments. Among them 2-pyridones and 2-quinolones have gained considerable attention. In this work, the tautomerism of 4-substituted phenylazo-4-hydroxyl-2-quinolones (Figure 1), their spectral characterization and quantum-chemical results of possible tautomers are studied. Experimental and calculated data were correlated and new facts on tautomerism in quinolone azo dyes are presented.



Slika 1. Najdominantniji tautomerni oblici kod ispitivanih hinolonskih azo boja
 Figure 1. The most dominant tautomeric forms of the investigated quinolone azo dyes
 (X = OH, MeO, Me, H, F, Cl, Br, CN, COCH₃, NO₂).

Acknowledgment. Authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project 172013) for the financial support of this work.

Solvatohromna svojstva azo boja na bazi 4-hidroksi-2-hinolona: Eksperimentalno i kvantno-hemijsko proučavanje

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UV-Vis apsorpcioni spektri, solvatohromizam i tautomerija serije 4-supstituisanih fenilazo-4-hidroksi-2-hinolona (Slika 1) analizirani su u dvadeset različitih rastvarača. Efekat polarosti rastvarača, kao i proton-donorskih i proton-akceptorskih interakcija rastvarača sa molekulima azo boja proučavan je metodom linearne korelacije energije solvatacije (LSER analiza) korišćenjem Kamlet-Taftove i Katalanove jednačine. Takođe, analiza uticaja supstituenata na apsorpcione maksimume urađena je pomoću metode linearne korelacije slobodnih energija (LFER model) i to primenom Hametove jednačine.

Solvatochromic properties of azo dyes derived from 4-hydroxyl-2-quinolone: Experimental and quantum-chemical study

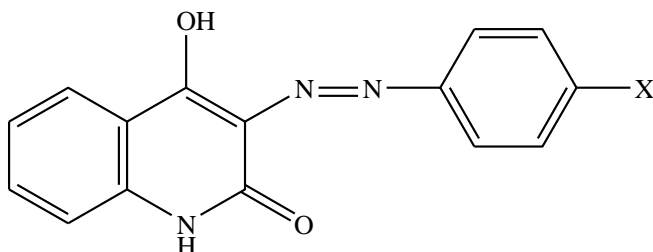
Violeta M. Arsovski, Jelena M. Mirković*, Julijana Tadić*, Bojan Đ. Božić*, Vesna D. Vitnik**, Željko J. Vitnik**, Gordana S. Ušćumlić*, Dušan Ž. Mijin*

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UV-Vis absorption spectra, solvatochromism and tautomerism of 4-substituted phenylazo-4-hydroxyl-2-quinolones (Figure 1) in twenty solvents have been analyzed. Effect of solvent polarity as well as proton-donating and proton-accepting interaction of solvent with azo dyes molecules have been investigated by means of linear solvation energy relationship (LSER) using the Kamlet-Taft and Catalán solvatochromic equations. Moreover, insight into substituent effects determining the absorption maxima shifts have been studied by the linear free energy relationship (LFER) concept proposed by Hammett.



X = -N(CH₃)₂, -OH, -OCH₃, -CH₃, -H, -F, -Cl, -Br, -COCH₃, -COOH, -CN, -NO₂

Slika 1. Struktura arilazo hinolonskih boja.

Figure 1. Structure of investigated arylazo quinolone dyes.

Acknowledgment: Authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project 172013) for the financial support of this work.

OH P05

Identifikacija proizvoda termolize metil-*N*-metil-*N*-nitrozoantranilata

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Poznato je da su *N*-nitrozo jedinjenja termalno nestabilna, ali se malo toga zna o reakcijama koje se odvijaju prilikom njihovog zagrevanja. Utvrđeno je da metil-*N*-metil-*N*-nitrozoantranilat (**1**), pri uslovima gasne hromatografije (GC-MS), podleže potpunoj termalnoj degradaciji dajući kao glavne proizvode metil-*N*-metilantranilat (**2**) i proizvod kuplovanja identifikovan kao 2,2'-(1,2-dimetilhidrazin-1,2-diil)dibenzoat (**3**). U cilju potvrde strukture proizvoda **3**, izvedena je preparativna termoliza jedinjenja **1**. Među 46 različitih sastojaka identifikovan je i potpuno spektralno okarakterisan novi proizvod kuplovanja metil-5-metil-6-okso-(5*H*)-fenantridin-4-karboksilat, dok proizvod **3** nije detektovan u termolizatu. Pažljivim razmatranjem struktura identifikovanih sastojaka termolizata predloženi su glavni putevi termolize jedinjenja **1** u parnoj i kondenzovanoj fazi. Generalno, identifikovani proizvodi bi mogli da se svrstaju u dve grupe, na one koji nastaju inicijalnim raskidanjem N–NO veze ili, neočekivano, Ar–NNO veze, tj. na proizvode koji su derivati antranilne i benzojeve kiseline. Strukturna raznolikost identifikovanih proizvoda i značajne razlike između termolize koja se odvija u parnoj i kondenzovanoj fazi ukazuju na mogući sintetski značaj termolize *N*-nitrozo jedinjenja.

Structural elucidation of thermolysis products of methyl *N*-methyl-*N*-nitrosoanthranilate

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Although it is common knowledge that *N*-nitroso compounds are thermally (and otherwise chemically) labile, little is known about the specific reactions that occur upon their heating. Methyl *N*-methyl-*N*-nitrosoanthranilate (**1**) was found to undergo complete thermal degradation under gas chromatographic (GC-MS) conditions yielding methyl *N*-methylantranilate (**2**) and a coupling product tentatively identified as dimethyl 2,2'-(1,2-dimethylhydrazine-1,2-diyl)dibenzoate (**3**), as the major ones. In an attempt to corroborate this find, a preparative scale thermolysis of compound **1** was carried out. Among 46 different products, a novel coupling product, methyl 5-methyl-6-oxo-(5*H*)-phenanthridine-4-carboxylate (**4**), was identified and fully spectrally characterized, while **3** was not detected in the thermolysate. A careful consideration of the structures of the identified thermolysate constituents led us to propose the major thermolysis pathways of **1** both in condensed and vapor phases. Generally, the identified products could be classified as those arising from fission of the N–NO bond or rather unexpectedly, the Ar–NNO bond, *i.e.* products related to anthranilic and benzoic acids, respectively. The structural diversity of the identified products and the noted marked differences between vapor and condensed phases point to the possible synthetic utility of thermolysis of *N*-nitroso compounds.

Acknowledgement: Ministry of Education, Science and Technological Development of Serbia (Grant No. 172061).

