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Српско хемијско друштво
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Serbian Young Chemists' Club

ЧЕТВРТА КОНФЕРЕНЦИЈА МЛАДИХ ХЕМИЧАРА СРБИЈЕ

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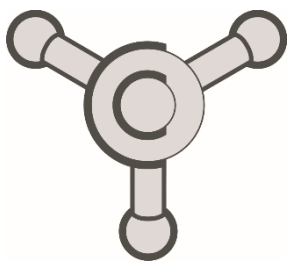
КРАТКИ ИЗВОДИ РАДОВА

Book of Abstracts

КЛУБ МЛАДИХ ХЕМИЧАРА СРБИЈЕ



Serbian Young Chemists' Club

Пленарно предавања / Plenary Lecture

PP 01

Termoplastični poliuretani na bazi poli(dimetilsiloksana): Sinteza, svojstva i biokompatibilnost

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Termoplastični poliuretanski (TPU) materijali na bazi poli(dimetilsiloksana) korišćeni su u različitim medicinskim uređajima, zahvaljujući njihovim dobrim mehaničkim svojstvima i biostabilnosti. Međutim, TPU na bazi PDMS, koji se trenutno koriste kao biomaterijali, imaju biokompatibilnost ispod optimalne što smanjuje njihovu efikasnost. Kako bi se poboljšala i proširila klinička primena TPU na bazi PDMS, cilj istraživanja je bio da se poboljša vezivanje endotelnih ćelija i svojstva ovih materijala u dodiru sa krvlju [1,2]. U ovom radu dat je pregled sinteze, karakterizacije strukture, površinskih, termičkih i mehaničkih svojstava, kao i ispitivanje biokompatibilnosti TPU na bazi PDMS. Sintetisani TPU na bazi PDMS pokazuju dobra površinska i temo-mehanička svojstva, kao i dobru biokompatibilnost jednaku komercijalnim TPU koji se trenutno koriste u biomedicini.

Thermoplastic polyurethanes containing poly(dimethylsiloxane): Synthesis, properties and biocompatibility

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Thermoplastic polyurethane (TPU) materials containing poly(dimethylsiloxane) (PDMS) segments have been used in various medical devices, primarily because of their good mechanical properties and biostability. However, PDMS-based TPUs, currently utilized for biomedical applications, have sub-optimal biocompatibility in terms of resistance to cell adhesion and relatively poor support for endothelial cell growth, which diminishes their efficacy. In order to significantly improve and extend clinical applications of PDMS-based TPUs, the aim of the research was to enhance the endothelial cell attachment and blood-contacting properties of these materials [1,2]. This study is focused on overview of the synthesis, characterization of the structure, surface, thermal, and mechanical properties, as well as investigation of biocompatibility of PDMS-based TPUs. The synthesized PDMS based TPUs exhibit good surface and thermo-mechanical properties, as well as good biocompatibility equal to current commercial biomedical TPUs.

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Предавања по позиву / Invited Lectures

PPP 01

Bioimitirajuće hibridne polimerne mreže sa lako promenljivim svojstvima

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Dizajn složenih polimernih materijala za postizanje unapred definisanih karakteristika sreće se sa izazovom: da uspostavi vezu sinteza-struktura-svojstva između komponenti, kao i da razume njihovu organizaciju i interakcije. Imitacija izuzetnih performansi prirodnih materijala predstavlja atraktivan, ali zahtevan pristup za njihovu sintezu. Hibridne mreže polielektrolita (poli(metakrilna kiselina)) i proteina (kazein) su sintetisane i njihovo bubrenje, mehaničke i strukturne karakteristike su ispitane u funkciji stepena neutralizacije i koncentracija kazeina. Dominacija različitih interakcija između komponenti je dovela do različitih oblika makromolekula kazeina (od micela do razvijenih lanaca) rezultirajući u veoma različitim materijalima: od poroznih, nebubrećih do veoma nabubrelih i ojačanih mreža. Pokazano je da postoji velika mogućnost da se lako menjaju karakteristike ovog hibridnog sistema da odgovori na potrebe specifične primene samo kroz promenu jednog parametra sinteze. Ovo daje mogućnost za njihovu primenu u različitim oblastima, od sorpcije, materijala za tretiranje rana i sistema za ciljano otpuštanje nerastvornih i slabo rastvornih lekova, do različitih pH osetljivih sistema i zahtevnih implantata i nosača.

Biomimic hybrid polymeric networks with easy tunable properties

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The design of complex polymeric materials to achieve predefined properties meets challenging issue: to establish synthesis-structure-properties relationship of the involved components, as well as to understand their arrangement and interactions. Mimicking the extraordinary performances of natural materials presents an attractive, but demanding approach in their synthesis. Hybrid networks of polyelectrolyte (poly(methacrylic acid)) and protein (casein) were synthesized and their swelling, mechanical and morphological properties were investigated as functions of neutralization degree and the concentrations of casein. The domination of different interactions between components led to diverse forms of casein macromolecules (from micelles to unfold chains) resulting in very different materials: from porous unswellable to highly swellable and reinforced networks. It was demonstrated that there was great opportunity to easily modulate the final characteristics of this hybrid system to fit the need of specific application just through the change of one synthesis parameter. This gives the opportunity for their application to various areas, from sorption, wound dressing and targeted delivery systems for water-insoluble and poorly soluble drugs, to diverse pH sensitive actuators and demanding implants and scaffolds.

PPP 02

Ekološke nezasićene poliestarske smole dobijene iz bio-obnovljivih sirovina

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Nezasićene poliestarske smole (NZPE) se koriste za izradu kompozitnih materijala u vojnoj i civilnoj industriji zbog svojih dobrih karakteristika, niske gustine i niske cene. Ove smole najčešće sarže visoke koncentracije reaktivnog rastvarača (npr. stirena) da bi mogle da se prerađuju tehnikom tečnog oblikovanja u kalupu kao i drugim jeftinim tehnikama tečnog oblikovanja. Pošto je stiren veliki zagađivač vazduha i lako isparljiva organska komponenta Federalna agencija za zaštitu životne sredine Amerike je uvela regulativu koja ograničava emisiju stirena pri izradi kompozita. Usled toga, slabo isparljivi reaktivni rastvarači imaju veliku prednost u odnosu na klasične reaktivne rastvarače. Shodno tome, usmerili smo istraživanje ka razvoju NZPE u potpunosti dobijenih iz bio-obnovljivih sirovina koristeći diestre itakonske kiseline kao zamenu za stiren. Itakonska kiselina i propilen glikol su korišćeni za sintezu predpolimera dok su dialkil itakonati upotrebljeni kao reaktivni rastvarači pri izradi NZPE. Ispitani su ispraljivost i viskozitet sintetisanih smola dok su nakon umrežavanja smole okarakterisane DMA, TMA, TGA i ispitivanjem na zatezanje. Detaljno je ispitan uticaj dialkil itakonata kao reaktivnih rastvarača na karakteristike sintetisanih smola. Značaj rezultata se ogleda u:

- dobijene su smole iz prirodnih izvora niže toksičnosti u odnosu na komercijalne
- aplikativne karakteristike dobijenih smola su slične karakteristikama komercijalnih
- dobijene su smole približno iste cene kao i komercijalne i njihova proizvodnja se može izvoditi na postojećim industrijskim postrojenjima.

Eco-friendly unsaturated polyester resins prepared from bio-based chemicals

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Unsaturated polyester resins (UPR) are used to make polymer matrix composites in military and commercial applications because of their good properties, low weight and low cost. These resins typically contain high concentrations of reactive diluents, such as styrene, to allow these resins to be molded using resin transfer molding and other inexpensive liquid molding techniques. Because styrene is a hazardous air pollutant and a volatile organic compound, the Federal Environmental Protection Agency of the United States of America introduced legislation to limit styrene emissions from composite manufacturing. Therefore, non-volatile reactive diluents offer a large advantage over current reactive diluents. In this context we directed our efforts to develop fully bio-based UPRs using the dialkyl esters of itaconic acid as a possible alternative to styrene. 100% biobased UPRs were synthesized using itaconic acid and propylene glycol for prepolymer and dialkylitaconates as reactive diluents. The so synthesized resins were characterized by volatility and viscosity measurements, while the cured samples were characterized by DMA, TMA, TG and tensile tests. The effect of dialkyl itaconate used as reactive diluent on properties of cured UPR was investigated in detail. The significance of our results comprises:

- prepared UPRs have biobased nature and far lesser toxicity compared to the commercial ones
- applicative properties of derived UPRs are comparable to that of the commercially available resins
- derived UPRs are competitive in price and adaptable to the existing manufacturing processes.

Саопштења / Contributions

Hemija makromolekula i nanotehnologije

Macromolecular Chemistry and Nanotechnology

MN O 01

Molekulski obeleženi polimeri za holesterol

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Tehnologija molekulskog obeležavanja (TMO) predstavlja korisnu metodu molekulskog prepoznavanja putem sinteze visoko umreženih molekulski obeleženih polimera (MOP) oko molekula templata, što dovodi do formiranja šupljina. Oblik, veličina i hemijska funkcionalnost formiranih šupljina komplementarni su molekulu analita (templatu) zahvaljujući različitim hemijskim interakcijama[1]. TMO je doživela veliki pomak u svojoj primeni, pa se osim u analitičke svrhe, danas koristi i u remedijaciji životne sredine, kao i u biotehnologiji[2]. Holesterol je značajan konstituent membrana životinjskih ćelija, takođe je i sintetički prekursor žučne kiseline, vitamina D i steroidnih hormona. Uloga holesterola ključna je i u nekim od najzastupljenijih bolesti, poput ateroskleroze i hipertenzije. U literaturi su opisani razni MOPovi za određivanje holesterola[3], premda ni u jednom od njih nije potpuno objašnjena fizičko-hemijska funkcionalnost ovih MOPova u smislu njihove selektivnosti i vezivne moći. Naše istraživanje je usmereno ka pronalaženju novih sintetičkih procedura za dobijanje MOPova sa većom selektivnošću i moći vezivanja. Istraživanje je pokazalo da povećanje hidrofobnih interakcija između molekula templata, funkcionalnog monomera i umreživača značajno utiče na vezivanje holesterola za MOP.

Molecularly imprinted polymers for cholesterol

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Molecular imprinting technology (MIT) provides an effective method for molecular recognition via the template-directed synthesis of highly cross-linked molecularly imprinted polymers (MIPs), producing cavities. The shape, size, and chemical functionality of the formed cavities are complementary to the target analyte (template) through different types of chemical interactions. MIT has undergone an enormous development, being applied not only in the analytical field, but also for environmental remediation and biotechnological processes. Cholesterol is an important part of animal tissue cell membranes, but is also a synthetic source of bile acid, vitamin D and steroid hormones. The role of cholesterol is important in some of the most widespread diseases, like atherosclerosis and hypertension. Various MIPs that can be used for the determination of cholesterol have been described in literature, yet none of them completely elucidate the physico-chemical functionality of these MIPs - their selectivity and sorptive power. The goal of this work was to investigate new synthetic procedures in order to obtain MIPs with higher selectivity and sorptive power. It was shown that the increase in hydrophobic interactions between the template, functional monomer and cross-linker molecules greatly affects its binding properties.

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MN O 02

Koordinacioni polimer Ag(I) sa 1,2,4,5-benzentetrakarboksilnom kiselinom i tiomorfolin-4-karbonitrilom

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Metal-organske umrežene strukture (engl. *Metal organic frameworks*, MOFs) predstavljaju potencijalno dobre materijale sa primenom u katalizi, odvajanju, skladištenju gasova i molekulskom prepoznavanju. U ovom radu opisana je sinteza i karakterizacija novog MOF-a srebra(I) dobijenog reakcijom srebro(I)-nitrata sa 1,2,4,5-benzentetrakarboksilnom kiselinom (H_4BTEC) i tiomorfolin-4-karbonitrilom (tmc). Rendgenska strukturna analiza je pokazala da srebro(I) centri imaju distorgovanu tetraedarsku geometriju, pri čemu dva koordinaciona mesta zauzimaju atomi kiseonika dva molekula H_4BTEC, dok su druga dva koordinacina mesta zauzimaju redom N-atom nitrilne grupe i S-atom tmc-a. Susedni srebro-karboksilatni lanci su povezani preko dva tmc liganda u 2D polimernu strukturu. Između 2D slojeva nalaze se molekuli vode koji grade vodonične veze sa karboksilatnim grupama iz susednih slojeva formirajući supramolekulsku 3D strukturu. Vodonične veze čine ovu strukturu fleksibilnom i pogodnom za apsorpciju gasova. Potencijalna primena ovog koordinacionog polimera za skladištenje vodonika će biti predmet daljih istraživanja.

Ag(I) coordination polymer of 1,2,4,5-benzenetetracarboxylic acid and thiomorpholine-4-carbonitrile

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Metal-organic frameworks (MOFs) are regarded as promising materials for applications in catalysis, separation, gas storage and molecular recognition. Here we report the synthesis and characterization of novel silver(I) MOF obtained by the reaction of silver(I) nitrate with 1,2,4,5-benzenetetracarboxylic acid (H_4BTEC) and thiomorpholine-4-carbonitrile (tmc). As shown by X-ray difraction analysis, silver(I) centers have distorted tetrahedral geometry with two coordination sites occupied by carboxylic oxygen atoms of two H_4BTEC, and the other two by N-atom from nitrile group and S-atom of tmc, respectively. Adjacent silver-carboxylate chains are connected by two tmc ligands into a 2D polymeric structure. Water molecules between these 2D layers are hydrogen bonded to carboxylic groups from adjacent layers and thus expanding the 2D structure into a supramolecular 3D structure. Hydrogen bonds make this structure flexible and suitable for gas absoption. Potential aplication of this coordination polymer as a hydrogen storage material will be the subject of further investigations.

MN O 03

Elektrohemijska sinteza i karakterizacija hidrogelova na bazi polivinil alkohola, hitozana i grafena sa inkorporisanim nanočesticama srebra

Katarina Nešović, Ivana Jevremović, Vesna Mišković-Stanković
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Nanokompozitni hidrogelovi srebro/polivinil alkohol/hitozan/grafen (Ag/PVA/CHI/Gr), pogodni za primenu u biomedicini, su dobijeni *in situ* elektrohemijskom sintezom nanočestica srebra u matrici hidrogelova polivinil alkohol/hitozan/grafen (PVA/CHI/Gr), koji su prethodno umreženi metodom uzastopnog zamrzavanja i odmrzavanja u 5 ciklusa. Radi ispitivanja uticaja koncentracije hitozana na svojstva hidrogelova, sintetisani su hidrogelovi sa 0,1 mas. % i 0,5 mas. % CHI. Ag/PVA/CHI/Gr hidrogelovi su karakterisani metodom UV–vidljive spektroskopije, kojom je potvrđeno prisustvo sfernih nanočestica srebra u strukturi hidrogela, kao i cikličnom voltametrijom, u cilju ispitivanja elektrohemijskih karakteristika hidrogelova. Infracrveni spektri hidrogelova sa i bez srebra pokazuju uočljive razlike u položaju i intenzitetu apsorpcionih traka, što ukazuje na koordinativno vezivanje srebra sa –OH i $–NH_2$ grupama na lancu polimera. Sa porastom koncentracije hitozana je primetan porast broja i jačine vodoničnih veza između funkcionalnih grupa PVA i CHI. Mikrofotografije površine uzoraka, dobijene skenirajućom elektronskom mikroskopijom, ukazuju na povećanje stepena amorfnosti i mikroporoznosti strukture hidrogela sa povećanjem koncentracije hitozana, ali i na postojanje krupnijih agregata srebra u matrici hidrogela.

Electrochemical synthesis and characterization of polyvinyl alcohol, chitosan and graphene based hydrogels with incorporated silver nanoparticles

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Silver/polyvinyl alcohol/chitosan/graphene (Ag/PVA/CHI/Gr) nanocomposite hydrogels for bio-medical applications were obtained by *in situ* electrochemical synthesis of silver nanoparticles in the matrix of polyvinyl alcohol/chitosan/graphene (PVA/CHI/Gr) hydrogels cross–linked by freezing–thawing method in 5 cycles. In order to investigate the influence of chitosan concentration, the hydrogels were synthesized with 0.1 wt. % and 0.5 wt. % CHI. The Ag/PVA/CHI/Gr hydrogels were characterized using UV–visible spectroscopy, which proved the presence of spherical silver nanoparticles in the hydrogel structure, and cyclic voltammetry, for determination of electrochemical properties. Infrared spectra of hydrogels with and without silver exhibited differences in positions and intensities of absorption bands, pointing to coordination bonding of silver and –OH and $–NH_2$ groups on the polymer chain. The increase in chitosan concentration increases the strength and quantity of hydrogen bonds between the functional groups of PVA and CHI. Scanning electron microscopy pointed to more amorphous and more porous structure of hydrogels with higher concentration of chitosan, but also to presence of larger silver aggregates in the hydrogel matrix.

MN O 04

Mikrosfere na bazi triblok kopolimera PCL/PEO/PCL za kontrolisano otpuštanje ibuprofena

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Biodegradabilni, alifatski poliestri, kao što je poli(ε-kaprolakton), PCL i njegovi kopolimeri i blende, se poslednjih decenija intenzivno ispituju kao sistemi za kontrolisano otpuštanje lekova. Mikrosfere na bazi triblok kopolimera, poli(ε-kaprolaktona) i poli(etilen-oksida), PEO, sa različitim sadržajem leka, ibuprofena, (10 i 20 mas%) su dobijene postupkom otparavanja lako isparljivog rastavarača iz emulzije. Ispitan je uticaj uvođenja kratkog, hidrofilnog, centralnog PEO segmenta u lance PCL-a na efikasnost inkapsulacije, veličinu mikrosfera i otpuštanje leka iz polimerne matrice. Kompatibilnost polimerne matrice i inkapsuliranog leka, kao i promene u vrednosti indeksa kristaliničnosti nakon inkapsulacije leka, ispitane su FTIR analizom. Optičkom mikroskopijom i SEM analizom je određena veličina čestica i njihova raspodela. Efikasnost inkapsulacije ibuprofena kao i otpuštanje leka iz polimernih mikrosfera je praćeno u fosfatnom puferu (pH 7,4 na 37 °C) tokom 72 h pomoću UV/Vis spektrofotometrije. Profili otpuštanja leka iz svih mikrosfera su pokazali inicijalno brzo otpuštanje leka ("burst" efekat), kao i ubrzano otpuštanje leka iz blok kopolimerne matrice sa većim sadržajem PEO. Primenom matematičkih modela na profile otpuštanja leka, potvrđeno je da se ibuprofen iz PCL/PEO/PCL matrice otpušta mehanizmom *Fikove* difuzije.

PCL/PEO/PCL block copolymer microspheres for controlled ibuprofen release

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Biodegradable, aliphatic polyesters, such as poly(ε-caprolactone), PCL, and its copolymers and blends, have been intensively investigated in a last few decades as a system for controlled drug release. Microspheres based on triblock copolymers, poly(ε-caprolactone) and poly(ethylene oxide), PEO, with different concentration of drug, ibuprofene, (10 and 20 mas%) were prepared by classical oil-in-water emulsion solvent evaporation technique. The influence of the introduction of a short, hydrophilic, central PEO segment in PCL chains on efficiency of encapsulation, microspheres' size and drug release from polymer matrix was also tested. Compatibility among the polymer matrix and encapsulated drug, as weel as the changes in crystallinity index after drug encapsulation, were investigated via FTIR analysis. Microspheres' size distribution was estimated by optical microscopy and SEM analysis. The efficiency of encapsulation as well as drug release from polymer microspheres was followed in phosphate buffer solution (pH 7.4 at 37 °C) during 72 h by using UV/VIS spectrophotometry. The drug release profiles of all polymer microspheres showed burst effect as well as faster release from the block copolymer matrix with higher PEO content. Applying different mathematical models for drug release profiles from polymer matrix, it was determined that the mechanism of ibuprofen release from PCL/PEO/PCL, was *Fickian* diffusion.

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MN P 01

Thermal stability of PMMA nanocomposites with carbon nanostructures

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The field of polymer nanocomposites in the last two decades has generated much interest due to the unique design possibilities and the surprising property combinations. In addition to being environmentally-friendly, their potential is promising for many diverse applications, such as aerospace components, automobiles, sensors, construction and electronics.
Poly(methyl methacrylate) (PMMA) nanocomposite with concentrations of single-walled nanocarbontubes (SWNCT), multi-walled nanocarbontubes (MWNCT) and graphene were synthesized by solvent casting method followed by 30-minute ultrasound treatment. The nanocomposites were evaluated for their thermal stability conducting thermogravimetric analysis (TGA) on PerkinElmer D7 System. The obtained data were analyzed for the effect of introducing the nanofillers in polymer matrix. The dispersion of carbon nanostructures within the polymer matrix was characterized by using SEM. It was determined that the morphology varies from spherulitic to fibrillar to undefined depending on the fraction of reinforcement. RAMAN spectra of the nanocomposites were scanned as well.

MN P 02

Razgranati poli(ε-kaprolaktoni) kao nosači za isporuku ibuprofena

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Biodegradabilni, alifatski poliestri, kao što je poli(ε-kaprolakton), PCL, poslednjih godina nalaze sve veću primenu u oblasti biomedicine. Serija razgranatih poliestara, sa različitim brojem grana (3R, 4R), sintetisana je polimerizacijom otvaranja prstena ε-kaprolaktona inicirana hidroksilnim grupama višefunkcionalnih alkohola: trimetilolpropana (TMP), pentaeritritola, (PERT) i di(trimetilolpropana), (diTMP), u prisustvu kalaj(II)-oktoata kao katalizatora. Dužina grana PCL-a je iznosila 5000 g/mol. Struktura i sastav dobijenih poliestara su ispitane NMR i GPC analizom, dok su termička svojstva analizirana DSC-om i TG-om. Dobijeni poliestri sa različitim brojem grana su korišćeni kao matrice za inkapsulaciju ibuprofena. Mikrosfere sa različitim sadržajem leka (10 i 20 mas %) dobijene su postupkom otparavanja lako isparljivog rastavarača iz emulzije. Ispitan je uticaj broja PCL grana i vrste jezgra na efikasnost inkapsulacije, veličinu mikrosfera i profil otpuštanja leka iz polimerne matrice. Efikasnost inkapsulacije ibuprofena je određena direktnom i indirektnom metodom pomoću UV/Vis spektrofotometrije. Dobijene mikrosfere su ispitivane FTIR analizom i optičkom mikroskopijom. Otpuštanje leka iz polimernih mikrosfera je praćeno u fosfatnom puferu (pH 7,4 na 37 °C) tokom 72 h pomoću UV/Vis spektrofotometrije na talasnoj dužini λ = 221 nm.

Star-shaped poly(ε-caprolactone)s as ibuprofen release carriers

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Biodegradable, aliphatic polyesters, such as poly(ε-caprolactone), PCL, have been intensively used in biomedical application in a last few years. Series of star-shaped polyesters with different number of branches, were synthesized by ring-opening polymerization initiated by hydroxy groups of multifunctional alcohols: trimethylolpropane (TMP), pentaerythritol (PERT), and di(trimethylolpropane) (diTMP) in the presence of tin(II) octoate as a catalyst. PCL branch lenght was fixed of 5000 g/mol. The structure and the composition of the obtained polyesters were determined by NMR and GPC anlysis, while thermal properties were analized by DCS and TGA. The obtained polyesters were used as matrix for ibuprofen encapsulation. Microspheres with different concentration of drug (10 and 20 wt%) were prepared by classical oil-in-water emulsion solvent evaporation technique. The influence of the number of PCL branches and type of the core on efficiency of encapsulation, microspheres' size and drug release profile was also tested. The efficiency of encapsulation was determined using direct and indirect method by UV/VIS spectrophotometry. Microspheres were investigated by FTIR analysis and optical microscopy. Drug release profiles from polymer microspheres was followed in phosphate buffer solution (pH 7.4 at 37 °C) during 72 h using UV/VIS spectrophotometry at wavelenght of λ = 221 nm.

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MN P 03

Uticaj organski modifikovanih nanočestica gline na svojstva poli(uretan-siloksanskih) nanokompozita

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Serija poli(uretan-siloksanskih) nanokompozita (PUSN) je sintetisana na bazi 4,4'-metilendifenil-diizocijanata i 1,4-bitandiola kao komonomera tvrdih segmenata i poli(propilenoksid)-*b*-poli(di-metilsiloksan)-*b*-poli(propilenoksida) kao dela mekih segmenata. Ispitan je uticaj dodatka nanočestica organomodifikovane gline (Cloisite 30B®) na termička, mehanička, površinska i mor-fološka svojstva ovih PUSN-a. TGA analiza je potvrdila da dodatak nanočestica gline u iznosu od svega 1 mas. % vodi do poboljšanja termičke stabilnosti PUSN-a za ~15 ºC. Vrednosti modula elastičnosti i zateznih čvrstoća su takođe bile povećane posle ojačanja poli(uretan-siloksanske) matrice sa nanočesticama gline. XPS analiza je potvrdila veliko prisustvo atoma Si na površini filmova, zbog čega ovi PUSN nanokompoziti poseduju izrazito veliku hidrofobnost površina. TEM analiza je pokazala homogenu disperziju nanočestica gline i njihovu mešovitu interkalarno-eksfoliranu morfologiju unutar strukture PUSN-a.

Effects of organically modified clay nanoparticles on the properties of poly(urethane-siloxane) nanocomposites

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Series of poly(urethane-siloxane) nanocomposites (PUSN) was synthesized based on 4,4'-methylenediphenyldiisocyanate and 1,4-butanediol as the comonomers of the hard segments and poly(propyleneoxide)-*b*-poly(dimethylsiloxane)-*b*-poly(propyleneoxide) as the part of the soft segments. The effect of the addition of nanoparticles of organomodified clay (Cloisite 30B®) on thermal, mechanical, surface and morphological properties of these PUSNs was investigated. TGA analysis confirmed that the addition of clay nanoparticles in the amount of only 1 wt. % leads to an improvement of the thermal stability of the PUSNs for ~15 ºC. Modulus of elasticity and tensile strength were also increased after the reinforcement of poly(urethane-siloxane) matrix with clay nanoparticles. XPS analysis confirmed the presence of a large quantity of Si atom on the surface of the films, which is why these PUSNs exhibit extremely high surface hydro-phobicity. TEM analysis revealed homogeneous dispersion of clay nanoparticles and existance of mixed intercalary-exfoliated morphology within the structure of PUSNs.

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Hemija hrane - Food Chemistry

HH P 01

Primena lekovitog bilja u pekarskim proizvodima

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Poslednjih godina u naučnim istraživanjima sve više pažnje se posvećuje hrani, koja pored unosa korisnih materija u cilju pravilnog rasta i razvoja organizma, ispoljava i blagotvorne efekte na ljudsko zdravlje. Usled svakodnevne konzumacije, hleb i pekarski proizvodi zauzimaju jedno od vodećih mesta u tehnologiji proizvodnje novih prehrambenih proizvoda i razvoja funkcionalnih proizvoda. U cilju istraživanja aktivnosti lekovitog bilja, u ove pekarske proizvode dodaju se ekstrakti biljaka koje se tradicionalno primenjuju u narodnoj medicini. Neke od njih su: kim, korijander, morač, nana, žalfija, divlja ruža i ruzmarin. Cilj ovog rada jeste prikaz mogućih primena lekovitog bilja u funkcionalnim pekarskim proizvodima sa dodatnom vrednošću. Zahvaljujući sinergističkom delovanju bioaktivnih metabolitia ovih biljaka, zapažen je pozitivan efekat na zdravlje ljudi, a posebno kod osoba koje imaju poremećaj u radu digestivnog trakta. Proizvodi koji su ispitani pokazuju dodatne aktivnosti, kao što su: antimikrobna, citotoksična, antitumorska i antiinflamatorna aktivnost.

Medical plant application in baking industry

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In recent years, one of the goal of scientific research is food, which, in addition to the rich nutritional value, manifest beneficial effects on human health. Due to the daily consumption of bread and bakery products occupy a leading position in the technology of new food products and the development of functional products. In order to investigate the activities of medicinal plants in the bakery products are added to extracts of plants that are traditionally used in medicine. Some of them are: cumin, coriander, fennel, mint, sage, wild rose and rosemary. The objective of this study is to show possible applications of medicinal plants in the functional bakery products with added value. Thanks to the synergistic effect of bioactive metabolites of these plants, there is a positive effect on human health, especially in people who have the disorder in the work of the digestive tract. Products that have been tested indicate other activities, such as antimicrobial, cytotoxic, antitumor and antiinflammatory activity.

HH P 02

Antiproliferativna aktivnost *G. applanatum* (Pers.) Pat. 1887

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Ganoderma applanatum, pripada familiji *Ganodermataceae* i smatra se višegodišnjom gljivom koja raste na panjevima listopadnog drveća. Poznato je da poseduje antimikrobne, antiproliferativne, antidijabetogene i antioksidantne efekte. Za ove aktivnosti se smatra da su od velikog značaja polisaharidi i fenolna jedinjenja.

Antiproliferativna aktivnost vodenih i etanolnih ekstrakata na estrogen-zavisnu ćelijsku liniju kancera dojke (MCF-7) je ispitana MTT testom. Rezultati ukazuju na jaču antiproliferativnu aktivnost primenjenih etanolnih u odnosu na vodene ekstrakte (748,79 μg/ml i 968,30 μg/ml nakon 24 h). Inhibicija proliferacije MCF-7 ćelija primenom etanolnih i vodenih ekstrakata nakon 72 h inkubacije ukazuje na inhibiciju ćelijske proliferacije pri koncentracijama od 177,46 μg/ml i 678,89 μg/ml.

Ukupni fenolni sastav ispitivanih ekstrakata varira od 18,73 mg ekv. GK /g s.m. do 265,38 mg ekv. GK/g s.m. (EtOH ekstrakt). Ukupni fenoli etanolnih ekstrakata pokazuju visoku korelaciju sa antiproliferativnom aktivnošću (r^2=0,98-0,99).

Dobra antiproliferativna aktivnost je direktno povezana sa sadržajem ukupnih fenola i ovi rezultati ukazuju na opravdanu tradicionalnu upotrebu ove vrste gljiva kao potencijalnog terapeutika.

Antiproliferative activity of *G. applanatum* (Pers.) Pat. 1887

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Ganoderma applanatum, which belongs to the *Ganodermataceae* family, is a perrennial fungal species growing as a saprotroph on the stumps of deciduous trees. It is known to possess antimicrobial, antiproliferative, antidiabetic and antioxidant effects. Most of these actions are believed to be due to its polysaccharidic and phenolic compounds.

Water and ethanolic extract's antiproliferative effect against estrogen dependent breast cancer cell line (MCF-7) were examined by MTT assay. The results showed higher antiproliferative activity of ethanolic than water extracts applied (748,79 μg/ml and 968,30 μg/ml after 24 h, respectively). The inhibition of proliferation of MCF-7 cells obtained for ethanolic and water extracts after 72 h of incubation achieved inhibition of cell proliferation at 177,46 μg/ml and 678,89 μg/ml, respectively.

Total phenol content in the examined extracts varied from 18,73 mg GA eq/g d.w. to 265,38 mg GA eq/g d.w. (EtOH extract). Total phenolics in ethanolic extracts showed high linear correlation with antiproliferative activity (r^2=0,98-0,99, respectively).

Good antiproliferative activity is directly related to content of total phenolics and these results could help justifying traditional use of these fungal species as potential therapeutics.

HH P 03

Toksični metali u biljnim čajevima: određivanje As, Cd i Pb upotrebom AAS

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Čaj predstavlja napitak koji se koristi širom sveta. Veoma je važno u samim biljkama čaja odrediti ukupan sadržaj metala, kao i sadržaj metala koji se oslobađa kuvanjem, kojem su ljudi izloženi prilikom konzumiranja. As, Cd i Pb smatraju se prioritetnim metalima čije koncentracije je neophodno kontrolisati zbog visoke toksičnosti, a samim tim i štetnih efekata po zdravlje ljudi. Svetska zdravstvena organizacija odredila je maksimalne dozvoljene vrednosti ovih metala u suvoj masi biljaka i to su 1.0 (As), 0.3 (Cd) i 10 (Pb) mg kg^{-1}. Cilj ovog rada je bio analiza devet uzoraka komercijalnih čajeva i određivanje sadržaja As, Cd i Pb (ukupnog sadržaja i sadržaja u vodenom rastvoru nakon kuvanja od 5 minuta) koristeći atomski apsorpcioni spektrometar. Ukupan sadržaj Pb i As je u svih devet uzoraka bio ispod maksimalne dozvoljene vrednosti, ali su zapažene varijacije između različitih uzoraka. Sa druge strane, Cd je imao veće vrednosti u nekoliko uzoraka, među kojima su se izdvojili kantarion i hajdučka trava. Ipak, te veće vrednosti ukupnog sadržaja kadmijuma ne moraju predstavljati opasnost po zdravlje jer je bitna ona koncentracija metala koja se otpusti u vodi tokom kuvanja čaja. U vodenim ekstraktima svih uzoraka, As i Pb su bili ispod limita detekcije, dok je Cd detektovan u kantarionu, majčinoj dušici i uvi. Ipak, njegova ekstrakciona efikasnost je bila niska, odnosno ispod 20 %.

Toxic metal in herbal teas: determination of As, Cd and Pb using AAS

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Tea is the popular beverage used worldwide. It is very important to determine the total metal content in these plants, as well as the extractable component of metals that is available to humans when consuming tea. As, Cd and Pb are considered toxic elements and due to their adverse effect on humans and high degree of toxicity, they rank among the priority metals concerning public health. Maximum permissible levels for As, Cd and Pb in the dry mass of plants has been established by the World Health Organization (WHO) (1.0, 0.3 and 10 mg kg^{-1}, respectively). The aim of this study was to analyze nine different samples of commercial herbal teas and to determine the content of As, Cd and Pb (the total metal content and the content in the tea infusion after boiling for 5 minutes) using the atomic absorption spectrometer. The total content of Pb and As in all nine tea samples were below the maximum permissible levels, but significantly varied among different tea samples. On the other hand, higher amounts of Cd were found in some samples, highest in St John's wort and yarrow. However, the higher total content of Cd may not be potential health hazards, since it's released content in the tea infusion represent the concentration of which man is exposed when consumed tea. In all herbal tea infusions, As and Pb were below our detection limit, while Cd, was detected in St John's wort, thyme and bearberry. However, its extraction efficiencies were low, below 20 %.

HH P 04

Određivanje fluorida u biljnim čajevima jonskom hromatografijom

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Poslednjih godina, čovečanstvo se sve više okreće tradicionalnoj medicini sa što manjom upotrebom komercjalno dostupnih lekova. Jedan od takvih načina lečenja je konzumiranje biljnih čajeva. Opšte je poznato da biljni čajevi imaju pozitivno dejstvo na ljudsko zdravlje zbog svojih esencijalnih elemenata, ali čak i supstance koje imaju pozitivni efekt na ljude mogu biti toksične ukoliko dođe do akumulacije u organizmu. Fluoridi su veoma značajni u malim koncentracijama, omogućavaju zdrav rast kostiju i učestvuju u očuvanju zubne gleđi. Međutim u velikim koncentracijama postaju veoma toksični izazivajući dentalnu i skeletnu fluorozu. U ovom radu ispitivali smo koncentraciju fluorida u vodenim ekstraktima biljnih čajeva (glog, hajdučka trava, kantarion, zova, kopriva, majčina dušica, nana i uva) jonskom hromatografijom. Posmatran je uticaj različitih načina pripreme i kiselosti (dodatkom limuna) na oslobađanje fluorida. Dobijeni rezultati pokazuju da se najniža koncentracija fluorida oslobađa kod hajdučke trave dok su se čaj od zove i glog izdvojili sa najvišim koncentracijama. Uočeno je da se koncentracija fluorida u nezakišeljenim i zakišeljenim vodenim ekstraktima biljnih čajeva značajno ne razlikuje u većini uzoraka.

