Srpsko hemijsko društvo
Serbian Chemical Society

Klub mladih hemičara Srbije
Serbian Young Chemists' Club

51. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA
i
2. KONFERENCIJA MLADIH HEMIČARA SRBIJE

PROGRAM
i
KRATKI IZVODI RADOVA

51st Meeting of the Serbian Chemical Society
and
2nd Conference of the Young Chemists of Serbia

Program
&
Book of Abstracts

Niš, 5-7. juni 2014.
Niš, Serbia, June 5-7, 2014

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2. KONFERENCIJA MLADIH HEMIČARA SRBIJE, NIŠ, 5-7. JUNI 2014.
PROGRAM I KRATKI IZVODI RADOVA

51ST MEETING OF THE SERBIAN CHEMICAL SOCIETY AND
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PROGRAM AND BOOK OF ABSTRACTS

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2. KONFERENCIJA MLADIH HEMIČARA SRBIJE
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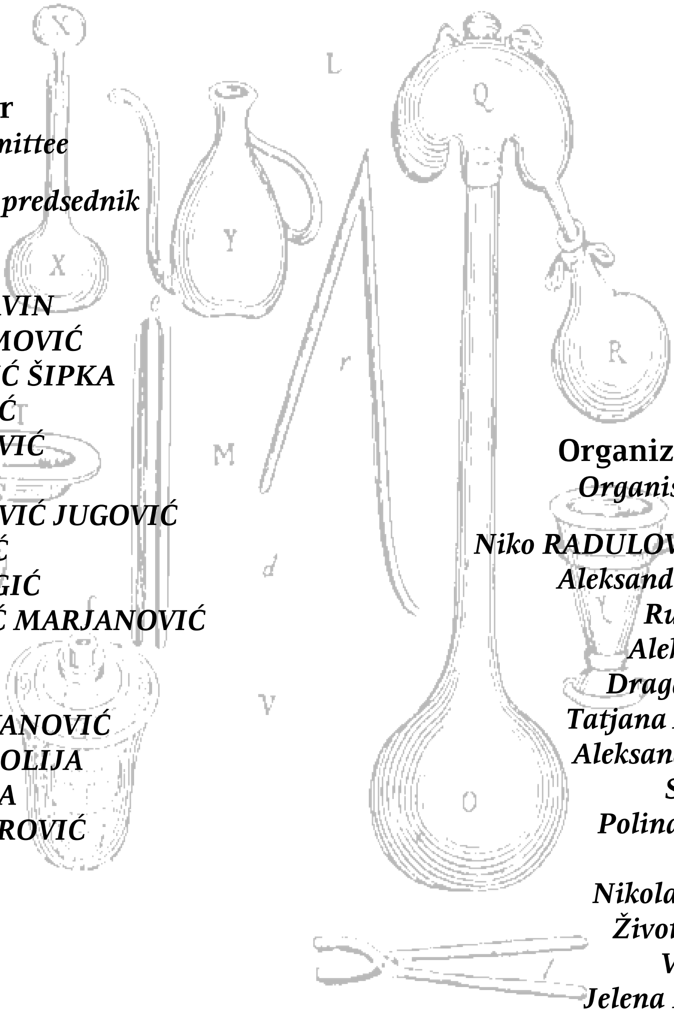

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Ova knjiga sadrži kratke izvode
plenarnih (PP) i predavanja po pozivu (PPP),
kao i usmenih (O) i posterskih (P) saopštenja prihvaćenih
za prezentovanje na Savetovanju i Konferenciji

Zbornik radova (svaki rad u obimu do četiri stranice)
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This book contains short abstracts of
Plenary (PP) and Invited Lectures (PPP),
as well as Oral (O) and Poster (P) contributions accepted
for the presentation at the Meeting, and at the Conference.

The Proceedings of the papers (consisting of four pages)
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as an integral part of the Meeting material.
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PRINT EXIT

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Elektrohemija / Electrochemistry

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Hemija životne sredine / Environmental Chemistry

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Biohemija / Biochemistry

Biotehnologija / Biotechnology

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Hemija i tehnologija makromolekula / Chemistry and Technology of Macromolecules

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2. konferencija mladih hemičara Srbije / 2nd Conference of the Young Chemists of Serbia
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PREDAVANJE PO POZIVU / INVITED LECTURE

SAOPŠTENJA / CONTRIBUTIONS

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Hemijska analiza

Hemijska sinteza

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PROGRAM

51. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA
51st Meeting of the Serbian Chemical Society

Četvrtak, 5. juni 2014. / *Thursday, June 5, 2014*

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Registration – Hall of Rectorate

Petak, 6. juni 2014. / *Friday, June 6, 2014*

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Registration – Hall of Rectorate

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Plenarna predavanja / *Plenary Lectures*
Predsedavajući / *Chairperson:* **Niko Radulović**

09.30–10.25 **PP1** **Matthias D hooghe,** *Department of Sustainable Organic Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, Belgium*
Application of small-ring azaheterocyclic building blocks for the construction of biologically relevant nitrogen compounds

10.30–11.25 **PP2** **Liudmil Antonov,** *Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria*
Tautomerism of azo dyes and Schiff bases: history, investigations and applications

Predsedavajući / *Chairperson:* **Slavica Ražić**

11.30–12.25 **PP3** **Zsanett Dorkó*, Tatjana Verbić**, Viola Horvath***, George Horvai*,***,**
**Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary, **Faculty of Chemistry University of Belgrade, Serbia, ***MTA-BME Research Group of Technical Analytical Chemistry, Budapest, Hungary*
Structure and composition of soft interfaces

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13.30 **Izlet /** *Excursion* **(okupljanje: ulaz u Tvrđavu /** *Meeting point: Fortress Entrance)*
15.00 **obilazak Tvrđave /** *Tour of the Fortress*
16.00 **odlazak memorijalnog kompleksa 12. Februar (logor na Crvenom krstu)**
Visit to memorijalniom complex February 12 (Concentration Camp at the Red Cross)
17.00 **obilazak Ćele kule /** *Visit to the Skull Tower*
18.00 **poseta Arheološkoj Sali /** *Visit to the Archaeological Hall*
19.00 **šetnja i razgledanje spomenika u centru Niša /** *Niš sightseeing*

20.00 **Zajednička večera /** *Social Dinner*
Restoren / *Restaurant* **Nišlijska mehana 2**

Subota, 7. juni 2014. / *Saturday, June 7, 2014*

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Svečana sala / *Ceremonial Hall* (SS)

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Synthesis of 1-aryl-4-ferrocenyl-3-phenyltetrahydropyrimidin-2(1H)-ones

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OH O 04 Marija N. Sakač, Katarina M. Penov Gaši
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Mala sala / *Small Hall* (MS)

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Predsedavajući / *Chairpersons:* Aleksandar Bojić i Aleksandra Pavlović
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PPP3 *Laboratorija za fiziku, Institut za nuklearne nauke „Vinča", Univerzitet u Beogradu, Srbija*
Primena membranske ekstrakcije u analitičkoj hemiji, zaštiti životne sredine i radiohemiji. Rezultati i perspektive
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Hol ispred SS / *Lobby in front SS*

10.45–11.00 **Postavljanje postera** / *Poster Mounting*
(Sesija I – OH i BH i Sesija II AH, BT, HTH i HTM)

11.00–13.00 **Poster sesija I i II**/ *Poster Sesion I i II* **(OH i BH - AH, BT, HTH i HTM)**
Osveženje – *Coffee Break*

13.00–13.15 **Skidanje postera** / *Poster Dismounting* **(Sesija I i II)**
(Sesija I – OH i BH i Sesija II AH, BT, HTH i HTM)

13.15–13.30 **Postavljanje postera** / *Poster Mounting*
(Sesija III – NH, HŽS, EH, FH, NM, TI, TH, HIN, NS)

Svečana sala / *Ceremonial Hall* (SS)

Sesija III / *Sesion I* **(NH, HŽS, EH, FH, NM, TI, TH, HIN, NS)**
Predsedavajući / *Chairperson:* **Miloš Đuran i Tatjana Anđelković**
Predavanje po pozivu / *Invited Lecture*

13.30–14.00
PPP1
Milica Kosović, Biljana Petrović*, Željko Jaćimović, Živadin D. Bugarčić*,
Metalurško-tehnološki fakultet, Univerzitet u Crnoj Gori, Cetinjski put, Podgorica,
**Prirodno-matematički fakultet, Univerzitet u Kragujevcu, R. Domanovića 12, Kragujevac*
Sinteza i karakterizacija novih kompleksa Pt(II) sa derivatima pirazola
Synthesis and characterization of the novel Pt(II) complexes with pyrazole derivatives

Usmena izlaganja / *Oral Presentations*

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Biljana Đ. Glišić, Beata Warżajtis, Niko S. Radulović, Urszula Rychlewska, Miloš I. Djuran
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14.15–14.30
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A photocatalytic degradation of sulfonylurea herbicide nicosulfuron in TiO_2 aqueous solution

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Danijela S. Slavnić, Luka V. Živković, Ana V. Bjelić, Branko M. Bugarski, Nikola M. Nikačević
Raspodela vremena zadržavanja u kontinulnom reaktoru sa oscilirajućim tokom fluida
Residence time distribution in continuous oscillatory flow reactor

15.00–15.15
NS O 01
Vesna D. Milanović, Aleksandar M. Đorđević, Milena R. Tošić
Muzej hemije – doprinos hemijskoj pismenosti
Museum of Chemistry - contribution of chemical literacy

15.30–17.15 **Poster sesija III** / *Poster Sesion III* **(NH, HŽS, EH, FH, NM, TI, TH, HIN, NS)**
Osveženje – *Coffee Break*

17.15–17.30 **Skidanje postera** / *Poster Dismounting* **(Sesija I i II)**

17.30 **Dodela IUPAC poster nagrada i zatvaranje Savetovanja**
IUPAC poster prize award and Closing Ceremony

DRUGA KONFERENCIJA MLADIH HEMIČARA SRBIJE
2nd Conference of the Young Chemists of Serbia

Subota, 7. juni 2014. / Saturday, June 7, 2014

08.00–12.00 Registracija – Hol rektorata

Mala sala (MS)

11.00–11.15 Svečano otvaranje

Predsedavajući: Vuk Filipović

Plenarno predavanje

11.15–11.45 **Jasmina Nikodinović-Runić**, *Institut za molekularnu genetiku i genetičko inženjerstvo, Univerzitet u Beogradu*
PP 1 Bakterijska ćelija – dizajnirani biokatalizator

Usmeno izlaganje

11.45–12.00 Jelena S. Radivojević
BB O 01 Majklova adicija različitih aldehida na β-nitrostiren katalizovana rekombinantnim ćelijama koje eksprimiraju 4-oksalokrotonat tautomerazu

12.00–12.15 Pauza

Predsedavajući: Života Selaković

Plenarno predavanje

12.15–12.45 **Milan B. Vraneš**, *Prirodno-matematički fakultet,Univerzitet u Novom Sadu*
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Usmeno izlaganje

12.45–13.00 Sofija P. Miškov, Ivona R. Radović
BB O 02 Sinteza i ispitivanje termofizičkih parametara biodizela dobijenog iz biootpada heterogenom tranesterifikacijom i karakterizacija katalizatora

13.00–13.15 Pauza

Predsedavajući: Jelena Radivojević

Predavanje po pozivu

13.15– 13.45 **Aleksandar Dekanski**, *IHTM - Centar za elektrohemiju, Univerzitet u Beogradu*
PPP 1 Kako prezentovati i publikovati rezultate naučnog istraživanja

Usmeno izlaganje

13.45–14.00 Marija Blažić, Radivoje Prodanović
BB O 03 Molekularno kloniranje celobiozo dehidrogenaznog gena iz *Phanerochaete chrysosporium* i ekspresija u kvascu *Saccharomyces cerevisiae*

Hol ispred SS / *Lobby in front SS*

14.00–14.15 Postavljanje postera

14.15–15.30 Poster sesija
Osveženje – *Coffee Break*

15.30–15.45 Skidanje postera

Mala sala (MS)

15.45–16.15 Dodela potvrda o učešću i zatvaranje Konferencije

PRINT EXIT

51. SAVETOVANJE
SRPSKOG HEMIJSKOG DRUŠTVA

51st Meeting of the Serbian Chemical Society

KRATKI IZVODI

ABSTRACTS

Plenarna predavanja / Plenary Lectures

PP 1

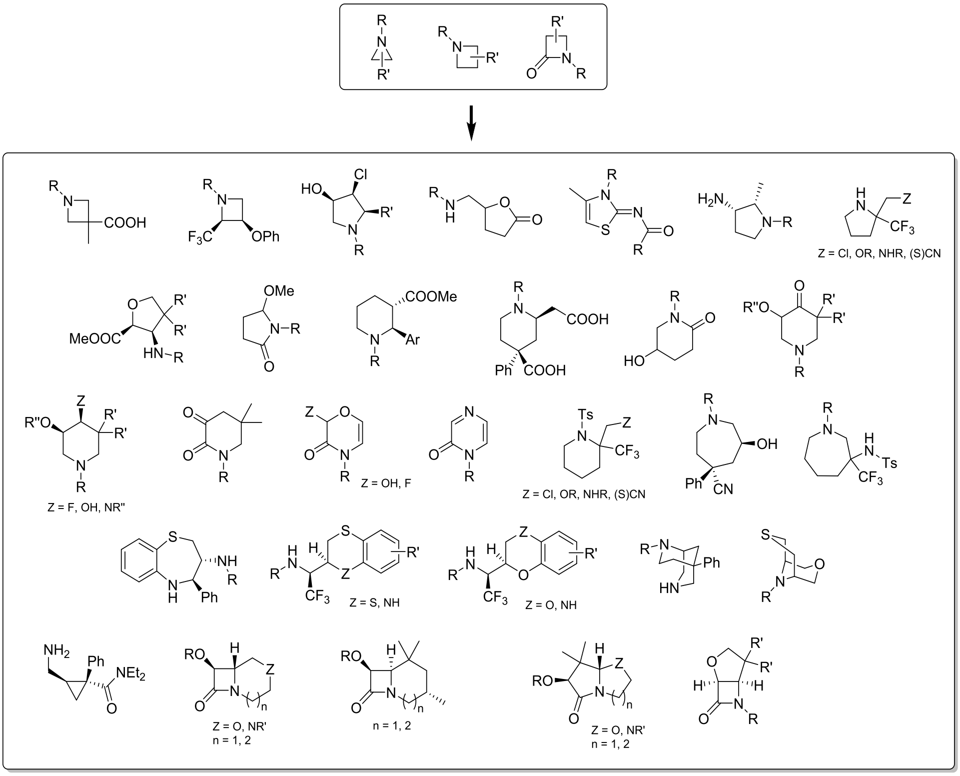
Application of small-ring azaheterocyclic building blocks for the construction of biologically relevant nitrogen compounds

Matthias D'hooghe

SynBioC Research Group, Department of Sustainable Organic Chemistry and Technology,
Faculty of Bioscience Engineering, Ghent University, Coupure Links 653, B-9000 Ghent, Belgium
matthias.dhooghe@UGent.be

Small-ring azaheterocyclic systems have acquired a pivotal position as building blocks in medicinal chemistry. In particular, aziridines, azetidines and beta-lactams have been shown to be eligible synthons for the construction of a broad variety of stereodefined (heterocyclic) frameworks, often endowed with pronounced biological activities. In this presentation, the synthetic flexibility of these three- and four-membered systems toward the preparation of different types of nitrogen-containing target structures will be explained.

In that respect, a number of novel synthetic strategies toward a broad set of important heterocyclic scaffolds will be discussed (see figure below). In particular, different new methods for the regio- and stereoselective rearrangement of aziridines, azetidines and beta-lactams into functionalized four- to seven-membered hetero(bi)cycles will be disclosed. All these compounds represent relevant moieties encountered as substructures in a variety of biologically active synthetic and natural products.



Furthermore, the application of aziridines, beta-lactams and other scaffolds for the preparation of specific types of bioactive compounds will be illustrated by means of selected examples. To that end, the synthesis and biological assessment (antimalarial, antiviral, antifungal, anticancer) of different classes of target molecules will be reviewed.

PP 2

Tautomerism of azo dyes and Schiff bases: history, investigations and applications

Liudmil Antonov

Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

http://www.orgchm.bas.bg/~i2mp

The tautomerism is a special case of equilibrium, which, due to the high rate of proton exchange, is especially difficult to be analysed. Even though tautomerism in azo dyes was first discovered in 1884 by Zincke and Bindewald, and has been studied by spectroscopic methods since 1899, more than hundred years of research has still left many questions unanswered. A major breakthrough was the development of chemometric methods to obtain the absorption spectra of the individual tautomers, even though these are never present in their pure form.

“Quantity” is an important detail concerning tautomeric mixtures, because it gives the possibility for clear explanation of the affecting factors (both structural and external) and for prediction of the properties of similar systems. The main requirement of analyitical chemistry, however, to perform quantitative analysis is the calibration, demanding physically separated individual tautomers. Such a requirement is impossible to be fulfilled in most tautomeric systems. As a result, a very interesting contradiction appeared after the rapid development of spectroscopy in the middle of the last century: on one hand, in most cases the tautomeric equilibrium could be shifted by changing the above mentioned external factors, but never to the end, pure tautomers; on the other hand, these changes could be measured using spectral instruments, but the collected data sets could never be processed in a strict mathematical way leading to quantitative information about the tautomeric constants. The impossibility of strict calibration gave rise to many chemometric approaches for treatment of the existing spectral data, all of them developed to overcome the lack of spectral data for the pure, individual, tautomers. The reliability of these approaches depends strongly on the mathematical and spectral approximations used.

However, as a final result, tautomeric constants as function of number of external parameters (temperature, irradiation, solvents, pH, concentration) can be estimated by using such chemometric data processing. Availability of this information makes it possible to obtain thermodynamic and kinetic picture of the equilibrium and to explain the solvent effects. The collected tautomeric constants give direct possibility to evaluate the reliability of the existing quantum-chemical methods and even to and to callibrate them.

The most interesting result of these tautomeric investigations is that the availability of clear picture about the tautomerism in the investigated compounds gives opportunities for their nontrivial application as molecular switches and design of sensing molecules.

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PP 3

Structure and composition of soft interfaces

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The interface between two phases is of prime importance in many branches of chemistry. Our studies of interfaces started from electroanalytical chemistry, where we wanted to understand the mechanism of the selective potentiometric response of plasticized polymer ion-selective membranes. A series of investigations with impedance spectroscopy, radiotracer methods, atomic force microscopy, small angle neutron scattering, ESCA and SIMS helped to discover that such membranes are selective ion exchangers with a complex internal and surface structure. Unexpected or unusual phenomena were encountered, e.g., that the surface of plasticized PVC is almost pure plasticizer, adsorption of several compounds near the surface occurs at different depth, surfactants can be trans-adsorbed from the liquid-liquid to a gas-liquid interface, and so on.

These studies had ramified then into different directions. The molecular level structure of fluid interfaces has been studied by Monte Carlo and molecular dynamics methods and had shown that the first molecular layer on the liquid surface has a similarly important role as on solids. In another research project we have investigated the selectivity of molecularly imprinted polymers. Since these polymers are being used in many different applications (adsorption, catalysis, sensors, etc.), their selectivity has been characterized by many, hardly comparable methods. We have found a very simple graphical method to overcome this difficulty. From this work we have also learned that selectivity, a central concept in chemistry, is very little understood. A method can be proposed now that tells us when selectivity can be meaningfully defined and when this is not possible.

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Predavanja po pozivu / Invited Lectures

PPP 1

Sinteza i karakterizacija novih kompleksa Pt(II) sa derivatima pirazola

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Istraživanja u oblasti kompleksnih jedinjenja platine su vrlo značajna sa biološke i medicinske tačke gledišta**.** Neki kompleksi Pt(II), kao što su cisplatina, karboplatina i oksaliplatina, se intenzivno koriste kao antitumorski lekovi u hemioterapiji. Klinički uspeh cisplatine je doveo do pojave interesovanja među istraživačima za sintezu novih strukturno različitih platinskih jedinjenja, koja mogu posedovati bolje citotoksične osobine.[1] Takođe, pirazol i njegovi derivati su vrlo značajni molekuli s obzirom da ulaze u sastav mnogobrojnih biomolekula i lekova.[2]

Ovaj rad opisuje sintezu i karakterizaciju proizvoda nastalih u reakciji između nekih Pt(II) kompleksa, kao što su: $K_2[PtCl_4]$, $K_2[PtCl_6]$, $[Pt(dach)Cl_2]$ i [Pt(bpma)Cl]Cl sa 3-amino-4-jodo pirazolom i 5-amino-4-bromo-3-metil pitazolom. Kompleksi su okarakterisani elementalnom analizom, UV-Vis, IR i NMR metodom. X-ray analizom kompleksa nastalog u reakciji između [Pt(bpma)Cl]Cl i bromo derivata pirazola potvrđena je koordinacija preko N1 atoma azota pirazolovog sistema.

Synthesis and characterization of the novel Pt(II) complexes with pyrazole derivatives

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The chemistry of platinum complexes is important from biological and medicinal point of view. Some Pt(II) complexes, *viz.* cisplatin, carboplatin and oxaliplatin, are extensively used as anticancer drugs in chemotherapy. The clinical success of cisplatin has produced an interest in synthesis of structurally different platinum metallodrugs that might exhibit better cytotoxic properties, hopefully accompanied by different antitumor specificities.[1] Also, pyrazole and its derivatives are also very important molecules due the facts that they are constituent of many biomelecules and medicaments.[2]

This work describes the synthesis and characterization of the products formed in the reaction between some Pt(II) complexes, such as $K_2[PtCl_4]$, $K_2[PtCl_6]$, $[Pt(dach)Cl_2]$ and [Pt(bpma)Cl]Cl with 3-amino-4-iodo-pyrazole and 5-amino-4-bromo-3-methyl-pyrazole. The complexes are characterized by elemental analysis, UV-Vis, IR and NMR. X-ray analysis of the complex obtained in the reaction between [Pt(bpma)Cl]Cl and bromo derivative confirms the coordination via N1 nitrogen atom.

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PPP 2

Analiza sekundarnih metabolita lišajeva - neočekivana iskustva

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Lišajevi (lichens) su simbiotički organizmi koji se sastoje od mikobionta (gljive) i fitobionta (alge) i imaju osobine koje nema ni jedna od udruženih vrsta ponaosob. Smatraju se najranijim kolonizatorima zemlje, njihovi fosilni ostaci su stari oko 400-600 miliona godina. Rastu vrlo sporo (oko 1 cm za godinu dana) i žive jako dugo, za neke arktičke lišajeve se smatra da su stari oko hiljadu godina. Lišajevi proizvode primarne (intracelularni) i sekundarne (ekstracelularni) metabolite. Sekundarne metabolite (tzv. lišajevske kiseline) sintetiše mikobiont i oni su jedinstveni za lišajeve. Njihovo izolovanje i identifikacija su čest predmet istraživanja hemičara. Dobijeni podaci se koriste u hemotaksonomiji a izolovane čiste supstanci za ispitivanja bioloških aktivnosti. Biće prezentovana neočekivana iskustva stečena prilikom izolovanja i identifikacije sekundarnih metabolita lišajeva Hypogymnia physodes i Umbilicaria crustulosa.

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Analysis of secondary metabolites of lichens-unexpected experiences

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Lichens are symbiotic organisms that consist of mycobiont (fungi) and photobiont (algae). They have the characteristics that are not specific to the species individually. Lichens are the earliest colonizers of land, their fossils are old around 400-600 million years. They grow very slowly (about 1 cm per year) and live very long, for some arctic lichen are believed to be about a thousand years old. Lichens produce primary (intracellular) and secondary (extracellular) metabolites. Mycobiont synthesizes secondary metabolites (called lichen acids) and they are unique to lichens. Their isolation and identification are often the subject of researches conducted by chemists. The obtained data are used in a taxonomy while isolated pure substances are used for biological activity assays. Unexpected experiences gained during the isolation and identification of secondary metabolites of lichens Hypogymnia physodes and Umbilicaria crustulosa will be presented.

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PRINT EXIT

PPP 3

Primena membranske ekstrakcije u analitičkoj hemiji, zaštiti životne sredine i radiohemiji. Rezultati i perspektive

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U ovom radu dat je pregled primene membranske ekstrakcije kao separacione metode u oblastima analitičke hemije, zaštite životne sredine i radiohemije. Membranska mikroekstrakcija se koristi kao metoda za pripremu uzoraka (istovremeno prečišćavanje i koncentrovanje) u analitičkoj hemiji. U radiohemiji, ova metoda još uvek nema praktičnu primenu za odvajanje radionuklida, ali neke njene osobine kao što su otpornost na zračenje, laka automatizacija i mali rizik od kontaminaacije je svrstavaju u separacione metode koje mogu biti primenje u rutinskim operacijama. Takođe je pokazano da membranska ekstrakcija može da ima značajnu ulogu u prečišćavanju otpadnih industrijskih voda, ova primena se uglavnom realizovala za uklanjanje metala iz otpadnih voda, ali u našim radovima je pokazano da i pesticidi mogu biti uklonjeni iz otpadnih voda i skoncentrisani na značajno manju zapreminu.

Ovaj rad je urađen u okviru projekta Fizika i hemija sa jonskim snopovima, Br. III 45006 koji je finansiran od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije.

Application of membrane extraction in analytical, environmental and radiochemistry. Results and perspective

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This work presents an outline of application of membrane extraction as separation methods in analytical, environmental and radiochemistry. Membrane microextraction has been used as sample preparation method (purification and preconcentration in a single step) in analytical chemistry. In radiochemistry, this technique have not applied yet in routine practice for separation of radionuclides, but the potential of its application is high due to good radiation resistance, easy automation and low risk of contamination. The results of purification of manufacturing waste water by membrane extraction in a hollow fibre contactors, shows a big potential of this method for removal of pesticides from waste waters.

We acknowledge the support to this work provided by the Ministry of Education, Science and Technological Development of Serbia through projects No. III 45006

Saopštenja / Contributions

Analitička hemija / Analytical Chemistry

AH O 01

Određivanje antibiotika anizomicina u tkivima metodom tečne hromatografije sa tandem masenom spektrometrijom

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Cilj ovog rada bio je razvoj osetljive analitičke metode za određivanje leka anizomicina u različitim tkivima. U optimizovanoj proceduri ekstrakcije, metanol je odabran kao rastvarač za ekstrakciju, a Oasis HLB kao kertridž za prečišćavanje ekstrakta. Prilikom validacije razvijene metode, anizomicin je efikasno ekstrahovan iz većine tkiva, kao što su srce, mozak, slezina, bubrezi i jetra, dok su za masno tkivo dobijeni niži prinosi. Niske granice detekcije (0,6–3,8 ng g^{-1}) i kvantifikacije (2,4–11,8 ng g^{-1}) ukazuju da je razvijena metoda pogodna za određivanje tragova anizomicina. U ispitivanom opsegu koncentracija (50–2500 ng g^{-1}) metoda je linearna ($R^2 > 0{,}975$). Značajan uticaj matrice eliminisan je upotrebom standarda koji odgovaraju matrici uzorka. Na osnovu rezultata validacije utvrđeno je da je razvijena metoda osetljiva i pouzdana za određivanje leka anizomicina u različitim tkivima korišćenjem tečne hromatografije sa tandem masenom spektrometrijom.

Determination of antibiotic anisomycin in tissue samples by liquid chromatography–tandem mass spectrometry

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The aim of this work was development of sensitive analytical method for determination of drug anisomycin in different tissue samples. The optimized extraction procedure included methanol as extraction solvent and Oasis HLB as extract clean up cartridge. In the method validation, anisomycin was efficiently extracted from most of tissues, such as heart, brain, spleen, kidney and liver, whereas lower recoveries were obtained for fat tissue. Low limits of detection (0.6–3.8 ng g^{-1}) and quantification (2.4–11.8 ng g^{-1}) indicate that developed method is suitable for determination of anisomycin trace levels. The method was linear ($R^2 > 0.975$) in the tested concentration range (50–2500 ng g^{-1}). Significant matrix effect was eliminated using matrix-matched standards. It was finally determined that the developed method is sensitive and reliable for determination of drug anisomycin in various tissue samples using liquid chromatography–tandem mass spectrometry.

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AH O 02

Kinetičko određivanje tragova tiocijanata

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U radu je predstavljena jednostavna i brza kinetičko-spektrofotometrijska metoda za određivanje tragova tiocijanatnih jona. Metoda se zasniva na aktivatorskom efektu SCN^- jona na brzinu redoks reakcije dinatrijum-6-hidroksi-5-[(4-sulfofenil)azo]-2-naftalensulfonata (azo boja"Sunset Yellow FCF", E110) i vodonik-peroksida u prisustvu tragova Cu(II) jona u alkalnoj sredini boratnog pufera. Radni eksperimentalni uslovi su optimizirani u pogledu dobijene maksimalne osetljivosti predložene kinetičke metode za određivanje tragova SCN^- jona. Oblast linearnosti se nalazi u opsegu koncentracija 0,29–5,81 μg/cm^3 , pod sledećim reakcionim uslovima: C(SY) = $4\cdot10^{-5}$ mol/dm^3; $C(H_2O_2)$ = 0,4 mol/dm^3; C(Cu(II)) = 318 ng/cm^3; pH = 10,5; i t = 25,0±0.1 °C. Relativna standardnadevijacija (n = 10), 2,32 μg/cm^3 SCN^- iznosi 3,36 %. Interferirajući efekti drugih jonskih vrsta su određeni u cilju ocene selektivnosti predložene metode. Metoda se može primeniti za određivanje tragova SCN^- jona u različitim kako biološkim vrstama, tako i uzorcima životne sredine, imajući u vidu njenu ekonomičnost, preciznost i tačnost**.**

Kinetic determination of traces of thiocyanates

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Simple and fast kinetic-spectrophotometric method for the determination of trace amounts of thiocyanates was presented in this paper. The method was based on the activation effect of traces of SCN^- ions the redox reaction between disodium-6-hydroxy-5-[(4-sulfophenyl)azo]-2-naphtalenesulfonate (artificial azo-dye "Sunset Yellow FCF", E110) and hydrogen peroxide, in presence of nano-amounts of Cu(II) ions, in alkaline media of borate buffer. Working experimental conditions are set by assuming the highest sensitivity of the proposed kinetic method for the determination of SCN^- ions. The linearity of the method was obtained in the concentration range 0.29–5.81 μg/cm^3 of SCN^- ions, under the following experimental conditions: C(SY) = $4\cdot10^{-5}$ mol/dm^3; $C(H_2O_2)$ = 0.4 mol/dm^3; C(Cu(II)) = 318 ng/cm^3; pH = 10.5; and t = 25.0±0.1 °C. The relative standard deviation (n = 10) determinations of 2.32 μg/cm^3 SCN^- was 3.36 %. The interference effects of the other ions were determined in order to assess the selectivity of the proposed kinetic method. Method could be useful for trace determination of thiocyanates in different kind of biological or environmental samples because of its cost-effectiveness, precision and accuracy.

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AH P 01

Determination of the herbicide linuron applying carbon paste electrodes based on boron doped carbonized hydrothermal carbons

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The voltammetry of herbicide linuron was investigated by using three kinds of hydrothermal carbon paste electrodes which we prepared in our laboratory. The electrodes were based on undoped carbonized hydrothermal carbon CHTC and boron doped samples CHTCB$_{0.2}$ and CHTCB$_{1}$ with paraffin oil as a binder. The CHTCB$_{0.2}$ exhibited the best analytical performance with respect to peak shape and signal intensity. The method, operated in differential pulse voltammetric mode, was applied to the determination of linuron in model samples in the concentration range from 2.5 to 30 μg cm^{-3} with LOD of 3.01 μg cm^{-3}. This appears to be the first application of a CHTCB$_{0.2}$ to the voltammetric determination of herbicide linuron.

We acknowledge the support to this work provided by the Ministry of Education, Science and Technological Development of Serbia through projects No. III 45006 and III 45012.

Određivanje herbicida linurona primenom elektroda od ugljenične paste dobijenih od karbonizovanih borom dopiranih hidrotermalnih karbona

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U ovom radu je ispitivano voltametrijsko određivanje herbicida linurona pomoću tri vrste elektroda od karbonizovane hidrotermalne ugljenične paste koje su pripremljene u našoj laboratoriji. Elektrode su pripremljene sa osnovnim hidrotermalnim karbonom CHTC, i borom dopiranim uzorcima CHTCB$_{0.2}$ i CHTCB$_{1}$ i parafinskim uljem kao vezivnim sredstvom. Elektroda CHTCB$_{0.2}$ je pokazala najbolji oblik pika i intenzitet signala. Razvijena je diferencijalno pulsna voltametrijska metoda za određivanje linurona u vodenom rastvoru u koncentracionom opsegu od 2,5 do 30 μg cm^{-3} sa granicom detekcije 3,01 μg cm^{-3}. U ovom radu je po prvi put prikazana primena CHTCB$_{0.2}$ za voltametrijsko određivanje herbicida linurona.

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AH P 02

Razrada UV spektroskopske metode za određivanje ketokonazola u farmaceutskim proizvodima

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Development of UV spectroscopic method for determination of ketoconazole in pharmaceutical formulations

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AH P 03

Uticaj organskih modifikatora na određivanje lipofilnosti nekih polidentatnih Šifovih baza pomoću RP-TLC

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Lipofilnost polidentatnih Šifovih baza je ispitivana pomoću reversno-fazne tankoslojne hromatografije. U cilju određivanja retencionog parametra kao mere lipofilnosti ispitivanih jedinjenja korišćena su tri različita binarna sistema rastvarača, sastavljena od vode i organskog modifikatora (metanol, acetonitril i tetrahidrofuran). Parametri lipofilnosti, zajedno sa 2D molekulskim deskriptorima su podvrgnuti multivarijantnoj statističkoj analizi. Analiza glavne komponente je upotrebljena da bi se utvrdili faktori koji najviše utiču na lipofilnost ispitivanih jedinjenja. Hemijske strukture ispitivanih jedinjenja, okarakterisane molekulskim deskriptorima su korelisane sa hromatografijski dobijenim parametrima. Primenom metanola kao organskog modifikatora postignuto je najbolje odvajanje strukturno sličnih jedinjenja, dok se primenom tetrahidrofurana ispitivana jedinjenja ponašaju kao homologa serija. Dobijeni rezultati mogu biti značajni pri sintezi i dizajnu novih jedinjenja.

Influence of organic modifiers on RP-TLC determination of lipophilicity of some polydentate Schiff bases

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The lipophilic character of polydentate Schiff bases was investigated by reversed-phase thin-layer chromatography. Three different binary solvent systems, composed of water and organic modifier (methanol, acetonitrile, and tetrahydrofurane) were used in order to determine retention parameter as a measure of the lipophilicity of the tested compounds. Lipophilicity parameters, together with 2D molecular descriptors, were subjected to the multivariate statistical analysis. Principal component analysis was employed to reveal the most influential factors governing the lipophilicity of the investigated compounds. The chemical structures of the investigated compounds characterized by molecular descriptors were correlated with chromatographically determined lipophilicity parameter. Optimal separation of structurally similar compounds was obtained by use of methanol, as organic modifier. Unlike methanol, when tetrahidrofuran was applied, investigated compounds could be regarded as a homologous series, regardless of the structural differences. Obtained results can help design and synthesis of new compounds.

AH P 04

Elektrohemijsko ponašanje bakra u rastvoru natrijum-tetraborata u prisustvu 2-amino-5-etil-1,3,4-tiadiazola

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Elektrohemijsko ponašanje bakra je ispitivano u 0,1 M $Na_2B_4O_7$ u prisustvu različitih količina 2-amino-5-etil-1,3,4-tiadiazola (AETD). Potenciodinamička merenja i merenje potencijala otvorenog kola su metode koje su korišćene tokom ispitivanja inhibitorskog uticaja AETD. Primenjene metode su pokazale da 2-amino-5-etil-1,3,4-tiadiazol deluje kao inhibitor mešovitog tipa sa nešto izraženijim uticajem na anodne korozione procese. Adsorpcija inhibitora na površini bakra se odvija spontano prema Lengmirovoj adsorpcionoj izotermi.

Electrochemical behaviour of copper in sodium tetraborate solution in the presence of 2-amino-5-ethyl-1,3,4-thiadiazole

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The electrochemical behavior of copper was studied in the presence of various amounts of 2-amino-5-ethyl-1,3,4-thiadiazole (AETD) in 0.1 M $Na_2B_4O_7$. The potentiodynamic measurements and the open circuit potential measurements were used for the AETD inhibition effect study. The applied methods showed that 2-amino-5-ethyl-1,3,4-thiadiazole acts as mixed-type inhibitor with more pronounced effect on anodic corrosion processes. The inhibitor adsorption on copper surface occurs spontaneously in accordance with Langmuir adsorption isotherm.

AH P 05

Испитивање равнотежа комплексирања у растворима бакра и неких антибиотика флуорохинолонског типа

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У овом раду проучаване су равнотеже комплексирања неких антибиотика флуорохинолонског типа (ципрофлоксацин, моксифлоксацин, левофлоксацин и ломефлоксацин) и бакар(II)-јона. Испитивања су вршена у воденим растворима потенциометријским мерењем у 0,15 M раствору NaCl на 37° C у инертној атмосфери азота при концентрационом односу метал : лиганд од 1:1 до 1:2. Константе стабилности за ове системе израчунате су помоћу рачунарског програма Hyperquad^{2006}. У испитиваним системима нађени су бинарни комплекси типа ML i ML_2 као и мешовити комплекси типа ML_pH_q у целокупној испитиваној области pH вредности ($2,0 \leq pH \leq 10,5$) где су p и q (1,1), (2,2), (2,1), (2,0) и (2,-1). Полинуклеарни комплески нису нађени.

Захвалница: *Захваљујемо се Министарству просвете, науке и технолошког развоја Србије на финансијској подршци у оквиру пројекта 172016.*

Complex formation equilibria between Cu(II)-ion and some fluoroquinolone antibiotics

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In this work, we studied the complexation equilibria between some fluoroquinolone antibiotics (ciprofloxacin, moxifloxacin, levofloxacin and lomefloxacin) and copper(II) ion. Investigation were conducted in aqueous solutions by potentiometric titrations in 0.15 M NaCl medium at 37 °C under inert atmosphere of nitrogen with metal to ligand concentration ratio from 1:1 to 1:2. Stability constants for these systems were calculated using the Hyperquad^{2006} software. In all systems the binary complexes ML, ML_2 and mixed ML_pH_q were found in whole accessible pH range ($2.0 \leq pH \leq 10.5$) where p and q were (1,1), (2,2), (2,1), (2,0) and (2,-1). Polynuclear complexes were not found.

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AH P 06

Hidrolitičko ponašanje itrijuma

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Poslednjih godina itrijum privlači veliku pažnju istraživača jer je našao primenu u PET (pozitronsko emisiona tomografija) dijagnostici, dok se generatorski dobijen Y-90 koristi u terapiji neoperativnih karcinoma. Može dospeti u krvnu plazmu preko različitih transportnih procesa gde pretežno postoji u obliku hidrolitičkih kompleksa. Tako, u ovom radu proučavana je specijacija hidrolitičkih kompleksa itrijuma. Potenciometrijske titracije su primenjene za određivanje identiteta i stabilnosti hidrolitičkih kompleksa itrijuma. Rezultati eksperimenata koji su rađeni na temperaturi od 25° C i u 0,15 M NaCl medijumu ukazuju na formiranje $Y(OH)$, $Y(OH)_2$, $Y_3(OH)_5$, $Y_4(OH)_6$ kompleksa sa konstantama stabilnosti od $-\log\beta = 7{,}71; 16{,}52; 34{,}2$ i $32{,}1$, respektivno.

Захвалница: *Захваљујемо се Министарству просвете, науке и технолошког развоја Србије на финансијској подршци у оквиру пројекта 172016.*

Hydrolysis behavior of yttrium

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In recent years yttrium attracted great attention of researchers because it found application in PET (positron emission tomography) diagnostics, and generator obtained Y-90 is used in the treatment of nonoperative cancers. It may get to blood plasma via various transporting processes where it predominantly exists in the form of hydrolytic complexes. Thus, in this work speciation of yttrium hydrolytic complexes was studied. Potentiometric titrations were conducted to determine identity and stability of yttrium hydrolytic complexes. The results obtained at a temperature of 25° C in 0.15 M NaCl media indicate formation of $Y(OH)$, $Y(OH)_2$, $Y_3(OH)_5$ and $Y_4(OH)_6$ with the stability constants $-\log\beta = 7.71; 16.52; 34.2$, and 32.1, respectively.

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AH P 07

Polifenolni profil lišća vinove loze

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Sekundarni metaboliti biljaka, naročito polifenoli, već duže vreme su predmet naučnih istraživanja. Za biljke koje se koriste u ishrani, sekundarni metaboliti predstavljaju markere botaničkog i geografskog porekla, a služe i za proveru autentičnosti. Cilj ovog ispitivanja bio je da se identifikuju i kvantifikuju pojedinačna polifenolna jedinjenja, da se odredi sadržaj ukupnih polifenola, njihova relativna antioksidativna aktivnost, kao i sadržaj metala u 23 uzorka lišća vinove loze. Tečni hromatograf visokih performansi (UHPLC) kuplovan sa DAD detektorom i masenim spektrometrom upotrebljen je za kvantifikaciju polifenola u ekstraktima lišća. Korišćenjem dostupnih standarda, kvantifikovano je 20 polifenolnih jedinjenja. Koncentracija ukupnih polifenola određena je pomoću Folin-Ciocalteu metode, a antioksidativna aktivnost pomoću DPPH·reagensa. Sadržaj ukupnih polifenola bio je u rasponu od 27,51 do 75,96 mg ekv. galne kiseline/g, a relativna antioksidativna aktivnost od 0,43 do 0,87 mmol ekv. troloksa/g suvog uzorka. Rezultati dobijeni za relativnu antioksidativnu aktivnost upoređivani su sa sadržajem ukupnih fenola (r = 0,92). U svim uzorcima pronađen je visok sadržaj Ca, K, Mg i S.

Phenolic profile of grape leaves

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Plant secondary metabolites, especially polyphenols, are the subject of research interest, for a long time. For plant-derived food, the secondary metabolites are markers of biological or geographical authenticity, as well as for adulteration and traceability studies. The aim of this study was to identify and quantify polyphenolic compounds, and to determine total phenolic content (TPC), radical scavenging activity (RSA), and mineral content in 23 leaf samples. Quantification of phenolics in grape leaves extracts was done using UHPLC coupled with a diode array detector (DAD) and connected to a triple-quadrupole mass spectrometer. A total of 20 compounds were quantified using the available standards. The concentration of total phenolics was determined using Folin-Ciocalteu method. Scavenging activity of leaf extracts was evaluated using DPPH reagent. TPC ranged from 27.51 to 75.96 mg GAE/g, and RSA ranged from 0.43 to 0.87 mmol TE/g of dried sample. The content of total phenolics was compared with RSA, and it was well correlated (r = 0.92). High contents of Ca, K, Mg and S were found in all samples.

AH P 08

Ispitivanje ekstrakcije ksantina iz vodenih rastvora

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Ispitivana je ekstrakcija ksantina (3,7-dihidro-purin-2,6-diona) iz vodenih rastvora u prisustvu neorganskih soli (NH_4Cl, NaCl i KCl) pomoću 1-butanola. Kod svih ispitivanih soli uočeno je smanjenje efikasnosti ekstrakcije (“salting-in” efekat) u odnosu na ekstrakciju iz čistog vodenog rastvora. Iako ovakvo ponašanje nije uobičajeno za većinu supstanci, izgleda da je to karakteristično za jedinjenja kod kojih se javlja tautomerna ravnoteža što je već uočeno kod nekih drugih derivata purina i pirimidina. Takođe je ispitivan efekat sinergizma kod ekstrakcije ksantina iz vodenog rastvora NaCl pomoću binarne smeše rastvarača dietil-etar/1-butanol. Kao i kod nekih drugih supstanci koje se slabo ekstrahuju, najbolja efikasnost ekstrakcije postignuta je smešom rastvarača sa malim udelom rastvarača koji je slabije ekstrakciono sredstvo (dietil-etar).

The study of xanthine extraction from aqueous solutions

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Extraction of xanthine (3,7-dihydro-purine-2,6-dione) from aqueous solutions in the presence of inorganic salts (NH_4Cl, NaCl and KCl) with 1-butanol was investigated. For all salts investigated in this study the decrease of extraction efficiency (salting-in effect) was observed in comparison to the extraction from pure aqueous solution. Although such behavior is not common for most substances, it seems to be peculiar for substances displaying tautomeric equilibrium since it was already observed for some other purine and pyrimidine derivatives. Also synergic effect was investigated for the extraction of xanthine from NaCl aqueous solutions with diethyl ether/1-butanol binary solvent mixture. As in the case of some other poorly extractable substances the best extraction efficiency was obtained with the solvent mixture containing small fraction of less efficient extractant (diethyl ether).