OH P06

Novi pirazolski pseudo-C-nukleozidi kao inhibitori rasta tumorskih ćelija

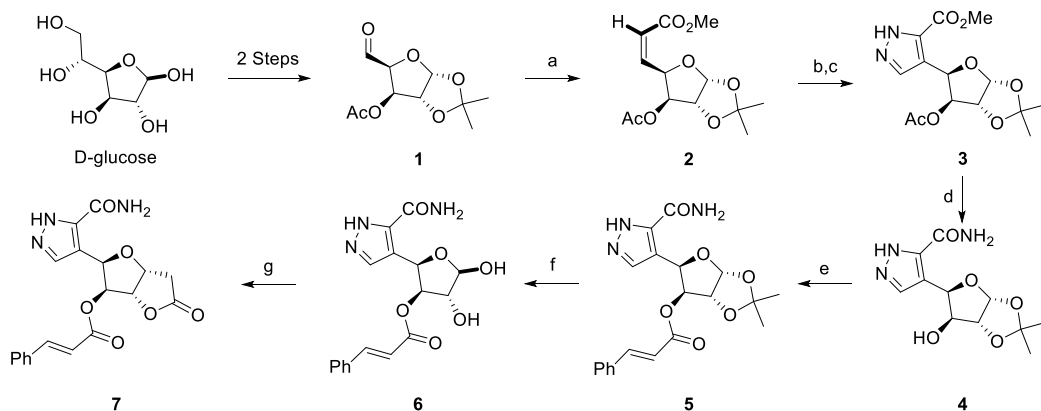
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U radu je ostvarena višefazna sinteza novih pseudo-C-nukleozida sa pirazolskim prstenom iz D-glukoze. Aldehyd **1** je uspešno preveden u ciljani molekul **7** nizom selektivnih hemijskih transformacija koje su prikazane na Shemi 1. Rezultati ispitivanja *in vitro* antiproliferativne aktivnosti jedinjenja **5** i **7** prema ćelijskim linijama odabranih humanih tumora biće takođe saopšteni i diskutovani.



Scheme 1. Reagents and conditions: (a) MCMP/MeOH, 0 °C → rt, 1.5 h; (b) CH₂N₂, Et₂O, 0 °C, 3 h; (c) Cl₂, CCl₄, 3 h; (d) NH₃, MeOH, 5 days; (e) cinnamic acid, DCC, DMAP, MeCN, rt, 45 h; (f) 90% aq TFA, rt, 1 h; (g) Meldrum's acid, DMF, Et₃N, 46 °C, 80 h.

Novel pyrazole pseudo-C-nucleosides as inhibitors of tumour cells growth

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Multi-step synthesis of novel pseudo-C-nucleosides containing pyrazole ring (compounds **5** and **7**) has been achieved starting from D-glucose. The aldehyde **1** was converted to the target **7** through a seven-step sequence outlined in Scheme 1. Results related to *in vitro* antiproliferative activity of **5** and **7** against a number of tumor cell lines will be presented and discussed.

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

OH P07

Azo-hidrazon tautomerija novih 5-arilazo-6(2)-hidroksi-4-metil-3-cijano-N(1)-fenil-2(6)-okso-piridin-3-karbonitrilnih boja

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Fizičko-hemijska svojstva arilazopiridonskih boja su usko povezana sa njihovim azo-hidrazo tautomerizmom. Pošto tautomeri imaju različita tehnička svojstva i performanse bojenja, proučavanje njihovog tautomerizma je važno kako sa teorijske, tako i sa praktične tačke gledišta. Mala razlika u energiji tautomera ih čini veoma osetljivim na uticaj sredine i efekata supstituenata. Tautomerna ravnoteža jedanaest arilazo piridonskih boja je proučavana na osnovu UV-Vis apsorpcionih spektara uz pomoć kvantno-mehaničkog modelovanja. NMR i teorijska izračunavanja korišćenjem PCM/xB97X-D/6-311G(d,p) metoda, potvrdili su da pripremljena jedinjenja postoje uglavnom u Hidrazo obliku. AIM topološka analiza i ukupna elektronska gustina na kritičnoj tački veze (BCP) potvrđuju su prisustvo jake intramolekulske vodonične veze koja doprinosi većoj stabilnosti Hidrazo oblika.

Azo-hidrazo tautomerism of novel 5-arylazo-6(2)-hydroxy-4-methyl-3-cyano-N(1)-phenyl-2(6)-oxo-pyridine-3-carbonitrile dyes

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The physico-chemical properties of arylazo pyridone dyes are closely related to their azo-hidrazo tautomerism. Since the tautomers have different technical properties and dyeing performances, studying the state of tautomeric equilibria is important from both theoretical and practical point of view. The small free energy difference between tautomers makes them sensitive to the influence of environment and substituent effects. The state of the tautomeric equilibria of eleven arylazo pyridone dyes was evaluated from UV-Vis absorption spectra with the aid of the quantum mechanical modeling. NMR analysis and theoretical calculations, by PCM/xB97X-D/6-311G(d,p) method, confirmed that prepared compounds exist mainly in Hydrazo form. AIM topological analysis and total electron density at the bond critical point (BCP) confirmed a presence of strong hydrogen bond which contributes to higher stability of Hydrazo form.

Ispitivanje kinetike i mehanizma fenilselenolaktonizacije 4-pentenske kiseline katalizovane trietilaminom

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U radu su predstavljeni rezultati ispitivanja kinetike i mehanizma fenilselenolaktonizacije 4-pentenske kiseline pomoću PhSeCl i PhSeBr, katalizovane trietilaminom. Glavni proizvod ove reakcije je γ -lakton koji u bočnom nizu sadrži PhSe-grupu koja posredstvom veoma jednostavnih hemijskih transformacija može lako biti prevedena u veliki broj korisnih funkcionalnih grupa. Takođe, značaj γ -laktona se ogleda i u tome što veliki broj molekula iz ove grupe predstavlja česte strukturne elemente mnogih biološki aktivnih jedinjenja.¹ Kinetika i mehanizam ovih reakcija ispitivani su UV-Vis spektrofotometrijski. Konstante brzine, kao i termodinamički parametri (ΔH^\ddagger , ΔS^\ddagger) su određeni koristeći UV-Vis metodu na tri različite temperature (288, 298 i 308K), u tetrahidrofuranu kao rastvaraču. Dobijeni rezultati ukazuju na veću efikasnost PhSeCl kao ciklizacionog reagensa u odnosu na PhSeBr. Takođe, visoke negativne vrednosti za entropiju aktiviranja i niske vrednosti entalpije aktiviranja sugerišu S_N2 mehanizam nukleofilne supstitucije.

Kinetic and mechanistic studies of triethylamine-catalyzed phenylselenolactonization of 4-pentenoic acid

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The aim of this work is exploration of kinetic and mechanistic aspects of triethylamine-catalyzed phenylselenolactonization of 4-pentenoic acid by means of phenylselenenyl halides (PhSeCl and PhSeBr). The major product of these reactions is γ -lactone with PhSe-functionalized side chain, which can be easily transformed in numerous useful functional groups by very simple chemical reactions. In addition, the importance of γ -lactones is reflected in the fact that a large number of these molecules present structural units of biologically active compounds.¹ The kinetic and mechanism for these reactions have been investigated by the UV-Vis spectrophotometry. The rate constants, as well as thermodynamic parameters (ΔH^\ddagger , ΔS^\ddagger) have been determined using UV-Vis method at three different temperatures (288, 298 and 308K) in THF as solvent. The large negative values for the entropy of activation and low enthalpy of activation with both reagents support the S_N2 mechanism, and obtained values for the rate constants have indicated higher reactivity of PhSeCl as reagent for cyclization.