Determination of fluoride in herbal teas by ion chromatography

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In the last few years, humanity is increasingly turning to traditional ways of treatment, with reduced use of common available drugs. One of those ways of treatment is the consumption of the herbal teas. It is known that herbal teas have a positive effect on human health because of its essential ingredients, but even substances that have a positive impact can become toxic due to their accumulation in organisms. Fluoride is very important in low concentrations, enabling healthy bone growth and participating in the preservation of tooth enamel. However, in high concentrations, fluoride become very toxic, causing dental and skeletal fluorosis. The aim of this study was to determine the concentration of fluoride in water extracts of herbal teas (hawthorn, yarrow, St John's wort, elder, nettle, thyme, mint and bearberry) using ion chromatography. The influence of different procedures of making tea and the acidity of the infusion (by adding lemon juice) on fluoride releasing was observed. The results show that the lowest concentration of fluoride was released from yarrow, while elder and hawthorn singled out with the highest concentrations. It is noticed that the concentracion of fluoride in unacidified and acidified herbal tea water extracts showed similar values in many samples.

HH P 05

Određivanje koncentracije srebra, selena i arsena u divljim pečurkama *Macrolepiota procera*

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Divlje pečurke mogu imati visok sadržaj esencijalnih, ali i za ljude toksičnih elemenata. One akumuliraju metale absorbujući ih iz podloge pomoću micela ili rizomorfi. U našem radu ispitan je sadržaj i bioakumulacija mikroelemenata (As, Se i Ag) u divljim, jestivim pečurkama *Macrolepiota procera* i u odgovarajućim podlogama zemljišta, koji su prikupljeni sa pet različitih lokacija u Rasinskom okrugu, centralna Srbija. Analizirani uzorci pečuraka su podeljeni na šešire i drške. Sadržaj Ag, As i Se u svim uzorcima je određen pomoću ICP-MS metode. Na osnovu dobijenih rezultata izračunati su biokoncentracioni i translokacioni faktori. U zavisnosti od lokacije uzorkovanja, sadržaj metala u pečurkama se razlikovao. U svim uzorcima u najvećim koncentracijama zastupljeno je srebro (4,1 mg/kg dw u šeširima i 8,3 mg/kg dw u drškama) dok se Se i As javljaju u znatno manjoj količini (1,0 mg/kg dw u šeširima i 0,9 mg/kg dw u drškama). BCF vrednosti za As i Se bile su ispod jedinice, što ukazuje da ova pečurka ne usvaja ove elemente iz zemljišnog supstrata. Sa druge strane, BCF vrednosti za Ag bile su veće od jedinice, ali stepen akumulacije zavisi od lokacije uzorkovanja. TF vrednosti pokazuju da ova vrsta pečurke akumulira Ag pre svega u drškama, dok su As i Se podjednako zastupljeni u telu pečuraka.

Determination of silver, selenium and arsenic concentration in wild mushrooms *Macrolepiota procera*

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Wild mushrooms may have high content of both essential and toxic elements to humans. They accumulate metallic elements by absorbing them from the soil substrate via mycelia and rhizomorphs. The content and bioaccumulation of trace elements (Ag, Se, As) in wild, edible mushroom *Macrolepiota procera* and its corresponding soil substrates, collected from five sites in the Rasina region in central Serbia, were investigated. In our study, all mushroom samples were separated into caps and stipes. The content of Ag, As and Se in all samples were determined by ICP-MS. Based on the given results, bioconcentration and translocation factors were calculated. Concentration of elements in mushrooms samples depends on location of collection site. In all samples, silver is element with highest content (4,1 and 8,3 mg/kg dw in caps and stripes, respectivly) while contents of Se and As were lower (1,0 i 0,9 mg/kg dw in caps and stripes, respectivly). For Se and As, BCF values were below 1, which means that these mushrooms have not ability to acumulate these element from soil. On the other hand, BCF values for silver in all the sites showed efficient accumulation of silver (BCF values higher than 1), but the extent of accumulation depended on the collection site. From the calculated TF values it was concluded that silver is more abundant in stipes compared to caps, while Se and As were equally distributed between two parts of mushroom.

HH P 06

Procena dnevnog unosa esencijalnih i toksičnih elemenata konzumirajući srpska vina

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Obzirom da je vino jedno od najpopularnijih pića na svetu, ali i činjenica da je bogatog elementarnog sastava, nameće se pitanje koliko se esencijalnih i toksičnih elemenata unese dnevnim konzumiranjem. Ispitivana vina potiču iz vinarije Radmilovac, Beograd. Koncentracije elemenata određene su ICP-OES i ICP-QMS metodom. Zapremina od 100 mL crvenog i belog vina, prosečna težina konzumera od 70 kg[1] i preporučeni dnevni unosi (RDA)[2] su korišćeni za računanje dnevnog mineralnog unosa (DMI) za esencijalne elemente (K, Ca, Mg, Mn i Cu); DMI=Cx100/RDA. Na osnovu dobijenih rezultata uočeno je da crveno vino obezbeđuje značajan unos K i Mg (3,38 %, 2,60 %, respektivno), dok je belo vino dobar izvor Ca, Cu i Mn (1,06 %, 6,75 % i 4,37 %, resektivno). Privremeno podnošljivi nedeljni unos (PTWI)[3] je korišćen za računanje dnevnog unosa toksičnih elemenata (As, Cd i Pb). Najveći doprinos dnevnom unosu daje Pb (2,06 % za crvena i 3,59 % za bela), dok za As i Cd dnevni unos u ispitivanim vinima ne prelazi 1,50 %. Stoga, procena dnevnog unosa toksičnih elemenata uz potrošnju od 100 mL crvenog i belog vina ne predstavlja toksikološki rizik.

The estimate of the daily intake of essential and toxic elements consuming Serbian wines

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Considering that wine is one of the most popular drinks in the world, but the fact that it is rich in elemental composition, the question is how is essential and toxic elements enter daily consumption. Analyzed wines originate from winery Radmilovac, Belgrade. Concentration of elements were determined by ICP-OES and ICP-QMS method. Volume of 100 mL of red and white wine, the average consumer with a body weight of 70 kg[1] and the Recommended Daily Intake (RDA)[2] were used for the calculation of Daily Mineral Intake (DMI) for essential elements (K, Ca, Mg, Mn and Cu); DMI=CX100/RDA. Based on obtained results, it was noted that red wine provides a significant intake of K and Mg (3.38 %, 2.60 %, respectively), while white wine good source of Ca, Cu and Mn (1.06 %, 6.75 % and 4.37 %, respectively). Provisional Tolerable Weekly Intake (PTWI)[3] is used to calculate the daily intake of toxic elements (As, Cd and Pb). The largest contribution to the daily intake provides Pb (2.06 % for red and 3.59 % for white), while for As and Cd daily intake in the studied wines do not exceed 1.50 %. Therefore, estimates of daily intake of toxic elements with a consumption of 100 mL of red and white wine does not represent a toxicological risk.

Reference:

1. European Food Safety Authority. (2012). *EFSA Journal*, *10*(3), 2579.
2. Official Journal of the European Union, Commission Directive 2008/100/EC.
3. N. Czipa, D. Andràsi and B. Kovàcs. (2015). *Food chemistry*, *175*, 536-542.

HH P 07

Uticaj vremena zrenja i botaničkog porekla na sadržaj elemenata u semenima gajenog i samoniklog voća

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Duga tradicija gajenja voća i povoljni klimatski uslovi u Srbiji omogućavaju veoma uspešnu i raznoliku proizvodnju bobičastog voća. Kako se seme ovog voća konzumira zajedno sa plodom njegova uloga u ljudskoj ishrani je značajana. Cilj ovo rada je utvrđivanje kriterijuma za klasifikaciju i razlikovanje gajenog od samoniklog voća, kao i potencijalnih razlika između pojedinih botaničkih vrsta, na osnovu sadržaja elemenata određenih induktivno spregnutom plazmom – optičko emisionom spektometrijom (ICP-OES) u kombinaciji sa nekoliko hemometrijskih tehnika. U uzorcima gajenog voća uočeno je postojanje tri različite grupe objekata. Sorte maline, kupine i borovnice formiraju prvi klaster, dok drugu grupu čine uzorci ribizle i ogrozda. Osatak uzoraka gajenog voća čini treću grupu. S druge strane uzorci semena samonikle borovnice, jagode i ribizle su jasno razdvojeni od odgovarajućih uzoraka gajenog voća. Drugi aspekt ovog rada je rešavanje problema industrijskog otpada i povećanje ekonomske efikasnosti eksploatacije različitih semenki voća, koje se odbacuju svake godine kao sporedni proizvodi u industrijskoj proizvodnji džema, soka, konzervirane hrane i alkoholnih pića.

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Effect of ripening time and origin on element profile in wild and cultivated friut seeds

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A long tradition of fruit cultivation and favourable climatic conditions in Serbia enables a very successful and diverse berry fruit production. Fruit seeds are consumed together with a fruit and hence they have important role in humans diet. Aim of this work was to establish criteria for classification and differentiation of cultivated and wild fruits, and different botanical species, based on elements content determinated by inductively coupled plasma – optical emission spectrometry (ICP-OES) in combination with several chemometric techniques. Based on element content cultivated fruit samples differentiated in three distinctive groups according to botanical origin. Cultivars of raspberry, blueberry and blackberry seeds formed first cluster, while the second compact group is made of gooseberry and currant seeds. The rest of the samples of cultivated fruit formed the third group. On the other side, samples of wild blueberry, strawberry and currant seeds were clearly separated offrom the appropriate cultivated fruit seeds. Another aspect of this work was to solve the problem of disposal of industrial waste and increase the economic efficiency of exploitation of different fruit seeds which are discarded every year, as a by-products, during the processing in the fruit industrial production of jam, juice, canned food and the beverage.

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HH P 08

Sadržaj minerala i teških metala u košticama šljiva različitog porekla i perioda zrenja

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Šljiva se najčešće konzumira u svežem obliku, ali se u značajnim količinama upotrebljava i u industriji kao sirovi materijal za različite proizvodne procese. Trenutno, velike količine semena se odbacuju svake godine tokom proizvodnje što predstavlja potencijalni gubitak resursa zbog značajnih količina ulja, proteina, vlakana, polifenola i minerala prisutnih u semenu šljiva, kao i ozbiljan problem odlaganja otpada. Cilj istraživanja je bio da istakne značaj semena šljiva kroz karakterizaciju statistički značajnog broja uzoraka različitog porekla i vremena zrenja kroz sadržaj esencijalnih i teških metala. Količine 20 elemenata (Ca, Mg, K, Na, P, Al, S, As, Ba, Cd, Co, Cr, Cu, Hg, Mn, Ni, Pb, Sr and Zn) određene su pomoću i*nduktivno spregnute* plazma atomskog emisionog spektrometra (ICP-OES), kao i i*nduktivno spregnute* plazme sa masenim spektrometrom (ICP-MS). Multivarijantnom obradom dobijenih rezultata analizirani uzorci su klasifikovani prema botaničkom poreklu i vremenu zrenja, a takođe je utvrđen uticaj poplava na sadržaj elemenata u uzorcima iz dve uzastopne godine.

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

Mineral and heavy metal composition of plum kernels differing in origin and ripening time

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Plum fruits are in most cases intended for fresh market consumption, but also they are largely used in the industry as raw material for various types of processing. Currently, large amounts of plum seeds are discarded yearly in different producing industries which is a potential waste of valuable resource due to the substantial amounts of oil, proteins, fibers, phenolics, and minerals, and serious disposal problem together. This study aim to emphasize the importance of plum seeds by characterization of essential and heavy metals composition of statistically significant number of cultivars differing in origin and ripening time. The amounts of 20 elements (Ca, Mg, K, Na, P, Al, S, As, Ba, Cd, Co, Cr, Cu, Hg, Mn, Ni, Pb, Sr and Zn) were determined by inductively coupled plasma optical emission spectrometer (ICP-OES) and inductively coupled plasma mass spectrometer (ICP-MS). Application of multivariate data analysis enabled us to differentiate particular botanical family and maturity stage, and to compare metal content in the same species of plum seeds from two differente years with the aim to investigate influence of flood on metal content.

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HH P 09

Uticaj herbicida na sadržaj karotenoida u listu kukuruza šećerca

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Karotenoidi predstavljaju jednu od najvažnijih klasa biljnih pigmenata i imaju važnu ulogu u foto-zaštiti prilikom procesa fotosinteze, prevenciji u foto-oksidativnim oštećenjima i prekusorsi su u sintezi fitohormonske abscisinske kiseline (ABA). Cilj ovog rada bio je ispitivanje promene sadržaja karotenoida u listu dva hibrida kukuruza šećerca u dve faze: faza I-48 h i faza II- 2 nedelje nakon primene dva herbicida (mezotrion i nikosulfuron). Sadržaj luteina + zeaksantina i β-karotena određen je primenom visoko efikasne tečne hromatografije (HPLC). U obe faze, nakon primene mezotriona, sadržaj luteina + zeakstantina u listu oba hibrida bio je viši u odnosu na kontrolu (bez primene herbicida). Suprotno, sadržaj β-karotena u listu hibrida I, bio je veći u fazi I, ali manji u fazi II. U listu hibrida II, sadržaj β-karotena bio je veći u obe faze u poređenju sa kontrolom. Nakon primene nikosulfurona, koncentracija karotenoida u listu hibrida I, bila je veća u fazi I, dok je u fazi II bila niža u odnosu na kontrolu. U listu hibrida II, sadržaj karotenoida bio je niži u fazi I, odnosno viši u fazi II. Promene u sadržaju karotenoida u listu, mogu se smatrati anti-oksidativnim mehanizmom odbrane biljke usled stresa prouzrokovanim primenom herbicida.

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Herbicide impact on carotenoids content in sweet maize leaves

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Carotenoids form one of the most important classes of plant pigments and play a crucial role in photo-protective functions during photosynthesis, prevention of photo-oxidative damage, and serving as precursors for the phytohormone abscisic acid (ABA). The aim of this study was to investigate the changes in carotenoids content in leaves of two sweet maize hybrids, in two phases: phase I -48 h and phase II- 2 weeks after application two herbicides (mesotrione and nicosulfuron). Content of lutein + zeaxanthin and β-carotene was determinate by high per-formance liquid chromatography (HPLC). In both phases, after mesotrione application content of lutein + zeaxanthin in leaves from both hybrids was higher compare to control (no herbicide application). Opposite, content of β-carotene in leaves from hybrid I, was higher in phase I and lower in phase II. In leaves from hybrid II content of β-carotene was higher in both phases compare to control. In phase I, after application of nicosulfuron, carotenoids concentration in leaves from hybrid I was higher, while in phase II was lower compared to control. In leaves from hybrid II, the content of carotenoids was lower in phase I and higher in phase II. Variations in carotenoids content in leaves can be considered as antioxidant defense mechanism of the plant due to the stress caused by the herbicide application.

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HH P 10

Određivanje sadržaja metala u listu koprive ICP-OES metodom analize

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Kopriva (*Urtica dioica* L.) je samonikla biljka sa izuzetno širokim spektrom biološke aktivnosti. Ova biljka ima široku primenu u narodnoj medicini, u ishrani, u prehrambenoj industriji za proizvodnju čajeva i kao izvor zelenog pigmenta hlorofila (E140). Sadržaj elemenata i minerala u listu koprive određen je primenom metode indukovane kuplovane plazme-optičke emisione spektroskopije (ICP-OES). Dobijeni rezultati ukazuju na veliku sadržaj makroelemenata: natrijuma, kalijuma, kalcijuma i magnezijuma u količinama od 0,30; 27,96; 9,57 i 2,00 mg/g, redom. Od mikroelemenata najzastupljenije je gvožđe (24,75 μg/g), dok je sadržaj mangana, cinka i bakra nešto niži (14,74; 3,84 i 1,78 μg/g, redom). Sa druge strane, analiza je pokazala izuzetno nizak sadržaj teških metala (olova i kadmijuma) i arsena. Njihov sadržaj u listu koprive bio je 0,04; 0,01 i 0,08 μg/g, redom, dok prisustvo žive nije dokazano. Ovakav hemijski profil lista koprive ukazuje na mogućnost njenog korišćenja u ishrani kao izvor za organizam neophodnih elemenata i minerala.

Elemental profile of stinging nettle leaves obtained by ICP-OES analysis

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Stinging nettle (*Urtica dioica* L.) is wild growing annual plant known for its wide range of biological activities. It has been used for a long time in human nutrition and folk medicine. In these days it founds its application in food industry as a source of green pigment chlorophyll (E140) and as a tea. Elemental analysis of stinging nettle leaves was performed using inductively coupled plasma atomic emission spectroscopy (ICP-OES). Obtained results revealed high contents of bulk elements sodium, potassium, calcium and magnesium (0.30, 27.96, 9.57 and 2.00 mg/g, respectively). Iron, manganese, zinc and copper were the most abundant microelements in stinging nettle leaves (24.75, 14.74, 3.84 and 1.78 μg/g, respectively). on the other hand, conducted analysis revealed presence of pollution elements (lead, cadmium and arsenic in rather trace levels (0.04, 0.01 and 0.08 μg/g, respectively), while presence of mercury was not confirmed. Such elemental composition of stinging nettle leaves indicated that this plant may be used as a significant source of essential elements for human organism.

Hemijska analiza - Chemical Analysis

HA P 01

Određivanje sadržaja vanadijuma u veštačkim jezerima u Srbiji

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Vanadijum je mikroelement široko rasprostranjen u zemljinoj kori u koncentraciji od ~100 μg/kg. U pijaćoj vodi sadržaj vanadijuma značajno zavisi od geografskog položaja i varira u opsegu od ~0,2 do preko 100 μg/L. Vanadijum u životnu sredinu uglavnom dospeva iz industrijskih izvora, posebno rafinerija nafte i energetskih postrojenja koja koriste mazut i ugalj bogat ovim elementom. Međunarodna agencija za istraživanje kancera (IARC) utvdila je da vanadijum ima potencijalno kancerogeno dejstvo na ljude (Grupa 2B).
Cilj istraživanja bio je određivanje sadržaja vanadijuma u slatkovodnim resursima u veštačkim jezerima u Srbiji: Savskom, Gružanskom, Ćelijama, Bovanskom, Garašima (centralna Srbija), Vrutcima (zapadna Srbija), Srebrnom (istočna Srbija), Vlasinskom i Prvoneku (južna Srbija). Sadržaj vanadijuma određen je analitičkom tehnikom induktivne kuplovane plazme sa optičkom emisionom spektrometrijom, ICP-OES. Koncentracija vanadijuma u ispitivanim uzorcima bila je u opsegu od 0,27 do 2,65 μg/L. U uzorcima vode jezera Ćelije, Vrutci i Gruža vanadijum je detektovan u koncentraciji od 1,39, 1,63 odnosno 2,65 μg/L, što je iznad maksimalno dozvoljene koncentracije (MDK) u vodi za ljudsku upotrebu (1μg/L). Dalje istraživanje biće usmereno na procenu uticaja ovog mikroelementa na zdravlje ljudi.

Determination of vanadium content in artificial lakes in Serbia

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Vanadium is a trace element widely distributed in the earth's crust at an average concentration of approximately 100 μg/kg. In drinking-water the content of vanadium depends significantly on geographical location, and may range from ~0.2 to more than 100 μg/L. Releases of vanadium to the environment are mainly associated with industrial sources, especially oil refineries and power plants using vanadium rich fuel oil and coal. The International Agency for Research on Cancer (IARC) has determined that vanadium is possibly carcinogenic to humans (Group 2B).
The aim of the study was to evaluate the content of vanadium in freshwater resources of the artificial lakes in Serbia: Savsko, Gruža, Ćelije, Bovan, Garaši (Central Serbia), Vrutci (West Serbia), Srebrno (East Serbia), Vlasina, and Prvonek (South Serbia). The content of vanadium was determined by the analytical technique inductively coupled plasma - optic emission spectrometry (ICP-OES). In water samples from the lake Ćelije, Vrutci, and Gruža vanadium was detected at a concentration of 1.39, 1.63 and 2.65 μg/L, respectively, which was above the maximum allowable concentration (MAC) in water for human use (1 μg/L). Further research will focus on the impact of this microelement to human health.

HA P 02

Primena zeolita tipa X izmenjenog jonima paladijuma za elektrolitičku proizvodnju vodonika

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Zeoliti se smatraju važnim katalizatorima zbog svoje jedinstvene strukture, mogućnosti da razmenjuju svoje jone, velike adsorpcione površine i visoke katalitičke aktivnosti. Uz to, paladijum se sve više istražuje kao zamena za skupu platinu. Zeolit tipa X izmenjen jonima paladijuma poslužio je kao materijal za izradu elektroda za ispitivanje reakcije izdvajanja vodonika u baznim uslovima. Elektroda je napravljena od zeolita i ugljenika, koji je dodat u cilju povećanja električne provodljivosti materijala. Struktura Pd X zeolita ispitana je rendgenskom strukturnom analizom. Elektrohemijska karakterizacija je urađena snimanjem ciklovoltamograma zeolit-ugljenik elektrode u 0,1 M rastvoru KOH. Elektrode su testirane za reakciju izdvajanja vodonika linearnom voltametrijom u 8 M KOH od potencijala otvorenog kola do -1,5 V brzinom od 10 mV s^{-1} i brzinom od 2 mV s^{-1} u temperaturskom opsegu od 25 °C do 85 °C. Impedansna merenja vršena su na tempereturi od 25 °C pri potencijalu otvorenog kola, -1,25 V, -1,35 V i -1,45 V, a zatim u temperaturskom opsegu od 25 °C do 85 °C pri potencijalu od -1,45 V. Test stabilnosti urađen je hronoamperometrijski. Na osnovu dobijenih rezultata su određeni kinetički parametri poput Tafelovog nagiba i energije aktivacije.

Application of zeolite X exchanged with Pd ions for electrolytical hydrogen generation

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Zeolites are important catalysts due to their unique structure, ability to exchange their ions, large adsorption area and high catalytic activity. Palladium is more and more investigated as a substitute for expensive platinum. Pd-ion exchanged form of X zeolite was used as material for the preparation of an electrode for hydrogen evolution reaction in alkaline conditions. Electrode was made of zeolite and carbon black, which was added in order to increase the electrical conductivity of the material. The structure of PdX was examined by X-ray diffraction analysis. Electrochemical characterisation was done by recording cyclic voltammogram of zeolite-carbon electrode in 0.1 M KOH solution. Electrode was tested for hydrogen evolution reaction using linear scan voltammetry in 8 M KOH from the open-circuit potential up to -1.5 V at a rate of 10 mV s^{-1} and 2 mV s^{-1} over a temperature range from 25 °C to 85 °C. The impedance measurements were conducted at temperature of 25 °C at the open circuit potential, -1.25 V, -1.35 V and -1.45 V, and then in range from 25 °C to 85 °C at a potential of -1.45 V. Stability test was done using chronoamperometry. Based on the obtained results, kinetic parameters such as Tafel slope and activation energy were determined.

HA P 03

Interkomparacijska merenja radioaktivnosti

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Laboratorija za zaštitu od zračenja i zaštitu životne sredine već godinama učestvuje u raličitim interkomparacijskim merenjima radioaktivnosti uzoraka iz životne sredine. Od specifičnih metoda koriste se spektrometrija gama emitera, određivanje ukupne alfa i beta aktivnosti, određivanje radona i određivanje beta emitera ^{90}Sr i ^{3}H. U ovakvoj vrsti međulaboratorijskih poređenja najvažnija je adekvatna priprema uzoraka. Primer jedne interkomparacije je IAEA-TEL-2015-03 world proficiency test za određivanje sadržaja prirodnih i proizvedenih radionuklida u vodi, pirinču i zemljištu koju organizuje Međunarodna Agencija za Atomsku Energiju. Za uzorke vode, pirinča i zemljišta uz zahtevanu analizu spektrometrije gama emitera, dobijena je ocena A (uspešan) (u jednoj vodi su detektovani proizvedeni radionuklidi ^{134}Cs, ^{137}Cs i ^{90}Sr, dok su u drugoj vodi detektovani ^{22}Na i ^{65}Zn, u pirinču su detektovani ^{134}Cs, ^{137}Cs i prirodni ^{40}K , a u uzorku zemljišta ^{137}Cs i ^{90}Sr i prirodni ^{238}U, ^{228}Ac, ^{214}Bi, ^{40}K, ^{214}Pb, ^{226}Ra i ^{235}U). Za uzorke vode uz zahtevanu analizu za merenje ukupne alfa i beta aktivnosti dobijena je ocena A (uspešan). Rezultati rada u okviru date interkomparacije ukazuju na to da je priprema uzoraka i kalibracija detektora HPGe za gamaspektrometrijsko merenje, kao i kalibracija gasnog proporcionalnog detektora za merenje ukupne alfa i beta aktivnosti urađena adekvatno.

Intercomparison measurements of radioactivity

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Radiation and Environmental Protection Department participate for years in various inter-comparison radioactivity measurements in environmental samples. Specific methods used for these measurements are gamma spectrometry, determination of gross alpha and gross beta activity, determination of radon and beta emitters ^{90}Sr and ^{3}H. In this kind of interlaboratory exercise the most important is an adequate sample preparation. An example of the inter-comparison is IAEA-TEL 2015-03 world-wide proficiency test for the determination of natural and anthropogenic radionuclides in water, rice and soil samples organized by the IAEA. With the required analysis of gamma spectrometry, the final score is A (accepted) (in the first water artifical radionuclides were detected ^{134}Cs, ^{137}Cs i ^{90}Sr, and in the second ^{22}Na and ^{65}Zn, in rice ^{134}Cs, ^{137}Cs and natural ^{40}K were detected, and in soil ^{137}Cs, ^{90}Sr and natural ^{238}U, ^{228}Ac, ^{214}Bi, ^{40}K, ^{214}Pb, ^{226}Ra i ^{235}U). For water samples with the required analysis gross alpha and beta activity final score was A (accepted). The results of this intercomparison indicate that the sample preparation and calibration of HPGe detectors for gamma spectrometry measurement and calibration of gas proportional detector for the measurement of gross alpha and beta activity performed adequately.

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HA P 04

Priprema uzoraka voda za merenje koncentracije tricijuma

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Tricijum (^{3}H), radioaktivni izotop vodonika, koji je dospeo u prirodu 60-tih godina veštačkim putem iz nuklearnih eksplozija, povećao je prirodni sadržaj ovog radionuklida u atmosferi i u vodama iz životne sredine. S obzirom na činjenicu da je srednja koncentracija tricijuma u vodama od 0,6 Bq l^{-1} do 2-3 Bq l^{-1}, uzorci moraju biti elektrolitički obogaćeni u cilju povećanja koncentracije. Parametri koji definišu sam proces elektrolize su: separacioni faktor, parametar obogaćenja, faktor obogaćenja. Priprema uzoraka obuhvata preliminarnu destilaciju, elektrolizu u setu elektrolitičkih ćelija koji sadrži uzorke voda i uzorke u kojima se nalazi poznata količina tricijuma, i sekundarnu destilaciju. Merenje se vrši na tečnom scintilacionom detektoru nakon mešanja 8 ml uzorka i 12 ml scintilacionog koktela. Pored uzoraka na detektoru se mere i mrtva voda za određivanje fona, voda obeležena tricijumom i standardni rastvor tricijuma. Na osnovu izmerenih koncentracija tricijuma mogu se odrediti parametri kao što su: sezonski indeksi, depozicija tricijuma na Zemljinu površinu i procena efektivne doze. Rezultati uzoraka dobijeni iz jedne elektrolize su sledeći: koncentracija tricijuma kreće se od 0,5 Bq l^{-1} do 3 Bq l^{-1} za 13 uzoraka padavina Zeleno Brdo, Zlatibor i Zaječar. Vrednost parametra obogaćenja za datu elektrolizu iznosi 0,9 dok je faktor obogaćenja 5. U Republici Srbiji postoji zakonska regulativa o dozvoljenim vrednostima koncentracije tricijuma jedino u vodi za piće (100 Bq l^{-1}).

Sample preparation for measurement of tritium concentration in water

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Tritium, which reached in the nature by nuclear explosions, increased the natural abundance of this radionuclide in the atmosphere and in the water. Tritium in natural water is very low and samples must be electrolytically enriched in order to increase the concentration. The parameters that define the process of electrolysis are: separation and enrichment factor and the enrichment parameter. Sample preparation includes a two distillations and electrolysis in a set of electrolytic cells. Measurement is carried out on a liquid scintillation detector (8 ml of the sample and 12 ml of scintillation cocktail). In addition to samples, dead water must be measured for background as well as standard solution of tritium. Based on the measured concentrations of tritium, parameters such as seasonal indices, tritium deposition, and effective dose can be determined. For 13 precipitation samples, tritium concentrations ranged from 0,5 Bq l^{-1} to 3 Bq l^{-1}. Enrichment parameter for a given electrolysis was 0,9 while the enrichment factor was 5. In Serbia there is legislation on allowable values for tritium concentration in drinking water (100 Bq l^{-1}).

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HA P 05

Ispitivanje uticaja alizarina na dinamiku Briggs-Rauscher oscilatorne reakcije

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Briggs-Rauscher (BR) oscilatorna reakcija je reakcija katalitičkog razlaganja vodonik-peroksida u kiseloj sredini u prisustvu organskog substrata-malonske kiseline, jodata i metalnog jona (Mn^{2+}) kao katalizatora. Nedavno je, primenom elektronske paramagnetne rezonantne (EPR) tehnike, detektovano prisustvo radikalskih vrsta ($HO^{\cdot}$, $IO_2^{\cdot}$, $HOO^{\cdot}$) u jodatnim oscilatorima. Alizarin (1,2- dihidroksiantrakinon, $C_{14}H_8O_4$) se koristi kao crveni pigment, najčešće u tekstilnoj industriji. S obzirom da su dva susedna atoma vodonika na antrakinonu zamenjena hidroksilnim grupa, ovaj analit ima potencijalno antiradikalsko dejstvo. U cilju procene antiradikalske aktivnosti, ali i konstruisanja kalibracionih krivih neophodnih za postavku analitičkog eseja i određivanje nepoznate konacentracije alizarina, u ovom radu, vršilo se ispitivanje uticaja različitih koncentracija alizarina na karakteristične parametare BR oscilatorne reakcije (indukcioni, oscilatorni i postoscilatorni period, kao i amplitudu i broj oscilacija).

The investigation of alizarin influence on Briggs-Rauscher oscillatory dynamics

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Briggs-Rauscher (BR) oscillatory reaction is the reaction of catalytic hydrogen-peroxide decomposition in an acidic medium in the presence of an organic substrate-malonic acid, iodate and metal ion (Mn^{2+}) as a catalyst. Recently, the presence of radical species ($HO\cdot$, $IO_2^{\cdot}$, $HOO\cdot$) has been detected in iodate oscillators by using electron paramagnetic resonance (EPR) techniques. The alizarin (1,2 dihydroxyanthraquinone, $C_{14}H_8O_4$) is frequently used as a red pigment, mostly in the textile industry. Considering the fact that two neighboring hydrogen atoms on the anthraquinone substituted by hydroxyl groups, this analyte has a potential scavenging effects. In order to assess antiradical activity, as well as constructing calibration curves necessary for determination the unknown alizarin concentration, in this paper, the influence of different alizarin concentration on the characteristic BR parameters (such as induction, oscillatory and post-oscillatory period, amplitude and the number of oscillations) is investigated.

HA P 06

Uticaj svetlosti na reakciju oksidacije joda vodonik-peroksidom u kiseloj sredini: Određivanje energije aktivacije

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Oksidacija joda vodonik-peroksidom u kiseloj sredini je važan reakcioni podsistem oscilatorne Bray-Liebhafsky (BL) reakcije. Iako je u BL oscilatoru ovo brz proces, ako se posmatra odvojeno (tj. izvan BL sistema) reakcija oksidacije joda može imati dug indukcioni period (IP), ili reakcija može da se ne odigra uopšte. Oksidacija joda vodonik-peroksidom u literaturi nije istražena dovoljno. Ovde je na brojnim temperaturama analiziran uticaj svetlosti na indukcioni period i dužinu trajanja reakcije. Praćena je apsorbancija joda na 460 nm UV/VIS spektrofotometrom. Takođe, energija aktivacije ove reakcije je određena po prvi put. Dobijeno je da je kinetika reakcije kompleksna i različita za eksperimente urađene na dnevnoj svetlosti i u totalnom mraku, kao i da je indukcioni period znatno smanjen u mraku. Stoga je zaključeno da su različiti reakcioni putevi dominantni zavisno od reakcionih uslova (svetlo/mrak) i da radikalske reakcije mogu imati važnu ulogu tokom IP.

Effect of light on the reaction of iodine oxidation with hydrogen peroxide in acidic medium: Determination of activation energy

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The iodine oxidation with hydrogen peroxide in acidic medium is the important subsystem of the oscillatory reaction known as Bray-Liebhafsky (BL) reaction. It has been noticed that, while in the BL oscillator it is fast process, if observed separately (ie. beyond BL system) it can be preceded by a long induction period (IP), or can even not start at all. Regardless, the iodine oxidation with hydrogen peroxide has not been investigated enough. Here, effect of light on IP and time in which reaction takes a place has been analyzed at numerous temperatures. The iodine absorption is followed by UV/VIS spectrometer at 460 nm. Also, activation energy, for this reaction, has been determined for a first time. It has been achieved that kinetics of reaction is complex and different for experiments done at daylight and in absolute dark, as well as that induction period is considerably decreased in the dark. Therefore, it has been concluded that different reaction pathways are dominant under this two reaction conditions (daylight/dark) and that radicals may play important role during the IP.

HA P 07

Određivanje odabranih steroida u uzorcima otpadnih komunalnih voda

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Određivanje tragova steroida u prirodnim i otpadnim vodama je predmet sve većeg interesovanja, jer se trenutno ne nalaze u postojećim propisima o kvalitetu voda. U zavisnosti od njihove toksičnosti i potencijalnih neželjenih efekata koje mogu imati na životnu sredinu i ljudsko zdravlje, mnogi steroidi se smatraju kandidatima za buduće zakonske regulative. Među najzastupljenijim steroidima u komunalnim otpadnim vodama nalaze se ljudski/životinjski i biljni steroli, kao proizvodi ljudskog metabolizma. Iz tog razloga, steroli se mogu koristiti kao indikatori humanog fekalnog zagađenja. U ovom radu uzorci otpadnih voda su pripremljeni korišćenjem ekstrakcije na čvrstoj fazi, a dobijeni ekstrakti su analizirani metodom tečne hromatografije visokih performansi sa tandem masenom spektrometrijom uz upotrebu hemijske jonizacije na atmosferskom pritisku. Rezultati su pokazali da su holesterol i koprostanol bili prisutni u najvećim koncentracijama, u opsegu 6290–43810 ng l^{-1} za holesterol i 12610–34910 ng l^{-1} za koprostanol. S obzirom na to da većina gradova u Srbiji nema postrojenja za prečišćavanje otpadnih voda, posebno je važno imati podatke o nalaženju steroidnih jedinjenja u životnoj sredini kako bi se procenio njihov uticaj na kvalitet vodenih resursa.