AH P 09

Selectivity of molecularly imprinted polymers

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Molecularly imprinted polymers (MIPs) are selective sorbents for a target molecule and they have versatile applications in analytical chemistry. Characterization of MIPs has been carried out in many different ways, but only adsorption isotherms appear to be easily comparable between laboratories. However, the selectivity of MIPs cannot be quantitatively extracted from them. Adsorption isotherms of different templates on their respective MIPs have been frequently measured and found to be nonlinear. The chromatographic peaks using HPLC column filled with MIP are unusually wide, characterized by extreme tailing.

New isotherm presentation method has been proposed, the selectivity of the polymers is easily evaluated with this kind of graph. It was found in batch rebinding studies that the isotherm of the template can be made linear if a suitable additive is added to the solution. An HPLC column was filled with spherical MIP particles in order to investigate if narrower and more symmetrical chromatographic peaks can be obtained in the presence of this additive in the eluent. The main aim is to, if possible, apply this phenomenon for separation of enantiomers (e.g. propranolol) using a column filled with chiral MIP particles.

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Selektivnost molekulski obeleženih polimera

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Karakterizacija molekulski obeleženih polimera (MIP) može se izvršiti na različite načine, ali su samo adsorpcione izoterme lako uporedive među različitim laboratorijama i načinima sinteze. Međutim, selektivnost MIP-ova se ne može kvantitativno odrediti sa adsorpcionih izotermi. Adsorpcione izoterme su često određivane za različite template – analite kojima su polimeri obeleženi i pokazuju nelinearnost. Hromatografski pikovi dobijeni korišćenjem HPLC kolona napunjenih MIP-ovima su veoma široki sa karakterističnom asimetrijom.

U okviru ovog rada određene su adsorpcione izoterme za seriju MIP-ova i neobeleženih polimera (NIP) i predložen je novi način njihovog prikazivanja. Na osnovu ovakvog prikaza, selektivnost polimera se može lako oceniti. Dobijeni rezultati pokazuju da izoterme mogu biti linearne u prisustvu odgovarajućeg aditiva. U planovima za dalji rad je da se pomoću HPLC kolone napunjene sfernim MIP česticama dobiju uži i simetričniji hromatografski pikovi, u prisustvu aditiva u eluentu. Ovaj fenomen bio bi iskorišćen za razdvajanje enantiomera (na primeru propranolola), koristeći kolonu napunjenu hiralnim MIP česticama.

AH P 10

Determination of stability constants of aryldiketo acid complexes with Zn(II)

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4-Aryl-4-oxo-2-butenoic acids (aryldiketo acids-ADK) are compounds able to coordinate divalent metal ions and inhibit many metalloenzymes. An example is carbonic anhydrase, enzyme that catalyzes conversion of CO_2 to hydrogencarbonate, with Zn^{2+} ion in an active site [1]. Conditional stability constants (K_s) of ten Zn(II)-ADK complexes were determined by UV/Vis spectrophotometry under physiological conditions (30 mM TBS, pH = 7.3, I = 0.15 M), using the mole-ratio method (Fig. 1). According to spectrophotometric results, all complexes were formed in 1:1 (ADK : Zn^{2+}) molar ratio with $\log K_s$ in the 4.13–5.76 range. In order to confirm the stoichiometry and stability of Zn(II)-ADK complexes, potentiometric titrations in combination with HYPERQUAD software data analysis were performed. Representative Zn(II)-ADK complex was synthesized and characterized by NMR, IR spectroscopy, and elemental analysis.

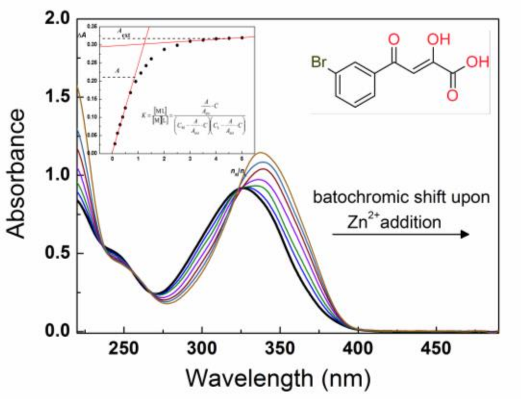

Figure 1. Molar ratio plot of 3-Br ADK

[1] M. Sechi, A. Innocenti, et al. *Bioorg. Med. Chem. Lett.* **22** (2012) 5801.

Одређивање константи стабилности Zn(II) комплекса са арилдикето киселинама

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4-Арил-2,4-диоксобутанске киселине (арилдикето киселине – АДК) су једињења која координативно везују двовалентне металне јоне и инхибирају многе металопротеазе. Један од примера је карбоанхидраза, ензим који катализује претварање CO_2 у хидрогенкарбонат и има Zn^{2+} у активном центру [1]. Условне константе стабилности (K_s) десет Zn(II)-АДК комплекса су одређене помоћу UV-Vis спектрофотометрије под физиолошким условима (30 mM TBS, pH = 7,3, I = 0,15 M) методом молског односа. UV-Vis спектри указују на формирање комплекса у молском односу 1:1 ($\log K_s$ 4,13–5,76). Равнотеже у воденом раствору комплекса проучаване су и потенциометријски уз обраду података софтвером HYPERQUAD. Репрезентативни Zn(II)-АДК комплекс (несупституисана АДК) синтетисан је и окарактерисан помоћу NMR, IR спектроскопије и елементалне анализе.

AH P 11

Human serum albumin binding of certain antimalarials

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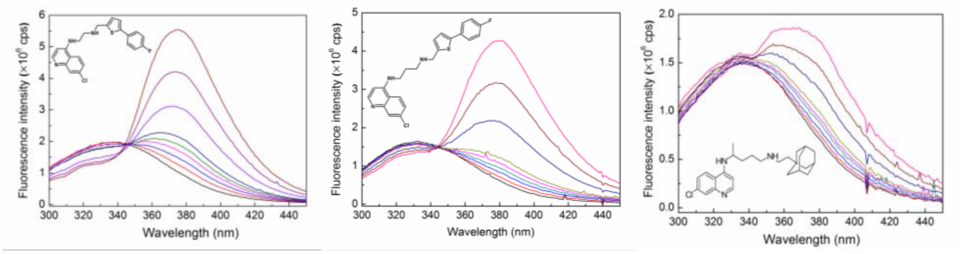
Human serum albumin (HSA) is the most abundant protein in blood plasma and it transports endogenous (fatty acids and bilirubin) and exogenous compounds (drugs) through the blood. In the present study binding of several derivatives of our new antimalarials, and chloroquine, to HSA was investigated by fluorescence spectroscopy (in 0.15 M HEPES, pH 7.35). Results show that among ten studied compounds only those with additional thiophene substructure bind to HSA, with moderate binding constants (comp. **1** $\log K_b = 4.33(\pm 0.46)$ and comp. **2** $\log K_b = 3.81(\pm 0.29)$), representative spectra shown on Fig. 1.



compound 1 **compound 2** **compound 3**

***Figure 1**. Changes in fluorescence emission of HSA upon addition of compounds **1**, **2**, and **3**.*

Competitive binding method with site specific probes (warfarin for Sudlow site I and ibuprofen for Sudlow site II) indicate that compounds **1** and **2** compete with both site probes, with slight preference toward Sudlow site I. Molecular docking studies were used to determine the binding mode of compounds **1** and **2** to HSA.

Везивање неких антималарика за хумани серум албумин

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Хумани серум албумин (ХСА) је најзаступљенији протеин у крвној плазми који преноси ендогене (масне киселине и билирубин) и егзогене супстанце (лекове) кроз крв. Флуоресцентном спектроскопијом је проучавано везивање ХСА са хлорокином и неколико наших нових аминохинолинских антималарика (у 0,15 М HEPES пуферу, pH 7,35). Показано је да се од испитиваних једињења за ХСА везују само једињења која садрже тиофенско језгро ($\log K_b = 4{,}33(\pm 0{,}46)$ за једињење **1** и $\log K_b = 3{,}81(\pm 0{,}29)$ за једињење **2**). Методом компетитивног везивања са специфичним пробама (варфарин и ибупрофен) показано је да се **1** и **2** везују за оба места, уз нешто већи афинитет према варфаринском месту. Докинг студије су коришћене у циљу утврђивања начина везивања једињења **1** и **2** за ХСА.

PRINT EXIT

AH P 12

Terfenadine pH-solubility profile

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The solubility–pH profile of drug substances is affected by pK_a values, ionic strength, buffer effects, aggregation, etc. A novel approach, based on the saturation shake-flask method, was described to address many of the challenges of salt solubility determinations. Terfenadine (Tf), antihistaminic drug formerly used for the treatment of allergic conditions, was used as a model compound, and its solubility determined at 25°C, in 0.15 M HEPES buffered solution (pH range 0.7–11.9). The pH – pc_H conversion is based on Avdeef-Bucher four parameter equation. The attention was paid to the total used mass of Tf, precise knowledge of all volumes and concentrations, time of equilibration and sedimentation, as this can make a significant difference in salt solubility experiments. Concentration of Tf in the supernatant was determined by HPLC-MS. The computer program p-DISOL-X^{TM} was used for data processing and refinement of equilibrium constants. The ionic strength ranged from 0.00 to 0.37 M and intrinsic solubility from 0.29 μg/mL to 0.35 mg/mL. Tf saturated solutions showed slight departure from the predictions based on Henderson-Hasselbalch equation. This might be caused by the Tf adsorption on hydrophobic PVDF membrane used for filtering; the solubility studies with hydrophobic *vs.* hydrophilic membrane filters are already in progress.

Proučavanje pH-zavisne rastvorljivosti terfenadina

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Rastvorljivost lekova zavisi od pK_a vrednosti, jonske sile, vrste pufera, agregacije molekula i sl. U ovom radu primenjen je nov pristup određivanju pH-zavisne rastvorljivosti zasnovan na postizanju zasićenja 'shake-flask' metodom i obradi podataka softverom p-DISOL-X^{TM}. Kao model jedinjenje izabran je terfenadin (Tf), ranije korišćen antihistaminik. Rastvorljivost je određivana na 25°C u 0,15 M HEPES puferu u pH intervalu 0,7–11,9. Konverzija pH u pc_H vrednosti izvedena je prema Avdeef-Bucher četvoro-parametarskoj jednačini. Ukupna masa Tf, zapremine i koncentracije korišćenih rastvora za podešavanje pH vrednosti, vreme uspostavljanja ravnoteže i sedimentacije su parametri o kojima je posebno vođeno računa jer značajno utiču na rastvorljivost. Koncentracija Tf u supernatantu je određena pomoću HPLC-MS, a podaci o ukupnoj jonskoj sili i rastvorljivosti dobijeni su obradom rezultata programom p-DISOL-X^{TM}. Jonska sila je u rastvorima varirala u intervalu 0,00–0,37 M, a rastvorljivost u zavisnosti od pH od 0,29 μg/mL do 0,35 mg/mL. Rastvorljivosti Tf u rastvorima različitih pH vrednosti odstupaju od predviđanja zasnovanog na Henderson-Hasselbalch jednačini. Ovo odstupanje može biti posledica adsorpcije Tf na hidrofobnoj membrani PVDF filtera; u toku su ispitivanja uticaja vrste membrane (hidrofobna *vs.* hidrofilna) na koncentraciju supstance u supernatantu.

AH P 13

Potenciometrijska karakterizacija i analitička primena piritne i halkopiritne elektrode za određivanje askorbinske kiseline

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Netoksični materijali koji potiču iz prirodnog okruženja, monokristali pirit i halkopirit, upotrebljeni su kao membrane elektroda čije su karakteristike ispitane u vodenoj i nevodenoj sredini. Navedene elektrode sa čvrstom membranom su jednostavne konstrukcije, pokazuju stabilan potencijal, kratko vreme odgovora (< 15 s), sub-Nernstovsku zavisnost sa nagibom od 48,0 mV po dekadi za piritnu i 42,4 mV po dekadi za halkopiritnu elektrodu u acetonitrilu, kao i mogućnost primene u velikom intervalu koncentracija ispitivanih vrsta u vodenoj i nevodenoj sredini. Osnovna namena piritne i halkopiritne indikatorske elektrode je njihova dalja primena za određivanje askorbinske kiseline u farmaceutskim proizvodima u vodi i acetonitrilu, uz bakar(II) jon kao titrant. Rezultati pokazuju da je najveća promena potencijala u okolini tački ekvivalencije u prisustvu helatnog, bidentatnog liganda, neokuproina (2,9-dimetil-1,10-fenantrolin). Standardna devijacija dobijenih rezultata je manja od 1,0%. Predložena potenciometrijska metoda za određivanje askorbinske kiseline je precizna, brza i reproduktivna, uz veliku osetljivost, selektivnost i pouzdanost primenjenih senzora.

Potentiometric characterisation and analytical application of pyrite and chalcopyrite electrode for determination of ascorbic acid

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Nontoxic materials that originate from natural environment, monocrystalline pyrite and chalcopyrite, were used as electrodes' membrane whose characteristics were investigated in aqueous and non-aqueous medium. These electrodes with solid state membrane have simple construction; they show stable potential, short response time (< 15 s), sub-Nernstian response, with a slope of 48.0 mV per decade for pyrite and 42.4 mV per decade for chalcopyrite in acetonitrile, as well as a possibility of their usage in wide concentration interval of examined species in aqueous and non-aqueous solution. The main purpose of the pyrite and chalcopyrite indicator electrode is their further application in determination of ascorbic acid in pharmaceutical products in water and acetonitrile, by using Cu(II) solution as the titrant. The results show that the largest potential change in the vicinity of the equivalence point was obtained in the presence of chelating bidentate ligand, neocuproine (2,9-dimethyl-1,10-phenanthroline). The standard deviation of obtained results is less than 1.0%. The potentiometric method proposed for ascorbic acid determination is precise, rapid and reproducible, with large sensitivity, selectivity and reliability of the applied sensors.

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AH P 14

Termohromno ponašanje i termodinamika hlorido kompleksa kobalta(II) u smeši amonijum-nitrat + *N*-metilformamid

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Snimljeni su apsorpcioni spektri kobalta(II) u ispitivanim sistemima NH_4NO_3 + zNMF (z = 3, 4, 5, 6 i 20) u vidljivoj oblasti spektra pri različitoj koncentraciji kobalta(II) i hloridnih jona na pet različitih temperatura: 308,15; 318,15; 328,15; 338,15 i 348,15 K. Analizom spektara izvedeni su zaključci o geometriji nagrađenih kompleksa. Poseban akcenat dat je na analizu uticaja temperature, kao i sastava binarne smeše na oblik i položaj apsorpcionih spektara. Analizom rezultata spektrofotometrijskih merenja, pomoću odgovarajućih kompjuterskih programa utvrđeno je postojanje sledećih kompleksnih čestica: $[Co(NO_3)_4(NMF)_2]^{2-}$, $[CoCl_3(NO_3)(NMF)_2]^{2-}$ i $[CoCl_4]^{2-}$. Određene su konstante stabilnosti navedenih kompleksa u svim sistemima na navedenim temperaturama. Na osnovu konstanti stabilnosti izračunati su termodinamički parametri za reakcije građenja kompleksa.

Termochromic behaviour and thermodynamics of cobalt(II) chlorido complexes in ammonium nitrate + *N*-metylformamide mixture

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Absorption spectra of cobalt(II) for the systems NH_4NO_3 + zNMF (z = 3, 4, 5, 6, and 20) were recorded in the visible wavelength range in the presence of different cobalt(II) and chloride concentrations at five selected temperatures: 308.15; 318.15; 328.15; 338.15, and 348.15 K. From the obtained spectra, geometry of the complexes was discussed. Influences of the temperature and mixture composition on the absorption spectra were also analyzed. From an analysis of the spectra using two computer programs, it was concluded that following complex species were formed: $[Co(NO_3)_4(NMF)_2]^{2-}$, $[CoCl_3(NO_3)(NMF)_2]^{2-}$ and $[CoCl_4]^{2-}$. For these complexes, stability constants were determined at all temperatures. Thermodynamic parameters were also calculated using the temperature dependence of stability constants.

Fizička hemija / Physical Chemistry

FH P 01

Effects of system parameters on decolorization of Reactive Orange 4 dye: comparison of Fenton and photo-Fenton processes

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In this work, the decolorization of textile azo dye Reactive Orange 4 (RO4) by Fenton and photo-Fenton process was investigated. For economic colour removal of dye wastewater by Fenton and photo-Fenton processes, there is a need to investigate the influence of various experimental parameters: effect of initial Fe^{2+}concentration, effect of initial H_2O_2 concentration and effect of initial dye concentration. Decolorization was faster for photo-Fenton process. The best working condition was found for an initial Fe^{2+} concentration of 0.1 mmol dm^{-3} for Fenton and photo-Fenton processes. The influence of initial concentration of H_2O_2 on decolorization of textile dye has been studied at initial concentrations of H_2O_2 from 5 to 50 mmol dm^{-3}. It is shown that the increase of concentration of H_2O_2 brings to an increase of decolorization process efficiency until the concentration of peroxide reaches approximately 25 mmol dm^{-3}, while above this concentration process rate decreases. Removal efficiency decreases with the increase of dye concentration from 10 to 100 mg dm^{-3}.

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Uticaj parametara sistema na dekolorizaciju boje Reactive Orange 4: poređenje Fenton i foto-Fenton procesa

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U ovom radu ispitivano je uklanjanje tekstilne azo boje Reactive Orange 4 (RO4) Fenton i foto-Fenton procesom. U cilju postizanja maksimalne efikasnosti procesa ispitivani su uticaji najznačajniji parametri procesa: uticaj inicijalne koncentracije Fe^{2+} jona, uticaj inicijalne koncentracije H_2O_2 i uticaj inicijalne koncentracije boje. Rezultati su pokazali da je efikasnost uklanjanja boje veća za foto-Fenton proces. Nađeno je da su najbolji uslovi rada pri koncentracijama Fe^{2+} jona od 0.1 mmol dm^{-3}. Uticaj inicijalne koncentracije peroksida na dekolorizaciju tekstilne boje proučavan je u opsegu od 5 do 50 mmol dm^{-3} H_2O_2. Pokazalo se da sa povećanjem koncentracije peroksida najpre raste efikasnost procesa, do koncentracije od oko 25 mmol dm^{-3}, dok iznad ove koncentracije brzina procesa se bitno ne menja. Sa porastom inicijalne koncentracije boje od 10 do 100 mg dm^{-3} smanjuje se brzina njenog razlaganja za oba procesa.

FH P 02

Uticaj polianilin/TiO_2 nanočestičnih katalizatora na fotokatalitičku razgradnju vodene suspenzije mezotriona primenom UV i simuliranog sunčevog zračenja

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Mezotrion {2-[(4-metilsulfonil)-2-nitrobenzoil]cikloheksan-1,3-dion, M_r = 339,3, CAS No 104206-82-8, $C_{14}H_{13}NO_7S$} je herbicid iz familije benzoil-cikloheksandiona, koji se koristi za kontrolu širokog spektra korovskih vrsta, naročito širokolisnih korova prilikom uzgajanja kukuruza. Razvijen je od strane kompanije Syngeta Crop Protection, a registrovan 2000. godine u Evropi, odnosno 2001. godine u SAD. Cilj rada je bio da se ispita fotokatalitička aktivnost sintetisanih polianilin/TiO_2 nanočestičnih katalizatora u različitim molarnim odnosima (TiO_2, TP-50, TP-100 i TP-150) na primeru razgradnje mezotriona primenom UV i simuliranog sunčevog zračenja. Rezultati su upoređeni sa komercijalno dostupnim katalizatorima TiO_2 Degussa P25 i TiO_2 Hombikat. Dobijeni rezultati ukazuju na to da je u UV oblasti najveću fotokatalitičku aktivnost pokazao sintetisani nanočestični katalizator TiO_2. Do sličnih rezultata se došlo primenom simuliranog sunčevog zračenja.

The influence of polyaniline/TiO_2 nanocomposite powders on photocatalytic degradation of aqueous suspension of mesotrione using UV and simulated sunlight

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Mesotrione {2-[(4-methylsulfonyl)-2-nitrobenzoyl]cyclohexane-1,3-dione, M_r = 339.3, CAS No 104206-82-8, $C_{14}H_{13}NO_7S$} is an herbicide from the family of benzoyl-ciclohexanedione, to control wide spectrum of broad leaf weeds, especially in corn farming. It was developed by the company Syngeta Crop Protection and it was registered in Europe in 2000, and in the United States in 2001. The object of this work was investigation of photocatalytic activity of the synthesized polyaniline/TiO_2 nanocomposite powders in different molar ratio (TiO_2, TP-50, TP-100 i TP-150) in the degradation of herbicide mesotrione by UV and simulated sunlight. These results were compared with those obtained using commercially available catalysts TiO_2 Degussa P25 and TiO_2 Hombikat. Obtained results indicate that the highest photocatalytic activity in UV region shows the synthesized catalyst TiO_2. Similar results were obtained using simulated sunlight.

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FH P 03

Volumetrijske osobine, električna provodljivost i viskoznost binarne smeše γ-butirolaktona i jonske tečnosti 1-butil-1-metilpirolidinijum bis(trifluorometilsulfonil)imida

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Gustina, električna provodljivost i viskoznost binarne smeše γ-butirolaktona (GBL) i jonske tečnosti 1-butil-1-metilpirolidinijum bis(trifluorometilsulfonil)imid, [bmim][NTf$_2$], su izmerene u temperaturnom intervalu T = 293.15 - 323.15 K na atmosferskom pritisku i u celom opsegu koncentracija. Iz eksperimentalnih podataka izračunate su dodatne molarne zapremine koje su zatim fitovane Redlich-Kisterovom polinomnom jednačinom. Izračunate su i druge volumetrijske osobine: termički koeficijent širenja, parcijalne molarne zapremine, dodatne molarne zapremine i parcijalne molarne zapremine pri beskonačnom razblaženju, a u cilju dobijanja informacija o interakcijama između GBL i odabrane jonske tečnosti.

Density, excess properties, electrical conductivity and viscosity of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + γ-butyrolactone binary mixtures

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Density, electrical conductivity and viscosity of binary liquid mixtures of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [bmim][NTf$_2$], with γ-butyrolactone (GBL) were measured at temperatures from (293.15 to 323.15) K and at atmospheric pressure over the whole composition range. Excess molar volumes have been calculated from the experimental densities and were fitted with Redlich-Kister polynomial equation. Other volumetric properties, such as isobaric thermal expansion coefficients, partial molar volumes, apparent molar volumes and partial molar volumes at infinite dilution have been also calculated, in order to obtain information about interactions between GBL and selected ionic liquid.

PRINT EXIT

Elektrohemija / Electrochemistry

EH P 01

Primena derivata tiazola kao inhibitora korozije bakra

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U ovom radu je ispitivana mogućnost primene 2-tiono-5-(4'-etoksibenziliden)-2,4-dioksotetrahidro-1,3-tiazola, TEBDT kao potencijalnog inhibitora korozije bakra u kiseloj sulfatnoj sredini (0,1 moldm^{-3} Na_2SO_4, pH=3,0). Primenjena potenciostatska polarizaciona merenja ukazuju na to da ispitivano jedinjenje raspolaže dobrim inhibitorskim osobinama u odnosu na koroziju bakra u kiseloj sredini pri datim uslovima. Utvrđeno je da TEBDT deluje kao mešoviti inhibitor, čija efikasnost u velikoj meri zavisi od primenjene koncentracije. Dobijeni rezultati takođe ukazuju i na to da se TEBDT molekuli pri datim eksperimentalnim uslovima adsorbuju na bakarnoj površini. Vrednosti dobijene za konstantu ravnoteže i promenu slobodne energije procesa adsorpcije ukazuju na to da se adsorpcija molekula tiazola na bakarnoj površini odigrava brzo i spontano prateći mehanizam Bokris-Svinkels-ove izoterme. Molekuli tiazola pri tome formiraju stabilan film u kome su organski molekuli koordinaciono vezani za atome bakra.

The application of thiazole derivative as a copper corrosion inhibitor

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In this paper the possibility of using 2-thiono-5-(4'-ethoxybenzylidene)-2,4-dioxotetrahydro-1,3-thiazole, TEBDT as potential copper corrosion inhibitor in acidic sulfate solution (0.1 moldm^{-3} Na_2SO_4, pH=3) was investigated. Applied potentiostatic polarization measurements confirmed that the tested compound has good inhibitory properties against corrosion of copper in acidic environment at the given conditions. It was found that TEBDT acts as a mixed inhibitor, whereby its effectiveness depends on the applied concentration. The results also indicate that the TEBDT molecules at the given experimental conditions are adsorbed on the copper surface. The values obtained for the equilibrium constant and standard free energy of adsorption indicates that the adsorption of thiazole molecules on copper surface is quick, spontaneous and follows the mechanism of Bockris-Swinkels isotherms. Thiazole molecules whereby form stable film, where are the organic molecules coordinative bound to copper atoms.

EH P 02

Elektrohemijska razgradnja azitromicina na DSA platina-oksid elektrodi

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Buduća istraživanja iz oblasti toksikologije i ljudskog zdravlja imaće za cilj da ispitaju stepen uticaja različitih antibiotika. Makrolidni antibiotici su značajni zagađivači vodenih resursa i različite metode njihove razgradnje su među najčešće proučavanim. Azitromicin, koji je indikovan u terapiji infekcija izazvanih osetljivim mikroorganizmima se izdvaja među makrolidima kao jedan od najviše prepisivanih, ali i najrasprostranjenijih u pogledu zagađivanja životne sredine.

U ovom radu je proučavana elektrohemijska razgradnja azitromicina indirektnom elektrolizom na DSA platina-oksid elektrodi u neutralnom elektrolitu. Brzina reakcije je praćena tečnom hromatografijom sa visokim performansama (HPLC), a dobijena reakciona smeša je analizirana tečnom hromatografijom-masenom spektrometrijom (LC-MS) u cilju utvrđivanja proizvoda razgradnje.

Electrochemical degradation of azithromycin on DSA platinum-oxide electrode

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Depending on their toxicity and human health, many antibiotics are regarded as candidates for future investigations. Macrolide antibiotics are outstanding water resources pollutants and as such they are subject of the investigation of degradation ability with different methods. Azithromycin is useful for the treatment of a number of bacterial infections and it is widely marketed although most harmful in environmental sample.

Its degradation was acomplished by indirect electrolysis on DSA platinum-oxide electrode in neutral electrolyte. The rate of electrodecomposition was monitored using HPLC measurements. The reaction mixture were analyzed by LC-MS technique in order to establish the products of degradation.

EH P 03

Elektrolitičko dobijanje mangana iz rastvora bogatog ureom

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Elektrolitičko dobijanje mangana u čistom, metalnom stanju, se uobičajeno vrši iz vodenog rastvora $(NH_4)_2SO_4$ i $MnSO_4$. Međutim, u tehnologiji proizvodnje mangana se neprekidno traga za poboljšanjem procesa, u cilju povećanja iskorišćenja struje i dobijanja glatkih taloga mangana.

U ovom radu je ispitivan proces elektrolize mangana iz novog rastvora, kome je pored uobičajenih soli $(NH_4)_2SO_4$ i $MnSO_4$, dodata urea, $CO(NH_2)_2$ u visokoj koncentraciji (8 mol dm^{-3}). Mangan je taložen iz rastvora sa i bez uree, na čeličnom supstratu, katodnim gustinama struje u opsegu između 40 i 90 mA cm^{-2}, pri čemu je vreme taloženja podešavano tako da talozi imaju debljinu najviše 10 μm. Poboljšanje iskorišćenja struje za taloženje mangana je potvrđeno merenjem mase i debljine dobijenih taloga. Analiza hemijskog sastava prevlaka EDS metodom je pokazala da se iz obe vrste rastvora taloži mangan u metalnom obliku, odnosno bez prisustva Mn-oksida. Pored toga, analizom skenirajućom elektronskom mikroskopijom pokazan je povoljan uticaj dodatka i na morfologiju i poroznost taloga mangana.

Manganese electrolysis from urea-rich solution

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Electrolytic manganese in metallic state is conventionally produced from water solution of $(NH_4)_2SO_4$ and $MnSO_4$. However, the development of technology for electrolytic Mn production has consistently sought more effective performance, in sense of higher current efficiency and smoother morphology of Mn deposit.

In the present article, the manganese electrolysis from a new solution was examined. The influence of additive, urea, $CO(NH_2)_2$, in high concentration (8 mol dm^{-3}), to the conventional deposition solution of $(NH_4)_2SO_4$ and $MnSO_4$ was examined. Manganese was deposited from solutions with and without urea, on steel substrate, at cathodic current densities in the range of 40 – 90 mA cm^{-2}. The deposition time was adjusted to obtain deposit thickness of up to 10 μm. The improvement in the current efficiency for Mn growth was shown by measuring both the mass and thickness of the deposits. The chemical analysis of Mn deposits by EDS, gave evidence that only metallic manganese, without Mn oxides, was deposited from both solutions. Furthermore, the beneficial effect of the additive on the morphology and porosity of the manganese layer was shown by scanning electron microscopy.

Hemijsko inženjerstvo / Chemical Engineering

HIN O 01

Raspodela vremena zadržavanja u kontinulnom reaktoru sa oscilirajućim tokom fluida

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Cilj ovog rada je ispitivanje hidrodinamike kontinualnog reaktora sa oscilirajćim tokom fluida u reaktoru sa pregradama (prstenovima). Dužina reaktora je 2 m, unutrašnji prečnik 44 mm i podeljen je pregradama na 30 jednakih segmenata. Za ispitivanje načina proticanja fluida kroz reaktor primenjena je metoda impulsne promene koncentracije obeležene supstance (OS) i praćenja odziva –OS na izlazu. Kao procesni fluid je korišćena voda atmosferskog pritiska i temperature, a koncentracija obeležene supstance je uzorkovana u vremenu i merana UV - VIS spektrofotometrom. Dobijeni rezultati su pokazali da se pri veoma malim površinskim brzinama proticanja fluida kroz reaktor (Re = 113,5 – 726,0) postiže približno klipno strujanje sa relativno uskom raspodelom vremena zadržavanja (RVZ). Raspodela vremena zadržavanja značajno zavisi od promene uslova oscilatornog toka. Sa povećanjem frekvencije i/ili amplitude oscilacija, aksijalna disperzija se smanjuje i krive RVZ postaju uže. Sličan trend je uočen i u slučajevima povećanja sekundarnog, neoscilatornog toka. Na osnovu eksperimentalnih rezultata razvijen je matematički model neidelanog strujanja sa povratnim tokom fluida kojim se opisuje raspodela vremena zadržavanja u kontinualnom reaktoru sa oscilirajućim tokom fluida.

Residence time distribution in continuous oscillatory flow reactor

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The aim of this study is investigation of hydrodynamics of continuous oscillatory flow baffled reactor. The reactor internal diameter is 44 mm, length of 2 m is divided by baffles in 30 cavities. Residence time distribution (RTD) of liquid phase is determined by the response on a pulse injection of the tracer at the inlet. The process fluid was water at atmospheric temperature and pressure and concentration of the tracer at the outlet was sampled in time and measured by UV - VIS spectrophotometer. The experimental results demonstrate very good internal mixing in compartments between baffles providing narrow residence time distribution. Further, it is shown that the RTD highly dependents on oscillatory flow conditions. Axial dispersion decreases with frequency or/and amplitude of fluid oscillation and thus the flow approaches the plug flow pattern. In addition, similar trend is observed in the case of increasing secondary non-oscillatory flow. Mathematical model that includes compartments and back-mixing is developed to describe non-ideal flow pattern. Back-mixing flow model parameters were obtained from experimental results. The model well describes residence time distribution in continuous oscillatory flow baffled reactor.

HIN P 01

Korelisanje konstante ravnoteže tečno-tečno sirćetne kiseline u sistemu sojino ulje-sirćetna kiselina-vodonik peroksid-voda

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Epoksidovano sojino ulje se koristi kao stabilizator za PVC materijale. Proizvodi se epoksidovanjem sojinog ulja persirćetnom kiselinom formiranom *in situ* iz sirćetne kiseline i vodonik peroksida u prisustvu kiselog katalizatora. Od ispitanih heterogenih katalizatora, kisele jonoizmenjivačke smole imaju najvišu aktivnost. Pri postavljaju matematičkog modela ovog tečno-tečno-čvrstog (ulje-voda-smola) reakcionog sistema, potrebno je uzeti u obzir raspodelu komponenata među fazama. Koeficijent raspodele između uljne i vodene faze se može izračunati iz uslova ravnoteže tečno-tečno i gustine faza.

U ovom radu konstanta ravnoteže tečno-tečno sirćetne kiseline u sistemu sojino ulje-sirćetna kiselina-vodonik peroksid-voda je korelisana sa sastavom smeše i temperaturom primenom UNIQUAC i NRTL modela za koeficijent aktivnosti. Binarni interakcioni parametri ovih modela su određeni fitovanjem eksperimentalnih podataka za konstantu ravnoteže tečno-tečno sirćetne kiseline dobijenih za devet smeša na četiri temperature. Za fitovanje je primenjena metoda Marquardt-a. Niska prosečna relativna greška, 2.93% za UNIQUAC, i 3.07% za NRTL, ukazuje na adekvantnost primene oba modela za proračun konstante ravnoteže tečno-tečno sirćetne kiseline u sistemu sojino ulje-sirćetna kiselina-vodonik peroksid-voda.

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Correlation of liquid-liquid equilibrium constant for acetic acid in a soybean oil-acetic acid-hydrogen peroxide-water system

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Epoxidized soybean oil is a stabilizer for PVC. It is produced by epoxidation of soybean oil with peracetic acid formed *in situ* from acetic acid and hydrogen peroxide in the presence of an acidic catalyst. Among investigated heterogeneous catalysts, acidic ion exchange resins have the highest efficiency. A partitioning of components among system phases has to be included in the kinetic model of this liquid-liquid-solid (oil-water-resin) reaction system. The partition coefficient between the oil and water phases may be calculated from a liquid-liquid phase equilibrium condition and known phase densities.

In this work, the liquid-liquid equilibrium constant for acetic acid in a system soybean oil-acetic acid-hydrogen peroxide-water was correlated with composition of the mixture and temperature using UNQUAC and NRTL models of activity coefficient. Binary interaction parameters of models were determined by fitting the experimental data of the equilibrium constant obtained for nine mixtures at four temperatures. Marquardt method was used for fitting. The low average relative errors, 2.93% for UNIQUAC, and 3.07% for NRTL, indicate the adequacy of both models for calculation of the liquid-liquid equilibrium constant for acetic acid.

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HIN P 02

Investigation of the Solid-liquid Equilibrium of PEG 2000 and PEG 35000 with Aniline and N,N-dimethylaniline

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Experimental determination of solid-liquid equilibrium of binary systems is very important for many industrial processes. In chemical industry, products of many processes are extremely toxic compounds whose use is necessary to regulate. Also, the measures for removing these substances from industrial waste streams have to be defined. Solid-liquid equilibrium is the basis for every crystallization process. It is very important, also, for other processes in chemical industry: separation of thermally unstable compounds and isomers, cooling processes, design of pipelines and production of high purity products. In this work, equilibrium of various organic solvents with poly(ethylene glycols) (PEGs) with molecular weight 2000 and 35000 is investigated, at atmospheric pressure. Aniline and N,N–dimethylaniline are considered as organic solvents. Results of this study indicate that these organic solvents could be treated with investigated solid polymers.

Ispitivanje ravnoteže čvrsto-tečno PEG 2000 i PEG 35000 u rastvoru anilina i N,N-dimetilanilina

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Poznavanje ravnoteže faza čvrsto-tečno pojedinih sistema je od izuzetno velikog značaja u različitim industrijskim procesima. U hemijskoj industriji, proizvodi mnogih procesa su izuzetno toksične supstance čiju upotrebu je potrebno regulisati i definisati mere uklanjanja tih supstanci iz otpadnih industrijskih tokova. Ravnoteža čvrsto-tečno predstavlja osnovu za svaki proces kristalizacije. Takođe, od velike je važnosti i u drugim procesima koji se odvijaju u hemijskoj industriji, kao što su: separacija termonestabilnih jedinjenja ili izomera, rashladni procesi, projektovanje cevovoda, dobijanje proizvoda visoke čistoće itd. U ovom radu ispitivana je ravnoteža pojedinih organskih rastvarača sa polietilen glikolima (PEG) molarne mase 2000 i 35000, na atmosferskom pritisku. Razmatrani organski rastvarači su anilin i N,N-dimetilanilin. Rezultati ove studije ukazuju na mogućnost tretiranja ovih organskih rastvarača ispitivanim čvrstim polietilen glikolima.

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HIN P 03

Merenje gustine etanola, n-heptana i njihovih smeša na visokim temperaturama i pritiscima

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Gustine etanola, n-heptana i njihove tri smeše (25 mol% etanola, 50 mol % etanola i 75 mol % etanola) su merene na Antoan Paar DMA HP gustinomeru. Gustine čistih supstanci su merene u širokom opsegu temperatura (288.15-433.15) K i na pritiscima do 60 MPa. Gustine smeša su merene na sedam izotermi u intervalu (293.15-373.15) K i pritiscima do 40 MPa. Rezultati su upoređeni sa literaturnim podacima u cilju provere eksperimentalne procedure i preciznosti kalibracione metode.

Dobijene gustine su poređene sa literaturnim vrednostima i predstavljene grafički pri čemu se zapaža da je slaganje dobijenih gustina i literaturnih prilično dobro. Prilikom poređenja određena su moeđusobna srednja procentualna odstupanja metenja: 0.052 % za etanol, 0.048 % za heptan, 0.052 % za smešu 25 mol % etanola sa n-heptanom, 0.023 % za smešu 50 mol % etanola i 0.017 % za smešu 75 mol % etanola sa n-heptanom. Dobijeni rezultati su veoma zadovoljavajući, s obzirom na to da je ispitivan veliki broj eksperimentalnih tačaka, kao i na veliki broj polinomskih zavisnosti koje su korišćene u ovom radu.

Density measurement of ethanol, n-heptane and their mixtures at high temperatures and high pressures

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Density of ethanol, n-heptane and their three mixtures (ethanol + n-heptane with 25 mol %, or 50 mol %, or 75 mol % of ethanol) were measured using Anton Paar DMA HP densimeter. The measurements for the pure substances were performed in the wide temperature range (288.15-433.15) K and at pressures up to 60 MPa. The mixtures' densities were measured at 7 isotherms in the interval (293.15-373.15) K and pressures up to 40 MPa.

The results were compared with the literature data in order to verify the experimental procedure and the accuracy of the selected calibration method.

From the presented results it can be concluded that densities determined in our laboratory, using previously described calibration equations3, are in very good agreement with literature data.

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HIN P 04

Viscosity measurements and viscosity deviations for binary systems 2-Butanol+TEGDME, 2-Butanol+NMP and NMP+TEGDME as potential solvents for SO_2 capture from flue gases

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Indirect greenhouse gas, SO_2, is released to atmosphere, due to burning of fossil fuels. Lately, flue gas desulphurization processes (FGD), especially SO_2 capture with physical or chemical absorption followed by solvent thermal regeneration, gained more importance. In this work, viscosities of binary mixtures, at atmospheric pressure, 2-Butanol + Tetraethylene Glycol Dimethyl Ether (TEGDME), 2-Butanol + N-Methyl-2-Pyrrolidone (NMP) and NMP+TEGDME, as potential solvents for SO_2 capture, have been measured and viscosity deviations have been calculated.

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Određivanje viskoznosti i promene viskoznosti binarnih sistema 2-Butanol+TEGDME, 2-Butanol+NMP i NMP+TEGDME kao potencijalnih solvenata za uklanjanje SO_2 iz dimnih gasova

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Usled sagorevanje fosilnih goriva u elektranama, u atmosferu se emituje gas sa efektom staklene bašte sa indirektnim uticajem – SO_2. U poslednje vreme, sve više dobijaju na značaju postupci za odsumporavanje dimnih gasova, sa fizičkom i hemijskom apsorpcijom i termičkom regeneracijom solventa. U radu su prikazane viskoznosti i promene viskoznosti binarnih smeša, 2-Butanol + Tetraetilen glikol dimetil etar (TEGDME), 2-Butanol + N-metil-2-pirolidon (NMP) i NMP+TEGDME, na atmosferskom pritisku, kao potencijalnih solvenata za uklanjanje SO_2.

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HIN P 05

Experimental measurements of volumetric properties, viscosity and refractive index of the binary system diethylsuccinate + 1-propanol

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Density, viscosity and refractive index data for the binary system diethylsuccinate + 1-propanol 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.

Eksperimentalno određivanje volumetrijskih svojstava, indeksa refrakcije i viskoznosti binarnog sistema dietilsukcinat + 1-propanol

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Eksperimentalno su određene gustine, viskoznosti i indeksi refrakcije binarnog sistema dietilsukcinat + 1-propanol 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.

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HIN P 06

Heat transfer from packed bed to an immersed spherical particle

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In this paper, heat transfer coefficients between the hot packed beds of particles and the larger cold immersed sphere were experimentally determined. The packed beds consisted of mono-sized spherical glass particles of d_p=1.2, 1.94 and 2.98 mm. The aluminium test spheres of D_p=6, 12 and 20 mm with K-type (Ni/Al) thermocouples inserted in them were immersed into the bed. The temperatures of the test spheres were recorded until the thermal equilibrium was reached. From these recordings, heat transfer coefficients were determined. The experiments were performed in the range of gas superficial velocity of ~0.3-0.8 m/s and the bed temperature from 90 to 320ºC. It was found that the measured heat transfer coefficients increased with the increase in gas superficial velocity. The heat transfer coefficients were generally larger for smaller test spheres, while they did not show significant dependence on the size of the bed particles.

The mean error between the experimentally determined heat transfer coefficients and the ones calculated from literature correlation was 12.7 %.

Prenos toplote sa pakovanog sloja na uronjenu sferičnu česticu

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U ovom radu, izvršeno je eksperimentalno određivanje koeficijenta prenosa toplote između pakovanog sloja povišene temperature i uronjene sfere sobne temperature. Pakovani sloj čestica su činile sferične staklene čestice prečnika d_p=1.2, 1.94 and 2.98 mm. Aluminijumske test sfere prečnika D_p=6, 12 and 20 mm sa ugrađenim Ni/Al termoparovima su uronjene u pakovani sloj na sobnoj temperaturi. Temperatura test sfera je merena u vremenskim intervalima od 1 s, do postizanja termičke ravnoteže. Korišćenjem ovih eksperimentalnih podataka izračunati su koeficijenti prelaza toplote. Eksperimenti su vršeni u opsegu površinskih brzina gasa od ~0.3-0.8 m/s i temperatura pakovanog sloja od 90 do 320ºC. Utvrđeno je da izmerene vrednosti koeficijenata prelaza toplote rastu sa porastom površinske brzine gasa. Koeficijenti prelaza toplote su bili veći za sitnije čestice, a nije primećena njihova značajna zavisnost od veličine čestica koje su činile pakovani sloj.

Srednje odstupanje između eksperimetalno određenih koeficijenata prenosa toplote i vrednosti izračunatih iz literaturne korelacije iznosila je 12.7 %.

HIN P 07

Solids circulation rate in water fluidized beds of spherical particles

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Liquid–solid fluidized beds represent a widespread type of contactors and are used in many industrial processes. Solids circulation rate is very important quantity in fluidized bed dynamics because it influences the overall agitation in the fluidized bed as well as the transport characteristics of the bed. In this paper, the equation for overall particle circulation rate in water-fluidized beds was proposed using the correlation for the mean particle speed from our previous paper. The optimal porosity of the fluidized bed was defined as the porosity at which the overall circulation rate shows its maximum, which is also the porosity at which the transport coefficients in the bed show their maximal values. The optimal porosity was calculated from the derivative of the proposed correlation. The calculated optimal porosity was in the range 0.68-0.72 for the overall circulation rate. The results obtained are in accordance with the experimental findings from the literature which show that heat and mass transport coefficients have maximal values in the range of porosities of the liquid fluidized beds of 0.6-0.8.

Cirkulacija čestica u fluidizovanom sloju tečnost-sferične čestice

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Fluidizacija tečno-čvrsto se u praksi koristi u različitim procesima kao što su, separacioni procesi, klasifikacija materijala, adsorpcija, jonska izmena, katalitički kreking, za tretman otpadnih voda i slično. Ukupna cirkulacija čestica predstavlja veoma značajnu veličinu u dinamici fluidizovanih slojeva, zato što utiče na mešanje čestica u fluidizovanom sloju, kao i na intenzitet prenosa toplote i mase unutar sloja. U ovom radu su predložene jednačine za ukupnu cirkulaciju čestica u fluidizovanom sloju tečnost (voda) – čestice. U jednačinama je korišćena korelacija za srednju brzinu kretanja čestica u fluidizovanom sloju, predložena u našem prethodnom radu. Definisana je optimalna poroznost fluidizovanog sloja, kao poroznost pri kojoj je cirkulacija čestica u sloju najintenzivnija, odnosno pri kojoj funkcija ukupne cirkulacije čestica ima maksimum. Pri ovoj poroznosti se javljaju i maksimalne vrednosti koeficijenata toplote i mase. Optimalna poroznost je izračunata iz izvoda predložene funkcije ukupne cirkulacije čestica u fluidizovanom sloju u zavisnosti od poroznosti. Izračunate vrednosti optimalne poroznosti fluidizovanog sloja tečnost-čestice su u intervalu od 0,68 do 0,72. Dobijeni rezultati su u skladu sa eksperimentalnim ispitivanjima drugih autora koja su pokazala da su maksimalne vrednosti koeficijenata prenosa toplote i mase dobijene u intervalu poroznosti sloja od 0,6 do 0,8.