Ovaj rad je finansijski potpomognut od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, projekat br. 172011.

1. T. Janecki, Natural Lactones and Lactams: Synthesis, Occurrence and Biological Activity, Wiley VCH, Verlag, 2013.

OH P09

Regioselektivnost i kinetika Co(II)hlorid katalizovane fenilselenociklizacije 6-metil-hept-5-en-2-ola

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Selenociklizacione reakcije verovatno predstavljaju najkorisniju primenu elektrofilnih seleno(II) reagenasa. Adicija ovih reagenasa na dvostruku vezu inicira nukleofilni napad pogodno orjentisane grupe, koja je sastavni deo supstrata, što rezultira stvaranjem cikličnog proizvoda. Zahvaljujući velikoj raznovrsnosti nukleofila koji se mogu upotrebiti, ove reakcije su našle rasprostranjenu primenu u sintezi prirodnih proizvoda, gde selenociklizacija predstavlja ključni korak u sintezi.¹ Iako ove reakcije imaju dobro utvrđenu sintetičku primenu, vrlo malo je učinjeno po pitanju boljeg razumevanja mehanizma i kinetike ovih reakcija. U ovom radu, mi smo pokušali da postignemo bolji uvid u mehanizam fenilselenoeterifikacije 6-metil-hept-5-en-2-ola kroz sintetičku i kinetičku studiju Co(II)hlorid-katalizovane ciklizacije pod uslovima reakcije *pseudo*-prvog reda uz pomoć UV-Vis spektrofotometrije. Poredeći sa rezultatima bazno katalizovanih reakcija, primećeno je da reakcije katalizovane sa CoCl₂ ispoljavaju mnogo bolju regioselektivnost. Dobijene vrednosti konstanti brzina reakcija potvrdile su katalitičku ulogu CoCl₂.

Regioselectivity and kinetics of Cobalt(II) chloride catalyzed phenylselenocyclization of 6-methyl-hept-5-en-2-ol

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Selenocyclization reactions are probably the most useful utilization of the electrophilic selenium(II) reagents. Addition of the reagents to the double bond triggers the nucleophilic attack of the suitably positioned pendant group resulting in the generation of a cyclic product. Due to the great diversity and versatility of pendant nucleophiles that can be used, these reactions have found widespread usage in some natural product synthesis, where the selenocyclization reaction represents the key step in their synthesis.¹ Although, these reactions have established synthetic utility, very little has been done in improvement of understanding the mechanism and kinetics of these reactions. In this work we tried to achieve better insight in the mechanism of phenylselenoetherification of 6-methyl-hept-5-en-2-ol through the synthetic and kinetic study of the Co(II) chloride catalyzed cyclization under *pseudo*-first order conditions by UV-Vis spectrophotometry. Compared to the Lewis base catalyzed reactions, of this alkenol, much better regioselectivity was expressed with CoCl₂. The obtained values for the rate constants have confirmed catalytic role of the CoCl₂.

Ovaj rad je finansijski potpomognut od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije, projekat br. 172011.

1. X. Jiang, H. Lui, in *Comprehensive organic synthesis*, P. Knochel, G. A. Molander, Ed(s)., Elsevier, 2014, p. 466.

OH P10

Sinteza, karakterizacija i citotoksičnost novih antrahinonskih amida

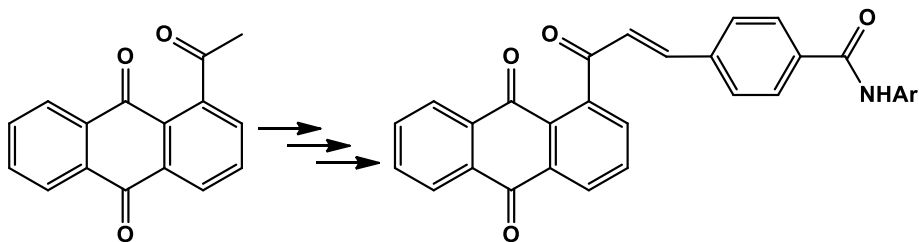
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Hibridni organski molekuli, koji u svojoj strukturi sadrže halkonsku i antrahinonsku farmakoforu, pokazali su izraženu citotoksičnost prema HeLa ćelijama uz relativno visoku selektivnost u odnosu na normalnu MRC-5 ćelijsku liniju.¹ Ovi rezultati podstakli su nas da sintetizujemo nove antrahinonske hibridne derivate koji sadrže α,β -nezasićeni konjugovani sistem u cilju poboljšanja citotoksične aktivnosti i selektivnosti dobijenih molekula. Dobijanje takvih jedinjenja ostvareno je polazeći od 1-acetil-antrahinona, koji u reakciji sa 4-formilbenzoeskom kiselinom daje odgovarajući halkonski prekursor koji se može dalje derivatizovati zahvaljujući prisustvu karboksilne grupe koja preko kiselinskog hlorida sa aromatičnim aminima daje finalne amidne derivate. Preliminarni rezultati citotoksične aktivnosti ukazuju na značajan antiproliferativni potencijal koji nameće potrebu daljeg ispitivanja mehanizma njihovog delovanja prema HeLa ćelijama.



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Synthesis, characterization and cytotoxicity of novel anthraquinone amides

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Hybrid organic molecules with chalcone and anthraquinone pharmacophores showed a pronounced cytotoxicity against HeLa cell line with good selectivity against normal MRC-5 cells.¹ These results encouraged us to prepare novel hybrid anthraquinone derivatives which contain α,β -unsaturated conjugated system, with intention to increase cytotoxicity and selectivity of obtained molecules. The synthesis of these compounds starts with the reaction of 1-acetyl-antraquinone with 4-formylbenzoic acid giving the corresponding chalcone precursor, which can be subjected to further derivatization due to the presence of carboxylic group which can be transformed into corresponding chloride and react with aromatic amines to give final amid derivatives. Preliminary results of cytotoxic activity show considerable antiproliferative potential which impose the necessity to further examine their mechanism of action against HeLa cell line.

This work has been funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172016 and 175011).

1. V. Marković et al. *Eur. J. Med. Chem.* **89** (2015) 401.

OH P11

Sinteza i karakterizacija 1,3,5-trisupstituisanog-1,2-azaboracikloheksana

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Visoko regioselektivnom reakcijom benzilamina i etil-propiolata moguće je dobiti δ -dienamino estar u neutralnim uslovima, ili β -*N,N*-dienamino estar u baznim uslovima. δ -Dienamino estar upotrebljen je kao supstrat za stereoselektivnu sintezu 1,3,5-trisupstituisanog-1,2-azaboracikloheksana. Dobijeno jedinjenje okarakterisano je na osnovu IC, HRMS, 1D i 2D NMR spektroskopije. NOE eksperiment ukazao je na *trans* konfiguraciju dve estarske grupe, pri čemu je grupa vezana za C-3 atom u ekvatorijalnom položaju, a grupa vezana za C-5 atom u aksijalnom položaju. Benzil-grupa vezana za atom azota je ekvatorijalno orijentisana.

