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18 RUŽIČKA DAYS

TODAY SCIENCE – TOMORROW INDUSTRY

September 16–18, 2020 | Vukovar, Croatia

BOOK OF ABSTRACTS

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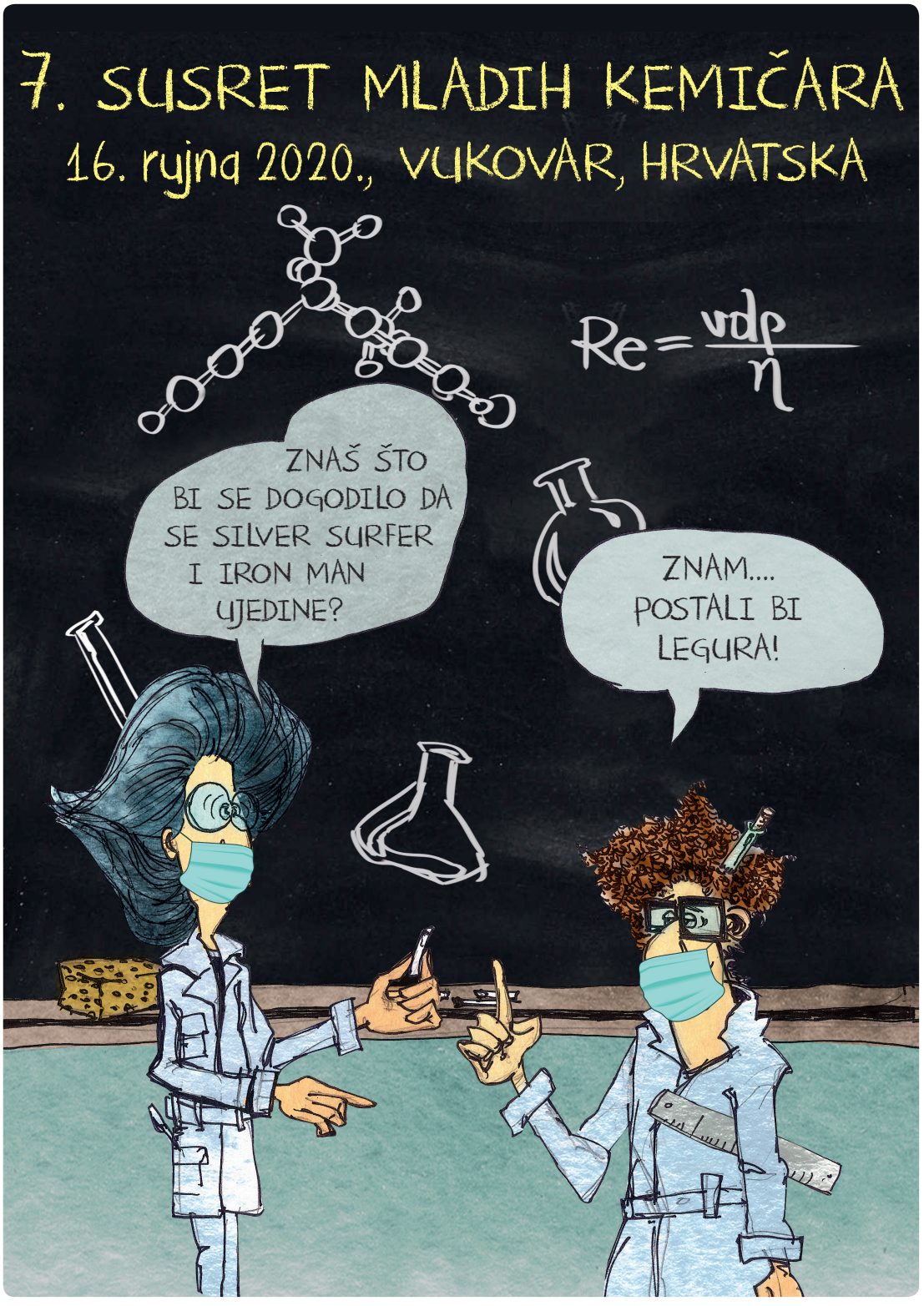
7. SUSRET MLADIH KEMIČARA
16. rujna 2020., VUKOVAR, HRVATSKA
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ZNAŠ ŠTO BI SE DOGODILO DA SE SILVER SURFER I IRON MAN UJEDINE?
ZNAM.... POSTALI BI LEGURA!

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18 RUŽIČKINI DANI

DANAS ZNANOST – SUTRA INDUSTRIJA

16. – 18. rujna 2020. | Vukovar, Hrvatska

KNJIGA SAŽETAKA

***BOOK OF ABSTRACTS* | KNJIGA SAŽETAKA**

18th Ružička Days
TODAY SCIENCE – TOMORROW INDUSTRY
18. Ružičkini dani
DANAS ZNANOST – SUTRA INDUSTRIJA

***Published by* | Izdavači**

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7. Susret mladih kemičara
7th Meeting of Young Chemists

18. RUŽIČKINI DANI – UVODNA RIJEČ

18th RUŽIČKA DAYS - FOREWORD

Poštovane kolege, dragi gosti i sudionici 18. Ružičkinih dana,

Zadovoljstvo mi je pozdraviti Vas i zahvaliti Vam na prijavi i sudjelovanju u ime Znanstveno-organizacijskog odbora i organizatora Skupa. Usprkos ovogodišnjim izvanrednim okolnostima pandemije novog koronavirusa, zahvaljujući razmjerno dobrome stanju u Hrvatskoj odlučili smo redovito održati Skup poštujući sve propisane mjere i zahtjeve epidemiološke struke i stožera civilne zaštite. Ipak, za razliku od prethodnih skupova, ovaj put su većinom sudionici iz Hrvatske. Po prvi puta uvodimo i istodobni video prijenos skupa uživo, kao i virtualnu, elektroničku izložbu posterskih priopćenja. Dio predavača će održati predavanja na daljinu, a i veliki broj sudionika će pratiti skup na isti način. Već preko deset godina slogan Skupa je Danas znanost – sutra industrija, čime se želi naglasiti i potaknuti suradnju znanosti i gospodarstva u našemu društvu i općenito. Upravo krizne situacije poput sadašnje, uključujući i nedavni jaki potres u Zagrebu, te ukupno, teško gospodarsko stanje, pokazuju koliko je čvrsta i stalna suradnja znanosti i industrije neophodna za prevladavanje krize i osiguranje brzog oporavka i daljnjeg razvoja društva. Zadnjih godina navedena suradnja u znatnom je porastu zahvaljujući velikim ulaganjima i sredstvima strukturnih fondova EU, a u sljedećem razdoblju (EU sljedeći naraštaj i zeleni plan) za očekivati je da će i dodatno narasti. Plodovi te suradnje trebaju povećati konkurentnost našeg gospodarstva i time opću društvenu dobrobit. Zbog toga je važno u takvim suradnjama sudjelovati i doprinijeti im, što skup Ružičkini dani od svoga utemeljenja i potiče. Zahvaljujući velikom broju prijava, program Skupa je prilično sadržajan. Biti će održano pet plenarnih i tri pozvana predavanja, uz deset usmenih i više od 140 posterskih priopćenja. Dodatno, na 7. susretu mladih kemičara s kojima skup počinje, održat će se i sedam predavanja učenika srednjih škola. Ovom prilikom pozivam sve autore da dio svojih rezultata svakako objave i u hrvatskim časopisima *Chemical and Biochemical Engineering Quaterly* i *Croatian Journal of Food Science and Technology*. Tijekom skupa, održat će se i prijem dobrodošlice uz razgledavanje postava Franjevačkog muzeja, kripte, podruma i obnovljene Crkve Sv. Filipa i Jakova u Vukovaru, te organizirani obilazak grada Iloka uz zajedničku večeru u hotelu Dunav.

Tradicionalno, pokrovitelj konferencije je Hrvatska akademija znanosti i umjetnosti, Razred za matematičke, fizičke i kemijske znanosti. Uz HAZU, na kraju zahvaljujem u ime organizatora i svim ostalim podupirateljima i sponzorima Ružičkinih dana, osobito zlatnim sponzorima, tvrtkama INA Industrija nafte i Pliva Hrvatska, srebrnim sponzorima, tvrtkama Xellia, Shimadzu i Tetra Pak, brončanim sponzorima, tvrtkama Kefo i Karolina, Ministarstvu znanosti i obrazovanja, Ministarstvu poljoprivrede, te naravno, tvrtci Borovo, gradu Vukovaru i Hrvatskom domu Vukovar.

Prof. dr. sc. Ante Jukić
Predsjednik Znanstveno-organizacijskog odbora i predsjednik HDKI

SUSRET MLADIH KEMIČARA

MEETING OF YOUNG CHEMISTS

Ivanka Miličić

Javna ustanova u kulturi Hrvatski dom Vukovar,
J. J. Strossmayera 20, p.p. 70, 32 000 Vukovar, Croatia

Dvanaest godina je prošlo od prvog Susreta mladih kemičara. Obnovom rodne kuće nobelovca Leopolda (Lavoslava) Ružičke 2008. godine stvoreni su uvjeti da se znanstveni skup „Ružičkini dani", započet u Vukovaru prije 42 godine, ponovno vrati na mjesto gdje je sve i počelo - u Vukovar; ovoga puta u obnovljenu rodnu kuću Nobelovca. Iste 2008. godine, Grad je osnovao Javnu ustanovu u kulturi Hrvatski dom Vukovar. Odredbom Osnivača, Ustanova skrbi i o rodnoj kući Nobelovca. Te se godine održavaju 12. Ružičkini dani i to po prvi put upravo u Ružičkinoj kući. Na sastancima organizacijskog odbora često se traže ideje kako skup približiti mladima, kako ih što aktivnije uključiti u rad i pridobiti ih kao sudionike. Odboru sastavljenom od stručnjaka, sveučilišnih profesora i dekana fakulteta, predložila sam pokretanje projekta Mladi kemičari. Radeći deset godina u školi, znala sam da među nastavnicima i učenicima ima onih, čije ambicije i znanje prelaze granice redovnog nastavnog programa i traže mjesto i mogućnost da to ostvare. Ideja je prihvaćena, stoga već 2008. godine skromno počinjemo s održavanjem 1. susreta mladih kemičara. Jedni od prvih sudionika su učenici Tehničke škole Nikola Tesla iz Vukovara, koji su od tada sudjelovali na svim Susretima, prezentirajući sve bolje radove. Vođenje ovog projekta preuzimaju stručnjaci – profesori s osječkog Tehnološkog fakulteta, što je garancija da će i kvaliteta prijavljenih i odabranih radova biti na razini skupa u čijem je programu. Broj sudionika iz godine u godinu sve je veći, pa možemo reći da ih ima iz cijele Hrvatske. Od 2016. godine na Susretu mladih kemičara sudjeluju i učenici Katoličkog školskog centra „Don Bosco" iz Žepča, čime Susreti postaju međunarodni.
Što reći na kraju? Ovo su 7. Susreti mladih kemičara. Održavaju se u godini kada ništa nije kao prije. Mjere, koje moramo provoditi zbog epidemije COVID-a 19 sigurno će imati utjecaja i na provođenje ovoga Skupa. Poželimo svima koji sudjeluju uspjeh u radu i svi zajedno učinimo sve da odgovornim ponašanjem zaštitimo i sebe i druge.

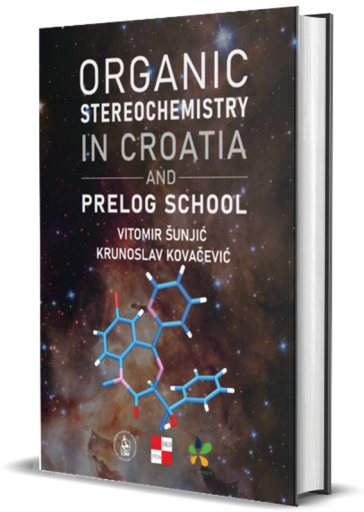
Plenarna predavanja
Plenary Lectures

ORGANSKA STEREOKEMIJA U HRVATSKOJ, OD ZNANOSTI DO TEHNOLOGIJE

ORGANIC STEREOCHEMISTRY IN CROATIA, FROM SCIENCE TO TECHNOLOGY

Vitomir Šunjić

Croatian Academy of Science and Arts,
Trg Nikole Šubića Zrinskog 11, 10 000 Zagreb, Croatia



Asymmetric synthesis of chiral compounds in the optically pure form represents highlight of organic stereochemistry. Scientific achievements in this field often turn to industrial methods for production of commercial products, primarily drugs and other biologically active compounds.

Various methods to approach pure enantiomers of racemic compounds were explored by generations of Croatian organic chemists that studied with prof. Prelog at Faculty of Chemistry in Zagreb (1935-1941) or spent doctoral or post-doctoral years in his laboratory at ETH in Zurich (1952-1989). They were over 25 and are known in Croatia as "Prelog school".

The authors of detailed overview [1, 2] decided to present development of organic stereochemistry in Croatia for the period 1960-2019. Collected data revealed approx. 400 papers published in this period by over 200 Croatian authors. Both, printed and electronic edition of the book are jointly edited and supported by the three national institutions; Croatian Academy of Science and Arts, Croatian Chemical Society and Faculty of Chemical Engineering and Technology, University of Zagreb. Research projects are presented either according to synthetic methods, e.g. stereoselective and asymmetric synthesis completed by organometallic catalysis, oganocatalysis or biocatalysis, or according to structural characteristics of the target chiral molecules. Examples are selected to illustrate how academic projects (new knowledge) extend to industrial (problem solving) approach and vice versa.

The authors expect this information to promote future international collaboration of academic projects from Croatia and support Croatian companies in the business-related activities.

Keywords: organic stereochemistry, Prelog school, stereoselective and asymmetric syntheses, structural characteristics, catalysis

[1] V. Šunjić, K. Kovačević, Organic Stereochemistry in Croatia and Prelog School, Zagreb, 2020.
[2] Web site (open access), https://prelog.hkd.hr/.

BIOPROSPECTING ISTRAŽIVANJA JADRANSKOG MORA: POTENCIJALI, USPJESI, OGRANIČENJA

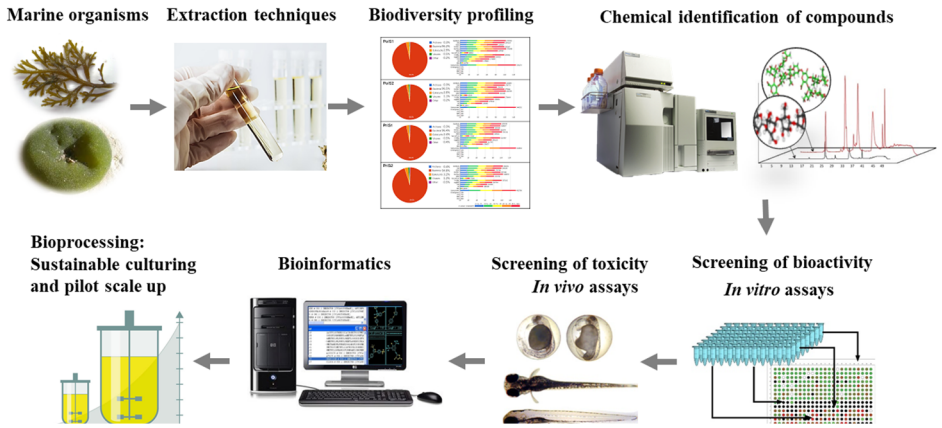
BIOPROSPECTING RESEARCH OF THE ADRIATIC SEA: POTENTIAL, SUCCESS AND COSTRAINTS

Rozelindra Čož-Rakovac, Marin Roje

Institut Ruđer Bošković, Bijenička 54, 10 000 Zagreb, Hrvatska

Bioprospecting Jadranskog mora predstavlja opsežno istraživanje njegovih bioloških potencijala koje će omogućiti stvaranje snažne znanstvene baze i održivog iskorištavanja biološkog i kemijskog potencijala jadranskih bioresursa u svrhu razvoja novih proizvoda u farmaceutskoj, prehrambenoj i kozmetičkoj industriji, kako za hrvatsko, tako i za europsko poslovno okruženje. Ova istraživanja će pozitivno utjecati na: unapređenje i poboljšanje sustava kultivacije morskih organizama, optimaliziranje *scale–up* laboratorija u pilot–skali do procesa industrijskih razmjera, razvoj novih protokola u analitici, akumuliranje znanja o eksploataciji metagenomskih resursa, biološku i kemijsku raznolikost, *in silico* predviđanja aktivnosti, biološki potencijal dobivenih bioaktivnih supstanci. Time će se generirati nova znanja i ekspertize te stvoriti snažna osnova za daljnji razvoj i dugoročnu održivost .