Determination of selected steroids in municipal wastewater samples

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Measuring of steroid residues in environmental and wastewaters is a subject of growing interest, since they are not covered by existing regulations on the water quality. Depending on their toxicity and potentially unwanted effects in the environment and on the human health, many steroids are regarded as candidates for future regulations. Among substances detected at the highest levels in wastewaters are human/animal and plant sterols as products of human metabolism. For this reason, sterols can be used as indicators of human fecal pollution. In this work, wastewater samples were prepared using solid-phase extraction and extracts were analyzed by high performance liquid chromatography-tandem mass spectrometry with atmospheric pressure chemical ionization. The results have shown that cholesterol and coprostanol were present at the highest concentrations, in the range 6290–43810 ng L^{-1} and 12610–34910 ng L^{-1}, respectively. Since the majority of cities in Serbia do not have wastewater treatment plants, it is especially important to collect data on steroid occurrence in environment in order to assess their impact on quality of the water resources.

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HA P 08

Ispitivanje stabilnosti anizomicina metodom tečne hromatografije sa tandem masenom spektrometrijom

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U cilju poboljšanja kvaliteta leka i unapređenja sigurnosti njegovog korišćenja, potrebno je praćenje stabilnosti i određivanje degradacionih proizvoda koji mogu nastati tokom proizvodnje, rukovanja ili čuvanja leka. Cilj ovog rada je ispitivanje stabilnosti i praćenje degradacije višefunkcionalnog leka anizomicina. Stabilnost anizomicina je ispitivana sprovođenjem studija forsirane degradacije, koje obuhvataju ispitivanje osetljivosti leka na hidrolizu (kiselu, baznu i neutralnu), oksidaciju, svetlost (vidljivu i UV) i povišenu temperaturu, u skladu sa ICH (eng. International Conference on Harmonization) smernicama. Za praćenje degradacije leka i identifikaciju degradacionih prozvoda korišćena je metoda tečne hromatografije sa tandem masenom spektrometrijom. Pokazano je da je anizomicin stabilan u prisustvu oksidacionog sredstva i svetlosti, umereno stabilan u kiseloj i neutralnoj sredini, jako nestabilan u baznoj sredini i termodegradabilan. Deacetilanizomicin je identifikovan kao glavni proizvod degradacije anisomicina.

Investigation of anisomycin stability using liquid chromatography coupled to tandem mass spectrometry

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In order to improve the quality of a drug and its safety usage, it is necessary to monitor stability of a drug and to determine degradation products that may form during production, usage and storage. Aim of this work was to investigate stability and monitor degradation of the multifunctional drug anisomycin. Stability of anisomycin was studied by performing force degradation that includes investigation of susceptibility of the drug to hydrolysis (acidic, alkaline and neutral), oxidation, light (visible and UV) and temperature, in accordance with ICH (International Conference on Harmonization) guidelines. Liquid chromatography coupled to tandem mass spectrometry was used for investigation of the drug degradation and identification of the degradation products. It was shown that anisomycin was stable in the presence of oxidizing agent and light, moderately stable under acidic and neutral conditions, very unstable under alkaline conditions and thermodegradable. Deacetylanisomycin was identified as the principal degradation product of anisomycin.

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HA P 09

Revizija stereohemije furanopingvizanola

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Seskviterpen α-furanopingvizanol je identifikovan kao glavni sastojak etarskog ulja jetrenjače *Porella cordaeana*. Iako je ovo jedinjenje izolovano i spektralno okarakterisano pre više od 20 godina [1], primećena su brojna neslaganja spektralnih podataka iz naše studije sa podacima koje su objavili Tori i sar. [1]. U ovom radu su izloženi argumenti koji pokazuju da je tim japanskih istraživača pogrešno pripisao strukturu α-furanopingvizanola drugom, srodnom jedinjenju. Najvažniji korak u određivanju relativne konfiguracije furanopingvizanola bila je analiza promene hemijskih pomeranja indukovane lantanidom (Δδ). Pomeranja protona H1 (0,26 ppm) i H4 (0,14 ppm) sa α strane molekula bila su skoro duplo veća od Δδ vrednosti H13 (Δδ 0,14) i H15 (Δδ 0,08 ppm) metil grupa sa β strane, što pokazuje da se ova dva protona nalaze na istoj strani molekula kao i OH grupa. Naše je mišljenje da su Tori i sar. [1] izolovali dijastereoizomerno jedinjenje (β-furanopingvizanol) i pogrešno odredili stereohemiju na C7 centru.

Revised stereochemistry of furanopinguisanol

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The major constituent of the essential oil of the liverwort *Porella cordaeana* was shown to be α-furanopinguisanol, a sesquiterpene with a very rare carbon skeleton. Although α-furanopinguisanol was previously reported in the literature [1], a number of significant discrepancies between the spectral data reported by Tori et al. [1] and the data obtained in our study were recognized. Herein, we present arguments that the Japanese team erroneously assigned the structure of α-furanopinguisanol to a different, related compound. The key step in the determination of the relative configuration of the compound was the analysis of shift changes produced by a lanthanide shift reagent. H1 and H4 protons (located on the α face of the molecule) showed almost two times larger Δδ values (0.26 and 0.14 ppm, respectively) compared to the H13 (Δδ 0.14) and H15 (Δδ 0.08 ppm) methyl groups on the β face, thus inferring that they were on the same face of the molecule as the OH group. We now believe that Tori and co-workers [1] actually isolated the diastereomeric compound –β-furanopinguisanol – and incorrectly assigned the stereochemistry at C7.

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HA P 10

Hemijski sastav etarskog ulja dobijenog iz cvasti I listova biljne vrste *Erigeron annuus* (L.) Pers. (Asteraceae) iz jugoistočne Srbije

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Erigeron annuus (L.) Pers., u Srbiji poznata kao krasolika, invazivna je jednogodišnja zeljasta biljka iz porodice glavočika (Asteraceae), koja se u narodnoj medicini koristi kao diuretik, za lečenje dijareje i kamena u bubrezima. Ova biljna vrsta je predstavljala predmet istraživanja nekoliko fitohemijskih studija, ali se do sada samo nekolicina njih fokusirala na hemijski sastav etarskog ulja. U ovom radu prezentujemo rezultate GC-MS analize etarskog ulja nadzemnog dela biljke *E. annuus* ubranog kod Oblačinskog jezeta, u blizini Niša. Hidrodestilacijom svežih nadzemnih delova biljke, skupljenih na početku perioda cvetanja, dobijena je mala količina zelenkastog etarskog ulja (0,105% prinosa), koje u velikom procentu sadržavalo poliacetilene. Glavni sastojci etaskog ulja su germakren D (38,6%), (*Z*)-lahnofilum estar (8-dihidromatrikarija estar; 25,2%) i (*Z,Z*)-matrikarija estar (3,7%). C_{10} poliacetileni predstavljavljaju tipične sastojke biljnih vrsta iz porodice glavočika (Asteraceae), sa matrikarija estrima i njima srodnim jedinjenjima kao najučestalijim.

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Chemical composition of the inflorescence and leaf essential oil of *Erigeron annuus* (L.) Pers. (Asteraceae) from southeastern Serbia

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Erigeron annuus (L.) Pers. (Asteraceae), daisy fleabane, is a widespread herbaceous annual plant species that has been used in traditional medicine as diuretic, as well as a treatment for diarrhoea and kidney stones. The plant has been the subject of several phytochemical studies, but up to this point only a few studies dealt with the composition of the essential oil of this plant taxon. Herein, we analyzed (by GC-MS) the composition of the essential oil from the above-ground parts of *E. annuus* from a wild-growing population in Serbia (Oblačina Lake, near Niš). Hydrodistillation of the fresh aboveground parts, collected in the beginning of the flowering phase, yielded a small amount of light green essential oil (0.105%) with polyacetylenes as one of the major chemical classes detected. The main constituents of the essential oil were found to be germacrene D (38.6%), (*Z*)-lachnophyllum ester (8-dihydromatricaria ester; 25.2 %) and (*Z,Z*)-matricaria ester (3.7%). C_{10} polyacetylenes seem to be typical of Astereae, with matricaria ester-related compounds as the most widespread ones.

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HA P 11

Proučavanje degradacije herbicida sa hlor dioksidom

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Cilj ovog rada je bilo ispitivanje i optimizacija degradacije herbicida (kao što su bentazon i tifensulfuron-metil) sa hlor dioksidom u dejonizovanoj vodi. Degradacija herbicida je ispitivana u dejonizovanoj vodi sa različitim količinama hlor dioksida (5 i 10 ppm), različitim vremenom degradacije (30 min, 1 h, 2 h, 3 h, 6 h i 24 h), pri različitim pH vrednostima (3, 7 i 9) i pod uslovima svetla ili mraka, dok je koncentracija herbicida bila 10 ppm. Efikasnost degradacije je praćena pomoću HPLC-DAD. Glavni degradacioni proizvodi su identifikovani pomoću GC/MS analize. Najbolja efikasnost degradacije bentazona postignuta je tretiranjem sa 10 ppm hlor dioksida na svetlu, nakon 24 h od početnog tretmana, pri pH 3 i 7, i iznosila je 92%. U slučaju tifensulfuron-metil herbicida, najbolja efikasnost degradacije postignuta je tretiranjem sa 10 ppm hlor dioksida na svetlu, nakon 24 h od početnog tretmana, i iznosila je 73%. Toksikološka analiza korišćenjem *Daphnia magna* je urađena za proizvode degradacije herbicida nakon tretmana hlor dioksidom od 1, 6 i 24 h.

Study on degradation of herbicides with chlorine dioxide

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The aim of this study was to investigate and optimize degradation of herbicides (such as bentazone and thifensulfuron-methyl) with chlorine dioxide in deionized water. Degradation of herbicides was examined in deionized water with different amount of chlorine dioxide (5 and 10 ppm), different time of degradation (30 min, 1 h, 2 h, 3 h, 6 h and 24 h), at different pH (3, 7 and 9) and under light or dark conditions, while concentration of herbicides was 10 ppm. Degradation efficiency of herbicides was followed using HPLC-DAD. Major degradation products were identified using GC/MS analysis. The best degradation efficiency of bentazone was achieved by treatment with 10 ppm of chlorine dioxide under light, after 24 h of initial treatment, at pH of 3 and 7, and it was 92%. In the case of a thifensulfuron-methyl herbicide, the best efficiency of degradation was achieved by treatment with 10 ppm of chlorine dioxide under light, after 24 h of initial treatment, and it was 73%. Toxicological analysis using *Daphnia magna* was performed for degradation products 1, 6 and 24 h after the treatment with chlorine dioxide.

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

HA P 12

Primena hromatografskih metoda u proceni lipofilnosti amida kortienske kiseline metilprednizolona

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Glukokortikoidi se često koriste u obliku preparata za lokalnu primenu na kožu ili oko. Jedna od najvažnijih fizičko-hemijskih osobina od koje zavisi permeabilnost ovih jedinjenja kroz biološke barijere i biološka raspoloživost na ciljnom mestu delovanja je lipofilnost. Cilj ovog rada je procena lipofilnosti četiri novosintetisana amida kortienske kiseline metilprednizolona u odnosu na tri konvencionalna glukokortikoida (hidrokortizon, metilprednizolon i fluocinolonacetonid) primenom dve hromatografske tehnike: reverzno-fazne hromatografije na tankom sloju (RP-TLC) i reverzno-fazne tečne hromatografije visokih performansi (RP-HPLC). Pri izvođenju RP-TLC metode korišćena su tri sistema sa četiri različita odnosa rastvarača: etanol/voda (50:50, 60:40, 70:30 i 80:20, V/V), aceton/voda (60:40, 70:30, 80:20 i 90:10, V/V) i acetonitril/voda (50:50, 60:40, 70:30 i 80:20, V/V). Pri izvođenju RP-HPLC metode kao mobilna faza korišćena je smeša acetonitril/voda sa četiri različita odnosa rastvarača (40:60, 50:50, 60:40 i 70:30, V/V). Sva novosintetisana jedinjenja pokazala su zadovoljavajuću lipofilnost, što je od značaja za njihovu potencijalnu lokalnu primenu na kožu.

Application of chromatographic methods for lipophilicity evaluation of amides of methylprednisolone-derived cortienic acid

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Glucocorticoids are often used in formulations for local application onto the skin or eye. Lipophicility is one of the most important physico-chemical properties of these drugs that influences permeability through biological barriers and bioavailability at the target site. The aim of this study was the estimation of lipophilicity of four newly synthesized amides of cortienic acid derived from methylprednisolone, in comparison to three traditional glucocorticoids (hidrocortisone, methylprednisolone and fluocinolone acetonide), using two chromatographic techniques: reversed - phase thin-layer chromatography (RP-TLC) and reversed - phase high-performance liquid chromatography (RP-HPLC). RP-TLC method was performed using three systems with four different ratios of solvents: ethanol/water (50:50, 60:40, 70:30 and 80:20, V/V), acetone/water (60:40, 70:30, 80:20 and 90:10, V/V) and acetonitrile/water (50:50, 60:40, 70:30 and 80:20, V/V). RP-HPLC method was performed using acetonitrile/water as mobile phases in four different ratios (40:60, 50:50, 60:40 and 70:30, V/V). All newly synthesized compounds have satisfactory lipophilicity, which is important for their potential local application onto the skin.

HA P 13

Estri (iregularnih) monoterpenola, karakteristika etarskog ulja korena biljne vrste *Artemisia absinthium* L.

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Etarsko ulje (EU) korena biljne vrste *Artemisia absinthium* L. prethodno je ispitivano svega nekoliko puta. Zato je cilj ovog rada bio detaljna analiza odgovarajućeg EU, uključujući detekciju i identifikaciju kako glavnih, tako i minornih isparljivih sastojaka korena. GC i GC/MS analize ulja korena belog pelina su kombinovane sa "dry flash" hromatografijom (DFH), što je omogućilo identifikaciju blizu 150 različitih komponenti; mnoge od njih su bile prisutne u niskim koncentracijama (<0.05%). Dominantne komponente ulja bile su α-fenhen (13.9%), β-mircen (9.0%) i bornil-acetat (9.0%). Lavandulol i njegovi estri čine 23.0% mase EU. Citronelol, geraniol, nerol, fragranol i njihovi estri čine dodatnih 12.0% mase uzorka. Kako su neki od pomenutih estara nove komponente, potvrdu identifikacije alkoholnog dela estra (dostupni standardi za ko-injekciju) dobili smo transesterifikacijom EU i DFH frakcija koje sadrže pomenute estre, pomoću natrijum-metoksida, nakon čega je ponovo vršena GC i GC/MS analiza. Ovo je prvi put da je potvrđeno prisustvo estara iregularnih monoterpenskih alkohola lavandulola i fragranola u etarskom ulju korena *A. absinthium*.

Esters of (irregular) monoterpenols, a hallmark of *Artemisia absinthium* L. root essential oil

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Artemisia absinthium L. root essential oil (EO) was previously investigated on only few occasions. Therefore, the aim of this study was to reinvestigate the corresponding EO and to try to detect and identify not only the major root volatiles, but also those present in trace amounts. GC and GC/MS analyses of *A. absinthium* root EO were combined with "dry flash" chromatography (DFC), which enabled a successful detection and identification of *ca.* 150 different constituents; many of these were present in low relative amount (<0.05%). The dominant EO constituents were α-fenchene (13.9%), β-myrcene (9.0%) and bornyl acetate (9.0%). Nonetheless, lavandulol and its esters comprised 23.0% of the EO. Citronellol, geraniol, nerol, fragranol and their esters made up for an additional 12.0% of the sample. As some of these seem to be new compounds, to confirm the identity of the alcohol moieties of the esters (pure standards available for co-injection), both the EO and its esters-containing DFC fractions were subjected to trans-esterification using sodium methoxide; the resulting mixtures were re-analyzed using GC and GC/MS. This is the very first time (esters of) irregular lavandulol and fragranol were found in *A. absinthium* root EO.

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

HA P 14

Određivanje elemenata u tragovima u svemirskoj hrani primenom spektroskopije laserski indukovane plazme

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Alga spirulina zbog svog izuzetno hranljivog sastava predstavlja idealni dodatak u ishrani. Kada je NASA predložila spirulinu kao hranu za astronaute na svemirskim putovanjima postala je veoma popularna i komercijalno dostupna. U ovom radu ispitana je mogućnost primene spektroskopije laserski indukovane plazme (LIBS) za kvalitativnu i kvantitativnu analizu uzoraka alge. Kao izvor laserskog zračenja korišćen je impulsni TEA CO_2 laser koji emituje zračenje u infracrvenom delu spektra (λ=10,6 μm). Primenom sintetičkih standarda konstruisane su kalibracione krive i postignuta je linearna zavisnost za Ba, Sr, Fe, Mn i Mg sa regresionim koeficijentom iznad 0,92 i sa preciznošću 1,9 % (Ba) i 8,6 % (Sr). Na osnovu dobijenih rezultata i upoređivanjem sa rezultatima iz literarature može se zaključiti da je predloženi LIBS sistem na bazi TEA CO_2 lasera pogodan za pouzdanu, brzu i jednostavnu kvalitativnu i kvantitativnu analizu ove vrste čvrstih uzoraka.

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

Analysis of trace elements in spacefood using Laser Induced Breakdown Spectroscopy

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Due to its remarkably nutrient composition, algae spirulina represents an ideal food supplement. Spirulina became very popular and commercially available when NASA proposed it as a food for astronaut on space travel. In this paper, application capability of Laser Induced Breakdown Spectroscopy (LIBS) for qualitative and quantitative analysis of algae samples was investigated. An impulse TEA CO_2 laser which emits irradiation in IR part of spectrum (λ=10.6 μm) was used as a laser irradiation source. Calibration curves were constructed based on a set of synthetic standards and linear dependence were obtained for Ba, Sr, Fe, Mn and Mg, with regression coefficients exceeding 0.92 and precision between 1.9 % (Ba) and 8.6 % (Sr). Based on the obtained results we may conclude that the proposed simple, cost effective, TEA CO_2 laser based LIBS system is suitable for qualitative and quantitative analysis of this type of solid samples.

Acknowledgement: *This research was supported by the Ministry of Education, Science and Technological Development of Republic Serbia (Project no. 172019).*

Hemijska sinteza - Chemical Synthesis

HS P 01

Sinteza, karakterizacija i biološka aktivnost kompleksa platine(II) i paladijuma(II) sa hinolinskim derivatima tiosemikarbazona

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Cilj ovog rada je ispitivanje strukture, geometrije i biološke aktivnosti kompleksa platine(II) i paladijuma(II) sa različitim hinolinskim derivatima tiosemikarbazona. Sintetisana su četiri nova kompleksa platine(II) i paladijuma(II) sa ligandnim sistemima: 2-hinolinkarboksaldehid tiosemikarbazonom (H2QATSC) i 8-hinolinkarboksaldehid tiosemikarbazonom (H8QATSC). Kompleksi platine(II) i paladijuma(II) sa H2QATSC ligandom, [PtCl(2QATSC)] **(1)** i [PdCl(2QATSC)] **(2)**, su dobijeni direktnom sintezom, a okarakterisani su primenom rendgenske strukturne analize. Kompleksi platine(II) i paladijuma(II) sa H8QATSC ligandom, [PtCl(8QATSC)] **(3)** i [PdCl(8QATSC)] **(4)**, su okarakterisani NMR spektroskopijom. U kompleksima **1**–**4** ligandi se koordinuju tridentatno preko hinolinskog i iminskog atoma azota i atoma sumpora iz tiosemikarbazona, obrazujući sa jonom metala dva petočlana helatna prstena. Geometrija oko metalnog jona je kvadratno-planarna, pri čemu hloridni jon zauzima četvrto koordinaciono mesto. Ispitana je antitumorska aktivnost kompleksa **1**–**4** i upoređena sa aktvinošću cisplatine.

Synthesis, characterization and biological activity of platinum(II) and palladium(II) complexes with quinoline derivatives of thiosemicarbazones

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The aim of this study was to elucidate the structure, geometry and biological activity of platinum(II) and palladium(II) complexes with different quinoline derivatives of thiosemicarbazones. Four novel platinum(II) and palladium(II) complexes with 2-quinolinecarboxaldehyde thiosemikarbazone (H2QATSC) and 8-quinolinecarboxaldehyde thiosemikarbazone (H8QATSC) were synthesized. The complexes of platinum(II) and palladium(II) with H2QATSC ligand, [PtCl(2QATSC)] **(1)** and [PdCl(2QATSC)] **(2)**, were synthesized by direct reaction and characterized by single crystal X-ray analysis. The complexes of platinum(II) and palladium(II) with H8QATSC ligand, [PtCl(8QATSC)] **(3)** and [PdCl(8QATSC)] **(4)**, were characterized by NMR spectroscopy. In the complexes **1**–**4** ligands are coordinated tridentately *via* the quinoline and imine nitrogen atoms and thiosemicarbazone sulfur atom, forming two five-membered rings with metal ion. The geometry around metal ions is square-planar, where chloride ion occupies fourth coordination site. Antitumor activity of the complexes **1**–**4** was investigated and compared with the activity of cisplatin.

HS P 02

Sinteza i antifungalna aktivnost tiofenskih i furanskih guanilhidrazona

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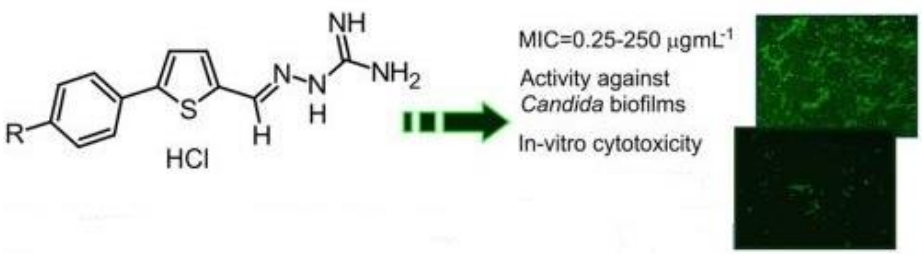
Koristeći jednostavne procedure sintetisali smo seriju novih tiofenskih i furanskih guanilhidrazona u visokim prinosima.[1] Antifungalna aktivnost je testirana na 8 sojeva gljivica, kao i na 3 soja mikromiceta. Antiproliferativni esej (citotoksičnost) rađen je na ćelijama humanih fibroblasta pluća (MRC5, ATCC kolekcija). Ispitan je efekat guanilhidrazona na rast hifa soja *C. albicans*. Takođe, ispitan je i uticaj guanilhidrazona na formiranje i rasturanje biofilmova koje formiraju klinički izolati soja *Candida*. Neki od guanilhidrazona testirani su i na embriotoksičnost (prema kičmenjačkom modelu *Danio rerio*.



Synthesis and antifungal activity of thiophene- and furane-based guanylhydrazones

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**Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Belgrade*

Using simple procedures series of new thiophene- and furane-based guanylhydrazones were synthesized in high yields. The antifungal activity was tested against 8 fungal strains, as well as on 3 mold strains. Antiproliferative assay (cytotoxicity) was tested on human lung fibroblasts (MRC5, ATCC collection). The effect of guanylhyrdazones on *C. albicans* yeast to hyphe transition was testes. Also, the effect of guanylhydrazones on *Candida* biofilm formation and disruption was tested. Some of the guanylhydrazones were assessed for zebrafish embryotoxicity.

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

References:

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HS P 03

Sinteza B-kondenzovanog tetrazolskog derivata holne kiseline

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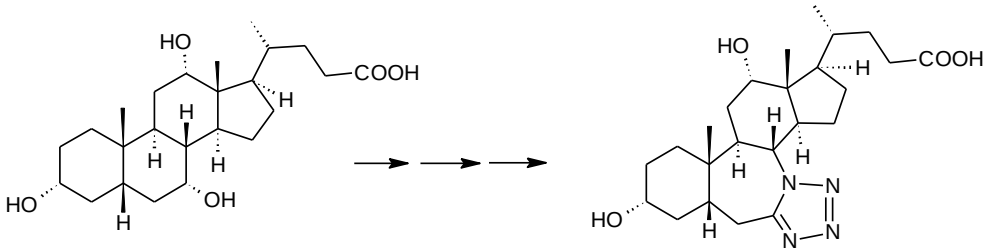
Imajući u vidu potencijal koji žučne kiseline i njihovi derivati pokazuju kao promotori transporta lekova sinteza novi derivata koji bi imali poboljšane osobine je vrlo važno polje istraživanja.
U ovom radu izvršena je višefazna sinteza tetrazolskog derivata holne kiseline: 7a-aza-3α,12α-dihidroksi-7a-homo-tetrazolo[5',1':7,7a]-5β-holanske kiseline (**1**). Polazeći od holne kiseline (**CA**) pomenuti tetrazol je sintetisan iz odgovarajućeg zaštićenog 7-okso prekursora pomoću Schmidt-ove reakcije. Struktura i čistoća novosintetizovanog B-kondenzovanih tetrazola potvrđena je spektroskopskim tehnikama, posebno analizom ^{1}H i ^{13}C NMR spektara.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja (broj projekta 172021) na finansijskoj pomoći.



CA **1**

Synthesis of a B-fused tetrazole derivate of cholic acid

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Since bile acids and their derivatives are promissing drug transport promoters synthesis of new derivatives becomes very important field of research.
In this study we presents the synthesis of a new steroidal tetrazole derivate: 7a-aza-3α,12α-dihidroxy-7a-homo-tetrazolo[5',1':7,7a]-5β-cholanoic acid (**1**). Starting from cholic acid the above mentioned tetrazole was synthesized employing Schmidt reaction on the protected 7-oxo precursor. Structure and purity of the newly synthetized B-fused tetrazole was confirmed by spectroscopic techniques, especialy with the analysis of ^{1}H i ^{13}C NMR spectra.

Autors acknowledge Ministry of Education, Science and Technological Developement of Republic of Serbia (project no. 172021) for financial support.

HS P 04

Novi derivati bis(alkilamino)diazahrizena aktivni na Ebola virus

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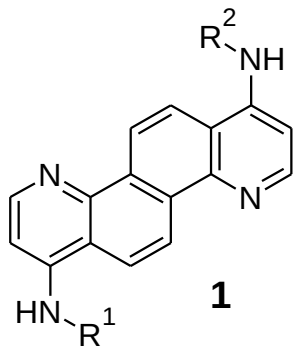
Ebola virus virulentan je patogen koji uzrokuje smrtonosnu hemoragijsku groznicu kod primata i ljudi. Mali molekuli predstavljaju jednu od obećavajućih vrsta potencijalnih terapeutika protiv ove, za sada neizlečive, bolesti. Raniji naši radovi sa diazahrizenskim strukturama simetrično supstituisanim dvema istovetnim alkilamino grupama pokazali su dobre rezultate[1]. Sada smo prvi put razvili metodu za sintetisanje derivata supstituisanih dvema različitim alkilamino-grupama **1**, sa ciljem ispitivanja efekta ove asimetrizacije molekula na aktivnost. Testirana jedinjenja pokazuju značajnu inhibitornu aktivnost u esijima sa Ebola virusom, nisku toksičnost po zdrave ćelije i ispoljavaju željeni trend zavisnosti aktivnosti od koncentracije. Najaktivniji derivat poseduje EC_{50} vrednost 0,26 μM, EC_{90} vrednost 0,85 μM i indeks selektivnosti 31.



1

Novel bis(alkylamino)diazachrysenes active againt the Ebola virus

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The Ebola virus is a virulent pathogen that causes a deadly hemorrhagic fever in humans and non-human primates. Small molecules present a promising class of potential therapeutics against this fatal illness. Our earlier research with diazachrysenes symmetrically substituted with two identical alkylamino groups gave positive results[1]. Now, for the first time, we have developed a method for the synthesis of derivatives with two different alkylamino substituents **1** in order to examine the effect of this structural asymmetrization. New compounds have been tested and showed significant inhibitory activity in Ebola virus based assays, low toxicity and exibit a satisfactory dose-response relationship. The most active derivative has an EC_{50} value of 0.26 μM, EC_{90} value of 0,85 μM with a selectivity index of 31.

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HS P 05

Inhibicija BoNT/A *in vitro* i zaštita SNAP-25 u ćeliji novih aminohinolinskih derivata tiofena

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Botulinum neurotoksin serotip A, jedan je od proizvoda metabolizma bakterije *Clostridium botulinum* i spada u najjače poznate otrove proteinske strukture. Trovanjem BoNT/A dolazi do hidrolize proteina SNAP-25 u neuronima i prekida se prenos neurotransmitera acetil-holina, što kod ljudi i životinja izaziva paralizu. Kako efikasan tretman ovog stanja ne postoji, potrebno je sintetisati nove molekule koji bi inhibirali dejstvo toksina posle intoksikacije. U nastavku naših istraživanja u ovoj oblasti,[1a,b] sintetisali smo nove 4-aminohinolinske derivate tiofena i analizirali njihovu *in vitro* inhibitornu aktivnost prema BoNT/A. Takođe, pokazali smo da novi derivati, u zavisnosti od koncentracije, štite SNAP-25 od hidrolize neurotoksinom u motornim neuronima, razvijenim iz embrionalnih matičnih ćelija miša. Ispitali smo uticaj povećanja dužine metilenskog niza i metilovanja benzilne amino-grupe na biološku aktivnost.

New aminoquinoline derivatives of thiophene as BoNT/A inhibitors *in vitro* and SNAP-25 cleavage protectors in cell-based assays

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Botulinum neurotoxin serotype A (BoNT/A) is one of *Clostridium botulinum* bacteria metabolic products. It is also one of the most potent protein toxins known. Toxic effects of BoNT/A include the cleavage of neural protein SNAP-25 and blocking the transmission of acetylcholine, resulting in paralysis. Due to the lack of an effective therapeutic treatment for this condition, identification of an appropriate compound that would inhibit the neurotoxin activity is of great importance. Following our previous results in this field,[1a,b] we have synthesized new 4-aminoquinoline thiophene-based derivatives and examined their *in vitro* inhibition of BoNT/A metalloprotease. In addition, we have shown that these compounds protect SNAP- 25 from cleavage in a dose-dependent manner in the cell-based experiments, performed on mouse embryonic stem cell-derived motor neurons. The structural modification influence on biological activity will be discussed.

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

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HS P 06

Citotoksični oktil estri iz etarskog ulja šizokarpa biljne vrste *Tordylium maximum* L. (Apiaceae)

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Vrste roda *Tordylium* (Umbelliferae) su se još u staroj Grčkoj koristile kao sastojci lekova, medicinskih vina i u kulinarstvu. Do sada nisu analizirani isparljivi sastojci plodova vrste *T. maximum*. U ovom radu, po prvi put, izvršena je analiza etarskog ulja dobijenih hidrodestilacijom suvih plodova ove biljne vrste. GC i GC-MS analizom ovog etarskog ulja utvrđeno je prisustvo estara 1-oktanola sa sirćetnom, propanskom, akrilnom, metakrilnom, butanskom, izobutanskom, pentanskom, izovalerijanskom, 2-metilbutanskom, senecio, tiglinskom i angelinka kiselinom. Svi ovi estri su sintetisani Šteglih-ovom metodom polazeći od 1-oktanola i odgovarajućih kiselina. 3-(4,5-Dimetiltiazol-2-il)-2,5-difeniltetrazolijum-bromidni (MTT) test je pokazano da oktil-tiglat, oktil-metakrilat i oktil-izobutanoat nemaju nikakvog efekta na peritonealne makrofage pacova, dok oktil-2-metilbutanoat, oktil-izovalerat i oktil-senecioat pokazuju značajnu toksičnost. Vrednosti srednjih letalnih doza (u moldm^{-3}) za ova tri aktivna estra su redom: 1,2×10^{-4}, 8,9×10^{-3} i 5×10^{-4} (pozitivna kontrola, 5-fluorouracil, LD_{50} = 1,5×10^{-5} mol dm^{-3}).

Cytotoxic octyl esters from the schizocarp essential oil of *Tordylium maximum* L. (Apiaceae)

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Tordylium taxa (Umbelliferae) were used in Greece in drugs and medicinal wines and also as culinary herbs. Up to date, there are no reports on the volatile constituents of the schizocarps of *T. maximum*. Herein, we wish to report on an analysis of the volatiles obtained by hidrodistillation from the dried fruits of *T. maximum*. Initial GC and GC-MS analyses of the essential oil revealed a series of esters of 1-octanol and acetic, propanoic, acrylic, methacrylic, butanoic, isobutanoic, pentanoic, isovaleric, 2-methylbutanoic, senecioic, tiglic and angelic acids. All of the twelve mentioned esters were prepared by a Steglich procedure starting from 1-octanol and the corresponding acids. An 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT)-assay, showed that octyl tiglate, octyl methacrylate and octyl isobutanoate were devoid of any effect towards rat peritoneal macrophages, while octyl 2-methylbutanoate, octyl isovalerate and octyl senecioate demonstrated prominent cytotoxicity with LD_{50} values (in mol dm^{-3}): 1.2×10^{-4}, 8.9×10^{-3}, 5×10^{-4}, respectively (cf. the positive control, 5-fluorouracil, LD_{50} = 1.5×10^{-5} moldm^{-3}).

Acknowledgements: *The authors were funded by the Ministry of Education, Science and Technological Development of Serbia (Grant No. 172061).*

HS P 07

Sinteza i kristalna struktura kompleksa nikla(II) sa 2-(2-(piridin-2-ilmetilen)hidrazinil)-4-(4-tolil)-1,3-tiazolom

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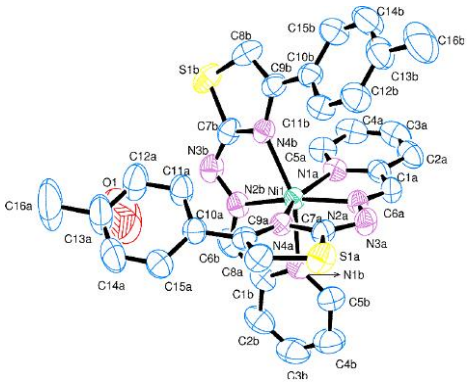

Sintetisan je novi kompleks nikla(II) sa ligandom 2-(2(piridin-2-ilmetilen)hidrazinil)-4-(4-tolil)-1,3--tiazolom (HL) sa ciljem ispitivanja biološke aktivnosti i razumevanja načina koordinacije ovog tipa ligandnih sistema. Kompleks je sintetisan direktnom reakcijom HL sa $Ni(CH_3COO)_2{\times}4H_2O$, pri čemu je dobijen u obliku monokristala i struktura kompleksa rešena je primenom rendgenske strukturne analize. Kompleks $[NiL_2]{\cdot}H_2O$ ima distorgovanu oktaedarsku geometriju pri čemu su za Ni(II) koordinovana dva liganda u deprotonovanom obliku. Ligandi su koordinovani tridendatno preko piridinskog, iminskog i tiazolovog atoma azota, formirajući dva petočlana helatna prstena oko centralnog metalnog jona. Koordinovani ligandi nisu kristalografski ekvivalentni. U spoljašnjoj sferi kompleksa nalazi se jedan molekul kristalne vode. Kristalno pakovanje kompleksa zasnovano je na vodoničnim i π-π steking interakcijama. Merenjem molarne provodljivosti utvrđeno da je kompleks neelektrolit, a magnetna merenja su pokazala da je kompleks paramagnetičan.