Zahvalnica: Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije za finansijsku podršku (Projekat br. 172020).

**Synthesis and Characterization of
1,3,5-Trisubstituted-1,2-azaboracyclohexane**

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The highly regioselective reaction of benzylamine and ethyl propiolate affords δ -dienamino ester under neutral conditions, or β -*N,N*-dienamino ester under basic conditions. The former was employed as a substrate for the stereoselective synthesis of 1,3,5-trisubstituted-1,2-azaboracyclohexane. It was characterized on the basis of IR, HRMS, 1D and 2D NMR techniques. The NOE experiment revealed *trans* relationship between the two ester groups, the one attached at the C-3 being in equatorial position and the one attached at the C-5 in the axial position. The *N*-Bn substituent is equatorially oriented.

Acknowledgement: Financial support from the Ministry of education, science and technological development of the Republic of Serbia is acknowledged (Project No. 172020).

Sinteza i antitumorska aktivnost (–)-kleistenolida

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(–)-Kleistenolid (**1**) je prirodni proizvod izolovan iz biljke *Cleistochlamys kirkii* poreklom iz Tanzanije i Mozambika. Jedinjenje **1** pokazuje antibakterijsku (*Staphylococcus aureus* i *Bacillus anthracis*) i antigljivičnu aktivnost (*Candida albicans*). Ovom prilikom želimo da saopštimo novu totalnu sintezu jedinjenje **1** polazeći iz diacetonida D-glukoze (**2**). Molekul **2** je preveden u finalni proizvod **1** primenom višefazne sintetičke sekvence prikazane na reakcionoj shemi. Kolorimetrijskim MTT testom je po prvi put utvrđeno da molekul **1** pokazuje *in vitro* antitumorsku aktivnost prema panelu malignih ćelijskih linija.

Synthesis and antitumour activity of (–)-cleistenolide

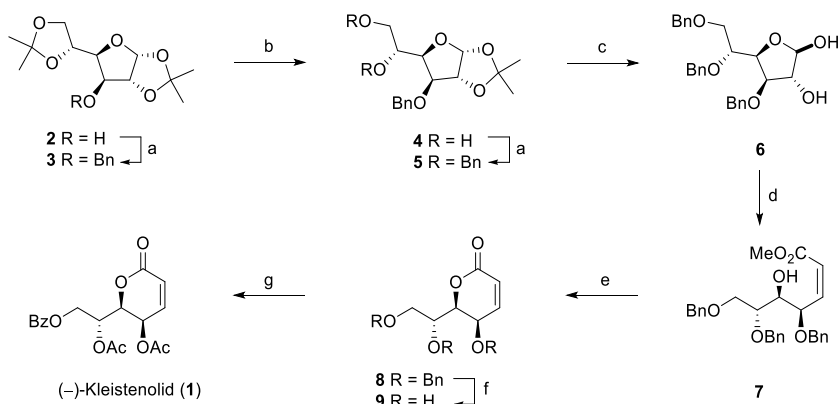
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(–)-Cleistenolide (**1**) is a natural product isolated from the plant *Cleistochlamys kirkii* originating from Tanzania and Mozambique. Compound **1** shows antibacterial activity against *Staphylococcus aureus* and *Bacillus anthracis*, as well as antifungal activity against *Candida albicans*. Herein we wish to report a new total synthesis of natural product **1** starting from diacetonide D-glucose (**2**). Molecule **2** was converted to the final product **1** through a multi-step sequence outlined in the reaction scheme. Using the MTT colorimetric assay it was found, for the first time, that molecule **1** shows *in vitro* antitumour activity against a panel of malignant cell lines.



Reagents and conditions: (a) *BnBr*, *NaH*, *DMF*, 0°C, rt; (b) aq 60% *AcOH*, rt; (c) aq 50% *TFA*, rt; (d) (i) *H₅IO₆*, *EtOAc/H₂O*; (ii) *MeOH*, *MCMP*, rt; (e) *TsOH*, *CH₂Cl₂*, rt; (f) *FeCl₃*, *CH₂Cl₂*, rt; (g) *BzCl*, *Ac₂O*, *CH₂Cl₂/Py*, rt.

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

OH P13

Sinteza novih anilidopiperidina kao potencijalnih opioidnih agonista

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U okviru našeg istraživanja o farmakološki aktivnim anilidopiperidinima sintetisali smo četiri nova analoga, *trans*-1-fenetil-4-(*N*-fenilpropionamido)piperidin-3-karboksamid (**3**), *trans*-metil (1-fenetil-4-(*N*-fenilpropionamido)piperidin-3-il)karbamat (**4**) i *cis* i *trans*-5-fenetil-1-fenilheksahidro-1H-imidazo[4,5-*c*]piridin-2(3H)-on (**5** i **6**). Ovde je predstavljena njihova parcijalna sinteza polazeći od *cis/trans* izomera 1-fenetil-4-(fenilamino)piperidin-3-karboksamida (**1** i **2**). Jedinjenja **4**, **5** i **6** dobijena su modifikovanom metodom Hofmann-ovog premeštanja, koju smo nedavno objavili, (put A odnosno put B). **Put A**: *N*-ptopionilovanjem karboksamida **1** propionil hloridom u prisustvu trietilamina, dobijen je karboksamid **3**, u skromnom prinosu (40%). U reakciji Hofmann-ovog premeštanja, pod sledećim reakcionim uslovima: *N*-bromoacetamid, litijum hidroksid, metanol, karbamat **4** dobijen je stereoselektivno u visokom prinosu (80%) iz karboksamida **3**. **Put B**: direktnim Hofmann-ovim premeštanjem karboksamida **1** i **2** pod već pomenutim uslovima, dobijene su ciklične uree, **5** i **6** stereoselektivno u visokom prinosu (~85%).

Reakcije su stereoselektivne (u oba reakciona puta), jednostavne za izvođenje, podrazumevaju laku obradu i izolovanje proizvoda reakcije i upotrebu jeftinih reagenasa.