Ključne riječi: bioprospecting istraživanja, morski organizmi, kemijska karakterizacija, biološke aktivnosti, *in silico* predviđanja



ULOGA BENZAZOLA KAO POVLAŠTENIH STRUKTURA U RAZVOJU NOVIH PREDVODNIH SPOJEVA S ANTITUMORSKIM DJELOVANJEM

THE ROLE OF BENZOAZOLES AS A PRIVILEGED SCAFFOLDS IN DEVELOPMENT OF NOVEL LEAD COMPOUNDS WITH ANTITUMOR POTENTIAL

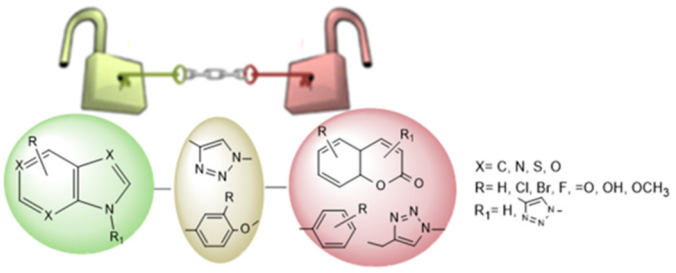
Tatjana Gazivoda Kraljević

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

One of the main trends in medical chemistry along with the rational design and development of new and more effective biologically active compounds is the development of modern strategies for their synthesis. Heterocyclic nuclei offer a huge area for new lead molecules for drug discovery and for generation of activity relationships with biological targets for enhance pharmacological effects. In general, heterocyclic compounds containing a nitrogen atom are a significant source of pharmacologically active compounds. Therefore, in the last 15 years the concept of privileged scaffolds was introduced into medicinal chemistry. Such structures exhibit drug-like properties and are selected as chemical entities in the preparation of compound libraries with potential biological activity [1, 2]. Privileged scaffolds include purine and purinomimetics such as benzothiazole, benzimidazole and benzoxazole ring that are present in a number of natural products, bioactive molecules and drugs [3].
During my talk, I will present the development of new chemical entities structurally related to purine applying the scaffold hopping approach based on benzoazoles as a privileged structures. With the aim to obtain new lead compounds with improved antitumor and antibacterial activities, benzoazole and pyrrolopyrimidine derivatives were synthesized by using modern synthetic methods including click chemistry, Pd-catalyzed cross-coupling and mechanochemical reactions.

Keywords: privileged structures, benzoazoles, scaffold hopping, click chemistry

[1] J. Kim *et. al*., *J Am Chem Soc* 136 (2014) 14629.
[2] Y. Wan *et al*., *Eur J Med Chem* 183 (2019) 111691.
[3] N. M. Meghani *et al.*, *Drug Discov Today* 22 (2017) 1604.



Plenarna predavanja / *Plenary Lectures*

PRIROĐENE LINIJE LIMFOCITA T U PSORIJAZI: UVID U IMUNOFENOTIP, TRANSKRIPTOM I REPERTOAR T STANIČNOG RECEPTORA

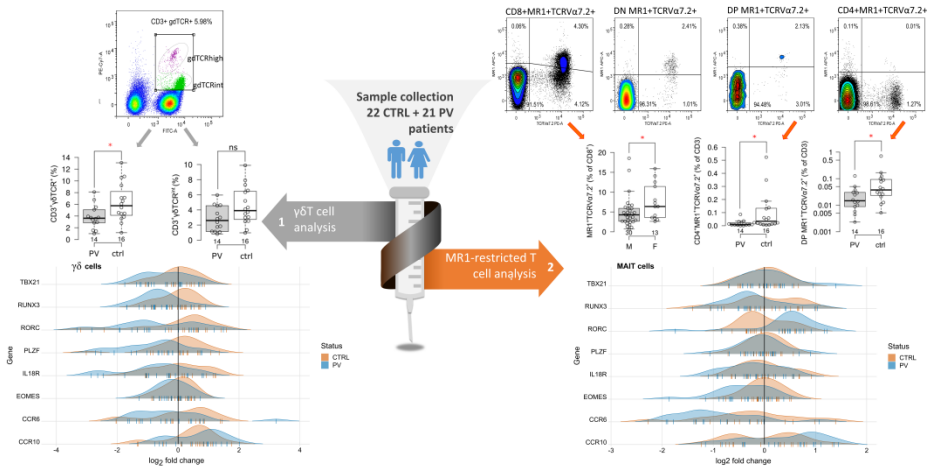
INNATE-LIKE LYMPHOID T CELLS IN PSORIASIS: CLUES ON IMMUNOPHENOTYPE, TRANSCRIPTOME AND TCR REPERTOIRE

Stana Tokić[1], Mario Štefanić[1], Vera Plužarić[2], Martina Mihalj[1], Peter Balogh[3], Martin Petrek[4], Ljubica Glavaš-Obrovac[1]

[1]*Faculty of Medicine, J. J. Strossmayer University of Osijek, 31 000 Osijek, Croatia*
[2]*University Hospital Osijek, 31 000 Osijek, Croatia*
[3]*Faculty of Medicine, University of Pecs, 7 600 to 7 636 Pecs, Hungary*
[4]*Faculty of Medicine and Dentistry, Palacký University, 77 900 Olomouc, Czech Republic*

Innate-like, MR1-restricted and γδ T cells are vital for maintaining homeostatic functions at barrier sites, but their regulation in psoriasis (PV), an autoinflammatory skin disease, is not well understood. Here, we identify an MR1-restricted CD4+CD8±TCRVα7.2+ T cell population, akin to mucosal-associated innate-like T (MAIT) cells, which is contracted in the blood of male patients, and track the sources of heterogeneity among circulating γδ T cells by identifying distinct γδint and γδhigh subsets that exhibit differential perturbations in relation to sex-disaggregated case-control status, serum content of skin-homing cytokines, and CMV exposure. In this context, transcriptional alterations of FACS-purified MR1+ and ydTCR+ T cells will be discussed, together with updated estimates of Vδ1 and Vδ2 T cell subcommunities in psoriasis. Future avenues for T cell receptor (TCR) clonality research using next-generation sequencing will be presented as well.

Keywords: MR1, mucosal associated invariant T cells, γδ T lymphocytes, psoriasis



VALORIZACIJA BIOAKTIVNIH SPOJEVA S ANTIOKSIDACIJSKIM KAPACITETOM IZ AGROINDUSTRIJSKIH NUSPRODUKATA

VALORISATION OF BIOACTIVE COMPOUNDS WITH ANTIOXIDANT ACTIVITY FROM AGROINDUSTRIAL BY-PRODUCTS

Carlo I. G. Tuberoso

University of Cagliari, S.P. Monserrato-Sestu km 0.700 - 09042 Monserrato (CA), Italy

The agroindustrial sector has great economic and commercial relevance in the Mediterranean area, and its by-products are a promising source of bioactive compounds with antioxidant activity. Major crops, such as olive and grapes, and other vegetable productions like saffron, herbs and shell fruits are a valuable raw source of phytochemicals [1-3]. Nowadays, there is an increasing interest in the capability of such compounds, especially polyphenols, to strengthen endogenous antioxidant defences in human tissues. Several studies demonstrated the potential beneficial effects of these phytochemicals both on the intestine and overall at a systemic level for the prevention of cardiovascular and neurodegenerative diseases. For all these reasons, pharmaceutical, cosmetic and food industries show a great deal of interest around the isolation, characterization, and biological activity investigation of these phytochemicals. This requires an interdisciplinary approch with contributions from researches belonging to all chemical fields. A crucial challenge is the development of green extraction technologies for a cheap, fast and eco-friendly procedure to obtain these bioactive molecules. Finally, many of these natural compounds have also been identified as valid models to design semisynthetic derivatives and/or synthetic analogs with enhanced health properties. Thus, the exploitation of the agroindustrial by-products represents an important source of bioactive compounds that can be used as ingredients or to produce functional ingredients.

Keywords: bioactive compounds, antioxidant activity, agroindustrial by-products

[1] P. Montoro *et al*., *J Food Sci Technol* 57 (2020) 2051.
[2] M. Manconi *et al*., *Colloids Surf B* 146 (2016) 910.
[3] C. I.G. Tuberoso *et al.*, *Food Chem* 199 (2016) 18.

Pozvana predavanja
Invited Lectures

LIGNOCELULOZA KAO NOVO CRNO ZLATO – SNOVI ILI STVARNOST?

LIGNOCELLULOSE AS A NEW BLACK GOLD – DREAMS OR REALITY

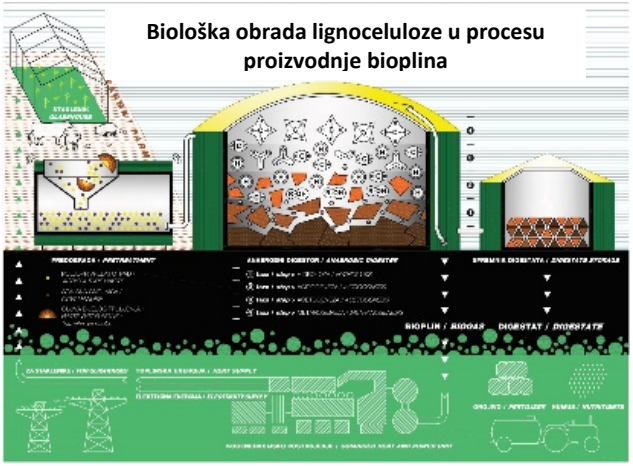
Marina Tišma

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Biorefineries are being developed as an answer to the instability of the petrochemical industry and as concern about sustainable energy development and climate change. By the definition, biorefineries are industrial processes that tend to produce a variety of value-added products, fuels and chemicals from different feedstocks. Compared to refineries, biorefineries use biobased raw materials such as agro-industrial lignocellulose-based materials, instead of the oil. The important step toward a low carbon future, which is the main aim of biorefineries, is the assessment of availability of biomass resources (lignocellulose). It is also important to know lignocellulose chemical composition and to assess the possibility to use them for biofuel production or to transform them into value-added products, including the assessment of concomitant emissions mitigation.

An integrated view of the possible use of filamentous fungi in biorefinery concept will be given in this lecture, as follows: *a)* Production and application of enzymes; *b)* Food and feed production, *c)* Environmental application. A special attention will be dedicated to solid-state fermentation (SSF) which imposed itself as a reliable method for biovalorization or reuse of lignocellulose in different purposes. The possibility to employ *Trametes versicolor* for lignocellulose degradation in SSF for large-scale biogas production will be specially emphasised.

Keywords: lignocellulose, biorefinery, sustainable development



NOVA ONEČIŠĆIVALA I NJIHOV UTJECAJ NA OKOLIŠ

EMERGING CONTAMINANTS AND THEIR INFLUENCE ON THE ENVIRONMENT

Šime Ukić, Marija Sigurnjak, Viktorija Prevarić, Matija Cvetnić, Mirjana Novak Stankov, Martina Miloloža, Marinko Markić, Dajana Kučić Grgić, Hrvoje Kušić, Ana Lončarić Božić, Marko Rogošić, Tomislav Bolanča

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

The global occurrence of numerous novel organic and inorganic substances in the environment has raised concern about their potential negative effects on the environment and human health. Many world countries, especially the "developed" ones, have recognized these substances as contaminants of emerging concern. The emerging contaminants (ECs) in environment can be more or less persistent, which depends on their chemistry, as well as on the environment conditions. In addition, the persistence might depend on applied treatments prior the discharge into the environment as well. Degradation/transformation of ECs might result with (by)products that are even more dangerous for the environment than the original molecules. Therefore, the origin, fate, behavior, and characterization of the ECs in the environment, as well as the related risk assessment and remediation modes, all have an increased attention of scientific community for some time.
This presentation will provide an insight in the problem of ECs in the environment. Pharmaceuticals, pesticides, and plastics (especially micro- or nano-sized one) will be especially discussed since these ECs are currently in the focus of scientific community. The authors will present benefits and deficiencies of actual approaches applied for risk assessment. Finally, an overview of strategies and current approaches for remediation of contaminated environment will be provided.

Keywords: environment, pesticides, pharmaceuticals, plastics

Acknowledgment
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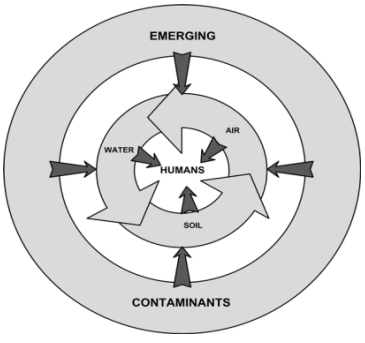


OTPAD KAO SIROVINA I ENERGENT ZA PROIZVODNJU „ZELENOG" AMONIJAKA

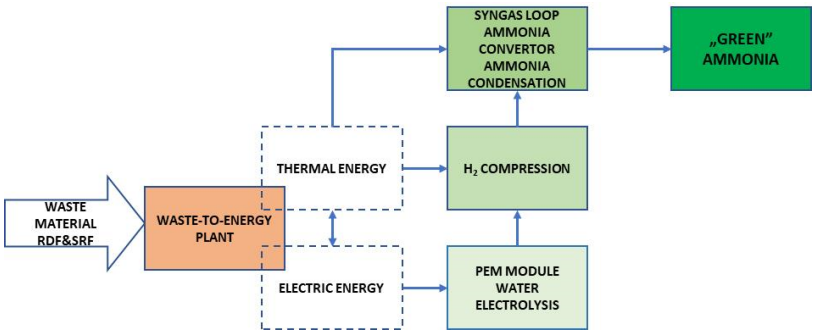
WASTE AS A FEEDSTOCK AND ENERGY SOURCE FOR "GREEN" AMMONIA PRODUCTION

Nenad Zečević[1], Elvira Vidović[2], Igor Dejanović[2]

[1]*Petrokemija d.d., Aleja Vukovar 4, 44 320 Kutina, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*

In 2030 developed countries drive to decarbonize the economy is expected to be well balanced. Chemical compounds which consist hydrogen without carbon will play a key factor in this process. Ammonia production as mature technology represents possible pathway towards that aim. However, the important issue on how to bypass ammonia production from the fossil fuels in order to avoid co-production of harmful carbon-dioxide should be resolved. Application of circular economy in order to optimize resources regarding use of a wide range of by-products and recycles of waste materials in ammonia production could be a valuable contribution to replacement of fossil fuels. In this work the new technological hybrid route in which use of waste fuel in the shape of Solid Recovered Fuel (SRF) and/or Refuse Derived Fuel (RDF) that ensures necessary thermal and electrical power, which could be used in subsequent production of "green" ammonia are presented. The renewable energy potential of this waste fuels serves as the backbone for the production of the hydrogen through well-established modular technology for industrial scale water electrolysis. Combining the clean molecules of hydrogen and nitrogen, transfer the classical and well proved Haber-Bosch process to sustainable operation for the future. The operating envelope of such unit was verified by the steady-state model which was compared with the traditional top-fired steam methane reforming ammonia unit. The results of the model are more than promising taking into account all premises of circular economy where the main task is delivery of the "green" ammonia within the incentive to switch to a low carbon economy. The model brings cost competitive production of sustainable "green" ammonia product as raw material for fertilizers and energy carrier for the power sector – both at world-scale and small-scale capacities as well as for green-field and brown-field projects.