Synthesis and crystal structure of nickel(II) complex with 2-(2-(pyridine-2-ylmethylene)hydrazinyl)-4-(4-tolyl)-1,3-thiazole

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New Ni(II) complex with 2-(2-(pyridine-2-ylmethylene)hydrazinyl)-4-(4-tolyl)-1,3-thiazole (HL) ligand was syntesized with the aim of evaluation of biological activity and understanding the modes of coordination of this type of ligand systems. The complex was syntesized by the reaction of HL with $Ni(CH_3COO)_2 \times 4H_2O$. It was obtained as a single crystal and its structure was determined by X-ray diffraction analysis. The complex $[NiL_2]{\cdot}H_2O$ has distorted octahedral geometry with two deprotonated HL ligands which are tridentately coordinated *via* pydidine, imine and thiazole nitrogen atoms, forming two five-membered chelate ring around the central metal ion. The coordinated ligands are not crystallographicaly equivalent. In outher sphere of the complex there is a water molecule. Crystal packings of the complex is based on hydrogen interactions and the π-π stacking interactions. Molar conductivity measurements showed that the complex is non-electrolyte, while magnetic measurements showed that the complex is paramagnetic.

HS P 08

Hiralnost kristala – kompleksi kobalta sa derivatima tiazola

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Hiralnost je izraženo svojstvo biološkog sveta. Mnogi organski molekuli su hiralni, uključujući većinu bioloških aminokiselina. Takođe, dvostruki heliks DNK u svom kanonskom obliku ima formu desnog zavrtnja. Međutim, značaj hiralnosti sagledan je tek nakon tragedije sa talidomidom [1]. S druge strane, postoje mnogi nebiološki hiralni kristali kojima nije razmatrana hiralnost, a oni uključuju važne enantioselektivne katalizatore i senzorske materijale, kao i enantioselektivne hromatografke materijale. Kada se radi o hiralnosti u kristalnim strukturama, važno je razlikovati tri različite grupe objekata koji mogu biti ili hiralni ili ahiralni: 1) molekulske komponente kristala, 2) same kristalne strukture, 3) simetrijske grupe kristalnih struktura. Hiralnost kristala će biti razmatrana na primerima kompleksa kobalta sa tiazolskim ligandima.

Crystal chirality – cobalt complexes with thiazole based ligands

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Chirality is a striking property of the biological world. Many organic molecules, including the most biological amino acids are chiral and the DNA double helix in its standard form twists like a right-handed screw. The importance of chirality in biological systems was brought to light by the thalidomide tragedy [1]. On the other hand, there are many non-biological chiral crystals which have not been treated in terms of chirality, which include important enantioselective catalysts and sensing materials, as well as enenatioselective chromatographic materials. In dealing with chirality in relation to crystal structures it is essential to distinguish between three different objects that may be either chiral or achiral: 1) the molecular components of the crystal, 2) the crystal structure itself and 3) the symmetry group of the crystal structure. Chirality of crystals will be discussed taking cobalt complexes with thiazole based ligands as examples.

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HS P 09

Magnetno-strukturne korelacije kod bakar(II) kompleksa sa hloridnim ligandima u mostu

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Obimna istraživanja su izvršena u cilju korelacije strukture i magnetnih svojstava velikog broja različitih bakar(II) kompleksa sa hloridnim ligandima u mostu. Magnetna svojstva ovakvih sistema zavise od prirode terminalnih liganada, koordinacione geometrije oko atoma bakra i strukturnih distorzija od idealne geometrije. Sintetisana su dva bakar(II) kompleksa sa kondenzacionim derivatom metilhidrazinoacetata i 2-acetilpiridina koja su okarakterisana metodom difrakcije X-zraka sa monokristala. Diskutovana su magnetna svojstva kompleksa na osnovu rezultata rendgenske strukturne analize i magnetnih merenja merenja SQUID tehnikom. Izvršena su magnetno-strukturna poređenja sa strukturno sličnim bakar(II) kompleksima i uspostavljena je moguća korelacija između strukture i magnetnih svojstava kompleksa.

Magneto-structural coorelations in chlorido-bridged copper(II) complexes

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A considerable amount of work has been carried out aiming at correlating structures of a large variety of chlorido-bridged copper(II) complexes and their magnetic properties. Magnetic properties of such systems depend on the nature of terminal ligands, the coordination geometry around the copper atoms, and structural distortions from an ideal geometry. Copper(II) complexes with the condensation derivative of methyl hydrazinoacetate and 2-acetylpyridine were synthesized and characterized by a single crystal X-ray diffraction. Magnetic properties of both complexes are discussed based on X-ray structures and SQUID measurements. Magneto-structural comparisons to structurally similar copper(II) complexes are provided, and a possible correlation has been established.

HS P 10

Sinteza novih ferocenskih derivata 1,3-tiazinan-2-imina

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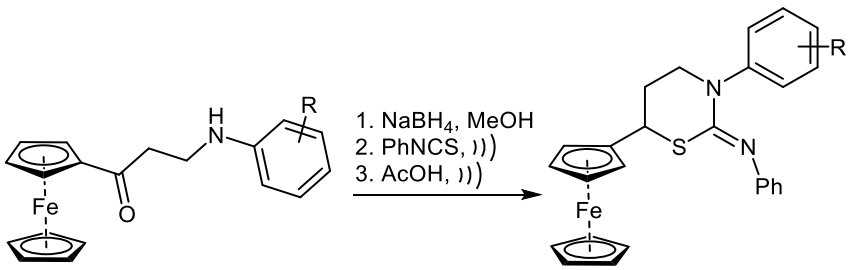
Heterociklični sistemi sa azotom i sumporom u prstenu su važne strukturne komponente koje se javljaju u prirodi i poseduju biološku aktivnost.[1] U skladu sa tim i našim prethodnim istraživanjima, koja se zasnivaju na sintezi heterocikličnih jedinjenja koja sadrže ferocen,[2] u ovom radu biće opisan postupak za dobijanje ferocenskih derivata 1,3-tiazinan-2-imina. Kao polazni supstrati za sintezu ovih heterocikala korišćeni su ranije opisani 3-(aminoaril)-1-ferocenilpropan-1-oni,[3] koji su redukovani pomoću $NaBH_4$ do odgovarajućih 1,3-aminoalkohola. Dobijeni 1,3-aminoalkoholi u reakciji sa fenil-izotiocijanatom pod dejstvom ultrazvučnih talasa daju hidroksitiouree, koje tretiranjem sa sirćetnom kiselinom grade 3-aril-*N*-fenil-6-ferocenil-1,3-tiazinan-2-imine (63-87%).



R = H, *o*-metil-, *m*-metil-, *p*-metil-, mezitil-

Synthesis of novel ferrocene-containing 1,3-thiazinan-2-imines

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Heterocyclic systems with nitrogen- and sulfur-containing ring are important structural components of natural products and possess biological activity.[1] In the present report, accordingly to our permanent interest in the synthesis of ferrocene-containing heterocyclic compounds,[2] the elegant synthesis of ferrocene-containing 1,3-thiazinan-2-imines will be described. This synthesis was achieved starting from 3-arylamino-1-ferrocenylpropan-1-ones (recently described by us),[3] which were reduced ($NaBH_4$) to the corresponding 3-arylamino-1-ferrocenylpropan-1-ols. The obtained 1,3-aminoalcohols later were submitted to the reaction with phenyl isothiocyanate (prompted by ultrasound irradiation) to give hydroxythioureas. Subsequent treatment of hydroxythioureas with acetic acid gave 3-aryl-6-ferrocenyl-*N*-phenyl--1,3-thiazinan-2-imines (63-87%).

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

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2. a) A. Pejović *et al., Polyhedron* **31** (2012) 789; b) A. Pejović *et al., Eur. J. Med. Chem.* **83** (2014) 57; c) A. Minić *et al., RSC Adv.* **5** (2015) 24915.
3. a) I. Damljanović *et al., J. Organomet. Chem.* **696** (2011) 3703; b) A. Pejović *et al., Helv. Chim. Acta*, **95** (2012) 1425.

HS P 11

Sinteza novih derivata N-(1-ferocenil-2-(metiltio)etil)-anilina

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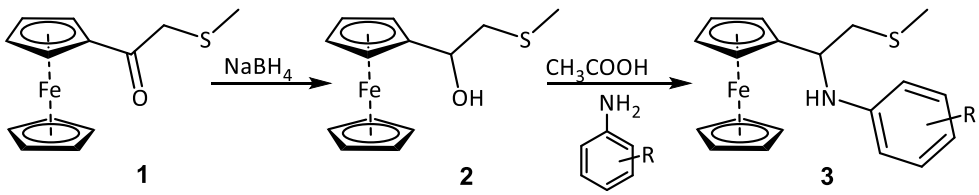
Derivati ferocena koji sadrže jedan ili više heteroatoma su se pokazali kao odlični ligandi za građenje kompleksa sa različitim jonima prelaznih metala. Veliki broj ovih kompleksa pokazuje antitumorsku aktivnost[1], a neki od njih se mogu koristiti i kao katalizatori u asimetričnoj sintezi[2]. U ovom radu biće predstavljena sinteza serije N-(1-ferocenil-2-(metiltio)etil)-anilina (**3**) koji predstavljaju potencijalne ligande za kompleksiranje sa prelaznim metalima. Ferocenski anilini **3** su dobijeni iz acilferocena **1** koji sadrži atom sumpora u bočnom nizu. U prvom koraku 1-ferocenil-3-tiabutan-1-on (**1**) je redukovan do odgovarajućeg alkohola **2**, koji je preveden u ciljne molekule **3** tretiranjem različito supstituisanim anilinima u kiseloj sredini. Dobijena jedinjenja će biti spektroskopski okarakterisana.



R= H, *p*-Cl, *m*-Cl, *o*-Cl, *p*-CH_3, *m*-CH_3, *o*-CH_3

Synthesis of novel derivatives of N-(1-ferrocenyl-2-(methylthio)ethyl)aniline

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**Technical Faculty Kosovska Mitrovica, University of Priština, Serbia*

Ferrocene derivatives that contain one or more heteroatoms are known as very good ligands for the synthesis of complexes with different transition metals ions. Many of these complexes show antitumor activity[1], and some of them can be used as catalyst in asymmetric synthesis[2]. In this report we will present the synthesis of series of novel N-(1-ferrocenyl-2-(methylthio)ethyl)anilines that are potential ligands for coordination to transition metal ions. Ferrocene-containing anilines **3** are obtained from acylferrocene **1** which contains sulfur atom in the alkyl chain. In the first step 1-ferrocenyl-3-thiabutan-1-one (**1**) is reduced to the corresponding alcohol **2** which is then converted to the target molecules **3** by treatment with different substituted anilines in an acidic medium. The obtained compounds will be spectroscopically characterized.

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

1. Susana S. Braga, Artur M. S. Silva; *Organometallics* 2013, **32**, 5626−5639
2. Li-Xin Dai, Xue-Long Hou; Chiral ferrocenes in asymmetric catalysis, 2010 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.

HS P 12

Sinteza i karakterizacija dinuklearnog kompleksa bakra(II) sa 4-(dietilamino)salicilaldehidom

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Kompleks bakra(II) (**1**) dobijen je reakcijom između 4-(dietilamino)salicilaldehida (deprotonovanog natrijum-metoksidom u metanolu), $Cu(BF_4)_2{\cdot}6H_2O$ i 1,10-fenantrolina u molskom odnosu 2:1:1. Kao rastvarač je korišćena smeša metanola i acetonitrila u zapreminskom odnosu 1:1. Kompleks **1** je okarakterisan elementalnom analizom, IC i UV-VIS spektroskopijom i magnetnim merenjima. Kristalna struktura kompleksa **1** određena je rendgenskom strukturnom analizom. Dobijeni paramagnetni kompleksni jon je dinuklearni. Za svaki jon bakra(II) bidentatno je koordinovan po jedan molekul 1,10-fenantrolina, preko dva atoma azota, i po jedan deprotonovani ligand. Deprotonovani ligand je, takođe, bidentatno koordinovan preko dva atoma kiseonika, od kojih je kiseonik iz hidroksilne grupe mostno vezan. Kao kontra joni se nalaze dva BF_4^- jona. Svaki metalni centar se nalazi u približno trigonalno-bipiramidalnom okruženju.

Synthesis and characterization of binuclear cupper(II) complex with 4-(diethylamino)salicyaldehyde

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Cupper(II) complex (**1**) was obtained in the reaction of 4-(diethylamino)salicyaldehyde (deprotonated with sodium methoxide in methanol), $Cu(BF_4)_2{\cdot}6H_2O$ and 1,10-phenantroline in molar ratio 2:1:1. Mixture of methanol and acetonitrile was used as a solvent in volume ratio 1:1. Complex **1** was characterized by elemental analysis, IR and UV-VIS spectroscopy and magnetic measurements. Crystal structure of the complex **1** was determineted by X ray crystallography. Obtained paramagnetic complex is binuclear. One molecule of 1,10-phenantroline is bidentately coordinated to each cupper(II) ion via two nitrogen atoms, as well as one deprotonated ligand. Deprotonated ligand is, also, bidentately coordinated, via two oxygen atoms of which one from hydroxyl group is bridging atom. Two BF_4^- ions are contra ions of complex cation. Each metal centre has approximately trigonaly-bipyramidal surroundings.

HS P 13

Sinteza steroidnih halohidrina

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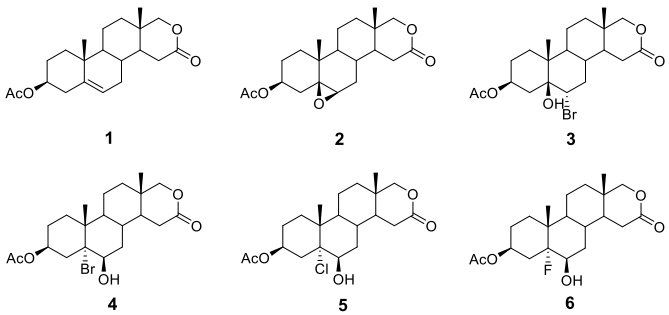
Hemijski modifikovana steroidna jedinjenja su našla primenu u lečenju niza oboljenja, od kojih se posebno ističu hormon-zavisni kanceri. Kod jedinjenja koja su pokazala značajnu citotoksičnu aktivnost kao farmakofore se ističu D-laktonski prsten, hidroksilne grupe i atomi halogena u A i B-steroidnim prstenovima. Imajući ovo u vidu sintetisani su različiti steroidni 5,6-halohidrini polazeći od dehidroepiandrosterona. Prvo je prema poznatom postupku sintetisan 17a-laktonski derivat **1** iz kog su potom dobijeni steroidni bromhidrini **3** i **4** i epoksid **2**. Epoksid **2** je upotrebljen za sintezu brom **4**, hlor **5** i fluorhidrina **6**. Biološka raspoloživost halohidrina **3**-**6** je ispitana poređenjem izračunatih molekulskih svojstava sa Lipinski i Veber pravilima.

Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije (br. projekta 172021) na finansijskoj podršci.



Synthesis of steroidal halohydrins

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Chemically modified steroid compounds have found application in treatment of a range of diseases, of which the most important are hormone-dependent cancers. In the compounds that have demonstrated significant cytotoxic activity as pharmacophores stand out D-lactone ring, a hydroxyl group and halogen atoms in the A and B-steroid ring. With this in mind various steroid 5,6-halohydrins were synthesized starting from dehydroepiandrosterone. 17a-lactone **1** was synthesized according to a known procedure and was further used for synthesis of steroidal bromohydrins **3** and **4** and epoxide **2**. Epoxide **2** was used for the synthesis of bromo **4**, chloro **5** and fluorhydrin **6**. Bioavailability of halohydrins **3**-**6** was assessed by comparing calculated molecular properties with the criteria for Lipinski and Veber rules.

Authors would like to thank the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 172021) for financial support.

HS P 14

Sinteza i biološka aktivnost novosintetisanih liganada arilpiperazinskog tipa

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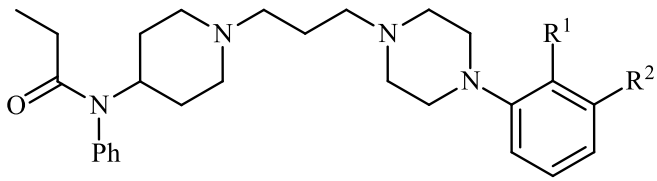
U cilju proučavanja interakcija između liganda i vezivnog mesta dopaminskog D2 receptora, sintetisana su tri nova liganda arilpiperazinskog tipa (**3**, **4** i **5)**.
Sinteza jedinjenja **3**, **4** i **5**, u tri faze, podrazumevala je: katalitičko debenzilovanje *N*-benzil fentanila uz pomoć Pd/C katalizatora u metanolnom rastvoru hlorovodonika, u toku 48 h na 25 °C, zatim selektivno alkilovanje soli sekundarnog amina **1** pomoću 1-brom-3-hlorpropana u MeCN na 25 °C pri čemu je dobijen alkil hlorid **2**, i alkilovanje *N*-arilpiperazina pomoću **2** u DMF, na 80°C. Oba alkilujuća koraka su izvedena u prisustvu K_2CO_3 kao baze, u toku 24 h. Proizvodi u visokim prinosima su dobijeni u sve tri faze. Za novosintetisane ligande ispitan je afinitet vezivanja za dopaminski D2 receptor u *in vitro* testovima kompeticije sa [^{3}H]-spiperonom kao radioaktivnim ligandom. Sinaptozomalne membrane izolovane su iz mozga pacova.
Ovi rezultati će doprineti boljem modelovanju dopaminskih D2 receptora.



3, R^1=R^2=H
4, R^1=R^2=Cl
5, R^1=OMe, R^2=H

Synthesis and biological activity of newly synthesized arylpiperazine ligands

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Three novel arilpiperazine ligands (**3**, **4** i **5)**, were synthesized in order to further examine the interaction between the ligand and the binding site of the dopamine D2 receptor.
The three step procedure for synthesis of compounds **3**, **4** and **5** involved: catalytic debenzylation of *N*-benzyl fentanyl using Pd/C catalyst in methanolic hydrogen chloride during 48 h at 25 °C, subsequent selective alkylaton of secondary amine salt **1** with 1-bromo-3-chloropropane in MeCN affording alkylchloride **2** and alkylation of *N*-arilpiperazine with **2** in DMF at 80°C. Both alkylation steps were conducted in the presence of K_2CO_3 as a base, during 24 h. All three steps provided products in high yields. Dopaminergic activities of newly synthesized ligands were estimated by *in vitro* competition experiments using [^{3}H]-spiperone as the radioligand.
These results will contribute to a better modeling of the dopamine D2 receptors.

HS P 15

Синтеза, карактеризација и кристална структура комплекса $[Ru(\eta^6\text{-}p\text{-cymene})(N\text{-MeIm})_3]Cl_2{\cdot}2H_2O$

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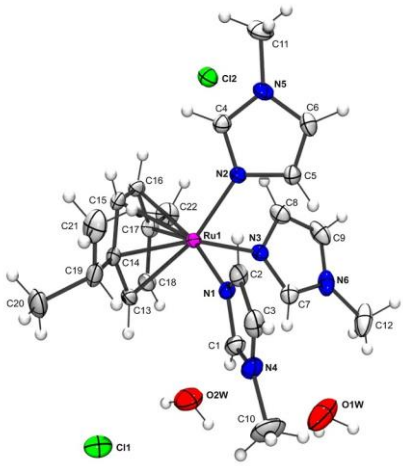
У овом раду приказана је синтеза, карактеризација и кристална структура комплекса Ru(II)-*p*-цимена и *N*-метилимидазола као лиганда. Смеша $[Ru\text{-}(\eta^6\text{-}p\text{-cimen})Cl_2]_2$ (0.122 g, 0.0002 mol) и *N*-метилимидазола (95.4 μL, 0.0012 mol) је растворена у 20 ml метанола и рефлуктована 2 сата на 65 °C. Након рефлуктовања, раствор је охлађен, процеђен и упарен до сува. Жути кристали су добијени након додатка ДМФ-а. Карактеризација синтетисаног комплекса $[Ru(\eta^6\text{-}p\text{-cimen})(N\text{-MeIm})_3]Cl_2{\cdot}2H_2O$ извршена је рендгенском структурном анализом, снимањем IR и NMR спектара и одређивањем тачке топљења.



Synthesis, characterization and crystal structure of $[Ru(\eta^6\text{-}p\text{-cymene})(N\text{-MeIm})_3]Cl_2{\cdot}2H_2O$ complex

Maja B. Đukić, Olivera Klisurić*, Zoran D. Matović

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This paper describes the synthesis, characterization and crystal structure of the complex Ru(II)-*p*-cymene with *N*-methylimidazole as a ligand. To a suspension of $[Ru\text{-}(\eta6\text{-}p\text{-cymene})Cl_2]_2$ (0.122 g, 0.0002 mol) and *N*-methylimidazole (95.4 μL, 0.0012 mol) was added methanol (20 mL). The resulting mixture was heated to reflux for 2 h on 65 °C, cooled and filtered. The solution was evaporated to dryness. Yellow crystals were obtained by the addition of DMF. Characterization of the synthesized complex $[Ru(\eta^6\text{-}p\text{-cymene})(N\text{-MeIm})_3]Cl_2{\cdot}2H_2O$ was performed by using X-ray analysis, IR and NMR spectroscopy and melting point determination.

HS P 16

Sinteza, karakterizacija i antimikrobna aktivnost kompleksa Ni(II) sa kondenzacionim proizvodom 2-hinolinkarboaldehida i Žirarovog T reagensa

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Ligand (**HL**Cl), (*E*)-*N*,*N*,*N*-trimetil-2-okso-2-(2-(hinolin-2-il-metilen)hidrazinil)etan-1-aminijum hlorid, dobijen je kondenzacionom reakcijom 2-hinolinkarboksaldehida i Žirarovog T reagensa. U reakciji liganda **HL**Cl sa $Ni(BF_4)_2{\cdot}6H_2O$ i NaN_3 u molskom odnosu 1 : 1 : 4 u metanolu dobijen je dinuklearni Ni(II) kompleks sa jednim azotovim atomom iz azida u svakom od dva mosta (**1**), opšte formule $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]$. Ligand (**HL**Cl) i kompleks **1** su okarakterisani elementalnom analizom, NMR (samo u slučaju liganda), IC i ULj/Vid spektroskopijom, konduktometrijom, a kristalna struktura kompleksa **1** je određena i rendgenskom strukturnom analizom. Antimikrobna aktivnost liganda **HL**Cl, kompleksa **1**, $Ni(BF_4)_2{\cdot}6H_2O$ i NaN_3 je ispitana korišćenjem mikrodilucionog metoda na tri linije Gram-pozitivnih bakterija, četiri linije Gram-negativnih bakterija i jedan soj glivica *Candida albicans*. Generalno, antimikrobna aktivnost je niska, zapažene MIK vrednosti su mnogo veće nego što su za ampicillin i amfotericin B. Od svih ispitivanih jedinjenja najizraženiju amtimikrobnu aktivnost ima kompleks **1**, što može biti posledica sinergističkog dejstva Ni(II) jona, hinolinskog hidrazona i azido liganda.

Synthesis, characterization and antimicrobial activity of Ni(II) complex with condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

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The ligand (**HL**Cl), (*E*)-*N*,*N*,*N*-trimethyl-2-oxo-2-(2-(quinolin-2-ylmethylene)hydrazinyl)ethan-1-aminium chloride, was obtained in the condensation reaction of 2-quinolinecarboxaldehyde and Girard's T reagent. In the reaction of the ligand **HL**Cl with $Ni(BF_4)_2{\cdot}6H_2O$ and NaN_3 in molar ratio 1 : 1 : 4 in methanol dinuclear double end-on azide bridged Ni(II) complex (**1**), with composition $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]$, was obtained. The ligand (**HL**Cl) and the complex **1** were characterized by elemental analysis, NMR (only for ligand), IR and UV/Vis spectroscopy, conductometric measurements, and structure of the complex **1** was defined by X-ray crystal analysis. Antimicrobial activity of **HL**Cl ligand, complex **1**, $Ni(BF_4)_2{\cdot}6H_2O$ and NaN_3 was tested against three strains of Gram-positive bacteria, four strains of Gram-negative bacteria and one strain of yeast *Candida albicans* using broth microdilution method. Generally, antibacterial activity of compounds was poor, the observed MIC values were much higher than that for ampicilin and amphotericin B. Among the investigated compounds complex **1** showed the most pronounced antimicrobial activity, which can be attributed to the synergistic effect of Ni(II) ion, quinoline hydrazone and azido ligands.

HS P 17

Flow sinteza kombretastatina A-4

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Kombretastatin A-4 (**1**) je prirodni spoj koji inhibira formiranje mikrotubula i pokazuje antiangiogenetsku aktivnost. 1995 godine izoliran je iz južnoafričkog stabla *Combretum caffrum*.[1-2]. Spoj **1** je potencijalni kandidat u liječenju raka. Nedavne studije uključuju razvoj novih derivata tog spoja kako bi se poboljšala svojstva poput topljivosti i stabilnosti te izučavao odnos između strukture i aktivnosti.[3]

Ovdje opisujemo razvoj sintetske strategije za dobivanje kombretastatina A-4 koristeći isključivo tehniku '*flow chemistry*'. Ova moderna metoda [4] ima niz prednosti u usporedbi s klasičnim tehnikama organske sinteze. Dosadašnja klasična sinteza ovog spoja uključuje niz problema kao što je stereo-selektivnost, opsežni postupci pročišćavanja te mala iskorištenja. Integracija svih koraka sinteze u kontinuirani proces '*flow chemistry*' značajno je skratila vrijeme reakcije i poboljšala iskorištenja.

Reakcije tipa Bestmann-Ohira [5a] i Sonogashira [5b] su optimizirane u uređajima marke VapourTec (R-, i modernijoj E-seriji). Eksperimenti katalitičke hidro-genacije [5c] provedeni su u uređaju H-Cube pri čemu je dobiven željeni spoj.

Priređeni derivati okarakterizirani su spektroskopskim metodama ^{1}H i ^{13}C NMR.

Rad je izrađen u Laboratoriju za organsku kemiju i sinteze, Université de Namur, u Belgiji.

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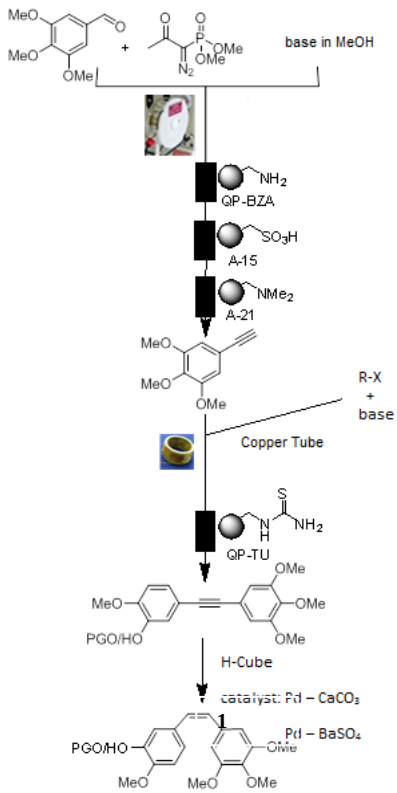

Shema 1. Predloženi sintetski put kombretastatina A-4

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5. a) Baxendale, I. R., *et al, Angew. Chem. Int. Ed*. **2009**, *48*, 4017; b) Zhang, Y., *et al, Org. Lett*. **2011**, *13*, 280; c) Chandrasekhar, S., *et al, Tetrahedron Lett*. **2011**, *52*, 3865.

HS P 18

Sinteza i karakterizacija kompleksa kobalta(III) sa 2-(2-(piridin-2-ilmetilen)hidrazinil)-4-(4-tolil)-1,3-selenoazolom

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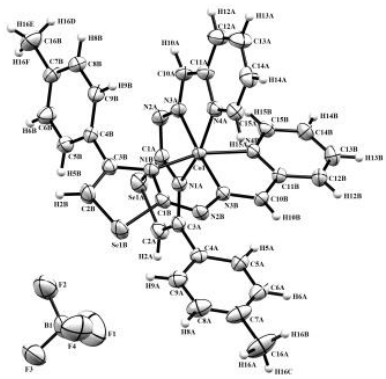
U cilju dobijanja biološki aktivnih kompleksnih jedinjenja sa biometalima, sintetisan je i strukturno okarakterisan novi kompleks kobalta(III) sa ligandom 2-(2-(piridin-2-ilmetilen)hidrazinil)-4-(4-tolil)-1,3-selenoazolom (HL). Kompleks je sintetisan reakcijom HL sa $Co(BF_4)_2 \times 6H_2O$. Na osnovu parametara dobijenih ^1H i ^{13}C NMR spektroskopijom pretpostavljena je tridentatna koordinacija liganda preko piridinskog atoma azota, iminskog atoma azota i atom azota koji potiče iz selenoazolovog prstena. Kako je kompleks dobijen u obliku monokristala, struktura mu je potvrđena primenom rendgenske strukturne analize. Kompleks $[Co(L)_2]BF_4$ ima distorgovanu oktaedarsku geometriju pri čemu su za Co(III) koordinovanaa dva liganda u monoanjonskom obliku, preko navedenog seta atoma. Koordinovani HL ligandi nisu kristalografski ekvivalentni. U spoljašnjoj sferi kompleksa nalazi se tetrafluoroboratni anjon. Kristalno pakovanje kompleksa zasnovano je na neklasičnim vodoničnim interakcijama, elektrostatičkim interakcijama i C–H···π interakcijama.



Synthesis and characterization of cobalt(III) complex with 2-(2-(pyridine-2-ylmethylene)hydrazinyl)-4-(4-tolyl)-1,3-selenoazole

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In order to obtain biologically active complexes with biometals, cobalt(III) complex with the ligand 2-(2-(pyridine-2-ylmethylene)hydrazinyl)-4-(4-tolyl)-1,3-selenoazole (HL) was synthesized and characterized. The complex was obtained by the reaction of HL with $Co(BF_4)_2 \times 6H_2O$. Based on the parameters obtained by ^1H i ^{13}C NMR spectroscopy tridentate ligand coordination *via* pyridine and azomethine nitrogen atoms and nitrogen atom from selenoazole ring is assumed. The complex was obtained as a single crystal and the structure was confirmed by X-ray structural analysis. The complex $[Co(L)_2]BF_4$ has distorted octahedral geometry with two deprotonated HL ligands coordinated *via* the mentioned set of atoms. The coordinated ligands are not crystallographicaly equivalent. In outher sphere of the complex there is tetrafluoroborate ion. Crystal packing of the complex is based on non-classical hydrogen interactions, electrostatic interactions and the C–H ··· π interactions.

HS P 19

Sinteza, struktura i svojstva 7,8-benzo-1,3-diazaspiro[4.5]dekan-2,4-diona i njegovih derivata

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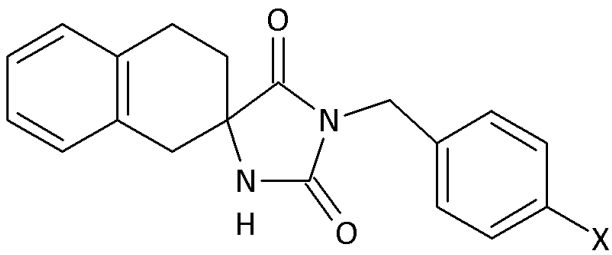
Derivati tetrantoina (7,8-benzo-1,3-diazaspiro[4.5]dekan-2,4-diona) (Slika) su jedinjenja širokog spektra biološke aktivnosti. Mnogi od njih su poznata antikonvulzivna, antivirusna i antikancerogena jedinjenja, a uspešno se koriste i u lečenju dijabetesa. U okviru ovog rada, sintetizovan je tetrantoin i njegovi derivati koji u položaju 3 hidantoinskog prstena sadrže supstituisanu benzil grupu (supstituent X: H, CH_3, OCH_3, Cl, Br, CN). Struktura navedenih jedinjenja potvrđena je temperaturama topljenja, ^{1}H i ^{13}C NMR, Ft-IR i UV spektroskopskim metodama. Na osnovu strukturnih i lipofilnih karakteristika diskutovana je potencijalna biološka aktivnost sintetizovanih jedinjenja.



X = H, CH_3, OCH_3, Cl, Br, CN

Derivati tetrantoina / Derivatives of tetrantoin

Synthesis, structure and properties of 7,8-benzo-1,3-diazaspiro[4.5]decane-2,4--dione and its derivatives

Željko Mandić, Anita M. Lazić, Bojan Đ. Božić, Gordana S. Ušćumlić
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Derivatives of tetrantoin (7,8-benzo-1,3-diazaspiro[4.5]decane-2,4-dione) (Figure) are the compounds of a wide range of biological activities. Many of them are known anticonvulsant, anticancer and antiviral compounds, and are successfully used in the treatment of diabetes. In this work, was synthesized tetrantoin and its derivatives which in the 3-position of the hydantoin ring containing a substituted benzyl group (the substituent X: H, CH_3, OCH_3, Cl, Br, CN). The structure of these compounds was confirmed by melting point, ^{1}H and ^{13}C NMR, FT-IR and UV spectroscopic methods. Based on structural lipophilic characteristics is discussed the potential biological activity of the synthesized compounds.

HS P 20

Dizajn, sinteza i antiproliferativna aktivnost novih cikloalkanspiro-5-hidantoinskih derivata: Veza između strukture i aktivnosti

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Spirohidantoini pripadaju grupi jedinjenja koja ispoljavaju širok spektar biološke aktivnosti. Do sada su derivati spirohidantoina identifikovani kao antikonvulzivi, antiaritmici, antidijabetici i antitumorni agensi. U cilju ispitivanja biološke aktivnosti, testirana je citotoksičnost novih serija jedinjenja: 3-(4-supstituisanih benzil)-1,3-diazaspiro[4.5]dekan-2,4-diona, 3-(2-(4-supstituisanih fenil)-2-oksoetil)-1,3-diazaspiro-[4.5]-dekan-2,4-diona, 3-(4-supstituisanih benzil)-1,3-diazaspiro[4.6]undekan-2,4-diona i 3-(2-(4-supstituisanih fenil)-2-oksoetil)-1,3-diazaspiro[4.6]undekan--2,4-diona. Citotoksična aktivnost određena je MTT testom prema ćelijskim linijama humane mijeloidne leukemije (K562), raka debelog creva (HCT-116) i raka dojke (MDA-MB-231). Testirana jedinjenja pokazala su značajnu citotoksičnost prema svim ćelijskim linijama, a naročito su se istakli derivati koji u okviru svoje strukture sadrže halogene kao supstituente. Uticaj sternih i elektronskih svojstava supstituenata na aktivnost proučavanih jedinjenja, analiziran je primenom QSAR modela.