Synthesis of novel anilidopiperidines as potencial opioid agonists

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As a part of our ongoing research on pharmacologically active anilidopiperidines, four new analogs namely *trans*-1-phenethyl-4-(*N*-phenylpropionamido)piperidine-3-carboxamide(**3**), *trans*-methyl (1-phenethyl-4-(*N*-phenylpropionamido)piperidin-3-yl)carbamate (**4**), and *cis* and *trans*-5-phenethyl-1-phenylhexahydro-1H-imidazo[4,5-*c*]pyridin-2(3H)-one (**5** and **6**) were synthesized. Herein we present their partial synthesis from *cis* and *trans* isomers of 1-phenethyl-4-(phenylamino) piperidine-3-carboxamide (**1** and **2**). Compounds **4**, **5** and **6**, were obtained by Hofmann rearrangement, a novel method that we published recently, pathway A and B, respectively. **Pathway A**: *N*-propionylation of carboxamide **1** with propionyl chloride in the presence of triethyl amine provided carboxamide **3** in moderate yields (~40%). In the reaction of Hofmann rearrangement under following reaction conditions: *N*-bromoacetamide, lithium hydroxide, methanol/, carbamate **4** was obtained from carboxamide **3**, in high yields (~80%). **Pathway B**: a direct Hofmann rearrangement of carboxamides **1** and **2**, under the aforementioned reaction conditions, afforded *cis* and *trans* cyclic ureas **5** and **6** (yield ~85%).

Reactions are stereoselective (in both pathways), and easy to perform. The products could be isolated by simple procedure and reagents are cheap.

Authors acknowledge the Ministry of Education, Science and Technological Development of the Republic of Serbia for financial support, grant No. 172032.

OH P14

Sinteza, antimikrobna i antioksidativna aktivnost novih benzociklobutan-2,5-diona

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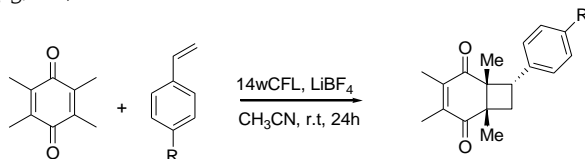
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Nekoliko novih benzociklobutan-2,5-diona je sintetisano reakcijom fotocikloadicije durohinona sa nekiloko različito supstituisanih etilena. Reakcija je izvedena u prisustvu 14W CFL lampe kao izvora svetlosti. Dobijena jedinjenja su testirana na antimikrobno i antioksidativno dejstvo. Antimikrobna aktivnost je testirana na Gram –pozitivnim bakterijama (*Bacillus spizizenii* ATCC 6633 and *Staphylococcus aureus* ATCC 6538) i tri Gram-negativne bakterije (*Escherichia coli* ATCC 8739, *Pseudomonas aeruginosa* ATCC 9027 and *Salmonella abony* NCTC 6017). Minimalne inhibitorne koncentracije (MIK) su varirale između 0.25 i 1 mg/ml. Svi testirani uzorci su bili aktivni na *B. spizizenii*, *S. aureus* i *P. aeruginosa* a neaktivni protiv *E. coli* i *S. abony*.

Lipidno peroksidativna aktivnost sintetisanih jedinjenja merena je TBA-MDA testom (tiobarbiturna kiselina-malondialdehid). Testirana jedinjenja su pokazala veoma dobra antioksidativna svojstva (sa IC₅₀ vrednostima između 53.88 i 81.51 µg/ml). Njihova antioksidativna svojstva su uporediva sa kvercetinom (IC₅₀ = 10.47 µg/mL).



Scheme 1. Synthesis of benzocyclobutane-2,5-diones

Synthesis, antibacterial and antioxidant activity of new benzocyclobutane-2,5-diones

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Several new benzocyclobutane-2,5-diones were synthesized using photocycloaddition reaction of duroquinone with various phenylsubstituted ethylenes. Reaction is performed in the presence of 14W CFL lamp i.e. reaction is catalyzed by visible light. Upon synthesis their antibacterial and antioxidant properties were examined.

Antimicrobial activity was evaluated against two Gram-positive bacteria (*Bacillus spizizenii* ATCC 6633 and *Staphylococcus aureus* ATCC 6538) and three Gram-negative bacteria (*Escherichia coli* ATCC 8739, *Pseudomonas aeruginosa* ATCC 9027 and *Salmonella abony* NCTC 6017). The minimal inhibitory concentrations (MICs) varied between 0.25 and 1.0 mg/mL. All tested samples were effective against *B. spizizenii*, *S. aureus* and *P. aeruginosa* but also inactive against *E. coli* and *S. abony*. Lipid peroxidation (LP) inhibition level in the presence of the synthesized compounds, was measured by thiobarbituric acid–malondialdehyde (TBA–MDA) test. Tested compounds possessed very good antioxidant properties (with IC₅₀ values between 53.88 and 81.51 µg/mL). Their antioxidant effects are comparable to that of quercetin (IC₅₀ = 10.47 µg/mL).

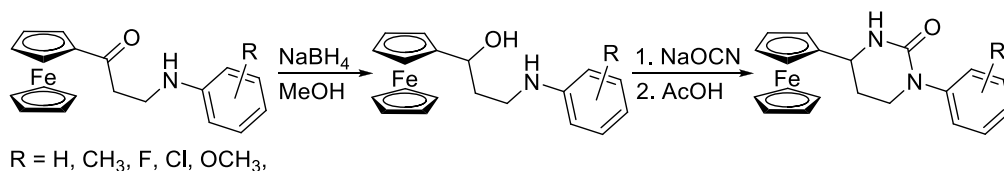
This work was supported by the Ministry of Education and Science of the Republic of Serbia (project No. 172020)

OH P15

Sinteza 1-aryl-4-feroceniltetrahidropirimidin-2(1H)-onaAleksandra Minić, Dragana Stevanović, Anka Pejović, Niko Radulović*, Rastko D. Vukićević
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Jedinjenja čije strukture obuhvataju tetrahidropirimidinonski prsten pokazuju različite oblike biološke aktivnosti,¹ pa postoji stalno interesovanje za njihovu sintezu. U ovom radu biće opisana sinteza serije derivata ovog heterocikla koji sadrže i ferocensko jezgro - 1-aryl-4-feroceniltetrahidropirimidin-2(1H)-ona, polazeći od ranije opisanih 3-amino-aryl-1-ferocenilpropan-1-ona.² Redukcija ovih pomoću NaBH₄ daje odgovarajuće 1,3-amino-alkohole, koji pod dejstvom ultrazvučnih talasa reaguju sa natrijum-cijanatom dajući hidroksiuree. Tetiranjem hidroksiurea sirćetnom kiselinom (preko stabilnog α -ferocenil-karbokatjona) nastaju ciljna jedinjenja.³

**Synthesis of 1-aryl-4-ferocenyltetrahydropyrimidin-2(1H)-ones**Aleksandra Minić, Dragana Stevanović, Anka Pejović, Niko Radulović*, Rastko D. Vukićević
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Compounds containing a tetrahydropyrimidinone ring exhibit different kinds of biological activity,¹ therefore, there is a permanent interest in their synthesis. In this work we wish to report on a protocol for the synthesis of a series of derivatives of this heterocycle containing also a ferrocene nucleus - 1-aryl-4-ferocenyltetrahydropyrimidin-2-(1H)-ones - starting from 3-aminoaryl-1-ferocenylpropan-1-ones, recently described by us.² The NaBH₄ reduction of these compounds gave the corresponding 1,3-aminoalcohols which were, then, submitted to the reaction with sodium cyanate under an ultrasound irradiation. This gave the corresponding hydroxyureas, which in a subsequent treatment with acetic acid gave (*via* a stable α -ferrocenyl carbocation) the target molecules.³

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project 172034).