Keywords: circular economy, "green" ammonia, renewable energy, waste fuel, water electrolysis



Usmena priopćenja
Oral presentations

MIKROESTRAKTORI I EUTEKTIČKA OTAPALA: ZAJEDNIČKO DJELOVANJE U UČINKOVITOM PROČIŠĆAVANJU BIODIZELA

MICROEXTRACTORS AND DEEP EUTECTIC SOLVENTS: JOINT ACTION TOWARDS EFFICIENT BIODIESEL PURIFICATION

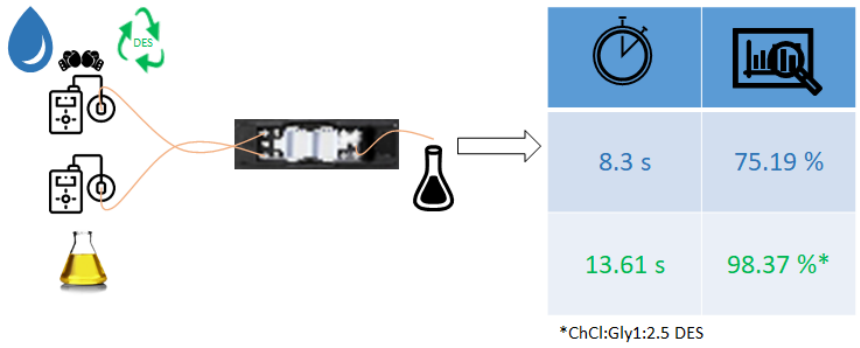
Martin Gojun[1], Anita Šalić[1], Ana Jurinjak Tušek[2], Bruno Zelić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*

With the increasing demand for the production of biodiesel, transesterification process took its place in the production line. On the other hand, the purification of crude biodiesel is still a bottleneck of downstream process. Because of that, and in order to satisfy international standard norms (EN 14214:2012/A2:2019), the removal of glycerol as the main challenge needs to be thoroughly explored. In this work, water and different deep eutectic solvents (DESs) based on ethylene glycol or glycerol mixed with choline chloride was used as extraction/purification medium. Three different microextractors were used and compared. With the usage of ChCl:$Gly_{1:2.5}$ DES, glycerol was almost completely removed from the crude biodiesel for the residence time of only 13.61 s [1]. This clearly demonstrates the application of DESs in micro-extractors as efficient methodology for glycerol removal during biodiesel purification.

Keywords: biodiesel, microextractor, glycerol, deep eutectic solvents

[1] A. Šalić *et al*., *Sep Purif Technol* 242 (2020) 116783.



PRIMJENJIVOST ALKOHOLA KAO BIOGORIVA ZA NAMJEŠAVANJE U DIZELSKO GORIVO

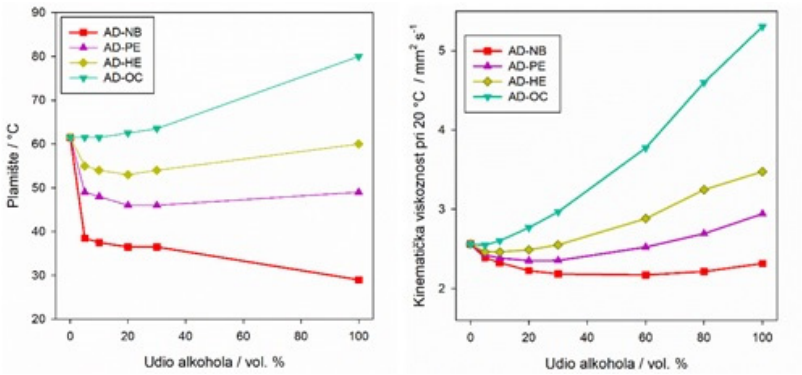
APPLICABILITY OF ALCOHOLS AS BIOFUEL COMPONENTS FOR FOSIL DIESEL

Lucija Konjević[1], Fabio Faraguna[2], Marko Racar[2], Marija Tirić-Unetić[1], Petar Ilinčić[3]

[1]INA Industrija nafte d.d., Razvoj rafinerija i marketinga, Centralni ispitni laboratorij, Lovinčićeva ul. 4, 10 000 Zagreb, Hrvatska
[2]Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Marulićev trg 19, 10 000 Zagreb, Hrvatska
[3]Fakultet strojarstva i brodogradnje, Sveučilište u Zagrebu, Ul. Ivana Lučića 5, 10 000 Zagreb, Hrvatska

Bioalkoholi su alkoholi koji se proizvode iz bioloških izvora ili biomase, direktnom ili indirektnom fermentacijom iz usjeva, lignoceluloznih ostataka te prehrambenog otpada. Prirodni ili genetski modificirani kvasci i bakterije direktnom fermentacijom iz šećera proizvode bioalkohole dok indirektnom fermentacijom acetogene bakterije proizvode bioalkohole iz plinova dobivenih prethodnom pirolizom biomase. Zbog sve većeg regulatornog pritiska za korištenje obnovljivih izvora energije, posebice biogoriva, dodavanje bioalkohola u tekuća fosilna goriva sve je više atraktivno naftnoj industriji. Bioetanol je već pronašao svoje mjesto u mješavinama s motornim benzinom, dok je uporaba drugih bioalkohola, zbog smanjene mogućnosti proizvodnje, tek u začetcima. U ovom istraživanju ispitana su svojstva mješavina butanola, pentanola, heksanola i oktanola s dizelskim gorivom. Dobiveni rezultati uspoređeni su sa zahtjevima norme vezane uz kvalitetu goriva te je ocijenjena primjenjivost pojedinih mješavina za pogon motornih vozila.

Ključne riječi: bioalkohol, dizelsko gorivo, mješavine



UTJECAJ SUMPOROVODIKA NA DEETIOLACIJU PŠENIČNE TRAVE (*Triticum aestivum L.)*

INFLUENCE OF HYDROGEN SULFIDE ON DE-ETIOLATION OF WHEATGRASS (*Triticum aestivum L.*)

Marija Kristić, Sanja Grubišić, Andrijana Rebekić, Marija Špoljarević, Tihana Teklić, Ana Šoštarić, Gabrijela Rebeka Stanković, Miroslav Lisjak

Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Hrvatska

Hydrogen sulfide (H_2S) as a component of cellular signal transduction is involved in a large number of physiological processes and responses to abiotic types of stress. It is known it increases photosynthesis by stimulating the carboxylation pathway of RuBISCO and increasing chlorophyll synthesis. The aim of the study was to determine the influence of sodium hydrogen sulfide (NaHS) and time of application on the physiological properties of etiolated wheatgrass plants. Wheatgrass was grown under controlled conditions for five days without light and then with a 12-hour photoperiod, watered for 3 days with 100, 200 and 500 mmol dm^{-3} of NaHS solutions. Plants were watered from 7^{th}-9^{th}, 10^{th}-12^{th} and 13^{th}-15^{th} day. The highest content of phenols (268.56 µgGA 100 $mgFW^{-1}$), flavonoids (153.72 µgQC 100 $mgFW^{-1}$) and hydrogen peroxide (9.617 nmol gFW^{-1}) was found in wheatgrass plants watered with 100 mM NaHS. The highest proline content and lipid peroxidation were found in plants at 500 mmol dm^{-3} NaHS. At 200 mmol dm^{-3} NaHS, the highest content of total chlorophyll (1.08 mg gFW^{-1}), vitamin C (0.897 mg $100gFW^{-1}$) and antioxidant activity (IC50 % 13.837 mgFW) were determined. Watering period significantly influenced the examined physiological parameters, as well. The results show that H_2S significantly affects the de-etiolation process in wheatgrass plants.

Keywords: etiolation, hydrogen sulfide, wheat grass

SINTEZA I BIOLOŠKA AKTIVNOST NOVIH HIBRIDA KUMARINA I KINOLINA PREMOŠTENIH 1,2,3-TRIAZOLNIM PRSTENOM

SYNTHESIS AND BIOLOGICAL ACTIVITY OF NOVEL COUMARIN AND QUINOLINE HYBRIDS BRIDGED BY 1,2,3-TRIAZOLE RING

Moris Mihovilović[1], Tatjana Gazivoda Kraljević[2]

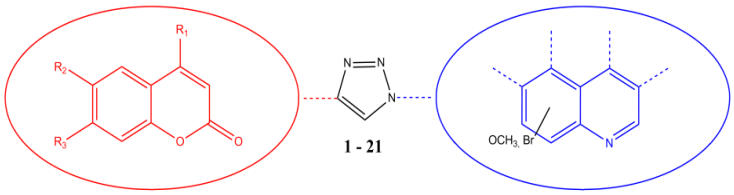
[1]*Pliva Croatia Ltd., Prilaz baruna Filipovića 25, 10 000 Zagreb, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*

The field of medicinal chemistry has numerous examples of heterocyclic molecules having a wide range of use and properties. In continuous efforts to find more potent and efficient molecules, development of molecular hybrids using combinations of moieties that are proven to be biologically active is an emerging trend in drug discovery [1]. Coumarin and quinoline are two heterocyclic scaffolds that have a wide range of biological activity and play an essential role in many pharmaceuticals. Their use in new hybrids using 1,2,3-triazole linkages has recently been reported in several studies [2,3],

In this work, we present novel, potentially biologically active, hybrids of coumarin and quinoline bridged with 1,2,3-triazole linkage that were synthesized using azidoquinoline and terminal alkyne bearing coumarin and quinoline precursors. Terminal alkyne coumarin and quinoline precursors that have an ether linkage were prepared from hydroxycoumarin derivatives *via* nucleophilic substitution with propargyl bromide. The 4-ethynylcoumarin for the synthesis of **1-4** was prepared from hydroxycoumarin derivatives by Sonogashira reaction of a previously synthesized coumarin triflate and trimethylsilylacetylene followed by deprotection using potassium carbonate. Coumarin and quinoline hybrids bridged with 1,2,3-triazole (**1-21**) were synthesized using a copper catalyzed Huisgen-1,3-dipolar cycloaddition and evaluated against Gram-positive and Gram-negative bacterial strains.

*Keywords:*quinoline, coumarin, 1,2,3-triazole, molecular hybrids

[1] G. Bérubé, *Expert Opinion on Drug Discovery* 11 (2016) 281.
[2] R. Reddyrajula *et al*., *Chemistry Select* 4 (2019) 2685.
[3] Kavita Bhagat *et. al., ACS Omega* 4 (2019) 8720.



R_1 = OH_2C---, H, ---
R_2 = OH_2C---, H
R_3 = OH_2C---, OCH_3, H

NANOPRAŠCI ČISTOG I CINKOM DOPIRANOG CERIJEVA(IV) OKSIDA KAO UV FILTERI U KREMAMA ZA SUNČANJE

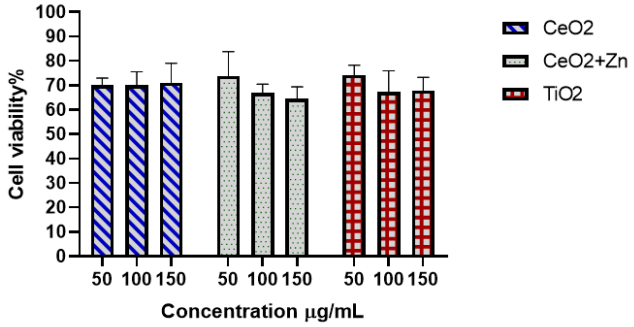
PURE AND ZINC DOPED CERIA NANOPOWDERS AS UV FILTERS IN SUNSCREENS

Katarina Mužina[1], Stanislav Kurajica[1], Sabina Keser[2], Goran Dražić[3], Marija Tirić-Unetić[4]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Pharmacy and Biochemistry, University of Zagreb, Ante Kovačića 1, 10 000 Zagreb, Croatia*
[3]*National Institute of Chemistry, Hajdrihova 19, 1 001 Ljubljana, Republic of Slovenia*
[4]*INA d.d., Central Testing Laboratory, Lovinčićeva 4, 10 000 Zagreb, Croatia*

Aside from environmental and energy related applications, ceria (CeO_2) possesses great potential as a sunscreen ingredient because it absorbs UV radiation while being relatively transparent to visible light. Additionally, it has lower photocatalytic activity in comparison to titania and zinc oxide which are currently main inorganic UV-blocking filters used in cosmetic industry. The problem is its high catalytic activity for oxidation of organic materials. The general idea of this work is to incorporate zinc into the ceria crystal lattice in order to get the advantages of both compounds in one material. Pure and zinc doped ceria were prepared by hydrothermal synthesis and characterized using transmission electron microscopy, electron energy lost spectroscopy, X-ray diffraction and UV-Vis diffuse reflectance spectroscopy. Fine ceria and doped ceria nanoparticles with particle sizes around 6 nm and band gap values of 3.23 and 3.14 eV were prepared. Their catalytic activity, as well cell toxicity in comparison to TiO_2 was also evaluated. The results indicate that prepared nanoparticles show no difference in cell viability and are biocompatible with human skin, while also being catalytically inactive, making them potential candidates for a new type of UV filters in sunscreens.

Keywords: doped ceria, citotoxicity, catalytic activity



UTJECAJ ROKA BERBE I KVASACA NA FIZIKALNA, KEMIJSKA I SENZORSKA SVOJSTVA VINA GRAŠEVINA

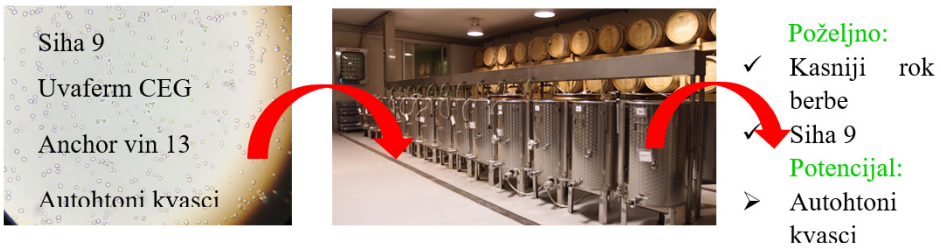
INFLUENCE OF HARVEST DATE AND YEAST STRAINS ON PHYSICAL, CHEMICAL AND ORGANOLEPTIC PROPERTIES OF GRAŠEVINA WINE

Valentina Obradović, Josip Mesić, Maja Ergović Ravančić, Brankica Svitlica, Helena Marčetić, Svjetlana Škrabal

Veleučilište u Požegi, Vukovarska 17, 34 000 Požega, Hrvatska

Graševina je najznačajnija vinska sorta u Republici Hrvatskoj, a Vinogorje Kutjevo je među najpoznatijim vinogorjima u kontinentalnoj Hrvatskoj, idealno za razvoj maksimalnih sortnih potencijala. Cilj ovog rada je utvrditi utjecaj različitih vrsta kvasaca i rokova berbe na fizikalno-kemijska i senzorska svojstva vina Graševina. Grožđe je uzgojeno u Vinogorju Kutjevo, na položaju Podgorje 2019. godine. Za proces fermentacije korištene su tri vrste komercijalnih kvasaca (Siha 9, Uvaferm CEG, Anchor vin 13), te autohtoni kvasac, a berba je provedena u dva termina početkom rujna i početkom listopada 2019. godine. U uzorcima je određen udio alkohola, ukupne kiseline, ukupni ekstrakt i ekstrakt bez šećera, reducirajući šećeri, pH, vinska i jabučna kiselina, antioksidativna aktivnost DPPH metodom, te gustoća boje. Senzorsko ocjenjivanje vina proveo je panel profesionalnih ocjenjivača metodom 100 bodova. Autohtoni kvasci nisu uspješno završili fermentaciju u svrhu dobivanja suhog vina, osobito u kasnijem roku berbe, te je takav stil poluslatkog vina ujedno i lošije senzorski ocijenjen. Najbolje ocijenjeno vino je vino iz kasnijeg roka berbe, uz upotrebu kvasca Siha 9, a isti kvasac je i u prvom roku berbe pokazao bolji rezultat senzorskog ocjenjivanja od ostalih. Kasniji rok berbe rezultirao je većim udjelom šećera u grožđu i posljedično većim sadržajem alkohola u suhim vinima, manjim vrijednostima ukupne kiselosti i jabučne kiseline, dok nema značajnije razlike u antioksidativnoj aktivnosti. S druge strane, vina dobivena fermentacijom pomoću autohtonih kvasaca su pokazala nešto veću antioksidatvnu aktivnost od vina dobivenih pomoću komercijalnih kvasaca.