Nauka o materijalima / Material Science

NM O 01

Smanjenje emisije slobodnog formaldehida iz veziva koja se koriste u proizvodnji ploča na bazi drveta

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Ovim radom se stavio akcenat na pregled veziva koja se koriste u proizvodnji ploča na bazi usitnjenog drveta, kao i na veziva koja bi mogla ući u upotrebu zbog svog ekološkog značaja.
Formaldehid se u velikoj meri koristi za proizvodnju sintetičkih veziva, reakcijom fenola, uree i melamina. UF - urea – formaldehidno vezivo je najviše korišćeno vezivo, posebno u proizvodnji ploča na bazi drveta. Za proizvodnju kompozitnih materijala na bazi drveta se koriste veziva na bazi formaldehida, čija kasnija emisija dovodi do ozbiljnih zdravstvenih problema. Formaldehid predstavlja najveću brigu, proteklih godina, jer je njegova emisija i kontrola emisije u vazduhu zatvorenog prostora važan faktor u rešavanju ekoloških i zdravstvenih problema, u smislu da je formaldehid opasan po zdravlje i glavni uzročnik iritacije respiratornih organa, dermatoloških problema, kao i uzročnik pojave kancera.

Emission reduction of formaldehyde from the adhesives used in the production of wood based panels

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Of this work is put emphasis on the review of binder used in the production of wood-based chopped wood, and the binder that could come into use because of its ecological importance.
Formaldehyde is used mainly for the production of synthetic adhesives, reaction of phenol, urea and melamine. UF - urea - formaldehyde resin is a resin used, especially in the production of wood-based panels. For the production of composite materials based on wood used formaldehyde-based resins, with subsequent emission leads to serious health problems. Formaldehyde is a major concern, in recent years, because its emissions and control emissions to the indoor air is an important factor in solving environmental and health problems, in the sense that formaldehyde is a health hazard and a major cause irritation of respiratory, dermatological problems and causes of cancer.

NM P 01

Fotokatalitička aktivnost hidrotermalno sintetisanih TiO_2-karbon kompozita

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Hidrotermalnom sintezom na 160 ^{o}C korišćenjem različitih molskih odnosa prekursora, Ti-izopropoksida i rastvora glukoze, dobijeni su kompoziti TiO_2/hidrotermalni ugljenik (TiO_2/HTC). Karakterizacija materijala izvršena je skenirajućom elektronskom mikroskopijom, rendgenskom difrakcijom i UV-vis refleksionom spektroskopijom. Proces razgradnje metilenskog plavog korišćen je za ispitivanje fotokatalitičke aktivnosti TiO_2/HTC karbon kompozita. Dobijeni rezultati pokazuju da sa povećanjem udela glukoze dolazi do povećanja udela anataz kristalne modifikacije. Najbolja fotokatalitička aktivnost postignuta je kod uzorka TiO_2/HTC_3, pri optimalnom molarnom odnosu prekusora Ti-izopropoksid : glukoza = 1 : 0,15.

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Photocatalytic activity of TiO_2-carbon composites hydrothermally synthesized

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In this work, TiO_2-carbon composites (TiO_2/HTC) were obtained by hydrothermal synthesis, using different ratios of precursors, Ti-isopropoxide and glucose solution. Obtained materials were characterized by scanning electron microscopy, X-ray diffraction and UV-Vis diffuse reflectance spectroscopy. The photocatalytic activity of TiO_2/HTC carbon composites was tested by photodegradation of methylene blue in aqueous solution. It was shown that the ratio of crystal modification anatase increased with increasing the share of glucose. The best photocatalytic activity was observed with optimal molar ratio of precursors Ti-isopropoxide : glucose = 1 : 0.15.

Neorganska hemija / Inorganic Chemistry

NH O 01

Kompleksi zlata(III) sa monodentatno koordinovanim hinoksalinom i fenazinom

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Heterociklična jedinjenja koja u svojoj strukturi sadrže atom azota predstavljaju veoma važne ligande u sintezi kompleksa zlata(III), kao potencijalnih antitumorskih i antimikrobioloških agenasa [1]. U ovom radu, ispitivane su reakcije između K[AuCl$_4$] kompleksa i dva heterociklična liganda, hinoksalina (qx) i fenazina (phz). Nađeno je da se u ispitivanim reakcijama, bez obzira na molski odnos reaktanata, uvek formiraju kompleksi zlata(III) sa monodentatno koordinovanim heterocikličnim ligandima. Dobijeni kompleksi su okarakterisani primenom NMR spektroskopije i rendgenske strukturne analize. Rezultati rendgenske strukturne analize su pokazali da, u kristalima ispitivanih kompleksa, postoje π···π interakcije, dok Au…Cl interakcije nisu utvrđene. Pored toga, u kristalima [AuCl$_3$(phz)] kompleksa, postoje intramolekulske Au…H–C i intermolekulske Cl…N interakcije, kao posledica C_2 molekulske simetrije kompleksa.

Gold(III) complexes with monodentate coordinated quinoxaline and phenazine

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Nitrogen-containing heterocycles represent an important class of ligands in the synthesis of gold(III) complexes that have been evaluated as potential antitumor and antimicrobial agents [1]. Considering this, in the present study, we have investigated the reactions of K[AuCl$_4$] complex with two diazaaromatic ligands, namely quinoxaline (qx) and phenazine (phz). Regardless of different stoichiometric ratio of the reactants, only gold(III) complexes with monodentate coordinated diazaaromatic ligands have been isolated and characterized by NMR and X-ray diffraction techniques. In crystals, [AuCl$_3$(qx)] and [AuCl$_3$(phz)] complexes are involved in columnar π···π stacking interactions, but are deprived of short Au…Cl contacts. Furthermore, short intramolecular Au…H–C and intermolecular Cl…N contacts, that appear in the crystals of [AuCl$_3$(phz)], have been interpreted as resulting from utilization of C_2 molecular symmetry of this complex in the crystal.

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NH P 01

Spektroskopsko ispitivanje interakcija M(II) jona biometala sa sirćetnom kiselinom

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U radu je ispitivana interakcija M(II) jona biometala (Cu, Co, Mn) na molarnom i milimolarnom nivou UV/VIS i FTIR spektroskopijom sa O-donor ligandom, sirćetnom kiselinom (AcA) koja se u svakodnevnoj ishrani koristi kao aditiv. Promene u UV/VIS spektrima ispitivanih model sistema M(II)-AcA (λ_{max}, Abs., Δ) u odnosu na rastvor jona biometala ukazuju da dolazi do interakcije između ispitivanog O-donor liganda i odgovarajućeg M(II) jona. Promene u FTIR spektrima ispitivanih model sistema, $\Delta\nu = \nu_{asim}(COO) - \nu_{sim}(COO)$, $\Delta\nu_{Cu\text{-}AcA}=215$ nm, $\Delta\nu_{Co\text{-}AcA}=175$ nm i $\Delta\nu_{Mn\text{-}AcA}=217$ nm, ukazuju da se AcA u sistemu sa Cu(II) i Mn(II) jonom ponaša kao monodentatni O- donor ligand. U sistemu sa Co(II) jonom ista se ponaša kao bidentanti ligand. Jačina interakcija metal ligand, prema položaju R–C–O---M(II) vibracija, opada u nizu Co–AcA > Cu–AcA > Mn–AcA, što je posledica osobina jona metala (jonski radijus, polarizabilnost, energija stabilizacije u ligandnom polju).

Spectroscopic investigation of interaction of M(II) biometal ions and acetic acid

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In this study was investigated a interaction between M(II) biometal ions (Cu, Co, Mn) and O-donor ligand acetic acid (AcA), which is used as daily diet aditive, on molar and milimolar level by UV/VIS and FTIR spectroscopy. The changes in the UV/VIS spectra of the investigated model systems M(II)-AcA (λ_{max}, Abs., Δ) with regard to the solution of biometal ions show that there is interaction between the investigated O-donor ligand and the corresponding M(II) ion. The changes in FTIR spectra of analyzed model systems $\Delta\nu = \nu_{asim}(COO) - \nu_{sim}(COO)$, $\Delta\nu_{Cu\text{-}AcA}=215$ nm, $\Delta\nu_{Co\text{-}AcA}=175$ nm and $\Delta\nu_{Mn\text{-}AcA}=217$ nm, indicate that AcA behave as monodentate ligand in system with Cu(II) and Mn(II) ion. In the system with Co(II) ion this O-donor ligand behave as a bidentate ligand. Stength of metal-ligand interaction, according to assignment of R–C–O---M(II) vibration, decreases in the series Co–AcA > Cu–AcA > Mn–AcA, as a result of properties of metal ions (ionic radius, polarizability, energy stabilization of the ligand field).

NH P 02

Korelacija u sadržaju biometala (Fe, K, Ca, Zn) biljne vrste koprive (*Urtica dioica L.*) iz zemljišta sa lokaliteta u okolini Niša

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U radu je ispitivan sadržaj Fe i drugih biometala K, Ca i Zn u biljnoj vrsti koprivi *(Urtica dioica L)* koja se u ovom podneblju tradicionalno koristi u ishrani i lečenju anemije, sa različitih staništa u okolini Niša (sela Cerje i Prosek). Sadržaj biometala određivan je u biljci i zemljištu na kome je rasla, zemljište bogato krečnjakom na nadmorskoj visini od 580 m (Cerje) i silkatno zemljište na nadmorskoj visini od 290 m (Prosek). Sadržaj metala određivan je tehnikom ICP-OES u rastvoru po proceduri koja se primenjuje za analizu biljnog materijala i zemljišta. Sa ispitivanih staništa ova biljka sadrži od 0,0252 do 0,0979 mg/g Fe, pri čemu je viši sadržaj vezan za biljke koje su rasle na zemljištu bogatom krečnjakom. Ova biljna vrsta je i dobar nutritijent za ostale biometale K (24,69 – 25,35 mg/g), Ca (16,00 – 21,05 mg/g) i Zn (0,0282 – 0,0352 mg/g).

Correlation of content of biometals (Fe, K, Ca, Zn) in plant species of Stinging nettle (*Urtica dioica* L.) from soil from sites in the surroundings of Niš

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This study examines the content of Fe and other biometals K, Ca and Zn in plant species of Stinging nettle *(Urtica dioica L)* which is traditionally used in nutrition and treatment of anemia in this region, from different habitats in the surroundings of Niš (village Cerje and Prosek). The content of biometals was determined in the plant and soil in which it grew, the soil that is rich with limestone at an altitude of 580 m (Cerje), and silicate soil at an altitude of 290 m (Prosek). The content of biometals (Fe, K, Ca, Zn) was determined by ICP-OES in the solution according to the procedure which is used for the analysis of plant material and soil. This plant contains from 0,0252 to 0,0979 mg/g Fe in investigated habitats, wherein the higher content is related with the plants which are grown in soils rich in limestone. This plant species is also a good nutrient for the other biometals K (24,69 – 25,35 mg/g), Ca (16,00 – 21,05 mg/g) and Zn (0,0282 – 0,0352 mg/g).

NH P 03

Kristalne strukture PLTSC·HCl·2H_2O i kompleksa [Fe(PLTSC)Cl_2(H_2O)]Cl

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Tiosemikarbazoni i njihovi kompleksi sa metalima predstavljaju važnu klasu jedinjenja sa širokim spektrom farmakoloških karakteristika. U poslednjih nekoliko decenija, posebna pažnja je posvećena tiosemikarbazonima derivatima biološki važnog supstrata piridoksala (forme vitamina B6). Nađeno je da kompleksi metala sa ligandima odgovarajućih tiosemikarbazona piridoksala (PLTSC) pokazuju antitumorno dejstvo.
U ovom radu, sintetisali smo i strukturno okarakterisali novo jedinjenje PLTSC·HCl·2H_2O (**1**) i prvi mono PLTSC oktaedarski Fe(III) kompleks formule *cis*-(Cl)-[Fe(PLTSC)Cl_2(H_2O)]Cl (**2**). PLTSC katjon u jedinjenju **1** zauzima konfiguraciju u kojoj su fenolni kiseonik *cis*, a atom sumpora *trans* u odnosu na hidrazinski atom azota. U jedinjenju **2**, Fe(III) se nalazi u deformisanom oktaedarskom okruženju jednog ONS tridentatnog PLTSC liganda i jednog hloridnog jona u ekvatorijalnoj ravni, dok aksijalna mesta zauzimaju drugi hloridni jon i molekul vode. Nađeno je da je ligand koordinovan u neutralnoj, ali cviter-jonskoj formi, preko atoma kiseonika fenolne OH-grupe, azometinskog atoma azota i atoma sumpora.

Crystal structure of PLTSC·HCl·2H_2O and complex [Fe(PLTSC)Cl_2(H_2O)]Cl

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Thiosemicarbazones (TSCs) and their metal complexes represent an important class of compounds with a wide range of pharmacological properties. In the last few decades, special attention has been devoted to the TSCs derived from biologically important substrate pyridoxal (form of vitamin B6). It has been found that the metal complexes of the corresponding pyridoxal thiosemicarbazone (PLTSC) ligands display antitumoral activity.
In this work, we have synthesized and structurally characterized novel compound PLTSC·HCl·2H_2O (**1**) and first mono PLTSC octahedral Fe(III) complex of the formula *cis*-(Cl)-[Fe(PLTSC)Cl_2(H_2O)]Cl (**2**). The PLTSC cation in **1** is found in a configuration where the phenolic oxygen is in *cis*, while the sulfur atom is in *trans* position with respect to hydrazine nitrogen. In **2**, the Fe(III) atom is six-coordinated by one tridentate ONS PLTSC ligand and one chloride in equatorial plane, while axial positions are occupied by another chloride and water. It was found that ligand is coordinated in its neutral but zwitterionic form, *via* oxygen atom of phenolic OH-group, azomethine nitrogen atom and sulfur atom.
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NH P 04

Kompleksi hroma(III) sa semikarbazonom piridoksala

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Dugi niz godina, a posebno u poslednje vreme, kompleksi prelaznih metala sa ligandima na bazi halkogensemikarbazida predmet su proučavanja mnogih autora, ne samo sa teorijskog, već i sa aspekta praktične primene. Sa tridentatnim ONO semikarbazonom piridoksala (PLSC), kao jednim iz ove klase liganada, do sada su opisani kompleksi sa mnogim prelaznim metalima kao što su bakar, gvožđe, nikal, vanadijum i platina. U ovom radu, po prvi put, opisane su sinteze oktaedarskih kompleksa hroma(III) formula $[Cr(PLSC)(PLSC-H)](NO_3)_2 \cdot H_2O$ (**1**), $K[Cr(PLSC-H)(NCS)_3] \cdot EtOH$ (**2**) i $[Cr(PLSC-H)(NCS)_2(NH_3)] \cdot 2H_2O$ (**3**). Kompleksi su okarakterisani elementalnom analizom, IR spektroskopijom, konduktometrijskim merenjima, a kompleks **2,** kao i PLSC·HNCS, koji nastaje pri sintezi ovog kompleksa i rendgeno-strukturnom analizom.

Complexes of chromium(III) with pyridoxal semicarbazone

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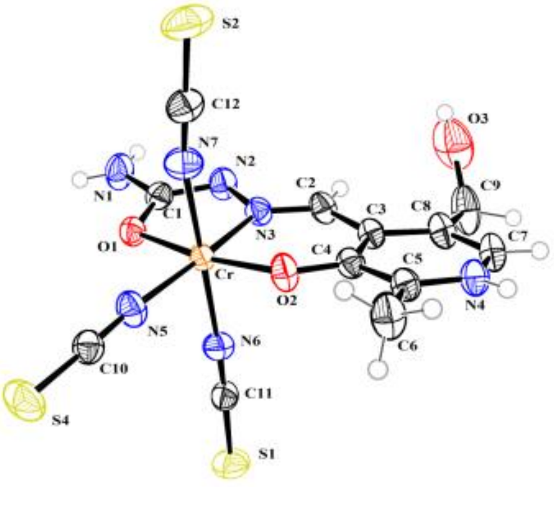
For many years, and particularly in recent time, transition metal complexes with ligands based on chalkogensemicarbazides are the subject of study by many authors, not only theoretically but also in terms of practical application. Complexes of a tridentate ONO pyridoxal semicarbazone (PLSC), as one belonging to this class of ligands, with many transition metals such as copper, iron, nickel, vanadium and platinum are hitherto described. This paper reports, for the first time, syntheses of octahedral chromium(III) complexes of the formulas: $[Cr(PLSC)(PLSC-H)]-(NO_3)_2 \cdot H_2O$ (**1**), $K[Cr(PLSC-H)(NCS)_3] \cdot EtOH$ (**2**) i $[Cr(PLSC-H)(NCS)_2(NH_3)] \cdot 2H_2O$ (**3**). The complexes are characterized by elemental analysis, IR spectroscopy and conductometry. Additionally, complex **2**, as well as PLSC·HNCS which is obtained during the synthesis of this complex, are characterized by X-ray crystallography.

The research was supported by the Ministry of Education and Science, of the Republic of Serbia (Grant no. 172014).



NH P 05

Hidroliza peptidne veze u *N*-acetilovanim L-metionil-glicin i L-histidil-glicin dipeptidima u prisustvu različitih dinuklearnih kompleksa platine(II)

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Raniji rezultati ispitivanja reakcija dinuklearnih kompleksa Pt(II) sa peptidima koji u bočnom nizu sadrže aminokiseline L-metionin i L-histidin su pokazali da ovi kompleksi predstavljaju dobre katalitičke agense za hidrolitičko raskidanje peptidnih veza u ovim molekulima.[1,2] U ovom radu, primenom ^{1}H NMR spektroskopije, ispitivane su reakcije hidrolize *N*-acetilovanih dipeptida L-metionil-glicina (Ac-L-Met–Gly) i L-histidil-glicina (Ac-L-His–Gly) u prisustvu $\{[Pt(L)(H_2O)]_2(\mu\text{-pz})\}^{4+}$ kompleksa (L je bidentatno koordinovan diamin: 1,3-pn, 1-Et-1,3-pn i 2,2-diMe-1,3-pn; pz je mostni pirazinski ligand). Dipeptid i odgovarajući Pt(II) kompleks su reagovani u 1:1 molskom odnosu, u pH oblasti 2,0–2,5 u D_2O i na 37 °C. Nađeno je da dinuklerani $\{[Pt(L)(H_2O)]_2(\mu\text{-pz})\}^{4+}$ kompleksi hidrolizuju Met–Gly peptidnu vezu u Ac-L-Met–Gly, pri čemu brzina hidrolize ne zavisi od sternog efekta Pt(II) kompleksa. Međutim, u reakciji Ac-L-His–Gly dipeptida i odgovarajućeg dinukleranog Pt(II) kompleksa, pri navedenim eksperimentalnim uslovima, brzina hidrolize His–Gly peptidne veze opada sa povećanjem sternog efekta kompleksa platine(II) (1,3-pn > 1-Et-1,3-pn > 2,2-diMe-1,3-pn).

Hydrolysis of the amide bond in *N*-acetylated L-methionylglycine and L-histidylglycine in the presence of different dinuclear platinum(II) complexes

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Recent studies of the reactions between dinuclear Pt(II) complexes and methionine- and histidine-containing peptides showed that these complexes can be promising reagents for hydrolytic cleavage of the amide bond.[1,2] In the present study, the hydrolytic reactions of Ac-L-Met–Gly and Ac-L-His–Gly dipeptides in the presence of dinuclear $\{[Pt(L)(H_2O)]_2(\mu\text{-pz})\}^{4+}$ complexes (L is bidentate coordinated diamine: 1,3-pn, 1-Et-1,3-pn and 2,2-diMe-1,3-pn; pz is bridging pyrazine ligand) were studied by ^{1}H NMR spectroscopy. All reactions were performed with equimolar amounts of the reactants in the pH range 2.0–2.5 in D_2O as solvent and at 37 °C. It was found that $\{[Pt(L)(H_2O)]_2(\mu\text{-pz})\}^{4+}$ complexes affect hydrolytic cleavage of the Met–Gly amide bond in Ac-L-Met–Gly and that the rate of this reaction does not depend on the steric bulk of the catalyst. However, in the reaction of dipeptide Ac-L-His–Gly with these complexes, under the above mentioned experimental conditions, the rate of hydrolysis of the His–Gly amide bond decreases as the steric bulk of the platinum(II) complex increases (1,3-pn > 1-Et-1,3-pn > 2,2-diMe-1,3-pn).

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NH P 06

Sinteza i spektroskopska karakterizacija kompleksa nikla(II) sa nekim diaminopolikarboksilatnim ligandima

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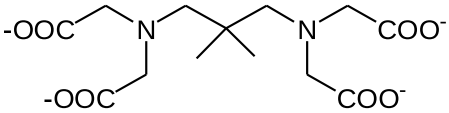
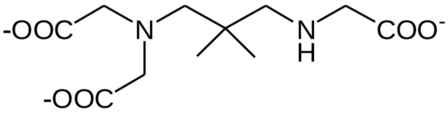
Sintetisani i okarakterisani su novi 2,2-diMe-1,3-pdta (2,2-dimetil-1,3-propandiamin-*N,N,N',N'*-teraacetat) i 2,2-diMe-1,3-pd3a (2,2-dimetil-1,3-propandiamin-*N,N,N'*-triacetat) ligandi. Barijumove soli ovih liganada su upotrebljene za sintezu odgovarajućih kompleksa nikla(II). Infra-crveni i elektronski apsorpcioni spektri sintetisanih Mg[Ni(2,2-diMe-1,3-pdta)]$\cdot 6H_2O$ i Mg[Ni$_2$(2,2-diMe-1,3-pd3a)$_2$]$\cdot 9H_2O$ kompleksa su poređeni sa odgovarajućim spektrima ranije okarakterisanih Mg[Ni(1,3-pdta)]$\cdot 8H_2O$ [1], Mg[Ni(1,3-pndta)]$\cdot 10H_2O$ [2] (1,3-pentandiamin-*N,N,N',N'*-teraacetat) i Mg[Ni$_2$(1,3-pnd3a)$_2$]$\cdot 8H_2O$ (1,3-pentandiamin-*N,N,N'*-triacetat) [2] kompleksa.



2,2-diMe-1,3-pdta



2,2-diMe-1,3-pd3a

Synthesis and spectroscopic characterization of nickel(II) complexes with some diaminopolycarboxylate ligands

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New 2,2-diMe-1,3-pdta (2,2-dimethyl-1,3-propanediamine-*N,N,N',N'*-teraacetate) and 2,2-diMe-1,3-pd3a (2,2-dimethyl-1,3-propanediamine-*N,N,N'*-triacetate) ligands have been synthesized and characterized. In the present study barium salts of these ligands have been used for preparation of the corresponding nickel(II) complexes. The infrared and electronic absorption spectra of the presently investigated Mg[Ni(2,2-diMe-1,3-pdta)]$\cdot 6H_2O$ and Mg[Ni$_2$(2,2-diMe-1,3-pd3a)$_2$]$\cdot 9H_2O$ complexes are discussed in comparison with those previously reported for the analogous Mg[Ni(1,3-pdta)]$\cdot 8H_2O$ (1,3-propanediamine-*N,N,N',N'*-tetraacetate) [1], Mg[Ni(1,3-pndta)]$\cdot 10H_2O$ (1,3-pentanediamine-*N,N,N',N'*-teraacetate) [2] and Mg[Ni$_2$(1,3-pnd3a)$_2$]$\cdot 8H_2O$ [2] complexes (1,3-pentanediamine-*N,N,N'*-triacetate).

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

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NH P 07

Uticaj kompleksa rutenijuma(II) na aktivnost enzima antioksidativne odbrane

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Reaktivne kiseonične vrste (ROS) su u niskoj koncentraciji neophodne za signalizaciju mnogih ćelijskih procesa, dok u visokoj koncentraciji uzrokuju oksidativni stres i oštećenja biomakromolekula. Organizam je razvio sistem antioksidativne odbrane preko enzima kao što su superoksidna-dismutaza (SOD) i katalaza (CAT). Ispitan je efekat dva kompleksa Ru(II), opšte formule TF.2H[$RuCl_3(DMSO)_3$] **(1)** i TF.2H[$RuCl_3(\eta^6$-p-cymen)] **(2)** (TF.2H je protonovani trifluoperazin), u tri različite doze (0.4, 4.5 i 90.4 μmol kg^{-1} TM) na produkciju ROS-a prateći aktivnost antioksidativnih enzima SOD i CAT u krvi pacova pod fiziološkim uslovima. Kompleks **(2)** smanjuje ukupnu aktivnost SOD u svim dozama u odnosu na kontrolnu grupu i nema uticaja na stvaranje $O_2^{\bullet -}$, dok kompleks **(1)** u nižim dozama pokazuje veliki zaštitni efekat. Značajno povećanje ukupne SOD aktivnosti i njenih izoenzima uočeno je dodatkom 90.4 μmol kg^{-1} TM kompleksa **(1)**. Najniža aktivnost CAT dokazana je primenom kompleksa **(1)** u dozi od 4.5 mmol kg^{-1} TM. Kompleks **(2)** ne utiče značajno na aktivnost CAT, ali njena aktivnost linearno opada sa povećanjem doze ovog kompleksa. Smanjenje aktivnosti CAT direktno je povezano sa smanjenjem aktivnosti SOD i ukazuje da manje doze kompleksa **(1)** ne dovode do proizvodnje $^{\bullet}OH$ u fiziološkim uslovima.

The effects of ruthenium(II) complexes on the activity of antioxidative enzymes

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Reactive oxygen species (ROS) in a low levels are vital for many cell signaling events, while the high concentrations as result have oxidative stress and damage of the biological macromolecules. Organisms developed a variety of antioxidant defenses that include antioxidant enzymes as superoxide dismutase (SOD) and catalase (CAT) to protect itself. We investigated the effects of two Ru(II) complexes of the general formulae TF.2H[$RuCl_3(DMSO)_3$] **(1)** and TF.2H[$RuCl_3(\eta^6$-p-cymen)] **(2)** (TF.2H is protonated trifluoperazine) applied in three different doses (0.4, 4.5 and 90.4 μmol kg^{-1} bw) on the production of ROS by following antioxidant enzymes activity of SOD and CAT in rats blood, under physiological conditions. Complex **(2)** is reduced the overall activity of SOD in all the applied doses comparing to the control group and does not affect the creation of $O_2^{\bullet -}$, while the complex **(1)** showed the greatest protect effect applied in the lower doses. Significant increasing of total SOD activity and their isoenzymes is noticed using 90.4 μmol kg^{-1} bw of complex **(1)**. The lowest value of CAT activity is observed using complex **(1)** at 4.5 mmol kg^{-1} bw. The complex **(2)** has no significant effect on CAT activity, but its activity decreases linearly with increasing of applied dose. Decreased CAT activity is directly associated with a reduced activity of SOD and indicates that the complex **(1)** in lower doses does not lead to the production of $^{\bullet}OH$ under physiological conditions.

NH P 08

Zlato(III) kompleks sa *O,O'*-di-*n*-butil-(*S,S*)-etilendiamin-*N,N'*-di-2-(4-metil)pentanoatom – ligandom R_2edda-tipa: sinteza i karakterizacija

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Kompleksi zlata(III) sa R_2edda-tip ligandima su već pokazali značajnu *in vitro* anti-tumorsku aktivnost[1].

Novi zlato(III) kompleks $[AuCl_2\{(S,S)\text{-}(n\text{-}Bu)_2eddl\}]PF_6$, ($(S,S)\text{-}(n\text{-}Bu)_2eddl$ = *O,O'*-di-*n*-butil-(*S,S*)-etilendiamin-*N,N'*-di-2-(4-metil)pentanoat), sintetisan je i okarakterisan elementalnom analizom, IC, ^{1}H i ^{13}C NMR spektroskopijom i masenom spektrometrijom.

Rezultati elementalne analize odgovaraju prikazanoj formuli. IC spektar pokazuje specifične apsorpcione trake: ν(C=O) na 1736 cm^{-1}, ν(C–O) na 1246 cm^{-1} i $\nu(CH_3)$ na 2963 cm^{-1}. U ^{1}H NMR spektru etilenski protoni iz etilendiaminskog dela molekula nalaze se na 3,55 ppm, što ukazuje na koordinaciju azotovih atoma. U ^{13}C NMR spektru karbonilni ugljenikovi atomi nalaze se na očekivanoj vrednosti hemijskog pomeranja za ovu klasu jedinjenja kod kojih kiseonik ne učestvuje u koordinaciji (170,3 ppm).

Gold(III) complex with *O,O'*-di-*n*-butyl-(*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)pentanoate – R_2edda-type ligand: synthesis and characterization

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Gold(III) complexes with R_2edda-type ligands have already shown significant *in vitro* antitumor activity[1].

A novel gold(III) complex, $[AuCl_2\{(S,S)\text{-}(n\text{-}Bu)_2eddl\}]PF_6$, ($(S,S)\text{-}(n\text{-}Bu)_2eddl$ = *O,O'*-di-*n*-butyl-(*S,S*)-ethylenediamine-*N,N'*-di-2-(4-methyl)pentanoate), was synthesized and characterized by elemental analysis, IR, ^{1}H i ^{13}C NMR spectroscopy and mass spectrometry.

Results of elemental analysis are in agreement with the proposed formula. IR spectrum shows specific absorption bands: ν(C=O) at 1736 cm^{-1}, ν(C–O) at 1246 cm^{-1} and $\nu(CH_3)$ at 2963 cm^{-1}. In ^{1}H NMR spectrum ethylene protons from ethylenediamine moiety are found at 3.55 ppm, indicating nitrogen coordination. In ^{13}C NMR spectrum, carbonyl carbon atoms show resonances at expected chemical shifts for this class of compounds where oxygen is not participating in coordination (170.3 ppm).

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Hemija životne sredine / Environmental Chemistry

HŽS O 01

Fotokatalitička degradacija nikosulfurona u vodenoj suspenziji TiO_2

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Zagađenje vodenih resursa pesticidima predstavlja problem za životnu sredinu zahvaljujući njihovoj postojanosti u zemljištu, visokoj rastvorljivosti u vodi i fotohemijskoj stabilnosti.

Sulfonilurea herbicidi se razlikuju od ostalih pesticida zbog svoje selektivnosti, minimalne doze primene i povoljnih ekoloških svojstava.

Fotokatalitička degradacija nikosulfurona, sulfonilurea herbicida proučavana je u prisustvu TiO_2 Degussa P25 kao fotokatalizatora i pri UV osvetljenju.

Uticaji različitih parametara, kao što su, početna koncentracija katalizatora i početna koncentracija nikosulfurona, uticaj različitih vrsta soli i pH vrednosti na brzinu degradacije ispitani su sa ciljem da se odrede optimalni uslovi za uklanjanje pesticida iz vodene sredine.

Brzina razgradnje praćena je UV spekroskofotometrijski i tečnom hromatografijom (HPLC) dok je mineralizacija analizirana jonskom hromatografijom (IC) i sadržajem ukupnog organskog ugljenika (TOC).

A photocatalytic degradation of sulfonylurea herbicide nicosulfuron in TiO_2 aqueous solution

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

Among other pesticides, sulfonylurea herbicides 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 TiO_2 Degussa P25 as photocatalyst under UV irradiation.

The influence of various parameters, such as, initial concentration of catalyst and initial nicosulfuron concentration, the pH and salt effect on the degradation rate was investigated in order to determine the optimum conditions for the pesticide removal from the aqueous solution.

The rate of photodecomposition was monitored using UV spectroscopy and HPLC measurements while the mineralization was followed with ion chromatography (IC) and total organic carbon (TOC) analysis.

HŽS P 01

Uklanjanje Cr(VI) jona iz vode biosorbentom kora *Lagenaria vulgaris*-ZrO_2

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U ovom radu je ispitivano uklanjanje hroma(VI) iz vode biosorbentom na bazi hemijski modifikovane kore biljke *Lagenaria vulgaris* (LV). Biosorbent je dobijen fizičko-mehaničkom preradom kore LV i hemijskom modifikacijom pomoću ZrO_2. Tretmani su rađeni u vodenim model-rastvorima Cr(VI) jona. Ispitivan je uticaj kontaktnog vremena i inicijalnog pH na efikasnost procesa uklanjanja metala. Veliko smanjenje koncentracije Cr(VI) jona u toku tretmana (95%) ukazuje na visoku efikasnost delovanja ispitivanog biosorbenta. Biosorpcija Cr(VI) jona u toku vremena se odvija u dve faze: inicijalna brza faza uklanjanja metala, nekon čega sledi sporija faza uklanjanja. Rezultati pokazuju da je najveća efikasnost sorpcije u prvih 60 minuta kontakta između sorbenta i sorbata, kada je uklonjeno 79.2% Cr(VI) jona. Nakon 240. minuta tretmana 94.7% ukupne količine Cr(VI) je uklonjeno iz vodenog rastvora. Efikasnost uklanjanja Cr(VI) jona biosorbentom značajno zavisi od inicijalne pH vrednosti rastvora, pri čemu je maksimalna sorpcija na pH vrednosti oko 2 i iznosi 95%. Rezultati ispitivanja pokazuju da se biosorbent na bazi hemijski modifikovane kore *Lagenaria vulgaris* može koristiti kao efikasno sredstvo za uklanjanje hroma(VI) iz zagađene vode.

Removal of Cr(VI) from water by *Lagenaria vulgaris* shell-ZrO_2 biosorbent

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The removal of chromium(VI) from aqueous solution using biosorbent based on *Lagenaria vulgaris* (LV) shell was studied. Biosorbent was prepared by drying, grounding, chemical purification and chemical modification of the shell with ZrO_2. The effect of contact time and initial pH on the sorption process was studied in a batch process mode. Significiant decrease of Cr(VI) concentration during the treatment indicated high efficacy of investigated material. Biosorption of Cr(VI) ions as a function of contact time occurs in two phases, a rapid initial uptake, followed by a slower process. The experimental results show that maximum adsorption efficiency was observed in the first 60 min of sorbent-sorbate contact, when removal of Cr(VI) ions was 79.2%. After 240 min of treatment 94.7 % of total Cr(VI) ions were removed from aqueous solution. Removal efficacy of Cr(VI) ions by biosorbent is significantly affected by solution pH and maximal sorption was achieved about pH 2 with value 95%. The obtained results showed that biosorbent based on chemically modified *Lagenaria vulgaris* shell with ZrO_2 could be used as the effective technology for removal of chromium(VI) from polluted waters.

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HŽS P 02

Ugljenične nanocevi kao nosači katalizatora na bazi Pd i Cu za reakciju katalitičke denitracije vodenog model sistema

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Katalitička denitracija predstavlja idealnu metodu za uklanjanje nitrata iz vode. Niska konverzija, visoka selektivnost u pogledu nitrita, kao i prisustvo amonijaka kao neželjenog proizvoda, najčešći su problemi katalizatora za denitraciju.

U radu su prikazani rezultati karakterizacije, aktivnosti i selektivnosti katalizatora na bazi Pd i Cu sa višeslojnim ugljeničnim nanocevima (VSUNC) kao nosačem u reakciji denitracije vodenog model sistema. VSUNC su sintetisane metodom katalitičke hemijske depozicije, prečišćene u cc HNO_3 i potom tretirane u struji N_2. Katalizator je sintetisan metodom vlažne impregnacije Pd-Cu aktivne faze na VSUNC i karakterisan metodama transmisione elektronske mikroskopije (TEM) i difrakcije X-zraka (XRD). U polušaržnom reaktoru sa mešanjem, uz prisustvo H_2 kao reduktanta i CO_2 radi regulisanja pH, postignuta je konverzija nitrata od 60%, dok su selektivnosti prema azotu, nitritnom jonu i amonijaku bile 0,87, 0,012 i 0,11, redom. Dobijeni rezultati ukazuju da performanse primenjenog Pd-Cu katalizatora u mnogome zavise od disperznosti metalnih čestica vezanih za površinu VSUNC, a formiranje željenog ili neželjenog proizvoda je određeno njihovim hemijskim sastavom, veličinom i geometrijom.

Carbon nanotubes as Pd-Cu-based catalyst support for water denitration

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Catalytic denitration is one of the most promising alternatives for nitrate removal from potable water. Nitrite, as intermediate and ammonium ion, as undesired product are regarded as the major limitations of this process.

In this study, we report results of characterization, as well as activity and selectivity of bimetallic Pd-Cu-based catalyst supported on multiwalled carbon nanotubes (MWCNTs) for the reduction of nitrates. MWCNTs were synthesized by catalytic chemical vapor deposition, purified in ccHNO_3 and heat treated under N_2. The Pd-Cu-based catalyst for water denitration was synthesized by impregnation of the MWCNTs with the Pd-Cu active phase and characterized by TEM and XRD. The reduction of nitrate was carried out in a semibatch reactor in the presence of H_2 and CO_2. The catalyst activity was expressed as degree of nitrate conversion presenting a value of 0.6, while the selectivities to nitrogen, nitrite and ammonium were 0.87, 0.012 and 0.11, respectively. The obtained results revealed that the performance of the tested Pd-Cu-based denitration catalyst is highly dependent on the dispersion of the metal particles attached to the MWCNTs. This particularly applies to their chemical composition, size and geometry which tailor the formation of desired or undesired product.

HŽS P 03

Degradacija triketonskih pesticida u dunavskoj vodi, primenom hlor-dioksida

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Hlor-dioksid je moćno sredstvo za dezinfekciju i izuzetno selektivan oksidans. Koristi se za smanjenje mikrobioloske kontaminacije a takođe je efikasan u uklanjaju ostataka pesticida na svežem voću i povrću. Degradacija triketonskih pesticida, mezotriona i sulkotriona, hlor-dioksidom ispitana je u realnom uzorku dunavske vode. Eksperimenti su rađeni u uslovima svetla i mraka, u zatvorenom sistemu, na konstantnoj temperaturi. Korišćene koncentracije hlor-dioksida su 5 i 10 ppm. Degradacija pesticida je praćena u vremenskim intervalima od 20 minuta, 1h, 2h, 3h i 24h. Efikasnost degradacije pesticida je praćena primenom tečne hromatografije visokih preformansi (HPLC-DAD), dok su proizvodi degradacije identifikovani primenom UHPLC–Orbitrap–MS analize. Predložen je mehanizam degradacije za oba pesticida. Za proizvode degradacije nakon 24h tretmana urađena je toksikološka i mikrobiološka analiza.

Degradation of triketone herbicides, in Danube water, with chlorine-dioxide

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Chlorine-dioxide is a powerful disinfectant and extremely selective oxidant. It is used for reduction of microbial contamination and for removal of pesticides residue on fresh fruits and vegetables. Degradation of triketone herbicides, mesotrione and sulcotrione, was studied using chlorine-dioxide, in light and dark condition, in real sample of Danube water. Degradation system was closed and the temperature was maintained constant. Used concentrations of chlorine-dioxide was 5 and 10 ppm. Degradations of pesticides were followed in time intervals of 20 minutes, 1h, 2h, 3h and 24h. Degradation efficiency was followed by high performance liquid chromatography (HPLC–DAD). Degradation products were identified with UHPLC–Orbitrap–MS analyses. A simple mechanism of degradation was proposed for both pesticides. Products of 24h chlorine-dioxide treatment were toxilogicaly and microbially tested.

HŽS P 04

Modelovanje NOx emisije na nacionalnom nivou veštačkim neuronskim mrežama

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Razvoj modela za predviđanje NOx emisije na nacionalnom nivou u evropskim državama u ovom radu je vršeno metodologijom koja kombinuje veštačke neuronske mrežame (*Artificial Neural Network* – ANN) i ekonomske i industrijske indikatore, kao i indikatore održivog razvoja. Modelom je obuhvaćen period od 2005. do 2011. godine, uz primenu dostupnih podataka za 31 evropsku državu. Dobijeni rezultati ANN modela su upoređeni sa modelom zasnovanim na višestrukoj linearnoj regresiji (*Multiple Linear Regression* – MLR). Nakon optimizacije ANN modela korelacionom analizom, umanjen je broj ulaznih promenljivih sa 18 na 11, što je redukcija od 40 %, čime se znatno smanjuje vreme potrebno za prikupljanje i pripremu ulaznih podataka. Poređenje najboljeg ANN modela sa MLR modelom, koji je kreiran i testiran sa istim setom podataka, pokazalo je da ANN model daje mnogo tačnije predviđanje NOx emisije na nacionalnom nivou.

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Modelling of national NOx emission using artificial neural networks

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This paper presents a development of an Artificial Neural Network (ANN) model for the prediction of NOx emissions at the national level for European countries, using available sustainability, economical, industrial and environmental indicators as inputs. The model was trained, validated and tested with the data for 31 European countries for the period from 2005 to 2011. The selection of available input variables was performed using correlation analysis. The optimization of model inputs resulted in the reduction of the number of inputs by 40%, from 18 to only 11. A comparison of the ANN model with a multi-linear regression (MLR) model, created and tested using the same dataset, showed that the ANN model has demonstrated considerably better forecast performance.

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HŽS P 05

Aktivni biomonitoring izotopa olova transplantiranim mahovinama u javnim garažama i tunelu u urbanom delu Beograda

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Aktivni biomonitoring primenom transplantiranih mahovina je pogodna tehnika za procenu kvaliteta vazduha. U ovom istraživanju vrećice sa mahovinom *Sphagnum girgensohnii* su bile postavljene u četiri javne garaže i tunelu u centru Beograda. Nakon izlaganja mahovina tokom 10 nedelja, u periodu jesen-zima 2011. godine, u uzorcima su mereni stabilni izotopi olova (^{206}Pb, ^{207}Pb i ^{208}Pb) na masenom spektrometru sa indukovano spregnutom plazmom. Određivanje izotopskog sastava olova u transplantiranim mahovinama je prvi put primenjeno u ovom radu, da bi se odredio izotopski sastav ovog elementa nakon zabrane upotrebe olova kao aditiva benzinu, od januara 2011. godine, u Republici Srbiji. U ispitivanim uzorcima su detektovane relativno niske koncentracije olova (oko 3 µg/g), a odnos ^{206}Pb i ^{207}Pb u uzorcima je bio 1,157-1,178. Na ovaj način određen je izotopski sastav olova koje potiče iz saobraćaja, za potrebe biomonitoringa aerozagađenja, nakon zabrane korišćenja benzina sa olovom kao aditivom.

Active moss biomonitoring of lead isotope ratio in public parking garages and tunnel in Belgrade urban area

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Mosses are among the most commonly used biomonitors of airborne pollutants due to their unique morphological and physiological features. Active biomonitoring with moss bags is a cost-effective method which provides a good preliminary overview of the air quality. In this study, moss bag technique survey of lead isotopic composition was performed in four parking garages and one city tunnel situated in the downtown of Belgrade. Moss *Sphagnum girgensohnii* was exposed for 10 weeks during autumn-winter season 2011. Stable lead isotopes were measured by inductively coupled plasma mass spectrometry. The aim of this research was to determine the lead isotope ratio after the legislation ban of leaded gasoline in the Republic of Serbia in January 2011. The moss bags were applied for the first time for this purpose. The average lead concentration in samples was low (3 µg/g) while the range of isotopic ratio ^{206}Pb/^{207}Pb was 1.157-1.178. Lead isotopic composition obtained in this way enables biomonitoring of lead originated from traffic after the lead gasoline phasing out.

Teorijska hemija / Theoretical Chemistry

TH P 01

Predviđanje BPK vrednosti na nacionalnom nivou primenom veštačkih neuronskih mreža uz odabir ulaznih promenljivih Monte Karlo simulacijama

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Evropske zemlje imaju obavezu izveštavanja o biološkoj potrošnji kiseonika (BPK) na godišnjem nivou u rekama, međutim praćenje BPK vrednosti je istovremeno finansijski i vremenski zahtevno. U ovom radu prikazan je razvoj modela za predviđanje BPK vrednosti u rekama na nacionalnom nivou, koji je zasnovan na veštačkim neuronskim mrežama, uz korišćenje dostupnih ekonomskih i industrijskih indikatora, kao i indikatora održivog razvoja, pri čemu je njihov krajnji odabir vršen Monte Karlo simulacijama (MCS). Primenom MCS tehnike broj potrebnih ulaza je smanjen za 25 %, pri čemu su performanse modela kod predviđanja BPK vrednosti poboljšane. Najbolji rezultati postignuti su korišćenjem neuronske mreže sa opštom regresijom, koja je takođe bila značajno preciznija od odgovarajućeg linearnog modela zasnovanog na višestrukoj linearnoj regresiji (MLR).