1. P. Babczinski *et al.*, *Pestic. Biochem. Phziol.*, **52** (1995) 33.
2. a) I. Damljanović *et al.*, *J. Organomet. Chem.* **696** (2011) 3703; b) A. Pejović *et al.*, *Helv. Chim. Acta*, **95** (2012) 1425.
3. A. Minić *et al.*, *RSC Adv.*, **5** (2015) 24915.

Primena acil-piruvata u sintetičkoj hemiji

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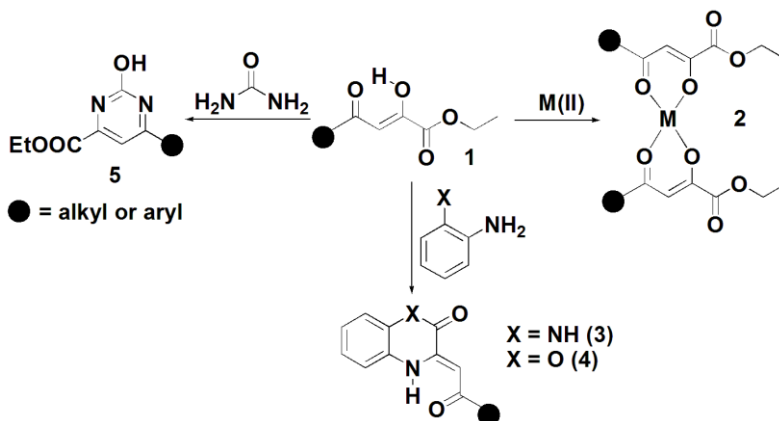
Acil-piruvati (1) predstavljaju klasu molekula koji imaju značajnu primenu u sintetičkoj hemiji.¹ Korišćeni su kao polazna jedinjenja u sintezi malih biblioteka novih M(II) kompleksa (2), hinoksalin-2(1H)-ona (3), benzo[b][1,4]oksazin-2-ona (4) i 2-hidroksi-pirimidina (5). Sva jedinjenja su dobijena u dobrim do odličnim prinosima.

Application of acyl pyruvates in sintethic chemistry

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Acyl pyruvates (1) represent a class of molecules that have attracted a considerable interest in synthetic chemistry.¹ These molecules were used as a starting compounds in synthesis small libraries of novel M(II) complexes (2), quinoxalin-2(1H)-ones (3), benzo[b][1,4]oxazin-2-ones (4) and 2-hydroxy-pyrimidines (5). Yields were good-to-excellent for all compounds.



Acknowledgements: The authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia for financial support (Grant 172011)

1. S. V. Ryabukhina et. al. *Tetrahedron Lett.* **51**(2010) 4229.



Biološki aktivno vlakno sa ceftriaksonom

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Osobine biološki aktivnih vlakna zavise od vrste nosača i od strukture samog lijeka. U ovom radu selektivnom oksidacijom celuloznog zavoja dobijena je oksidovana celuloza (OC) sa različitim sadržajem karboksilnih grupa koja je iskorištena za hemijsko vezivanje antibiotika ceftriaksona.

Vezivanje lijeka vršeno je iz vodenog rastvora antibiotika koncentracije $c=3,4 \cdot 10^{-3}$ mol/L na sobnoj temperaturi (22 ± 1 °C), a desorpcija lijeka u fiziološkom rastvoru. Količine vezanog i otpuštenog lijeka određene su spektrofotometrijski u UV području. Maksimalna količina vezanog lijeka (0,1032 mmol/g) dobijena je sorpcijom na modifikovani zavoj sa 2,276 mmol/g COOH, a maksimalna količina desorbovanog ceftriaksona iznosila je 0,0060 mmol/g. Antimikrobno djelovanje uzoraka zavoja sa vezanim ceftriaksonom testirano je *in vitro* na kulture *Staphylococcus aureus*, *Bacillus subtilis* i *Escherichia coli* metodom difuzije na agarnoj ploči. Najveća zona inhibicije dobijena je u odnosu na *Staphylococcus aureus*.

U radu se proučava uticaj hemijske strukture ceftriaksona, pH vrijednosti rastvora iz koga se vrši sorpcija kao i sadržaja karboksilnih grupa OC na količinu vezanog lijeka. Ustanovljeno je da se vezivanje ostvaruje jonskim i vodoničnim vezama lijeka sa oksidovanim celuloznim zavojem.

Biologically active fiber containing ceftriaxone

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Properties of biologically active fiber depend on the type of carrier and the structure of the drug. In this paper oxidized cellulose (OC) with different carboxylic group content is obtained by selective oxidation and used for chemical bonding of antibiotic ceftriaxone.

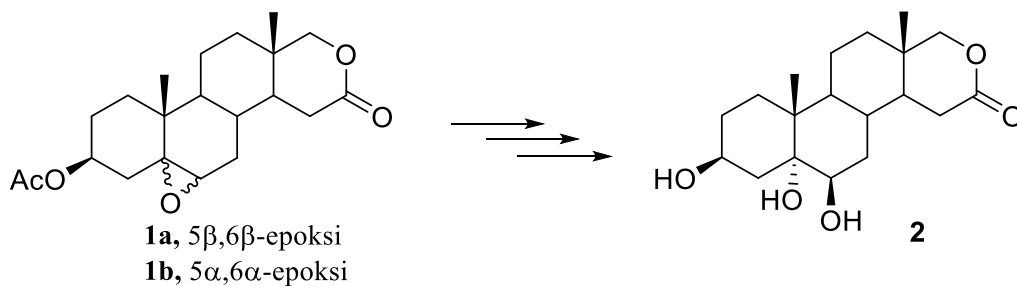
The bonding was performed in antibiotic water solution concentration of $c=3,4 \cdot 10^{-3}$ mol/L at room temperature (22 ± 1 °C), while desorption was performed in physiological solution. The amounts of bonded and released antibiotic were determined spectrophotometrically in UV range. Maximum amount of bound drug (0,1032 mmol/g) was obtained during the sorption on the oxidized bandage with 2,276 mmol/g COOH and the maximum amount of released ceftriaxone was 0,0060 mmol/g. Antimicrobial activity of the samples with bonded ceftriaxone was tested *in vitro* against *Staphylococcus aureus*, *Bacillus subtilis* and *Escherichia coli* by agar diffusion test. The biggest zone of inhibition was obtained for *Staphylococcus aureus*.

The paper studies the influence of ceftriaxone chemical structure, solution pH in which sorption is performed and content of carboxyl group OC, on the amount of bonded drug. It was established that the drug bonding was achieved by ionic bonds and the hydrogen bonds of the drug functional groups with oxidised cellulose bandage.