Ključne riječi: graševina, Kutjevo, kvasci, rok berbe



UTJECAJ KOLIČINE SAHAROZE I TREHALOZE NA AROMATSKI PROFIL PUNILA NA BAZI KUPINA TIJEKOM SKLADIŠTENJA

INFLUENCE OF SUCROSE AND TREHALOSE AMOUNT ON FLAVOUR PROFILE OF BLACKBERRY CREAM FILLINGS DURING STORAGE

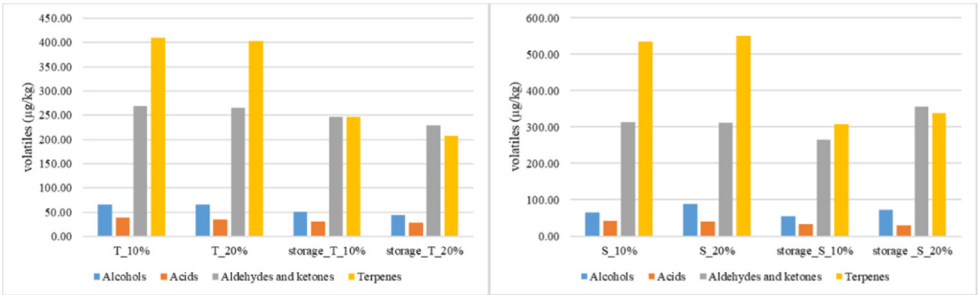
Anita Pichler[1], Ivana Ivić[1], Josipa Vukoja[1], Iva Horvatić[1], Josip Šimunović[2], Mirela Kopjar[1]

[1]Faculty of Food Technology Osijek, J. J. Strossmayer University in Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia
[2]North Carolina State University, Department of Food, Bioprocessing and Nutrition Sciences, Raleigh, NC 27 695, USA

Blackberry cream fillings were prepared from blackberry juice, citrus fiber and disaccharides. Two disaccharides, sucrose and trehalose, were used in amount of 10% and 20% in order to investigate influence of disaccharides amount on retention of blackberry volatiles during preparation of cream fillings as well as during 4 months of storage. GC-MS analyses were conducted for evaluation of volatile compounds amount. Overall, 29 volatiles were detected in samples and they were divided into 4 groups; alcohols, acids, terpenes and aldehydes and ketones. After preparation, there was no difference in volatiles amount between samples with 10 % and 20 % of trehalose addition. In the case of sucrose addition, alcohols and terpenes were detected in higher amount when 20% of disaccharide was used for preparation of samples while amount of other two volatile groups did not depend on sucrose amount. During storage, amount of majority volatiles decreased but there were some exceptions in aldehydes and ketones probably due to their formation during storage. Terpenes as volatiles that highly influence flavour profile of fruits, had the highest retention in samples with 10 % of trehalose addition and 20 % of sucrose addition (in both cases 60 %).

Keywords: blackberry cream fillings, sucrose, trehalose, volatiles, storage

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *IP-2019-04-5749*.



DERIVATI PEPTIDA KAO INHIBITORI SARS-CoV-2-S PROTEINA

PEPTIDE DERIVATIVES AS INHIBITORS OF SARS-CoV-2-S PROTEIN

Vesna Rastija, Domagoj Šubarić, Maja Karnaš

Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Hrvatska

Spike surface glycoprotein (S protein) is a component of coronavirus virion particle and it is responsible for viral recognition of Angiotensin Converting Enzyme 2 (ACE2). S protein binds with to human ACE2 and uses it as an entry receptor to invade target cells. S1 subunit is responsible for binding to the host cell receptor, while S2 subunit for the fusion of the viral and cellular membranes. SARS-CoV infection could be blocked by inhibitors that bind to the RBD and induced conformational changes in S glycoprotein and prevents binding to the ACE2 [1]. Peptide-type compounds were found to have promising activity against SAR-CoV. Consequently, these molecules attracted the attention of researchers to prepare and test their more derivatives [2].

In order to screen the abilities for binding to the SARS-CoV-2 spike glycoprotein (S protein) of previously proven peptide-type SARS-CoV 3CL protease inhibitors [2], we performed the molecular docking study. The three dimensional structure of the SARS-CoV-2 spike glycoprotein in complex with N-acetyl-D-glucosamine as ligand (NAG) (pdb: 6VSB) was downloaded from the Protein Data Bank. Molecular docking was performed on 62 optimized structures of compounds (**1**-**62**) and antiviral drug Remdesivir. The highest binding affinity towards S protein has compound **21** (E = -127.2 kcal mol^{-1}). Compound **21** is in conformation that forms a cluster of H-atom acceptor (O and N atoms), which allows stronger biding to S1 subdomain. Antiviral drug Remdesivir demonstrated low binding affinity to the S protein.

Ključne riječi: SARS-CoV-2, spike glycoprotein, peptide-type compounds, molecular docking

[1] A.C. Walls *et al*., *Cell* 180 (2020) 1.
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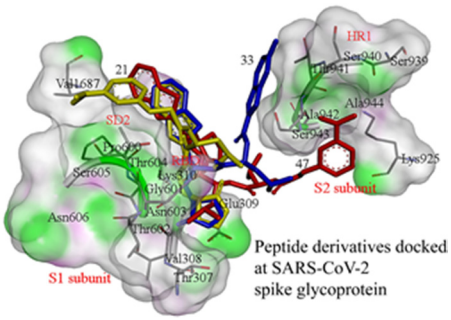


POLUVODIČKA SVOJSTVA $BiVO_4$ ZA OBRADU VODE VIDLJIVOM I SUNČEVOM SVJETLOSTI

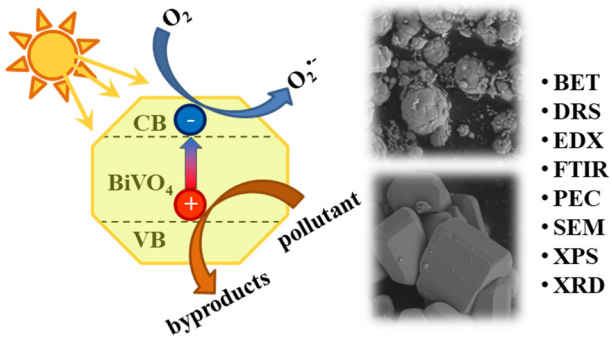
SEMICONDUCTING PROPERTIES OF $BiVO_4$ FOR VISIBLE- AND SOLAR-LIGHT DRIVEN WATER TREATMENT

Tayebeh Sharifi[1], Marin Kovačić[1], Marin Popović[2], Igor Peternel[2], Dražan Jozić[3], Marijana Kraljić Roković[1], Hrvoje Kušić[1], Urška Lavrenčič Štangar[4], Ana Lončarić Božić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Karlovac University of Applied Sciences, Trg J.J. Strossmayera 9, 47 000 Karlovac, Croatia*
[3]*Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21 000 Split, Croatia*
[4]*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1 000 Ljubljana, Slovenia*

$BiVO_4$ is considered to be a perspective photocatalyst due to its low band gap (2.34-2.90 eV). However, photocatalytic performance of pristine $BiVO_4$ is limited due to high electron-hole recombination rate and low electron mobility. Hence modifications are necessary to mitigate these drawbacks. In this work, several methods were employed to synthesize $BiVO_4$.The photocatalysts were characterized using techniques such as BET, DRS, FTIR, SEM/EDX, XPS and XRD to inspect their structure, morphology, composition, surface and optical properties. In addition, photoelectrochemical performance of the new photocatalysts was investigated. Photostability of the photocatalysts was studied using chronoamperometric technique as well. To further asses the performance of as-prepared photocatalysts, their activity was examined for the treatment of diclofenac, one of the common contaminants of emerging concern.

Keywords: $BiVO_4$, semiconducting properties, visible photocatalysis



ZELENA INA

GREEN INA

Maja Fabulić Ruszkowski[1], Bernard Suknjov[1], Ivana Čović Knezović[1], Vesna Kučan Polak[1], Lucija Konjević[2]

[1]INA Industrija nafte d.d., Razvoj rafinerija i marketinga, Avenija Većeslava Holjevca 10, 10 000 Zagreb, Croatia
[2]INA Industrija nafte d.d., Razvoj rafinerija i marketinga, Centralni ispitni laboratorij, Lovinčićeva ul. 4, 10 000 Zagreb, Hrvatska

INA Industrija nafte započela je transformaciju iz klasične naftne kompanije u kompaniju koja koristi obnovljive izvore energije, kontinuirano poboljšava energetsku učinkovitost te smanjuje intenzitet emisija stakleničkih plinova. Vezano uz sadašnje i nadolazeće EU zakonodavstvo, INA kao glavni proizvođač i distributer motornog goriva u RH ispunjava/ispunjavati će zahtjeve Direktive o obnovljivim izvorima energije (eng. *Renewable Energy Directive* - RED 2) vezane uz uvođenje obnovljivih i naprednih biogoriva te Europski zeleni plan (eng. *European Green Deal*) vezano uz dekarbonizaciju gospodarstva. U proteklom periodu INA - Razvoj, kao glavni pokretač promjena vodio je niz projekata koji su pokazali mogućnosti dobivanja energije i goriva iz obnovljenih izvora energije. Tako su provedeni sljedeći projekti: Ugradnja fotonaponske elektrane u RN Rijeka, Studija o korištenju CO_2 s naglaskom na kemijsku konverziju, *Test run* na FCC postrojenju u RN Rijeka s bio pirolitičkom uljem, *Test run* na HDS postrojenju s biljnim i rafiniranim biljnim uljem u RN Rijeka i RN Sisak, Sakupljanje otpadnih jestivih ulja iz kućanstava te Ispitivanje mogućnosti dobivanja biogoriva iz algi. Ujedno se razmatraju i novi projekti s čijom implementacijom bi INA doživjela preobrazbu prema spomenutim ciljevima: zeleni vodik; hvatanje, korištenje i skladištenje ugljika (engl. *Carbon Capture, Utilisation and Storage for* RR – CCUS), proizvodnja bio avionskog goriva; proizvodnja naprednih biogoriva (projekt Biorafinerija koja će proizvoditi bioetanol 2G, FCC *co-processing*, HDS *co-processing*) te korištenje motornih goriva dobivenih iz otpadne plastike i automobilskih guma. Navedeni projekti primjer su kako INA primjenjuje nove tehnologije za proizvodnju obnovljivih goriva s ciljem smanjenja emisija stakleničkih plinova i očuvanja okoliša.

Ključne riječi: obnovljivi izvori energije, dekarbonizacija, biogoriva

Posterska priopćenja
Poster presentations

Sekcija: Kemijska analiza i sinteza
Topic: Chemical Analysis and Synthesis

PREDNOST OTOPINSKIH METODA ZA SINTEZU $Sr_3Fe_2WO_9$

ADVANTAGE OF SOLUTION METHODS TOWARDS SYNTHESIS OF $Sr_3Fe_2WO_9$

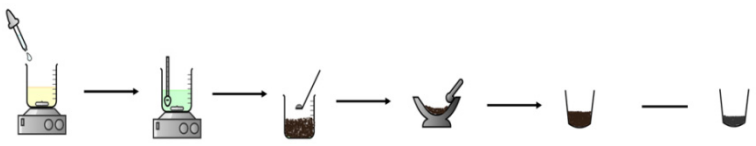
Jelena Bijelić[1], Dalibor Tatar[1], Anna-Marija Milardović[1], Antonia Vicić[1], Anamarija Stanković[1], Pascal Cop[2], Sebastian Werner[2], Zvonko Jagličić[3,4], Bernd Smarsly[2], Igor Djerdj[1]

[1]*Department of Chemistry, J. J. Strossmayer University of Osijek, Ul. cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Institute for Physical Chemistry, Justus Liebig University of Giessen, Heinrich-Buff-Ring 17, Giessen, Germany*
[3]*Institute of Mathemathics, Physics & Mechanics, University of Ljubljana, Jadranska 19, 1 000 Ljubljana, Slovenia*
[4]*Faculty of Civil and Geodetic Engineering, University of Ljubljana, Jamova 2, 1 000 Ljubljana, Slovenia*

The properties of materials have appeared to be size- and shape-dependent which is why in this work we compare two synthesis routes: sol-gel solution synthesis and solid state synthesis of triple $Sr_3Fe_2WO_9$ perovskite. This material has been prepared in form of semi-spherical particle agglomerates using a modified aqueous sol–gel citrate route and as a bulk material using solid state synthesis by means of planetary ball milling. Structural investigation has been conducted by ambient and in situ X-ray powder diffraction (XPRD), X-ray photoelectron spectroscopy (XPS), high resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED), thermogravimetric analysis (TGA) and unpolarized Raman spectroscopy. Results of powder X-ray diffraction show phase pure nanocrystalline $Sr_3Fe_2WO_9$ prepared by sol-gel route, while compounds prepared by solid state method contained larger amount of impurities. It has been revealed that synthesized compound crystalizes in tetragonal system (space group *I*4/*m*) with crystallite size of 36 nm and high crystallinity. Magnetic properties have been determined using SQUID measurements and have shown ferrimagnetic ordering with gradual transition around Curie temperature of 213 K as opposed to bulk $Sr_3Fe_2WO_9$ with sharp transition at 373 K. Optical properties have been estimated using Tauc method which revealed band gap values of 2.71 eV for direct band gap and 2.10 eV for indirect band gap.

Keywords: nanocrystalline, triple perovskite, sol-gel synthesis, solid state reactions

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *IP-2016-06-3115*.



SINTEZA 1,2,3-TRIAZOLNOG DERIVATA BENZOFENONA KLIK KEMIJOM

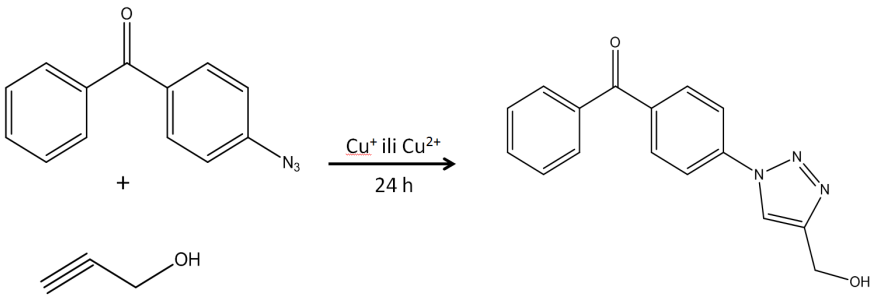
SYNTHESIS OF 1,2,3-TRIAZOLE DERIVATE OF BENZOPHENONE BY CLICK CHEMISTRY

Roko Blažic, Elvira Vidović

Fakulet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Molekulna hibridizacija pomoću poznatih farmakofora novi je pristup sintezi biološki aktivnih spojeva. Jedan od poznatih farmakofora je benzofenon. Derivati benzofenona javljaju se u prirodi i specifični su za porodicu biljaka kluzijevki (*Clusiaceace*), a pokazuju biološku aktivnost (antibakterijska svojstva, anti-HIV aktivnost, protuupalno djelovanje, inhibiciju rasta stanica karcinoma). Biološka aktivnost je utvrđena i kod sintetskih derivata benzofenona. Primjerice, ketoprofen dostupan je na tržištu kao protuupalni lijek. Također, poznati farmakofor je 1,2,3-triazolna skupina. Otporan je na metaboličku degradaciju, omogućava stvaranje vodikovih veza i poboljšava vezanje pripadajuće molekule na biološke mete. Jednostavna sinteza 1,2,3-triazola kroz reakciju azid-alken cikloadicije, koja je katalizirana solima bakra, uzrok je čestog odabira triazolne skupine prilikom sinteze novih biološki aktivnih spojeva. U ovom radu provedena je sinteza 4-(4-(hidroksimetil)-1H-1,2,3-triazol-1-il)benzofenona (**1**) iz 4-azidobenzofenona i propagil alkohola uz primjenu Cu^{+} ili Cu^{2+} soli kao katalizatora. Upotrebom Cu^{2+} soli u različitim otapalima (metanol, tetrahidrofuran) uspješno je sintetiziran spoj **1**. Nasuprot tome, u sustavu s Cu^{+} kao katalizatorom u otapalu *N*,*N*-dimetilformamid/voda nije došlo do nastanka spoja **1**. Sintetizirani spoj karakteriziran je spektroskopijom nuklearne magnetne rezonancije i infracrvenom spektroskopijom.