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Prediction of national BOD level in rivers using Artificial Neural Networks and Monte Carlo Simulations

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European countries are annually reporting the Biological Oxygen Demand (BOD) values in rivers, however BOD monitoring is both costly and time consuming. This study presents the development of an Artificial Neural Network (ANN) model for the prediction of national BOD level in rivers using available sustainability, economical, industrial and environmental indicators as inputs, while the selection of inputs was based on Monte Carlo Simulation (MCS) technique. The best results were achieved with General Regression Neural Network (GRNN) which had 25% less inputs than the initial model and also had significantly higher accuracy in comparison with the conventional Multiple Linear Regression (MLR) model.

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Biohemija / Biochemistry

BH O 01

Soj *Streptomyces* sp. NP10 biosintetiše velike količine *n*- i razgranatih slobodnih masnih kiselina kao odgovor na prisustvo kratkolančanih masnih kiselina

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Bakterije roda *Streptomyces* biosintetišu više od polovine od 10.000 poznatih biološki aktivnih jedinjenja, pa su preko 50 godina u žiži interesovanja naučnika i industrije. Nova vrsta roda *Streptomyces*, označena kao NP10, je izolovana iz uzorka zemljišta sela Čumić, kod Kragujevca. Ova vrsta, gajena pod različitim uslovima (vreme inkubacije, hranljiva podloga, temperatura, itd.) je biosintetisala velike količine slobodnih dugolančanih masnih kiselina (C_7-C_{31}). Detaljna analiza lipidnog profila ovog soja, koja je usledila (hromatografska razdvajanja, derivatizacija, hemijske transformacije i GC-MS ko-injekcija sa standardima), je omogućila identifikaciju preko 50 masnih kiselina *n*-, *iso*- i *anteiso*-niza uključujući zasićene, nezasićene i ciklopropanske kiseline. Najzastupljenije, kako slobodne, tako i vezane, su bile 12-metiltetradekanska, 14-metilpentadekanska, heksadekanska i oktadekanska kiselina. U prisustvu (u hranljivoj podlozi ili atmosferi) izomernih butanskih i pentanskih kiselina dolazi do hiperprodukcije pomenutih slobodnih masnih kiselina. Ovakva prirodna adaptacija može da predstavlja odbrambeni mehanizam protiv drugih mikroorganizama u zemljištu koji produkuju ove kratkolančane masne kiseline.

Streptomyces sp. NP10 produces a large amount of *n*- and branched free fatty acids as a response to the presence of short-chain fatty acids

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Representatives of *Streptomyces* genus, producers of more than half of the 10,000 documented bioactive compounds, are attracting interest of both industry and academia for more than 50 years. A new *Streptomyces* sp. isolate designated as NP10 was discovered in soil sampled from the village Čumić, near Kragujevac. Under varying cultivation conditions (incubation time, nutritive medium, temperature, etc.) the species was found to accumulate considerably large amounts of free long-chain fatty acids (C_7-C_{31}). A detailed lipidomics study (chromatographic isolation, derivatization, chemical transformations and GC-MS co-injections) that followed enabled identification of over 50 different fatty acids of *n*-, *iso*- and *anteiso*- chains including both saturated, unsaturated and cyclopropyl acids. The free and bound lipid profile of *Streptomyces* sp. NP10 was dominated by 12-methyltetradecanoic, 14-methylpentadecanoic, hexadecanoic and octadecanoic acids. Interestingly, the presence (in both nutritive medium and headspace) of isomeric butanoic and pentanoic acids caused a hyperproduction of the mentioned free fatty acids by this bacterium. This environmental adaptation might be a defense mechanism against other soil microorganisms that produce these short-chain acids.

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BH P 01

Citotoksični efekat biljne vrste *Reseda lutea* L.: Slučaj zaboravljenog leka

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Autolizati dobijeni iz različitih organa (korena, cvetova i plodova) biljne vrste *R. lutea* analizirani su pomoću GC i GC-MS, kao i IR, 1D i 2D NMR spektroskopijom. Glavni sastojak autolizata korena bio je benzil-izotiocijanat, dok je u autolizatu cveta najzastupljeniji bio 2-(α-L-ramnopiranoziloksi)benzil-izotiocijanat (koji predstavlja novi prirodni proizvod). Autolizati i njihovi glavni sastojci podvrgnuti su MTT testu na dve humane ćelijske linije: A375 (melanom) i MRC5 (fibroblast). Mehanizam citotoksičnog dejstva proučavan je pomoću analize ćelijskog ciklusa i Aneksin V testa. Izotiocijanati su pokazali značajnu antiproliferativnu aktivnost u slučaju obe ćelijske linije, što objašnjava uočenu citotoksičnost testiranih autolizata. Analizom ćelijskog ciklusa utvrđeno je da je najverovatniji mehanizam ćelijske smrti apoptoza. Dobijeni rezultati idu u prilog antitumorskoj aktivnosti koja je u istorijskim tekstovima pripisivana ovoj biljnoj vrsti.

Cytotoxic effect of *Reseda lutea* L.: A case of forgotten remedy

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The composition of autolysates obtained from different organs (root, flower and fruit) of *R. lutea* was investigated by GC and GC-MS analyses, as well as IR, 1D and 2D NMR spectroscopy. Benzyl isothiocyanate and 2-(α-L-rhamnopyranosyloxy)benzyl isothiocyanate were identified as the major constituents the root and flower autolysates, respectively (the later represents a new natural product). Autolysates and their major constituents were submitted to an MTT-dye reduction cytotoxic assay on human A375 (melanoma) and MRC5 (fibroblast) cell lines. Mechanism of the cytotoxic effects was studied by cell cycle analysis and Annexin V assay. The isothiocyanates showed significant antiproliferative effects against both cell lines, which could also explain the observed high cytotoxic activity of the tested autolysates. Cell cycle analysis revealed apoptosis as the probable mechanism of cell death. Tumor healing properties attributed to *R. lutea* in the pre-modern texts were substantiated by the herein obtained results.

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BH P 02

Hemoselektivna bioredukcija ferocenil-halkona od strane kvasca *Saccharomyces cerevisiae*

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U ovom radu su izneti rezultati sinteze nekoliko ferocenil-halkona i njihove, po prvi put izvedene, reduktivne biotransformacije od strane kvasca *Saccharomyces cerevisiae*. Sinteza ferocenil-halkona je izvršena bazno ili kiselo katalizovanom reakcijom aldolne kondenzacije formil- ili acetil-ferocena sa odgovarajućim aril- ili alkil-ketonom, odnosno aldehidom. Bioredukcijom ovih α,β-nezasićenih karbonilnih jedinjenja hemoselektivno se formiraju putem konjugovane Michael-ove adicije samo odgovarajući zasićeni ketoni (ferocenil,aril-1-propanoni). Kinetika reakcije je praćena periodično, uzimanjem alikvota koji su analizirani pomoću GC-MS i UV/Vis. Stopa konverzije je bila 50% za 24 h. Budući da se redukcija odvija upotrebom suspenzije pekarskog kvasca u vodenom rastvoru u prisustvu male količine etanola (za rastvaranje polaznog halkona), ova reakcija se može svrstati u domen „zelene hemije“. Strukture halkona i proizvoda biotransformacije potvrđene su analizom njihovih MS, NMR i IR spektara.

Chemoselective bioreduction of ferrocenyl chalcones by the yeast *Saccharomyces cerevisiae*

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Herein we report the chemical synthesis and the first reductive biotransformation of several ferrocenyl chalcones by the yeast *Saccharomyces cerevisiae*. The synthesis of ferrocenyl chalcones was performed by a base or acid catalyzed aldol condensation of formyl or acetyl ferrocene with appropriate aryl or alkyl ketones/aldehydes. The biotransformation of these α,β-unsaturated carbonyl compounds was a chemoselective one and yielded only the corresponding saturated ketones (ferrocenyl,aryl-1-propanones) in a Michael-type conjugated addition. The reaction progress was monitored periodically by taking aliquots further analyzed by GC-MS and UV/Vis. The 50% conversion was reached in 24 h. Such a reduction of ferrocenyl chalcones using baker's yeast is an example of a "green reaction" since the reaction is carried out in aqueous medium with only a small amount of ethanol used for the dissolution of the starting chalcones. The structures of the prepared chalcones and their biotransformation products were confirmed through the analysis of their MS, NMR and IR spectra.

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BH P 03

Da li je gljiva *Ganoderma resinaceum* (Boud. in Pat.1889) novi izvor anti-inflamatornih agenasa?

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Gljive su atraktivan izvor fiziološki aktivnih supstanci i prekursora lekova, i od davnih vremena pa do danas predstavljaju za ljude značajan izvor funkcionalne hrane. Različite biaktivne supstance poreklom iz gljiva pokazuju širok spektar farmakoloških aktivnosti kao što su: antikancerogena, anti-inflamatorna i imunomodulatorna. Gljive roda *Ganoderma* obuhvataju basidiomicete bele truleži (*G. lucidum*, *G. applanatum* i druge) koje se koriste u medicinske svrhe vekovima naročito u azijskim zemljama dalekog Istoka: Kini, Japanu i Koreji. U cilju određivanja antiinflamatorne aktivnosti hloroformskih i etanolnih ekstrakata *G. resinaceum* korišćen je optimizovani *in vitro* test za određivanje potencijala inhibicije ciklooksigenaze-1 (COX-1) i lipooksigenaze-12 (12-LOX). Trombociti su korišćeni kao izvori COX-1 i 12-LOX, dok je visoko osetljiva i specifična LC–MS/MS tehnika korišćena za određivanje metabolita arahidonske kiseline. Aktivnost hloroformskih ekstrakata *G. resinaceum* za inhibiciju COX-1/12-LOX (IC50 = 1,84 i 0,63 mg/mL) je bila daleko bolja u odnosu na aktivnost etanolnih ekstrakata *G. resinaceum* (IC50 = 153,07 i 2,05 mg/mL), pokazujući da su nepolarna jedinjenja doprinela ispoljavanju navedene aktivnosti.

Is the fungus *Ganoderma resinaceum* (Boud. in Pat.1889) a new source of anti-inflamatory agents?

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Fungi are an attractive sources of physiologically active substances and drug precursors since ancient times until nowadays thus representing functional foods for humans. Their diverse biactive substances display a wide range of pharmacological activities such as anticancer, anti-inflammatory and immunomodulating. Fungal genus *Ganoderma* comprises white rot basidiomycete fungi (*G. lucidum, G. applanatum* and others) which have been used for medicinal purposes for a centuries particularly in far eastern asian countries China, Japan and Korea. Optimized *in vitro* assay for determination of cyclooxygenase-1 (COX-1) and 12-lipoxygenase (12-LOX) inhibition potency was undertaken in order to evaluate the anti-inflammatory activity of chloroform and ethanolic extracts of *G. resinaceum* species. Platelets were used as a source of COX-1 and 12-LOX enzymes while highly sensitive and specific LC–MS/MS technique was used for detection of main arachidonic acid metabolites. Activity of chloroform extract of *G. resinaceum* towards COX-1/12-LOX inhibition (IC_{50}=1,84 and 0,63 mg/mL, respectively) was superior to the obtained activity of ethanolic extract of *G. resinaceum* (IC_{50} = 153,07 and 2,05 mg/mL, respectively) giving more nonpolar compounds dedicated to the manifested activities.

BH P 04

Antitumorski potencijal 17α-pikolil A-modifikovanih 5-androstenskih derivata

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Zbog visoke stope smrtnosti od malignih bolesti istraživanja u cilju pronalaženja terapeutika za lečenje obolelih su veoma značajna. Ova istraživanja obuhvataju sintezu i proučavanje uticaja novosintetizovanih jedinjenja na proliferaciju, morfologiju, ekspresiju gena, indukciju apoptoze, inhibiranje ćelijskih enzima, kao i promene ćelijskog ciklusa tumorskih ćelija. Među novosintetizovanim steroidnim jedinjenjima, 17α-pikolil A-modifikovani derivati 5-androstena su ispoljili značajnu antiproliferativnu aktivnost, naročito prema estrogen receptor pozitivnim (ER+) ćelijama adenokarcinoma dojke (MCF7). U ovom radu su predstavljeni rezultati ispitivanja uticaja odabranih 17α-pikolil A-modifikovanih 5-androstenskih derivata na ćelijski ciklus MCF7 ćelija, kao i sposobnosti ovih jedinjenja da indukuju apoptozu tumorskih ćelija.

Antitumor potential of 17α-picolyl A-modified 5-androstene derivatives

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Due to the high mortality rates associated with cancer, researches to find therapeutics for the treatment of patients suffering from these diseases are of great importance. This research includes studying the effects of newly synthesized compounds on the proliferation, morphology, gene expression, induction of apoptosis, inhibition of cellular enzymes, as well as the changes of cell cycle of tumor cells. Among newly synthesized steroidal compounds 17α-picolyl A- modified derivatives of 5-androstene exhibited significant antiproliferative activity, in particular against the estrogen receptor positive (ER+) breast adenocarcinoma cells (MCF7 cell line). This paper presents the effects of selected 17α-picolyl A- modified 5-androstene compounds on the cell cycle of MCF7 cells, and their ability to induce apoptosis of tumor cells.

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BH P 05

Antimikrobna aktivnost ekstrakta kore drveta bele jove (*Alnus Incana* (L.) Moensch)

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Alnus Incana (L.) Moensch, poznata pod nazivom bela jova, je listopadno drvo veoma rasprostranjeno u severnoj Evropi koje može služiti kao izvor tzv. „ zelenih“ hemikalija, kao i biološki aktivnih jedinjenja. *A. Incana* poseduje visok sadržaj ektrakta kore u poređenju sa drugim listopadnim vrstama, a koji se koriste u narodnoj medicini za lečenje bakterijskih i gljivičnih infekcija. Najkaraktestičnija osobina roda *Alnus* je visok sadržaj diarilheptanoida i njihovih glikozida u različitim morfološkim delovima drveta. Uzorci kore bele jove su prikupljeni sa stabla starog 25 godina iz sliva Jošaničke reke u Raškoj na Kopaoniku (Srbija). Da bi se odredio sadržaj hidrofilnih i lipofilnih ektrakta, vršena je ekstrakcija usitnjene kore osušene na vaduhu u Soxhlet-ovom aparatu upotrebom četiri rastvarača različite polarnosti: etanol, etil-acetat, dietiletar i voda. Ispitana je antimikrobna aktivnost ekstrakta kore na 15 različitih sojeva Gram-pozitivnih i Gram-negativnih bakterija pomoću mikrodilutacionog metoda. Ekstrakti kore bele jove pokazuju umerenu antimikrobnu aktivnost na ispitane sojeve bakterija, a najveću aktivnost pokazuju na soj *Bacillus cereus*. Dobijene minimalne inhibirajuće koncentracije (MIC) su poređene sa ukupnim sadržajem fenola koji je određen Folin-Ciocalteu metodom.

Antimicrobial activity of grey alder (*Alnus Incana* (L.) Moensch) bark extracts

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Alnus Incana (L.) Moensch, commonly known as grey alder, is a deciduous tree widely distributed in northern Europe that could represent a potential source of valuable „green“ chemicals, including biologically active compounds. *A. Incana* posses high content of the bark extracts compared to the other deciduous species, that have been used in traditional medicine for treating bacterial and fungal infections. The most characteristic feature of the *Alnus* genus is the occurrence of large quantities of diarylheptanoids and their glycosides in different morphological parts of the tree. *A. Incana* bark samples were collected from Jošanička river basin in Raška, Kopaonik (Serbia) from 25 years old normal wood. Air-dried powdered material was extracted in Soxhlet apparatus using four solvents of different polarities: ethanol, ethyl-acetate, diethyleter and water in order to determine the contents both of lipophilic and hydrophilic extracts. Antimicrobial activity of bark extracts was screened against 15 different Gram-positive and Gram-negative bacteria strains using the broth microdilution method. *A. Incana* bark extracts show moderate activities against the investigated bacteria expressing the highest activity on *Bacillus cereus* strain. The obtained minimal inhibitory concentrations (MIC) were correlated to the total phenolics contents determined by the Folin-Ciocalteu method.

BH P 06

Hemijski sastav etarskog ekstrakta cvetova biljne vrste *Daphne blagayana* Freyer (Thymelaeaceae)

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Jeremičak, *Daphne blagayana* Freyer (Thymelaeaceae), je biljna vrsta cenjena zbog intenzivnog mirisa svojih cvetova. Da bi se identifikovali sastojci cvetova koji su odgovorni za njen miris, u ovom radu po prvi put je izvršena GC i GC-MS analiza hemijskog sastava dietil-etarskog ekstrakta svežih cvetova ove vrste. Cvetovi su sakupljeni kod mesta Leposavić, na Kosovu (Srbija), marta 2014. godine. Više od 100 jedinjenja je uspešno identifikovano, među kojima veliki broj potencijalnih nosioca mirisa. Cvetni isparljivi sastojci su najvećim delom bili sačinjeni od oksigenovanih monoterpenoida (48,9%) i benzenoidnih jedinjenja (37,0%). Benzil-benzoat (7,6%) i linalool (5,5%) su bili glavni sastojci. Detektovan je veći broj jedinjenja strukturno povezanih sa linaloolom, a među njima: *trans*-hotrienol, *cis*- i *trans*-ruža oksidi, dijastereomeri furanoidnih i piranoidnih linalool-oksida, jorgovan alkoholi i aldehidi, kao i nekoliko izomera hidroksilinaloola. Pošto se biljne vrste koje biosintetišu benzenoidne estre i alkohole, linalool i/ili oksigenovane monoterpene kao mirisne komponente oprašuju od strane ljiljaka, ovo je mogući način razmnožavanja jeremička.

Chemical composition of the diethyl ether extract of *Daphne blagayana* Freyer (Thymelaeaceae) flowers

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Daphne blagayana Freyer (Thymelaeaceae) is a highly appreciated plant taxon ("Jeremičak" in Serbian) because of heady fragrance of its flowers. In order to detect and identify its odoriferous constituents, in this study we performed the first GC and GC-MS analysis of the chemical composition of the diethyl ether extract of fresh *D. blagayana* flowers. The inflorescence were collected at a location near Leposavić, Kosovo, Serbia, in March, 2014. Over 100 compounds were successfully identified, many of which were easily recognized as having odorous properties. The floral volatiles were made up largely of oxygenated monoterpenoids (48.9%) and benzenoid compounds (37.0%). The major components were found to be benzyl benzoate (7.6%) and linalool (5.5%). A number of linalool-related compounds were detected: *trans*-hotrienol, *cis*- and *trans*-rose oxides, diastereomers of furanoid and pyranoid linalool oxides, lilac alcohols and aldehydes, and several hydroxylinalool isomers. Interestingly enough, species producing benzenoid esters, benzenoid alcohols, linalool and/or oxygenated monoterpenes are known to be moth-pollinated flowers. This fact suggests to a possible reproductive way of *D. blagayana*.

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PRINT EXIT

BH P 07

Antitumorska aktivnost novih steroidnih tetrazola

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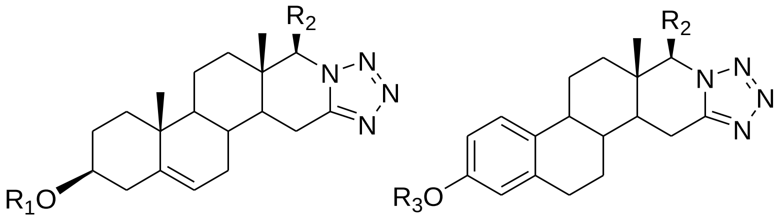
Istraživanja povezana sa jedinjenjima koja sadrže tetrazolski sistem izuzetno su aktuelna zbog široke mogućnosti njihove primene u medicinske svrhe. Novosintetizovani androstanski i estranski tetrazoli **1-8** smanjuju proliferaciju estrogen receptor pozitivnih (ER+) ćelija adenokarcinoma dojke (MCF7).

Predmet ovog istraživanja bilo je proučavanje antitumorskog potencijala tetrazola **1-8** ispitivanjem njihovog uticaja na ćelijski ciklus i indukovanje apoptoze tumorskih ćelija.



1: R_1=H, R_2= H
2: R_1=H, R_2=CH_3
3: R_1=OAc, R_2=H
4: R_1=OAc, R_2=CH_3

5: R_2=H, R_3= H
6: R_2=CH_3, R_3=H
7: R_2=H, R_3=Bn
8: R_2=CH_3, R_3=Bn

Antitumor activity of new steroidal tetrazoles

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Research related to the compounds containing tetrazole system is in focus because of their widespread use for medical purposes. Newly synthesized androstane and estrane tetrazoles **1-8** reduce the proliferation of estrogen receptor positive (ER +) breast adenocarcinoma cells (MCF7).

The subject of this research was to study the antitumor potential of tetrazoles **1-8** by examining their effects on the cell cycle and inducing of apoptosis in tumor cells.

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Biotehnologija / Biotechnology

BT O 01

Elicitacija sekundarnih metabolita u izdancima dve vrste roda *Nepeta* gajenim *in vitro* primenom sintetičkih jedinjenja (DO63 i DOVF15)

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Istraživanje je usmereno ka ispitivanju produkcije glavnih sekundarnih metabolita u izdancima dve vrste roda *Nepeta* izloženim dejstvu potencijalnih elicitora, sintetičkih jedinjenja iz grupe 1,2,4,5-tetraoksana (DO63) i 2,5-difenil-tiofena (DOVF15). Ispitivan je efekat DO63 i DOVF15, u opsegu koncentracija od 0,1 do 2 mg/L, na produkciju *cis,trans-* nepetalaktona i ruzmarinske kiseline u izdancima *Nepeta pannonica* L. i *N. cataria* L. gajenim u *in vitro* uslovima, na ½ MS hranljivim podlogama. Uočena je zavisnost efekta ispitivanih jedinjenja od primenjene koncentracije, kao i od vrste biljaka na koju se primenjuju. Rezultati ukazuju na mogućnost primene ispitivanih jedinjenja iz grupe 1,2,4,5-tetraoksana (DO63) i aminohinolina (DOVF15) kao elicitora, a u cilju stimulacije produkcije sekundarnih metabolita iz grupe fenolnih kiselina i naročito monoterpenoida kod vrsta roda *Nepeta*.

Ovo istraživanje je finansirano od strane MPNTR R Srbije (projekti 172008 i 173024).

Elicitation of secondary metabolites in shoots of two *Nepeta* species grown *in vitro* by synthetic compounds (DO63 and DOVF15)

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The present study was concentrated on the elicitation of the main secondary metabolites production in *in vitro* grown shoots of two *Nepeta* species, by exposing them to synthetic compounds from the group of 1,2,4,5-tetraoxanes (DO63) and 2,5-diphenyl-tiophenes (DOVF15). The effect of DO63 and DOVF15 on the production of *cis,trans*-nepetalactone and rosmarinic acid in shoots of *Nepeta cataria* L. and *N. pannonica* L., was investigated by treating the shoots grown on ½ MS culture medium with synthetic compounds in concentrations ranging from 0.1 to 2 mg/L. The content of targeted metabolites in shoots was dependent on the applied concentration of DO63 and DOVF15, and on the plant species. The results highlight the possibility of DO63 and DOVF15 application for the elicitation of the main secondary metabolites production in species from the genus *Nepeta*.

This work was financially supported by MESTD of the R Serbia (Projects 172008 and 173024).

BT P 01

Inovativni biodegradabilni filmovi na bazi pektina za ambalažu prehrambenih proizvoda

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Cilj ovog rada je dobijanje novih biodegradabilnih filmova namenjenih pakovanju hrane, koji bi zamenili konvencionalne filmove od polipropilena, polietilena i sl. čime bi se značajno smanjila količina otpada. Kao polazna komponenta za sintezu filmova korišćen je visoko-esterifikovani pektin i poli(etilen glikol) (PEG) kao plastifikator. Pektin/PEG 400 filmovi dobijeni su izlivanjem rastvora u kalupe i otparavanjem rastvarača. FT-IR spektroskopija je korišćena kako bi se ispitale strukturne karakteristike filmova. Takodje, ispitana su mehanička i termijska svojstva pektin/PEG 400 filmova. Rezultati FT-IR spektroskopije ukazuju na formiranje vodoničnih veza izmedju pektina i PEG-a. Dodavanjem PEG-a u sistem dobijaju se filmovi poboljšanih mehanički i termijskih svojstava u poređenju sa filmovima u čiji sastav ulazi samo pektin.

Novel pectin biobased films for food packaging application

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The aim of this work was to obtain biodegradable films intended for food packaging with the final result that the conventional films such as polypropylene, polyethylene etc. can be replaced. Samples were prepared using high methoxyl (HM) pectin and poly(ethylene glycol) as plastisizer. The pectin/PEG 400 films were obtained by a casting/solvent evaporation technique. FT-IR spectroscopy was used to examine structural properties of films. Also, mechanical and the thermal properties of pectin/PEG 400 films were analyzed. FT-IR spectroscopy confirmed the establishment of hydrogen bonds between pectin and poly(ethylene glycol). All the obtained films show enhanced mechanical properties and thermal stability compared to the starting components.

BT P 02

Dekolorizacija antrahinonskih boja peroksidazom iz rena imobilisanom na kaolin

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Antrahinonske boje su veoma značajne za tekstilnu industriju i, odmah nakon azo boja, imaju najveću primenu. Nažalost, kao i azo boje, i antrahinonske boje predstavljaju ozbiljan problem zagađenja životne sredine. Većina njih je toksična, mutagena, karcinogena i rezistentna na degradaciju. Osnovni cilj ovog rada je razvoj efikasnog, ekološki prihvatljivog imobilisanog biokatalizatora za primenu u procesima dekolorizacije antrahinonskih boja. Ispitivanje je fokusirano na primenu kaolina, i to njegovog aktiviranog oblika, kao nosača za imobilizaciju peroksidaze iz rena. Peroksidaza je imobilisana adsorpcijom i ispitan je uticaj početne koncentracije enzima na masu vezanog enzima kao i na aktivnost dobijenog imobilisanog preparata. Koncentracija enzima varirana je u opsegu 0,5 – 3 mg cm^{-3} pri čemu su dobijeni visoki prinosi imobilizacije, a fitovanje dobijenih eksperimentalnih podataka Lengmirovom adsorpcionom izotermom (R^2=0,911) ukazuje na to da se na površini nosača formira monosloj. Dobijeni biokatalizatori su ispitani u reakciji dekolorizacije dve antrahinonske boje (C.I. Acid violet 109 i C.I. Acid blue 225). Ostvareni rezultati ukazuju na veliki potencijal pripremljenih biokatalizatora. Biokatalizator dobijen pri početnoj koncentraciji enzima od 1,5 mg cm^{-3} već nakon 30 min ukloni preko 90 % C.I. Acid violet, a nakon 60 min preko 80 % C.I. Acid blue boje. Dobijeni biokatalizatori su takođe pokazali dobru operativnu stabilnost i mogućnost ponovne upotrebe.

Decolorization of antraquinone dyes using horseradish peroxidase immobilized onto kaolin

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Anthraquinone dyes are very important compounds and constitute the second most important class of textile dyes. Unfortunately, these compounds cause serious environmental pollution. Most of them are toxic, mutagenic and carcinogenic and resistant to degradation. The objective of this work was to develop an efficient, ecofriendly immobilized biocatalyst for the decolorization of antraquinone dyes. The study was focused on the application of kaolin, in its activated form, as a carrier for the immobilization of horseradish peroxidase. Peroxidase was immobilized by adsorption, and the influence of the initial enzyme concentration on the enzyme coupling yield and the activity of the immobilzed preparation was investigated. Initial enzyme concentration was varied in the range 0.5 – 3 mg cm^{-3} and high enzyme loadings were obtained. Monolayer formation of enzyme on the kaolin surface was approved by fitting experimentall data with Langmuir adsorption isotherm model (R^2=0.911). The obtained biocatalysts were tested directly in the decolorization reaction of two antraquinone colors (CI Acid Violet 109 and CI Acid Blue 225) and showed great potential for their removal. Biocatalyst obtained at the initial enzyme concentration of 1.5 mg cm^{-3}, removed more than 90% of C.I. Acid Violet after 30 min, and more than 80% C.I. Acid blue after 60 min. Obtained biocatalysts also showed good operational stability and the possibility of re-use in the reaction.

BT P 03

Biološko luženje gomile

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Različite sirovine sa niskim sadržajem metala kao i koncentrati mogu biti podvrgnuti biološkom luženju na gomili. Komercijalno biolužženje odlagališta može se ekonomski opravdati, ali planskim formiranjem gomile nastaju uslovi za optimizaciju procesa bioluženja. Udrobljavanjem rude (ili nekih drugih sirovina) i stavljanjem na nepropusnu podlogu efikasnija je raspodela rastvora luženja, aerisanost i sistem prikupljanja. Temperatura unutar gomile je određena različitim faktorima. Postoje različiti modeli za luženje gomile koji se mogu koristiti za procenu operativnih uslova za rad jedne auto-termičke gomile. U radu su dati neki od njih. Njihovo dobro poznavanje može doprineti povećanju prinosa željenih metala.

Heap bioleaching

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Different raw materials with a low metal content as well as the concentrates can be treated by heapbioleaching. Commercial bioleaching of dumps can be economically justified, but by planned forming of the heap creates the conditions for the optimization of the bioleaching. Crushing ore (or other raw materials) and putting it on an impervious surface is more efficient distribution the leach solution, aeration and collection system. The temperature inside the heap is determined by various factors. There are various models for the leaching of heaps, which can be used to estimate the operating conditions for the process of auto-thermal heap. In this paper are presented some of them. Their good knowledge can contribute to increase the yield of desired metals.

BT P 04

Majklova adicija različitih aldehida na β-nitrostiren katalizovana rekombinantnim ćelijama koje eksprimiraju 4-oksalokrotonat tautomerazu

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Razvijen je novi sistem biokatalize sa čitavim bakterijskim ćelijama zasnovan na rekombinantno eksprimiranoj 4-oksalokrotonat tautomerazi (4-OT) i pokazano je da je ovakav sistem efikasan biokatalizator za asimetrične Majklove adicije acetaldehida na β-nitrostiren.[1] Pokazano je da su čitave bakterijske ćelije bolje u odnosu na prečišćen enzim jer prevazilaze problem inicijalne inhibicije količinom prisutnog supstrata te je detaljna optimizacija odnosa supstrata aldehida i β-nitrostirena, kao i biokatalizatora određena. Takođe, ispitivani su i razliciti načini dodavanja supstrata u reakcionu smesu, kao i recikliranje biokatalizatora. Pod optimizovanim uslovima ispitana je reaktivnost različitih aldehida. Dobijena je odlična enantioselektivnost (> 99 % ee) proizvoda sa prinosima do 60%. Pokazano je da je ovaj biokatalizator efikasan i u adiciji cikličnih i acikličnih razgranatih aldehida na β-nitrostiren, pri čemu se dobijaju sintetički vredni γ-nitroaldehidi koji sadrže kvaternarni ugljenikov atom u α-polo~aju.

Michael-type addition of different aldehydes to β-nitrostyrene by recombinant 4-oxalocrotonate tautomerase whole-cell biocatalyst

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A novel whole cell system based on recombinantly expressed 4-oxalocrotonate tautomerase (4-OT) was developed and shown to be an effective biocatalyst for the asymmetric Michael addition of acetaldehyde to β-nitrostyrene.[1] It was shown that whole-cell biocatalyst is more efficient in comparison to purified 4-OT as much higher initial concentrations of substrates could be tolerated. Therefore, the optimal ratio of substrates and biocatalyst was determined and various substrate feeding strategies and biocatalyst recycling were examined. Reactivity of different aldehydes were determined under optimal conditions. Excellent enantioselectivity (>99% ee) and product yields of up to 60% were obtained. Furthermore, it was shown that various cyclic and acyclic branched aldehydes can be used as donors in this system yielding synthetically valuable γ-nitroaldehydes containing quaternary carbon.

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Hemija i tehnologija hrane / Chemistry and Technology of Food

HTH O 01

Korelacija između antioksidativne aktivnosti i sadržaja ukupnih i pojedinačnih polifenolnih jedinjenja u crnoj čokoladi

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Crna čokolada je proizvod sa visokim sadržajem polifenolnih jedinjenja, kao što su katehin, epikatehin i procijanidini. Upravo prisutni polifenoli koji imaju ulogu antioksidanata su odgovorni za preporuku korišćenja crne čokolade u ishrani. Ukupni polifenoli su određeni Folin-Ciocalteu metodom. Sadržaj ukupnih polifenola, dat kao miligram ekvivalent galne kiseline (GAE) po gramu crne čokolade, kreće se u intervalu od 7,09 do 40,42 mg GAE/g. Ukupni sadržaj flavonoida je određen metodom koja se zasniva na afinitetu flavonoida da formiraju kompleks sa $AlCl_3$. Ukupni sadržaj flavonoida, dat kao miligram ekvivalent katehina (CE) po gramu crne čokolade, kreće se u intervalu od 2,41 do 30,42 mg CE/g. Antioksidativna aktivnost je određena primenom četiri spektrofotometrijska testa: DPPH (21,37-33,96 µmol TE/g), ABTS (0,11-0,17 µmol TE/g), FRAP (73,78-317,40 µmol FE/g) i RP test redukcione moći Fe(III) u Fe(II) (93,95-495,59 µmol TE/g). Sadržaj pojedinačnih polifenola je određen HPLC metodom. Dobijeni rezulati su pokazali da postoji visok stepen korelacije između antioksidativne aktivnosti i sadržaja pojedinačnih polifenolnih jedinjenja.

Correlation of antioxidative activity with total and individual polyphenolic compounds of dark chocolate

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Dark chocolate is product with a high content of organic compounds such as catechin, epicatechin and procyanidins. Polyphenols, which act as antioxidants, are responsible for the recommendation the use of dark chocolate in the diet. Total polyphenols were determined by Folin-Ciocalteu method. Content of total polyphenolics, expressed as miligram of gallic acid equivalents (GAE) per gram of dark chocolate, was ranged from 7.09 to 40.42 mg GAE/g. Total flavonoid content was measured by method based on flavonoid affinity to form complex with $AlCl_3$, using catechin (CE) as a standard. Content of total flavonoids was ranged from 2.41 to 30.42 mg CE/g. Antioxidant activity was determined using four spectrophotometric assays: DPPH (21.37-33.96 µmol TE/g), ABTS (0.11-0.17 µmol TE/g), FRAP (73.78-317.40 µmol FE/g) and RP reducing power assay Fe(III) to Fe(II) (93.95-495.59 µmol TE/g). Individual polyphenolic compounds were determined using HPLC method. Obtained results showed high correlation between antioxidant activity and individual polyphenolic compounds.

HTH P 01

Migracija ftalata iz polietilenskih infuzionih boca niske gustine u fiziološki rastvor

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Ftalati su grupa hemijskih jedinjenja koja se koriste kao plastifikatori u proizvodnji plastične ambalaže zbog njihove sposobnosti da povećaju mekoću i fleksibilnost plastike. Medicinska oprema proizvedena od PVC plastike, može da sadrži čak i 20-40% di-(2-etilheksil) ftalata (DEHP). Pacijeni podvgnuti bolničkim tretmanima, kao što su transfuzija, infuzija, dijaliza itd. mogu biti izloženi štetnim uticajima DEHP. Detekcija i određivanje ftalata u uzorcima plastičnih boca, napravljenih od polietilena niske gustine (LDPE), u kojima se nalazio fiziološki rastvor, ali iz različitih serija proizvodnje, vršeno je ekstrakcijom čvrsto-tečno pomoću heksana. Tečno-tečno ekstrakcija je primenjena za ekstrahovanje ftalata iz tečnih uzoraka, fizioloških rastvora. I u čvrstim i u tečnim uzorcima detektovani su dibutil ftalat (DBP) i di-(2-etilheksil) ftalat (DEHP), dok benzil butil ftalat (BBP) nije detektovan ni u jednom uzorku. Koncentracija DEHP u uzorcima je do 10 puta viša u odnosu na koncentraciju BBP. Istraživanje je pokazalo da su BBP i DEHP prisutni u uzorku LDPE plastike, iako se za ovu vrstu plastike ftalati ne bi trebalo koristiti kao plastifikatori.

Zahvalnica: *Ovaj rad je realizovan u okviru Projekta III 41018, finansiranog od strane MPNTR Srbije.*

Migration of phthalates from low density polyethylene infusion bottles into physiological saline solutions

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Phthalates are group of chemical compounds which are widely used as polymer additives in plastics due to the ability to improve the softness and flexibility of plastics. PVC medical devices contain on average 20-40% DEHP (bis(2-ethylhexyl) phthalate) by weight. Patients who are undergoing medical procedures, such as blood transfusions and hemodialysis potentially can be exposed to DEHP. Determination of phthalates in infusion bottles which are made of low density polyethylene (LDPE) and in physiological saline solution samples stored in LDPE infusion bottles was performed by liquid extraction and GC/MS analysis. Only DEHP and DBP were found in the obtained extracts from the samples of infusion bottles, although in low amounts. Percentage of DBP in each sample was about 0.002%. The concentration of DEHP is 10 times higher than concentration of DBP. Even though, the investigated plastic material commonly does not possess plasticizers, the DEHP and/or DBP are found in the infusion bottles. However, the contamination of physiological saline solution is probably not only from the bottles where they are stored but from the tubing material that are used in their industrial preparation.

PRINT EXIT

HTH P 02

Određivanje di-*n*-butil ftalata i di-*n*-oktil ftalata u uzorcima vode pomoću GC/MS metode

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Di-*n*-butilftalat (DnBP) i di-*n*-oktilftalat (DnOP) se koriste kao plastifikatori koji se dodaju plastičnim materijalima, kako bi se postigla njihova veća elastičnost. Polietilentereftalat (PET) je uobičajena plastična ambalaža za komercijalno flaširanu vodu. Određivanje koncentracija DnBP i DnOP je izvršeno u 6 uzoraka vode pomoću gasne hromatografije kuplovane sa masenom spektrometrijom (GC/MS), kako bi se ispitala njihova migracija iz PET ambalaže. Analiza je vršena u Full Scan modu (FS) i Single Ion Monitoring modu (SIM), kako bi se uporedila osetljivost ovih metoda. Rezultati ukazuju na prisustvo DnBP i odsustvo DnOP u vodi, što je posledica njihove različite rastvorljivosti u vodi. DnBP sa kraćim alkil lancem je rastvorljiviji u vodi od DnOP sa dužim alkil lancem. Srednje vrednosti DnBP u uzorcima vode su analitički detektovane u opsegu 0.0786-1.0359 µg/L. Koncentracije DnBP koje su detektovane u uzorcima vode, odgovaraju standardima higijenske ispravosti vode, jer su ispod MDK vrednosti za ftalate, koja iznosi 6 µg/L.

Zahvalnica: *Ovaj rad je realizovan u okviru Projekta III 41018, finansiranog od strane MPNTR Srbije.*

Determination of di-*n*-butyl phthalate and di-*n*-octyl phthalate in water samples by GC/MS

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Di-n-butyl phthalate (DnBP) and di-n-octyl phthalate (DnOP) are widely used as polymer additives in plastics due to the ability to improve the softness and flexibility of plastics. Polyethylene terephthalate (PET) are widely used materials for bottled drinking water. The analysis was performed in full scan mode and in the single ion monitoring mode (SIM), in order to compare the sensitivity of these methods. The presence of DnBP and DnOP in six water samples was investigated. The results indicate the presence of DnBP and absence of DNOP in water, as a result of their differing solubility in water. Average values for DnBP in water samples were detected in the range of 0.0786-1.0359 mg /L. DnBP concentrations that are detectable in samples of water are below the values for the maximum allowed concentration for phthalates, that is 6 µg /L.

HTH P 03

Sadržaj toksičnih elemenata u voćnim infuz čajevima

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Cilj ovog rada bio je određivanje sadržaja potencijalno toksičnih elemenata u voćnim infuz čajevima. Koncentracije aluminijuma, arsena, kadmijuma, bakra, hroma, gvožđa, mangana, olova, nikla i cinka su određene u jedanaest voćnih infuz čajeva (trešnja, jagoda, malina, šumsko voće, marelica, trešnja, borovnica, jabuka, nar, egzotično voće i ananas) metodom atomske emisione spektrometrije sa induktivno spregnutom plazmom (ICP-AES). Al, Mn, Fe, Zn i Cu su elementi sa najvećim sadržajem u svim uzorcima. Ukupni sadržaj ispitivanih metala u infuz čajevima je u intervalu: Al (24,7-753 mg/kg), Mn (51-611 mg/kg), Fe (4,7-172 mg/kg), Zn (1,8-26,6 mg/kg), Cu (2,92-9,44 mg/kg), Ni (0,74-3,95 mg/kg), Cr (0,24-2,34 mg/kg), Pb (nije detektovan-1, 06 mg/kg), As (0,42-0,74 mg/kg) i Cd (0,055-0,165 mg/kg). Koncentracije nekih toksičnih metala kao što su As i Cd u infuz čajevima su ispod maksimalno dozvoljenih vrednosti (1 mg/kg za As i 0,3 mg/kg za Cd) koje preporučuje Svetska zdravstvena organizacija (WHO). Prema Pravilniku Republike Srbije, maksimalne koncentracije olova u čaju i domaćem čaju su 2 mg/kg i 5 mg/kg. Dobijene vrednosti za Pirsonov koeficijent korelacije ukazuju na dobru korelaciju između sadržaja elemenata, osim u slučaju As i Cd. Ovo može da ukaže na eventualnu razliku u poreklu As i Cd uzorcima u odnosu na ostale ispitivane elemente.

Toxic elements content of fruit tea infusions

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This paper intends to provide information about the content of potentially toxic elements in fruit tea infusions. Therefore, aluminum, arsenic, cadmium, copper, chromium, iron, manganese, lead nickel and zinc were determined in the eleven infusions of fruit tea (cherry, strawberry, raspberry, forest fruits, apricot, sweet cherry, blueberry, apple, pomegranate, exotic fruits and pineapple) by ICP-AES. Al, Mn, Fe, Zn and Cu are the elements with a major content in all samples. The total contents of investigated metals determined in tea infusions arranged in the following order: Al (24.7 to 753 mg/kg), Mn (51 to 611 mg/kg), Fe (4.7 to 172 mg/kg), Zn (1.8 to 26.6 mg/kg), Cu (2.92 to 9.44 mg/kg), Ni (0.74 to 3.95 mg/kg), Cr (0.24 to 2.34 mg/kg), Pb (not detected to 1.06 mg/kg), As (0.42 to 0.74 mg/kg) and Cd (0.055 to 0.165 mg/kg). It should be noted that the concentrations of some toxic heavy metal such as As and Cd in tea infusions are below the maximum permissible limits in foods recommended by the World Health Organization; which are 1 mg/kg and 0.3 mg/kg for As and Cd respectively. According to Serbian regulative, the maximum levels for Pb in tea and homemade tea is of 2 mg/kg and 5 mg/kg, respectively. According to the values of Pearson correlation coefficient all metals except As and Cd are significantly correlated with each other. The statistical results may indicate that As and Cd, possibly, originated from sources that were different from the other elements.

HTH P 04

Određivanje polifenolnog profila krompira

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Krompir (*Solanum tuberosum L.*) se, po lekovitosti sastojaka, sadržaju ugljenih hidrata, proteina, minerala i polifenolnih jedinjenja, ubraja u red najvažnijih prehrambenih proizvoda. Količina ovih komponenata u krompiru varira u zavisnosti od klimatskih faktora, podneblja i sezone gajenja i ubiranja. Sadržaj pojedinih fitohemikalija je različit u različitim delovima krtole. U skladu sa prethodnim sistematskim ispitivanjima autentičnosti hrane, predmet ovog rada je određivanje polifenolnog profila različitih sorti krompira. Iz različitih delova pomenutih uzoraka krompira pripremljeni su metanolni ekstrakti i analizirani ultraefikasnom tečnom hromatografijom spregnutom sa masenom spektrometrijom visoke rezolucije (*UPLC-LTQ-orbitrap MS/MS)* u cilju dobijanja pomenutog fenolnog profila. Fenolna jedinjenja su identifikovana i kvantifikovana prema odgovarajućim spektralnim karakteristikama: masenim spektrima, tačnim masama, karakterističnoj fragmentaciji i karakterističnim retencionim vremenima. Dobijeni rezultati pokazuju da ljuska krompira, koja je otpad iz industrije čipsa i pomfrita, može biti značajan izvor fitohemikalija korisnih za ljudsko zdravlje.