Design, synthesis and antiproliferative evaluation of novel cycloalkane-spiro-5-hydantoin derivatives: A structure-activity relationship study

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**Faculty of Biology, University of Belgrade, Studentski trg 16, Belgrade, Serbia*

Spiroydantoins belong to a group of compounds exhibiting a wide range of biological activities. Until now, the spirohydantoin derivatives are identified as anticonvulsants, antiarrhythmic drugs, antidiabetic agents and antitumor agents. In order to investigate the biological activity was tested on the cytotoxicity of the new series of compounds: 3-(4-substituted benzyl)-1,3-diazaspiro[4.5]decane-2,4-dione, 3-(2-(4-substituted phenyl)-2-oxoethyl)-1,3-diazaspiro[4.5]decane-2,4-dione, 3-(4-substituted benzyl)-1,3--diazaspiro-[4.6]undecane-2,4-dione and 3-(2-(4-substituted phenyl)-2-oxoethyl)-1,3-diazaspiro[4.6]-undecane-2,4-dione. Cytotoxic activity was assessed by MTT assay cell lines of human myeloid leukemia (K562), colon (HCT-116) and breast cancer cells (MDA-MB-231). The test compounds showed a significant cytotoxicity to all cell lines, and in particular the derivatives containig within its structure halogens as substituents. The effect of steric and electronic properties of the substituents on activity of studed compounds, was analyzed by QSAR models.

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HS P 21

Sinteza i karakterizacija kompleksa srebra(I) sa *N*-heterocikličnim aromatičnim jedinjenjima

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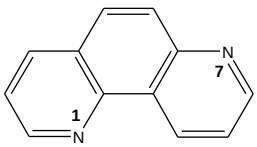
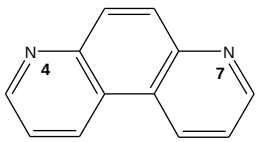


1,7-fenantrolin



4,7-fenantrolin

Raniji rezultati bioloških ispitivanja kompleksa srebra(I) sa *N*-heterocikličnim aromatičnim ligandima su pokazali da ovi kompleksi imaju značajnu atimikrobiološku i antitumorsku aktivnost [1]. U ovom radu, opisana je sinteza i strukturna karakterizacija dva nova kompleksa srebra(I) sa 1,7- i 4,7-fenantrolinom kao ligandima. Struktura ovih kompleksa je određena na osnovu NMR, IR i UV-vis spektroskopije, kao i metodom difrakcije rendgenskih zraka sa kristala. Nađeno je da u reakcijama ovih liganada sa $AgNO_3$ nastaju nuklearni $[Ag(NO_3)(1,7\text{-fenantrolin})_2]$ i polinuklearni $\{[Ag(4,7\text{-fenantrolin})](NO_3)\}_n$ kompleksi.

Synthesis and characterization of silver(I) complexes with aromatic *N*-heterocycles

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Recent results from biological evaluation of silver(I) complexes with aromatic nitrogen-containing heterocycles showed that these complexes have significant antimicrobial and antitumor activity [1]. In this study, two new silver(I) complexes with 1,7- and 4,7-phenanthroline as ligands were synthesized and structurally characterized. The structures of these complexes were elucidated from NMR, IR and UV-vis spectroscopy and single-crystal X-ray diffraction analysis. It was found that the reactions between 1,7- and 4,7-phenanthroline and $AgNO_3$ resulted in the formation of mononuclear $[Ag(NO_3)(1,7\text{-phenanthroline})_2]$ complex and 1D coordination polymer, $\{[Ag(4,7\text{-phenanthroline})](NO_3)\}_n$.

Acknowledgements: *This work was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172036) and the SupraMedChem@Balkans.Net SCOPES Institutional Partnership (Project No. IZ74Z0_160515).*

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HS P 22

Sinteza, biološka aktivnost i DNK interakcija novih bakar(II) kompleksa sa 2-hidroksi-4-aril-4-okso-2-butenoatima

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Sintetisana je serija novih kvadratnopiramidalnih bakar(II) kompleksa [Cu(L)2H2O] (3a–d) sa O,O-bidentatnim ligandima [L = etil-2-hidroksi-4-aril-4-okso-2-butenoati; aril = 3-metoksifenil-2a, (E)-2-fenilvinil-2b, (E)- 2-(4'-hidroksi-3'-metoksifenil)vinil-2c, 3-nitrofenil-2d, 2-tienil-2e] i okarakterisani spektroskopskim (UV-Vis, IR, ESI-MS i EPR), elementalnom i X-ray analizama. Koristeći MTT metodu citotoksična aktivnost je testirana na nekoliko ćelija tumora (HeLa ćelijskim linijama, kacinoma pluća A549 ćelijskim linijama i karcinoma debelog creva LS174 ćelijskim linijama). Svi kompleksi su pokazali dosta bolju citotoksičnu aktivnost u odnosu na cisplatinu koja je upotrebljena kao standard. Kompleks 3d je pokazao najbolju aktivnost na svim testiranim ćelijskim linijama (IC_{50} vrednosti 7.45 - 7.91 μg mL^{-1}). Ispitivanja vezana za interakcija između odabranih kompleksa (**3d** i **3e**) i CT-DNK su vršena fluorimetrijskom metodom sa etidijum-bromidom kao interkalatorom. Eksperiment je pokazao da 3d i 3e interkalacijom mogu izbaciti EB iz EB-DNK komleksa i pokazuju jaku konkurentnost za vezevinje [Ksv = (1.4 ± 0.2) i (2.9 ± 0.1) × 104 M^{-1}]. Dobijene Ksv vrednosti ukazuju da se ovi kompleksi vezuju za DNK kovalentno i nekovalentno.

Synthesis, biological activity and DNA binding study of novel copper(II) complexes with 2-hydroxy-4-aryl-4-oxo-2-butenoate

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A serie of novel square pyramidal copper(II) complexes [Cu(L)2H2O] (3a–d) with O,O-bidentate ligands [L = ethyl-2-hydroxy-4-aryl-4-oxo-2-butenoate; aryl = 3-methoxyphenyl-2a, (E)-2-phenylvinyl-2b, (E)- 2-(4'-hydroxy-3'-methoxyphenyl)vinyl-2c, 3-nitrophenyl-2d, 2-thienyl-2e] were synthesized and characterized by spectral (UV-Vis, IR, ESI-MS and EPR), elemental and X-ray analysis. The cytotoxic activity was tested using the MTT method on human epithelial carcinoma HeLa cells, human lung carcinoma A549 cells and human colon carcinoma LS174 cells. All complexes showed extremely better cytotoxic activity compared to cisplatin at all tested concentrations. Compound 3d expressed the best activity against all tested cell lines with IC_{50} values ranging from 7.45 to 7.91 μg mL^{-1} . The interactions between selected complexes (**3d** and **3e**) and CT-DNA were investigated by the fluorescence spectroscopic method. Competitive experiments with ethidium bromide (EB) indicated that 3d and 3e have a propensity to displace EB from the EB–DNA complex through intercalation suggesting strong competition with EB [Ksv = (1.4 ± 0.2) and (2.9 ± 0.1) × 104 M^{-1} , respectively]. Ksv values indicate that these complexes bind to DNA covalently and non-covalently.

HS P 23

Biokatalizovana sinteza novih 2-okso-1,2,3,4-tetrahidrohinoksalina i benzo-[*b*][1,4]oksazin-2-ona: limunov sok kao alternativa štetnim rastvaračima i katalizatorima

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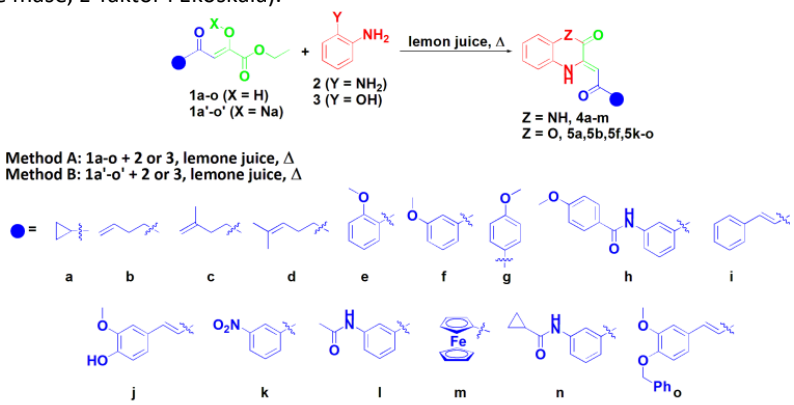
Dve male biblioteke novih 2-okso-1,2,3,4-tetrahidrohinoksalina (**4a-m**) i benzo-[*b*][1,4]oksazin-2-ona (**5a**, **5b**, **5f** i **5k-o**) sintetisane su ciklizacijom etil-2-hidroksi-4-alkil(alil)-4-okso-2-butenoata (**1a-o**) ili njihovih odgovarajućih soli (**1a'-o'**) sa *o*-fenilendiaminom (**2**) ili *o*-aminofenolom (**3**) u limunovom soku kao rastvaraču i katalizatoru. Postignuti su veoma dobri do odlični prinosi u svim reakcijama (do 95%). Sintetička metoda sa limunovim sokom proizvela je manje količine otpada, bez nusproizvoda i sa odličnim vrednostima eko-parametara (atomska efikasnost, efikasnost reakcione mase, *E*-faktor i Ekoskala).[1]



Biocatalytic synthesis of novel 2-oxo-1,2,3,4-tetrahydroquinoxalines and benzo[*b*][1,4]oxazin-2-ones: lemon juice as an alternative to hazardous solvents and catalysts

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Two small libraries of novel 2-oxo-1,2,3,4-tetrahydroquinoxalines (**4a-m**) and benzo[*b*][1,4]oxazin-2-ones (**5a**, **5b**, **5f** and **5k-o**) were synthesized by cyclization of ethyl 2-hydroxy-4-alkyl(aryl)--4-oxo-2-butenoate (**1a-o**) or their corresponding salts (**1a'-o'**) with *o*-phenylenediamine (**2**) or *o*-aminophenol (**3**) in lemon juice as a solvent and catalyst. Very good to excellent yields were achieved in all reactions (up to 95%). Lemon juice synthetic strategy has produced less amounts of waste without by-products and with excellent values of green chemistry metrics (atom efficency, reaction mass efficiency, *E*-factor and EcoScale).[1]

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

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HS P 24

Sinteza i karakterizacija novih rutenijum(II) polipiridil kompleksa i ispitivanje njihovih interakcija sa DNK

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U okviru ovog istraživanja sintetisana je serija novih monofunkcionalnih Ru(II) kompleksa opšte formule [Ru(Cl-Ph-tpy)(*N-N*)Cl]Cl, gde je Cl-Ph-tpy 4'-(4-hlorofenil)-2,2':6',2''-terpiridin, *N-N* helatni bidentatni ligand (1,2-diaminoetan (en, **1**), 1,2-diaminocikloheksan (dach, **2**), ili 2,2'-bipiridin (bpy, **3**)).[1] Pomenuti kompleksi su okarakterisani elementalnom analizom i spektroskopskim tehnikama (IR, UV-Vis, ^{1}H NMR). Lipofilnost sva tri hlorido kompleksa je određena izračunavanjem podeonog koeficijenta (log Po/w). Na osnovu dobijenih rezultata kompleks **3** je najhidrofobniji što može olakšati njegov prolazak kroz ćelijsku membranu i povećati njegovu antitumorsku aktivnost. DNK vezivanje je ispitano pomoću UV-Vis spektroskopije i merenjem fluorescencije. U konkuretnoj reakciji sa etidijum bromidom (EB) pokazano je da kompleksi mogu zameniti EB vezan za DNK ukazujući na jaku konkurenciju sa EB (K_{sv}= 3,7 - 9,6 x 10^4 M^{-1}). Ova ispitivanja pokazuju da rutenijum kompleksi interaguju sa DNK kovalento i preko interkalacije. Citotoksičnost hlorido kompleksa određena je pomoću MTT testa. Rezultati ukazuju na to da je kompleks **3** najreaktivniji.

Istraživanje je finansijski pomoglo Ministarstvo prosvete, nauke i tehnološkog ražvoja projekat broj 172011.

Synthesis and characterization of new ruthenium(II) polypyridyl complexes and their interactions with DNA

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In this study we have synthesized a series of new monofuctional Ru(II) complexes of the general formula [Ru(Cl-Ph-tpy)(*N-N*)Cl]Cl in which Cl-Ph-tpy is 4'-(4-chlorophenyl)-2,2':6',2''-terpyridine, *N-N* is a bidentate chelating ligand (1,2-diaminoethane (en, **1**), 1,2-diaminocyclohexane (dach, **2**) or 2,2'-bipyridine (bpy, **3**)).[1] These complexes were characterized by elemental analysis and spectroscopic techniques (IR, UV-Vis, ^{1}H NMR). Lipophilicity of all three chlorido complexes was determined by calculating the octanol-water partition coefficients (log Po/w). The obtained results showed that complex **3** is the most hydrophobic which may facilitate its cell uptake efficiency and enhance its anticancer activity. DNA binding was studied using UV-Vis spectroscopy and fluorescence quenching measurements. Competitive studies with ethidium bromide (EB) showed that investigated complexes can displace DNA-bound EB, suggesting strong competition with EB (K_{sv}= 3.7 – 9.6 x 10^4 M^{-1}). These experiments show that the ruthenium complexes interact with DNA covalently and via intercalation. Cytotoxicity was determined using the MTT test and complex **3** was the most reactive.

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HS P 25

Novi steroidni 4-aminohinolinski derivati kao antagonisti BoNT/A primenjeni posle intoksikacije u motornim neuronima razvijenim iz embrionalnih matičnih ćelija miša

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Botulinum neurotoksini (BoNTs) su proteini koje luči bakterija *Clostridium botulinum*. Jedni su od najjačih bioloških neurotoksina i mogu da izazovu smrtonosnu bolest botulizam.[1] U okviru naših istraživanja sintetisani su novi steroidni 4-aminohinolinski derivati i ispitana njihova inhibitorna aktivnost prema kratkom nizu BoNT/A i holotoksinu BoNT/A u motornim neuronima razvijenim iz embrionalnih matičnih ćelija miša (mES-MNs) (Slika 1). Kada se primene 30 minuta posle intoksikacije, uspešno štite SNAP-25 od dejstva toksina i do 99%. Za jedinjenje koje pokazuje najveći stepen inhibicije, izvršena je detaljna farmakokinetička analiza. Pregledom literature, ustanovljeno je da je ovo prvi primer malih molekula kao inhibitora kratkog niza BoNT/A, koji vrše zaštitu SNAP-25 u mES-MNs, kada se primene posle intoksikacije.

New steroidal 4-aminoquinolines antagonize BoNT/A in mES-MNs in post-intoxication model

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Botulinum neurotoxins (BoNTs) are proteins produced by the bacterium *Clostridium botulinum*. They are among the most potent toxins known and can cause a serious and life-threatening illness called botulism.[1] In this study we report on the synthesis and detailed evaluation of inhibitory potencies of new steroidal 4-aminoquinoline derivatives against BoNT/A light chain and full length BoNT/A in mouse ES-cell derived motor neurons (mES-MNs) (Figure 1). In a post-exposure model, where compounds were added 30 minutes following holotoxin administration, these derivatives were found to protect SNAP-25 from cleavage by up to 99%. For the most promising compound, detailed pharmacokinetic analysis has been carried out. To the best of our knowledge, this is the first example of LC inhibitors antagonizing BoNT intoxication in mES-MNs in a post-exposure model.

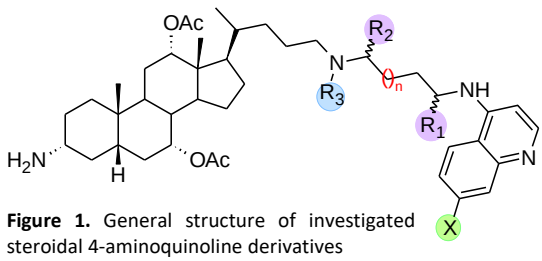

Figure 1. General structure of investigated steroidal 4-aminoquinoline derivatives

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HS P 26

Sinteza azepina nukleofilnom aromatičnom supstitucijom u mikrotalasnim reakcionim uslovima

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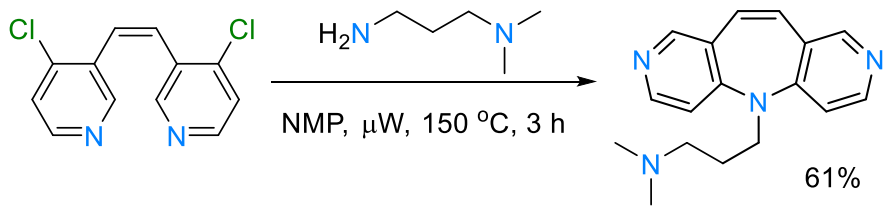
Nedavno, razvili smo novu metodologiju za sintezu 5*H*-diaril[*b*,*f*]azepina iz odgovarajućih *Z*-stilbena, građenjem dve C-N veze uz pomoć paladijuma kao katalizatora.[1] Ovde je predstavljena nova metoda za sintezu dipiridoazepinskih derivata. Azepinski prsten formiran je dvostrukom nukleofilnom aromatičnom supstitucijom, reakcijom primarnog alifatičnog amina i 3,3'-(*Z*)-eten-1,2-diilbis(4-hlorpiridina). Prednost nove metode u odnosu na ranije opisane sinteze azepina je što se reakcija odvija bez prisustva katalizatora na bazi prelaznih metala, a reakciono vreme je značajno skraćeno primenom mikrotalasnih reakcionih uslova.



Microwave-assisted synthesis of azepines via nucleophilic aromatic substitution

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We recently reported the preparation of 5*H*-dipyrido[4,3-*b*][1]azepines using the palladium-catalyzed *N*-arylation-cyclization reaction of primary amines with *ortho*-halogensupstituted *Z*-stilbenes.[1] Here we report the first microwave-assisted synthetic procedure for the formation of same azepine derivatives based on the double S_NAr reaction of 3,3'-(*Z*)-ethene-1,2-diylbis(4-chloropyridine) with primary aliphatic amines. The novel methodology was also successfully applied for the synthesis of new azepines. This procedure has the great advantage for being transition metal-free, and the time of the reaction was significantly shortened by microwave heating.

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

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HS P 27

Identifikacija i sinteza novih estara iz etarskog ulja hmelja (*Humulus lupulus* L.)

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Šišarke hmelja (*Humulus lupulus* L., Cannabaceae) se koriste za poboljšanje ukusa piva, a mnogi narodi ovu biljku koriste i u medicinske svrhe. Etarsko ulje hmelja se dobija hidrodestilacijom ženskih cvasti biljke (strobuli lupuli), u kojima se nalaze žlezde pune ulja. Do sada je identifikovano više od 200 različitih sastojaka ovog etarskog ulja, međutim, veliki broj jedinjenja je ostao neidentifikovan. Motivisani ovim, izolovano je etarsko ulje hidrodestilacijom svežih šišarki hmelja (prinos: 0,6%, w/w), sakupljenih u blizini Niša (jugo-istočna Srbija), a sastojaci etarskog ulja su preparativno razdvojeni gradijentnom "dry flash" hromatografijom na silika-gelu. Detaljna GC i GC-MS analiza dobijenih frakcija, pokazala je da je jedna od njih (eluirana sa 2% (v/v) dietil-etra u pentanu) bogata mnoštvom metil-estara alifatičnih karboksilnih kiselina normalnog i račvastog niza. Na osnovu njihovih masenih spektara i retencionih indeksa identifikovana je čitava serija metil-2-metilalkanoata (C_8-C_{11}). Kako metil-2-metilnonanoat i metil-2-metildekanoat nisu do sada identifikovani u etarskom ulju hmelja, izvršena je njihova sinteza. Odgovarajući litijum-enolati, dobijeni u reakciji metil-nonanoata i metil-dekanoata sa litijum-bis(trimetilsilil)amidom na -78 °C, alkilovani su metil-jodidom. GC ko-injekcija sintetisanih estara sa uzorkom etarskog ulja je potvrdila prisustvo metil-2-metilnonanoata i metil-2-metildekanoata u etarskom ulju hmelja.

Identification and synthesis of new esters from the essential oil of *Humulus lupulus* L.

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For hundreds of years strobiles from *Humulus lupulus* L. (Cannabaceae) have been used to flavor beer and in the enthnopharmacology of many nations. The essential oil is produced by the female inflorescences (strobuli lupuli) which contain the oil bearing glands. Up to now, more than 200 essential-oil constituents have been identified; however, a large number still remained unknown. Prompted by this, we subjected a sample of hydrodistilled essential oil of fresh hop cones (yield: 0.6%, w/w), collected from a wild-growing population of *H. lupulus* near the city of Niš (SE Serbia), to gradient "dry flash" SiO_2 chromatography. Initial GC and GC-MS analyses revealed a fraction (eluded with 2% (v/v) diethyl ether in pentane) that consisted of a myriad of methyl esters of normal and branched aliphatic carboxylic acids. A series of methyl 2-methylalkanoates (C_8-C_{11}) was tentatively identified based on their mass spectra and retention data. Since methyl 2-methylnonanoate and methyl 2-methyldecanoate were never previously reported for *H. lupulus*, we decided to prepare the two compounds by synthesis. The corresponding lithium enolates, obtained in the reaction of methyl nonanoate and methyl decanoate with lithium bis(trimethylsilyl)amide at -78 °C, were alkylated with methyl iodide. The subsequent co-injection experiments corroborated the initial tentative identifications, i.e. this is the first report on the occurrence of methyl 2-methylnonanoate and methyl 2-methyldecanoate in *H. lupulus* essential oil.

Acknowledgements: *The authors acknowledge the Ministry of Education, Science and Technological Development of the Republic of Serbia for the financial support (Project 172061).*

Biohemija i biotehnologija - Biochemistry and Biotechnology

BB P 01

Interakcije aminokiselinskih derivata *tert*-butilhinona sa biomakromolekulima

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Ispitane su interakcije devet aminokiselinskih derivata *tert*-butilhinona sa biomakromolekulima. SDS gel–elektroforezom i masenom spektrometrijom su praćene modifikacije lizozima ispitivanim derivatima hinona. Spektrofotometrijskim ispitivanjima je ispitano postojanje interakcija između hinona i CT-DNA. Praćeno je i smanjenje intenziteta fluorescencije etidijum–bromida i boje Hoechst 33258 u kompleksu sa CT-DNA, nastalo kao posledica dejstva sintetisanih jedinjenja na DNA iz timusa govečeta. Elektroforetskim ispitivanjem je proverena sposobnost derivata da narušavaju strukturu plazmida pUC19. DPPH testom je ispitana mogućnost hinonskih derivata da deluju kao hvatači slobodnih radikala.

Interactions of amino acid derivatives of *tert*-butylquinone with biomacromolecules

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The interactions of nine amino acid derivatives of *tert*-butylquinone with biomacromolecules were reported. Modifications of lysozyme by any of the synthesized compounds were characterized by SDS electrophoresis and mass spectrometry. Existence of interactions between the quinones and CT-DNA were observed using spectrophotometric studies. The quenching of fluorescence of intercalator ethidium bromide from EB–CT-DNA system and of minor groove binder Hoechst 33258 from H–CT-DNA system by the synthesized derivatives was examined. The cleavage of pUC19 plasmid in the presence of any of the synthesized compounds was examined by electrophoretic pattern. The ability of the derivatives to scavenge radicals was confirmed by DPPH test.

BB P 02

Sinteza fruktooligosaharida specifičnom inulinazom iz *Aspergillus awamori*

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Fruktooligosaharidi (FOS) su oligosaharidi fruktoznih jedinica međusobno povezanih β(1→2) vezom. Poslednjih godina je povećana potreba za FOS-ovima u industriji hrane i pića. Jedan od najefikasnijih načina za dobijanje FOS-ova je upotrebom enzima (inulinaze) iz mikroorganizama, kao što je mikrogljiva roda *Aspergillus*. U ovom radu je produkovana inulinaza gljive *A. awamori* koja je okarakterisana specifičnom zimogramskom tehnikom. Ispitani su i optimizovani uslovi reakcije sinteze FOS-ova korišćenjem izolovane izoforme inulinaze (A) kao što su pH, temperatura i vreme trajanja reakcije. Dobijeni proizvodi reakcije su detektovani tankoslojnom hromatografijom (TLC-om). Pokazano da uslovi reakcije diktiraju tok reakcije u smislu hidrolize inulina ili sinteze FOS-ova uporebom iste izoforme inulinaze.

Synthesis of fructooligosaccharides by using specific inulinase from *Aspergillus awamori*

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Fructooligosaccharides (FOS) represents a polymer of D-fructose residues linked by β(2→1) bonds. Need for FOSs increased in the last few years, especially in food and beverage industry. One of the most efficient way to obtain FOSs is enzymatically, using fungal inulinase, particularly the one produced by microfungi from genus *Aspergillus*. In this study, inulinase, produced by fungi *A. awamori,* is characterized by a specific zymogram technique. Identified isoforms are separated by gel chromatography on a FPLC system. Synthetic reaction of FOS was optimized (pH, temperature and reaction time). The obtained reaction products were detected by thin layer chromatography (TLC). It was shown that the reaction conditions dictate the course of the reaction in terms of hydrolysis of inulin or FOS synthesis's by using is the same isoform.

BB P 03

Enzim-inhibitorna aktivnost ekstrakta ploda aronije dobijenog ekstrakcijom subkritičnom vodom

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Poslednjih nekoliko godina, sve je veći interes za funkcionalnom hranom i dodacima ishrani na biljnoj bazi, a sve u cilju pomoći u prevenciji dijabetesa, gojaznosti, kardiovaskularnih i drugih bolesti. Aronija (*Aronia melanocarpa*) je višegodišnja biljka bogata polifenolima, intenzivno proučavana zbog znatnog lekovitog potencijala. Brojne studije pokazale su pozitivno dejstvo ploda aronije u kontroli i prevenciji dijabetesa i komplikacija povezanih sa dijabetesom. U okviru ovog rada ispitana je aktivnost ekstrakta ploda aronije, dobijenog ekstrakcijom subkritičnom vodom, ka inhibiranju odabranih enzima. Ekstrakcija subkritičnom vodom izvedena je u trajanju od 25 minuta na temperaturi od 125°C i pritisku od 35 bara. Inhibitorna aktivnost ispitivanog ekstrakta određena je merenjem njegove sposobnosti da inhibira aktivnost α-amilaze, α-glukozidaze i tirozinaze. Ekstrakt ploda aronije je pokazao najveću aktivnost ka inhibiciji tirozinaze gde je vrednosti inhibitorne koncentracije iznosila 10,94±0,89 mg EKK/g ekstrakta. U slučaju α-amilaze i α-glukozidaze vrednosti inhibitornih koncentracija bile su 0,45±0,01 mmol EA/g ekstrakta i 1,40±0,15 mmol EA/g ekstrakta, redom. Prikazani rezultati mogu doprineti razvoju novih dijetetskih suplemenata i dodataka ishrani.

Enzyme-inhibitory activity of subcritical water extract of aronia berries

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In recent years, substantial interest in functional food and plant-based supplements that can be utilized as an aid in prevention of diabetes, obesity, cardiovascular and other diseases, has arisen. Aronia (*Aronia melanocarpa*) is a polyphenol-rich perennial plant and has been intensively studied for its medicinal potential. Numerous studies have shown favorable effect of aronia berries in control and prevention of diabetes and diabetes-associated complications. In this study, ability of subcritical water extract of aronia berries to inhibit the activity of selected enzymes was evaluated. The subrcritical water extraction was carried out for 25 min at temperature of 125°C and pressure of 35 bar. The enzyme inhibitory effects of tested extract were investigated against α-amylase, α-glucosidase and tyrosinase enzymes. The aronia berries extract exhibited the highest inhibitory activities against tyrosinase with the inhibitory concentration of 10.94±0.89 mg KAEs/g extract. In the case of α-amylase and α-glucosidase, inhibitory concentrations were 0.45±0.01 mmol ACEs/g extract and 1.40±0.15 mmol ACEs/g extract, respectively. Reported results could be valuable in order to consider bioactive compounds from aronia extracts as a model of new supplement formulations.

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BB P 04

Антибактеријска и цитотоксична активност нафтохинонских пигмената из корена биљке *Onosma visianii*

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У овом раду приказана је антибактеријска и цитотоксична активност једињења изолованих из корена биљке *Onosma visianii*. Дескрипција седам изолованих једињења деоксишиконина (***1***), изобутирилшиконина (***2***), α-метилбутирилшиконина (***3***), ацетилшиконина (***4***), β-хидроксиизовалерилшиконина (***5***), 5,8-O-диметил изобутирилшиконина (***6***) и 5,8-O-диметил деоксишиконина (***7***) урађена је различитим хроматографским и спектроскопским методама. Међу тестираним једињењима ***3*** и ***4*** су показали најбољу антибактеријску активност према тестираним бактеријама. Најбољу цитотоксичну активност према MDA-MB-231 ћелијској линији показала су једињења ***3*** и ***4***, док су ***1***, ***3***, ***4*** и ***5*** значајно смањила вијабилност HCT116 ћелијске линије. Наши резултати указују на то да су сви тестирани нафтохинонски пигменти потенцијални кандидати за клиничку употребу као антибактеријски и цитотоксични агенси.

Antibacterial and cytotoxic activities of naphthoquinone pigments from *Onosma visianii* Clem

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In this study, the antibacterial and cytotoxic activities of isolated compounds from the roots of *Onosma visianii* were investigated. By using different chromatographic techniques and appropriate spectroscopic methods, the seven naphthoquinones were described: deoxyshikonin (***1***), isobutyrylshikonin (***2***), α-methylbutyrylshikonin (***3***), acetylshikonin (***4***), β-hydroxyisovalerylshikonin (***5***), 5,8-O-dimethyl isobutyrylshikonin (***6***) and 5,8-O-dimethyl deoxyshikonin (***7***). Among the tested compounds ***3*** and ***4*** exhibited the highest antibacterial activities toward all tested bacterial species. Also, naphthoquinones ***3*** and ***4*** exhibited strong cytotoxic activity against MDA-MB-231 cells, while compounds ***1***, ***3***, ***4*** and ***5*** significantly decreased viability of HCT116 cells. Our results indicated that all tested naphthoquinone pigments are potential candidates for clinical uses as antibacterial and cytotoxic agents.

BB P 05

Isparljiva jedinjenja korena biljne vrste *Conium maculatum* L.

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Conium maculatum L. (Apiaceae; *kukuta*) spada u najpoznatije otrovne biljne vrste. Kukuta je višegodišnja zeljasta biljka evropskog porekla, ali je danas rasprostranjena na svim kontinentima. Smatra se da je koniin, isparljivi alkaloid iz svežih listova, plodova i cvetova kukute, odgovoran za Sokratovu smrt. Interesantno je da su do sada sastav i biološke aktivnosti etarskog ulja kukute bile predmet svega nekoliko studija – tek je nedavno objavljen sastav etarskih ulja listova i cvetova kukute iz Srbije i Irana. U ovom radu je po prvi put (pomoću gasne hromatografije (GC) i gasne hromatografije/masene spektrometrije) ispitan hemijski sastav etarskog ulja dobijenog hidrodestilacijom korena biljne vrste *C. maculatum.* Prinos etarskog ulja je bio vrlo nizak (0,08 % u odnosu na svež biljni materijal, ubran u okolini Leskovca). Uspešno je identifikovano 100 sastojaka koji čine oko 90% ukupne površine pikova u GC hromatogramu. Glavni sastojci etarskog ulja su bili (*Z*)- β -ocimen (25, 3%), β-pinen (17, 8%), (*Z*)-falkarinol (17,2 %), mircen (13,1 %), β-seskvifelandren (3,2 %) i elemicin (2,4 %). Piperidinski alkaloidi nisu detektovani.

Volatile metabolites of the underground parts of *Conium maculatum* L.

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Conium maculatum L. (Apiaceae; poison hemlock) is one of the most renowned poisonous plant species. Hemlock is a perennial herbaceous flowering plant of European origin found throughout many parts of the world. The fresh leaves, fruits and flowers contain a volatile alkaloid, coniine, historically associated with the death of Socrates. Strangely, the composition and the associated activities of its essential oils of hemlock were the subject of only several previous studies. Recently, the chemical compositions of the leaf and flower essential oils of *C. maculatum* from Serbia, as well as the essential oil of Iranian hemlock, were published. Herein, we describe the first analysis by GC and GC-MS of the hydrodistilled essential oil of *C. maculatum* L. roots. The yield of the root essential oil was rather low (0.08 %, based on fresh root weight, collected near the city of Leskovac). One hundred constituents were successfully identified, representing ca. 90% of the total detected GC-peak areas. The main constituents of the essential oil were (*Z*)- β -ocimene (25.3%), β-pinene (17.8 %), (*Z*)-falcarinol (17.2 %), myrcene (13.1 %), β-sesquiphellandrene (3.2 %) and elemicin (2.4 %). No traces of piperidine alkaloids were detected in the roots.

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BB P 06

Uporedna studija profila alkana iz voska cveta i lista biljne vrste *Draba lasiocarpa* Rochel (Brassicaceae)

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Draba L. je najveći rod porodice Brassicaceae (Cruciferae) i sadrži više od 370 biljnih vrsti poznatih kao gladnice. *Draba lasiocarpa* Rochel cveta u rano proleće na području Karpata i planina Balkanskog poluostrva. Sekundarni metaboliti biljne vrste *D. lasiocarpa* nisu nikada ranije ispitivani, a voskovi biljaka porodice Brassicaceae proučavani su vrlo retko. U ovom radu, po prvi put, analizirali smo hloroformski ispirak cveta i lista biljne vrste *D. lasiocarpa*. Biljni materijal je sakupljen u Jelašničkoj klisuri, jugoistočna Srbija. Hromatografsko razdvajanje ispiraka je dalo frakciju sastavljenu isključivo od *n*-, *iso*- i *anteiso*-alkana. Sastav alkana listova i cvetova se kvalitativno i kvantitativno značajno razlikovao. Dominirali su *n*-alkani (C_{23}-C_{35}) sa neparnim brojem ugljenikovih atoma, što je uobičajeno za više biljke. Najzastupljeniji alkan u cvetu je bio nonakozan (C_{29}), a u listu hentriakontan (C_{31}). Zanimljivo je da su *iso*-alkani bili zastupljeni u velikom procentu u vosku cveta. U cvetu, približni odnos *n*-:*iso*-:*anteiso*- alkana je iznosio 59:40:1, dok u vosku listova praktično nije bilo alkana račvastog niza. Ovakva distribucija je sa biosintetskog/ekološkog aspekta zanimljiva i zaslužuje dalje istraživanje.