Ključne riječi: derivati benzofenona, triazol, klik kemija



OPTIMIRANJE PRIPRAVE SINTETSKIH GEOPOLIMERA U KONFIGURACIJI TANKOG FILMA

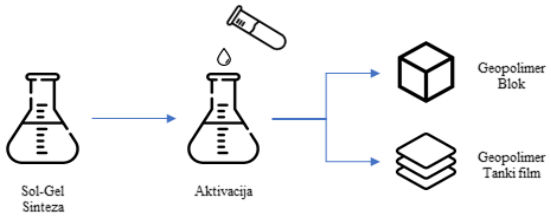
OPTIMISATION OF PREPARATION OF THE SYNTHETIC GEOPOLYMERS IN A THIN-FILM CONFIGURATION

Filip Brleković, Lucija Višić, Arijeta Bafti, Juraj Šipušić, Vilko Mandić

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Geopolimerni materijali dobivaju na značaju u području specijalnih cemenata (veziva). Za razliku od ostalih vrsta cemenata, očvršćivanje se ne temelji na procesu hidratacije, već na procesu geopolimerizacije. Tijekom tog procesa alumosilikatni prekursori se zapravo aktiviraju s alkalnim otopinama pri čemu se mikrostruktura s karakterističnim nano i mikro domenama, slično kao u zeolitima, što omogućuje razmatranje šire primjene. Sintetski prekursori i konačno sintetski geopolimeri omogućuju bolju kontrolu priprave, što omogućuje njihovo razmatranje u području naprednih i funkcionalnih materijala gdje je reproducibilnost materijala puno značajnija. Stoga su u ovom radu korišteni alumosilikatni prekursori pripravljeni različitim varijantama sol-gel metode. Korišteni su alkoksidi (tetraetoksi silan i aluminij-tri-sec-butoksid) i kelatori (etil acetoacetat) u reakcijama na različitim temperaturama kako bi se pripravili gelovi različite kemijske homogenosti. Dobiveni gelovi su žareni pri različitim temperaturama, što je utjecalo na različite stupnjeve uklanjanja organskih ostataka kao i različita strukturna i morfološka svojstva prekursora. Termički tretirani alumosilikatni prekursori aktivirani su smjesom vodenog stakla i natrijevog hidroksida u širem rasponu koncentracija na različitim temperaturama. Pripravljeni su blokovi geopolimera. Prekursori i geopolimeri su detaljno karakterizirani rendgenskom difrakcijskom analizom (XRD), analizom infracrvenom spektroskopijom s Fourierovom transformacijom (FTIR) te diferencijalnom termalnom i termogravimetrijskom analizom (DTA-TGA). Rezultati analize omogućili su razumijevanje doprinosa kemijskog sastava i homogenosti konstituanata kao i njihovih morfoloških karakteristika na geopolimerizaciju uzoraka, a sve s ciljem optimiranja procesa priprave geopolimera u konfiguraciji tankog filma. Temperatura odvijanja reakcije aktivacije pokazala je značajan utjecaj na reproducibilnost dobivenih geopolimera. Geopolimerni filmovi slijede svojstva geopolimernih blokova što otvara mogućnost njihove napredne upotrebe.

Ključne riječi: geopolimeri, sol-gel, sintetski alumosilikati, tanki film



DIAMANTOIDNI ESTERI U DIZAJNU NANOMATERIJALA

DIAMONDOID ESTERS IN NANOMATERIAL DESIGN

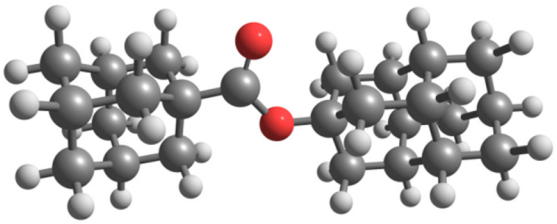
Nataša Burić, Marina Šekutor

Ruđer Bošković Institute, Bijenička 54, 10 000 Zagreb, Croatia

Diamondoids are cage hydrocarbons with a spatial arrangement of carbon atoms resembling the diamond crystal lattice. Unlike bulk diamond, diamondoids possess great capability for derivatization and their functionalized derivatives found application in medicine, material science, nanotechnology, supramolecular chemistry, etc [1, 2]. Investigation of diamondoid self-organized structures has been of great interest recently as they are promising building blocks in nanotechnology [3-5]. We have synthesized new diamondoid derivatives by connecting two diamondoid cages *via* a carboxyl moiety. We have also prepared adamantane methyl and *tert*-butyl esters as standards for further investigation that will include the use of atomic force microscopy for studying the influence of structure on self-organization behaviour on metal surfaces. The experimental findings will be supported by computational chemistry tools to further clarify the relationship between the structure and the self-assembly capability.

Keywords: diamondoids, ester derivatives, nanomaterials, computations

[1] H. Schwertfeger *et al., Angew Chem Int Ed* 47 (2008) 1022.
[2] M. A. Gunawan *et al*., *New J Chem* 38 (2014) 28.
[3] D. Ebeling, *et al*., *ACS Nano* 11 (2017) 9459;
[4] E. M. King *et al*., *Langmuir* 35 (2019) 16062;
[5] H. Yan *et al*., *Nat Mat* 16 (2016) 349.



FOTODINAMIČKI UČINAK AMFIFILNIH TRIPIRIDILPORFIRINA NA STANICAMA MELANOMA

PHOTODYNAMIC ACTIVITY OF AMPHIPHILIC TRIPYRIDYLPORPHYRINS ON MELANOMA CELLS

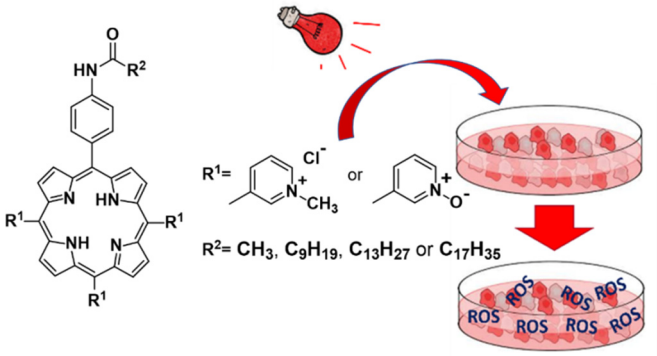
Anamarija Cindrić, Laura Penić-Ivanko, Martina Mušković, Ivana Ratkaj, Nela Malatesti

Department of Biotechnology, University of Rijeka, Radmile Matejčić 2, 51 000 Rijeka, Croatia

Melanomas are difficult to treat due to variety of resistance mechanisms, such as defects in apoptotic pathways, ABC transporters and melanin [1, 2]. Photodynamic therapy (PDT) shows some encouraging results against melanoma, thanks to multitarget mechanism of action [1].
Amphiphilic porphyrins have been widely investigated due to their possibility to pass through membrane, as well as being water soluble. Our research group has previously described activity of pyridylporphyrins on several cell lines, and amphiphilic porphyrins showed significantly higher PDT activity compared to their hydrophilic analogues [3].
Here we study the impact of conjugation of hydrophobic chains of various length within *N*-methylated and *N*-oxidised pyridylporphyrins. Physicochemical differences between groups are investigated on singlet oxygen production, stability, spectroscopic properties, and lipophilicity of the photosensitizers (PSs). Photodynamic activity will be evaluated on MEWO melanoma cell line by testing cytotoxicity and localization of the PSs inside cells.

Keywords: photodynamic therapy, amphiphilic porphyrins, melanoma cell line

[1] I. Baldea *et al*., *J Photoch Photobio B* 151 (2015) 142.
[2] Y.-Y. Huang *et al*., *Biol Chem* 394 (2013) 239.
[3] M. Jelovica *et al*., *Chem Med Chem* 13 (2018) 13 360.



RAZVOJ MEHANOKEMIJSKE METODE ZA SINTEZU METALO-ORGANSKIH MREŽA

EVOLUTION OF MECHANOCHEMICAL METHOD TOWARDS SYNTHESIS OF METAL-ORGANIC FRAMEWORKS

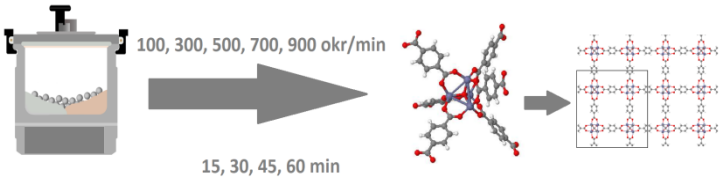
Ivan Ćorić, Kristina Janđel, Jelena Bijelić, Elvira Kovač-Andrić

Odjel za kemiju, Sveučilište J. J. Strossmayera u Osijeku,
Ul. cara Hadrijana 8/A, 31 000 Osijek, Hrvatska

Metalo-organske mreže, poglavito MOF-5 zbog svoje se porozne strukture najčešće koriste za uklanjanje štetnih plinova iz zraka adsorpcijom. Klasična sinteza kompleksnih spojeva, posebno organskih spojeva, redovito zahtijeva upotrebu organskih otapala i utrošak velike količine energije. Napredak sintetske kemije donosi nove metode sinteze uz minimalnu upotrebu otapala te sa značajnim uštedama energije. Primjer takve metode je mehanokemijska sinteza [1]. Dobro poznati porozni materijal MOF-5 (eng. *metal-organic frameworks*, MOF) moguće je dobiti klasičnom sintezom iz cinkovog nitrata heksahidrata i tereftalne kiseline. No taj postupak zahtjeva višesatno zagrijavanje i uporabu otapala poput dimetilformamida (DMF). Molekule otapala nakon sinteze ostaju ukomponirane u metalo-organskoj mreži, što rezultira slabijom adsorpcijom. Za dobivanje aktiviranog MOF-5 koji bi mogao adsorbirati različite plinove potrebni su dodatni postupci uklanjanja otapala, što oduzima vrijeme i povećava cijenu proizvodnje. Mehanokemijskom sintezom u planetarnom kugličnom mlinu višesatna sinteza može se svesti na manje od jednog sata. Ušteda energije je značajna, a moguće je u rednom koraku dobiti aktivirani produkt budući da se ne koristi otapalo. Smanjena upotreba otapala znači i manju količina otpadnog materijala koji potencijalno može dospjeti u okoliš. U ovom radu provedene su serije sinteza u kojima je proučavan utjecaj vremena sinteze i brzine okretaja na nastanak MOF-5. Dobiveni su uzorci analizirani spektroskopskim i termičkim metodama kako bi se utvrdila prisutnost ciljanog spoja u uzorcima.

Ključne riječi: MOF-5, mehanokemijska sinteza, optimizacija sinteze

[1] G.-W. Wang, *Chem. Soc. Rev.* 42 (2013) 7668.



REAKCIJA KOPULACIJE FEROCENA I C5-SUPSTITUIRANIH DERIVATA URACILA

THE COPULATION REACTION OF FERROCENE AND C5-SUBSTITUTED URACIL DERIVATIVES

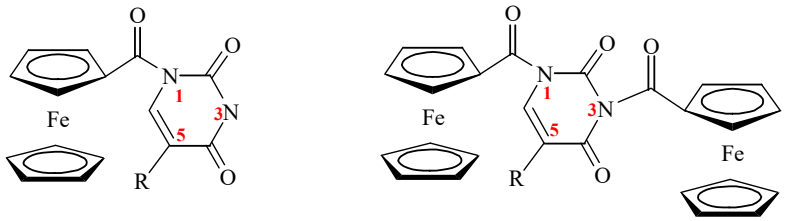
Senka Djaković,[1] Jasmina Lapić,[1] Ivana Kuzman,[1]
Mateja Toma,[2] Valerije Vrček[2]

[1]*Prehambeno-biotehnološki fakultet, Sveučilište u Zagrebu, Pierottijeva 6, 10 000 Zagreb, Hrvatska*
[2] *Farmaceutsko-biokemijski fakultet, Sveučilište u Zagrebu, Ante Kovačića 1, 10 000 Zagreb, Croatia*

Istraživanja interakcije ferocena i biomolekula, poput DNA i RNA, su značajna za razumijevanje kompleksnih mehanizama aktivnosti koji mogu poslužiti za sintezu novih lijekova te se stoga u zadnjih desetak godina povećao interes za konjugate ferocena s nukleobazama, nukleozidima i nukleotidima [1]. Vezanje supstituenata na molekulu ferocena omogućeno je rotacijom ciklopentadienilnih prstenova ferocena koji poprima biološke karakteristike kada se na njega veže neka biološka molekula poput nukleobaze. Naša prethodna istraživanja vezanja ferocenske podjedinice preko karbonilnog mosta na purinske derivate ukazuju na nastajanje N7 i N9-produkata [2]. Ovdje ćemo se fokusirati na sintezu ferocenoil-pirimidiskih konjugata **I** i **II**, a posebna pozornost biti će usmjerena na nastajanje N1 i/ili N1, N3 produkata. Regioselektivnost reakcija pratit će se pri različitim reakcijskim uvjetima, kao što je korištenje različitih deprotekcijskih baza, otapala, kao i vrijeme aktivacije (60 i 120 minuta). Nastali kopulati biti će karakterizirani 1D, 2D-NMR i FTIR spektroskopijom.

Ključne riječi: ferocen, C5-derivati uracila, N1 i/ili N1/N3-kopulati

[1] A. A. Simenel *et al*., *Appl Organomet Chem* 23 (2009) 219.
[2] M. Toma *et al*., *J Org Chem* 84 (2019) 12471.



I **II**

R = H, CH_3, F, Cl, Br, I, CN

MODIFIKACIJA I PRIMJENA GRAĐEVINSKIH MATERIJALA ZA IZGRADNJU ZDRAVIH ZGRADA

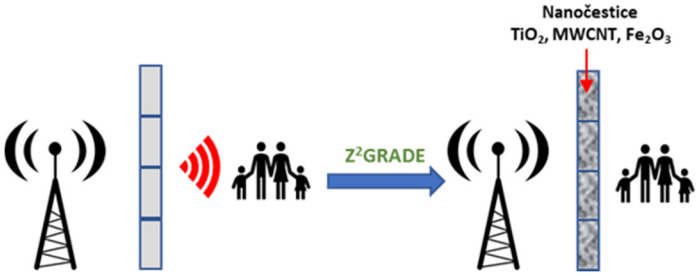
MODIFICATION AND APPLICATION OF CONSTRUCTION MATERIALS FOR HEALTHY BUILDINGS

Nikolina Filipović[1], Jelena Brdarić[1], Berislav Marković[1], Dalibor Tatar[1], Milan Pajičić[1], Damir Varevac[2], Ivana Miličević[2]

[1]Odjel za kemiju, Sveučilište J. J. Strossmayera u Osijeku,
Ulica cara Hadrijana 8/A, 31 000 Osijek, Hrvatska
[2]Građevinski i arhitektonski fakultet, Sveučilište J. J. Strossmayera u Osijeku,
Vladimira Preloga 3, 31 000 Osijek, Hrvatska

Onečišćenje elektromagnetskim (EM) zračenjem, kao posljedica ubrzanog tehnološkog razvoja predstavlja jedno od važnijih pitanja (problema) modernog svijeta. Kako bi se ono smanjilo, teži se izgradnji stambenih objekata modifikacijom materijala koji apsorbiraju EM valove. Beton, kao kompozitni građevinski materijal, miješa se s raznim nanočestičnim tvarima koje imaju svojstvo apsorpcije EM valova. Komponente koje su korištene u ovom radu su: titanijev dioksid (u dvije kristalne modifikacije - anatas i rutil), lebdeći pepeo, ugljikove nanocjevčice (MWCNT-višestjenčane) te oksidi željeza i feritni materijali. Spomenute komponente potrebno je detaljno karakterizirati. Termogravimetrijskom analizom i razlikovnom pretražnom kalorimetrijom (TGA/DSC) određene su fazne transformacije, sadržaj vlage te udio organskih komponenata u ispitivanim materijalima. Akustičnom spektroskopijom određene su veličine čestica i njihov zeta potencijal nakon raspršivanja u prikladnoj tekućoj fazi. Također je analizirana poroznost, odnosno izmjerena specifična površina čestica adsorpcijom dušika odnosno Brunauer-Emmet-Teller (B.E.T.) metodom. Detaljno karakterizirani materijali dodavat će se u beton različitih sastava te se očekuje mogućnost potpune ili selektivne apsorpcije EM zračenja.