Hemijske modifikacije 5 α ,6 α - i 5 β ,6 β -epoksida u cilju dobijanja 3 β ,5 α ,6 β -trihidroksi derivata steroidnog D-homo laktona

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Budući da su se steroidni derivati sa hidroksilnim funkcijama u A- i B-prstenovima pokazali kao potentni citotoksični agensi, 3 β -acetoksi-5 β ,6 β -epoksi-17-oxa-17a-homoandrost-16-on (**1a**) i njegov 5 α ,6 α -epoksi derivat (**1b**)¹, podvrgnuti su nizu hemijskih modifikacija u cilju dobijanja 3 β ,5 α ,6 β -trihidroksi-17-oxa-17a-homoandrost-16-ona (**2**). Nakon oksidativnog otvaranja epoksida **1a** i **1b**, usledile su redukcija dobijene karbonilne grupe u položaju C6 i deacetilovanje u položaju C3 steroidnog skeleta. Redosled poslednje dve faze u sintezi je menjan radi utvrđivanja najefikasnijeg reakcionog puta, a u cilju povećanja prinosa željenog trihidroksilnog proizvoda **2**.



Chemical modifications of the 5 α ,6 α - and the 5 β ,6 β -epoxide in the purpose of obtaining 3 β ,5 α ,6 β -trihydroxy steroidal D-homo lactone

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Considering that steroidal derivatives with the hydroxyl functions in the A and B-rings have shown themselves as potent cytotoxic agents, 3 β -acetoxy-5 β ,6 β -epoxy-17-oxa-17a-homoandrost-16-one (**1a**), as well as its 5 α ,6 α -epoxy derivative (**1b**)¹, were subjected to a series of chemical modifications in the purpose of obtaining 3 β ,5 α ,6 β -trihydroxy-17-oxa-17a-homoandrost-16-one (**2**). Oxidative opening of the epoxide **1a** i **1b** was followed by the reduction of the resulting carbonyl group in the position C6 and the deacetylation in position C3 of the steroid skeleton. The order of the last two phases of the synthesis was changed in order to determine the most efficient reaction pathway and to increase the yield of the desired product **2**.

1. E. A. Đurendić, M. P. Savić, O. R. Klisurić, M. N. Sakač, G. M. Bogdanović, D.S. Jakimov, K. M. Penov Gaši, Struct. Chem. **23** (2012) 1761–1767

OH P19

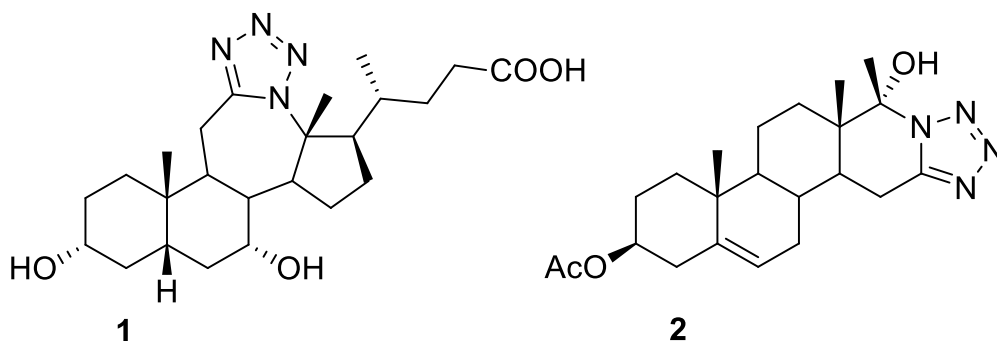
Sinteza novih C i D kondenzovanih steroidnih tetrazola

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Tetrazoli poseduju različite biološke, kao i jedinstvene fizičko-hemijske i farmakološke osobine. Imajući ovo u vidu, cilj ovog rada bio je sinteza steroidnih tetrazola.

Holna kiselina, odnosno dehidroepiandrosteron su poslužili kao polazna jedinjenja u sintezi željenih tetrazola. Ključni korak u sintezi tetrazola **1** je reakcija odgovarajućeg 12-okso intermedijera sa hidrazoinском kiselinom (HN_3), u prisustvu bortrifluorid-eterata kao katalizatora, a u slučaju sinteze tetrazola **2** je reakcija 16,17-seko-16-nitrila sa natrijum-azidom.

Struktura novosintetisanih jedinjenja potvrđena je NMR spektroskopskom analizom.

**Synthesis of new C and D fused steroidal tetrazoles**

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Tetrazoles possess various biological, and unique physicochemical and pharmacological properties. Having that in mind the aim of our work was to synthesise steroidal tetrazoles. Holic acid and dehydroepiandrosterone were used as starting compounds for synthesis of desired tetrazoles. The key step in synthesis of tetrazole **1** is the reaction between 12-oxo intermediate and hydrazoic acid (HN_3) in the presence of borontrifluoride-etherate as a catalyst, while in synthesis of tetrazole **2** is reaction between 16,17-seco-16-nitrile and sodium azide.

Structures of newly synthesized compounds were confirmed by NMR analysis.

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

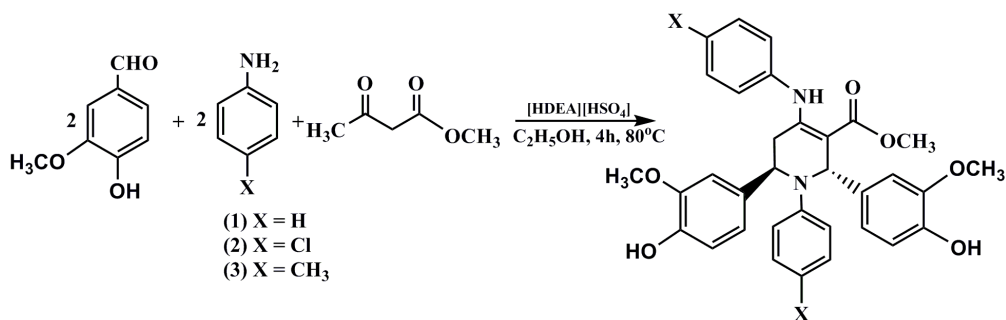
OHP 21

Diastereoselektivna one-pot sinteza vanilin-piperidinskih derivata i ispitivanje njihove antioksidativne aktivnosti

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U efikasnoj dvostrukoj one-pot Manihovoj reakciji između vanilina, metil-acetoacetata i različitih supstisuanih anilina dobijeni su visoko funkcionalizovani piperidinski derivati u dobrom prinosu (Shema 1). Kao reciklabilan katalizator ove reakcije upotrebljena je jonska tečnost dietanolamonijumhidrogensulfat. Važno je istaći da je ova ekonomična reakcija *anti*-diastereoselektivna, odnosno da je u njoj nastao samo *anti*-diastereoisomer.