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Comparative study of wax alkane profiles from the flower and leaf of *Draba lasiocarpa* Rochel (Brassicaceae)

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Draba L., the largest genus in the family Brassicaceae (Cruciferae), comprises over 370 species, commonly known as whitlow-mustards. *Draba lasiocarpa* Rochel flowers in early spring throughout Carpathians and the mountains of the Balkan Peninsula. The secondary metabolites of *D. lasiocarpa* have never been investigated previously, and, in general, the epicultricular compounds from Brassicaceae have received little attention. In this work, for the first time, we analyzed the chloroform leaf and flower surface washings of *D. lasiocarpa*. The plant material was collected from the gorge of the river Jelašnica, near Niš (SE Serbia). A chromatographic separation of the washings yielded a fraction representing a mixture of solely *n*-, *iso*- and *anteiso*-alkanes. Both qualitatively and quantitatively, the composition of the leaf and flower alkanes differed significantly. The alkane profiles were dominated by *n*-alkanes (C_{23}-C_{35}) with the usual higher plant odd-even ratio, and showed a maximum at C_{29} and C_{31} for the flowers and leaves, respectively. Interestingly, *iso*-alkanes were present in a significant share in the flower wax with the approximate ratio of *n*-:*iso*-:*anteiso*- alkanes 59:40:1, while the leaf waxes were practically devoid of branched alkanes. Such a distribution is of a biosynthetic/ecological significance and deserves further study.

BB P 07

Oksidativna stabilnost celobiozo dehidrogenaze

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Celobiozo dehidrogenaza (CDH, EC 1.1.99.18) iz *Phanerochaete chrysosporium* pripada grupi oksidoreduktaza i ima sposobnost da degraduje različite komponente drvenastih biljaka. CDH je zbog svojih osobina našla primenu u industrijskim i biotehnološkim procesima kao i u proizvodnji biosenzora i biogorivnih ćelija. Enzimi koji se koriste u biosenzorima trebalo bi da imaju povećanu stabilnost, posebno u odnosu na kiseonične reaktivne vrste. Za poboljšanje oksidativne stabilnosti CDH, uvedene su mutacije i testirana je stabilnost enzima u prisustvu vodonik peroksida. Nakon uspešnog kloniranja u pYES2 vektor, saturaciona mutageneza je korišćena za dobijanje biblioteka mutanata. Rezidualna aktivnost mutanata je merena nakon inkubacije enzima u 0.3 M vodonik peroksidu u 0, 2 i 6 času. Nakon analize velikog broja mutanata, tri mutanta su pokazala veću oksidativnu stabilnost u poređenju sa wild – type enzimom. Rezidualne aktivnosti ova tri mutanta nakon šestog časa inkubacije u vodonik peroksidu su bile iznad 50%, dok ta vrednost za wild – type iznosi 30%. Selektovani mutanti su eksprimirani u *S. cerevisiae* i prečišćeni na DEAE koloni. Stepen prečišćenosti i aktivnost enzima su detektovani na elektroforeznom gelu.

Oxidative stability of cellobiose dehydrogenase

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Cellobiose dehydrogenase (CDH, EC 1.1.99.18) from *Phanerochaete chrysosporium* belongs to a group of oxidoreductases and has the ability to degrade different components of woody plants. This makes her an important enzyme for applications in industrial and biotechnological processes, as well as biosensors and biofuel cells. Enzymes used in biosensors should have high stability, especially toward reactive oxygen species. In order to improve oxidative stability of CDH, we mutated CDH and tested its stability in presence of hydrogen peroxide. After successful cloning of the CDH gene in pYES2 vector, saturation mutagenesis was used to make library mutants. Residual activity of mutants was measured after the enzyme incubation in 0.3 M hydrogen peroxide for 0, 2 and 6h. After analysis of large number of mutants, it was observed that three mutants are showing higher oxidative stability compared to the wild – type enzyme. Residual activities of these mutants after 6 hour incubation in the hydrogen peroxide were over 50 %, whereas wild-type has 30%. Selected mutants were expressed in *S.cerevisiae* and purified on DEAE column. Purity and activity of the enzymes were detected on the electrophoresis gel.

BB P 08

Хемијски састав етарског уља листа мотрике пореклом из Црне Горе

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Crithmum maritimum L., мотрика или морски коморач, једини је представник рода Crithmum, породице Apiaceae, са стаништем на каменитом приобаљу Европе. Од давнина користи се као зачин и храна, а познатаје и његова етнофармаколошка примена (антискорбутик, диуретик итд). За благо слан и ароматичан укус листова заслужно је присуство етарског уља, за које су досадашња истраживања показала висок степен варијабилности, како у приносу, тако и у саставу, у зависности од станишта биљне врсте. У овом раду, по први пут, анализиран је хемијски састав етарског уља листова C. maritimum пореклом са стеновитих плажа полуострва Луштица, у републици Црној Гори. Свеж биљни материјал, прикупљен током периода цветања, подвргнут је хидродестилацији, дајући 0,14 % етарског уља, w/w. ГХ-МС анализом је идентификовано преко 60 састојака, од којих су доминантни били: лимонен (66,7 %), сабинен (8,7 %), дилапиол (6,1 %), α-пинен (4,8 %) и γ-терпинен (4,0 %). Добијено етарско уље се и квалитативно и квантитативно разликовало од досада анализираних, што даје простора за могућност постојања различитих хемотипова C. maritimum.

Захвалност: *Овај рад финансиран је од стране Министарства просвете, науке и технолошког развоја Србије [евиденциони број пројекта 172061].*

Chemical compositionof the leaf essential oil of sea fennel from Montenegro: the first report

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Crithmum is a genus of the Apiaceae plant family with the sole species *Crithmum maritimum* L., known as samphire or sea fennel. This plant taxon, characteristic of the beaches in the Old World, has been used for various purposes, as a medicinal herb (anti-scorbutic agent, diuretic, etc.), as a spice and also as everyday food. Eaten raw, the leaves have a slightly salty, spicy taste, due to the volatile oil present therein. Up to now, a number of researchers have analyzed the composition of the essential oil of *C. maritimum*, and these studies have revealed a great variation in the content and identity of volatile secondary metabolites. In this study, we analyzed, for the first time, the chemical composition of the hydrodistilled essential oil of *C. maritimum* leaves from Montenegro. Fresh plant material, collected during the flowering period, from rocky coastsof the peninsula Luštica, yielded a yellowish fragrant essential oil (0.14 %, w/w). A GC-MS analysis enabled the identification of more than 60 constituents, among which limonene (66.7 %), sabinene (8.7 %), dill-apiole (6.1 %), α-pinene (4.8 %) and γ-terpinene (4.0 %) were the major ones. Both qualitatively and quantitatively the currently analyzed essential oil differed from those previously published indicating the possible existence of different chemotypes of *C. maritimum*.

BB P 09

Peroksidaze trave *Mischantus x giganteus* koje razlažu boje Coomassie Brilliant Blue i Ponso S

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Miscanthus x giganteus je biljka sa velikim prinosom biomase, koja se koristi kao biogorivo. Vrlo je otporna je na negativne uticaje sredine zahvaljujući odbrambeinim sistemima, u koje spada i enzim perkosidaza. U ovom radu je ispitano dejstvo peroksidaza trske na razlaganje boja. Boje koje se koriste u tekstilnoj industriji u velikoj meri zaršavaju u otpadnim vodama, a toksične su. Jedan od postupaka za nihovo uklanjanje je razlaganje oksidoreduktazama. Perksidaze imaju široku supstratnu specifičnost i primenjuju se u biotehnologiji uklanjanja fenolnih jedinjenja i organskih boja. Analizom sirovog ekstrakta rizoma *M. x giganteus* izoelektričnim fokusiranjem i zimografijom detektovane su dve grupe perkosidaznih izoformi, kisele i bazne, koje su dalje izolovane jonoizmenjivačkom hromatografijom. Optimalno pH obe grupe izoformi je 6, prema gvajakolu. Testirano je njihovo dejstvo na boje, u koncentraciji 50 μg/mL, u kiseloj, neutralnoj i baznoj sredini. Razlaganje boja je rađeno na sobnoj temperaturi tokom 2 h. Korišćena je aktivnost enzima 0,5 U/mL i 240 mM vodonik peroksid. Obe izoforme su efikasno razlagale boju Coomassie Brilliant Blue R-250 u neutralnoj i baznoj sredini, potpuno je uklanjajući. Bazna izoforma je razložila 40 % boje Ponceau S, i to samo u baznoj sredini. Dalja karakterizacija enzima i optimizacija uslova delovanja je neophodna za procenu mogu li se industrijski primeniti.

Coomassie Brilliant Blue and Ponso S degrading peroxidases from the grass *Miscanthus x giganteus*

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Miscanthus x giganteus is a plant with high yield of biomass, which is used as biofuel. It can overcome negative environmental influences due to its defence systems, which include enzyme peroxidase. The ability of peroxidases to degrade dyes was investigated in this study. Dyes used in textile industry often end up in waste waters, although they are toxic. Oxidoreductases are used for bioremediation of waters which contain phenolic compunds and organic dyes. In this work, isoelectric focusing followed by zymograme analyses of crude extract of *Miscanthus x giganteu*s rhizome demonstrated existance of two groups of peroxidases, acidic and alkaline, which were further isolated by ion-exchange chromatography. The optimal pH value for both groups was 6, according to guaiacol. Their activity on dyes (50 μg/mL) was tested, at acidic, neutral and alkaline pH. Tests were performed at room temperature during 2 h, with enzyme activity of 0.5 U/mL and hydrogen peroxide concentration of 240 mM. Both isoforms were efficient in decomposing the dye Coomassie Brilliant Blue R-250 at neutral and alkaline pH, completely removing it. Alakline isoform removed 40 % of the Ponceau S dye, but only at alkaline pH. Further characterisation of these enzymes and optimisation of their working conditions is necessary to estimate whether they can be applied on the industrial scale.

BB P 010

In vitro proučavanje citotoksičnih efekata odabranih karbamata i urea

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Karbamati i uree su važne hemijske strukture koje se mogu naći u velikom broju biološki aktivnih jedinjenja. Karbamatni derivati poseduju karakterističnu -O-CO-NH- grupu koja ima različitu primenu u medicinskoj hemiji. Ciklične uree su korisni sintetički intermedijeri, posebno u sintezi farmakološki aktivnih imidazola.

Rezultati ispitivanja citoksičnosti trinaest cikličnih urea i karbamata u *in vitro* eksperimentu prema tri odabrane ćelijske linije humanog kancera, adenokarcinoma cerviksa HeLa, karcinoma pluća A549 i karcinoma dojke MDA-MB-453 pokazuju umerenu aktivnost kod četiri jedinjenja (**1**, **2**, **3** and **4**). Među njima, *trans*-5-fenetil-1-fenilheksahidro-1*H*-imidazo[4,5-*c*]piridin-2(3*H*)-on (**1**) je ispoljio najjaču aktivnost prema MDA-MB-453 ćelijama (IC_{50}=83,41μM). Ostala jedinjenja iz ispitivane serije bila su neaktivna prema sve tri testirane ćelijske liije. Najaktivnija jedinjenja su dalje testirana za procenu tipa ćelijske smrti na HeLa ćelijama pod fluorescentnim mikroskopom. Morfološka procena ćelija pokazala je da došlo do apoptoze nakon što su ćelije kancera tretirane sa koncentracijama IC_{50} četiri najaktivnija jedinjenja. Ova jedinjenja predstavljaju vodeće strukture za dizajn novih analoga sa poboljšanom citotoksičnom aktivnošću.

In vitro study on cytotoxic effects of selected carbamate and urea derivatives

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The carbamate and urea are an important chemical moieties which can be seen in the molecular scaffold of a large number of biologically active molecules. Carbamate derivatives with a recognizable –O-CO-NH– moiety encompass multiple applications in medicinal chemistry. Cyclic ureas are synthetically useful intermediates, particularly as precursors to pharmacologically active imidazoles.

The results of *in vitro* cytotoxic study of thirteen cyclic urea and carbamate derivatives toward three human cancer cell lines, cervix adenocarcinoma HeLa, non-small cell lung carcinoma A549 and human breast carcinoma MDA-MB-453 indicated moderate activities of four compounds (**1**, **2**, **3** and **4**). Amongst them *trans*-5-phenethyl-1-phenylhexahydro-1*H*-imidazo[4,5-*c*]pyridin-2(3*H*)-one (**1**) was the most active against MDA-MB-453 cells (IC_{50}=83.41μM). The other compounds from the series were inactive regarding all three studied cell lines. The most active compounds were further tested to evaluate cell death type on the HeLa cells under the fluorescent microscope. The morphological evaluation of cells revealed that apoptosis occurred after cancer cells were treated with IC_{50} concentrations of four the most active compounds, so they should be further investigated in the sense of structural modifications and cytotoxic activity enhancement.

BB P 11

Procena antioksidativnog kapaciteta ekstrakata kamilice koristeći elektrohemijske DNK-biosenzorne i spektrofotometrijske metode

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Kamilica (*Matricaria recutita* L.) je široko rasprostranjena biljka sa različitom terapeutskom primenom koja se vekovima koristi kao lekovita biljka. Pored tradicionalne upotrebe, nedavna istraživanja potvrdila su da čaj kamilice poseduje antioksidativno, antiinflamatorno, antikancer i mnoga druga delovanja. U okviru ovog rada ispitana je antioksidativna aktivnost subkritičnih vodenih ekstrakta kamilice dobijenih pri različitim pritiscima. Uticaj pritiska na biološki potencijal kamilice ispitan je u opsegu pritiska od 10 do 90 bar pri temperaturi od 115°C. Iako se optičke metode baziraju na donaciji vodonika ili elektrona između antioksidanasa i radikala, biosenzorne DNK metode simuliraju *in vivo* testove izlaganjem DNK molekula sistemu sa antioksidantima i ROS molekulima. Tokom ovog istraživanja ukupni antioksidativni kapacitet subkritičnih vodenih ekstrakata kamilice određen je spektrofotometrijskim (DPPH i Reducing Power) kao i DNK biosenzornim metodama naspram $HO^{\bullet}$ radikala.

Assessment of antioxidant capacity of chamomile extracts using electrochemical DNA-based biosensor and spectrophotometric methods

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Chamomile (*Matricaria recutita* L.) is a widely available herb with diverse therapeutic uses that has been used for centuries as a medicinal plant. Apart from its traditional use, recent investigations on health promoting efficacy of chamomile tea have also revealed its antioxidant, anti-inflammatory, anticancer activities, etc. In the frame of this research antioxidant activity of subcritical water extracts of chamomile obtained under different pressure were evaluated. Impact of pressure on biological potential of chamomile extracts was observed at five different pressures in the range from 10 to 90 bar, applying a temperature of 115°C. Although the optical methods are based on the donation of hydrogen or electrons between antioxidants and radicals, the DNA-based biosensor intends to simulate an *in vivo* assay by exposing DNA layer to biological ROS and antioxidants. During this research, total antioxidant capacity of subcritical water extracts of chamomile was determined by spectrophotometric methods (DPPH and Reducing Power assay) and DNA-based biosensors against the reactive oxygen species: $HO^{\bullet}$.

BB P 12

Efikasnost *Candida rugosa* lipaza u sintezi kapsinoida tokom transesterifikacije kokosovog ulja

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Kapsinoidi su fiziološki aktivni estri vanilil-alkohola (VA) i masnih kiselina (MK) i strukturno su slični kapsaicinu. Ova studija je bazirana na pokazanoj supstratnoj specifičnosti *Candida rugosa* lipaza (CRL) ka masnim kiselinama (MK) srednje dužine niza tokom esterifikacije VA. Kako trigliceridi kokosovog ulja (KU) obiluju baš ovim MK, ono je odabrano kao acil-donor. U optimalnim reakcionim uslovima (rastvarač *n*-heksan, molski odnos VA/MK = 1,5/1; 48 h, 45 °C, 600 o/min) KU je obogaćeno smešom kapsinoida: vanilil-kaprilat, vanilil-dekanat i vanilil-laurat (prinosi konverzije VA: 26 %, 13 % i 41 %, redom). ^{1}H i ^{13}C NMR strukturnom karakterizacijom je zaključeno da se esterifikuje isključivo primarna (benzilna) –OH grupa VA. Pored toga što je znatno unapredio medicinsku i prehrambenu vrednost KU, naš postupak ima i veliki potencijal za obradu sličnih složenih supstrata.

Efficacy of *Candida rugosa* lipases in synthesis of capsinoids during transesterification of coconut oil

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Capsinoids are physiologically active esters of VA and fatty acids (FA), structurally related to capsaicin. This study is based upon CRL substrate specificity towards medium-chain length FA during esterification of VA. Since coconut oil's (CO) triglycerides are rich in these particular FA, it was chosen as an acyl-donor. Under optimal conditions (solvent *n*-hexane; mol ratio VA/FA = 1,5/1; 48h, 45°C, 600 rpm), CO was enriched with capsinoid mixture: vanillyl-caprylate, vanillyl-decanoate and vanillyl-laurate (VA conversion yields:26 %, 13 % and 41 %, respectively). ^{1}H and ^{13}C NMR structural analysis revealed that esterification of VA occurs exclusively through its primary (benzyl) –OH group. In addition to significant improvement of medicinal and nutritive value of CO,our procedure also therefore has a great potential for processing of simillar complex substrates.

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BB P 13

Ispitivanje interakcija bimetalskih kompleksa platine(II) i paladijuma(II) sa DNK i BSA

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Bimetalski kompleksi spadaju u novu generaciju potencijalnih antitumorskih lekova. Razlog velikog interesovanja za izučavanjem ovih kompleksa je njihova sposobnost da sa molekulom DNK formiraju proizvode koji se strukturno razlikuju od onih koje formiraju cisplatina i slični kompleksi.[1]
Ispitivane su interakcije tri bimetalska dinuklearna kompleksa platine(II) i paladijuma(II), [{PdCl(N-N)}(μ-L){PtCl(N-N)}]Cl(ClO_4) (gde je N-N = 2, 2'-bipiridin; L = pirazin ili 1, 6-diaminoheksan) i [{PdCl(N-N)}(μ-L){PtCl(N-N)}]Cl(ClO_4) (gde je N-N = etilendiamin; L = pirazin) sa molekulom DNK i BSA (govođim serum albuminom) primenom različitih eksperimentalnih metoda. Visoke vrednosti konstanti vezivanja ukazuju na veoma jake interakcije bimetalskih kompleksa sa molekulom DNK. Svi ispitivani kompleksi pokazuju veliki afinitet vezivanja za serum albumin, pri čemu kompleks sa etilendiaminom kao inertnim i pirazinom kao mostnim ligandima ispoljava najveći. Rezultati ispitivanja takođe pokazuju da postoji samo jedno mesto u albuminu pogodno za vezanje kompleksa.[2]

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Study of the interactions of bimetallic complexes of platinum(II) and palladium(II) with DNA and BSA

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Bimetallic complexes represent a novel generation of potential antitumor drugs. The reason for huge interest in studying of these complexes is their capability to interact with DNA forming compounds which are distinctly different from compounds that form cisplatin and similar complexes.[1]
The interactions of three bimetallic dinuclear complexes of platium(II) and palladium(II), [{PdCl(N-N)}(μ-L){PtCl(N-N)}]Cl(ClO_4) (where N-N = 2, 2'-bipyridine; L = pyrazine or 1,6-diaminohexane) and [{PdCl(N-N)}(μ-L){PtCl(N-N)}]Cl(ClO_4) (where N-N = ethylenediamine; L = pyrazine) with DNA and BSA (bovine serum albumine) were investigated using different experimental methods. High values of binding constants indicate very strong interactions of bimetallic complexes with DNA molecule. Additionaly, all studied complexes showed a high binding affinity for BSA, esspecially for complex with ethylenediamine as inert and pyrazine as bridge ligands. The results also showed that there is only one site in albumine capable for binding of complex.[2]

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Nauka o materijalima - Materials Science

NM P 01

Uticaj uslova sinteze na stepen bubrenja pH osetljivih hidrogelova na bazi kopolimera poli(akrilamid-ko-akrilna kiselina)

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Hidrogel na bazi kopolimera poli(akrilamid-ko-akrilna kiselina) sintetisan je radikalnom polimerizacijom iniciranom sistemom inicijatora i akceleratora. Za sintezu hidrogelova korišćene su dve vrste inicijatora - kalijumpersulfat (KPS) i amonijumpersulfat (APS) i akcelerator N,N,N',N'-tetrametil etilendiamin (TEMED), dok je kao umreživač korišćen N,N'-metilen bisakrilamid (MBAM). Pored vrste inicijatora u sintezi je variran odnos monomera akrilne kiseline i akrilamida i udeo umreživača (1 i 3% umreživača u odnosu na ukupnu masu monomera). Kinetika bubrenja dobijenih hidrogelova ispitana je u kiseloj (pH=5) i alkalnoj sredini (pH=10) na temperaturi 35 – 37 °C. Dobijeni rezultati pokazali su postojanje korelacije između strukture hidrogela i količine apsorbovane vode. Gelovi sa manjim udelom umreživača pokazali su očekivano veću sposobnost apsorpcije vode. Na kinetiku bubrenja uticao je i odnos monomera, tip primenjenog inicijatora, ali i pH vrednost sredine u kojoj je vršeno određivanje stepena bubrenja. To implicira mogućnost primene hidrogelova na bazi poli(akrilamid-ko-akrilne kiseline) u širokom spektru područja kao što su medicina, farmacija, kozmetika, prečišćavanje vode.

Autori se zahvaljuju docentu dr Ivanu Ristiću.

The influence of synthesis condition on the swelling behaviour of pH sensitive poly(acrylamide-co-acrylic acid) based hydrogels

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Poly (acrylamide-co-acrylic acid) (poly(Aam-co-AA)) based hydogels were prepared by free radical polymerization initiated by system of initiator and accelerator. Two types of initiators - potassium persulfate (KPS) and ammonium persulfate (APS), accelerator N,N,N',N'-tetramethyl ethylene diamine (TEMED) and crosslinking agent N,N'-methylene bisacrylamide (MBAM) were employed in syntehsis of hydrogels. The type of initiator as well as monomers ratio and amount of crosslinking agent (1 and 3% per total weight of monomers) were varied in the synthesis of copolymer hydrogels. The swelling kinetics of obtained hydrogels has been investigated in acidic and alkaline medium at 35-37 °C. Obtained results have showed strong correlation between hydrogel composition and swelling behaviour. Gels with lower amount of crosslinking agent have showed expected greater ability to absorb water. Swelling kinetics is affected by monomers ratio, initiator type as well as pH value of the environment. That implies the possibility of applying (poly(Aam-co-AA)) based hydogels in a wide range of fields such as medicine, pharmacy, cosmetics, water treatment.

The authors wish to thank docent dr Ivan Ristić.

NM P 02

Evaluacija pletenina namenjenih za izradu letnje odeće

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Polazeći od činjenice da optička svojstva tekstilnih materijala predstavljaju bitan parametar koji uslovljava toplotni komfor i bezbednost (zaštita koju odevni predmet pruža), u okviru ovog rada se pristupilo evaluaciji odabranog asortimana pletenina namenjenog za izradu letnjih majica. Radi se o četiri varijante desno-levih (DL) pletenina izrađenih od mešavine vlakana konoplje (55 %) i organskog pamuka (45 %). Ove pletenine su ispitivane u pogledu sposobnosti propuštanja ultraljubičastog (UV) i vidljivog (VIS) dela sunčevog spektra. Pored toga, meren je stepen zagrevanja pletenina pod dejstvom sunčeve svetlosti. Rezultati sposobnosti propuštanja vidljive svetlosti i stepena zagrevanja pletenina poslužili su za njihovu evaluaciju u pogledu toplotnog komfora, dok je ispitivanje intenziteta propuštanja UV zraka bilo usmereno na ocenu pletenina u pogledu bezbednosti, odnosno zaštite od štetnog UV zračenja. Dobijeni rezultati ističu pleteninu izrađenu od sirovih vlakana konoplje i organskog pamuka kao pleteninu sa najvećim potencijalom u pogledu ispitivanih performansi.

Evaluation of knitted fabrics for summer clothing

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Bearing in mind that the optical properties of textile materials represents important parameter which influences the level of thermal comfort and safety (concerning health) of a garment, the evaluation of the selected assortment of knitted fabrics for summer T-shirt was conducted in this study. Four variants of plain jersey knitted fabrics produced from blended hemp 55 % and organic cotton 45 % fibres were evaluated. The knitted fabrics were investigated in terms of the ability to transfer ultraviolet (UV) and visible (VIS) light. In addition, the temperature of the knitted fabrics under sunlight was measured. The selected assortment of knitted fabrics was evaluated in terms of thermal comfort according to their VIS transmittance and ability to produce heat. Investigation of the ability of the knits to transmit UV radiation was focused on their evaluation in terms of protection against harmful UV radiation. According to the results obtained, the grey knitted fabric was chosen from the selected assortment since it has the greatest potential in terms of investigated performances.

NM P 03

Sensors activity followed through conductivity changes in PMMA/CNTs nanocomposite as a potential sensor material

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With unique structure and transport properties, carbon nanotubes (CNTs) have attracted much interest as the reinforcement for polymer matrix composites. The CNTs/polymer nanocomposites hold the promise of delivering exceptionally mechanical properties and multi-functional characteristics. Therefore in the recent years, CNTs nanocomposites are increasingly being thought of as a realistic alternative to conventional smart materials, largely due to their superior electrical properties. When CNTs are incorporated into polymers, the result is electrically conductive composites with high electrical conductivity at very low CNTs content. Great interest has been generated for carbon nanotubes (CNTs) as a result of their properties that may be exploited to develop next generation of sensors as highly selective, sensitive, responsive, and cost effective sensors. These sensors could make significant impact in everyday life, as a result of modulation of the conductance due to their changes in chirality, when CNTs are subjected to a mechanical strain. For this research, biocompatible polymer matrix based on PMMA, was used to provide a medium between the CNTs. For the preparation of the polymer nanocomposites with different content of CNTs, were used SWCNT mixed in 1 and 0.5 % w/w content and MWCNT mixed in 1, 0.5 and 0.25 % w/w content. The PMMA/CNT nanocomposites were prepared by mixing the CNT and PMMA in a dichloromethane solution. Sensors activity was followed through the conductivity changes in PMMA/CNTs nanocomposite films with different type of CNT (SWCNT and MWCNT) and various surface treatments (by acid or base). Our results demonstrate the proof-of-concept for the new detector to be used in several applications as an accurate gas sensor for CO detection, including indoor and atmosphere air quality monitoring, industrial uses, automobile exhaust monitoring, gas leak detectors, home food spoilage monitors etc.

NM P 04

PANI/CNT and PANI/GR nanocomposites as nanosensors

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Because of their light weight, conductivity, mechanical flexibility and low cost, conductive polymers have potential for different applivations. Polyaniline (PANI) has very interesting properties such as excellent environmental stability, tailorable and reversible electrical properties by controlled charge transfer processes. The capability of this polymer to switch between conducting and insulating states enables this material to be use in many applications such as chemical and biological sensors.

Recently, a new class of composite materials with PANI as a matrix reinforced with nanoparticles has shown unique synergism in properties. Furthermore, CNT, graphene and other carbon based nanomaterials are of particular interest because of their exceptional structural, mechanical and electronic properties.

It is expected that GR and CNT nanocomposites should display different properties because of the monoatomic thickness and planar structure of GR. These two types of nanocomposites are also expected to have differences in the morphology and the interactions between their components.

In this work, we investigate the morphology of PANI/CNT and PANI/GR nanocomposites, which have the potential to be used as nanosensors.

NM P 05

Testing of SPE lectrode sensor based on PANI/CNT nanocomposites

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Traditional sensing devices have been produced with inorganic semiconductors, solid electrolytes and metals. Polymer nanocomposites have entered the sensor market thank to their ease of process and versatility, as chemical and physical properties of polymers can be tailored by chemical manipulation to fit specific requirements. As most polymers are unable to conduct electricity, their insulating properties have been widely utilized by the electronic industry, to immobilize and protect actively sensing materials. With the discover of conducting polymers and carbon nanostructures, organic macromolecules have found increasing application as active materials in sensors. In this work, PANI/MWCNT nanocomposites were used as a sensing component.
Electro-polymerization of MWCNT/PANI systems was performed directly on the screen printed gold electrode surface optimizing previously the necessary conditions in order to obtain the correct PANI form. After that, the obtained nano-sensor electrodes were backed in order to obtain stable nanocomposite film on the electrode wires . The surface of the nano composites directly electro-polymerzied on the electrodes was studied by SEM and ATF-FTIR spectroscopy. The changes in electrical resistivity were followed due to the pH changes of the water.

NM P 06

Fizičko-mehaničke i strukturne osobine biorazgradivih biofilmova na bazi pogače uljane tikve

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Poslednjih godina proizvodnja biorazgradivih ambalažnih materijala, dobijenih iz agro-industrijskog otpada, je u ekspanziji. Zbog sposobnosti da se razgrade u spoljašnjoj sredini i činjenice da se dobijaju iz prirodnih izvora, ovi materijali predstavljaju veoma dobru alternativu za polimerne ambalažne materijale, koji su trenutno vodeći materijali u industriji pakovanja. Cilj istraživanja je da se ispitaju fizičko-mehaničke i strukturne osobine biorazgradivih filmova na bazi pogače uljane tikve (PuOC). Pogača uljane tikve je nusproizvod dobijen nakon hladnog ceđenja ulja iz semena tikve. PuOC predstavlja najmanje obrađen oblik semena tikve, koja sadrži približno 63 % proteina, 12 % ugljenih hidrata, 4,5 % vlakana, 8,4 % uljai 13 % ostalih komponenti. Zbog ovakvog sastava, cela PuOC pogača predstavlja odgovarajući materijal za dobijanje biofilmova. Različite koncentracije najčešće korišćenog plastifikatora, glicerola (30, 40 i 50 %) i stabilizatora, guar-ksantana (0,1; 0,3 i 0,5 %) su dodate u PuOC filmove kako bi se dobile optimalne fizičko-mehaničke osobine filmova. Pored ispitivanih fizičko-mehaničkih osobina (zatezna jačina, izduženje pri kidanju, bubrenje, rastvorljivost i sadržaj vlage), strukturne osobine dobijenih filmova su takođe ispitane. Dobijeni filmovi su imali debljine od 0,15 do 0,24 mm. Filmovi su imali različita mehanička svojstva u zavisnosti od koncentracije dodatog glicerola i guar-ksantana. Optimalne vrednosti mehaničkih osobina je pokazao film sa najmanjom koncentracijom glicerola i najvećom koncentracijom guar-ksantana. Veće koncentracije glicerola nisu imale uticaj na bubrenje i ukupnu rastvorljivost dobijenih filmova, dok je sa povećanjem koncentracije glicerola primećeno i povećanje sadržaja vlage u filmovima. Ispitivani film je pokazao pikove karakteristične za veze prisutne u molekulima proteina.

Physico-mechanical and structural properties of biodegradable biofilms based on pumpkin oil cake

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Nowadays, production of packaging materials based on biopolymers obtained from agro industrial waste is in expansion. Because of their ability to decompose in environment and fact that they are isolated from natural sources, these materials are very good alternative for polymer packaging materials that are currently leading materials in packaging industry. The objective of this study was to examine physico-mechanical and structural properties of biodegradable film based on whole pumpkin oil cake (PuOC). Pumpkin oil cake (PuOC) is a by-product, obtained after cold-pressing oil extraction from pumpkin seed. PuOC contains the least-processed form of pumpkin seed protein having approximate composition 63 % proteins, 12 % carbohydrates, 4.5 % crude fibers, 8.4 % oils and 13 % other components. Because of its content, the whole PuOC is suitable material for the production of bio-based films. Different concentrations of glycerol (30, 40 and 50 %), as the most commonly used plasticizer, and guar-xanthan (0.1, 0.3 and 0.5 %), as a stabilizer, were added in PuOC films in order to obtain optimal physico-mechanical film characteristics. Beside physico-mechanical (tensile strenght, elongation at break, swelling deegre, total soluble matter and moisture content), structural properties of obtained PuOC films were investigated. Results showed that obtained film thicknesses varied form 0.15 to 0.24 mm. Films had different mechanical properties, depending on concentrations of added glycerol and guar-xanthan. The optimal mechanical properties had film with the lowest concentration of glycerol and the highest concentration of guar-xanthan. The addition of glycerol did not have influence on deegre of swelling and total solubility of obtained films, however with higher concentration of glycerol the increase of moisture content was observed. In examined film, peaks characteristic for bonds present in protein molecules were observed.

NM P 07

Hidrotermalna sinteza mikročestica hematita (α-Fe_2O_3), morfološka i magnetna karakterizacija

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Metodom hidrotermalne sinteze dobijene su mikročestice hematita. Vršene su sinteze na temperaturama od 140^{0}C i 180^{0}C, sa trajanjem od 12-90 sati. Prekursor za sve sinteze bio je vodeni rastvor gvožđe(III)hlorid heksahidrata, kao izvor gvožđa, dok je za određene uzorke korišćen glicin kao surfaktant, u različitim molarnim odnosima Fe^{3+}/glicin. Dobijene su različite morfologije mikročestica: kubne, poliedarske, elipsoidne, što je potvrđeno skenirajućom elektronskom mikroskopijom (SEM). Veličine čestica hematita su bile u intervalu od jednog do nekoliko mikrometara. Metoda energijske disperzije rendgenskog zračenja (EDS), potvrdila je prisustvo gvožđa i kiseonika u svim uzorcima, u masenim odnosima koji približno odgovaraju stehiometriji Fe_2O_3. Magnetne osobine proučavane su magnetometrom sa vibrirajućim uzorkom (VSM). Snimljene su histerezisne petlje sa širokim opsegom koercitivnosti (70-3850 Oe) za različite uzorke. Koercitivnost značajno raste kod uzoraka sintetisanih u prisustvu glicina. Dalja istraživanja mikročestičnog hematita bi trebalo da idu u pravcu elektrohemijske karakterizacije, ka potencijalnoj primeni za skladištenje energije. Netoksičnost hematita ima potencijal za eventualne praktične primene.

Hydrothermal synthesis of hematite (α-Fe_2O_3) microparticles, morphological and magnetic characterization

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The hematite microparticles were prepared by a hydrothermal synthesis method. Syntheses were carried out under temperatures 140^{0}C and 180^{0}C, with durations in range from 12 to 90 hours. General precursor was ferric chloride hexahydrate as source of iron and glycine was used as surfactant, with various Fe^{3+}/glycine molar ratios. SEM (scanning electron microscopy) measurements confirmed different microparticle mophologies: cubic, polyhedral, eliptical. Particle sizes were in interval from one to few micrometers. Energy dispersive X-ray spectroscopy (EDS) confirmed presence of iron and oxygen in every sample, with mass ratios approximately corresponding to Fe_2O_3 stoichiometry. Magnetic properties have been studied with vibrating sample magnetometer (VSM). Recorded hysteresis loops showed wide range of the coercivity values (70-3850 Oe) for various samples. Samples synthesized with glycine assisted method had significantly higher coercivity. Further investigations of microparticle hematite should include electrochemical characterization, towards energy storage applications. Hematite, as non-toxic material, offers potential in practical applications.

NM P 08

Teorijska studija uticaja nabiranja i dopiranja grafenske ravni na njenu reaktivnost

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Grafen je poslednjih godina zaokupio pažnju zajednice koja se bavi Naukom o materijalima, usled jedinstvenih mehaničkih i elektronskih svojstava. Od svog otkrića, grafen je predlagan kao pogodan materijal za različite primene. Dodatne mogućnosti primene otvaraju se modifikacijom elektronske strukture grafena funkcionalizacijom, dopiranjem i nabiranjem njegove ravni. Koristeći proračune bazirane na Teoriji funkcionala gustine, pokazano je kako nabiranje grafena (pri različitim nivoima naprezanja) utiče na elektronsku strukturu, a time i na reaktivnost bazalne ravni. Uticaj dopiranja ovakvih sistema azotom i fosforom na njihovu reaktivnost takođe je ispitan, na primeru adsorpcije atomskog vodonika na ove sisteme. Pokazano je da se topologija površine može kontrolisati izborom dopanta.