Ključne riječi: zdrave zgrade, neionizirajuće elektromagnetsko zračenje, kompozitni građevinski materijali



PRIMJENA PEKTINA IZ KORE MANDARINE *(C. reticulata)* U BIOGENOJ SINTEZI SELENOVIH NANOČESTICA

APPLICATION OF MANDARIN *(C. reticulata)* PEEL PECTINS IN BIOGENIC SYNTHESIS OF SELENIUM NANOPARTICLES

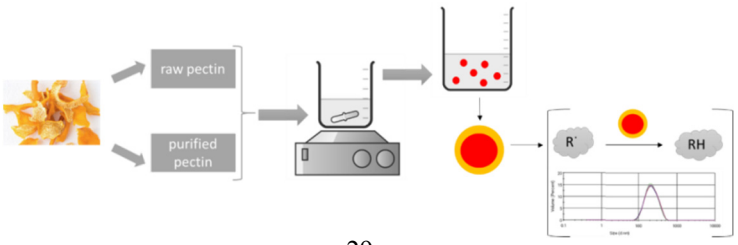
Emerik Galić[1], Nikolina Golub[2], Kristina Radić[2], Dubravka Vitali Čepo[2], Nikolina Kalčec[3], Ivana Vinković Vrček[3], Tomislav Vinković[1]

[1]*Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia*
[2]*Faculty of Pharmacy and Biochemistry, University of Zagreb, Ante Kovačića 1, 10 000 Zagreb, Croatia*
[3]*Institute for Medical Research and Occupational Health, Ksaverska cesta 2, 10 000 Zagreb, Croatia*

Mandarin peel has been recognized as the valuable source of functional ingredients such as polyphenols (hesperidin, tangeretin and nobiletin) and dietary fibres (pectin). In this study, we optimized the procedure of extraction and purification of pectin from mandarin peel extract for using raw pectin fraction (RP) and purified pectin fraction (PP) in biogenic synthesis of selenium nanoparticles (bnSeNPs). Obtained SeNPs were compared to chemically synthesised particles (cnSeNPs) in terms of size distribution, zeta potential, stability and functional properties (antiradical and reductive ability). The bnSeNPs stabilized with 0.7 % RP and PP showed particle size distribution comparable to cnSeNPs with average diameter of 230 nm and 290 nm, respectively. Surface charge of bnSeNPs showed more negative values than for cnSeNPs (-35 mV in relation to -10 mV) indicating better stability of obtained colloidal system. Also, in comparison to cnSe, bnSe coated with 0.7 % RP and PP showed significantly higher antioxidant activity (24.5 and 46.3 gTE $molSe^{-1}$, respectively) in comparison to cnSeNPs (1.91 gTE $molSe^{-1}$) that were probably associated to polyphenols remaining in pectin fractions. Obtained results revealed the potential of mandarin peel as a source of natural coating materials for development of green synthesis processes of SeNPs achieving improved functional properties.

Keywords: pectin, selenium nanoparticles, mandarin peel, biogenic synthesis, antioxidant activity

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grants HRZZ-*IP-2018-01-8119* and HRZZ-*PZS-2019-02-4323*.



PRIPREMA UZORAKA I ANALIZE SADRŽAJA NUTRICINA U KONZUMNIM JAJIMA

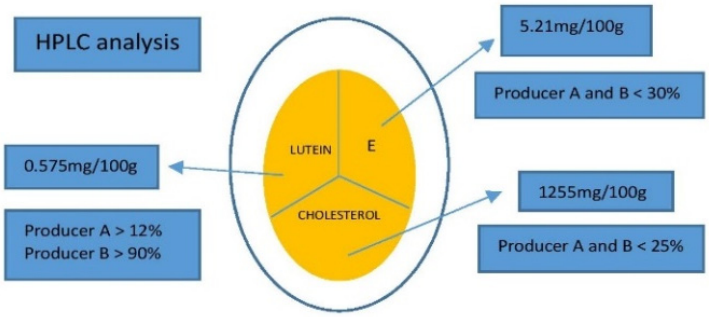
SAMPLE PREPARATION AND ANALYSIS OF NUTRICINES CONTENT IN TABLE EGGS

Olivera Galović[1,3], Maria Elena Nikolić[1], Luka Dornjak[1], Matea Marunica[1], Zlata Kralik[2,3]

[1]*Department of Chemistry, J. J. Strossmayer University of Osijek, Ulica cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia*
[3]*Scientific Center of Excellence for Personalized Health Care, J. J. Strossmayer University of Osijek, Trg sv. Trojstva 3, 31 000 Osijek, Croatia*

Egg is a food rich in various nutrients, which is why it can be used daily in human consumption. Due to the large number of nutrients, eggs are a complex matrix for sample preparation and analysis of nutricines. In this study the content of nutricines (lutein, vitamin E) and cholesterol from laying hens eggs of two producers available at Croatian market (A, B) was determined. The eggs were purchased at the mall where they were stored at 4 ˚C. Nutricines and cholesterol were determined on a total of 20 L-weight class egg yolks (egg mass 63 g – 73 g). For the analysis 10 egg yolks of each producer was used. For the extraction and measurement of concentration of nutricines and cholesterol the previously described methods were used but with minor modifications. The concentrations was determined by means of high resolution liquid chromatography (HPLC). According to the literature, the concentration of total vitamin E is 5.21 mg (α tocopherol 5.16 mg), lutein 0.575 mg and cholesterol 1255 mg 100 g^{-1} of egg yolk. In the analyzed samples, vitamin E content in both groups was 30 % lesser than in the literature, the lutein content in group A was 12 % and in group B 90 % higher, and the cholesterol content in both groups was 25 % lesser than the literature data.

Keywords: eggs, lutein, vitamin E, cholesterol, HPLC



UTJECAJ ABIOTIČKIH ČIMBENIKA NA KOLOIDNU STABILNOST SREBRNIH NANOČESTICA PRI VISOKOJ IONSKOJ JAKOSTI

INFLUENCE OF ABIOTIC PARAMETERS ON SILVER NANOPARTICLE COLLOIDAL STABILITY IN HIGH STRENGTH ELECTROLYTES

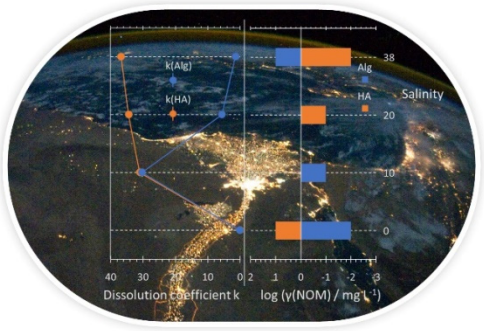
Ivana Hazdovac, Lara Jurković, Dijana Pavičić-Hamer,
Bojan Hamer, Daniel Mark Lyons

Center for Marine Research, Ruđer Bošković Institute,
G. Paliage 5, 52 210 Rovinj, Croatia

The increasing use of silver nanoparticles (AgNP) in a wide range of consumer and medical products represent a growing risk due to the potential for their release into the environment. However, there are few data on the fate of these nanoparticles as they transition from freshwater to brackish to marine waters, particularly as the abiotic characteristics of these environmental compartments are complex and dissimilar. Thus, in this study, the influence of abiotic parameters including electrolyte strength, oxygen saturation and light intensity, and their complex interplay, on AgNP colloidal stability in freshwater, brackish waters and seawater was determined. Further, the modulating role of natural organic matter including humic and alginic acids, and proteinaceous matter was investigated. Data indicate AgNP agglomeration with increasing electrolyte strength may be greatly reduced depending on the nature of organic matter coronas formed around the nanoparticles and the kinetics of oxidative dissolution are significantly altered. Further, ultraviolet light irradiation has been shown to act against the dissolution process leading to reduction of silver ions at the surfaces of the AgNPs. These results show the complex behaviour of AgNPs as they transition from riverine to coastal waters, with a concomittant impact on their potential toxicity to biota.

Keywords: nanoparticle, kinetics, oxidative dissolution, natural organic matter

Acknowledgement
This study was financially supported by the Croatian Science Foundation through grant *IP-2018-01-5351 NanoEMC2*.



UTJECAJ INERTNOG ELEKTROLITA NA OKSIDO-REDUKCIJSKA SVOJSTVA KOMPLEKSA CINKA SA HIDRAZIDNIM DERIVATOM DIPIKOLINSKE KISELINE

THE EFFECT OF INERT ELECTROLYTE ON OXIDO-REDUCTION PROPERTIES OF ZINC COMPLEX WITH DIPICOLINIC ACID HYDRAZIDE DERIVATIVE

Klara Iličić, Tatjana Šafarik, Ivana Balić, Tomislav Balić, Martina Medvidović-Kosanović

Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8A, 31 000 Osijek, Croatia

Hydrazide derivatives of dipicolinic acid contain a large number of potential donor atoms which are capable of coordinating to the metal center in diverse arrangements [1]. Previous studies have shown that Zn dipicolinic acid complexes exhibit effective insulin-mimetic activity [2]. The main goal of this study was to examine the effect of three different inert electrolytes (LiCl, KNO_3 and KCl) on the oxido-reduction properties of zinc complex with dipicolinic acid hydrazide derivative (Zn_2L_2), with two voltammetric techniques (cyclic and differential pulse voltammetry). The measurements were performed using the three electrode system which included a working glassy carbon electrode, counter electrode platinum wire and Ag/AgCl reference electrode. Before each measurement, the surface of the working electrode was polished with α-Al_2O_3 suspension. The system was purged with high purity argon Ar 5 (φAr = 99.999 %) to accomplish the inert atmosphere.
Cyclic voltammograms of the studied zinc complex showed one oxidation peak in all three investigated electrolytes indicating an irreversible oxidation process as shown in graphical abstract. The oxidation peak current increased with the increase of scan rate and the highest oxidation peak current was observed for KCl. Differential pulse voltammograms also revealed one oxidation peak, in all three electrolytes. The oxidation peak decreased with successive scans, which confirmes adsorption of the zinc complex oxidation product on the surface of the glassy carbon electrode.

Keywords: inert electrolyte, voltammetry, metal complexes

[1] R. A. Al-Salahi *et al*., *Molecules* 15 (2010) 6588.
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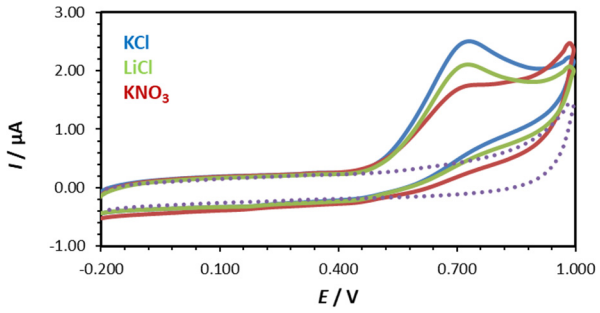


EKSTRAKCIJA I RAZDVAJANJE POLIFENOLNIH SKUPINA BOBICA ARONIJE I BAZGE

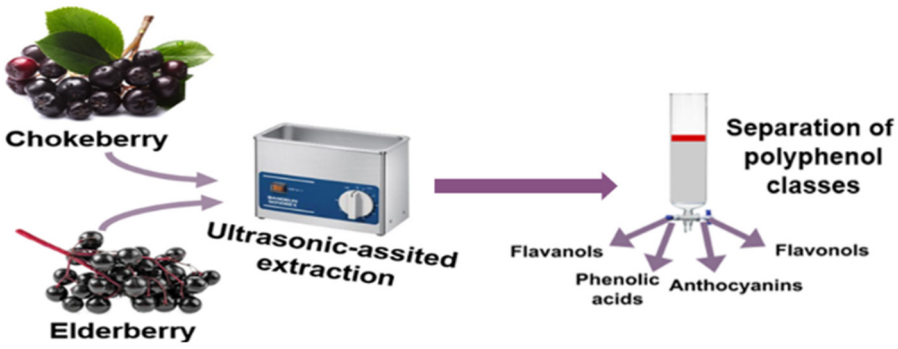
EXTRACTION AND SEPARATION OF POLYPHENOL CLASSES IN CHOKEBERRY AND ELDERBERRY FRUIT

Jozo Ištuk, Lidija Jakobek, Ivica Strelec

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Chokeberry (*Aronia melanocarpa*) and elderberry *(Sambucus nigra L.*) fruits are one of the richest dietary sources of polyphenols, a natural bioactive compounds. Anthocyanins are the most prevalent polyphenols in these fruits although other classes such as phenolic acids, flavonols, and flavanols are present as well. Those phenolic subgroups can show different bioactivities. That is why it can often be apropriate to examine bioactivities of these subgroups separately. The aim of this study was to to extract and determine polyphenols from chokeberry and elderberry and to separate polyphenol subgroups present in the extracts. The extraction was conducted using 80 % methanol as a solvent with the help of ultrasonic bath, and repeating the extraction step four times. Polyphenol subgroups found in extracts were separated using gel chromatography fractionation with Sephadex LH-20 as a stationary phase and different percentages of methanol in water as a mobile phase. Polyphenols in extracts and fractions were analysed using reversed-phase high performance liquid chromatography (RP-HPLC). The amount of polyphenols extracted from chokeberries and elderberries was 15557 and 10009 mg kg^{-1} of fresh fruit weight, respectively. Four fractions were separated for each fruit. Flavanols were eluted in fraction 1 (100 % and 100 %) and phenolic acids in fraction 2 (100 % and 100 %), anthocyanins were dominant in fraction 3 (91 % and 55 %), while flavonols were prevalent in fraction 4 (53 % and 100 %) for chokeberry and elderberry, respectively. Using gel-chromatography fractionation, four fractions containg different polyphenol subgroups were seeparated which could be useful in further research.

Keywords: berries, polyphenols, extraction, separation



SINTEZA I KARAKTERIZACIJA NANOČESTICA BAKRA STABILIZIRANIH PREVLAKOM METALNOG SREBRA

SYNTHESIS AND CHARACTERIZATION OF SILVER-PROTECTED COPPER NANOPARTICLES

Irena Ivanišević, Stjepan Milardović

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

Recently, copper nanoparticles (CuNPs) have attracted wide attention in printing conductive features for application in printed electronics, due to low price of copper precursor material, together with its high conductivity [1] A major problem in utilizing CuNPs is their instabillity in air and aqueous solutions, therefore, coating the nanoparticles by a proper protective layer is of outmost importance [2].
This study reports the aqueous synthesis of copper core – silver shell nanoparticles. Process was conducted in reduction atmosphere, with addition of poly(acrylic acid) (PAA) as a nanograin stabilizer, nanosilver material for reduction kinetics improvement, and silver(I) nitrate for transmetalation reaction. Characterization of the polymer- and silver-protected nanocopper suspension was performed using cyclic voltammetry (CV) and ultraviolet-visible (UV-Vis) measurements.
In alkaline media (ammonium buffer solution, pH = 10.10), addition of Cu(II) and Ag(I) results in ammine-complex formation, which is easily detected by glassy carbon electrode. The increment of anodic current response regarding Cu(II)-complex species with addition of silver(I) salt confirmed transmetalation reaction. Furthermore, absorption maximum of pure CuNPs (λ = 590 nm) has been shifted towards lower values (λ = 418 nm), which is in agreement with silver shell formation. By this method, the obtained bimetallic particles have optical and electric properties of both metals, while the oxidation of the copper core is prevented.