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

Determination of polyphenolic profile of potato

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Potato (*Solanum tuberosum L.*) is considered as one of the most important food product because of its healing ingredients, contents of carbohydrates, proteins, minerals, and polyphenolic compounds. The amount of these components varies depending on climate factors, region of cultivation and harvesting season. The content of the individual phytochemicals is different in various parts of tubers. In accordance to our systematic investigations of the food authenticity, the main goal of this paper is determination of polyphenolic profiles of different potato cultivars. The methanol extracts from different parts of the mentioned samples of potatoes have been prepared and analyzed by using ultra-preformance liquid chromatography coupled to Orbitrap mass spectrometry (*UPLC-LTQ-orbitrap MS/MS)* in order to gain the mentioned phenolic profile. Phenolic compounds have been identified and quantified according to appropriate spectral characteristics: mass spectra, accurate mass, characteristic fragmentation, and characteristic retention time. The obtained results suggest that the potatoes peel, waste from the potato chips and fries industry, may be an important source of phytochemicals useful for human health.

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Hemija i tehnologija makromolekula
Chemistry and Technology of Macromolecules

HTM O 01

Ispitivanje morfoloških i površinskih svojstava segmentiranih poli(uretan-urea-siloksanskih) kopolimera

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U ovom radu su ispitana morfološka i površinska svojstva segmentiranih poli(uretan-urea-siloksanskih) kopolimera (PUUS) na bazi 4,4'–metilendifenildiizocijanata (MDI) i etilendiamina (ED) kao komponeti tvrdog segmenta i α,ω–dihidroksipropil-poli(dimetilsiloksana) (PDMS, M_n = 1000 g mol^{-1}) kao mekog segmenta. Serija PUUS kopolimera sa sadržajem tvrdih segmenata u opsegu 38 do 65 mas. % je sintetisana postupkom dvostepene poliadicije u rastvoru, uz kalaj-oktoat kao katalizator. Struktura i sastav PUUS kopolimera su potvrđeni ^{1}H NMR i FTIR spektroskopijom. Na osnovu rezultata analize rasipanja X-zraka na velikim (WAXS) i malim uglovima (SAXS), kao i FTIR analize vodoničnog vezivanja, utvrđeno je da sintetisani PUUS kopolimeri pokazuju mikrofazno razdvojenu strukturu. Globularne superstrukture, zapažene u filmovima uzoraka kopolimera pomoću skenirajuće elektronske mikroskopije (SEM) i mikroskopije atomskih sila (AFM), bile su posledica mikrostrukturne organizacije MDI–ED segmenata, zavisno od njihovog udela i dužine. PUUS kopolimeri su pokazali veliku otpornost na vodu, pri čemu se hidrofobnost i hrapavost njihove površine neznatno povećavala sa povećanjem masenog udela PDMS segmenta

Examination of morphological and surface properties of segmented poly(urethane-urea-siloxane) copolymers

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Morphological and surface properties of segmented poly(urethane-urea-siloxane) copolymers (PUUS), based on 4,4′-methylenediphenyl diisocyanate (MDI) and ethylene diamine (ED) as the hard segment components and α,ω-hydroxypropyl-poly(dimethylsiloxane) (PDMS, M_n = 1000 g mol^{-1}) as the soft segment are investigated. A series of PUUS copolymers with the hard segment content in the range from 38 to 65 wt. % was prepared by a two-step polyaddition procedure in a solution in the presence of stannous octoate as a catalyst. The structure and composition of the PUUSs were confirmed by ^{1}H NMR and FTIR spectroscopy. Wide and small-angle X-ray scattering (WAXS and SAXS, respectively) and hydrogen bonding analyses by FTIR indicated the formation of the microphase-separated copolymers. Globular superstructures observed in the copolymer films by scanning electron microscopy (SEM) and atomic force microscopy (AFM) were probably arisen from the microstructural organization of the MDI–ED segments, depending on their content and length. The PUUS copolymers showed high water resistance, their surface became more hydrophobic and the values of the surface roughness slightly increased with increasing the weight fraction of the PDMS segment.

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HTM P 01

Degradacija PS-g-skrob kopolimera u otpadnoj vodi

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PS-g-skrob kopolimeri dobijeni emulzionom polimerizacijom uz korišćenje novog inicijator/aktivator para (KPS/različiti amini) podvrgnuti su degradaciji u otpadnoj vodi reke Save. Stepen degradacije je praćen gubitkom mase uzoraka, a broj mikroorganizama Kohovom metodom. Eksperiment je trajao 27 dana, a procenti degradacije kopolimera su se kretali između 45,8 i 93,1 % u odnosu na masu kopolimera ili između 66,6 i 100 % u odnosu na masu skroba prisutnu u kopolimerima. Degradacija je potvrđena IR spektroskopijom i skenirajućom elektronskom mikroskopijom. Razlike u stepenu biodegradacije su posledica različite strukture uzoraka. Utvrđeno je postojanje značajne negativne korelacije između udela polistirena u kopolimeru (stepena kalemljenja) i stepena degradacije. Procenat kalemljenja PS neophodan da spreči biodegradaciju iznosio je 54 %. Razlog za nepotpunu degradaciju verovatno leži u činjenici da je u ovakvim kopolimerima skrob potpuno prekriven polistirenom i samim tim ne podleže degradaciji. U kopolimerima gde je skrob delimično prekriven dolazi do delimične degradacije koja zavisi od sposobnosti mikroorganizama, prisutnih u otpadnoj vodi, da degraduju skrob.

Zahvalnica: Ovo istraživanje je podržalo Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije kroz projekte 172001 i 172062.

Degradation of PS-g-starch copolymers in waste water

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PS-g-starch copolymers obtained by emulsion polymerization using new initiator/activator pair (PPS/different amines) were subjected to degradation in waste water from Sava River. Percentage of degradation was monitored by mass decrease and number of microorganisms by Koch’s method. Experiment lasted 27 days and the percentage of degraded copolymers varied between 45.8 and 93.1 % of total mass of copolymer or between 66.6 and 100 % of starch mass present in the copolymers. Degradation was confirmed by IR spectroscopy and Scanning electron microscopy. The differences in the degree of biodegradation are the consequences of the different structures of the samples, and there was a significant negative correlation between the share of polystyrene in the copolymer (degree of grafting) and the degree of degradation. The grafting degree of PS necessary to prevent biodegradation was 54 %. The reason that degradation is limited is probably due to the fact that in such copolymer, starch is completely covered by polystyrene, and thus non-degradable, while where starch is only partially covered, can be partially degraded, depending of the capabilities of microorganisms present in waste water system.

HTM P 02

Karakterizacija hidrogelova na bazi poli(metakrilne kiseline) i natrijum kazeinata

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Sintetisani su hibridni hidrogelovi na bazi poli(metakrilne kiseline) (PMAA) i natrijum kazeinata (CS). Glavni cilj ove sinteze je pronalaženje veze između reakcionih parametara sinteze hibridnih hidrogelova (stepen neutralizacije monomera, udeo metakrilne kiseline i kazeina, koncentracija umreživača) i karakteristika dobijenog materijala (strukture, bubrenja, mehaničkih karakteristika). Morfologija dobijenih PMAA/CS hibridnih hidrogelova je karakterisana skenirajućom elektronskom mikroskopijom i Furijeovom transformisanom infracrvenom spektroskopijom. Pored toga ispitano je i bubrenje i dinamičko-mehaničke karakteristike sintetisanih gelova. Utvrđeno je da se variranjem reakcionih parametara mogu dobiti materijali značajno različitih svojstava: sa ili bez mogućnosti bubrenja, različitih oblika kazeina, značajno poboljšanih mehaničkih svojstava itd.

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Characterization of poly(methacrylic acid) and sodium caseinate hybrid hydrogels

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Hybrid hydrogels based on poly(methacrylic acid) (PMAA) and sodium caseinate (CS) were synthesized. The major prerequisite to develop the synthesis of these materials with predetermined properties, the so-called conducted synthesis, is to find the relationships between synthesis parameters, structure of materials and desired material properties. Having that in mind, the main goal of this work was to investigate the possibility of establishing relations between the parameters of synthesis of PMAA/CS hybrid hydrogels (neutralization degree of monomer, hydrogel composition and concentration of crosslinker) and their properties (structure, swelling behavior and mechanical properties). PMAA/CS hybrid hydrogels were, therefore, characterized with Fourier transform infrared spectroscopy and scanning electron microscopy to confirm the morphology. Additionally, dynamical-mechanical analysis and swelling experiments were conducted. Varying mentioned parameters, we obtained significantly different materials: with and without ability to swell, with different casein forms, notably improved dynamical-mechanical features, etc.

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HTM P 03

Termička i morfološka svojstva termoplastičnih poliuretana na bazi poli(propilenoksida)-*b*-poli(dimetilsiloksana)-*b*-poli(propilenoksida)

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U ovom radu ispitan je uticaj sadržaja mekih poli(propilenoksida)-*b*-poli(dimetilsiloksana)-*b*-poli(propilenoksida) (PPO-PDMS) segmenta na termička i morfološka svojstva novih termoplastičnih poliuretana pomoću TGA, DSC i AFM analiza kao i dekonvolucijom FTIR spektara. Termička stabilnost kopolimera se povećavala, dok se stepen kristaliničnosti smanjivao sa povećanjem sadržaja PPO-PDMS segmenata. AFM i FTIR analize su potvrdile da se sa smanjivanjem sadržaja PPO-PDMS segmenata povećavao stepen mikrofaznog razdvajanja kopolimera.

Thermal and morphological properties of thermoplastic polyurethane-based on poly(propylene oxide)-*b*-poly(dimethylsiloxane)-*b*-poly(propylene oxide)

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In this paper was investigated the influence of the content of soft poly(propylene oxide)-*b*-poly(dimethylsiloxane)-*b*-poly(propylene oxide) (PPO-PDMS) segments on the thermal and morphological properties of new thermoplastic polyurethane with TGA, DSC and AFM analyses as well as deconvolution of FTIR spectra. The thermal stability of the copolymers increased, while the degree of crystallinity decreased with increasing content of PPO-PDMS segments. AFM and FTIR analysis confirmed that with decreasing of the content of PPO-PDMS segments the degree of microphase separation in copolymers increased.

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HTM P 04

Uticaj punila i procesnih ulja na svojstva hibridnih materijala na osnovu EPDM kaučuka

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Izbor prekursora mreže u kombinaciji sa adekvatnim punilima i procesnim uljima su ključni kriterijumi u proizvodnji elastomernih zaptivki izuzetnih svojstava. Zahvaljujući odličnoj stabilnosti u vodi elastomer na osnovu terpolimera etilena, propilena i dienske komponente (EPDM) je jedan od najčešće korišćenih materijala za celularne izolacione materijale sa zatvorenim porama za zaptivke u automobilskoj, farmaceutskoj i prehrambenoj industriji. Materijali na osnovu EPDM ispoljavaju stabilnost u toploj vodi, pari, kiselinama i alkalnim rastvorima i preporučuju se za sve polarne medije. Cilj ovog rada je bio da se ispita uticaj punilaca i procesnih ulja na svojstva materijala na osnovu EPDM. Mehanička svojstva materijala su odredjena pre i posle starenja, a dinamičko-mehaničko ponašanje je praćeno u opsegu od -120°C do 100°C. Temperaturni opseg u kome je tanδ > 0,3 je korišćen kao arbitrarni kriterijum za kapacitet prigušenja pripremljenih hibridnih materijala.

The influence of filler and oil-extender on the properties of hybrid materials based on EPDM rubber

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The choice of the network precursors in combination with an adequate selection of fillers and oil-extender are the key criteria for producing the advanced elastomeric sealing products. Thanks to its excellent stability in water the materials based on terpolymer of ethylene, propylene and a diene-component (EPDM) are very convinient material for closed cell elastomeric thermal insulators and for sealant in automotive, pharmaceutical and food industry. Materials based on EPDM have high stability in hot water, steam, acids and alkaline solutions and are recommended for all polar media. The aim of this work was to estimate the influence of fillers and oil-extender on the properties of EPDM elastomeric materials. Mechanical properties were assessed before and after ageing of materials. Dynamic-mechanical behavior of samples was determined at a temperature range from -120 °C to 100 °C. The temperature range with tanδ > 0.3 was used to assess the damping capacity of prepared hybrid materials.

HTM P 05

Sinteza i karakterizacija kopolimernih hidrogelova na bazi metakrilne kiseline i 2-akrilamido-2-metilpropansulfonske kiseline

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U ovom radu su sintetisani novi kopolimerni hidrogelovi na bazi metakrilne kiseline i 2-akrilamido-2-metilpropansulfonske kiseline radikalnom kopolimerizacijom na 70 °C tokom 5 h. Ovi hidrogelovi su karakterisani FTIR spektroskopijom, ravnotežnim stepenom bubrenja u vodi i sorpcijom boja Basic Yellow 28 i Basic Red 46 u pojedinačnom i binarnom sistemu. Odnos komonomera utiče na krajnja svojstva dobivenih kopolimera. Stepen bubrenja ovih kopolimera u vodi raste sa porastom udela AMPS-a u hidrogelu. Sintetisani hidrogelovi poseduju bolja sorpciona svojstva u binarnom sistemu, zbog različitog afiniteta interakcije prisutnih funkcionalnih grupa u hidrogelu sa bojom. Maksimalni stepen sorpcije boje Basic Yellow 28 i Basic Red 46 je dobiven na hidrogelu P(MAA-co-AMPS)50/50 i iznosi 96,4% i 98,3%, pojedinačno. Stepen desorpcije boja u pojedinačnom i binarnom sistemu raste sa porastom udela AMPS-a u hidrogelu.

Synthesis and characterization of copolymer hydrogels based on methacrylic acid and 2-acrylamido-2-methylpropane sulfonic acid

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In this study novel copolymer hydrogels based on methacrylic acid and 2-acrylamido-2-methylpropane sulfonic acid were synthesized by free-radical aqueous copolymerization at 70°C for 5 hours. These hydrogels were characterized by FTIR spectroscopy, equilibrium swelling degree and sorption of Basic Yellow 28 and Basic Red 46 dye in single and binary system. The ratio of comonomers in reaction mixture affected the properties of resulting copolymers, as the equilibrium swelling degree increased with the increase in AMPS content in hydrogel. The synthesized hydrogels showed better sorption in binary system compared to the sorption of these dyes in single system, probably due to different ability of hydrogel functional groups to interact with cationic dyes. The maximal percent removal of Basic Yellow 28 and Basic Red 46 dyes were observed by P(MAA-co-AMPS) 50/50 hydrogel and reached values of 96.4% and 98.3%, respectively. Desorption of BY28 and BR46, in both, single and binary system increased with the increase of AMPS content in hydrogel.

HTM P 06

Sinteza *n*-amil-izobutirata pomoću lipaze iz *Candida rugosa* imobilisane u hidrogel *N*-izopropilakrilamida i itakonske kiseline

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U radu je izvedena sinteza mirisnog estra, *n*-amil-izobutirata, esterifikacijom izobuterne kiseline i *n*-amil alkohola u *n*-heksanu. Kao biokatalizator korišćena je lipaza iz *Candida rugosa* imobilisana u hidrogel poli(*N*-izopropilakrilamid-*ko*-itakonska kiselina) sintetisan kopolimerizacijom preko slobodnih radikala u atmosferi azota na 25 °C, pri čemu je sadržaj uklopljenog proteina bio visok. Morfologija sintetisanog biokatalizatora je ispitana skenirajućom elektronskom mikroskopijom (SEM) i mikroskopijom atomskih sila (AFM). Ispitan je uticaj temperature, pH, sadržaj dodate vode i mase biokatalizatora na prinos estra, kao i mogućnost ponovne upotrebe biokatalizatora. Imobilisana lipaza je pokazala veliku otpornost na denaturaciju i poboljšanu stabilnost prilikom skladištenja.

Production of *n*-amyl isobutyrate using lipase from *Candida rugosa* immobilized into *N*-isopropylacrylamide and itaconic acid hydrogel

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The study of ester synthesis, *n*-amyl isobutyrate, via esterification of isobutyric acid and *n*-amyl alcohol in *n*-hexane has been performed. Lipase from *Candida rugosa* immobilized into poly(*N*-isopropylacrylamide-*co*-itaconic acid) hydrogel was used as the biocatalyst. The biocatalyst was synthesized by free radical copolymerization in the nitrogen atmosphere at 25 °C, after which high protein-loading level was also achieved. The inner/outer morphology of the synthetized biocatalyst was confirmed by Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The esterification reaction parameters, such as temperature, pH, added water content and biocatalyst amount, as well as the reusability study have been evaluated in order to achieve very high ester yield. The immobilized lipase possessed high resistance to denaturation and enhanced storage stability.

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PRINT EXIT

HTM P 07

Hidrolitička i enzimska degradacija PCL-PEO-PCL blok kopolimera

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Alifatski poliestri, kao što je poli(ε-kaprolaktnon), PCL, predstavljaju najznačajniju klasu biodegradabilnih materijala za biomedicinsku primenu. Kopolimerizacijom PCL sa poli(etilen-oksidom), PEO, se može povećati hidrofilnost, a time podešavati kinetika biodegradacije materijala. Pored uticaja na biodegradabilnost, prisustvo netoksičnog i biokompatibilnog PEO u biomaterijalima na bazi PCL sprečava imuni odgovor organizma smanjenjem nespecifične adsorpcije proteina. U radu su prikazane dve serije triblok kopolimera sastavljenih od PEO kao centralnog bloka (M_n 400 i 1000 g/mol) i PCL-a kao spoljašnjeg bloka (M_n od 20000 do 40000 g/mol), dobijenih polimerizacijom otvaranja prstena ε-CL. Sintetisani kopolimeri su karakterisani ^{1}H NMR, GPC, DSC i WAXS tehnikama. Polimerni filmovi su pripremani iz rastvora hloroforma. Površinska svojstva filmova kopolimera su karakterisana statičkim kontaktnim uglom i određivanjem raspodele veličina PCL sferulita. Hidrolitička degradacija polimernih filmova je ispitivana na 37 ^{o}C u fosfatnom puferu pH 7,4 tokom 8 nedelja, a enzimska u prusustvu *Pseudomonas* lipaze tokom 2 nedelje. Stepen degradacije polimernih filmova je praćen gravimetrijski, analizom promene molarne mase (GPC), stepena kristaliničnosti (DSC i WAXS), a promena morfologije površine optičkom mikroskopijom.

Hydrolitic and enzymatic degradation of PCL-PEO-PCL block copolymers

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Aliphatic polyesters, such as poly(ε-caprolacton), PCL, are one of the most important biodegradable materials for biomedical application. The hydrophilicity and kinetics of bio-degradation PCL based materials can be tuned by copolymerization with poly(ethylene oxide), PEO. In addition, the presence of nontoxic, biocompatible PEO in PCL biomaterials prevents the immune response of body by decreasing unspecific adsorption of proteins. In this study, two series of triblock copolymers, which consist of PEO as a central block and PCL as lateral blocks are presented. The copolymers with different lenght of central PEO (400 and 1000 g/mol) and lateral PCL block (M_n from 20000 to 40000 g/mol) were synthesized by a ring opening polymerization of ε-CL. The resulting block copolymers were characterized by ^{1}H NMR, GPC, DSC and WAXS. Polymer films were prepared by casting from chloroform solutions. The surface properties of polymer films are characterized by measuring the static water contact angles and size distribution of PCL spherulites. The hydrolitic degradation of polymer films was investigated at 37 ^{o}C in a pH 7.4 phosphate buffer during 8 weeks and enzymatic degradation in the presence of *Pseudomonas* lipase during 2 weeks. The degree of degradation of these films was characterized by mass loss, change of molar masses by GPC, degree of crystallinity (DSC and WAXS) and change of surface morphology by optical microscopy.

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HTM P 08

Priprema i svojstva antikorozivnih epoksidnih kompozita na bazi nanoglina

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Izrada nanokompozita polimer/nanoglina (NC) i njihova primena u polimernim premazima je postala predmet brojnih istraživanja usled pozitivnog uticaja nanoglina na antikorozivna i barijerna svojstva polimera. Dispergovanje gline u hidrofobnoj polimernoj matrici podrazumeva raslojavanje slojevite strukture gline, što se postiže modifikovanjem površine gline organskim modifikatorima. U ovom radu, serija nanokompozita na bazi epoksidne smole (diglicidil-etar bisfenola A), poliamido-amina kao umreživača i hemijski modifikovane gline Cloisite 30B (C30B) je pripremljena polimerizacijom u rastvoru, pri čemu je variran sadržaj gline (1-10 mas.%). Zatim, su nanokompoziti inkorporirani u osnovni i završni sloj dvoslojnog premaza sa sadržajem gline 1-3 mas.%. Eksperiment bubrenja i analiza reoloških svojstava disperzije na bazi gline C30B i komercijalnog razređivača su potvrdila visok stepen bubrenja gline u smeši rastvarača i formiranje fizičke mreže. Reološka analiza neumreženih nanokompozita je pokazala da porast sadržaja gline dovodi do porasta vrednosti reoloških parametara. Značajno povećanje reoloških parametara je primećeno iznad perkolacionog sastava ($\Phi^* = 4{,}2$ mas.%) usled jakih interakcija između čestica gline. Na osnovu ogleda u slanoj komori, prisustvo gline u osnovnom i završnom premazu je povećalo antikorozivnu zaštitu dvoslojnog premaza, zahvaljujući barijernom efektu gline prema korozivnim vrstama.

Preparation and properties of anticorrosive epoxy/clay nanocomposites

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Preparation of polymer/clay nanocomposites (NCs) and its insertion in the commercial coatings became the topic of numerous papers due to the positive impact of nanoclays on the anticorrosive and barrier properties of polymers. In order to disperse clay nanolayers in the hydrophobic polymeric matrix, clay must be modified by organic modifiers. In this work epoxy/clay NCs based on diglycidyl ether of bisphenol A (DGEBA) epoxy resin, polyamidoamine curing agent and 1-10 wt% of commercial organoclay Cloisite 30B (C30B) were prepared by the solution intercalation method. Also, epoxy NCs with 1-3 wt% organoclay content were incorporated in epoxy primer and topcoat. The “free swelling” test and rheological analyses of C30B/thinner dispersion confirmed the high swelling capacity of C30B in a thinner and a formation of organoclay physical network. The rheological properties of epoxy NCs at uncured state were improved, where the rheological parameters increased as the organoclay content increased. The significant improvement of rheological behavior was seen above the percolation threshold ($\Phi^* =$ 4.2 wt%) due to the strong physical interactions between clay particles. Two layer coating systems, obtained with NC-based primers and topcoats, had higher corrosion stability in a salt spray chamber, in comparison to unmodified system, due to the barrier effect of nanoclay against corrosive species.

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HTM P 09

Kompoziti biodegradabilnog poliestra sa nanoglinama: uticaj organskog modifikatora nanoglina na reološko ponašanje rastopa

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Poli(ε-kaprolakton), PCL, je biodegradabilni poliestar pogodan ne samo kao zamena za nedegradabilne polimere koji se koriste u širokoj potrošnji, već i za različite primene u biomedicini. Atraktivan način da se poboljšaju svojstva ovog polimera je i priprema kompozita sa nanoglinama. Glavni cilj je poboljšanje mehaničkih svojstava, posebno kod primena gde je materijal izložen velikim naponima. Da bi se postiglo najveće poboljšanje svojstava kod nanokompozita sa glinama, neophodno je postići disperziju gline do nano--nivoa, tj. eksfolijaciju slojeva gline. U okviru ovog rada pripremljeni su nanokompoziti PCL sa organomodifikovanim glinama, iz rastvora. Korišćene su dve vrste nanoglina: Cloisite®30B i Cloisite®15A, modifikovane organskim jedinjenjima različite polarnosti, koje ostvaruju različite interakcije sa PCL matricom. XRD merenjima je utvrđeno da se u slučaju C30B dobija eksfolirana, a u slučaju C15A interkalarna struktura, pri većim udelima nanogline. Dinamičko-mehaničkim merenjima uočen je očekivani trend porasta dinamičkog viskoziteta rastopa obe serije nanokompozita, sa izraženim pseudoplastičnim ponašanjem koje prati povećanje udela gline. Poređenjem reoloških parametara rastopa za uzorke nanokompozita sa eksfoliranom strukturom utvrđeno je da su oni funkcija ne samo stepena dispergovanosti, već i vrste organskog modifikatora nanogline koja se koristi.

Biodegradable polyester/nanoclay composites: Effect of clay organic modifier on melt rheological behavior

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Poly(ε-caprolactone), PCL, is a biodegradable polyester suitable not only as a replacement for nondegradable commodity plastics currently in use, but also for various biomedical applications. Preparation of PCL/nanoclay composites is an attractive solution for the properties improvement. One of the properties usually targeted for the improvement, is its mechanical strength, especially for the high bear loading applications. In order to achieve the best properties improvement, in the case of nanoclay as a filler, the full dispersion at the nanometer scale, i.e. exfoliation, is required. In a framework of this study organically modified natural nanoclays were used to prepare PCL based nanocomposites by solution casting. Two types of nanoclays were used: Cloisite®30B and Cloisite®15A, different in respect to organic modifier, thus having different interactions with PCL matrix. By XRD measurements an exfoliation was confirmed for the nanocomposites with C30B, and for the C15A nanoclay an intercalation occurred, for the higher clay loadings. The nanocomposite samples were further subjected to the dynamic-mechanical measurements in the melt. A general trend of increased dynamic viscosity with the increase in the clay content, accompanied with pronounced shear thinning is observed. For the nanocomposites with supposed exfoliated structure, it was observed that rheological properties depend not only on the dispersion of the clay, but also on the type of the organic modifier of the nanoclay.

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Organska hemija / Organic Chemistry

OH O 01

Sinteza 1-aril-3-fenil-4-feroceniltetrahidropirimidin-2(1*H*)-ona

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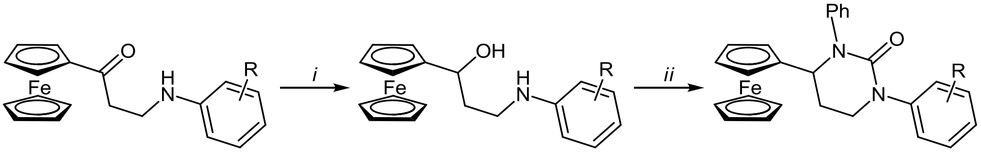
Konstantno interesovanje istraživača za sintezu cikličnih urea, uključujući tetrahidropirimidinone, posledica je njihove raznovrsne biološke aktivnosti.[1] U ovom radu biće opisan postupak za dobijanje derivata ovog heterocikličnog jedinjenja koji sadrže ferocensko jezgro (1-aril-3-fenil-4-feroceniltetrahidropirimidin-2(1*H*)-ona). Kao polazni materijal za tu sintezu upotrebljeni su ranije opisani 3-aminoaril-1-ferocenilpropan-1-oni,[2] koji su redukcijom pomoću $NaBH_4$ dali ogovarajuće 1,3-aminoalkohole. Reakcijom ovih jedinjenja sa fenilizocijanatom pod dejstvom ultrazvučnih talasa i tretiranjem tako nastalih hidroksiurea (bez izolovanja) sirćetnom kiselinom dobijeni su 1-aril-3-fenil-4-feroceniltetrahidropirimidin-2(1*H*)-oni u visokim prinosima (78-99%).



i) $NaBH_4$, MeOH; *ii*) PhNCO, AcOH; R= H, CH_3, Cl, F

Synthesis of 1-aryl-4-ferrocenyl-3-phenyltetrahydropyrimidin-2(1*H*)-ones

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Permanent researchers' interest in synthesis of cyclic ureas, including tetrahydropirimidinones, is a consequence of their diverse biological activities.[1] In the present report a protocol for the synthesis of ferrocene containing derivatives of tetrahydropirimidinone (1-aryl-4-ferrocenyl-3-phenyl-tetrahydropyrimidin-2(1*H*)-ones) will be described. 3-Aminoaryl-1-ferrocenylpropan-1-ones (recently described by us)[2] were used as the starting materials in this synthesis. The reduction of these compounds with $NaBH_4$ gave the corresponding 1,3-aminoalcohols, which submitted to reaction (prompted by ultrasound irradiation) with phenylisocyanate. Subsequent treatment of the obtained hydroxyureas (without its isolation) with acetic acid gave 1-aryl-4-ferrocenyl-3-phenyl-tetrahydropyrimidin-2(1*H*)-ones in high yields (78-99%).

1. C. O. Kappe, *Acc. Chem. Res.* **33** (2000) 879
2. a) I. Damljanović *et al., J. Organomet. Chem.* **696** (2011) 3703; b) A. Pejović *et al., Helv. Chim. Acta,* **95** (2012) 1425

OH O 02

Derivati tiazola i kumarina: kristalno pakovanje određuje tautomerni oblik

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Zarad boljeg razumevanja uočene antimikrobne aktivnosti 4-[(4-metil-1,3-tiazol-2-il)amino]- (**1T1**) i 4-[(5-metil-1,3-tiazol-2-il)amino]-3-nitro-2*H*-hromen-2-ona (**2T1**), izvršena je kristalografska analiza odgovarajućih monokristala. Utačnjavanje strukture je pokazalo da smo umesto **1T1**/**2T1** dobili kristale njihovih tautomera: (*Z*)-4-((4-metiltiazol-2(3*H*)-iliden)amino)- (**1T2**) i (*Z*)-4-((5-metiltiazol-2(3*H*)-iliden)amino)-3-nitro-2*H*-hromen-2-on (**2T2**). Rezultati prethodnih proučavanja 2-aminotiazol/2-iminotiazolin-tautomerije, kao i teorijska (DFT) i NMR (^{1}H, ^{13}C and 2D; u različitim rastvaračima) analiza jedinjenja **1T1/1T2** i **2T1/2T2**, pokazali su da je supstituisani 2-aminotiazol (**1T1**, **2T1**) dominantni tautomerni oblik u rastvoru; najviši **T2**/**T1** odnos (1/3) zabeležen je u DMSO-u. Neslaganje vezano za hemiju proučavanih jedinjenja u rastvoru i čvrstom stanju bi moglo biti posledica efekta kristalnog pakovanja.

Thiazole-coumarin hybrids: crystal packing determines tautomeric form

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In order to get a better understanding of the observed antimicrobial activity of 4-[(4-methyl-1,3-thiazol-2-yl)amino]- (**1T1**) and 4-[(5-methyl-1,3-thiazol-2-yl)amino]-3-nitro-2*H*-chromen-2-ones (**2T1**), we performed X-ray analysis of the corresponding monocrystals. X-ray data refinement revealed that instead of **1T1/2T1** we obtained crystals of their tautomeric forms (*Z*)-4-((4-methylthiazol-2(3*H*)-ylidene)amino)- (**1T2**) and (*Z*)-4-((5-methylthiazol-2(3*H*)-ylidene)amino)-3-nitro-2*H*-chromen-2-ones (**2T2**). The results of previous studies on 2-aminothiazole/2-iminotiazoline tautomerism, as well as theoretical (DFT) and NMR (^{1}H, ^{13}C and 2D; in different solvents) analyses on compounds **1T1/1T2** and **2T1/2T2**, pointed out to substituted 2-aminothiazoles (**1T1**, **2T1**) as the predominant tautomeric form in solution; the highest **T2**/**T1** ratio (1/3) was observed in DMSO. The discrepancies between solution and solid state chemistries of the title compounds might be due to crystal packing effects.

Acknowledgment. *Authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172061) for the financial support of this work.*

OH O 03

Spektroskopsko proučavanje *N,N'*-bisarilmalonamida: uticaj rastvarača i strukture

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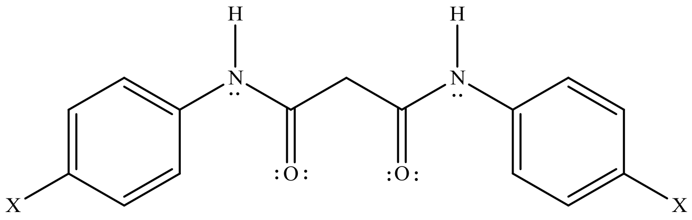
UV apsorpcioni spektri deset *N,N'*-bisarilmalonamida snimljeni su u opsegu od 200 do 400 nm u setu različitih rastvarača. Interakcije između rastvorka i rastvarača analizirani su korišćenjem metode linearne korelacije solvatacionih energija predložene od strane Kamleta i Tafta. Uticaj supstituenata na apsorpcione spektre ispitivan je Hametovom jednačinom. U nastavku istraživanja, urađeni su kvantno-hemijski proračuni energija, geometrija i talasnih brojeva ispitivanih amida primenom DFT metode.



X: OH, MeO, Me, H, Cl, Br, COOH, CH_3CO, CN, NO_2

Slika. *Struktura ispitivanih N,N'-bisarilmalonamida*
Figure. *Structure of the investigated N,N'-bisarylmalonamides*

Spectroscopic investigation of *N,N'*-bisarylmalonamides: Solvent and structural effects

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UV absorption spectra of ten *N,N'*-bisarylmalonamides have been recorded in the range 200–400 nm in the set of selected solvents. The solute–solvent interactions have been analyzed on the basis of linear solvation energy relationships (LSER) concept proposed by Kamlet and Taft. The effects of substituents on the absorption spectra have been interpreted by correlation of absorption frequencies with Hammett substituent constants. In addition, quantum chemical calculations of energies, geometrical structure and vibrational wavenumbers of the investigated amides have been performed using density functional theory.

The work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172006).

OH O 04

Sinteza novog steroidnog izoksazola

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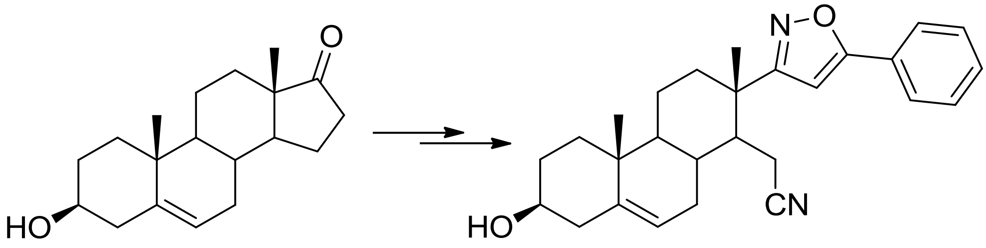
Izoksazoli spadaju u grupu jedinjenja od farmakološkog značaja, zahvaljujućim svojim antiproliferativnim, analgetičkim, anti-inflamatornim ili antiviralnim aktivnostima. Cilj ovog rada bio je sinteza novog steroidnog izoksazolskog derivata, potencijalnog antitumorskog agensa. Polazno jedinjenje u ovoj višefaznoj sintezi bio je dehidroepiandrosteron.



A synthesis of a new steroidal isoxazole

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Isoxazoles belong to a group of pharmacologically important compounds, thanks to their antiproliferative, analgesic, anti-inflammatory or antiviral activities. The goal of this work was a synthesis of a new steroidal isoxazole derivative with potential antitumor activity. The starting compound in this multistep synthesis was dehydroepiandrosterone.

Realizacija ovog rada finansirana je iz sredstava projekata ON172021 i 114-451-3600/2013-03

OH P 01

Sinteza, karakterizacija i antimikrobna aktivnost male biblioteke acetoacetata koji sadrže ferocen i njihovih fenil analoga - novi antikandidalni agensi

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Biblioteka od šesnaest 2-supstituisanih metil-acetoacetata koji sadrže ferocenil i/ili fenil grupu je dizajnirana u cilju utvrđivanja razlike u antimikrobnoj aktivnosti ferocenskih jedinjenja i njihovih fenil analoga. Sintetisani acetoacetati su potpuno okarakterisani spektralnim (MS, IR, UV-Vis, 1D i 2D-NMR) i elektrohemijskim (ciklična voltametrija) tehnikama. Sva jedinjenja su pokazala *in vitro* antimikrobnu aktivnost protiv šest bakterijskih sojeva (tri Gram-pozitivna i tri Gram-negativna) i dva soja gljiva sa vrednostima minimalne inhibitorne koncentracije 0,0050–20,6 µmol mL^{-1}. Aglomerativna hijerarhijska klaster statistička analiza podataka iz testova antimikrobne aktivnosti je pokazala da jedinjenja koje sadrže ferocensko jezgro imaju statistički različitu i veću antimikrobnu aktivnost u poređenju sa njihovim fenil analozima.

Synthesis, characterization and antimicrobial evaluation of a small library of ferrocene-containing acetoacetates and phenyl analogs - the discovery of a potent anticandidal agent

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Dragana Stevanović**, Rastko D. Vukićević**

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A library of sixteen 2-substituted methyl acetoacetates containing ferrocenyl and/or phenyl units was designed to disclose differences in the antimicrobial activity of ferrocene-containing compounds and their phenyl analogs. The acetoacetates were fully characterized by spectral (MS, IR, UV-Vis, 1D and 2D-NMR) and electrochemical (cyclic voltammetry) techniques. All compounds have demonstrated *in vitro* antimicrobial activity against six bacterial (three Gram-positive and three Gram-negative) and two fungal strains with minimal inhibitory concentration values of 0.0050–20.6 µmol mL^{-1}. Agglomerative hierarchical clustering statistical analysis of the antimicrobial assay data demonstrated that ferrocene-containing compounds have statistically different and greater antimicrobial activity when compared to their phenyl analogs.

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

OH P 02

Sinteza Pt(II) kompleksa sa 2-(fenilselanilmetil)oksolanom kao ligandom

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Kompleksi prelaznih metala sa organo-selenovim jedinjenjima kao ligandima su privukli posebnu pažnju zahvaljujući svojim biološkim i biomedicinskim primenama. Oni mogu ispoljavati citotoksična, antimalarijska, antileukemijska i antitumorska svojsta.[1] U prethodnom radu ispitivali smo antioksidativnu i antiproliferativnu aktivnost 2-(fenilselanilmetil)oksolana (L) na ćelijama raka debelog creva (HCT-116) i raka dojke (MDA-MB-231).[2] Koordinovanjem za Pd(II) dobijen je kompleks sa citotoksičnim i citostatičkim dejstvom. U cilju daljih istraživanja sintetisali smo njegov Pt(II) analog ne bi li uporedili biološku aktivnost sa odgovarajućim Pd(II) kompleksom.
U ovom radu predstavljamo sintezu novog Pt(II) kompleksa sa organo-selenovom grupom. Ligand L je dobijen po već opisanoj proceduri.[3] Jedinjenje L je potom tretirano sa K_2PtCl_4 u višku, na 40 °C, i EtOH/MeOH sistemu rastvarača, pri čemu je dobijen kompleks C (Shema 1).

Synthesis of a Pt(II) complex with 2-(phenylselanylmethyl)oxolane as a ligand

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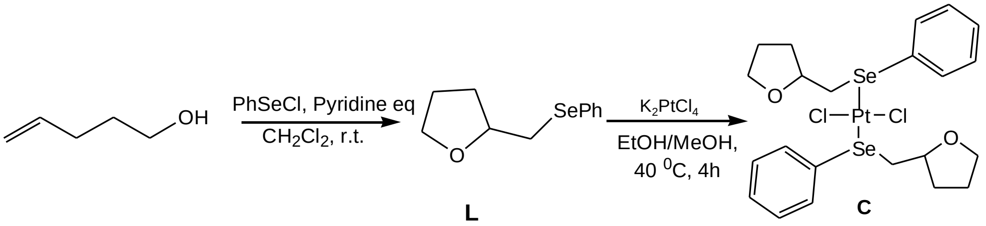
Transition metal complexes with organo-selenium compounds as ligands have attracted considerable interest due to their biological and biomedical applications. They can display cytotoxic, antimalarian, antileucemic and antitumor properties.[1] In our previous work we have screened 2-(phenylselanylmethyl)oxolane (L) for its antioxidant and antiproliferative efect on colon cancer cell line HCT-116 and breast cancer cell line MDA-MB-231.[2] Coordinating L to Pd(II) gave complex which exhibits cytostatic and cytotoxic abilities. To continue this line of work, we have synthetisized its Pt(II) analog, in order to compare its biological activities with those of Pd(II) complex.
Herein we report the synthesis of a new Pt(II) complex bearing organo-selenium moiety. Ligand L was created using a described method.[3] Compound L was then treated with an excess of K_2PtCl_4 at 40 °C, in EtOH/MeOH mixture as a solvent system, and afforded complex C (Scheme 1).



Shema 1, Scheme 1

1. T.R. Todorović, A.Bacchi, D.M. Sladić, N.M. Todorović, T.T. Božić, D.D. Radanović, N.R. Filipović, G. Pelizzi, K.K. Andjelković, *Inorg. Chim. Acta,* **362** (2009) 3813–3820.
2. J.V. Kosaric at all, *JBUON,* **19** (2014)283-290
3. Z.M. Bugarčić, B.M. Mojsilović, V.M. Divac, *J. Mol. Catal. A: Chem.* **272** (2007) 288-292.

OH P 03

Sinteza i spektralna karakterizacija biblioteke 1-fenilpirazola koji sadrže ferocen i njihovih fenil analoga

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Rastuća pojava otpornosti mikroorganizama na postojeće antibiotike učinila je pronalaženje novih antimikrobnih agenasa jednim od osnovnih ciljeva medicinskih hemičara. Jedna od strategija koja omogućava dobijanje jedinjenja sa pojačanom ili novom biološkom aktivnošću je uvođenje ferocenil grupe u jedinjenja sa već dokazanom biološkom aktivnošću. U ovom radu, u cilju budućeg ispitivanja potencijalne biološke aktivnosti, izvršena je sinteza 1*H*-1-fenil-3-ferocenil-pirazol-4-karboksaldehida (jedinjenja za koje je poznato da poseduje antibiotske osobine), a zatim i biblioteke alkohola adicijom Grignard-ovih reagenasa na ovaj aldehid. Sintetisani su i njihovi fenil analozi radi uporednog ispitivanja njihove aktivnosti, tj. utvrđivanja doprinosa ferocenskog jezgra utvrđenoj aktivnosti. Prinosi reakcija sinteze alkohola su bili u opsegu od 74 do 96%. Sva jedinjenja iz biblioteke (ukupno 24 sintetisanih jedinjenja) predstavljaju potpuno nova jedinjenja koja su potpuno spektralno okarakterisana (MS, IR, UV-Vis, 1D- i 2D-NMR).

Synthesis and spectral characterization of a library of 1-phenylpyrazoles containing a ferrocene unit and their phenyl analogues

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Due to an increasing emergence of microbial resistance to existing antimicrobial drugs, the design and discovery of new antimicrobial agents has become one of the main investigational goals of many medicinal chemists. A synthetic strategy that frequently leads to the discovery of new biologically active compounds or those with potentiated biological properties is the introduction of a ferrocenyl group into a compound with an already established biological effect. In this work, with an aim of finding new antimicrobial agents, a library of alcohols was synthesized by the addition of different Grignard reagents to the aldehyde group of 1*H*-3-ferrocenyl-1-phenyl-pyrazole-4-carbaldehyde (a compound with already demonstrated antimicrobial activity), itself obtain in a Vilsmeier-Haack reaction starting from the phenylhydrazone of acetophenone. The library included phenyl analogues of the prepared ferrocene-containing alcohols (formed by a formal exchange of the ferrocenyl group with a phenyl one). The phenyl analogues allowed determining the extent the ferrocene core contributes to the overall activity. All prepared alcohols (24 in total) were new compounds obtained in 74-96% yield. All of the synthesized compounds were fully spectrally characterized (MS, IR, UV-Vis, 1D- and 2D-NMR).

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

OH P 04

Nova sintetska metoda za dobivanje *N*-metil aromatičnih imina bez upotrebe rastvarača

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Sinteza *N*-metil aromatičnih imina bez prisustva rastvarača vršena je homogenizacijom aromatičnih aldehida, metilamin-hidrohlorida i baze, u tarioniku pistilom. Najbolji prinosi ostvareni su kada je reakcija izvođena u prisustvu viška $CH_3NH_2{\cdot}HCl$ i $NaHCO_3$ (najčešće u odnosu 1:5:5 = $ArCHO{:}CH_3NH_2{\cdot}HCl{:}NaHCO_3$), a reakciona smeša ostavljena nakon homogenizacije da stoji na sobnoj temperaturi od 1 h (u slučaju aldehida sa elektron-akceptorskim supstituentima) do 24 h (u slučaju aldehida sa elektron-donorskim supstituentima). Nakon jednostavne obrade reakcione smeše dobijeni proizvodi su bili uglavnom dovoljno čisti za spektralnu karakterizaciju. Na ovaj način sintetisan je 31 imin, od kojih osam predstavljaju potpuno nova jedinjenja, a njihove strukture su potpuno spektralno okarakterisane (^{1}H- i ^{13}C-NMR, IR, MS). U slučaju salicilaldehida i 4-hlorbenzaldehida izvršena je sinteza sa gramskim količinama reaktanata. Ovaj način sinteze *N*-metil aromatičnih imina ne samo da obezbeđuje dobre prinose, već i eliminiše nedostatke tradicionalne sinteze *N*-metil imina, kao što su: upotreba opasnih rastvarača, manje ili više skupih katalizatora i rad sa anhidrovanim gasovima pod pritiskom.