Corrugation and doping effects on the reactivity of the graphene basal plane - a theoretical study

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Graphene has captured the attention of the Materials Science community in the recent years owing to its unique mechanical and electronic properties. It has been explored for many possible applications ever since its discovery, but even more application possibilities arise from additional tuning of its electronic structure through functionalization, doping and corrugation. Using Density Functional Theory calculations, we have demonstrated how graphene corrugation (with different per cents of strain) affects the electronic structure and therefore the reactivity of the graphene basal plane as well, which was demonstrated on the example of atomic hydrogen adsorption. We have also explored doping these corrugated systems with nitrogen and phosphorus, and demonstrated that the surface topology can be tuned by dopants.

NM P 09

Teorijska analiza adsorpcionih svojstava dopiranih heksagonalnih nanotuba MgO

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Oksidni materijali imaju širok spektar primena u različitim poljima tehnologije. Oksidi pokazuju raznovrsnost elektronskih i kristalnih struktura, i njihova provodna svojstva mogu varirati od izolatora do provodnosti slične metalima. MgO je jedan od oksida čija se svojstva intenzivno ispituju. Usled njegove dostupnosti, stabilnosti i slabe reaktivnosti, predmet je mnogih studija koje proučavaju mogućnost njegove funkcionalizacije za primene kao što su selektivni adsorbensi ili podloga za katalizatore.
Ovde će biti prikazani rezulati DFT proračuna svojstava heksagonalnih nanotuba MgO različitih veličina. Svojstva ovih nanotuba menjana su dopiranjem Li, B, C, N, i F, na različitim mestima duž nanotube. Promena elektronske strukture i stvaranje magnetizacije na mestu dopanta upućuje na moguću upotrebu ovakvih sistema kao adsorbenata ili katalizatora, ili za dobijanje novih magnetnih nanostruktuiranih materijala. Adsorpciona svojstva su ispitana koristeći CO kao probni molekul. Dopiranjem dolazi do značajne promene energije adsorpcije, pri čemu je ova promena lokalizovana na i u blizini mesta dopanta.

Theoretical analysis of adsorption properties of doped hexagonal MgO nanotubes

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Oxide materials have a wide range of application in various fields of technology. Oxides exhibit diverse electronic and crystalline structures, and their conductive properties can vary from insulators to conductivity similar to those of metals. MgO is one of the oxides whose properties are being intensively studied. Due to its availability, stability and chemical inertness, it's a subject of many studies that are investigating the possibilities of functionalizing it for applications such as selective adsorbents or catalyst support.
Here we will show the results of DFT calculations of the properties of hexagonal MgO nanotubes of varying sizes. The properties of these nanotubes were altered by doping with Li, B, C, N, and F, at various sites along the nanotube. Change of electronic structure and the induction of magnetization at the dopant site points towards the possible use of these systems as adsorbents or catalysts, or as new nanostructured magnetic materials. Adsorption properties are tested using CO as a probe molecule. It is shown that adsorption energy is drastically changed by doping, the change being localized at and around the dopant site.

NM P 10

Efekat oblaganja nanočestica CeO_2 na stabilnost njihove suspenzije

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Nanočestice CeO_2 (nanoceria) su interesantan biomaterijal zbog istovremenog postojanja Ce^{3+} i Ce^{4+} jona i formiranja kiseoničnih praznina na njihovoj površini. Dvojno ponašanje ovih nanočestica predstavlja veliki farmakološki potencijal, kao što je poboljšanje tretmana kancera, isporuka lekova i kataliza. Nanoceria može da štiti zdrave ćelije od oksidativnog stresa jer su moćni sakupljači slobodnih radikala, ali takođe pokazuju citotoksičnost nakon produženog izlaganja ćelija višim koncentracijama. Glavni problem dalje biomedicinske primene je njihova slaba ratvorljivost u vodi, koja može biti poboljšana oblaganjem nanočestica. Cilj ovog istraživanja je razvijanje odgovarajuće metode za oblaganje nanočestica CeO_2 sa tri različita ugljenim hidratima i ispitivanje efekta oblaganja na stabilnost njihove suspenzije. Za karakterizaciju nanočestica su korišćene X-Ray i FTIR spektroskopija i SEM (skenirajući elektronski mikroskop). Efekat oblaganja nanočestica na stabilnost suspenzije je ispitan merenjem turbiditeta.

The effect of nanoceria's coating on their suspension stability

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Cerium oxide nanoparticles CeO_2 (nanoceria) is interesting biomaterial due to coexistence of Ce^{3+} and Ce^{4+} ions and formation of oxygen vacancies on its surface. This dual behavior of nanoceria represents a great pharmacological potential, such as improving the treatment of cancers, drug delivery and catalysis. Nanoceria can protect healthy cells from oxidative stress because they are potent free radical scavenger, but they also show cytotoxicity after prolonged exposure of cells to higher concentrations. The main problem of their further biomedical application is their low solubility in water, which could be improved by coating of nanoparticles. The aim of this study was to develop appropriate methods for coating CeO_2 nanoparticles with three different carbohydrates and testing the effect of coating on their suspension stability. For nanoparticles characterisation were used X-Ray and FTIR spectroscopy and SEM (scanning electron microscopy). The effect of nanoparticles' coating on their suspension stability were investigated by measuring turbidity.

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NM P 11

Influence of pH value on reduction of graphene oxide by olive mill wastewater

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The main goal of this research was the preparation of graphene by means of chemical reduction with phenolic compounds present in olive vegetation water at various pH values. The reduction of GO has been carried out at pH 7 and 10 and temerature of 80°C using olive leaf extract (ELM) solution and olive mill wastewater (OMW). The duration of the experiments was five hours, resulting in rGO(ELM, pH 7), rGO(ELM, Ph 10) and rGO(OMW, Ph 10) products. The course of the reduction was monitored using UV/Vis. The obtained products were characterized using cyclic voltametry, EIS, TGA, IR spectroscopy and *four point probe* method. Three different samples of rGO have been examined by cyclic voltametry during which a glassy carbon (GC) electrode was used as a current collector. rGO(ELM, pH 10) sample has shown the best capacitive properties. Some residual polyphenolic compounds have been noticed in rGO(OMW, pH 10) sample, as a result, anodic and cathodic current peaks were formed in the cyclic voltammogram. The highest specific capacitance, 25,11 F g^{-1}, has been registered for rGO(OMW, pH 10) sample. By comparing capacitance of rGO(ELM, pH 10) and rGO(ELM, pH 7) samples it has been found that materials obtained by reduction at a higher pH value have better specific capacitance values.

NM P 12

Sinteza i fotokatalitičke osobine koloidnih čestica $BiVO_4$

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U cilju rešenja problema zagađenja životne sredine, fotokataliza pomoću poluprovodnika privlači sve više pažnje. Zbog odgovarajuće strukture zabranjene zone, bizmut-vandat ($BiVO_4$) je pogodan za apsorpciju vidljivog dela spektra. Sinteza koloidnog $BiVO_4$ u etilen glikolu uz PEG-200 kao dirigujući agens uspešno je postignuta. Optimizovani su različiti uslovi sinteze kao što su pH vrednost, koncentracija prekursora i molekulska težina PEG-a. Dobijeni koloidi okarakterisani su UV-VIS spektroskopijom. Izmereni apsorpcioni spektri , za niže koncetracije prekursora, pokazuju plavi pomak i izračunata energija zabranjene zone E_g je u opsegu od 2.55 do 2.76 eV. Nakon sinteze, dobijeni koloidi se mešaju sa vodom, centrifugiraju i dobijeni talog ispira metanolom. Difraktogrami koji odgovaraju prahovima nakon sinteze, pokazuju da nanočestice $BiVO_4$ imaju čistu tetragonalnu strukturu. U cilju poboljšanja kristaliničnosti i detaljnijeg ispitivanja strukture i fotokatalitičkih osobina, dobijene nanočestice žarene su na 450 °C u toku 3 sata. Kako bi se ispitala fotokatalitička aktivnost uzoraka, testirana je njihova sposobnost za degradaciju organske boje. Nanočestice dobijene na ovaj način pokazuju izuzetnu fotokatalitičku aktivnost i dalje unapređenje efikasnosti kao i druge primene se mogu očekivati u budućnosti.

Synthesis and photocatalytic properties of colloid particles of $BiVO_4$

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In order to solve the pollution problem, semiconductor photocatalysis has gained a lot of attention. Because of its corresponding band structure, bismuth-vanadate ($BiVO_4$) is well suited for harvesting the visible part of the spectrum. Herein, colloid synthesis of $BiVO_4$ in ethylene-glycol with PEG-200 as a directing agent has been successfully achieved. Various synthesis conditions such as pH value, concentration of precursors and molecular weight of PEG have been optimized. Prepared colloid solutions have been characterized by UV-VIS spectroscopy. Measured absorption spectra, for lower concentrations of the precursors, showed blue shift and calculated band gap E_g of the colloid particles ranged from 2.55 to 2.76 eV. Obtained colloid solutions have been mixed with water, centrifuged, and the residue washed with methanol. X-ray diffraction (XRD) patterns show that the $BiVO_4$ nanoparticles crystallize in pure tetragonal phase. In order to improve their crystallinity and to investigate in more detail the structural and photocatalytic properties, the obtained $BiVO_4$ nanoparticles have been annealed at 450°C for 3 hours. In order to investigate photocatalytic activity of the samples, their ability to degrade organic dyes has been tested. $BiVO_4$ nanoparticles prepared via colloid synthesis show great photocatalytic activity and further improvements as well as some other applications are to be expected in the future.

NM P 13

Dokaz funkcionalnosti recikliranog katodnog materijala Li(Co-Mn-Ni)O_2 u vodenim elektrolitičkim rastvorima litijumove i natrijumove soli

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Potreba za zaštitom životne sredine od otpada litijum jonskih baterija je motivisala ovo istraživanje. Studija je fokusirana na reciklaži Li(Co-Mn-Ni)O_2 katodnog materijala. Metod koprecipitacije je korišćen za resintezu katodnog materijala $LiCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$. Njegov hemijski sastav, struktura i morfologija je određivana AAS-om, XRD, Ramanskom spektroskopijom i SEM-EDS-om. Funkcionalnost recikliranog materijala je proverena u vodenom rastvoru litijumove i natrijumove soli cikličnom voltametrijom i galvanostatskim merenjem. Početne vrednosti kapaciteta $LiCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$ i $NaCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$ u $LiNO_3$ i $NaNO_3$ iznose ~54 mAh g^{-1} i ~30 mAh g^{-1}, redom, na veoma velikoj brzini polarizacije 20 mV s^{-1}. Bolja cikličnost se pokazala u natrijumovoj soli, a razlog za to je diskutovan i povezan sa strukturnim preuređenjem materijala za vreme cikliranja.

The proof of functionality of the recycled Li(Co-Mn-Ni)O_2 cathode material in aqueous lithium and sodium electrolytic solutions

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This research addresses the need for better protecting the environment from the waste of spent Li-ion batteries. The study is focused on recycling of Li(Co-Mn-Ni)O_2 cathode material. The co-precipitation method is used to resynthesize the cathode material $LiCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$. Its chemical composition, structure and morphology were characterized by AAS, XRD, Raman spectroscopy and SEM-EDX methods. The applicability of recovered material was checked in an aqueous solution of lithium and sodium salts by CV and galvanostatic measurements. The initial capacity values of $LiCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$ and $NaCo_{0.415}Mn_{0.435}Ni_{0.15}O_2$ in $LiNO_3$ and $NaNO_3$ amount to ~54 mAh g^{-1} and ~30 mAh g^{-1}, respectively, at very high scan rate of 20 mV s^{-1}. Better cyclability was found for sodiated form, and the reason for this was discussed and correlated to the structural rearrangement of material during cycling.

NM P 14

Formiranje nanotubularnog oksidnog sloja na Ti-13Nb-13Zr leguri u funkciji vremena anodizacije

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Legure titana imaju veliku primenu u biomedicini zbog velike zatezne čvrstoće, visoke otpornosti na koroziju i izvanredne biokompatibilnosti, koje su posledica formiranja zaštitnog oksidnog sloja na površini materijala koji pre svega sprečava oslobađanje jona i štiti materijal od degradacije. U cilju dobijanja optimalnih svojstava implanata, površina implantnog materijala se često modifikuje primenom različitih hemijskih površinskih tretmana uključujući elektrohemijsku anodnu oksidaciju. Cilj ovog istraživanja je dobijanje nanotubularnog oksidnog sloja na površini Ti-13Nb-13Zr (TNZ) legure krupnozrne (coarse-grained, CG) i sitnozrne (ultrafine-grained, UFG) mikrostrukture postupkom anodizacije, kao i poređenje morfologije nanotuba dobijenih pri različitom vremenu anodizacije. Nanotubularni oksidni sloj na površini CG TNZ i UFG TNZ legura formiran je postupkom elektrohemijske anodizacije u elektrolitu koji sadrži fluoridne jone na sobnoj temperaturi tokom različitog vremena. Karakterizacija formiranih nanotuba je izvedena primenom skenirajuće elektronske mikroskopije. Rezultati su pokazali da vreme anodizacije ima veliki uticaj na debljinu zida i prečnik, kao i na raspored nanotuba, kod oba ispitivana materijala. Osim toga, nanotube formirane na UFG TNZ leguri su uniformnije raspoređene u odnosu na nanotube na CG TNZ.

Nanotubular oxide layer formation on Ti-13Nb-13Zr alloy as a function of anodizing time

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Titanium alloys are widely used in biomedicine due to their great tensile strength, high corrosion resistance and extraordinary biocompatibility, which are consequence of protective oxide layer formation on the materials surface which prevents ion release and protects the surface from degradation. In order to optimize the implants properties, the implants surfaces have been modified by different chemical surface-treatments including electrochemical anodic oxidation. The aim of this study was to obtain nanotubular oxide layer on the Ti-13Nb-13Zr (TNZ) alloy surface, with both coarse-grained (CG) and ultrafine-grained (UFG) microstructure using anodization, and to compare nanotube morphology obtained during different anodizing time. Nanotubular oxide layer on CG TNZ and UFG TNZ alloys was formed using electrochemical anodization in electrolyte which contains fluoride ions at room temperature during different time. The characterisation of formed nanotubes was performed using scanning electron microscopy. The results shown that anodizing time has significant influence on the wall thickness and diameter of nanotubes, as well as nanotubes arrangement, for both examined materials. Furthermore, nanotubes formed on UFG TNZ alloy are more uniformly arranged compared to nanotubes on CG TNZ alloy.

NM P 15

Sinteza, morfološke i optičke osobine novih crvenih fosfora $RE_2Hf_2O_7$: 1at. % Eu^{3+} (RE^{3+} =Y^{3+}, Gd^{3+}, Lu^{3+})

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Hafnati retkih zemalja su obećavajući kandidati za matrice luminiscentnih materijala zbog svojih visokih tački topljenja (oko 2700 K) i stabilnosti kristalne rešetke. U ovom radu, po prvi put su sintetisani $RE_2Hf_2O_7$:Eu^{3+} (RE^{3+} =Y^{3+}, Gd^{3+}, Lu^{3+}) hemijskom sintezom. Hafnati su dopirani sa 1at. % Eu^{3+} koji se ugrađuje na mesto RE jona u matrici. Kristalna struktura i čistoća faze su određeni difrakcijom X zraka (XRD). $RE_2Hf_2O_7$: 1at. % Eu^{3+} fosfori kristališu u kubičnu fluoritnu strukturu (Fm3m (2 2 5)) koja potpuno odgovara referentnoj kartici ICDD 00-024-1406 za kompaktni materijal itrijum-hafnata. Takođe, odredili smo veličinu kristalita u svim ispitivanim sistemima. U cilju proučavanja kako različiti RE^{3+} u $RE_2O_2O_7$ utiču na emisiju 1at. % Eu^{3+} pratili smo emisiju Eu^{3+} na talasnoj dužini od 612 nm pri pobudi na talasnoj dužini od 464 nm. Vreme života i CIE koordinate su određene za sve sintetisane fosfore.

Synthesis, morfological and optical properties of new red phosphors $RE_2Hf_2O_7$: 1at. % Eu^{3+} (RE=Y, Gd, Lu)

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Rare earth hafnates are promising candidates for luminiscent hosts because its high melting point (around 2700 K) and stability of crystal lattice. In this work, at the first time, it is synthesized $RE_2Hf_2O_7$: Eu^{3+} (RE^{3+} =Y^{3+}, Gd^{3+}, Lu^{3+}) by soft chemical synthesis. Hafnates are doped with 1 at. % Eu^{3+} where Eu^{3+} was replaced RE ions in matrix. The crystal structure and phase purity were investigated by X-ray diffraction (XRD). $RE_2Hf_2O_7$: 1at. % Eu^{3+} phosphors crystallize in cubic fluorite type of crystal structure (Fm3m (2 2 5)) and all of them are corresponding with referent card ICDD 00-024-1406 for bulk material of $Y_2Hf_2O_7$. Also, we determined the crystallite size in all examined systems. In order to study how different RE^{3+} in $RE_2Hf_2O_7$ influence on emission of 1at. % Eu^{3+} we monitored emission at 612 nm under the excitation wavelength of 464 nm. Life time and CIE coordinates was determined for all synthesized phosphors.

NM P 16

Mikrostrukturna karakterizacija Al-Mg-Si legure posle termičke obrade starenjem

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U ovom radu je sproveden metalografski postupak ispitivanja uzoraka aluminijumske legure EN-AW 6060 posle termičke obrade starenjem. Priprema uzoraka obuhvatila je termičku obradu uzoraka žarenjem na temperaturi 550 ºC u trajanju od 6 časova radi uklanjanja polazne strukture i dobijanja strukture homogenog čvrstog rastvora. Nakon toga usledilo je rastvorno žarenje na istoj temperaturi u trajanju od 1 časa i kaljenje u vodi sa ledom radi dobijanja prezasićenog čvrstog rastvora (α_{ssss}) u strukturi. Uzorci su zatim stareni na temperaturi 200 ºC u trajanju od 1-8 časova. Za mikrostrukturnu karakterizaciju izabran je uzorak sa najvećom izmerenom tvrdoćom koji je staren na temperaturi 200 ºC u trajanju od 4 časa. Stareni uzorci su pripremljeni za metalografsku analizu postupcima koji su uključivali brušenje, poliranje i nagrizanje. Na metalografski pripremljenim uzorcima napravljena je mikroskopska analiza snimanjem struktura. Analizirana je mikrostruktura uzoraka pomoću optičke mikroskopije (OM) i skenirajuće elektronske mikroskopije (SEM) sa energetsko disperzivnim spektrometrom. Ispitivan je hemijski sastav, morfologija i raspored prisutnih faza, dobijenih posle termičke obrade uzoraka starenjem. Metalografska analiza je potvrdila postojanje promena u precipitacionom ojačavanju kod aluminijumske legure.

Microstructural characterization of the Al-Mg-Si alloy after aging heat treatment

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In this paper, metalographic investigation of aluminum EN-AW 6060 samples was carried out following an aging heat treatment. Sample preparation included annealing at 550 °ºC for 6 hours in order to remove the initial structure and to obtain a homogeneous solid solution. This was followed by heat treatment of the solution at the same temperature for 1 hour and quenching in ice water to obtain the super saturated solid solution (α_{ssss}). Samples were then artificially aged at 200 °C for 1-8 hours. For microstructural characterization, the sample with the highest hardness value was selected and then aged at 200 °C for 4 hours. The aged samples were prepared for metallographic characterization by using standard grinding, polishing and etching techniques. On prepared samples microscopic analysis was done by recording the structures. Sample microstructures were analyzed using optical microscopy (OM) and scaning electron microscopy (SEM) with energy dispersive spectrometer (EDS). The chemical composition, morphology and distribution of the phases which occured in the aged samples were investigated. Metallographic analysis confirmed the existence of changes in the precipitation hardening of the investigated aluminum alloy.

NM P 17

Uticaj talka i polietilen glikola na termalna i mehanička svojstva polimlečne kiseline

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S obzirom na sve veći problem odlaganja otpada usled preteranog korišćenja plastike, nameće se potreba za razvijanjem novih biorazgradivih materijala koji će zameniti tradicionalnu plastiku. Biorazgradivi polimeri imaju izuzetnan potencijal, a savremena istraživanja koja se tiču modifikacije njihovog sastava mogu u velikoj meri da smanje njihovu cenu i poboljšaju termalne i mehaničke osobine, što će doprineti njihovoj ubrzanoj komercijalizaciji. U ovom radu pripremljeni su kompoziti polimlečne kiseline (PLA), polietilen glikogla (PEG) i različitih udela talka u rastvoru hloroforma sa ciljem utvrđivanja uticaja talka i polietilen glikola na termalna i probojna svojstva kompozita polimlečne kiseline. Termalna svojstva, temperatura kristalizacije, temperatura topljenja, temperatura prelaza u staklasto stanje i stepen kristalizacije polimlečne kiseline ispitivani su sa diferencijalnom skenirajućom kalorimetrijom, a praćena su i mehanička svojstava pripremljenih kompozita probojnom sondom, jačina proboja i deformacija pri proboju. Dobijeni rezultati su potvrdili nukleirajući efekat talka na kristalizacione osobine polimlečne kiseline. Utvđeno je da je efekat talka u kristalizaciji polimlečne kiseline i poboljšanju mehaničkih svojstava u odnosu na čist polimer najbolji pri na nižim udelima talka (2-5 %).

Influence of talc and polyethylene glycol on thermal and mehanical properties of poly lactic acid

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Regarding to the rising problem of waste disposal due to profusely usage of plastics, there is a certain need to develop new biodegradable materials which will be able to replace traditional plastics. Biodegradable polymers have significant potential and are being widely investigated nowadays for the modification of their composition which contributes the improvement of their thermal and mechanical properties, lowering the price and fastening the commercialization. In this work, composites based on poly lactic acid (PLA), polyethylene glycol (PEG) and different content of talc (0-15%) were prepared by solution casting technique from chloroform. Thermal properties, temperatures of crystallization (T_c) , melting (T_m), glass transition temperature (T_g) and degree of crystallinity (x_c) of poly lactic acid were examined with differential scanning calorimetry (DSC). The mechanical properties, strength and deformation were determined as well using puncture probe.
The obtained results confirmed, the nucleation effect of talc on crystallization behavior of PLA. It is established that improved mechanical properties where noticed at lower talc content of (2-5 %) related to pure PLA matrix.

NM P 18

The use of surfactants for electrochemical exfoliation of natural graphite flakes

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The aim of this work was to perform electrochemical exfoliation of natural graphite in order to obtain graphene. The electrolytes (0.1 mol dm^{-3}) were prepared by the dissolution of sodium dodecyl sulfate (SDS) and sodium dodecyl benzenesulfonate (SDBS) in de-ionized water. Graphite electrode was alternately polarized at positive and negative potentials by using two electrode system. During positive polarization SDS and SDBS are intercalated within the structure of graphite, and oxygen evolution as well as carbon oxidation takes place. By applying negative potential cations are intercalated into graphite working electrode and also hydrogen evolution takes place.

Electrodes were characterized by using cyclic voltammetry and the exfoliation process was followed by monitoring current transients. The exfoliated products were characterized by employing UV/Vis spectrophotometry and atomic force microscopy. The brown color of the electrolyte indicates that the graphite was exfoliated and UV/Vis spectra of graphene/SDS suspensions has proved that obtained product was graphene oxide. Atomic force microscopy has shown that bi- or trilayer graphene was present within the solution.

NM P 19

Zinc benzenepolycarboxylato complexes as a source for photocatalytic active ZnO

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The synthesis of ZnO *via* thermal decomposition of a single-source precursor such as ternary Zn complex represents a nonconventional and novel synthetic methodology. Thermally induced changes provide the ability to control the crystal structure, phase composition, morphology and crystallite size of the resulting ZnO nanomaterial. As a precursors for obtaining photocatalytic active ZnO, four Zn complexes with various benzenepolycarboxylates [1] were used. Main aims of this work were to investigate the influence of precursors on particle size and morphology of obtained ZnO nanoparticles, along with its photocatalytic activity. In addition, the mechanism and kinetics of thermal degradation of Zn benzenepolycarboxylato complexes is analyzed under non-isothermal conditions in N_2 atmosphere.

Benzenpolikarboksilato-kompleksi cinka kao izvor za dobijanje fotokatalitički aktivnog ZnO

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Dobijanje ZnO termičkom degradacijom prekursora kao što su ternarni Zn-kompleksi predstavlja nekonvencionalnu i novu metodu sinteze. Termički indukovane promene omogućavaju kontrolu kristalne strukture, faznog sastava, morfologije i veličine kristalita ZnO. Četiri kompleksa Zn sa različitim benzenpolikarboksilatima [1] korišćena su kao prekursori za dobijanje fotokatalitički aktivnog ZnO. Glavni ciljevi ovog rada su utvrđivanje uticaja prekursora na veličinu i morfologiju tako dobijenih nanočestica ZnO, kao i ispitivanje fotokatalitičke aktivnosti. Mehanizam i kinetika termičke degradacije benzenpolikarboksilato-kompleksa Zn analizirana je u neizotermskim uslovima u N_2 atmosferi.

1. L. Radovanović, J. Rogan, D. Poleti, M. Milutinović, M.V. Rodić, *Polyhedron* **112** (2016) 18.

NM P 20

Ефекат механичке активације летечи пепео врз осовина цемента

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Циљ ове студије био је добијање цемент са механичким активираним пепелом и да истраже особине добијеног цемента. Летећи пепео из термоелектране РЕК Битола, Македонија, механички је активиран 20 min у млину са куглама у циљу повећања реактивности честица пепела. Садржај пепела у цементу је био 16 % mass. Анализиран је ефекат механичке активације цемента на хемијски и гранулометриски састав, густину, специфичну површину и механичке особине (снага везивања и чврстоћа).

Effects of mechanically activated fly ash on the properties of the cements

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The aim of this study was to fabricate cements with mechanically activated fly ash and to investigate the properties of the obtained cements. Fly ash from the thermal power plant REK Bitola, Macedonia was mechanically activated for 20 min in a planetary ball mill to increase the reactivity of the fly ash particles. The fly ash content in the cement was 16 wt. %. The effect of the mechanical activation on the cements was followed by determine the chemical and granulometric composition, density, specific surface area and mechanical properties (bending strength and compressive strength).

Teorijska hemija - Theoretical Chemistry

TH P 01

Mehanistički pristup ispitivanju antiradikalske aktivnosti dopamina, epinefrina i norepinefrina prema DPPH

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Kateholamini predstavljaju značajnu klasu biološki aktivnih molekula koji u organizmu imaju funciju prenošenja signala (neurotransmisije). Intenzivno se ispituje njihova antiradikalska aktivnost zbog pretpostavke da predstavljaju prvu liniju odbrane od oksidativnog stresa u mozgu. U ovom radu je kvantno-hemijskim metodama ispitana kinetika prenosa atoma vodonika (HAT) u reakciji dopamina (DO), epinefrina (EP) i norepinefrina (NE) sa DPPH. Termodinamički parametri prenosa atoma vodonika u gasnoj fazi su izračunati za sve aktivne centre i prelazno stanje je nađeno za najpovoljniju poziciju, *p*-OH grupu. Energije aktivacije iznose 77.1, 56.4 i 60.1 kJ/mol za DO, EP i NE. Konstante brzina bez uključenih dodatnih efekata iznose $1.9x10^{-1}$, $8.2x10^{2}$ i $1.8x10^{2}$ za isti raspored molekula. Relativno niske vrednost posledica su stabilnosti DPPH. Dodatna istraživanja su potrebna kako bi opisao mehanizam antiradikalske aktivnosti kateholamina prema biološki važnim radikalima. Autori se zahvaljuju Ministarstvu prosvete, nauke i tehnološkog razvoja Republike Srbije na finansijskoj pomoći kroz projekte 172015, 174028 i 172040.

The mechanistic approach in the antiradical activity investigation of dopamine, epinephrine and norepinephrine towards DPPH

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Catecholamines present a class of biologically active molecules which have the function of signal transmission (neurotransmission). The antiradical activity of these molecules has been intensively investigated due to the assumption that they represent the first line of defense against the oxidative stress in brain. In this contribution the kinetics of hydrogen atom transfer (HAT) between dopamine (DO), epinephrine (EP) and norepinephrine (EP) with the DPPH was explored by the means of quantum-chemical methods. Thermodynamic parameters in gaseous phase were calculated for the atom transfer for all of the active centers and transition state was obtained for the most favorable position, *p*-OH group. The activation energies are 77.1, 56.4 and 60.1 for DO, EP and NE. The rate constants without additional effects are $1.9x10^{-1}$, $8.2x10^{2}$ i $1.8x10^{2}$ for the same position of molecules. Relatively low values are due to the stability of DPPH. Additional research is needed for the proper description of the antiradical activity of catecholamines towards the biologically relevant radicals. Authors would like to acknowledge the Ministry of Education, Science and Technological Development of the Republic of Serbia through projects No. 172015, 174028 and 172040.

TH P 02

Teorijska studija vibronske i spin-orbitne sprege u $X\ ^2\Pi_u$ elektronskom stanju bakar dikarbonil kompleksa $Cu(CO)_2$

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Ova studija ima za cilj da putem *ab initio* računa predvidi vibronsku i spin-orbitnu strukturu $X\ ^2\Pi_u$ elektronskog stanja $Cu(CO)_2$ molekula, koji predstavlja prvi neutralni petoatomski molekul koj ispoljava Rener-Telerov efekat. Za računanje vibronskog spektra primenjen je varijacioni pristup za tretiranje Rener-Telerovog efekta u molekulima sa proizvoljnim broje jezgara i linearnom ravnotežnom geometrijom, relativno skoro razvijen u našoj grupi. Primenjeni modelni hamiltonijan isključuje iz razmatranja istežuće vibracije i rotaciju molekula u celini. Sa druge strane, uključuje međusobni uticaj vibronske i spin-orbitne sprege. Sedam parametara (plus spin-orbitna konstanta), koji se mogu dobiti iz *ab initio* izračunatih potencijalnih površi molekula koje koreliraju sa $X\ ^2\Pi_u$ pri linearnoj geometriji, su dovoljni za kontrukciju matrice hamiltonijana, čijom dijagonalizacijom se dobija kompletan kompletan nisko-energetski vibronski spektar. Rezultati su upoređeni sa relativno nedavno objavljenom eksperimentalnom studijom.

Theoretical study of vibronic and spin-orbit coupling in the $X\ ^2\Pi_u$ electronic state of copper dicarbonyl complex $Cu(CO)_2$

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The aim of the present study is to predict by means of *ab initio* calculations the vibronic and spin-orbit structure in the $X\ ^2\Pi_u$ electronic state of $Cu(CO)_2$ molecule which represents the first neutral five-atomic spicies exibiting the Renner-Teller effect. Recentely developed variational approach in our group for handling the Renner-Teller effect in molecules with arbitrary number of nuclei and linear equilibirum geometry is applied for calculation of the vibronic spectrum. The applied model Hamiltonian excludes the stretching vibrations and end-over-end rotations. On the other hand, it considers the interplay between the vibronic and spin–orbit couplings. Seven parametars (plus the spin-orbit constant), which can be extracted from the *ab initio* calculated potential energy surfaces of the $Cu(CO)_2$ molecule correlating at linear nuclear arrangements with $X\ ^2\Pi_u$ state, are sufficient for building up the Hamiltonian matrix whose diagonalization results in the complete low-energy (bending) vibronic spectrum. The results of the present study are compared with recently published experimental data.

TH P 03

Теоријска анализа димера повезаних протоном

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Резултати представљени у овом раду су добијени теоријском анализом система општег облика X⋯H^+⋯Y (X, Y = N_2, CO) који су познати и као димери повезани протоном. Димери повезани протоном се јављају само у екстремним условима попут оних остварених у међузвезданим маглинама. Познавање спектралних особина оваквих система омогућава одређивање концентрација елемената C, N, O и H у међузвезданим маглинама као и одређивање брзина кретања маглина. Добијени резултати су потврђени постојећим експерименталним подацима за системе N_2⋯H^+⋯N_2/N_2⋯D^+⋯N_2 и указују на високу делокализованост протона услед постојања водоничне везе са ниском енергетском баријером. Оптимизације структура и прорачуни хармонијских фреквенција су извршени *Ab initio,* до нивоа CCSD/6-311++G(3df,3pd). Слагање добијених резултата са експерименталним подацима за системе N_2⋯H^+⋯N_2/N_2⋯D^+⋯N_2, попут енергија дисоцијација и карактеристичних фреквенција, омогућава потврду тачности добијених резултата за системе за које не постоје експериментални подаци. Резултати добијени за системе CO⋯H^+⋯CO/CO⋯D^+⋯CO и CO⋯H^+⋯N_2/CO⋯D^+⋯N_2 могу послужити као претходница експерименталне провере.

Theoretical analysis of proton bridged dimers

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Results presented in this work were obtained by theoretical analysis for systems of a general form X⋯H^+⋯Y (X, Y = N_2, CO) which are also known as proton bridged dimers. Proton bridged dimers exist only in extreme conditions like those appearing in the interstellar nebulas. Knowing spectral characteristics of such systems allows concentration determination of elements C, N, O и H in the interstellar nebulas as well as determining the speed of interstellar nebulas. Acquired results are verified by existing experimental data for systems N_2⋯H^+⋯N_2/N_2⋯D^+⋯ N_2 and show a high proton delocalization as a consequence of existing low barrier hydrogen bond. Structure optimization and harmonic frequency calculation were done *Ab initio*, up to the CCSD/6-311++G(3df,3pd) level. Correspondence of attained results with the experimental data for systems N_2⋯H^+⋯N_2/N_2⋯D^+⋯N_2, such as dissociation energies and characteristic frequencies, allows accuracy confirmation of attained results for systems that lack experimental data. Results presented for CO⋯H^+⋯CO/CO⋯D^+⋯CO and CO⋯H^+⋯N_2/CO⋯D^+⋯N_2 systems can be used as a spearhead for experimental research.