Keywords: copper nanoparticles synthesis, transmetalation reaction, UV-Vis spectroscopy, cyclic voltammetry.

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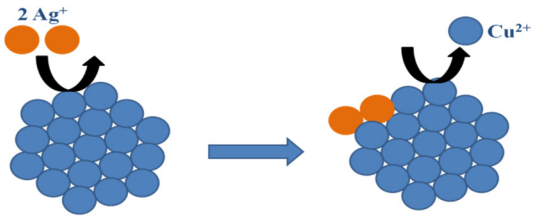
[2] M. Grouchko *et al*., *J Mater Chem* 19 (2009) 3057.



MIKROČIP KAPILARNA ELEKTROFORETSKA ANALIZA β-ALANINA i L-HISTIDINA S C^4D DETEKTOROM

MICROCHIP CAPILLARY ELECTROPHORETIC ANALYSIS OF β-ALANINE AND L-HISTIDINE WITH C^4D DETECTOR

Marija Jakić[1], Nikola Sakač[2], Brunislav Matasović[1], Marija Jozanović[1]

[1]*Department of Chemistry, J. J, Strossmayer University of Osijek, Cara Hadrijana 8, 31 000 Osijek, Croatia*
[2]*Faculty of Geotechnical Engineering, University of Zagreb, Hallerova 7, 42 000 Varaždin, Croatia*

β-Alanine and L-histidine supplementation results in elevated intramuscular carnosine content, enhancing human physical performance [1]. Thus, aforementioned amino acids are important constituent of animal feeds used in production of functional food with elevated levels of carnosine and also in various preworkout supplements. Therefore, it is necessary to develop fast and reliable analytical methods for the detection of these amino acids. Microchip capillary electrophoresis (MCE) using capacitively coupled contactless conductivity detector (C^4D) in various acidic electrophoretic buffers provides high resolution and short separation time for quantitative determination of β-alanine and L-histidine. The influence of the injection and separation parameters on the separation ability was investigated. The electrophoretic buffer composition were thoroughly studied in order to optimize the separation. The linear response region for each particular amino acid investigated, both single and in a mixture, was determined using linear regression. Detection limits for β-alanine and L-histidine were below 1 mg mL^{-1}.

Keywords: amino acids, β-alanine, C^4D detector, L-histidine, microchip capillary electrophoresis

[1] R. Hannah *et al*., *J Appl Physiol* 118 (2015) 604.

RAZVOJ I VALIDACIJA SFC METODE ZA ODREĐIVANJE ONEČIŠĆENJA U ELVITEGRAVIRU

DEVELOPMENT AND VALIDATION OF SFC METHOD FOR DETERMINATION OF IMPURITIES IN ELVITEGRAVIR

Zlata Lasić[1], Irena Radić[1], Antonija Radić[1], Asja Čulina[1], Nives Galić[2]

[1]*Pliva Croatia Ltd., Prilaz Baruna Filipovića 25, 10 000 Zagreb, Croatia*
[2]*Faculty of Science, University of Zagreb, Horvatovac 102a, 10 000 Zagreb, Croatia*

Elvitegravir (ELV) is a novel class of anti-retroviral agents, belongs to integrase strand transferase inhibitor, inhibits the integrase enzyme and prevents the virus replication [1]. In combination with other drugs, ELV is used to treat human immunodeficiency virus (HIV). The chemical name of ELV is 6(3-chloro-2-fluorobenzyl)-1-[(2*S*)-1-hydroxy-3-methylbutane-2-yl]-7-methoxy-4-oxo-1,4-dihydroquinoline-3-carboxylic acid.
Analytical method represents a critical lifecycle parameter of a pharmaceutical product due to their role in the early phase of the product development as well as their key role in the finished product quality control. In this study, a fast and efficient supercritical fluid chromatography (SFC) method for the analysis of impurities in ELV has been developed by using a diode array detector. The developed method was validated by determining the following validation parameters: specificity, limit of quantification, precision, linearity and accuracy [2, 3].

Keywords: Elvitegravir, SFC, impurities, validation

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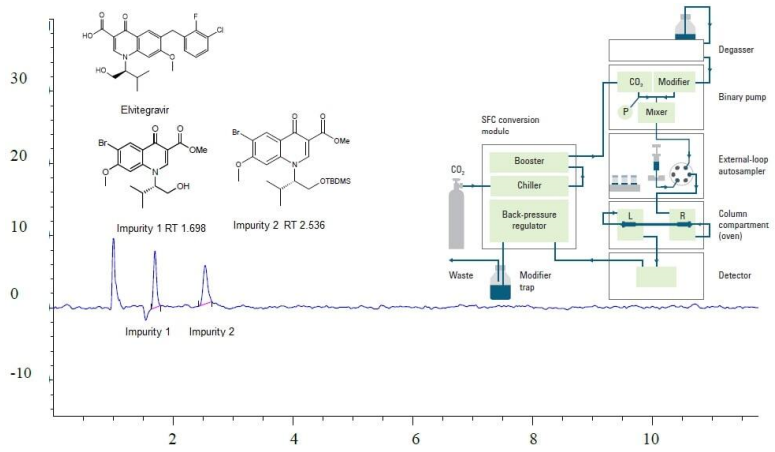

EUTEKTIČKA OTAPALA NA BAZI KOLIN-KLORIDA KAO PRIKLADAN ZELENI MEDIJ ZA SINTEZU KUMARINSKIH SCHIFFOVIH BAZA

CHOLINE CHLORIDE BASED DEEP EUTECTIC SOLVENTS AS SUITABLE GREEN MEDIA FOR SYNTHESIS OF COUMARINYL SCHIFF BASES

Mirjana Lončar, Melita Lončarić, Mario Komar, Maja Molnar

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Coumarin and its derivatives as highly bioactive heterocycles possess a wide range of biological, pharmacological, biochemical and therapeutic properties, which are strongly structure dependent. Schiff bases bearing coumarin moiety in conjunction with imino group (-C=N-), form a significant compounds in medicinal and pharmaceutical chemistry [1].
Deep eutectic solvents (DESs) have proven to be a suitable media for many synthetic pathways. DESs are often described as green mixtures, whose properties can be adjusted for various applications using different molar ratios of initial components [2].
The aim of this study was to synthesize coumarinyl Schiff bases utilizing ChCl-based DES as a reaction media and a catalyst, as well. Hereby, we applied an environmentally friendly approach, utilizing a solvent made of biodegradable components, with low toxicity and vapor pressure, which can be easily recycled and reused [3]. DESs are proven the excellent media for all these reactions, while the isolation of the final product was easy, and included the addition of water and filtration.

Keywords: deep eutectic solvents, coumarin, Schiff base

[1] M. Molnar *et al*., *Der Pharma Chem* 6 (2014) 313.
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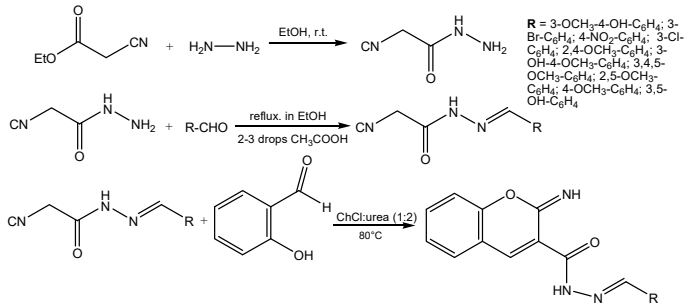
Acknowledgments
This study was financially supported by the Croatian Science Foundation through grant *UIP-2017-05-6593*.



SINTEZA NOVIH *N*-HETEROCIKLIČKIH DERIVATA 1,1'-DISUPSTITUIRANIH FEROCENA PRIMJENOM MEHANOKEMIJE I EUTEKTIČKIH OTAPALA

SYNTHESIS OF NEW *N*-HETEROCYCLE 1,1'-DISUBSTITUTED FERROCENE CONJUGATES USING MECHANOCHEMISTRY AND DEEP EUTECTIC SOLVENTS

Silvija Maračić[1], Martina Piškor[1], Ivona Čipor[1], Jasmina Lapić[2], Senka Djaković[2], Silvana Raić-Malić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*

In recent years, medicinal chemistry has faced a significant evolution in both approaches and methodologies because of the advent of new and innovative technologies. In this context, mechanochemistry does not only provide an access to reactivity of materials that are difficult or even impossible to reach from solution, but fulfils the demands of pharmaceutical industry for greener and more efficient alternative to a majority of conventional transformations [1, 2]. On the other hand, the use of deep eutectic solvents (DESs), as alternative environmentally benign solvents for organic synthesis, have found increased attention because of their high thermal stability, non-flammability and practically no vapour pressure [3]. Novel conjugates of purine, purine bioisosteres and 1,1'-disubstituted ferrocenes were synthesized using Cu(I) catalysed 1,3-dipolar cycloaddition reaction in sorbitol/urea/NH_4Cl deutectic mixture, while 1,1'-disubstituted ferrocene quinoline derivatives bridged *via* 1,2,3-triazole unit were prepared under solvent-free mechanochemical conditions.

Keywords: ferrocene, 1,2,3-triazole, mechanochemistry, deep eutectic solvents

[1] D. Tan *et al*., *Chem Commun* 52 (2016) 7760.
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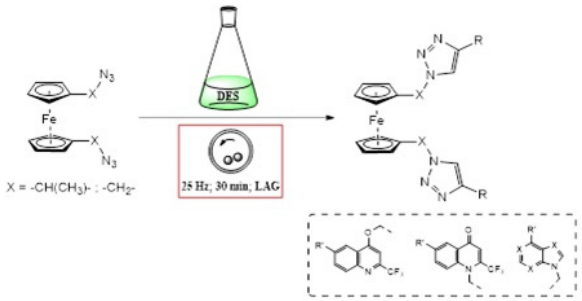

HLAPLJIVI SPOJEVI LISTA KOPRIVE

VOLATILE COMPOUNDS OF NETTLE LEAVES

Zvonimir Marijanović[1], Ani Radonić[1], Mladenka Šarolić[2], Verica Dragović-Uzelac[3], Maja Repajić[3], Ivana Gobin[4]

[1]*Kemijsko-tehnološki fakultet, Sveučilište u Splitu, Ruđera Boškovića 35, 21 000 Split, Hrvatska*
[2]*Veleučilište „Marko Marulić" u Kninu, Petra Krešimira IV. 30, 22 300 Knin, Hrvatska*
[3]*Prehrambeno-biotehnološki fakultet, Sveučilište u Zagrebu, Pierottijeva ul. 6, 10 000, Zagreb, Hrvatska*
[4]*Medicinski fakultet, Sveučilište u Rijeci, Braće Branchetta 20, 51 000, Rijeka, Hrvatska*

Kemijski sastav hlapljivih spojeva lista koprive ovisi o nekoliko faktora, kao što su: sorta, sezona, stanje lišća, geografski i klimatski uvjeti. U ovom radu analiziran je kemijski profil hlapljivih spojeva tri komercijalna uzorka suhog lista koprive. Analiza je provedena mikroekstrakcijom vršnih para na krutoj fazi (HS-SPME) koristeći vlakno s prevlakom DVB/CAR/PDMS (divinilbenzen/karboksen/polidimetilsiloksan, 50-30 μm). Ukupno je identificirano 38 spojeva, od čega u prvom uzorku 26, u drugom 20 i u trećem 22 spoja. Glavni spojevi vršnih para izolirani HS-SPME metodom s DVB/CAR/PDMS prevlakom bili su: *trans*-anetol (25,66-52,55 %), *trans-β*-kariofilen (2,41-13,37 %), limonen (0,81-12,92 %), karvon (1,28-10,74 %), *α*-kopaen (1,05-6,37 %) i estragol (1,54-3,57 %). Općenito, isparljivi spojevi lista koprive prethodno su pokazali antioksidacijsko, antibakterijsko i antigljivično djelovanje koje može biti korisno za prehrambenu, farmaceutsku i kozmetičku industriju.

Ključne riječi: kopriva, list, HS-SPME, GC-MS, hlapljivi spojevi

Zahvala
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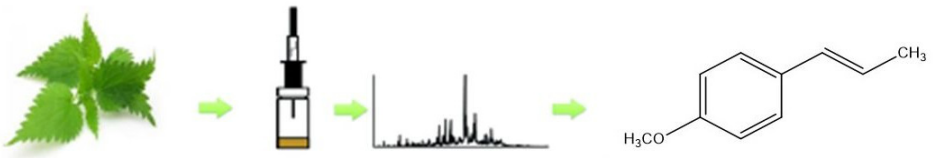

trans-anetol

International Conference *18th Ružička days*
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UČINKOVITA PET STUPANJSKA SINTEZA BIOLOŠKI AKTIVNIH KARBAMATA

EFFICIENT FIVE-STEP SYNTHETIC PATHWAY TOWARD BIOLOGICALLY ACTIVE CARBAMATES

Ana Matošević[1], Anamarija Knežević[2], Anita Bosak[1]

[1]*Institute for Medical Research and Occupational Health, Ksaverska cesta 2, 10 000 Zagreb, Croatia*
[2]*Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia*

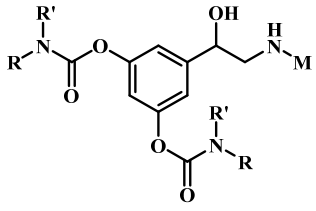
Compounds containing a carbamate group have found their application in various fields; they are valuable intermediates and protecting groups for amines in organic synthesis, linkers in combinatorial chemistry, and biologically active compounds such as insecticides or drugs and prodrugs. The use of carbamates as drugs has attracted much attention since some recent studies have shown that the incorporation of a carbamate group into the structure of biologically active compounds could lead to an improvement of their biological activity. More precisely, compounds bearing a carbamate group are characterized by conformational and metabolic stability, the ability to pass through cell membranes, and for some carbamates through the blood-brain barrier, which has led to the fact that carbamate groups have become a desirable part of the structure of many pharmacologically important compounds. Therefore, in recent years considerable efforts have been invested in the design of biologically active carbamate derivates as well as in the development of efficient methodologies for the synthesis of new carbamates.

Our goal was to prepare a series of aromatic amino alcohols with carbamate moiety on the phenyl ring with varying carbamate moieties, as well as a varying amine group. We have applied a five-step synthetic pathway for the preparation of these biologically active carbamates starting from 3,5-dihidoxyacetophenone.

We successfully synthesized 27 carbamates with an alkyl chain of different size (diethyl, ethyl/methyl or 1- pyrrolidine) on the nitrogen atom of a carbamate group, and a different amine moieties (aniline, piperidine, *p*-toluidine, cyclohexylamine, *tert*-amylamine, 1-adamantylamine, *tert*-butylamine, 2-phenylethylamine, 1-phenylethylamine). For all of the synthesized carbamates, the cholinesterase inhibition potency will be determined as a key feature of drugs for treating Alzheimer's disease.

Keywords: synthesis, carbamates, cholinesterases

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *IP-01-2018-7683*.