Simple and efficient one-pot solvent-free synthesis of *N*-methyl imines of aromatic aldehydes

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A one-pot solvent-free synthesis of *N*-methyl imines in good to excellent yields was performed by grinding together aromatic aldehydes and methylamine hydrochloride in the presence of a base. The best yields were achieved when an excess of $CH_3NH_2{\cdot}HCl$ and $NaHCO_3$ was used (usually in a molar ratio 1:5:5 = $ArCHO{:}CH_3NH_2{\cdot}HCl{:}NaHCO_3$), allowing the reaction to proceed for 1 h (in the case of aromatic aldehydes containing electron-withdrawing substituents) or overnight (in the case of electron-rich aldehydes). After a simple work-up the obtained products were mostly pure enough for spectral characterization. In this way, 31 *N*-methyl imines were prepared, among which 8 were synthesized for the first time. All synthesized products were fully spectrally (^{1}H- and ^{13}C-NMR, IR, MS) characterized. In the case of salicylaldehyde and 4-chlorobenzaldehyde the synthesis of the corresponding imines was also conducted on a gram-scale. This approach not only provides good to high yields, but also eliminates the disadvantages of the traditional synthesis of *N*-methyl imines, such as the use of hazardous solvents and more or less expensive catalysts and the necessity of work/handling with an anhydrous gas in pressurized containers.

Acknowledgment. *Authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172061) for the financial support of this work.*

OH P 05

Sinteza i antiproliferativna aktivnost androstanskih 16,17-seko-16,17a-dinitrila sa 4-en-3-on i 1,4-dien-3-on sistemom

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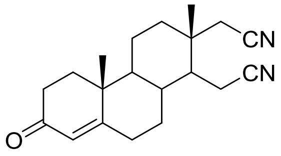
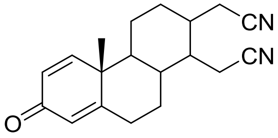
Dizajniranje i dobijanje novih antitumorskih agenasa ima za cilj pronalaženje takvih jedinjenja koja pokazuju što veći stepen inhibicije rasta neoplastičnih ćelija, pri što nižim koncentracijama, deluju specifično i selektivno samo na maligne ćelije, a da pri tome ne oštećuju zdrave. Tragajući za novim antitumorskim agensima sintetizovani su androstanski 16,17-seko-16,17a-dinitrili sa konjugovanim 4-en-3-on i 1,4-dien-3-on sistemom i ispitana je njihova antiproliferativna aktivnost prema sedam ćelijskih linija humanih tumora i jednoj zdravoj humanoj ćelijskoj liniji. Kako bi se ispitao uticaj konjugovanih sistema u novosintetizovanim jedinjenjima na antiproliferativnu aktivnost, analizom dobijenih rezultata uspostavljeni su korelacioni odnosi između strukture i aktivnosti ispitivanih jedinjenja.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (br. projekta 172021) i Pokrajinskom sekretarijatu za nauku i tehnološki razvoj Autonomne Pokrajine Vojvodine (br. projekta 114-451-2713/2012-01) na finansijskoj podršci .



1



2

Synthesis and antiproliferative activity of 16,17-seco-16,17a-dinitriles with 4-en-3-one and 1,4-dien-3-one system

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Searching for new antitumor agents, we have synthesized new androstane 16,17-seco-16, 17a-dinitrile with 4-en-3-one and 1,4-dien-3-one system, and tested for their antiproliferative activity against seven human tumor cell lines and a healthy human cell line. In order to investigate the effect of conjugated systems in newly synthesized molecules in antiproliferative activity, an analysis of the results have been established correlations between structure and activity of the tested compounds.

Authors would like to thank the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 172021) and the Provincial Secretariat for Science and Technological Development of the Autonomous Province of Vojvodina (Grant No. 114-451-2713/2012-01) for financial support.

OH P 06

Alkilovanje oksazolinskog derivata holne kiseline

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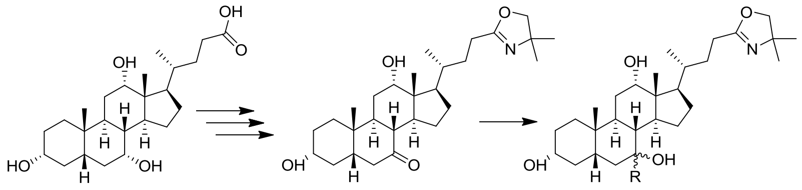
Bolje razumevanje uloge žučnih kiselina kao signalnih, transportnih i holelitolitskih molekula dovelo je do povećanja interesovanja za sintetske modifikacije ovih molekula u cilju dobijanja potencijalnih medikamenata. Soli žučnih kiselina su amfifilni molekuli koji mogu da formiraju micele sposobne da vežu i prenose hidrofobne lekove. Povećanje hidrofobne površine žučne kiseline može poboljšati sposobnost za vezivanje hidrofobnih molekula. Mi smo modifikovali hidrofobnost molekula uvođenjem butil i oktil bočnog niza u položaj C-7 steroidnog jezgra holne kiseline upotrebom Grignard-ove reakcije. Nukleofilna adicija Grignard-ovog reagensa na 7-keto grupu derivata žučne kiseline se dešava stereoselektivno.



Holna kiselina

R= *n*-Bu, *n*-Oktil

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

Alkylation of cholic acid oxazoline derivative

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Better understandings role of bile acids as a signalling, transport and cholelitholytic molecules yielded increase in interest for synthetic modifications of these molecules in order to obtain potential medicaments. Bile acid salts are amphiphilic molecules able to form micelles that can bind and transport liphophilic drugs. Increase in hydrophobic area of bile acid can benefit better binding of hydrophobic drugs. We have modified hidrophobicity of molecules by introduction of butyl and octyl side chain in position C-7 of steroid skeleton using Grignard reaction. Nuceleophilic addition of Grignard reagent on 7-keto group of bile acid occurs stereoselectivly.

Acknowledgement: *The work was supported by a grant from the Ministry of Education, Science and Technological development (Project ON172021).*

OH P 07

Homologo modelovanje 5HT1A receptora

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Homologo modelovanje proteina, ili komparativno modelovanje kako se još naziva, je tehnika koja koristi matricu poznate kristalne strukutre jednog proteina, za modelovanje strukture, sličnog (homologog) proteina, čija je strukutra nepoznata. Kvalitet homologog modela zavisi od više faktora, od kojih je najbitniji - izbor matrice, prema kojoj će se vršiti modelovanje. Tipičan model dobijen ovom tehnikom, ima grešku od oko 1-2A u slučaju kada je sličnost sa matricom 70%, ali sličnost od 25%, dovodi do greške od 2-4A. Greška je još veća u predelu petlji, gde njihova neuređena strukutra umnogome ometa modelovanje.

Homologo modelovanje 5HT1A receptora je za sada jedini način pomoću koga možemo predstaviti njegovu trodimenzionalnu strukuru. Do nedavno, jedine matrice za homologo modelovanje 5HT1A su bile krustalne strukture baketeriorodopsina i rodopisa, ali je danas taj izbor proširen na oko 60 novokristalisanih matrica, koje sa 5HT1A dele visok procenat sličnosti.

Cilj ovoga rada je da da poređenje različitih matrica i njihovu upotrebnu vrednost u homologom modelovanju novih modela 5HT1A receptora.

Homology Modeling of 5HT1A Receptor

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Homology modeling, also known as comparative modeling of protein, refers to constructing an atomic-resolution model of the "target" protein from its amino acid sequence and an experimental three-dimensional structure of a related homologous protein (the "template"). Homology modeling relies on the identification of one or more known protein structures likely to resemble the structure of the query sequence and on the production of an alignment that maps residues in the query sequence to residues in the template sequence . It has been shown that three-dimensional protein structure is evolutionarily more conserved than would be expected on the basis of sequence conservation alone. The quality of the homology model is dependent on the quality of the sequence alignment and template structure. Model quality declines with decreasing sequence identity; a typical model has ~1–2 Å root mean square deviation between the matched Cα atoms at 70% sequence identity but only 2–4 Å agreement at 25% sequence identity. However, the errors are significantly higher in the loop regions, where the amino acid sequences of the target and template proteins may be completely different.

OH P 08

Sinteza i *in vitro* antitumorska aktivnost novog pseudo-*C*-nukleozida sa pirazolskim prstenom

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U radu je ostvarena višefazna sinteza novog pseudo-*C*-nukleozida sa pirazolskim prstenom iz D-glukoze. Parcijalno zaštićena dialdoza **1** poslužila je kao pogodno polazno jedinjenje u ovoj sintezi. Aldehid **1** je uspešno preveden u ciljni molekul **7** nizom slektivnih hemijskih transformacija koje su prikazane na Shemi 1. Rezultati ispitivanja *in vitro* antiproliferativne aktivnosti jedinjenja **7** prema ćelijskim linijama odabranih humanih tumora biće takođe saopšteni i diskutovani.

Synthesis and *in vitro* antitumour activity of novel pseudo-*C*-nucleoside containing pyrazole ring

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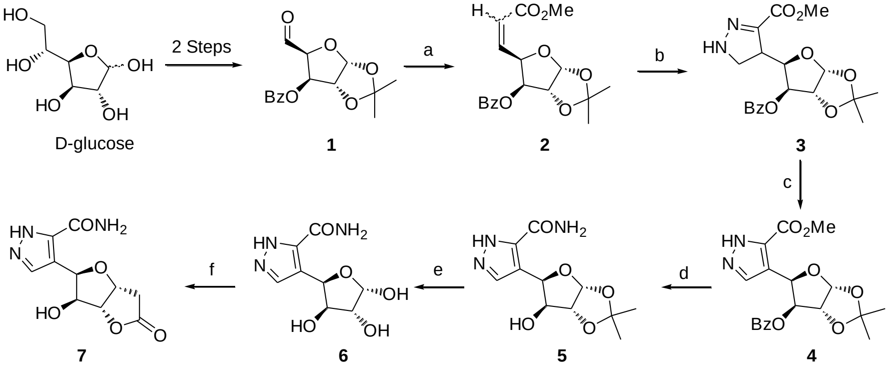
Multi-step synthesis of novel pseudo-*C*-nucleoside containing pyrazole ring (compound **7**) has been achieved starting from D-glucose. Partially protected dialdose **1** was used as a suitable starting compound. The aldehyde **1** was converted to the target **7** through an eight-step sequence outlined in Scheme 1. Results related to *in vitro* antiproliferative activity of **7** against a number of tumour cell lines will be presented.



Scheme 1. *Reagents and conditions: (a) MCMP/MeOH, 0 °C→ rt, 1.5 h; (b) CH_2N_2, Et_2O, 0 °C, 3 h; (c) Cl_2, CCl_4, rt, 3 h; (d) NH_3, MeOH, 9 days; (e) 90% aq TFA, 0 °C, 2 h; (f) Meldrum's acid, DMF, Et_3N, 46−50 °C, 70 h.*

***Acknowledgement**: The work was supported by a grant from the Ministry of Education, Science and Technological Development (Project 172006) as well as by Provincial Secretariat for Science and Technological Development of the Autonomous Province of Vojvodina.*

OH P 09

Sinteza, bioloska aktivnost i doking analiza novosintetisanih (2-metoksifenil)piperazina

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Slađana Kostić-Rajačić

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Dopaminski D2 receptor sadrži dva mesta vezivanja liganda: primarno mesto vezivanja - unutar samog receptora, izmedju transmembranskih heliksa TM 3,5 i 7 i sekundardno mesto vezivanja smesteno između TM 5, 6 i druge ekstracelularne petlje. Za postizanje visokog afiniteta prema D2 receptoru, ligand formira višestruke interakcije sa oba vezivna mesta. Kako bismo ispitali uticaj dužine, oblika i fleksibilnosti liganda na afinitet vezivanja za D2 receptor, sintetisali smo 12 derivata (2-metoksifenil)piperazina. Za sva novosintetisana jedinjenja određen je afinitet vezivanja u in vitro eksperimentima kompeticije sa 3H-spiperonom (Tabela 1.). Doking analizom određene su interakcije, receptora i liganada, kao i uticaj strukutre liganada na jačinu formiranja kompleksa receptor-ligand.

Synthesis, biological evaluation and docking analysis of new (2-methoxyphenyl)piperazines

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Dopamine D2 receptor binding cavity consists of two distinct binding pockets: orthosteric binding site (OBS), deep inside the receptor interior, located between transmembrane helices (TM) 3, 5 and 7, and second binding pocket (SBP) located in second extracellular loop (ecl) part of D2DR, bordering extracellular environment. This organization of binding cavity, facilitates D2DR to accommodate for different size and shape of the ligands. OBS is formed by Asp 114, Ser 167, Ser 194, Ser 197, Phe 386, Trp 390, and Tyr 420. During ligand binding, ASP 114 plays anchor point, and interacts with ligand protonated nitrogen atom, while Ser 167, Ser 194 and Ser 197 ensure correct ligand orientation in OBS via hydrogen bonding. Phe 386, Trp 390, and Tyr 420 form hydrophobic pocket, for ligands with corresponding hydrophobic groups .
SBP has different composition and role. It's primary role is to define top part of D2DR binding cavity, and separate it from extracellular space. SBP is formed from amino acid residues from TM 5 and 6, together with residues from ecl2. Ile 166, Leu 170, Leu 171, Ile 184, Phe 189, Val 190, His 397 and Ile 398 provide hydrophobic environment for the ligand corresponding groups, while polar interactions could be formed with Asn 186.

This work was supported by the Ministry of Education and Science of the Republic of Serbia (Project No. 172006).

OH P 10

Novi konformaciono kruti mimetik goniofufurona kao inhibitor rasta tumorskih ćelija

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Ostvarena je sinteza novog konformaciono krutog mimetika goniofufurona sa 5,7-*O*-metilidenskom i 7-hloro funkcijom (jedinjenje **4**), primenom dva nezavisna puta, polazeći iz D-glukoze. Takođe je ispitivana *in vitro* citotoksična aktivnost ovog mimetika prema nekoliko malignih i jednoj zdravoj ćelijskoj liniji, a rezultati su poređeni sa rezultatima dobijenim za vodeće jedinjenje **1** i za komercijalni antitumorski agens doksorubicin.

A novel conformationally constrained goniofufurone mimic as inhibitor of tumour cells growth

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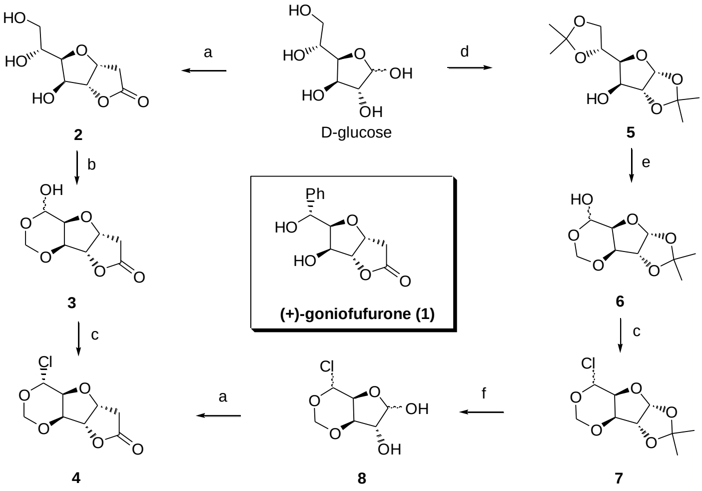
The synthesis of a conformationally constrained goniofufurone mimic with 5,7-*O*-methylidene and 7-chloro functions (compound **4**) is completed by using two independent multi-step sequences, both having D-glucose as a starting compound. In vitro cytotoxicities of target molecule against a number of human tumour cell lines were recorded and compared with those observed for the lead **1**, as well as for the commercial antitumour agent doxorubicin.



Scheme 2.
Reagents and conditions:
(a) Meldrum's acid, DMF, Et_3N, 46–48 °C;
(b) $NaIO_4$, CH_3CN, rt ;
(c) MsCl, CH_2Cl_2, Et_3N, 0 °C → +4 °C;
(d) conc. H_2SO_4, Me_2CO, rt,
(e) H_5IO_6, EtOAc, rt; (f) 90% aq TFA, 0 °C.

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172006) as well as by Provincial Secretariat for Science and Technological Development of the Autonomous Province of Vojvodina

OH P 11

Uticaj rastvarača i supstituenata na položaj azo-hidrazon tautomerije 5-(4-supstituisanih fenilazo)-3-cijano-6-hidroksi-1-hidroksietil-4-metil-2-piridona

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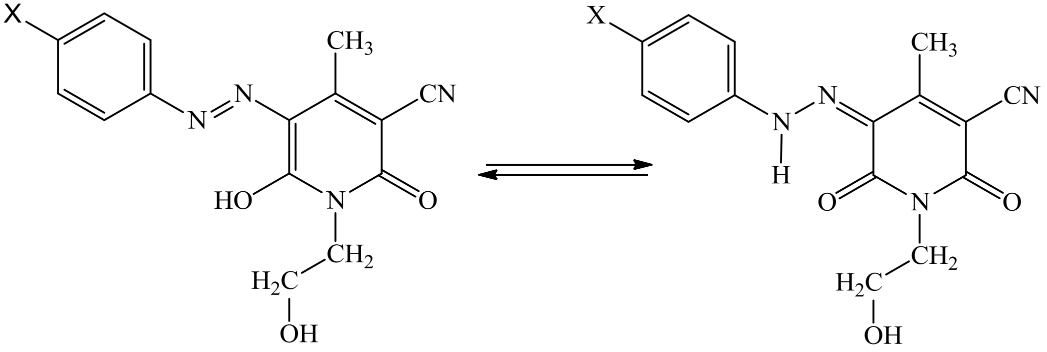
U okviru rada sintetisana je serija od deset 5-(4-supstituisanih fenilazo)-3-cijano-6-hidroksi-1-hidroksietil-4-metil-2-piridona i u potpunosti okarakterisana temperaturom topljenja, FTIR, ^{1}H NMR i ^{13}C NMR spektroskopijom. Solvatohromizam i tautomerija ovih jedinjenja je ispitana u dvadeset dva rastvarača različite polarnosti. Uticaj polarnosti i sposobnosti građenja vodoničnih veza rastvarača na položaj UV-Vis apsorpcionih traka analizirani su metodama linearne korelacije solvatacionih energija, Kamlet-Taftovom i Katalanovom jednačinom. Uticaj supstituenata na apsorpcione spektre ispitivan je Hametovom jednačinom.



X= OCH_3, NO_2, COOH,$COCH_3$, Br, H, CN, OH, Cl, CH_3

Slika. Azo-hidrazon tautomerija kod ispitivanih arilazo piridonskih boja
Figure. Azo-hydrazone tautomerism of the investigated arylazo pyridone dyes

Solvent and substituent effects on azo-hydrazone tautomerism of 5-(4-substituted phenylazo)-3-cyano-6-hydroxy-1-hidroxyethyl-4-methyl-2-piridones

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In this work, ten dyes having the same 3-cyano-6-hydroxy-1-ethylhydroxy-4-methyl-2-pyridone have been synthesized and fully characterized by melting point, FTIR, ^{1}H and ^{13}C NMR spectroscopy. Solvatochromism and tautomerism of these dyes have been investigated in twenty two solvents of different polarity. The effects of solvent dipolarity/polarizability and solvent-solute hydrogen bonding interactions on the position of their UV-Vis absorption bands have been analysed by means of linear solvation energy relationships (LSER) concepts, proposed by Kamlet-Taft and Catalan. Furthermore, substituent effects on the UV-Vis maxima have been evaluated using Hammett equation.

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OH P 12

Синтеза 1-арил-3-фенил-1-(3-фероценил-3-оксопропил)уреа

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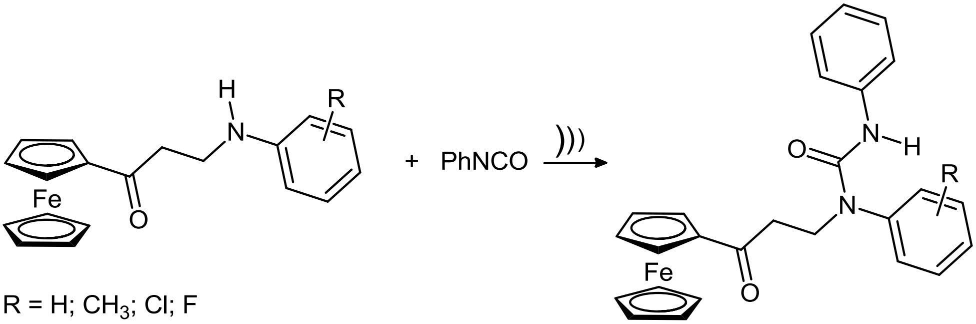
Синтезом уреа бави се велики броја хемичара, пошто ова једињења имају имају широку примену у разним областима органске синтезе и индустрије.[1] У овом саопштењу биће приказано добијање (и спектроскопска карактеризација) серије уреа које у свом саставу садрже фероценоил групу. Ова синтеза остварена је рекцијом фенилизоцијаната и одговарајућих 3-аминоарил-1-фероценилпропан-1-она под дејством ултразвучних таласа.



Synthesis of 1-aryl-1-(3-ferrocenyl-3-oxopropyl)-3-phenylureas

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Synthesis of ureas is permanently intriguing for chemists since these compounds are widely used in many fields of organic synthesis and industry.[1] In this report will be presented preparation (and spectroscopic characterization) of a series of ureas containing ferrocenoyl group. This synthesis was achieved by reacting of pfenylisocyanate with the corresponding 3-aminoaryl-1-ferrocenylpropan-1-ones prompted by ultrasonic irradiation.

1. T. P. Vishnyakova, I. A. Golubeva and E. V. Glebova, *Russ. Chem.Rev. (Engl. Transl.),* **54 (**1985) 249

OH P 13

Hemijske transformacije D-modifikovanih androstanskih derivata

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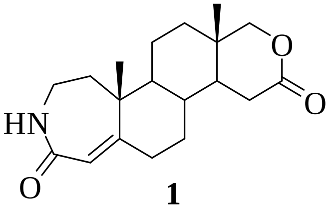
Steroidi su veoma značajna jedinjenja, koja privlače pažnju naučnika. Poznato je da su uključeni u regulaciju širokog spektra bioloških procesa i zato imaju potencijal da služe kao templati za razvoj lekova za lečenje velikog broja bolesti. Trenutno, mnogi steroidni lekovi, koji su u upotrebi, su polu-sintetski proizvodi, koji su nastali uvođenjem specifičnih funkcionalnih grupa u steroidno jezgro polaznog jedinjenja.

U ovom radu su u višefaznoj sintezi iz polaznog dehidroepiandrosterona dobijeni novi 3-aza-17-oksa-A,D-dihomoandrost-4a-en-4,16-dion (**1**) i 17(*E*)-pikoliniliden-3-aza-A-homoandrost-4a-en-4-on (**2**), kao potencijalno biološki aktivni derivati. Naime, cilj naših istraživanja je usmeren ka razvoju novih citotoksičnih agenasa, koji bi bili primenljivi u lečenju raznih hormon-zavisnih bolesti, kao što su kancer dojke ili kancer prostate.



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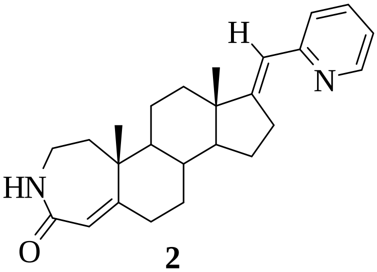

2

Chemical transformations of D-modified androstane derivatives

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Steroids are a fundamental class of molecules which continue to attract attention from the scientific community. Moreover, because steroids are involved in the regulation of a wide range of biological processes, they have the potential to serve as templates for the development of drugs for the treatment of a large number of human diseases. Currently, most steroid-based pharmaceuticals are semi-synthetic compounds prepared by connecting specific functional groups to a core steroid scaffold.

Because of that, in this work, starting from dehydroepiandrosterone in multistage synthesis new 3-aza-17-oxa-A,D-dihomoandrost-4a-en-4,16-dion (**1**) and 17(*E*)-picolinylidene-3-aza-A-homoandrost-4a-en-4-on (**2**) were obtained, as potential biological active compounds. Namely, the aim of our investigation was directed to development of some new steroidal cytotoxic agents, which can be applied against different hormone-dependent diseases (such as breast and prostate cancers).

Authors would like to thank the Provincial Secretariat for Science and Technological Development (Project No. 114-451-3600/2013-03) and the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. ON172021) for financial support.

OH P 14

Sinteza, struktura i svojstva novih 3-(supstituisanih benzil)-5,5'-cikloalkan spirohidantoina

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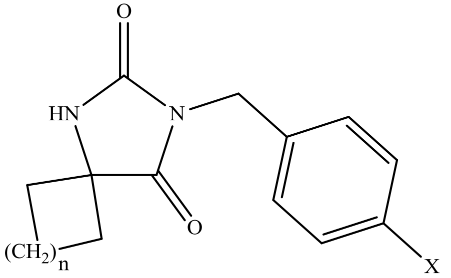
U radu je sintetizovano dvadeset novih 3-(supstituisanih benzil)-5,5'-cikloalkan-spirohidantoina čija je struktura određena temperaturama toplenja, FT-IR, ^{1}H i ^{13}C NMR i UV spektroskopijom. Solvatohromizam ovih jedinjenja je proučavan metodom linearne korelacije energija solvatacije. Kvantitativna procena uticaja rastvarača na pomeranje apsorbcionih maksimuma je nedvosmisleno ukazala na vezu između lipofilnosti i relevantnih farmakoloških karakteristika proučavanih jedinjenja sa njihovim proton-akceptorskim svojstvima.



n = 2, 3, 4 X = H, CH_3, OCH_3, Cl, Br, CN, NO_2

Slika. Struktura proučavanih jedinjenja
Figure. Structure of the investigated compounds

Synthesis, structure and properties of novel 3-(substituted benzyl)-5,5'-cycloalkanespirohydantoins

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In this work twenty novel 3-(substituted benzyl)-5,5'-cycloalkanespirohydantoins have been synthesized and fully characterized by melting point, FT-IR, ^{1}H and ^{13}C NMR and UV spectroscopy. Solvatochromism of these compounds have been analysed by means of linear solvation energy relationships (LSER) concept. The quantitative relationships beetwen hydrogen bonding interaction and the correspodenting pharmacologically relevant propereties of the studied compounds have been discussed.

OH P 15

Uticaj rastvarača na tautomernu ravnotežu 6(2)-hidroksi-4-metil-2(6)-okso-1-(supstituisanih fenil)-1,2(1,6)-dihidropiridin-3-karbonitrila

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Proučavanje tautomerne ravnoteže 6(2)-hidroksi-4-metil-2(6)-okso-1-(supstituisanih fenil)-1,2(1,6)-dihidropiridin-3-karbonitrila vršeno je primenom UV/Vis spektroskopije i kvantno-hemijske analize. Tumačenje eksperimentalnih podataka je upotpunjeno primenom teorijskog TD-DFT metoda. Uticaj rastvarača na tautomernu ravnotežu analiziran je primenom metoda linearnih korelacija solvatacionih energija (LSER). Rezultati su ukazali da stepen konjugacije i intramolekulski transfer naelektrisanja (ICT) zavisi od prirode prisutnih supstituenata. Proučavanjem položaja tautomerne ravnoteže sagledan je uticaj molekulske konformacije na prenos elektronskih efekata substituenata, kao i na različite interakcije rastvarač-rastvorena supstanca. Eksperimentalna i teorijska analiza su potvrdile postojanje oba tautomerna oblika (**2-PY**/**6-PY**) kod većine ispitivanih jedinjenja, osim jedinjenja sa hidroksi grupom u *para* položaju (**2-PY**), i trifluorometil-grupom u *meta* položaju (**6-PY**).

Solvent effects on tautomeric equilibria of 6(2)-hydroxy-4-methyl-2(6)-oxo-1-(substituted phenyl)-1,2(1,6)-dihydropyridine-3-carbonitriles

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The state of the tautomeric equilibria of 6(2)-hydroxy-4-methyl-2(6)-oxo-1-(substituted phenyl)-1,2(1,6)-dihydropyridine-3-carbonitriles were evaluated from UV/Vis and quantum chemical study. The experimental data were interpreted with the aid of time-dependent density functional (TD-DFT) method. Linear solvation energy relationships (LSER) rationalized solvent influence on tautomeric equilibria. It was found that substituents change the extent of conjugation, and affect intra-molecular charge transfer (ICT) character. Theoretical calculations and obtained correlations gave insight into the influence molecular conformation on the transmission of substituent effects, as well as on different solvent–solute interactions on state of tautomeris equilibria. Experimental and theoretical analysis confirm that the prepared compounds exists in both tautomeric forms (**2-PY**/**6-PY**), except compounds with *para*-hydroxy, **2-PY** form, and *meta*-trifluoromethyl substituent, **6-PY** form.

OH P 16

Halogenovani derivati krasalaktona D kao potencijalni antitumorski agensi: sinteza i SAR ispitivanja

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Krasalakton D je prirodni citotoksični spiro-lakton.[1] U ovom radu želimo da saopštimo sintezu jedanaest novih halogenovanih (I, Cl, Br) derivata krasalaktona D primenom reakcija haloeterifikacije na goniobutenolide A (**1**), B (**2**) i njihove 7-epimere **5** i **6**, ranije sintetizovane u našoj laboratoriji.[2] Ispitvana je *in vitro* antiproliferativna aktivnost **3a–d**, **4a–b**, **3a–c** i **4a–b** prema humanim tumorskim ćelijama. Detaljno će biti diskutovan uticaj novouvedenih atoma halogena na antitumorsku aktivnost analoga.

Halogenated crassalactone D derivatives as potential antitumour agents: synthesis and SAR study

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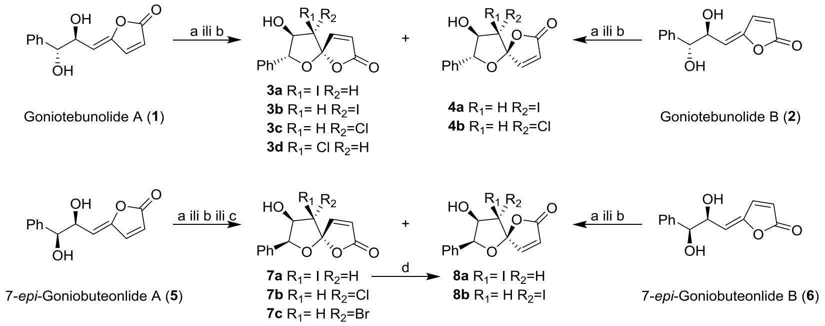
Crassalactone D is a naturally occurring cytotoxic spirolactone.[1] Herein we want to report synthesis of eleven novel halogenated (I, Cl, Br) crassalactone D derivatives by haloetherification of goniobutenolides A (**1**), B (**2**) and their 7-epimers **5** and **6**, that are previously synthesized in our laboratory.[2] *In vitro* antiproliferative activities of **3a–d**, **4a–b**, **3a–c** and **4a–b** against a number of human tumour cell lines were recorded. The influence of newly-introduced halogen atoms on antitumour activity will be presented and discussed in details.



Scheme 1. *(a) I_2, $NaHCO_3$, anh. CH_3CN, 21% (3a), 8% (3b), 29% (4a) from 1; 27% (3a), 10% (3b), 14% (4a) from 2, 40% (7a), 9% (8b) from 5; 51% (7a), 3 % (8b) from 6. (b) NCS, anh. DMF, 40% (3c) from 1; 17% (3d), 20% (4b) from 2; 13% (7b) from 5; 17% (7b) from 6. (c) NBS, anh. DMF, atm. N_2, 29% (7c). (d) TFA, $CHCl_3/H_2O$, 42% (8a), 43% (7a).*

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

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OH P 17

Fluorne izostere goniofufurona: sinteza i biološka aktivnost

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Jedna od često primenljivanih metoda za dizajn novih lekova je izosterna zamena OH grupe sa atomom halogena. U ovom radu želimo da saopštimo primenu ove metode za dizajn fluornih izostera goniofufurona (**1**-**4**), dobijenih višefaznom sekvencom prikazanom na reakcionoj shemi. Analozima je ispitana *in vitro* citotoksičnost na nekoliko malignih ćelijskih linija, kao i na jednu zdravu ćelijsku liniju (fetalni fibroblasti pluća, MRC-5).

Fluorine isosteres of goniofufurone: synthesis and biological activity

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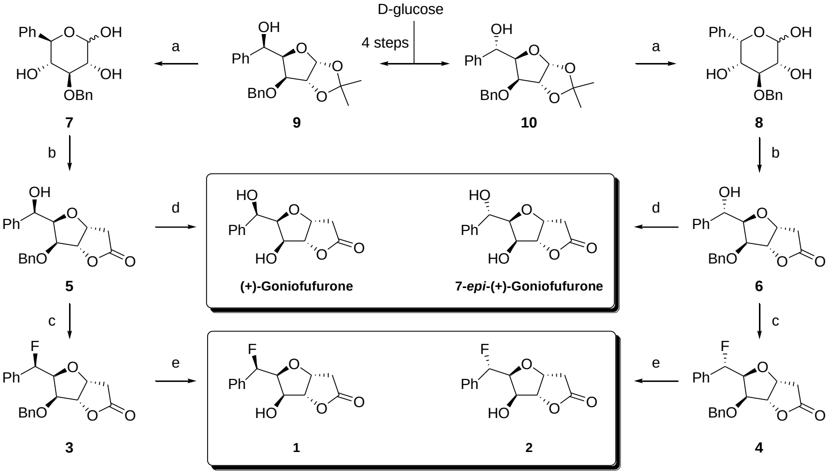
The isosteric replacement of an OH group with a halogen atom is widely used in the design of new drugs. Herein we want to report the implementation of this method for design of fluorine isosteres of goniofufurone (**1**-**4**), trough a multi-step sequence outlined in reaction scheme. The analogues were evaluated for their *in vitro* citotoxicity against several human tumour cell lines, as well as against normal foetal lung fibroblasts (MRC-5).



Reagents and conditions: (a) 90% aq TFA, rt, 40 min, 88% of 7; 30 min, 83% of 8;
(b) Meldrum's acid, Et3N, DMF, 46 °C, 65 h, 51% of 5; 70 h, 48% of 6; (c) DAST, CH2Cl2,
0 °C→rt, 4 h, 63% of 3, 12% of 4 (from 5); 3 h, 76% of 4, 24% of 3 (from 6);
(d) H2-Pd/C, MeOH, rt, 7.5 h, 69% of goniofufurone; 49 h, 84% of 7-epi-goniofufurone;
(e) H2-Pd/C, EtOAc+1% of conc. HCl, rt, 30 h, 70% of 1; 21 h, 79% of 2.

The work was supported by the Ministry of Education of the Republic of Serbia (Project No. 172006)

OH P 18

Hemijski sastav isparljivih komponenti korena *Chaerophyllum aureum* L.

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Rod *Chaerophyllum* L. (Apiaceae) je taksonomski složen rod koji obuhvata oko 40 vrsta rasprostranjenih u Evropi, Aziji i Severnoj Americi. Cilj ovog istraživanja bio je određivanje hemijskog sastava etarskog ulja i lako isparljivih komponenti korena *Chaerophyllum aureum* dobijenih "head space" (HS) tehnikom. Biljni materijal je prikupljen na Vlasinskom jezeru (Srbija) u toku jula meseca 2013. godine. Uzorci su analizirani na 7890/7000B GC/MS/MS tripl kvadropol uređaju u skanirajućem MS1 modu (Agilent Technologies, USA) koji je opremljen Combi PAL injektorom i Headspace sistemom G6501B/G6509B. U etarskom ulju je identifikovano 46 komponenti, što predstavlja 93.7% ulja dok 10 identifikovanih komponenti dobijenih HS tehnikom čini 97.6% ukupnog sadržaja isparljivih jedinjenja. Kao glavne komponente etarskog ulja korena identifikovana su monoterpenoidna jedinjenja: limonen (9.1%), sabinen (8.6%) i terpinen-4-ol (7.1%). *p*-Cimen (45.2%), α-pinen (21.1%) i mircen (14.5%) čine preko 80% lako isparljivih komponenti korena.

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Chemical composition of *Chaerophyllum aureum* L. root volatiles

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The genus *Chaerophyllum* L. (Apiaceae) is taxonomically complex genus and comprises about 40 species which occur commonly throughout Europe, Asia and North America. The present study reports the chemical composition of essential oil and HS volatiles isolated from the root of *Chaerophyllum aureum*. The plant material was collected on Vlasina plateau (Serbia), in July 2013. The samples were analyzed by a 7890/7000B GC/MS/MS triple quadrupole system in MS1 scan mode (Agilent Technologies, USA) equipped with a Combi PAL sampler and Headspace for G6501B/G6509B. For hydrodistilled oil, 46 components were identified representing 93.7% of the total, while 10 identified components, representing 97.6% of total HS root volatiles. The root essential oil showed the dominant presence of monoterpenoids with limonene (9.1%), sabinene (8.6%) and terpinen-4-ol (7.1%) as major constituents. *p*-Cymene (45.2%), accompanied by α-pinene (21.1%) and myrcene (14.5%), make up over 80% of the root HS volatiles.

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OH P 19

Sinteza novih tiepinskih derivata

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Jedinjenja koja sadrže tiepinski prsten, mogu pokazati značajnu biološku aktivnost. Nedavno, razvili smo novu metodologiju za sintezu tiepinskog prstena, građenjem dve C-S veze, uz korišćenje kalijum-tioacetata kao izvora sumpora i *tris*(*dibenziliden-aceton*)dipaladijumakao katalizatora.[1] U nastavku isrtaživanja, polazeći iz odgovarajućih *Z*-stilbena, optimizovani reakcioni uslovi primenjeni su u sintezi novih tiepinskih derivata. Takođe, pokazali smo da se novosintetisani derivati mogu dalje transformisati primenom jednostavnih sintetičkih metoda.

Synthesis of new thiepine derivatives

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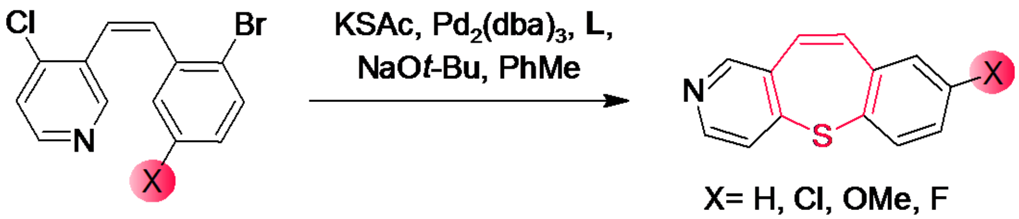
Thiepines, seven-membered heterocyclic rings containing sulfur, are known to showsignificant pharmaceutical activity. Recently, we have developed a simple and efficient palladium-catalyzed method for the synthesis of thiepine core.[1] In this work, under optimized reaction conditions, *Z*-stilbeneswere subjected to coupling reactions to obtain corresponding thiepines. Additional experiments were conducted to explore possibilities for further transformations of newly synthesized thiepines.



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OH P 20

Biblioteka 4-alkilamino-3-nitrokumarina sa jakom antimikrobnom aktivnošću protiv gastrointestinalnih patogena

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Biblioteka derivata kumarina koja se sastoji od devet novih 4-alkilamino-3-nitrokumarina je sintetisana sa ciljem da pruži dodatni uvid u antimikrobni potencijal kumarinskih jedinjenja. Antimikrobna aktivnost sintetisanih jedinjenja je određena za ukupno 24 soja, među kojima i za laboratorijske kontrolne sojeve i rezistentne (gastrointestinalni izolati) bakterijske i fungalne patogene. Sva sintetisana jedinjenja su pokazala određeni stepen selektivne aktivnosti, koja je u nekim slučajevima bila veoma izražena, dostižući vrednost minimalne inhibitorne koncentracije od 0,04 nmol/ml (12 ng/ml) protiv gljivice *Candida albicans*. Radi lakšeg povezivanja strukture i aktivnosti urađena je multivarijantna statistička analiza podataka dobijenih u ovom radu i onih iz prethodnih studija antimikrobne aktivnosti strukturno sličnih kumarina.

A library of 4-alkylamino-3-nitro-coumarin derivatives with potent antimicrobial activity against gastrointestinal pathogens

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A library of nine new 4-alkylamino-3-nitro-coumarins was designed and synthesized with an aim to provide further insight into the already established antimicrobial potential of coumarin derivatives. The antimicrobial activity of the library compounds was evaluated against a panel of in total 24 laboratory strains and resistant (gastrointestinal isolates) bacterial and fungal pathogens. All compounds showed some degree of selective activity that was very pronounced in some cases reaching the value of 0.04 nmol/ml (i.e. 12 ng/ml) for the minimal inhibitory concentration against *Candida albicans*. Finally, a multivariate statistical analysis of the herein obtained and previous results on the antimicrobial activity of related selected coumarins was performed to allow an easier structure-activity discussion.

Acknowledgment. *Authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172061, and 45022) for the financial support of this work.*

OH P 21

Pirolitička GC-MS analiza 4-arilamino-3-nitrokumarina sa različitim aril supstituentima

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Prilikom GC-MS analize 4-arilamino-3-nitrokumarina, sa različitim elektron-donorskim i electron-akceptorskim grupama na aril supstituentu, dolazi do izražene termalne degradacije ovih jedinjenja. Retencione osobine i maseni spektri glavnih proizvoda pirolize (dva po polaznom kumarinu) ukazuju da degradacioni proizvodi nastaju gubitkom fragmenata jednake mase, uz analogne promene retencionih vremena. Relativne količine nastalih proizvoda pirolize i pomenute spektralne karakteristike sugerišu da termalna degradacija ispitivanih jedinjenja pod datim uslovima nije vezana za aril suptituente, već se dešava na kumarinskom jezgru molekula.

Pyrolytic GC–MS analysis of 4-arylamino-3-nitrocoumarin derivatives with differing aryl side groups

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GC-MS analysis of 4-arylamino-3-nitrocoumarins, with different electron-donor and electron-acceptor substituents on the aryl side group, is accompanied with extensive thermal degradation of these compounds. GC retention features and the mass spectra of the corresponding major degradation products (two per coumarin derivative) indicate that these degradation products are formed by the loss of the same chemical species and have a constant difference in retention times. Based on the relative abundances of the products and on the mentioned spectral characteristics, the degradation of the studied compounds does not include the substituent of the arylamino moiety but it should be linked to the coumarin core.

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OH P 22

Dizajn i sinteza malih molekula kao inhibitora botulinum neurotoksina tipa A

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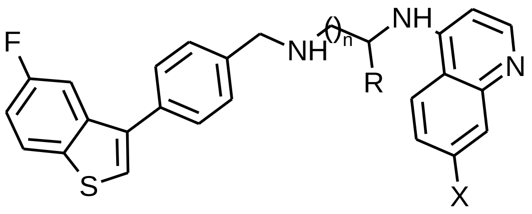
Botulinum neurotoksini su najjači biološki toksini i poznati su kao agensi najvišeg prioriteta u bioterorizmu. Zbog toga su načinjeni značajni napori kako bi se razvili mali molekuli, inhibitori, za tretman i prevenciju botulizma. Ovde je opisana sinteza novih malih molekula, koji pokazuju značajan procenat *in vitro* inhibicije BoNT/A. Polazeći od komercijalno dostupnih jedinjenja, sintetisano je nekoliko derivata benzotiofena, koji pokazuju inhibitornu aktivnost oko 30-40%, pri niskoj µM koncentraciji. Ispitan je uticaj malih strukturnih izmena na aktivnost, pri čemu je molekulsko modelovanje bilo od velike pomoći i dalo nam korisne smernice u sintezi. Promena supstituenta na aminohinolinskom delu strukture, u kombinaciji sa menjanjem dužine linkera, rezultovala je otkriću derivata koji poseduju značajno višu aktivnost, >50%.



X: H, Cl
R: H, Me
n = 2-5

BoNT/A LC % inhibicije: 56,37 (20 mM)

Design and synthesis of small molecules as inhibitors of botulinum neurotoxin type A

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Botulinum neurotoxins are the most potent of the biological toxins, and are listed as highest priority bioterror agents. Thus, substantial efforts have been made to develop small molecule inhibitors for the treatement and prevention of botulism. Herein we describe the synthesis of new small molecules, which show quite good *in vitro* inhibitory potency against BoNT/A light chain. In few steps, starting from commercially available compounds, we synthesized benzothiophene derivatives, with inhibitory activity around 30-40%, which are effective in the low µM range. That’s why we examined how some small modifications in structure affect inhibitory efficiency. Molecular modeling was very helpful tool that gave us a good guidance. Changing substituents on aminoquinoline moiety, combined with different length of the linker, provided derivatives possessing significantly higher activity, >50%.

Acknowledgement: This research was supported by the Ministry of Education, Science and Technology Development of Serbia (grant no. 172008) and National Institute of Health, (1U01AI082051-01).