Sintetizovana jedinjenja reaguju dobro sa DPPH radikalom i ispoljavaju visoku aktivnost, malo nižu u odnosu na referentno jedinjenje NDGA. Jedinjenja **1-3** imaju slične IC₅₀ vrednosti i one iznose 10.9, 12.5 i 11.1 μM.



Diastereoselective one-pot synthesis of vanillin-piperidine derivatives and investigation of their atioxidative activity

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In the efficient one-pot double Mannich reaction of vanillin, methyl acetoacetate and different substituted anilines were obtained highly functionalized piperidine derivatives in good yield (Scheme 1). The ionic liquid diethanolammonium hydrogensulfate was used as recyclable catalyst. It is worth pointing out that this economical reaction is *anti*-diastereoselektivna, namely in this reaction was formed only *anti*-diastereomer.

The synthesized compounds interact well with DPPH radical, and exhibit high activity, slightly lower than the reference compound NDGA. Compounds **1-3** have similar IC₅₀ values 10.9, 12.5 i 11.1 μM, respectively.

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

Reference

1. Hamid Reza Shaterian, Kobra Azizi, *Journal of Molecular Liquids* **180** (2013) 187-191

OH P22

Sinteza i antifungalna aktivnost novih izokumarinskih i tioizokumarinskih derivata

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Izokumarini su sekundarni metaboliti biljaka, gljiva i nekih bakterija. Ovi prirodni proizvodi pokazuju širok spektar farmakološkog dejstva, uključujući antimikrobno, citotoksično, antimalarijsko i antiinflamatorno dejstvo. Naša prethodna istraživanja su pokazala da sintetski izokumarini supstituisani azolima u položaju 3 pokazuju značajnu antifungalnu aktivnost. Cilj ovog rada je sinteza novih izokumarinskih i tioizokumarinskih derivata i evaluacija njihove *in vitro* antifungalne aktivnosti prema gljivici *Candida albicans*. Rezultati su pokazali da dobijeni tioizokumarinski derivati pokazuju antifungalnu aktivnost uporedivu sa vorikonazolom, dok se aktivnost nitro-izokumarina nije pokazala značajnom.

Zahvalnica: Ovo istraživanje je podržano od strane Ministarstva prosvete, nauke i tehnološkog razvoja Srbije (projekti br. 172009 i 173048).

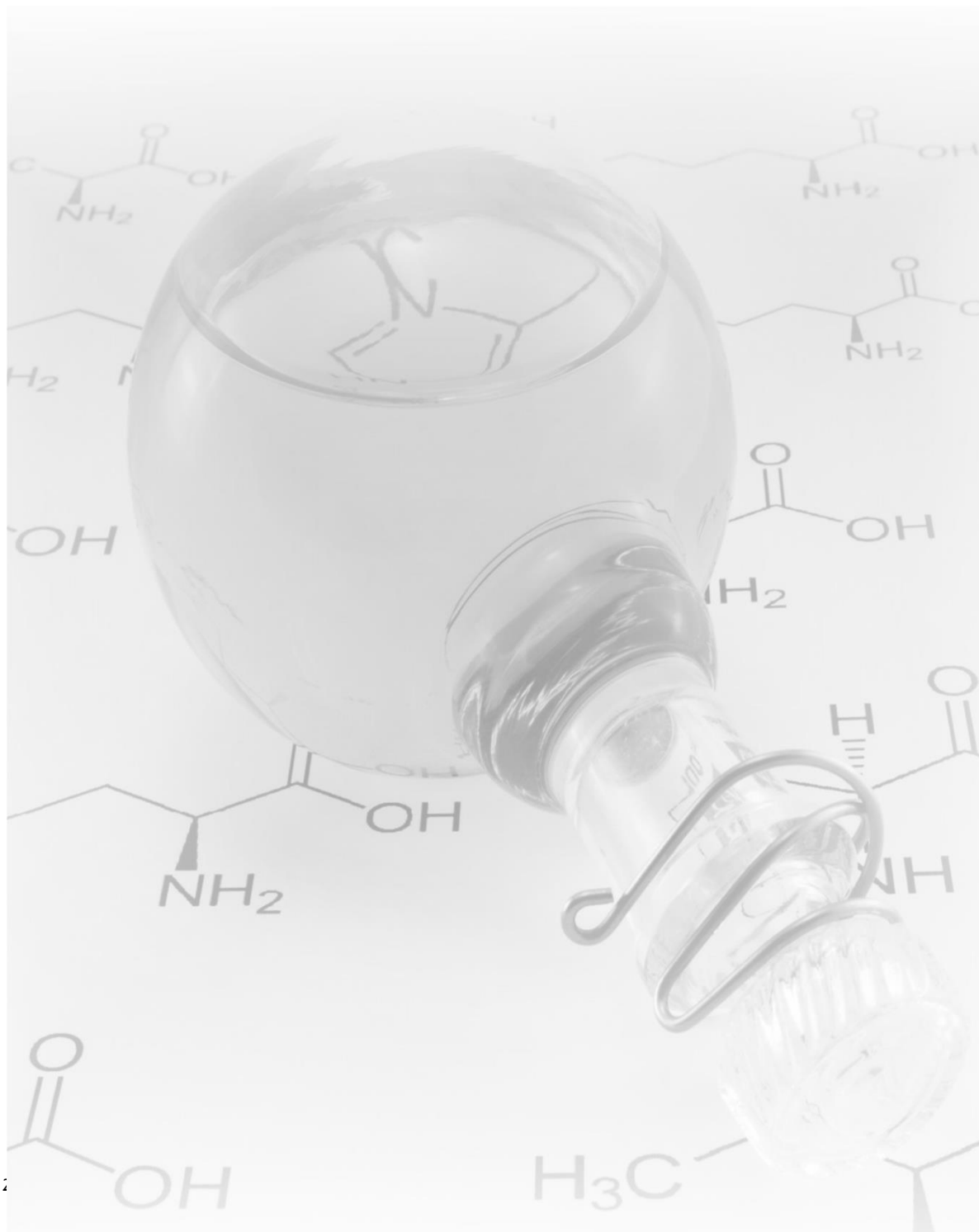
Synthesis and antifungal activity of novel isocoumarin and thioisocoumarin derivatives

Milena Simic, Ivan Boric, Sandra Vojnovic*, Jasmina Nikodinovic-Runic*, Gordana Tasic, Milos Petkovic, Predrag Jovanovic, Vladimir Savic
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Isocoumarins are secondary metabolites of the plants, fungi, and some bacteria. These natural products exhibit a broad range of pharmacological activities, including antimicrobial, cytotoxic, antimalaric and antiinflammatory activity. Our previous work showed that azol-substituted isocoumarins have significant antifungal activity. The aim of his study was the synthesis of new isocoumarins and thioisocoumarins (1*H*-isochromen-1-thion) substituted in position 3 and evaluation of their *in vitro* antifungal activity against *Candida albicans*. Synthesised thio derivatives showed antifungal activity comparable with voriconazole.

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