TH P 04

Racionalni dizajn agonista I_1 imidazolinskih receptora

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Derivati imidazolina sa centralnim hipotenzivnim dejstvom ostvaruju svoj farmakološki efekat aktiviranjem α_2-adrenergičkih receptora (α_2-AR) i imidazolinskih I_1-receptora (I_1-IR). Dalja istraživanja su ograničena nedovoljnim poznavanjem strukture I_1-IR i njegovih signalnih puteva. Jedini do sada predloženi kandidat za I_1-IR je citosolni protein-nisharin. U našoj studiji primenjen je VS (eng. *virtual screening*) protokol koji intergriše metode *Ligand-* i *Structure-Based Drug Design*-a i selektovano je šest jedinjenja koja su slično rilmenidinu, agonisti I_1-IR, sposobna da interaguju sa nisharinom i ispolje antikancersku aktivnost na K562 ćelijama. Dalje biološke studije su selektovale jedno *hit* jedinjenje koje ima proapoptotski profil sličan rilmenidinu. Veoma nizak afinitet izabranih jedinjenja za α_2-AR isključuje mogućnost sinergističkog uticaja ovog signalnog puta.[3]

Rational design of imidazoline I_1-receptor agonists

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Central hypotensive imidazoline derivates act on the α_2-adrenoceptors (α_2-AR) and the imidazoline I_1-receptors (I_1-IR). Advancements in this field are limited by the lack of of IR structure and ignorance of IR signaling pathways. The only I_1-IR candidate proposed so far is the cytoplasmic protein-nischarin. In our study we applied an approach that integrates ligand- and structure-based virtual screening protocols and identified the six ligands that similary to an I_1-IR agonist, rilmenidin, could interact with nischarin and manifest anticancer activity on K562 cells. Further biological studies selected one most promising compound as a hit, that exibits a proapoptotic profile similar to that of rilmenidine. Very low affinity of the candidate ligands for α_2-AR indicated on lack of synergistic influences mediated by this receptor pathway.[3]

TH P 05

Teorijsko proučavanje interakcija između HDAC-1 i HDAC-6 enzima i *in silico* dizajniranih inhibitora

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Nesrazmerna posttranslaciona deacetilacija histona je povezana sa nastankom tumora i neurodegenerativnim bolestima. Do sada, FDA je registrovala 5 inhibitora histon deacetilaze (HDAC), koji su okarakterisani kao neselektivni HDAC inhibitori. Koristeći virtuelni dizajn zasnovan na hemijskoj strukturi liganda (3D-QSAR), na primeru naftalimidnog derivata skriptaida, utvrdili smo molekulske karakteristike značajne za selektivnu inhibiciju histon deacetilaze 6. Nakon *in silico* dizajna novih inhibitora, primenili smo molekulski doking koristeći kristalnu strukturu HDAC-1 enzima (5ICN) i kristalnu strukturu drugog katalitičkog domena HDAC-6 enzima (5EDU). Molekulski doking je proučavan u GOLD 5.4.0 softveru, koristeći ChemScore kao skoring funkciju, i dva *in silico* dizajnirana jedinjenja D-48 I D-34 su odabrana kao potencijalni selektivni HDAC-6 inhibitori za sintezu. Kraći linker odabranih jedinjenja omogućuje hidroksamskoj grupi da bude dostupnija Zn^{2+} jonu pri dnu aktivnog mesta enzima. Oba jedinjenja su pokazala poboljšanu selektivnost predviđenu razvijenim 3D-QSAR modelima.

A theoretical study of interaction between HDAC-1 and HDAC-6 enzymes and *in silico* designed inhibitors

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The disproportionate posttranslational histone modification as deacetylation has been associated with tumorigenesis and neurodegenerative diseases. Currently, there are five approved histone deacetylase (HDAC) inhibitors by FDA, which are defined as pan-HDAC inhibitors. By using ligand based virtual design approach (3D-QSAR) based on naphthalimide derivative scriptaid, we found molecular determinants important for selectivity towards histone deacetylase 6 isoform. After in silico design of novel inhibitors, we performed molecular docking studies using crystal structure of HDAC-1 enzyme (5ICN) and crystal structure of second human catalytic domain of HDAC-6 enzyme (5EDU). Molecular docking procedure was performed in GOLD 5.4.0 Software and ChemScore as scoring functions, and two *in silico* designed compounds D-48 and D-34 were selected as potential selective HDAC-6 inhibitors for synthesis. The shorter linker of selected compounds allows hydroxamic group to be more accessible to Zn^{2+} ion at the bottom of the active pocket. Both of them shown improved predicted selectivity according to the developed 3D-QSAR models.

TH P 06

Analiza Jahn-Teller-ovog efekta u organskim i neorganskim sistemima

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Po Jahn-Teller-ovoj (JT) teoremi svi nelinearni molekuli sa degenerisanim elektronskim stanjem spontano se distorguju duž vibracija koje nisu totalno simetrične, pri čemu dolazi do uklanjanja degeneracije uz sniženje energije. JT efekat je analiziran i izračunati su JT parametri za ciklopentadienil radikal ($C_5H_5^{\bullet}$), benzen katjon ($C_6H_6^{+}$) i benzen anjon ($C_6H_6^{-}$), anjone i katjone koranulena i koronena ($C_{20}H_{10}^{-}$, $C_{20}H_{10}^{+}$, $C_{24}H_{12}^{-}$ i $C_{24}H_{12}^{+}$), anjonski magnezijum ftalocijanin ($MgPc^{-}$) i mangan(II) ftalocijanin (MnPc) primenom teorije funkcionala gustine. Izvedena je analiza uticaja većeg broja vibracija odgovornih za distorziju molekula primenom modela Svojstvenog puta distorzije. Sve potrebne informacije pri izračunavanju koeficijenata vibronske sprege sadržane su u strukturi minimalne energije koja predstavlja pravi minimum na površini potencijalne energije, pa je vibraciona analiza jednoznačna. Ovim modelom moguće je direktno odvojiti doprinose različitih vibracija JT distorziji, njihov energetski doprinos JT stabilizacionoj energiji duž puta distorzije i odrediti sile odgovorne za JT distorziju, dajući bolji uvid u poreklo i mehanizam vibronske sprege.

Analysis of the Jahn-Teller effect in organic and inorganic systems

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The Jahn-Teller (JT) theorem states that a molecule with a degenerate electronic state spontaneously distorts along a non-totally symmetric vibrational coordinates. This removes the degeneracy and lowers the energy. The JT effect was analysed and the JT parameters were determined for cyclopentadienyl radical ($C_5H_5^{\bullet}$), benzene cation ($C_6H_6^{+}$), benzene anion ($C_6H_6^{-}$), anions and cations of corannulene and coronene ($C_{20}H_{10}^{-}$, $C_{20}H_{10}^{+}$, $C_{24}H_{12}^{-}$ i $C_{24}H_{12}^{+}$), anionic magnesium phthalocyanine ($MgPc^{-}$) and manganese(II) phthalocyanine (MnPc) by the means of Density Functional Theory (DFT) approach. The analysis of the multimode JT problem was performed by the means of the Intrinsic Distortion Path (IDP) model. All the required information, to calculate the vibronic coupling coefficients is contained in the minimum energy lower-symmetry structure. This structure is the real minimum on the potential energy surface, allowing normal mode analysis in the straightforward manner. With this model, it is possible to directly separate the contributions of the different normal modes to the JT distortion, their energy contributions to the JT stabilization energy along a relevant particular path of distortion and the forces responsible for the distortion, giving further insight into the origin and mechanism of the vibronic coupling.

Industrijska i primenjena hemija - Industrial and Applied Chemistry

IP P 01

Biodiesel production from higher alcohols with guanidine catalyst

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Biodiesel is produced by transesterification of vegetable oil (triglycerides) with alcohol, mainly methanol and ethanol. Usually NaOH and KOH are used as catalyst, but they cause saponification, if a higher content of water or free fatty acids is present, which is common for waste cooking oils. This study examines the application of *N*,*N*′,*N*″-tris(3-dimethylaminopropyl)-guanidine as a catalyst for the transesterification of waste cooking oil with methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, *iso*-butanol, 1-pentanol, *iso*-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-decanol, 1-dodecanol, and benzyl-alcohol. Conversions in the range from 70 up to 99 mol % (except for 2-propanol and 2-buthanol) were obtained after 5 h at 50°C with 3 wt. % of catalyst and at 1:6.2 molar ratio of vegetable oil and alcohol. Phase separation of biodiesel and glycerol immediately after the transesterification was present only for biodiesel produced with methanol, ethanol and 1-butanol.

IP P 02

Ispitivanje kinetike i ravnoteže adsorpcije naproksena na ekonomski isplativim adsorbentima od koštica kajsije

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U ovom radu je ispitivana adsorpciona sposobnost ekonomski isplativog aktivnog uglja dobijenog iz koštice kajsije (*Prunus armeniaca)* termohemijskom aktivacijom pomoću fosforne kiseline. Pomoću serije ispitivanja, određene su kinetika i ravnoteža uklanjanja naproksena iz vodenog rastvora adsorpcijom na sintetisanom aktivnom uglju. Eksperiment je pokazao veoma brzu adsorpciju tokom prvih 20 minuta i optimalnu adsorpciju tokom prvih 30 minuta. Za opisivanje adsorpcionih procesa korišćena su četiri kinetička modela. Podaci su se dobro uklopili (R^2=0,9999) u pseudo-drugi red reakcije, iz čega se može zaključiti da je u pitanju hemijski tip adsorpcije. Takođe je ispitivan uticaj početnih koncentracija (1-50 mg/L). Najbolji rezultati su postignuti pri pH vrednosti 6 sa 50 mg adsorbenta, koncentracijom naproksena 10 mg/L i kontaktnim vremenom od 60 minuta, gde je efikasnost uklanjanja bila više od 96%. Adsorpcija se može opisati pomoću Lengmirove izoterme, koja pokazuje maksimalni adsorpcioni kapacitet od 17,27 mg/g. Ovaj rad je pokazao da aktivni ugalj dobijen od koštica kajsije može biti korišćen kao efikasan ekonomski isplativ adsorbent prilikom uklanjanja naproksena iz vode.

Kinetic and equilibrium studies of naproxen adsorption onto low-cost adsorbent prepared from apricot stone shells

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This study was conducted to test adsorption ability of low-cost activated carbon derived from apricot (*Prunus armeniaca*) stone shells by thermo-chemical activation using phosphorous acid. Kinetics and equilibrium of naproxen removal from aqueous solutions by sorption onto synthesized activated carbon have been investigated using batch adsorption experiments. Time dependent assays show rapid adsorption in first twenty minutes and optimal adsorption in first thirty minutes. Four kinetic models were used in this study to describe the adsorption process. The data fitted very well (R^2=0.9999) to a pseudo-second-order kinetic model, suggesting that the adsorption is a chemisorption process. Using apricot stone shells activated carbon in batch mode, the effects of initial naproxen concentration (1-50 mg/L) was studied. The best result was obtained at pH 6, with an adsorbent dosage of 50 mg, naproxen concentration of 10 mg/L and a contact time of 60 min, with over 96% of the naproxen being adsorbed. The adsorption behavior was well described by the Langmuir isotherm model, showing a maximum adsorption capacity of 17.27 mg/g. The conducted study has shown that activated carbon prepared from apricot stone shells can be effectively used as low-cost adsorbent for the removal of naproxen from aqueous solution.

IP P 03

Supercritical fluid extraction of *Salvia officinalis* L. and process optimization

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During the manufacture of herbal tea, approximately 10-20% herbal dust is being generated as by-product. Herbal dust represents the material that contains smaller particles compared to pore size of a regular tea bag, therefore, it is discarded as by-product. This by-product is often used as a raw material for extraction of various bioactive compounds. Lipid compounds can be extracted by using one of the solid/liquid extraction methods such as hydrodistilation or extraction using an organic solvent. For extraction of volatile lipid compounds, supercritical fluid extraction (SFE) represents alternative clean and green technology. The aim of this work was utilization of sage herbal dust as raw material for extraction of lipid compounds by SFE. Extractions were performed using designed experiments with pressure (100, 200 and 300 bar), temperature (40, 50 and 60 °C) and CO_2 flow rate (0.2, 0.3 and 0.4 kg/h) as independent variables. Total extraction yield was response variable and optimization was performed using response surface methodology (RSM). Observed optimal conditions were pressure of 295 bar, temperature of 55 ˚C and CO_2 flow rate 0.38 kg/h, while predicted value of total extraction yield at this set of SFE conditions was 9.75%. According to analysis of variance (ANOVA), applied second-order polynomial model was successfully used for description of experimental results.

Superkritična ekstrakcija žalfije (*Salvia officinalis* L.) i optimizacija procesa

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Prilikom proizvodnje čaja nastaje 10-20% nus-proizvoda koji se naziva „biljna prašina“. Herbalna prašina sadrži čestice čiji je prečnik čestica manji od prečnika pora na filter kesici čaja. Ovaj nus-proizvod se često koristi kao biljna sirovina za ekstrakciju bioaktivnih komponenata. Lipidne komponente se mogu ekstrahovati primenom jedne od ekstrakcionih tehnika čvrsto/tečno kao što je hidrodestilacija ili esktrakcija organskim rastvaračima. Za ekstrakciju isparljivih lipidnih komponenata dobru alternativu predstavlja zelena tehnologija superkritične ekstrakcije. Cilj ovog rada bio je iskorišćenje herbalne prašine žalfije kao sirovine za ekstrakciju lipidnih komponenata primenom superkritične ekstrakcije. Ekstrakcije su vršene na upotrebom posebnog dizajna eksperimenta na pritisku (100, 200 i 300 bar), temperaturi (40, 50 i 60°C) i protoku CO_2 (0,2, 0,3 i 0,4 kg/h) kao nezavisnih promenljivih. Ukupan prinos ekstrakcije predstavlja zavisnu promenljivu, optimizacija procesa je izvršena upotrebom metode odzivne površine (RSM – Response Surface Methodology). Dobijeno je da su optimalni uslovi procesa pri pritisku od 295 bar, temperaturi od 55°C i protoku CO_2 od 0,38 kg/h. Predviđena vrednost ukupnog prinosa ekstrakcije pri datim uslovima jeste 9,75%. Prema analizi varijansi (ANOVA), polinom drugog reda se uspešno može koristiti za opisivanje eksperimentalnih rezultata.

IP P 04

Novi dvofazni sistemi zasnovani na poli(etilen glikol) diakrilatu i različitim solima

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Zeleni rastvarači, poznati kao dvofazni vodeni sistemi, su pogodni za uklanjanje zagađivača iz otpadnih voda ili vodenih rastvora korišćenjem ekološki benignih separacionih tehnologija. Karakterizacija faznog ponašanja ovih sistema je neophodna za definisanje procesnih uslova u separacionim procesima. U ovom radu eksperimentalno su određeni fazni dijagrami na 298.15 K i na atmosferskom pritisku za nove dvofazne sisteme poli(etilen glikol) diakrilat (PEGDA)+soli ($MnSO_4$/$Na_3C_6H_5O_7$/K_3PO_4/$ZnSO_4$). Velika prednost ovih rastvarča je niska isparljivost polimera i soli, i mala količina tih supstanci potrebna za efikasnu separaciju. Moguće interakcije u ovim sistemima su: *i)* polimer-joni; *ii)* joni-voda i *iii)* polimer-voda. U ovom slučaju joni soli (agensi za isoljavanje) stvaraju hidratacione komplekse sa vodom i udaljavaju se od površine polimera (tj. vrši se ekskluzija polimera u drugu fazu). Na taj način dobijaju se dve vodene faze, jedna bogata solju i druga polimerom. Pritom, dolazi samo do delimične dehidratacije rastvoraka (PEGDA i soli); delimične - zato što su obe faze bogate vodom i rastvorci su hidratisani do određenog stepena. U so-bogatoj oblasti sve soli imaju isti uticaj, dok se određeni trend može uspostaviti u PEGDA-bogatoj oblasti: $MnSO_4 \approx Na_3C_6H_5O_7 \approx K_3PO_4 < ZnSO_4$. Iako je razlika u ovim uticajima mala, ipak se može zaključiti da $ZnSO_4$ pokazuje najjači efekat isoljavanja.

Novel biphasic systems formed by poly(ethylene glycol) diacrylate and various salts

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Green solvents, known as aqueous biphasic systems, are suitable for removal of pollutants from wastewaters or from aqueous solutions using environmentally benign separation technologies. Investigations on phase behavior of these systems are necessary for defining process parameters in separation processes. In this work phase diagrams of novel biphasic systems poly(ethylene glycol) diacrylate (PEGDA)+salts ($MnSO_4$/$Na_3C_6H_5O_7$/K_3PO_4/$ZnSO_4$) are experimentally determined at 298.15 K and at atmospheric pressure. Advantage of these solvents is low volatility of polymer and salts, and small amounts of those substances necessary for efficient separations. Possible interactions in these systems are: *i)* polymer-ion; *ii)* ion-water and *iii)* polymer-water. In this case salt ions (salting-out agents) form hydration complexes with water and in that way make exclusion of polymer into another phase. In that way two phases are formed, one rich in salt and another rich in PEGDA. Thereby, only partial dehydration of solutes (PEGDA and salts) happens; partial – because both phases are rich in water and solutes are hydrated only to some extent. In salt-rich phase investigated salts have similar influence and salting-out effect, while certain trend can be established in PEGDA-rich phase $MnSO_4 \approx Na_3C_6H_5O_7 \approx K_3PO_4 < ZnSO_4$. Although the difference in salting out effects of four salts is small, still it can be concluded that $ZnSO_4$ exhibit the strongest salting out effect.

IP P 05

Određivanje elemenata u uzorcima umetničkih glina i glazura. Procena rizika za ispitivane elemenata po ljudsko zdravlje

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Glina i glazure su dva najbitnija i najznačajnija materijala koja koriste umetnici iz oblasti keramike i grnčarije. U radu je ukupno analizirano 24 uzorka. Uzorci su prikupljeni u srednjoj umetničkoj školi „Tehnoart“. Kvalitativni i kvantitativni sastav uzoraka određen je Talasno disperzivno rendgensko fluorescentnom analizom (WD-XRF). Detektovano je ukupno 52 elementa, a fokus je dat na metalima Al, Ba, Cd, Co, Cr, Cu, Fe, Mn, Mo, Ni, Pb, Sn, V, Zn i metaloidima Si i Se. Za navedene metale i metaloide procena rizika po zdravlje učenika je računata. Rizik je računat korišćenjem detektovane koncentracije elemenata i formula koje se koriste za procenu rizika (EPA). Rezultati dobijeni istraživanjem pokazuju da je ingestivni nekancerogeni rizik najveći za metale Ba, Cr, Co i Cd u 6 uzoraka glazura. Kancerogeni metali su Cr(VI), Co, Cd, Ni, Pb i V (EPA) i navedeni metali utiču na povećani ukupni kancer rizik reda veličine 10^{-4} u 7 uzorka glazura, reda veličine 10^{-5} u 3 uzorka glazura i reda veličine 10^{-6} u 5 uzorka glazura i u jednom uzorku gline. Uočen je ingestivni, inhalacioni i dermalni kancer rizik. Ovo istraživanje je pokazalo koliko je bitno poznavanje hemijskog sastava materijala, koji učenici koriste tokom četvorogodišnjeg obrazovanja, i rizika kojem su izloženi pri radu sa potencijalno opasnim materijalom.

Determination of elements in artistic clay and glaze samples. Risk assessment for human health is performed

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Clay and glazes are the most important materials used by artists in the field of ceramics and pottery. In this paper, 24 samples of clay and glazes were analyzed. Samples were collected from the High school of Arts, "Tehnoart". Qualitative and quantitative composition of the samples was determined by Wavelength dispersive X-ray fluorescence spectrometry (WD-XRF). A total of 52 elements were detected and the focus was on the fallowing metals: Al, Ba, Cd, Co, Cr, Cu, Fe, Mn, Mo, Ni, Pb, Sn, V, Zn and metalloids Si and Se. For the mentioned metals and metalloids the risk assessement for student’s health was established. The risk was calculated using the obtained element concentrations and formulas that are suggested from the EPA. The results obtained by this research show that in 6 samples of glazes a oral non – cancer risk is the highest for metals: Ba, Cr, Co and Cd. Metals that have a carcinogenic toxicological profiles are Cr(VI), Co, Cd, Ni, Pb and V (EPA), and these metals affect the overall increased risk of cancer in the order of 10^{-4} in 7 samples of glazes, while risk of 10^{-5} was achived in 3 samples of glazes and of 10^{-6} in 5 samples of glazes and 1 sample of clay. The oral, inhalation and dermal cancer risk was noted. This research has shown how important is the knowledge of the chemical composition of materials that students use during the four-year education, and the risks to which they are exposed to when working with potentially hazardous materials.

IP P 06

Gustine i izvedene termodinamičke veličine metil i etil laurata na visokim pritiscima

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Biodizeli predstavljaju smeše estara viših masnih kiselina. Poslednjih decenija se znatno povećala njihova upotreba kao zamena za dizel goriva, što u cilju smanjenja zagađenja životne sredine što zbog iscrpljenosti neobnovljivih izvora energije. Vlade većine zemalja su uvele i posebne mere kojima se dodatno podstiče upotreba biodizela i drugih obnovljivih izvora energije.
Pošto se paljenje goriva u dizel motorima odvija na povišenim temperaturama i pritiscima, to bitno utiče na njihova termodinamička svojstva, što dalje dovodi do promena u procesu atomizacije i paljenja goriva. Stoga je neophodno ispitati ponašanja biodizela pri različitim uslovima pre njegove upotrebe u dizel motorima. U ovom radu su predstavljene gustine metil i etil estara laurinske kiseline, koji ulaze u sastav većine biodizela, na temperaturama 293.15-413.15 K i pritiscima do 60 MPa. Gustine su merene na DMA HP uređaju proizvođača Anton Paar, i korelisane pomoću modifikovane Tammann-Tait-ove jednačine na osnovu čega su izračunati i izotermska kompresibilnost i koeficijent izobarskog toplotnog širenja ispitivanih estara.

Densities and derived thermodynamic properties of methyl and ethyl laurate at high pressures

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Biodiesel represents a mixture of esters of fatty acids. In recent decades, their use as a substitute for diesel fuel has been significantly increased because of a reduction of environmental pollution as well as the exhaustion of non-renewable energy sources. Governments in most countries have introduced special regulations to further encourage the use of biodiesel and other renewable energy sources.
The fuel combustion in diesel engines occurs at elevated temperatures and pressures, and those conditions influence significantly their thermodynamic properties, which further leads to changes in the fuel atomization and combustion processes. Therefore, it is necessary to examine the behavior of biodiesel in different conditions prior to its use in diesel engines. Density of methyl and ethyl esters of lauric acid, which are part of the most of biodiesels, at temperatures 293.15-413.15 K and pressures up to 60 MPa will be presented here. Densities were measured on DMA HP measuring cell, produced by Anton Paar, and correlated using the modified Tammann-Tait equation which further provided the calculation of the isothermal compressibility and the isobaric thermal expansivity of the studied esters.

IP P 07

Ekstrakti žalfije (*Salvia officinalis* L.) dobijeni savremenim metodama ekstrakcije

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Prilikom proizvodnje jednokomponentnog ili mešavine čaja u filter vrećice koji sadrži žalfiju, proizvede se oko 10-20% sporednog proizvoda/otpada od žalfije tzv. „herbalne prašine“. Herbalna prašina predstavlja materijal čije su čestice manjeg prečnika od prečnika pora na filter vrećici. S obzirom na visok sadržaj fenola i fenolnih jedinjenja u nativnom materijalu, pretpostavlja se da se odgovarajućim metoda čvrsto-tečne ekstrakcije i sušenjem dobijenih tečnih ekstrakata iz ovakvog materijala može dobiti visokokvalitetan proizvod u formi suvog ekstrakta. Tečni ekstrakti su dobijeni pomoću pet prethodno optimizovanih metoda, i to maceracijom, ultrazvučnom ekstrakcijom, mikrotalasnom ekstrakcijom, ekstrakcijom subkritičnom vodom, a peti ekstrakt je predstavljao ostatak od destilacije žalfije vodenom parom. Tečni ekstrakti su sušeni *spray drying* tehnikom, i dobijenim suvim ekstraktima su određene fizičke karakteristike (sadržaj vlage, higroskopnost, indeks adsorpcije vode, indeks rastvorljivosti u vodi, zapreminska masa i rehidratacija) i hemijske karakteristike (sadržaj ukupnih fenola i flavonoida i antioksidativno delovanje primenom DPPH metode). U dobijenim suvim ekstraktima žalfije sadržaj ukupnih fenola se kreće 90,20-307,85 mg EGK/g, a sadržaj ukupnih flavonoida 56,98-154,88 mg EK/g. Suvi ekstrakti su pokazali visoku antioksidativnu aktivnost (IC_{50} od 2,297 do 10,499 μg/ml).

Sage (*Salvia officinalis* L.) extracts obtained by the modern extraction methods

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During the production of single or mixture of tea in filter bags containing sage produces around 10-20% of by-product/ waste form the so-called „herbal dust“. Herbal dust is a material with a particle diameter smaller than the filter bag pore diameter. Due to the high content of phenols and phenolic compound in native material, it is assumed that the appropiate methods of solid-liquid extraction and drying of liquid extracts obtained form such material can get a high quality product in the form of dry extract. Liquid extracts were obrained using the five previously optimized methods: maceration, ultrasonic assisted extraction, microwave assisted extraction, subcritical water extraction, and the fifth extract was a distillation residue. Liquid extracts are dried spray drying technique, and dry extracts obtained physical characteristis (moisture content, hygroscopicity, water adsroption index, index of solubility in water, density and rehydration) and chemical characteristics (content of total phenols and flavonoids and antioxidant activity using the DPPH method). The obrained dry extracts of sage total phenol content ranging from 90,20 to 307,85 mg GAE/g, a content of total flavonoids 56,98 to 154,88 mg CE/g. Dry extracts showed high antioxidant activity (IC_{50} from 2,297 to 10,499 mg/ml).

IP P 08

Viscosity modeling of binary mixture diethyl tartrate + 1-propanol

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Viscosity data for the binary system diethyl tartrate + 1-propanol have been measured in temperature range 288.15 - 323.15 K and at atmospheric pressure, using Anton Paar SVM 3000 digital viscometer. Data for pure diethyl tartrate are not available in the literature, and also for the investigated mixture. Modelling of viscosity was done using predictive UNIFAC-VISCO and ASOG-VISCO models. Group contribution based models are suitable for obtaining quick evaluations of thermophysical properties under different conditions of temperature, pressure and composition. The significance of the predictive approach is that the mixture viscosity could be calculated from the pure component data and the interaction parameters between functional groups present in the system. However, having in mind the fact that correlative models often lead to better results, the viscosity data were also correlated by Teja-Rice, Grunberg-Nissan, McAlister, Eyring-UNIQUAC and Eyring-NRTL models. Correlative models involve interaction parameters (one or more) obtained by some optimization technique. These models require some experimental data in order to establish the value of an interaction parameter specific for each mixture for the defined temperature and pressure. All models for investigated mixture give very good results. In most cases, percentage deviations (PD_{max}) are within 1%, till even below 0.05%.

Modelovanje viskoznosti binarne smeše dietil tartarat + 1-propanol

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Vrednosti viskoznosti za binarni sistem dietil tartarat + 1-propanol izmerene su u temperaturnom opsegu 288.15 – 323.15 K i na atmosferskom pritisku, na digitalnom viskozimetru Anton Paar SVM 3000. Podaci za čist dietil tartarat nisu dostupni u literaturi, kao ni za ispitivanu smešu. Modelovanje viskoznosti urađeno je koristeći prediktivne UNIFAC-VISCO i ASOG-VISCO modele. Modeli doprinosa grupa su pogodni za brzo izračunavanje termofizičkih veličina pri različitim uslovima temperature, pritiska i udela. Njihov značaj je u tome što se viskoznost smeše može izračunati samo iz podataka za čiste komponente i interakcione parametre između funkcionalnih grupa prisutnih u sistemu. Međutim, imajući u vidu da korelativni modeli uglavnom daju bolje rezultate, podaci za viskoznost su takođe korelisani Teja-Rice, Grunberg-Nissan, McAlister, Eyring-UNIQUAC i Eyring-NRTL modelima. Korelativni modeli koriste interakcione parametre (jedan ili više), dobijene nekom od optimizacionih tehnika. Ovi modeli zahtevaju eksperimentalne podatke da bi se odredile vrednosti interakcionih parametara posebne za svaku smešu za definisane uslove temperature i pritiska. Svi modeli za ispitivanu smešu daju veoma dobre rezultate. U većini slučajeva vrednosti procentualnih devijacija su do 1 %, čak ispod 0.05 %.

IP P 09

Life-cycle assessment of plastic bottles

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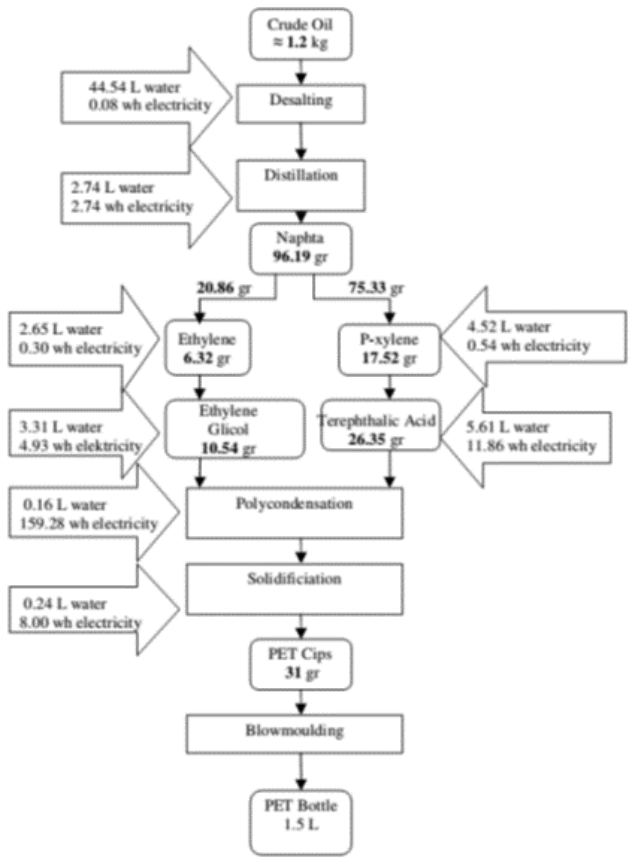
One of the plastic product with remarkable environmental effects are conventional plastic bottles. Manufacturing process of PET bottles have started 1973 and from that time it has rapidly progressed. The production chain consists of crude oil winning, taking naphtha by refining crude oil, getting terephthalic acid and ethylene glycol from naphtha, polymerization of terephthalic acid and ethylene glycol, all the stages of PET production and the usage and disposal phases. Types of wastes, environmental fate due to manufacturing process and methods of production wastes dispose have been evaluated and also feedback mechanisms after the usage of productions are examined and the necessity of feedback is investigated in this study. The aim is to evaluate LCA (Life-cycle assessment) of PET numerically with material-energy-waste-environmental impact circle. LCA is a special technique which includes: making a list of the incomes and outcomes of the manufacturing process, evaluation of the potential impacts on the environment and interpretation of the results from the analysis of the incomes and outcomes.

LCA technique has five stages:

1. Determing and geting the raw materials
2. The proces of manufacturing
3. The main use of the plastic bottles
4. Recycling
5. Transport



Hemija u nastavi - Chemistry Teaching

HN P 01

Ispitivanje studentskih sposobnosti za tumačenje hemijskih termina i simboličkih prikaza

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Cilj ovog istraživanja je bio da se ispita sposobnost studenata da razumeju i interpretiraju reči i simboličke prikaze koji se koriste u sklopu hemijskog jezika. Uzorak istraživanja su činili studenati Osnovnih akademskih studija hemije, Prirodno-matematičkog fakulteta u Novom Sadu. Za potrebe ovog istraživanja konstruisan je test koji se sastojao od pet blokova pitanja. U prvom bloku se tražilo da studenti sastave rečenice u kojima će upotrebiti navedene termine u hemijskom kontekstu. U drugom bloku se tražilo da studenti objasne značenje podvučene reči u okviru zadatih rečenica. U trećem bloku se tražilo da studenti na liniju pored hemijskog simbola upišu njegovo značenje. U četvrtom bloku se tražilo da studenti zaokruže rečenicu u kojoj je podvučena reč upotrebljena pravilno i u petom bloku se tražilo da studenti za svaku navedenu reč sastave po dve rečenice gde će u prvoj navedenu reč upotrebiti u naučnom kontekstu a u drugoj navedenu reč upotrebiti u kontekstu svakodnevnih životnih situacija. Na osnovu rezultata istraživanja utvrđeno je da su studenti u velikom procentu sposobni da reprodukuju definicije zadatih termina, ali da su daleko manje uspešni u njihovoj interpretaciji. Po pitanju tumačenja simboličkih prikaza, utvrđeno je da postoje parovi prikaza koje studenti mešaju, pa bi na to trebalo dodatno obraditi pažnju.

Testing students' ability to interpret chemical terms and symbolic representations

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The aim of this study was to investigate students' ability to understand and interpret words and symbolic representations used within chemical language. The study sample consisted of students of Undergraduate academic studies in chemistry at the Faculty of Sciences, Novi Sad. Test, that consisted of five blocks of questions, was constructed for the purpose of this study. In the first block, students were asked to compose a sentence using the given word. In the second block, they were asked to explain the meaning of the underlined words within the given sentences. In the third block, students were required to explain the meaning of the given symbolic representations. In the fourth block, students were asked to circle the sentence in which underlined word is used properly and in the fifth block, they were given a specific terms and were requested to compose two sentences wherein the given term would be used in the scientific context and in the context of everyday life situations. Based on the results it was found that a large percentage of students were able to reproduce the definitions of the given terms, however, they were far less successful in their apprehension. Regarding the interpretation of symbolic representations, it was found that there were pairs of representations mixed by students, so that should be further considered.

HN P 02

Analiza tipova i apstraktnosti ilustracija u udžbenicima Hemije za VII razred

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U radu je izvršena analiza ilustracija tri odabrana udžbenika Hemije za 7. razred, pri čemu je ispitana relativna zastupljenost ilustracija u udžbeniku, dok su prikupljene ilustracije analizirane prema tipu i sadržaju. U nastavku rada analiziran je stepen apstraktnosti ilustracija različitog tipa. Rezultati su pokazali da kod različitih izdavača nema većeg odstupanja u prosečnoj gustini ilustracija, a najveća gustina je zabeležena u udžbeniku izdavača „Zavod za udžbenike", nakon čega slede „Bigz" i „Klett". Analizirane ilustracije su uglavnom konvencionalne i realistične, dok je hibridnih ilustracija veoma malo kod sva tri udžbenika. Ilustracije u odabaranim udžbenicima Hemije za 7. razred najviše pripadaju podkategorijama: laboratorijska oprema i eksperimenti, modeli i ilustracije iz svakodnevnog života. Posmatrajući stepen apstraktnosti, najviše su zastupljene umereno apstraktne ilustracije. Na osnovu rezultata analiziranih udžbenika može se zaključiti da ilustrativni materijal u udžbenicima na adekvatan način dopunjuje tekst, pomažući učenicima prilikom razumevanja i usvajanja apstraktnih hemijskih sadržaja.

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The analysis of illustrations' type and abstraction in 7th grade Chemistry textbooks

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This paper analyses illustrations of three 7th grade chemistry textbooks, observing the relative density of illustrations in textbook and classification of illustrations based on their type and the content. In addition, the abstraction degree of different type illustrations was analysed. The results showed that there was no significan difference in average density of illustrations in observed textbooks, however the highest density was found in the textbook by „Zavod za udžbenike", followed by „Bigz" and „Klett". The illustrations in textbooks are mostly coventional and realistic, while there are only few hybrid illustrations in all three analysed textbooks. The illustrations in chemistry textbooks for 7th grade are mostly in subcategory of laboratory equipment and experiments, models and illustrations from everyday life. Observing the degree of abstraction, the illustrations are mostly moderately abstract. Based on the results, it could be concluded that illustrations represented in the analysed textbooks adequately complement the written text, helping the students in undrestanding of school material and abstract chemical concepts.

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