OH P 23

Reakcije enonskog sistema kod O-alkilovanih dehidrozingerona sa hidrazinom

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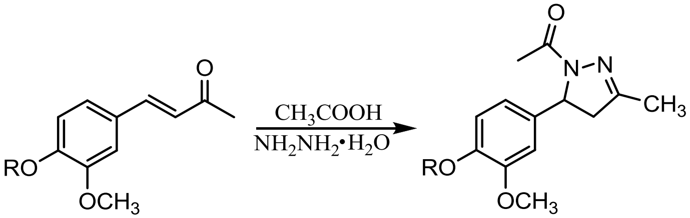
Dehidrozingeron i njegovi derivati pokazuju različite aktivnosti (antimikrobna, antiinflamatorna, antikancerogena, antioksidantna,...). Enonski sistem je vrlo pogodan za transformacije različitim reagensima. Ovde je opisana reakcija O-alkilovanih dehidrozingerona sa hidrazinom u ključaloj sirćetnoj kiselini. Dobijena je serija 1-(5-(4-alkoksi-3-metoksifenil)-3-metil-4,5-dihidro-1H-pirazol-1-il)etanona.



R=Me, Et, Pr, *i*-Pr, Bu

Rad je finansiran sredstvima Ministarstva prosvete i nauke u okviru projekta OI 172034

Reaction at enone systems of O-alkylated dehydrozingerones with hydrazine

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Dehydrozingerone and their derivatives exhibit various activities (antimicrobial, antiinflammatory, anticancer, antioxidant, ...). Their enone system is very suitable for the transformation with various reagents. Here is described the reaction of O-alkylated dehydrozingerones with hydrazine in boiling acetic acid. The series of 1-(5-(4-hydroxy-3-methoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazol-1-yl)ethanones were obtained.

This work has been supported by Serbian Ministry of Education and Science, grant 172034

OH P 24

Sinteza novih 1,4-dihidropirimidina bez prisustva rastvarača

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3,4-Dihidropirimidin-2-(1*H*)-oni (DHPM-i) i njihovi sumporni analozi predstavljaju klasu heterocikličnih molekula koji su privukli veliko interesovanje medicinske hemije[1]. Uprkos činjenici da DHPM derivati imaju širok spektar bioloških aktivnosti poznato je samo nekoliko metoda za sintezu 1,4-dihidropirimidina preko C-2 funkcionalizacije DHPM-a. Zbog toga, mi predstavljamo brzu metodu bez upotrebe rastvarača za C-2 funkcionalizaciju DHPM-a pri sintezi različitih 1,4-dihidropirimidina (2a-d). Sintezu 1,4-dihidropirimidina izvršili smo homogenizacijom različitih DHPM-a (1a-d), fenacil-bromida i baze u avanu na sobnoj temperaturi (Šema 1).

Synthesis of novel 1,4-dihydropyrimidines under solvent-free conditions

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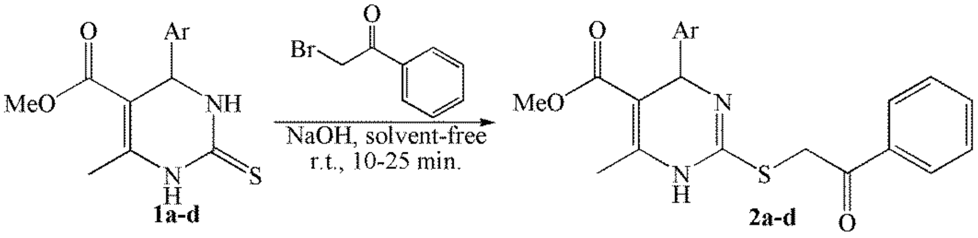
3,4-Dihydropyrimidin-2(1*H*)-ones (DHPMs) and their sulfur analogs, which represent a class of heterocyclic molecules, have attracted a considerable interest in medicinal chemisty[1]. Despite the fact that DHPM derivatives have a wide range of biologically activities, there are only few know methods for the synthesis of the 1,4-dihydropyrimidines through the C-2 position funcionalization of the DHPM[2]. In the light of this, we presented a fast solvent-free method for C-2 functionalization of DHPM for synthesis of different 1,4-dihydropyrimidines (2a-d). Synthesis of the 1,4-dihydropyrimidines was performed by homogenization of different DHPMs (1a-d), phenacyl-bromide and base in mortar at room temperature (Scheme 1).



Ar= 2'-furyl **(a)**, benzylidene **(b)**, 3'-nitrophenyl **(c)**, phenyl **(d)**

Scheme 1. Solvent-free synthesis of the 1,4-dihydropyrimidines

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

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OH P 25

Sinteza i ispitivanje biološke aktivnosti novih aminokiselinskih derivata avarona

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U ovom radu je prikazana sinteza i biološka aktivnost deset novih aminokiselinskih derivata seskviterpenskog hinona avarona. Ispitivana je antimikrobna aktivnost svih jedinjenja prema Gram-pozitivnim i Gram-negativnim bakterijama kao i aktivnost na kulture gljiva. Antitumorska aktivnost ispitivanih jedinjenja je određena MTT testom prema pet humanih tumorskih linija (HeLa, A549, FemX, K562, MDA-MB-453) i jedne humane netumorske ćelijske linije (MRC-5). Sintetisanim jedinjenjima je ispitana toksičnost na račiće *Artemia salina*.

Autori su zahvalni Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije na finansijskoj podršci (Projekt 172055).

Synthesis and biological activity investigation of new amino acid avarone derivatives

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In this paper, synthesis and biological activity of ten new amino acid derivatives of sesquiterpene quinone avarone is reported. Antimicrobial activity of all the compounds was investigated against Gram-positive and Gram-negative bacteria and against fungi cultures. Antitumor activity of investigated compounds towards five human cancer cell lines (HeLa, A549, FemX, K562, MDA-MB-453) and a non-cancerous human cell line (MRC-5), was determined by MTT assay. For all synthesized compounds toxicity against *Artemia salina* nauplii was determined by brine shrimp assay.

The authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia for financial support (Project No. 172055).

Nastavna sekcija / Chemistry Education

NS O 01

Muzej hemije – doprinos hemijskoj pismenosti

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Hemijska pismenost je glavni ishod hemijskog obrazovanja. Istorija hemije je sastavni deo te pismenosti. Zbog toga je važno da se kroz učenje hemije sagleda i njen istorijski razvoj. Prema kurikulumima redovne nastave hemije, na svim nivoima obrazovanja, nije predviđeno dovoljno prostora i vremena za ovaj aspekt hemije, ali se on može sagledati kroz posete muzejima nauke. Posete se mogu realizovati u okviru slobodnih aktivnosti koje su planirane nastavnim programima. Srbija je jedna od zemalja koja u okviru Muzeja nauke i tehnike ima i Muzej hemije (Zbirku velikana srpske hemije). U okviru istraživanja čiji je predmet povezivanje hemije sa drugim naukama, a jedan od ciljeva upoznavanje sa hemijskom baštinom, od marta 2012. godine organizuju se grupne učeničke posete Zbirci velikana srpske hemije. Posete vode studenti završnih godina Hemijskog fakulteta Univerziteta u Beogradu. Nakon posete koja traje 60 minuta, učenici pojedinačno i anonimno popunjavaju anketu u kojoj iznose svoje stavove i mišljenja o poseti. U ovom radu prikazani su stavovi i mišljenja 600 anketiranih učenika iz različitih škola sa teritorije Srbije. Rezultati ankete pokazuju da se kroz saznanja o nasleđu srpske hemije može uticati na saznajni, emotivni i socijalni razvoj učenika.

Museum of Chemistry - contribution of chemical literacy

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The main outcome of chemical education is chemical literacy. History of Chemistry is an integral part of the chemical literacy. Therefore it is important to percive the teaching of Chemistry through historical development of Chemistry. According to regular chemistry curriculum at all levels of education not provided enough space and time to this aspect of Chemistry, but it can be carried through a visit to the Museum of Science. Visits may be carried out under the extracurricular activities that are predicted in the curriculum of Chemistry. Serbia is one of the countries which have Museum of Chemistry (The Great Serbian Chemists' Collection) within the Musem of Science and Technics. Within the research which subject is connecting Chemistry with other sciences, and one of the aims is introducing the chemical heritage, the group students visits to the Great Serbian Chemists' Collection were organizing since March 2012. Museum group tours have been led by senior university students of the Faculty of Chemistry. After the visit, which lasts 60 minutes, the students individually and anonymously fill out a survey in which present their views and opinions on the visit. In this paper, we present views and opinions of 600 surveyed students from different schools in Serbia. The survey results show that the knowledge about the legacy of Serbian chemistry can affect cognitive, emotional and social development of students.

This report is an outcome of participation in the project „Theory and Practice of Science in Society: Multidisciplinary, Educational and Intergenerational Perspectives“, No. 179048, financed by the Ministry of Education, Science and Tehnological Development of the Republic of Serbia.

Tekstilno inženjerstvo / Textile Engineering

TI P 01

Uticaj perjodatne oksidacije na kapilarnost i parametre kvašenja viskozne pređe

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U ovom radu proučavan je uticaj oksidacije natrijum-perjodatom na kapilarnost viskozne pređe. S obzirom da se perjodatnom oksidacijom uvode aldehidne grupe u celulozu, promene u kapilarnosti i parametrima kvašenja viskozne pređe nakon oksidacije su očekivane. Kapilarnost je merena očitavanjem visine tečnosti na viskoznoj pređi uronjenoj jednim krajem u 0,1% rastvor eozina. Rezultati merenja kapilarnosti, visina tečnosti (h) i vreme penjanja (t), mogu poslužiti za izračunavanje parametara kvašenja: koeficijenta difuzije D (mm^2/s), koeficijenta radijusa pora C (mm/s) i koeficijenta R (odnos između ugla kvašenja pri određenoj visini tečnosti (h) i ugla kvašenja pri maksimalnoj (ravnotežnoj) visini (h_{eq})). Najveće vrednosti h_{eq}, D i R su izračunate za uzorak tretiran 0,2 % $NaIO_4$ tokom 45 min. Najmanja vrednost h_{eq} nađena je kod uzoraka tretiranih 0,2 % i 0,4 % $NaIO_4$ tokom 360 min, što je očekivano obzirom da je kod ovih uzoraka uvedena i najveća količina aldehidnih grupa oksidacijom. Kod ovih uzoraka je zabeležen i porast koeficijenata C i D, u odnosu na netretirani uzorak, što znači da je tokom oksidacije uvedena ne samo značajna količina aldehidnih grupa, već je morfologija uzoraka izmenjena, u smislu povećanog radijusa pora.

Zahvalnost: Ovaj rad je proistekao iz rada na projektu koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije (projekat OI 172029).

Influence of periodate oxidation onto capillarity and wettability parameteres of viscose yarn

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In this paper, influence of oxidation with sodium periodate onto capillarity of viscose yarn was studied. Considering that during oxidation aldehyde groups are introduced into cellulose, changes in capillarity and wettability parameters due to oxidation are expected. Capillarity was measured by reading of liquid height on viscose yarn dipped with one end into 0.1% solution of eosin. Results of capillarity measurements, height of liquid (h) and time of ascent (t), can serve for calculation of wettability parameters: diffusion coefficient D (mm^2/s), coefficient related to pore radius C (mm/s) and coefficient R (ratio of wetting angle at height (h) and wetting angle at the maximum (equilibrium) height (h_{eq})). The highest values h_{eq}, D and R are calculated for sample treated using 0.2 % $NaIO_4$ for 45 min. The lowest value h_{eq} was found in samples treated with 0.2 % and 0.4 % $NaIO_4$ for 360 min which was expected since under these oxidation conditions, the highest amount of aldehyde groups was introduced. Increase of coefficients C and D was also found in these samples compared with untreated sample, which means that during oxidation, not only significant amount of aldehyde groups was introduced, but morphology of samples was also affected, in terms of increased pore radius.

2. KONFERENCIJA MLADIH HEMIČARA SRBIJE

2nd Conference of the Young Chemists of Serbia

KRATKI IZVODI

ABSTRACTS

Plenarna predavanja / Plenary Lectures

PP 1

Bakterijska ćelija – dizajnirani biokatalizator

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Biokataliza u kojoj se koriste čitave bakterijske ćelije je pristup koji se pokazao kao jako važan i primenljiv za sintezu velikog broja vrednih jedinjenja.[1] Danas se ovaj pristup kreće ka sve kompleksnijem dizajnu rekombinantnih bakterijskih ćelijskih sistema koji obuhvataju heterologne pojedinačne enzime i čitave biosintetske puteve koji omogućavaju biokatalizu u više sintetskih koraka. Kako bi se dizajnirao produktivan bioproces baziran na čitavim bakterijskim ćelijama kao katalizatorima, moraju se sistematično i detaljno razmotriti svi biosintetski procesi koji se u tim ćelijama odvijaju.[2]

Koncepti koji su primenljivi u čitavim bakterijskim ćelijama kreću se od iskorišćavanja puteva već prisutnih u samim bakterijama, njihovog racionalnog inženjeringa i proširivanja kroz dodavanje rekombinantnih (jednog ili više) enzima. Ovi generalni koncepti će biti uvedeni i prodiskutovani na nekoliko primera, uključujući inženjering bakterijske tirozinaze[3].

The microbial cell – 'designer' biocatalyst

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Whole–cell biocatalysis has emerged as a useful alternative to the use of pure enzymes and an important tool for the synthesis of a variety of valuable products. Today it moves towards the more complex design of recombinant cell factories comprising heterologous enzymes or pathways enabling multistep biocatalysis. In order to design productive bioprocesses based on whole microbial cells as catalysts, concurrent biological processes must be considered in detail.

Concepts applied for whole-cell biocatalysis range from the exploitation of native pathways, their engineering and extension to multistep biocatalysis based on a single heterologous enzyme or enzyme combinations. These general concepts will be introduced and discussed on the basis of several examples, including engineering of bacterial tyrosinase.

Acknowledgments. *Author is grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia Projects No 173048 for the financial support of this work.*

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PP 2

Jonske tečnosti – zeleni rastvarači budućnosti

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Do danas, najčešće su se hemijske reakcije proučavale u molekulskim rastvaračima. Skoro dva milenijuma,većina našeg razumevanja hemije zasnovana je na ponašanju organskih i neorganskih jedinjenja u rastvorima molekulskih rastvarača. Međutim, nedavno je pronađena nova klasa rastvarača – jonske tečnosti. Ovi rastvarači su tečni na sobnoj temperaturi i sastoje se samo od jona. Jonske tečnosti imaju mnoge jedinstvene osobine koje su od fundamentalnog značaja za hemičare. Jedna od njihovih najvažnijih osobina je gotovo zanemarljiv napon pare i za razliku od konvencionalnih organskih rastvarača ne isparavaju. Zbog toga su, sasvim opravdano, privukle pažnju za “zelene” sinteze. Jonske tečnosti su označene i kao dizajnirani rastvarači, a to znači da se njihova svojstva mogu prilagoditi zahtevima određenog procesa. Osobine kao što su tačka topljenja, viskoznost, gustina i hidrofobnost mogu se varirati jednostavnim promenama u strukturi jona. Zbog njihove niske toksičnosti, visoke provodljivosti i značajne elektrohemijske stabilnosti, jonske tečnosti se mogu koristiti kao zeleni rastvarači i kao zamena za isparljive organske rastvarače u brojnim industrijskim procesima.

Ionic liquids – green solvents for the future

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To date, most chemical reactions have been carried out in molecular solvents. For two millennia, most of our understanding of chemistry has been based upon the behavior of organic and inorganic compounds in the solution phase in molecular solvents. Recently, however, a new class of solvent has emerged – ionic liquids. These solvents are liquid at room temperature, and consist entirely of ionic species. Ionic liquids have many unique properties which make them of fundamental interest to all chemists. One of their most important characteristics is almost immeasurable vapor pressure, and hence can emit no volatile organic compounds (VOCs). Therefore, they have attracted enormous attention as media for green synthesis. Ionic liquids have been described as designed solvents, which means that their properties can be adjusted to suit the requirements of a particular process. Properties such as melting point, viscosity, density, and hydrophobicity can be varied by simple changes to the structure of the ions. Due to their low toxicity, high conductivity and a significant electrochemical stability, ionic liquids can be used as green solvents and as a replacement for volatile organic compounds in many industrial processes.

Predavanje po pozivu / Invited Lecture

PPP 1

Како презентовати и публиковати резултате научног истраживања

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Научни рад је написани извештај који садржи приказ резултета оригиналног научног рада. Његов формат је дефинисан вишевековном традицијом писања радова, уређивачком праксом издавача, научном етиком, усвојеним стандардима и захтевима савремене штампе и публиковања. Нажалост искуства издавача и уредника научних публикација говоре да велики број радова који се подносе за штампу не задовољавају минималне услове да буду чак и узети у разматрање. Упадљиво је да са правом експлозијом научних истраживања у целом свету, огромним бројем радова који се сваке године публикује, издавачи бивају преплављени лоше написаним, лоше технички припремљеним и по квалитету дискутабилним радовима. Очигледно је да многи аутори радова, нарочито они млађи, нису стекли знање о томе како треба да се напише и технички припреми ради.

Ово саопштење указује на најбитније принципе које треба имти у виду при креирању рукописа рада или при презентовању научних резултата.

Пре одлуке о публиковању резултата научног истраживања, две ствари се морају имати на уму: прва је да постоји јасна и логична поруку за читаоце, и друга, да се садржај презентује у одговарајућој, од стране издавача захтеваној форми.

Прва је, наравно, много важнија. Без обзира колико је приказ резултата пажљиво и лепо припремљен, ако нема шта важно и значајно да се саопшти, рад може бити одбијен. Зато и пре почетка писања рада или припреме резултата за приказивање, треба продискутовати резултате са другима који се баве истом или сличном облашћу истраживања, било у непосредној околини или ван ње.

How to present and publish results of scientific research

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The end of each research is to present its results to the public, especially to those who are engaged in similar research. This is particularly true for scientific research. Scientific paper is written report that contains a presentation of the results of the original scientific research. Its format is defined by centuries-old tradition of writing, the editorial practices of the publishers, scientific ethics, accepted standards and requirements of modern printing and publishing. Unfortunately, the experience of the publishers and editors of scientific books and journals show that a large number of submitted contributions are not meeting the minimum requirements to be even considered. This presentation indicates the most important principles that one should have in mind during creation of full text paper or presentation of scientific results.

Saopštenja / Contributions

Biohemija i biotehnologija[‡]

BB O 02

Sinteza i ispitivanje termofizičkih parametara biodizela dobijenog iz biootpada heterogenom tranesterifikacijom i karakterizacija katalizatora

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U korak sa svakodnevnim povećanjem zahteva za gorivom i njegovim ograničenim prirodnim nalazištima nametnula se potreba za pronalaženjem i implementiranjem održivih, ekonomičnih i obnovljivih goriva. Pogodno rešenje je uvođenje biogoriva u masovnu potrošnju, za čije uvođenje nije neophodno izvršiti izmene na postojećim dizel motorima. Poseban akcenat je stavljen na ekološki prihvatljive sirovine za dobijanje biogoriva i na zakonom regulisane količine biogoriva u tradicionalnoj vrsti dizel goriva. Ovim radom su istraživane mogućnosti sinteze biodizela iz otpada prehrambene industrije, tranesterifikacijom biljnog ulja i metanola, katalizovane heterogenim katalizatorom na bazi kalcijum oksida dobijenim kontrolisanim zagrevanjem sprašenih pilećih kostiju i ljuske kokošijeg jajeta. U cilju potvrde kvaliteta dobijenog biogoriva, ispitivani su njegovi termofizički parametri (gustina, viskoznost i indeks refrakcije) dok je karakterizacija katalizatora izvršena SEM i BET analizama.

Synthesis and examining thermo physical properties of biodiesel produced from waste materials with heterogeneous transesterification and catalyst characterization

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With limited natural fuel resources and expanding energy demands there is a request for finding and implementing sustainable, economical and renewable fuels. Adequate solution is bio fuel introduction in wholesale consumption, which does not necessitate require any changes in existing diesel motors. Environmentally friendly sources for biodiesel production and amount of biodiesel in diesel fuel required by law are main concerns. Possibilities for synthesis of biodiesel from industrial bio waste by transesterification of vegetable oil and methanol with heterogeneous calcium-oxide based catalyst, made from powdered chicken bones and eggshells under controlled heating were tested in this work. For the purpose of evaluation of a produced biodiesel quality, termophysical properties of biodiesel were investigated (density, viscosity and refractive index) while the structure of produced catalyst was determined with SEM and BET analysis.

Autor se zahvaljuje na odličnoj saradnji Katedre za hemiju, Fakulteta za nauku, Mahasarakam univerziteta u Tajlandu i Katedre za hemijsko inženjerstvo, Tehnološko-metalurškog fakulteta, Univerziteta u Beogradu, iz koje je proizašlo ovo istraživanje.

[‡] Postersko saopštenje u okviru 51. savetovanja SHD sa oznakom **BT P 04** - **Majklova adicija različitih aldehida na β-nitrostiren katalizovana rekombinantnim ćelijama koje eksprimiraju 4-oksalokrotonat tautomerazu**, autora *Jelena S. Radivojević, Predrag Jovanović, Tanja Narančić, Branka Vasiljević, Veselin Maslak, Jasmina Nikodinović Runić,* biće usmeno prezentovano u okviru **2. Konferencije MHS** sa oznakom **BB O 01.** Kratki izvod saopštenja nalazi se na stranici **71.**

BB O 03

Kloniranje i ekspresija celobiozo dehidrogenaze iz *Phanerochaete chrysosporium* kao himere sa modifikovanim zelenim fluorescentnim proteinom iz *Aequoera victoria*

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Celobiozo dehidrogenaza (CDH, EC 1.1.99.18) pripada grupi oksidoredukcionih enzima i ima sposobnost da degraduje različite komponente drvenastih biljaka, zbog čega je našao primenu u industrijskim i biotehnološkim procesima. Zeleni fluorescentni protein (GFP) poseduje hromoforu koja je izgrađena od 3 aminokiselinska ostatka čime se obezbeđuje ispoljavanje fluorescencije bez obzira na organizam u kom je eksprimiran. Nakon uspešnog kloniranja CDH gena u pCTCON2 vektor i ekspresije enzima na površini ćelije kvasca, kloniran je i eksprimiran GFP – CDH konstrukt u istom sistemu. Ekspresija CDH obezbeđuje razvoj *high througtput screening* metoda u dirigovanoj evoluciji ovog enzima, dok GFP – CDH konstrukt omogućava indirektno određivanje količine eksprimiranog CDH na osnovu fluorescencije GFP molekula pomoću FACS-a. Nakon optimizacije fermentacije, uočeno je da je najveća aktivnost dobijena u 30 satu nakon indukcije. Dobijena aktivnost za CDH iznosi 0,00452 U/mL, dok je konstrukt GFP – CDH imao aktivnost od 0,00369 U/mL. Uočeno smanjenje aktivnosti GFP – CDH konstrukta ukazuje na sternu zaklonjenost aktivnog mesta CDH.

Cloning and expression cellobioso dehydrogenase from *Phanerochaete chrysosporium* as himera with enhanced green fluorescent protein from *Aequoera victoria*

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Cellobiose dehydrogenase (CDH, EC 1.1.99.18) belongs to a group of oxidoreduction enzymes and have an ability to degrade differente components of woody plants, due to which has applications in industrial and biotechnological processes. Green fluorescent protein (GFP) has a chromophore, constructed of 3 amino acid residues which ensure the expression of fluorescence, regardless of the organism in which it is expressed. After the successful cloning of a CDH gene in pCTCON2 vector and expression of the enzyme on the surface of yeast cells, was cloned and expressed GFP – CDH construct in the same system. Expression of CDH provides development high throughput screening methods in the orchestrated evolution of the enzyme, while the GFP - CDH construct enables an indirect determination of the amount expressed CDH based on the fluorescence of GFP molecule using a FACS. After optimization of the fermentation, it was observed that the maximum activity obtained at 30 hours after induction. The resulting activity of the CDH is 0.00452 U/mL, while the GFP – CDH construct had an activity of 0.00369 U/mL. The observed reduction in activity GFP – CDH construct indicates steric shelter of active site CDH.

BB P 01

Molekularno kloniranje celobiozo dehidrogenaznog gena iz *Phanerochaete chrysosporium* i ekspresija u kvascu *Saccharomyces cerevisiae*

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Celobiozo dehidrogenazni (CDH) gen iz *Phanerochaete chryosporium* je kloniran u pYES2 vektor i eksprimiran u kvascu *S.cerevisiae* InvSc1. Ekspresija konstrukta je optimizovana i prečišćen je jonoizmenjivačkom hromatografijom i ultrafiltracijom. Prečišćeni CDH konstrukt je pokazao jednu široku traku na SDS elektroforezi u opsegu molekulskih masa od 110 do 130 kDa. Na nativnoj elektroforezi je dobijena traka visoke molekulske mase što odgovara traci na zimogramu. Vrednosti k_{cat} za CDH kostrukt je 0.34 s^{-1} i K_m vrednost za laktozu je 1.23 mM i celobiozu 0.029 mM. Optimum pH je između 4 i 4,5. Kinetičke osobine za CDH su niže od konstrukata dobijenih kloniranjem u *Pichia pastoris*. Ovim radom smo omogućili dalji rad u pravcu dirigovane evolucije ovog enzima.

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Molecular cloning of the cellobiose dehydrogenase gene from *Phanerochaete chrysosporium* and expression in yeast *Saccharomyces cerevisiae*

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The cellobiose dehydrogenase (CDH) gene from *Phanerochaete chrysosporium* has been cloned in pYES2 vector and expressed in yeast *S. cerevisiae* InvSc1. Expression of the construct was optimized and he was purifed by ion-exchange chromatography and ultrafiltration. The purified CDH construct showed a broad band on SDS-PAGE with an apparent molecular weight between 110 and 130 kDa. On native electrophoresis he showed band with high molecular weight corresponding to the activity bands on zymogram. k_{cat} values for CDH construct was 0.34 s^{-1} and the K_m values for lactose was 1.23 mM and for cellobiose 0.029 mM. pH optimum was between 4 and 4.5. Kinetic properties for CDH are lower than those obtained from CDH construct from *Pichia pastoris.* This project enabled further development of directed evolution of CDH enzyme.

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BB P 02

Efekat tretmana naftenskim kiselinama na antioksidativni status biljaka krastavca

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U ovom radu proučavan je uticaj tretmana različitim koncentracijama kalijum-naftenata (0,1 – 400 μmol/dm^3) na antioksidativni status biljaka krastavca (*Cucumis sativus* L.). Parmetri oksidativnog stresa određivani su na ekstraktima listova tretiranih biljaka. Mereni su sadržaj rastvorljivih proteina, sadržaj ukupnih fenola, lipidna peroksidacija (LP) i aktivnost nekoliko enzima antioksidantne zaštite: superoksid-dismutaze (SOD), katalaze (CAT), gvajakol-peroksidaze (GPx). Svi rezultati ukazuju da je antioksidativni sistem biljaka krastavca osetljiv na tretman kalijum-naftenatom. Aktivnost enzima antioksitantne zaštite i intenzitet LP značajno se povećala kod tretmana visokim koncentracijama kalijum-naftenata (100, 200, 400 μmol/dm^3). Biljke krastavca koje su tretirane najvećom koncentracijom kalijum-naftenata imale su značajno veću aktivnost SOD, CAT i GPx enzima (89, 20.1 i 775.1%), kao i intenzitet LP (49.6%) u poređenju sa biljkama kontrole. Suprotno tome, tretmani nižim koncentracijama (0,1 μmol/dm^3) delovali su stimulativno na biljke, što se ogleda u porastu sinteze ukupnih fenolnih jedinjenja (26.8%).
S obzirom na dvojni efekat naftenskih kiselina (stimulativan i inhibitoran) na antioksidantni sistem biljaka krastavca, dalja istraživanja na fiziološkom i biohemijskom nivou bi preciznije ukazala na tačan mehanizam delovanja ovih jedinjenja na metabolizam ove povrtarske kulture.

Effect of naphthenic acids treatment to antioxidative status of cucumber plants

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This work presents a study of the effect of different concentrations of potassium naphthenate (0,1 – 400 μmol/dm^3) on the antioxidative status of cucumber (*Cucumis sativus* L.) assessed on leaves of treated plants. The content of soluble proteins, total phenolic content, lipid peroxidation (LP) and activities of several antioxidant enzymes: superoxide dismutase (SOD), catalase (CAT), guaiacol peroxidase (GPx) were determined. All obtained results indicate that the antioxidative system of cucumber plants is sensitive to such a treatment. The activities of antioxidant enzymes and the intensity of lipid peroxidation were significantly higher when plants were treated with very high concentrations of potassium naphtenate (100, 200, 400 μmol/dm^3). Plants treated with the highest concentration of potassium naphtenate had enhanced SOD, CAT and GPx activity (89, 20.1 and 775.1%,), as well as LP intensity (49.6%) in comparison to control. On the other hand, lower naphthenate concentrations (0,1 μmol/dm^3) showed stimulatory effect on cucumber plants, which is presented through increase in total phenolic content (26.8%).
Due to such an effect of potassium naphthenate (stimulatory and inhibitory) on antioxidant system of cucumber plants, further research of physiology and biochemistry of treated plants could give exact explanation of these compounds impact on investigated vegetable crop.

BB P 03

Ekstrakti četiri kultivara soje kao potencijalni inhibitori biosinteze eikozanoida

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Soja (*Glycine Max*) je najistaknutiji predstavnik *Fabaceae* familije biljaka. U okviru rada ispitan je anti-inflamatorni potencijal ekstrakata herbi četiri kultivara soje (*Sava*, *Maksimus*, *Favorit* i *Galina),* uzgajanih na Institutu za ratarstvo i povrtarstvo u Novom Sadu. Ispitivanje je vršeno *ex vivo* metodom zasnovanom na određivanju inhibicije produkcije metabolita arahidonske kiseline, 12-HHT, TXB_2, PGE_2, $PGF_{2\alpha}$ i 12-HETE, u humanim trombocitima. Inflamacija je izazvana dodatkom Ca^{2+} i kalcijumove jonofore, a zatim su praćeni efekti različitih koncentracija biljnih ekstrakata. Koncentracija produkovanih eikozanoida određena je visoko selektivnom LC-MS/MS tehnikom. Aktivnost uzoraka je izražena kao koncentracija ekstrakta koja ispoljava 50% inhibicije produkcije odabranih metabolita arahidonske kiseline. Sojini ekstrakti pokazali su dobar inhibitorni potencijal sa niskim IC_{50} vrednostima (3,83-4,38 mg/ml za 12-HHT, 4,68-5,50 mg/ml za 12-HETE i 3,43-4,41 mg/ml za TXB_2). Samo za PGE_2 nije postignuta 50% inhibicija u datom opsegu koncentracija. Sposobnost ekstrakata da inhibira produkciju eikozanoida koji su uključeni u razvoj različitih oboljenja poput kancera, alergije i astme, ukazuje da se ove biljke mogu koristiti kao potentni fitofarmaceutici i komponente funkcionalne hrane.

Projekat osnovnih istraživanja Ministarstva prosvete i nauke Republike Srbije br. 172058

Four soy cultivars as potential inhibitors of eicosanoids biosynthesis

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Soy (*Glycine max*) is the most important representative of the *Fabaceae* plant family. Over the course of this paper, herb extracts of four different soy cultivars (*Sava*, *Maximus*, *Favorit* and *Galina),* grown on Novi Sad Institute of Field and Vegetable Crops, were investigated for potential anti-inflammatory activity. Evaluation was carried out using *ex vivo* method based on observation of inhibitory potential of examined extracts on production of arachidonic acid metabolites, 12-HHT, TXB_2, PGE_2, $PGF_{2\alpha}$ and 12-HETE, in human platelets. The inflammatory response was induced by Ca^{2+}/calcium ionophore, and the effect of various levels of plant extracts was evaluated. The concentration of selected eicosanoids was monitored by highly selective LC-MS/MS technique. Activity was expressed as extract concentration resulting in 50 % inhibition of metabolite production. All extracts showed significant activity with low IC_{50} values (3,83-4,38 mg/ml for 12-HHT, 4,68-5,50 mg/ml for 12-HETE and 3,43-4,41 mg/ml for TXB_2), while for PGE_2 50% of inhibition was not reached in the selected range of concentrations. Since these eicosanoids are involved in development of various diseases such as cancer, allergies and asthma, and soy cultivars are shown to act as inhibitors of their production, these plants can be used as potent phytopharmaceuticals, as well as components of functional foods.

Research grant from the Ministry of Education and Science, Republic of Serbia No. 172058

Hemijska analiza

HA P 01

Analiza devet vrsti mahovina iz Nacionalnog parka Mavrovo

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Mahovine pripadaju klasi Bryophytes, koja je druga najveća grupa biljnog carstva. Nalaze se u svim staništima gde je moguća fotosinteza. Njihov hemijski sastav se razlikuje u zavisnosti od vrste, životnog staništa i sezone i mogu da igraju značajnu ulogu kao indikatori zagađenja životne sredine. Analizirano je devet vrsti mahovina: *Ctenidium molluscum, Neckera menziesii, Rhytidiadelphus triquetrus, Syntrichia ruralis, Cirriphyllum crassinervium, Abietinella abietina, Anomodon viticulosus, Hylocomium splendens, Brachythecium salebrosum* koje su prikupljene u Nacionalnom parku Mavrovo, Makedonija. Određena je antioksidativna aktivnost, etanolnih i vodenih ekstrakata, primenom DPPH (2,2-difenil-1-pikrilhidrazil) eseja. Pored toga određen je sadržaj 21 metala (Al, As, Ca, Cd, Co, Cr, Cu, Fe, K, Mg, Mn, Mo, Na, Ni, P, Pb, S, Sb, Se, V, Zn) primenom ICP-OES metode. Cilj rada je kvantifikacija antioksidativnog potencijal dobijenih ekstrakta, kao i sadržaja metala u cilju određivanja bioidikatorskih sposobnosti ispitivanih vrsta.

Analysis of nine moss species from Nacional park Mavrovo

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Mosses belong to Bryophytes, which are the second largest group in the plant kingdom. Can be found in any habitat, where photosynthesis is possible. The chemical composition differs depending on species, growth environment and season and can play a significant role as indicators of environmental pollution. We analyzed nine species of mosses: *Ctenidium molluscum, Neckera menziesii, Rhytidiadelphus triquetrus, Syntrichia ruralis, Cirriphyllum crassinervium, Abietinella abietina, Anomodon viticulosus, Hylocomium splendens, Brachythecium salebrosum*, which were collected at Mavrovo National Park, Macedonia. Antioxidant activity of ethanol and water extract were determinated using DPPH (2,2-diphenyl-1-picrylhydrazyl) assay. Additionally, concentration of 21 metals (Al, As, Ca, Cd, Co, Cr, Cu, Fe, K, Mg, Mn, Mo, Na, Ni, P, Pb, S, Sb, Se, V, Zn) were determinated using ICP-OES method. Aim of this study was to quantify antioxidant potential obtained extracts and metal content with objective of getting bioindicator potential of examinated mosses species.

HA P 02

Sirup, džem i ekstrakti ploda vrste *Rosa canina* L. kao potencijalni izvori fenolnih jedinjenja

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Plod vrste *Rosa canina* L. (šipak) smatra se bogatim izvorom fenolnih jedinjenja i vitamina C. Šipak se koristi u obliku namirnica i napitaka kao što su čaj, marmelada, žele i džem, a takođe se od nedavno primenjuje i kao dijetetski suplement. Cilj prikazanih ispitivanja bilo je određivanja fenolnog profila vodenih i metanolnih ekstrakata svežeg ploda, kao i tradicionalno pripremljenog sirupa i džema. Ispitivano je prisustvo i kvantitativni sadržaj 45 odabranih fenolnih jedinjenja primenom LC-MS/MS tehnike. Indentifikovana su 22 fenolna jedinjenja, pri čemu je uočen sličan kvalitativni sastav ispitanih ekstrakata, dok se količina detektovanih jedinjenja razlikuje. Najzastupljenija jedinjenja predstavljaju prekursori u biosintezi tanina, klase fenolnih jedinjenja karakterističnih za rod *Rosa*. Hinska kiselina bila je dominantna u svim ekstraktima, a zatim slede kvercitrin u metanolnom i vodenom ekstraktu, galna kiselina u sirupu, dok su u džemu nakon hinske kiseline najzastupljeniji epikatehin i galna kiselina. Poredeći ispitivane ekstrakte, sirup se odlikuje najvećim sadržajem ispitanih fenolnih jedinjenja, dok džem ima najmanji sadržaj. Prikazani rezultati podržavaju upotrebu svežeg šipka, džema i sirupa kao hrane visokog nutritivnog kvaliteta i podržavaju dalja istraživanja.

Rad je finansiran od strane Ministarstva prosvete, nauke i tehnološkog razvoja RS (OI 172050)

Syrup, jam and extracts of *Rosa canina* L. fruits as a potential sources of phenolic compounds

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Rosa canina L. fruits (rose hips) are known as valuable source of phenolic compounds and vitamin C. Rose hips have also been used as food and drinks: tea, marmalades, jellies and jams, followed by recently use as a food supplement. Therefore, the aim of this study was to define phenolic profile of water and methanolic extracts of fresh fruits and traditionally made syrup and jam. The presence and content of 45 plant phenolics were studied using LC-MS/MS. Twenty two compounds were found, the qualitative composition of the examined extracts was similar, but the content of phenolics varied. The most abundant were precursors in biosynthesis of tannins, a class of phenolic compounds present in genus *Rosa*. Quinic acid was the most dominant in all extracts, followed by quercitrin in water and metanolic extracts, while galic acid followed epicatehin in syrup and jam. Among examined samples, the syrup was the richest in phenolics, whereas jam was the poorest. Presented results support traditional use of fresh fruits and rose hip products as a food with high nutritional benefits and encourage new studies in the future.

The Ministry of Education, Sciences and Technological Development RS (OI 172050) supported this research work

HA P 03

Određivanje sadržaja elemenata u uzorcima bebi kašica primenom ICP-OES spektrometrije

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U ovom radu je određen sadržaj 28 elemenata (esencijalnih i neesencijalnih) u uzorcima 25 bebi kašica domaćeg proizvođača. Odabrani uzorci su različite voćne kašice (jabuka, breskva, kruška, kajsija, banana, šljiva, brusnica, borovnica, višnja); kašice od povrća (spanać, grašak, šargarepa, kukuruz, krompir, brokoli, muskatna tikva) kao i mesne kašice (piletina, junetina, teletina, ćuretina) pripremljeni postupkom digestije azotnom kiselinom. Primenjena je savremena, brza i osetljiva emisiona spektrometrijska metoda sa induktivno spregnutom plazmom kao izvorom zračenja (ICP-OES). Dobijeni rezultati pokazuju da su u najvećem sadržaju prisutni K, Na, Ca i Mg dok As, Cd, Hg i Sn, čiju maksimalno dozvoljenu koncentraciju (MDK vrednost) propisuje Pravilnik o zdravstvenoj ispravnosti dijetetskih proizvoda Republike Srbije, nisu detektovani. Olovo je detektovano u svim uzorcima sa vrednostima ispod MDK. Dobijeni sadržaji statistički su obrađeni u cilju izvođenja korelacija između sadržaja elemenata i vrste bebi kašice.

Determination of elements' content in baby food using ICP-OES spectrophotometry

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In this paper, the content of 28 elements (essential and non-essential) in 25 samples of baby food by a domestic producer were determined. Selected samples of different fruit purees (apple, peach, pear, apricot, banana, plum, cranberry, blueberry, cherry); purees of vegetables (spinach, peas, carrots, corn, potatoes, broccoli, pumpkin muscatel) and meat baby purees (chicken, beef, veal, turkey) were prepared by the process of digestion with nitric acid. The modern, rapid and sensitive emission spectrometric tecnique with inductively coupled plasma as radiation source (ICP-OES) was applied. The results show that K, Na, Ca i Mg are present at the highest content while As, Cd, Hg and Sn, whose maximum allowed concentrations (MAC values) are prescribed by national legislation of Republic of Serbia (Regulation on the health safety of dietary products), were not detected. Lead was detected in all samples with valus below the MAC. The obtained results were statistically analyzed in order to determine the possible correlation between the content of elements and the types of baby food.

HA P 04

Langelier-ov indeks zasićenja vode za piće – studija slučaja

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Stabilnost vode je značajna osobina proizvedene vode za piće radi procene nepromenljivosti standardizovanog kvaliteta tokom transporta vodovodnim sistemom do slavine krajnjeg potrošača. U toku probnog rada, od maja 2011. godine do maja 2012. godine, fabrika vode „Gorina” Leskovac proizvela je vodu vrhunskog kvaliteta. Na osnovu kvantitativnih vrednosti Langelier-ovog indeksa zasićenja (LSI) analizirana je sklonost agresivnog karaktera ove vode za piće. Utvrđena vrednost u opsegu, -0.38<LSI<0.99, katakteriše finalnu vodu PPV „Gorina” Leskovac, kao vodu bez sklonosti ili neznatno karozivnu, čime se postavlja pitanje potrebe potencijalne korekcije. Konačan odgovor, predviđanje realne tendencije, daće izračunavanje vrednosti Ryzner-ovog indeksa stabilnosti (RSI), što je naredni korak istraživanja.

Langelier's saturation index of drinking water - a case study

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Water stability is very important characteristic of potable water production for the purpose of evaluation of constancy of standardized quality during the water transportation through water system to the faucet of a final user. During the trial operation, from May 2011 to May 2012, water factory „Gorina” Leskovac have produced high quality water. According to quantitative values of Langelier saturation index (LSI) tendency to aggressive character of this water has been analyzed. Determined value in range, -0.38<LSI<0.99, characterizes the final water of water treatment plant (WTP) „Gorina” Leskovac, as water with no tendency to or slightly corrosive, thus raising an issue for the need of potential correction. Final answer, predicted real tendencies, shall be given by calculation of value of Ryznar stability index (RSI), which is the next research step.

HA P 05

Uklanjanje smetnji koje potiču od jona gvožđa(III), "u liniji", pri određivanju bakra protočno injekcionom (FIA) metodom sa amperometrijskom detekcijom

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Određivanje bakra se zasniva na merenju signala cijanida na radnoj srebrnoj elektrodi, sa i bez prisustva bakra, na potencijalu 0,0 V *vs.* Ag/AgCl [1]. FIA sistem je opremljen sa dva ventila za ubrizgavanje, jedan se koristi za ubrizgavanje rastvora cijanida (reagensa), a drugi za ubrizgavanje uzorka (bakra). Kao nosač za cijanide je korišćen rastvor natrijum-hidroksida (0,02 mol/l), a za bakar je rastvor hlorovodonične kiseline (0,01 mol/l). U ovakvom FIA sistemu bakar gradi stabilne cijano komplekse. Sistem sadrži i gasno-difuzionu jedinicu kroz koju difunduje cijanovodonik. Ovo određivanje ometaju svi joni koji grade stabilne cijano komplekse i koji se, najčešće, uklanjaju prethodnom pripremom uzorka što produžava vreme analize. Integrisanjem kolone napunjene celulozom u FIA sistem, uticaj ometajućeg jona gvožđa je potpuno uklonjen. U radu je ispitivan uticaj različitih koncentracija gvožđa, kao i broj ubrizgavanja na stabilnost kolone.

On-line elmination of Fe(III) during determination of copper flow injection analysis (FIA) with amperometric detection

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Determination of copper was based on measuring of the cyanide signal, without and in the presence of copper on working silver electrode at 0,0 V *vs* Ag/AgCl [1]. FIA manifold was equipped with two injection valves, one for injection of cyanide solution (reagent) and another one for the sample injection (copper solution). The carrier for cyanide solution was sodium-hydroxide (0,02 mol/l), and the carrier for copper solution was hydrochloric acid (0,01 mol/l). In such system copper forms stable cyano complexes. The system is equipped with gas-diffusion unit which enables diffusion of hydrogen-cyanide. Copper determination in such system was interfered with ions which form stable cyano complexes, which were removed off-line, therefore increasing the analysis time. By integrating the column filled with cellulose interferences by iron were completely removed. The effect of concentration of iron (III) was investigated, as well as the number of injections on stability of the cotton filled column.

1. A. Lolić, T. Tripković, R. Baošić, S. Nikolić-Mandić, B. Stanimirović, *J. Serb. Chem. Soc.* **77(11)** (2012) 1641

HA P 06

Ispitivanje uticaja rastvarača na apsorpcione spektre odabranih arilazo-pirimidinskih boja

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Azo boje su jedinjenja sa širokim spektrom primene. Najčešće se koriste za bojenje različitih vrsta materijala, u medicini, organskoj sintezi i mnogim drugim granama industrije. U ovom radu ispitivan je uticaj rastvarača i supstituenata na apsorpcione spektre novosintetisanih aril-azo boja radi dobijanja informacija o njihovim solvatohromnim svojstvima, koje u većini slučajeva imaju veliki uticaj na aktivnost molekula. Snimljeni su apsorpcioni spektri novosintetisanih derivata 4-hidroksi-6-metil-5-(2-fenilhidrazono) pirimidin-2(5H)-tiona u osam različitih rastvarača u oblasti od 300-500 nm. Ispitivan je uticaj prirode rastvarača i supstituenta na apsorpcione spektre ovih jedinjenja. Uticaj rastvarača analiziran je na osnovu Katalanovog solvatohromnog modela. Priroda interakcija rastvorak-rastvarač tumačena je i analizom Hansenovih parametara korišćenih rastvarača primenom metode višestruke linearne korelacije solvatohromnih energija, predložene od strane Kamleta i Tafta.

Investigation of the solvent effects on the absorption spectra of some arylazo-pyrimidines dyes

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Azo dyes are compounds with a broad spectrum of applications. Commonly they are used for dyeing of different types of materials, in medicine, in organic synthesis, and in many other industries. The aim of this work was investigation of the influence of solvent and substituents on the absorption spectra of the newly synthesized aryl-azo dye in order to obtain information about their solvatochromic properties, which in the most cases have a major impact on the activity of the molecule. Absorption spectra of newly sinthesized derivatives of 4-hydroxy-6-methyl-5-(2-phenylhidrazone) pyrimidine-2(5H)-thione have been recorded in eight different solvents in the range 300-500 nm. The solvent effect was interpreted on the basis of Catalan solvatochromic models. The solute-solvent interactions were interpreted by analysis of Hansen parameters of used solvent applying the method of multiple linear correlation solvatohromnih energy, proposed by Kamlet and Taft.

HA P 07

Proučavanje solvatohromnih svojstava novosintetizovanih derivata uracila

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Fizičko-hemijska karakterizacija čini važan segment u proučavanju potencijalno biološki aktivnih derivata uracila. U ovom radu je ispitivana serija novosintetisanih derivata 6-fenil-iminometil-1H-uracila, primenom spektrofotometrijske metode. Apsorpcioni spektri ispitivanih jedinjenja snimljeni su u UV oblasti, u osam različitih rastvarača. U radu je tumačen uticaj prirode rastvarača na apsorpcione spektre ovih jedinjenja primenom Kamlet-Taftovog i Katalanovog solvatohromnog modela. Priroda interakcija rastvorak-rastvarač analizirana je i primenom metode višestruke linearne korelacije Hansenovih parametara korišćenih rastvarača sa apsorpcionim maksimumima ispitivanih derivata.

Studying of the solvatohromic properties of newly synthesized uracile derivatives

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Physicochemical characterization is an important segment in studying of potentially biologically active derivatives of uracil. In this worek a group of newly synthesized derivates of 6-phenil-iminomethyl-1H-uracile were investigated using spectrophotometric methods. Absorption spectra of tested derivates were recorded in the UV range in eight different solvents. In this work the effect of the solvent's nature on the absorption spectra of this compound was interpreted by applying two solvatochromic models: Kamlet-Taft and Catalan. The nature of the solute-solvent interaction was also analyzed using the method of multiple linear correlation of Hansen parameters of used solvents with absorption maximum of tested derivatives.

HA P 08

Fenolni profil metanolnog i vodenog ekstrakta suvog ploda *Rosa canina* L.

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Plod šipka (*Rosa canina* L.) je veoma poznat u narodnoj medicini, gde se, najviše kao čaj, koristi u terapiji infekcija, inflamatronih stanja, kao i antidiabetik i diuretik. Uprkos velikoj popularnosti u našoj tradicionalnoj medicini, postoji malo podataka o fenolnom profilu ove biljne vrste sa teritorije Srbije. S obzirom na to, cilj ovog rada bilo je određivanje fenolnog profila vodenog i metanolnog ekstrakta suvog ploda šipka vrste *R. canina*. iz Sajana. Primenom LC-MS/MS metode izvršena je kvalitativna i kvantitativna analiza 45 odabranih fenolnih komponenti u uzorcima, pri čemu je dokazano je prisustvo 20 fenolnih jedinjenja. Sadržaj fenolnih kiselina je sličan u oba ekstrakta, a najzastupljenije su protokatehinska i 2,5-dihidrokisbenzoeva kiseline. Suprotno tome, sadržaj flavonoida se između ekstrakata veoma razlikuje. U vodenom ekstraktu najzastupljeniji flavonoidi su kvercitrin, katehin i kvercetin. Metanolni ekstrakt je kako u kvantitativnom, tako i u kvalitativnom sastavu pokazao bogatiji sadržaj flavonoida, pri čemu su dominantno prisutni flavonoidi kvercitrin hiperozid i kvercetin-3-*O*-glukozid. Dobijeni rezlutati pokazuju da *R. canina* sadrži značajne količine biološki aktivnih fenolnih jedinjenja i ukazuju na potrebu za daljim ispitivanjima šipka, u cilju potvrde njegove primene u tradicionalnoj medicini i ishrani.

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Phenolic profile of methanolic and aquatic extracts of dry fruits of *Rosa canina* L.

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Rosa canina L. (rose hip) fruit is well known in folk medicine, where is mostly as a tea, used in the treatment of infections, inflammatory diseases, as well as diuretic and antidiabetic agent. Despite the huge popularity in traditional medicine, there is little data about the phenolic profile of this plant species from the territory of Serbia. Therefore the aim of this research was to characterise phenolic profil of methanolic and aquatic extracts of dry fruits of *R. canina* collected in Sajan. Using the LC-MS/MS method a qualitative and quantitative analysis of the 45 selected phenolic components in extracts was carried out, whereby it has been proved the presence of 20 phenolic compounds. The content of phenolic acid was similar in both extracts and the most frequent acids were protocatechuic and 2,5-dihidrobenzoic acid. On the other hand, the differences in the content of flavonoids between extracts were more noticeable. Most abundant flavonoids in the aqueous extract were quercitrin, catechin and quercetin. While the methanol extract showed richer flavonoid content in both quantitative and qualitative analysis, with dominant flavonoid compounds quercitrin, hyperoside and quercetin-3-*O*-glucosid. The obtained results indicate that *R. canina* L. contains significant amounts of bioactive phenolic compounds and suggest a need for further investigation, in order to confirm its use in traditional medicine and nutrition.

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HA P 09

Hemijski sastav acetonskog ekstrakta lišaja *Parmelia sulcata* Taylor

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Cilj ovog rada bio je određivanje hemijskog sastava acetonskog ekstrakta lišaja *Parmelia sulcata* Taylor i izolovanje njegovih glavnih komponenti. Ekstrakt je dobijen maceracijom acetonom. Tankoslojna hromatografija je koriščena za izbor eluenta i identifikaciju frakcija, hromatografija na koloni silika-gela za razdvajanje komponenata i hromatografija pod visokim pritiskom (HPLC) za identifikaciju i određivanje čistoće izolovanih jedinjenja.
Maceracijom je dobijen acetonski ekstrakt u prinosu od 3,3%. HPLC analiza je pokazala da se ekstrakt sastoji od salazinske kiseline (65,5%), atranorina (21,7%) i hloratranorina (6,5%) u odnosu 10:3:1. Hromatografijom na koloni izolovano je 162,9 mg salazinske kiseline (HPLC čistoće 89,2%) i 183,9 mg smeše atranorina i hloratranorina. Uzastopnom reekstrakcijom acetonskog ekstrakta benzenom i acetonom dobijeno je 290,8 mg salazinske kiseline HPLC čistoće 78,1%.
Dobijeni rezultati o sastavu acetonskog ekstrakta su u skladu sa prethodno objavljenim. Primenom sukcesivnih ekstrakcija suvog acetonskog ekstrakta, benzenom i acetonom, postignuto je izolovanje salazinske kiseline zadovoljavajuće čistoće uz znatne uštede u vremenu i materijalu u odnosu na hromatografiju na koloni.

Zahvalnica: Prezentovani rezultati su deo istraživanja u okviru projekta br. 172047 koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije.

Chemical composition of *Parmelia sulcata* Taylor acetone extract

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The aim of this study was to determine the chemical composition of acetone extract of lichen *Parmelia sulcata* Taylor and isolate its main components.
The extract was obtained by maceration with acetone. Thin layer chromatography was used for eluent selection and fractions collection. The components were separated by atmospheric pressure column chromatography. Identification and determination of the purity of isolated compaunds was performed by high pressure liquid chromatography (HPLC).
The yield of the acetone extract was 2.6%. HPLC analysis showed that the extract consists of salazinic acid (65.5%), atranorin (21.7%) and chloratranorin (6.5%), in the ratio 10:3:1. In this study 162.9 mg of salazinic acid (HPLC purity 89.2%) and 183.9 mg of the mixture of atranorin and chloratranorin were isolalated by chromatography on column. By successive re-extraction of acetone extract with benzene and acetone 290.8 mg of salazinic acid (HPLC purity 78.1%) was obtained.
The obtained results of chemical composition of the acetone extract are consistent with previously published data. Isolation of salazinic acid of satisfying purity was achived by successive extraction of dry acetone extract with benzen and aceton. The applied procedure enabled considerable savings in time and material in relation to the chromatography column.

HA P 10

Hemijski sastav acetonskog ekstrakta lišaja *Flavoparmelia caperata* (L.) Hale

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Lišajevi (*Lichenes*) su jedinstvena grupa živih organizama koji su sastavljeni od gljiva (mikobionti) i algi (fotobionti). Hemijska ispitivanja lišajeva su fokusirana pretežno na njihove sekundarne metabolite, jer sintetišu aromatična jedinjenja koja su karakteristična samo za njih, dok ih više biljke ne sintetišu.

Cilj ovog rada bio je određivanje hemijskog sastava acetonskog ekstrakta lišaja *Flavoparmelia caperata* (L.) Hale i izolovanje njegovih glavnih komponenti.

Ekstrakt je dobijen maceracijom acetonom. Tankoslojna hromatografija je korišćena za izbor eluenta i identifikaciju frakcija, hromatografija na koloni silika-gela za razdvajanje komponenata i hromatografija pod visokim pritiskom (HPLC) za identifikaciju i određivanje čistoće izolovanih jedinjenja.

Maceracijom dobijen je acetonski ekstrakt u prinosu od 2,6%. HPLC analiza je pokazala da se ekstrakt sastoji od protocetrarične kiseline (64,5%), usninske kiseline (23,8%) i atranorina (1,3%). Hromatografijom na koloni izolovano je 145,8 mg protocetrarične kiseline (HPLC čistoće 95,4%) i 80,4 mg usninske kiseline (HPLC čistoće 98,6%).

Dobijeni rezultati o sastavu acetonskog ekstrakta su u skladu sa prethodno objavljenim. Postepenom promenom polarnosti eluenta postignuto je dobro razdvajanje komponenti ispitivanog ekstrakta što je potvrđeno stepenom njihove čistoće.

Zahvalnica: Prezentovani rezultati su deo istraživanja u okviru projekta br. 172047 koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja Republike Srbije

Chemical composition of *Flavoparmelia caperata* (L.) Hale acetone extract

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Lichens (*Lichenes*) are a unique group of living organisms consisting of fungi (mycobiont) and algae (photobiont). Chemical analysis of lichens are mainly focused on their secondary metabolites which are unique to them and differs them from higher plants. The aim of this study was to determine the chemical composition of the acetone extract of the lichen *Flavoparmelia caperata* (L.) Hale and isolate its main components.

The extract was obtained by maceration with acetone. Thin-layer chromatography was used for eluent selection and fractions collection. The components were separated by atmospheric pressure column chromatography. Identification and determination of the purity of isolated compounds was performed by high pressure liquid chromatography (HPLC).

The yield of the acetone extract was 2.6%. HPLC analysis showed that the extract consists of protocetraric acid (64.5%), usnic acid (23.8%), and atranorin (1.3%). In this study protocetraric acid (158.7 mg, HPLC purity 95.4%) and usnic acid (80.4 mg, HPLC purity 98.6%) were isolated.

The obtained results of extract chemical composition are consistent with previously published data. Good separation of extract's components was achieved by gradual chromatography and that was confirmed by HPLC purity of isolated compounds.

HA P 11

Izolovanje i identifikacija alkaloida iz biljke *Sedum acre* L.

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Sedum acre L. je višegodišnja biljka iz porodice *Crassulaceae* koja sadrži veliku količinu alkaloida koji uzrokuju blago toksično dejstvo. Može se naći na prostorima Evrope, Severne Amerike i Novog Zelanda, a raste na peskovitim i stenovitim podlogama.
Svež i zamrznut uzorak biljke je usitnjen i izvršena je ekstrakcija metanolom u prisustvu hlorovodonične kiseline. Filtrat je uparen na vakuum uparivaču do određene zapremine. Nakon dodatka rastvora NaOH do pH 11, izvršena je ekstrakcija dihlormetanom. Dihlormetanski rastvor je osušen pomoću Na_2SO_4 i uparen na vakuum uparivaču do suva. Ostatak je rastvoren u dihlormetanu i analiziran pomoću gasne hromatografije-masene spektroskopije na HP-5MS koloni.
Analizom dobijenog hromatograma utvrđeno je prisustvo 13 piperidinskih alkaloida: 2-monosupstituisani sa alifatičnim (peletierin, sedridin, N-metilpeletierin, 1-(2-N-metilpiperidil)-propan-2-ol, (1-metilpiperidin-2-il)sirćetna kiselina) i aromatičnim bočnim nizom (norsedamin, alosedamin, sedamin); hidroksipiperidinski (3-hidroksialosedamin, 4-hidroksisedamin) i 2,6-disupstituisani alkaloidi (sedakrin, sedinin, sedinon). Najzastupljeniji alkaloidi su sedinon (37.1%), 3-hidroksialosedamin (13.3%) i (1-metilpiperidin-2-il)sirćetna kiselina (9.5%). Udeo ostalih alkaloida je manji od 5%.

Zahvalnica: Istraživanje je finansirano od strane Ministarstva prosvete, nauke i tehnološkog razvoja (projekat ON 172047).

Isolation and identification of alkaloids from plant *Sedum acre* L.

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Sedum acre L. is a perennial plant of the family *Crassulaceae* which contains high quantities of alkaloids making it slightly toxic. It can be found in Europe, North America and New Zealand and it grows on sandy and rocky soils.
Fresh and frozen plant material was homogenized and extracted with methanol in the presence of hidrochloric acid. The filtrate was concentrated in vacuo. After addition of NaOH to pH 11, the solution was extracted with dichloromethane. The organic layers were dried with Na_2SO_4 and evaporated in vacuo. The residue was dissolved in dichloromethane and analyzed with gas chromatography-mass spectrometry on HP-5MS column.
The analysis of the obtained chromatogram shows the presence of 13 piperidine alkaloids: 2-monosubstituted with aliphatic (pelletierine, sedridine, N-methylpelletierine, 1-(2-N-methylpiperidyl)-propan-2-ol, (1-methylpiperidin-2-yl)acetic acid) and aromatic side chain (norsedamine, allosedamine, sedamine), hydroxypiperidine (3-hydroxyallosedamine, 4-hydroxysedamine) and 2,6-disubstituted alkaloids (sedacrine, sedinine, sedinone). The major components are sedinone (37.1%), 3-hydroxyallosedamine (13.3%) and (1-methylpiperidin-2-yl)acetic acid (9.5%). The abundance of other identified alkaloids is less than 5%.

Acknowledgments: The research was supported by Ministry of Education, Science and Technological Development of Serbia (Project No. 172047).

Hemijska sinteza

HS P 01

Sinteza novih azepinskih derivata kao potencijalnih antibakterijskih agenasa

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Triciklično iminostilbensko jezgro ulazi u sastav značajnih biološki aktivnih jedinjenja, od kojih mnoga deluju na centralni nervni sistem. Nedavno je primenjena nova metodologija za formiranje azepinskog prstena u prisustvu paladijuma kao katalizatora, iz odgovarajućih *Z*-stilbena.[1] Koristeći ovaj postupak, sintetisali smo seriju piridobenzoazepina i dipiridoazepina, u cilju ispitivanja antibakterijske i antifugalne aktivnosti.

Synthesis of new azepine derivatives with potential antibacterial activity

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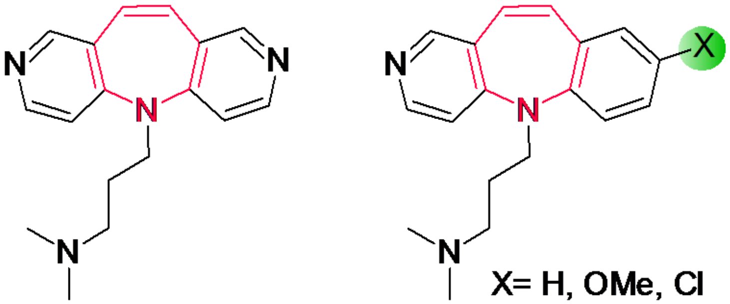
Iminostilbene (5H-dibenz[b,f]azepine) derivatives are important biologically active compounds, usually with the effects on central nervous system. Recently, new methodology for the synthesis of azepine ring was developed, using as a key step palladium-catalyzed amination–cyclization reaction.[1] Using this methodology, we have synthesized a series of pirydobenzazepine and dipirydoazepine derivatives in order to examine their antibacterial and antifungal activity.



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

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HS P 02

Nova metoda za sintezu acetala iz aldehida i ketona pomoću PPh_3-CCl_4

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Najčešće korišćena metoda za dobijanje acetala je reakcija aldehida ili ketona sa alkoholima, ali ona ima veliki broj nedostataka: nepovoljna termodinamika, prisustvo kiselog katalizatora i složena obrada reakcione smeše. Do sada je PPh_3 u kombinaciji sa CCl_4, kao reagens za dehidrataciju-hlorovanje, korišćen uspešno u supstitucionim reakcijama alkohola, reakcijama esterifikacije, građenja amida itd. U ovom radu ispitana je mogućnost primene PPh_3-CCl_4 u sintezi acetala iz aldehida/ketona i alkohola. U reakciji u kojoj je korišćen višak PPh_3 i alkohola, u odnosu na aromatični aldehid, u refluktujućem CCl_4, dobijen je željeni acetal i $OPPh_3$, ali i značajne količine odgovarajućih benzal-hlorida i 2,2-dihlorstirena. Varirani su odnosi reaktanata, kao i reakcioni uslovi (redosled dodavanja, temperatura i vreme refluktovanja), da bi se maksimalizovao prinos reakcije, a sporedni proizvodi sveli na minimum. Reakcija stehiometrijskih količina aldehida, alkohola i PPh_3 (1:2:1) je dala najbolje rezultate. U većini slučajeva reakcija je bila kvantitativna. Ovaj odnos reagenasa je omogućio da pored $OPPh_3$ i acetala u reakcionoj smeši nema drugih proizvoda. $OPPh_3$ je iz reakcione smeše u potpunosti uklanjan jednostavnim taloženjem pomoću hladnog pentana. Pod ovim reakcionim uslovima pripremljen je veći broj poznatih i novih acetala iz supstituisanih aromatičnih i alifatičnih aldehida i ketona. Svi proizvodi su potpuno spektralno (NMR, MS, UV, IR) okarakterisani. Pored kvantitativnosti i selektivnosti, pomoću ove reakcije je moguće, zbog neutralnih uslova odvijanja, pripremiti acetale aldehida i alkohola osetljivih na kiseline.

A new synthesis of acetals from aldehydes and ketones using PPh_3-CCl_4

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The most frequently utilized method for the preparation of acetals is the addition of alcohols to aldehydes or ketones, but it suffers from a number of shortcomings: bad thermodynamics, the presence of an acid catalyst and a complicated reaction workup. Up to now PPh_3 in combination with CCl_4 has been successfully used in the Appel reaction and for the preparation of esters and amides as a dehydrating-chlorinating agent. In this work we studied the possible use of PPh_3-CCl_4 reagent in the synthesis of acetals from carbonyl compounds and alcohols. When an excess of PPh_3 and an alcohol were used, in refluxing CCl_4, the aromatic aldehyde was converted to the target acetal along with benzal chloride and 2,2-dichlorostyrene. By varying the stoichiometric ratio of the reactants and reaction conditions (order of reagent addition, temperature and reaction time), the reaction yield was optimized while the side products were reduced to a minimum. The ratio 1:2:1 (aldehyde/alcohol/PPh_3) gave the best results, which was a quantitative conversion in most cases. This reagent ratio also resulted in reaction mixtures that besides $OPPh_3$ and the acetal contained no other products. Cold pentane was used to efficiently precipitate $OPPh_3$ from the reaction mixtures. In this way we prepared a number of known and new acetals of substituted aromatic and aliphatic aldehydes and ketones. All synthesized were fully spectrally (NMR, MS, UV, IR) characterized. Due to essentially neutral conditions during the reaction, this procedure, besides being quantitative and selective, can be readily employed for the preparation of acetals of acid-sensitive aldehydes and alcohols.

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Nauka o materijalima

NM P 01

Uticaj parametara procesa rasta kristala iz rastopa na oblik granice faza tečno - čvrsto

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Ispitivana je mogućnost određivanja temperaturnog gradijenta u rastopu sistema Al – Cu, na osnovu merenja rastojanja između sekundarnih grana dendrita analizom njihovih mikroskopskih fotografija. Uzorak je dobijen metodom Vertikalni Bridžmen (Bridgman) sa spuštanjem suda na dole. Pretpostavljeno je da je brzina rasta kristala jednaka brzini kretanja ampule i usvojeno je da je temperaturni gradijent u rastopu jednak temperaturnom gradijentu u peći, koji je dobijen eksperimentalno. Dobijeni uzorak je podvrgnut metalografskom ispitivanju strukture. Dobijene digitalne fotografije su obrađene u programu za anlizu slike Image – Pro Plus, verzija 4. Iz dobijenog temperaturnog gradijenta pri određenoj brzini rasta kristala i sastavu legure, a na osnovu Kriterijuma konstitucionalnog pothađenja, dobijena je konstanta koja je funkcija sastava. Na ovaj način moguće je merenjem rastojanja između sekundarnih dendrita odrediti temperaturni gradijent u rastopu pri manjim brzinama rasta kristala, a zatim i ustanoviti zavisnost temperaturnog gradijenta od brzine kretanja uzorka.

The influence of the crystal growth conditions in the melt on the shape of solid – liquid interface

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The possibility to determinate the temperature gradient in the molten Al-Cu alloy based on measurements of the distance between the secondary branches of dendrites was investigated. The sample was obtained using Vertical Bridgman while ampoule was moving downwards in a furnace. It was assumed that the crystal growth rate was equal to the temperature gradient in the furnace, which was obtained exerimentally. The structure of the resulting sample was metallographically examined. The sample was photographed with a digital camera and a resulting digital image is processed in image analysis program Image – Pro Plus, ver 4. According to the Criteria of Constitutional Supercooling and experimentally obtained temperature gradient in a melt for a certain crystal growth rate, constant that depends of composition of alloy was calculated. This method allows determination of the temperature gradient in the melt during the slow crystal growth from the measurement of the distance between the secondary dendrite.. In addition, it allows the determination of the temperature gradient as a function of ampule speed.

NM P 02

Određivanje uticaj azotne i fosforne kiseline na zateznu čvrstoću u obimnom pravcu staklo-poliester cevi

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Cevi od polimernih kompozita sa staklenim ojačanjem danas imaju široku primenu u hemijskoj i procesnoj industriji. Predmet ovog rada je određivanje uticaja azotne i fosforne kiseline na raspodelu napona i deformaciju u obimnom (tangencijalnom pravcu) staklo-poliester cevi pri ispitivanju zatezanjem. Uzorci cevi su tretirani ovim kiselinama 30, 60 i 90 dana ,a zatim je određena zatezna čvrstoća u obimnom pravcu. Ispitivanje zatezanjem je izvedeno na elektromehaničkoj kidalici na prstenovima sečenim od cevi koje proizvedenih metodom namotavanja, sa namotavanjem stklenog ojačanja pod uglom ±55°.

Determination of effect of nitric and phosphoric acid to a tension strength in the circumferentional direction in glass-polyester pipes

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Polymer composite pipes with glass fiber reinforcement have today a wide usage in the chemical and process industries. The basic subject of this paper is the determination of effect of nitric and phosphoric acid on distribution of stresses and strains in circumferentional directions of glass-polyester pipes under tension test. Sapmples were treated with this acids for 30, 60, 90 days after that the tension strengths in circumferentional directions are determined out. Tension test was performed on an electro-mechanical test machine on flat samples and rings obtained by cutting of pipes produced by the method “Filament winding” with glass fibers reinforcement ±55°.

NM P 03

UV zaštitna svojstva pletenina

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Odeća odnosno, tekstilni materijali predstavljaju jedno od najefikasnijih vidova UV zaštite. Polazeći od činjenice da relaksacioni procesi koji se neminovno dešavaju tokom prerade i upotrebe tekstilnih materijala izazivaju promene njihovih konstrukcionih karakteristika nameće se potreba analize uticaja ovih promena na UV zaštitna svojstva materijala. Zbog toga je cilj ovog rada bio ispitivanje uticaja dimenzione stabilnosti pletenina na njihovu sposobnost UV zaštite. Odabrane su glatke pletenine budući da su one najpodložnije relaksacionim promenama. Eksperimentalno ili računski su određeni strukturni parametri pletenina, kao i promene nastale nakon potpune relaksacije i nakon perioda nege i nošenja. UV zaštitna sposobnost delimično i potpuno relaksiranih pletenina, kao i pletenina koje su bile podvrgnute testu nege i nošenja, kvantitativno je ocenjena pomoću parametra – UV zaštitni faktor (UPF), koji predstavlja meru sposobnosti materijala da zaštiti čovekovu kožu od UV zračenja, prema evropskom standardu EN 13758-1:2002. Sprovedena ispitivanja su pokazala da se sa relaksacionim procesima u DL pleteninama menjaju njihova UV zaštitna svojstva. S obzirom da uočene promene strukture pletenina nisu bile istog intenziteta, efekat povećanja UPF-a posle relaksacije i perioda nege i nošenja nije bio isti za sve ispitivane pletenine.

UV protection properties of knitted fabrics

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Clothing is considered to be one of the most important tools for UV protection. Starting from the fact that the relaxation processes inevitably occurring during processing and usage of textile materials changes their structural characteristics, the investigation of the impact of these changes on their UV protective properties seems essential. Therefore, the aim of this study was to investigate the effect of dimensional stability of knitted fabrics on their UV protection ability. The plain knitted fabrics were chosen since they are particularly susceptible to relaxation. Structural parameters of the knitted fabrics were determined as well as the changes caused by full relaxation and/or after wear and care cycles. The Ultraviolet Protection Factor (UPF), as a quantitative measure of the effectiveness of the material to protect human skin against UV radiation, was determined for the knitted fabrics (partially and full relaxed, and after undergoing usage cycles) by *in vitro* test method according to European standard EN 13758-1:2002. According to the investigation conducted it can be concluded that relaxation processes in knitted fabrics changes their UV protection properties. Relaxation and shrinkage of the knitted fabrics due to relaxation caused the reduction of macroporosity increasing the UPF of the knitted fabrics. However, the effects of relaxation and “using the fabric” influenced to a different extent the increase of photoprotective qualities of the knitted fabrics.

NM P 04

Dobijanje pamučne pređe poboljšanih sorpcionih svojstava

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U ovom radu proučavan je uticaj TEMPO- oksidacije na hemijski sastav, strukturu i svojstva pamučne pređe. Nemodifikovana i modifikovana pamučna pređa okarakterisana je sa aspekta gubitka mase, sadržaja vlage, sadržaja karbonilnih i karboksilnih grupa, indeksa kristalnosti i sposobnosti zadržavanja vode. Promene u svojstvima modifikovanih pređa u odnosu na polazni uzorak su praćene u funkciji koncentracije oksidacionog sredstva i vremena modifikovanja. TEMPO-oksidacija pamučne pređe uticala je na smanjenje mase, povećanje sadržaja vlage i indeksa kristalnosti modifikovanih uzoraka. Oksidacijom pomoću TEMPO radikala dolazi do povećanja sorpcionih svojstava pamučne pređe usled značajnijeg povećanja sadržaja karboksilnih grupa, od 0,024 mmol/g celuloze za polazni uzorak do 0,679 mmol/g celuloze za uzorak oksidisan pri najrigoroznijim uslovima. Dobijeni rezultati omogućavaju optimizaciju selektivne TEMPO-oksidacije u cilju dobijanja pamučne pređe poboljšanih sorpcionih svojstava, koja predstavlja polaznu sirovinu za dobijanje širokog spektra tekstilnih proizvoda specijalne namene.

Zahvalnost: *Ovaj rad je proistekao iz rada na projektu koji finansira Ministarstvo prosvete, nauke i tehnološkog razvoja RepublikeSrbije (projekat OI 172029).*

Obtaining of cotton yarn with improved sorption properties

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In this paper, influence of TEMPO- oxidation onto chemical composition, structure and properties of cotton yarn was studied. Unmodified and modified cotton yarn was characterized from the aspect of weight loss, moisture content, carbonyl and carboxyl group content, crystallinity index and capability to retain water. Changes in the properties of modified yarns, compared to untreated sample, were monitored as a function of oxidizing agent concentration and time of oxidation. TEMPO- oxidation of cotton yarn had influence on weight loss, increase of moisture content and crystallinity index of the modified samples. Oxidation using TEMPO radical leads to an increase in sorption properties due to the significant increase in carboxyl group content, from 0.024 mmol/g cellulose for untreated sample to 0.679 mmol/g cellulose for sample oxidized under the most rigorous conditions. Obtained results allow optimization of selective TEMPO-oxidation in order to obtain a cotton yarn with improved sorption properties, which represents a starting raw material for the preparation of a broad spectrum of high performance textile products.

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Teorijska hemija

TH P 01

Kvantno-hemijsko modelovanje protolitičkih ravnoteža 4-aril-2,4-dioksobutanskih kiselina u vodenom medijumu

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Arildiketo kiseline (ADK) mogu helirati metalne jone, kritične kofaktore katalitičkog centra enzima, te mogu inhibirati enzimsku aktivnost. ADK, poznate po β-dikarbonilnoj strukturi, mogu postojati u jednom diketo, kao i u dva enolna oblika. Raspodela mogućih keto-enolnih tautomera ADK je pH-zavisna, i važna je za ADMET (apsorpcija, distribucija, metabolizam, izlučivanje i toksičnost) osobine. Stoga je poznavanje pK_a vrednosti ADK od velikog značaja jer različiti tautomeri mogu koordinisati katjone drugačijim afinitetima. Rastvorljivost ADK u vodi je veoma niska, te je eksperimentalno određivanje pK_a vrednosti često jako teško. Zbog toga smo proučavali set malih, strukturno jednostavnih ADK sa eksperimentalno određenim pK_a vrednostima, kako bismo razvijeni model mogli da primenimo na veće, u vodi nerastvorne ADK. U okviru ovog rada izvedena su kvantno-hemijska modelovanja protolitičkih ravnoteža sedam jedinjenja iz klase 4-aril-2,4-dioksobutanskih kiselina u vodenom medijumu. Predloženi su najstabilniji keto-enolni tautomeri i izračunate su odgovarajuće pK_{a1} vrednosti. Predviđanje pK_{a2} vrednosti pokazalo je jako velike devijacije, jer čak i male energetske razlike mogu dovesti do velikih pK_a grešaka. Modelovanja su izvedena na B3LYP/6-311++G(d,p) i CAM-B3LYP/6-311+G(d,p) nivoima teorije sa PCM i CPCM modelima rastvarača.

Quantum chemical modeling of the protolytic equilibria of 4-aryl-2,4-dioxobutanoic acids in aqueous media

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Aryldiketo acids (ADK) can chelate metal ions, critical cofactors at the enzyme catalytic core, so they can inhibit enyzme activity. ADK, known for β-dicarbonyl structure, can exist in one diketo, as well as in two enol forms. Distribution of the possible ADK keto-enol tautomers is pH dependent, and is important for ADMET properties (absorption, distribution, metabolism, excretion, and toxicity). For this, knowing pK_a values of ADK is very significant since diverse tautomers may coordinate cations with different affinities. The water solubility of ADK is very modest, so pK_a values are usually hard to be determined experimentally. Therefore we studied a set of small, structurally simple ADK with experimentally determined pK_a values so that we can apply the developed model on larger, water insoluble ADK. We performed quantum chemical modeling of the protolytic equilibria of seven 4-aryl-2,4-dioxobutanoic acids in aqueous media. The most stable keto-enol tautomers have been proposed, and appropriate pK_{a1} values have been computed. Prediction of pK_{a2} values shows very high deviation, since even small energy difference can lead to high pK_a errors. Calculations were performed at B3LYP/6-311++G(d,p) and CAM-B3LYP/6-311++G(d,p) levels of theory with PCM and CPCM solvation models.

TH P 02

Elektrostatički i topološki deskriptori kao prediktori antifungalne aktivnosti odabranih heterocikličnih jedinjenja prema *Candida albicans*

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U ovom radu su analizirana 24 derivata benzoksazola i oksazolo[4,5-*b*]piridina. Glavni cilj rada je bio da se primenom metode veštačkih neuronskih mreža dobiju modeli za precizno predviđanje antifungalne aktivnosti prema *Candida albicans* ($\log(1/c_{\mathrm{mic}})$) ispitivanih jedinjenja na osnovu izračunatih elektrostatičkih i topoloških deskriptora. Pored toga, dobijen je i uvid u elektrostatičke i strukturne karakteristike ovih jedinjenja koje najviše doprinose njihovoj antifungalnoj aktivnosti (minimalnoj inhibitornoj koncentraciji, c_{mic}). Nakon softverskog modelovanja i računanja deskriptora, primenjena je metoda višeslojnih veštačkih neuronskih mreža sa Brojden-Flečer-Goldfarb-Šano algoritmom. Formirano je 5 mreža sa odličnim statističkim karakteristikama i prediktivnom sposobnošću. Model sa deset ulaznih parametara i devet neurona u skrivenom sloju se pokazao kao najefikasniji sa greškom treniranja od 0,00015, greškom testiranja od 0,00106, greškom validacije od 0,00203 jedinica antifungalne aktivnosti i Pirsonovim koeficijentom korelacije od 0,9774. Dobijeni rezultati ukazuju na mogućnost preciznog predviđanja antifungalne aktivnosti ispitivanih jedinjenja primenom formiranih neuronskih mreža.

Zahvalnica: *Rezultati ovog rada finansirani su od strane Ministarstva prosvete, nauke i tehnološkog razvoja Republike Srbije u okviru projekata br. 172012 i 172014, i projekta br. 114-451-2373/2011 finansiranog od strane Pokrajinskog sekretarijata za nauku i tehnološki razvoj Autonomne Pokrajine Vojvodine.*

Electrostatic and topological descriptors as predictors of antifungal activity of some heterocyclic compounds against *Candida albicans*

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In the present paper 24 derivatives of benzoxazoles and oxazolo[4,5-*b*]pyridines were analysed. The main aim of this study was precise prediction of antifungal activity ($\log(1/c_{\mathrm{mic}})$) of the analysed compounds against *Candida albicans* using artificial neural networks and calculated electrostatic and topological descriptors. Besides, we determined the most significant electrostatic and topological characteristic for the compounds which mostly contribute to their minimum inhibitory concentration, c_{mic}. After molecular modelling by suitable software and calculation of descriptors, the obtained values were submitted to multilayer perceptron artificial neural networks modelling with Broyden-Fletcher-Goldfarb-Shanno training algorithm. Five outstanding networks were established. The best model is characterized by 10 input data, 9 hidden neurons, training error of 0.00015, test error of 0.00106, validation error of 0.00203 and Pearson's correlation coefficient of 0.9774. The obtained results indicate very good predictive ability of the established neural networks for prediction of antifungal activity of the analysed compounds.

TH P 03

Teorijska analiza rastvaranja ((E i Z)-N'-[1-(2-hidroksifenil)etiliden]izonikotinoilhidrazida)

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Strukture E i Z izomera N'-[1-(2-hidroksifenil)etiliden]izonikotinoilhidrazida), kao i njihovih deprotonovanih formi u vakuumu i vodi su optimizovane na cam-B3LYP/cc-pVTZ nivou pomoću programskog paketa Gausijan. Stabilnost izomera, harmonijske vibracione frekvencije i vertikalni elektronski prelazi svih vrsta su diskutovani sa posebnom pažnjom na promene koje se dešavaju prilikom rastvaranja u vodi. Elektronski spektri za sve vrste su izračunati korišćenjem TDDFT pristupa. Kao model rastvarača koriščen je model polarizabilnog kontinuuma (PCM). U vakuumu i vodi, stabilniji je E-izomer, dok je deprotonovana forma Z-izomera stabilnija od deprotonovane forme E-izomera. Prilikom rastvaranja E-izomera dolazi do rotacije fenilnog prstena, što dovodi do promena u infracrvenom (IC) spektru. U IC spektru protonovanih formi posebno su intenzivne trake O-H, N-H i C=O istežućih vibracija, s tom razlikom da je traka koja odgovara istežućoj O-H vibraciji Z-izomera mnogo manjeg intenziteta zbog toga što se fenilna grupa nalazi van ravni molekula i nije moguće građenje vodonične veze sa azotom hidrazonske grupe i kiseonikom karbonilne grupe. Dobijeni elektronski spektri su upoređeni sa eksperimentalnim podacima i izvršena je asignacija traka.

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Theoretical analysis of (E and Z)-N'-[1-(2-hydroxyphenyl)etiliden]isonicotinoylhydrazide) solvation

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Structures of E and Z isomers of N'-[1-(2-hydroxyphenyl)etiliden]isonicotinoylhydrazide), and their deprotonated forms in vacuum and water were optimized at cam-B3LYP/cc-pVTZ level with the Gaussian program package. Stability, harmonic vibrational frequencies and vertical electronic transitions of all species are discussed with emphasis on the changes that arise from solvation in water. Electronic spectra were computed for all species using TDDFT approach. As a model for solvent, Polarizable Continuum Model (PCM) was used. In vacuum and water, E-isomer is more stable than Z-isomer, while deprotonated E-isomer is less stable than deprotonated form of Z-isomer. In water solution, the phenyl ring in E-form rotates, which is reflected in the infrared (IR) spectrum. IR spectra of protonated species have very intense peaks that belong to O-H, N-H and C=O stretching vibrations, but the peak that corresponds to O-H stretch is less intense peak because this group is out of the molecule plane and no hydrogen bonds are formed between hydrogen and oxygen from carbonyl group and nitrogen from hydrazone group. The computed electronic spectra were compared with the experimental data the corresponding peaks assigned.

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TH P 04

Geometrijsko predstavljanje eksponenta politrope u radnom i toplotnom dijagramu

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U ovom radu, prikazana su tri načina grafičkog određivanja eksponenta politrope, odnosno njegovog predstavljanja u toplotnom i random dijagramu.U radu smo koristili karakteristične dijagrame *p-v* i *T-s* i u njima konstruisali određene politropske promene koje smo u daljim razmatranjima koristili za određivanja eksponenta politrope. Prvi način se zasniva na konstruisanju dijagrama *log p=f(log v)* i iz nagiba prave očitavamo vrednost traženog eksponenta. Drugi način se zasniva na konstruisanju politrope u *p-v* dijagramu, na koju, u proizvoljnoj tački politrope, povlačimo tangentu i diferencijalnom metodom dolazimo do eksponenta politrope. A treći način zasniva se na konstruisanju politrope u *T-s* dijagramu, korišćenju osnovnih teorema diferencijalnog računa, odnosno I i II zakona termodinamike za uočene izotermske promene i pisanju osnovne jednačine politropske zavisnosti u diferencijalnom obliku. Prikazana grafička rešenja omogućuju efikasnijije teorijsko izučavanje politropskih promena stanja i znatno pomažu jasnijiem sagledavanju problema koji su u vezi sa ovom vrstom promene stanja. Ove metode, određivanja eksponenta politrope, omogućavaju jednostavnija izračunavanja na polju hemijsko-inženjerske termodinamike.

Geometrical presentation of polytropic exponent in work and heat diagram

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In this paper , using existing knowledge of thermodynamics , we show three graphical ways of determining the polytropic index, as well as classical analytical method. In this paper we have used the characteristic *p-v* and *T-s* diagrams, and in these diagrams we have constructed some polytropic changes that are further considerations for the determination of the polytropic index. The first method is based on constructing a diagram *log p = f (log v)* from the slope of the line and we read the value of the polytropic index. The second method is based on the construction of the polytropic change in*p-v*diagram, to which, in an arbitrary point of polytropic, tangent is drawn and differential method come to the polytropic index. The third method is based on the construction of the polytropic change in *T-s*diagram, using the basic theorem of the calculus , and first and second laws of thermodynamics for isothermal change, which we observe and writing the basic equation of polytropic change in differential form. Displayed graphics solutions enable efficient theoretical study of polytropic change of the state and it significantly helps to a clearer consideration of problems that are related to this kind of change of state. This methods are suitable for some calculation in field of chemical-engineering thermodynamic.

Nastava hemije

NH P 01

Povećanje zainteresovanosti učenika sedmog razreda na primeru nastavne teme „Hemijska veza“

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U cilju povećanja zainteresovanosti učenika 7. razreda na primeru nastavne teme „Hemijska veza“ u okviru koje se izučavaju jonska i kovalentna veza, predložena je odgovarajuća dopuna nastavnih sadržaja vezanih za koordinativno-kovalentnu vezu sa odgovarajućim primerima vezanim za jone i molekule prisutne u svakodnevnom životu i materiju koja nas okružuje. Pedagoški eksperiment je obuhvatio uvodno testiranje učenika nakon obrađenih nastavnih sadržaja propisanih udžbenikom zatim upoznavanje sa primerima građenja koordinacione veze (molekuli vode; dokazivanje $Cl^{-,}$ Ca^{2+}, Mg^{2+} jona u vodi; Mg jon u hlorofilu, Fe u hemoglobinu, lekovi na bazi koordnacionih jedinjenja), demonstraciju eksperimenata, podelu materijala i završno testiranje. Rezultati pedagoškog eksperimenta u okviru nastavne teme „Hemijska veza“ u osnovnoj školi dokazali su da je nivo znanja učenika nakon obrade dopuna nastavnih sadržaja sa odgovarajućim demonstracionim ogledima značajno poboljšan. Procenat učenika koji su na uvodnom testu imali manje od 50% urađenog testa je 81.82% dok se na drugom testu ovaj procenat znatno smanjio i iznosi 40.91%.

Increasing interest in seventh grade pupils in the example of teaching topic “Chemical bond”

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In order to increase the interest in seventh grade pupils in the example of teaching topic "chemical bond" within the studied ionic and covalent bonds, the proposed amendment is appropriate teaching materials related to the coordinative-covalent bond with some examples related to ions and molecules present in everyday life and a substance that surrounds us. Pedagogical experiment included introduction test, after processed curriculum content prescribed by textbook, then introduction with examples of forming coordination bond (water molecules; determination of Cl^{-}, Ca^{2+}, Mg^{2+} ions in water; Mg ion in chlorophyll; Fe in hemoglobin; drugs based on coordination compounds), demonstration of experiments, the division of teaching material and final testing. Results of pedagogical experiment within the topic "chemical bond" in elementary school proved that the level of pupils' knowledge after treatment supplement teaching materials with appropriate demonstration experiments significantly improved. Percentage of pupils who are in the preliminary test had less than 50% of test, was 81.82%, while in the second test, this percentage is significantly reduced and it is 40.91%.

NH P 02

Indeksi težine i diskriminativnosti proceduralnih i deklarativnih zadataka u osnovnoškolskoj nastavi hemije

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U ovom radu ispitivani su indeksi težine i diskriminativnosti deklarativnih i proceduralnih zadataka na testovima iz hemije za osmi razred osnovne škole kao i relijabilnost i koeficijent korelacije između indeksa diskriminativnosti i indeksa težine zadataka. Ovim istraživanjem obuhvaćeno je 128 učenika osmog razreda osnovne škole „Kosta Trifković“ u Novom Sadu. U okviru ovog istraživanja korišćeno je pet različitih standardizovanih testova znanja kao merni instrument. Na osnovu dobijenih rezultata zaključeno je da su učenici imali veće teškoće u rešavanju proceduralnih zadataka, nego pri rešavanju deklarativnih zadataka na šta ukazuje znatno viša vrednost indeksa težine deklarativnih zadataka. Generalno gledano svi analizirani testovi spadaju u grupu srednje teških testova za rešavanje i imaju dobru diskriminativnost.

Difficulty and discrimination indices of the procedural and declarative tasks in the primary chemistry education

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In this study, the difficulty and discrimination indices of the declarative and procedural tasks in the eighth grade chemistry tests, as well as the reliability coefficient and correlation between index of task difficulty and index of task discrimination had been investigated. A research sample included 128 eight grade students who attended primary school "Kosta Trifković" in Novi Sad. In this study five different standardized tests of knowledge were used as measuring instruments. Based on the results obtained, it can be concluded that students have major difficulties when solving procedural tasks, in comparison to declarative tasks which had significantly higher value for difficulty index. Generally, all the applied tests belong to a group of medium-heavy tests and all of them have a good discrimination index.

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