R, R` = diethyl, ethyl/methyl or 1- pyrrolidine
M= aniline, piperidine, *p*- toluidine, cyclohexylamine, *tert*-amylmine, 1-adamntylamine, *tert*-butylamine, 2- phenylethylamine, 1- phenylethylamine

MOLEKULSKI TISKANI POLIMERI ZA ODREĐIVANJE GALNE KISELINE

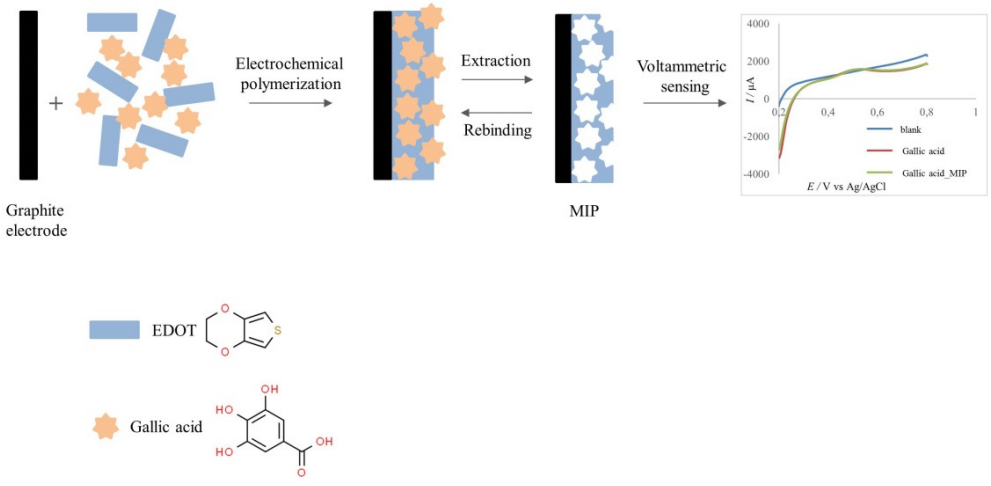
MOLECULARLY IMPRINTED POLYMERS FOR DETERMINATION OF GALLIC ACID

Filipa Mrčela[1], Ivana Smoljko[1], Rolando C. S. Dias[2], Catarina Gomes[2]

[1]Faculty of Chemistry and Technology, University of Split,
Ruđera Boškovića 35, 21 000 Split, Croatia
[2]LSRE-Instituto Politécnico de Bragança, Quinta de Santa Apolónia,
5 300 Bragança, Portugal

Molecularly imprinted polymers (MIP) are synthetic polymers with specific recognition for targeted molecules. Herein, a facile and efficient approach is presented for the preparation of MIP capable of recognizing polyphenol, i.e. gallic acid in aqueous system. Gallic acid (3,4,5 trihydroxybenzoic acid) is a secondary metabolite present in most plants and it was selected as a template due to its range of bioactivities including antioxidant, antimicrobial, anti-inflammatory, and anticancer. In this paper, MIP was prepared by electrochemical polymerization of 3,4-ethylenedioxythiophene (EDOT) monomer on graphite electrode templated with gallic acid by multiple scan cyclic voltammetry. The surface feature of the prepared MIP was characterized by cyclic voltammetry and linear sweep voltammetry. All results indicated that the prepared imprinted electrode with high affinity and stereo-selectivity toward gallic acid in the solution might offer a method for determination of gallic acid in the natural extracts.

Keywords: gallic acid, molecular imprinting, cyclic voltammetry, linear sweep voltammetry

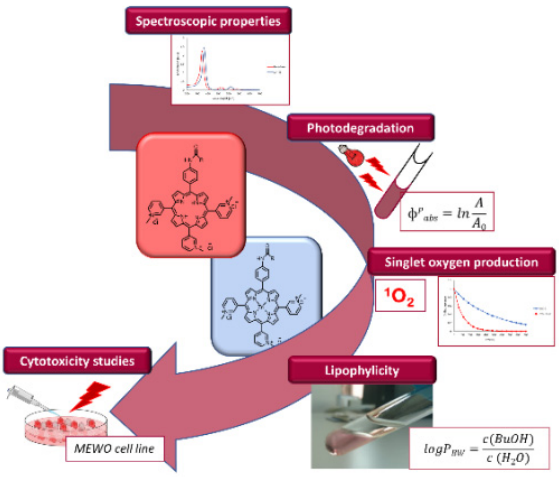


FOTODINAMIČKI POTENCIJAL AMFIFILNIH Zn(II) TRIPIRIDILPORFIRINA I NJIHOVIH ANALOGA SLOBODNE BAZE

PDT POTENTIAL OF AMPHIPHILIC FREE-BASE AND Zn(II) TRIPYRIDYLPORPHYRINS

Martina Mušković, Ivana Ratkaj, Nela Malatesti

Department of Biotechnology, University of Rijeka,
Radmile Matejčić 2, 51 000 Rijeka, Croatia



Photodynamic therapy (PDT) is a treatment modality used for malignant diseases where the combination of light, photosensitizer (PS) and molecular oxygen produces reactive oxygen species (ROS), which leads to cytotoxic effect and tumour destruction [1].
Characteristics of a good PS include good absorption of light in the red region of the spectrum, stability, negligible dark toxicity, and good production of singlet oxygen [1]. Increased production of singlet oxygen can be achieved by chelation with paramagnetic metals, such as zinc(II), since they increase the lifetime of the PS's triplet state (^{3}PS*)[2].
Lipophilicity also plays an important role in effectiveness of a PS in PDT. Hydrophobic moieties in PS facilitate passing through the membrane lipid bilayer, however, they reduce solubility in water and tend to aggregate. Hydrophilic moieties, on the other side, impair membrane penetration and cell internalization [3].
In this work, we investigate free-base, and Zn(II) chelated, amphiphilic tripyridylporphyrins, conjugated with chains of various length. Physiochemical properties of the prepared porphyrins will be analysed and compared. The relationship between these properties and PDT activity of the compounds will be shown using cytotoxicity test.

Keywords: amphiphilic porphyrins, cytotoxicity, lipophilicity, singlet oxygen production, Zn(II) chelation

[1] L. B. Josefsen *et al*., *Met-Based Drugs* 2008 (2008) 276109.
[2] L. Benov *et al*., *Anticancer Agents Med Chem* 2011 (11) 233.
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SINTEZA I STRUKTURNA KARAKTERIZACIJA NOVIH 1,2,3-TRIAZOLNIH DERIVATA BENZOKSAZOLA

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF NOVEL 1,2,3- TRIAZOLE DERIVATIVES OF BENZOXAZOLE

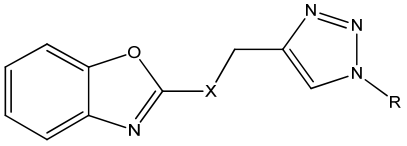
Robert Ostrički[1], Tatjana Gazivoda Kraljević[2]

[1]Pliva Hrvatska d.o.o., Prilaz baruna Filipovića 25, 10 000 Zagreb, Croatia
[2]Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

A great number of deaths are occurring throughout the world because of infectious diseases which are now hard to treat with traditional antibiotic drugs and clinicians have to depend on limited drugs such as vancomycin. Because of that there is an increased demand to develop newer antimicrobial agents. Benzoxazoles are structural isosters of natural nucleotides which interact easily with biopolymers, and represent an important class of heterocyclic compounds exhibiting remarkable pharmacological activities such as antibacterial, antifungal, anticancer, antiviral, anti-inflammatory, antimycobacterial and antihistaminic. Besides, some of them have found applications as fluorescent whitening agents and functional materials. Furthermore, a number of available marketed drugs posses benzoxazole ring, *i.e.* nonsteroidal anti-inflammatory drug (NSAID)-flunoxaprofen, benoxaprofen and antibiotic-calcimycin, roxazone. Benzoxazole moieties also act as tyrosinase inhibitor and cholesterol ester transfer protein inhibitor [1-3].
In order to evaluate i*n vitro* antimicrobial activity against Gram-positive and Gram-negative bacteria the novel derivatives with benzoxazole as a privileged scaffold have been synthesized by conventional and modern green synthetic methods. Benzoxazole derivatives with 1,2,3-triazole ring were performed by Cu(I) catalysed click reaction. The structures of synthesized benzoxazole derivatives were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry as well.

Keywords: benzoxazole, 1,2,3-triazole, green chemistry, click reaction

[1] S. Kakkar *et al*., *Chem C J* 12 (2018) 92.
[2] R. Sattar *et al*., *J Het Chem* 57 (2020) 2079.
[3] M. Kale *et al*., *Mini-Rev Org Chem* 16 (2019) 111.



R: alkyl, aryl
X: NH, S

IONSKO-SELEKTIVNE ELEKTRODE ZA ODREĐIVANJE ŽELJEZOVIH(III) KATIONA

ION-SELECTIVE ELECTRODES FOR FERRIC(III) CATIONS DETERMINATION

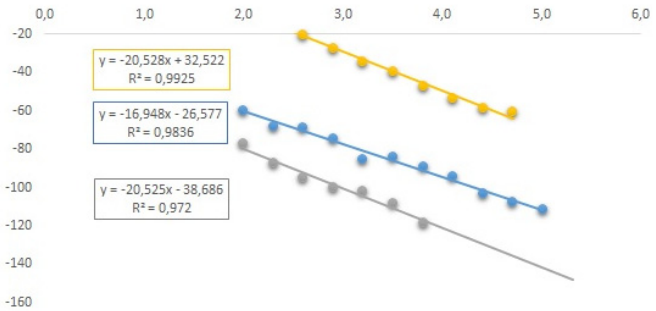
Andrea Paut[1], Ante Prkić[1], Ivana Mitar[2], Josipa Giljanović[1], Lucija Gućˇ[1]

[1]Kemijsko-tehnološki fakultet, Sveučilište u Splitu,
Ulica Ruđera Boškovića 35, 21 000 Split, Hrvatska
[2]Prirodoslovno-matematički fakultet, Sveučilište u Splitu,
Ulica Ruđera Boškovića 33, 21 000 Split, Hrvatska

Ionsko-selektivne membrane u svrhu potenciometrijskog određivanja koncentracije željezovih(III) kationa u otopinama, sastavljene su od laboratorijski pripravljenih taloga željezovog(III) fosfata i srebrovog sulfida uz dodatak komercijalnog politetrafluoretilena (PTFE). S obzirom da je senzor (M1) sastava $FePO_4$: Ag_2S : PTFE = 1:1:2 prilikom testiranja u laboratorijski pripremljenoj otopini željezovih(III) kationa prema istima pokazao promjenu potencijala u ovisnosti o promjeni koncentracije Fe^{3+} kationa u skladu sa zahtjevima Nernstove jednadžbe, membrana je zatim primijenjena za određivanje Fe^{3+} kationa u otopinama realnih uzoraka lijekova koji se koriste za nadomještanje manjka koncentracije željeza u krvi.
Predložena metoda određivanja željeza validirana je usporedbom rezultata s rezultatima predočenim na deklaraciji samog lijeka te određivanjem nasumično pripremljene koncentracije željezovih(III) kationa u laboratorijski pripremljenoj otopini. Tako je mikrovalnom digestijom jedne tablete farmaceutika potenciometrijski potvrđena koncentracija u iznosu od $1{,}8 \cdot 10^{-3}$ molL^{-1} dok je deklaracijom istaknuto $2{,}5 \cdot 10^{-3}$ molL^{-1} Fe^{3+} kationa pri pH vrijednosti 1. S druge strane, određivanjem koncentracije Fe^{3+} kationa u laboratorijski pripravljenoj otopini, potvrđena je očekivana koncentracija i to uz podudarnost od 100%. Sve navedeno ukazuje kako su ovdje prikazani laboratorijski pripravljeni senzori pogodni za određivanje Fe^{3+} kationa u realnim uzorcima [1] [2].

Ključne riječi: ionsko-selektivne elektrode, potenciometrija

[1] M. Bralić, A. Prkić, J. Radić, I. Pleslić, *Int J Electrochem Sci* 13 (2018) 1390-1399.
[2] A. Prkić, T. Vukušić, I. Mitar, J. Giljanović, V. Sokol, P. Bošković, M. Jakić, A. Sedlar, *Int J Electrochem Sci* 14 (2019) 861-874.



SINTEZA I SPEKTROSKOPSKA KARAKTERIZACIJA NOVIH 1,2,3-TRIAZOLIL-BENZTIAZOLA

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF NOVEL 1,2,3-TRIAZOLYL-BENZOTHIAZOLES

Kristina Pršir, Lidija Furač, Ivana Steinberg, Svjetlana Krištafor

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

Benzothiazole is an attractive building block in the design of novel fluorescent dyes because of its π-bridging and electron-withdrawing properties as well as high chemical and photophysical stability [1]. In addition, 1,2,3-triazoles have great potential in chemical sensing as they can act as a covalent linker between benzothiazole and corresponding functional group or can participate in binding of the target analyte [2]. In this work we present the synthesis of novel 1,2,3-triazolyl-benzothiazoles as potential chemosensing molecules for pH and/or heavy metal cations. To further investigate the use of fluorophores in the design of novel sensing materials, the most promising candidate was drop casted on paper strips and examined as pH probe as continuation of our ongoing research [3].

Keywords: benzothiazole, 1,2,3-triazole, fluorescent chemosensor

[1] M. S. Filho *et al*., *New J Chem* 41 (2017) 13760.
[2] Y. H. Lau *et al*., *Chem Soc Rev* 40 (2011) 2848.
[3] E. Horak *et al*., *Specrochim Acta A* 178 (2017) 225.

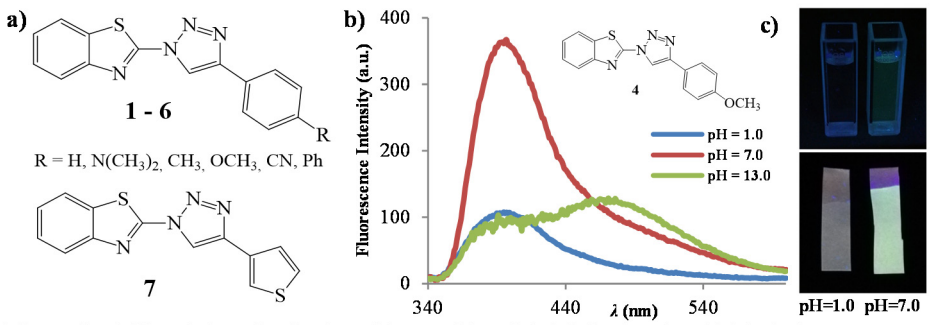


Figure 1. a) Novel 4-aryl-substituted benzothiazolyl-1,2,3-triazoles. b) Emission spectra of **4** in buffer solutions in different pH. c) Effect of pH on optical properties of **3**.

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INTERAKCIJE NOVIH AMIDINO-SUPSTITUIRANIH ARYL-BIS(BENZAZOLA) S DNA/RNA

INTERACTIONS OF NOVEL AMIDINO-SUBSTITUTED ARYL-BIS(BENZAZOLES) WITH DNA/RNA

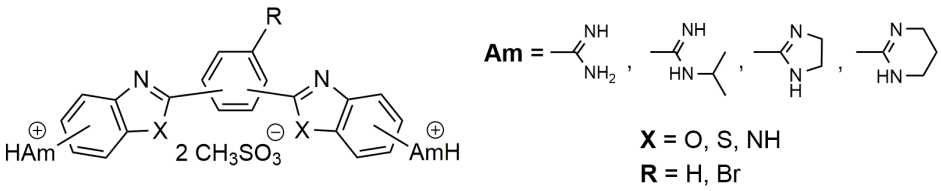
Lucija Ptiček[1], Livio Racané[1], Iva Zonjić[2],
Lidija-Marija Tumir[2], Marijana Radić Stojković[2]

[1]*Faculty of Textile Technology, University of Zagreb,*
Prilaz baruna Filipovića 28a, 10 000 Zagreb, Croatia
[2]*Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia*

Series of eleven novel amidino-substituted bis(benzazoles), differing in heteroaromatic scaffolds as well as in type and position of amidine moiety, were studied for their binding abilities for DNA and RNA. By introducing different types of amidinic substituents and heteroaromatic substructure, namely benzothiazole, benzimidazole and benzoxazole, presented compounds were synthesized by condensation reaction of amidino-substituted 2-aminothiophenols, 2-aminophenols or *o*-phenylenediamines with isomeric aromatic dialdehydes or dicarboxylic acids by our previously developed method [1, 2]. Noncovalent binding interactions with DNA and RNA like intercalation, groove and electrostatic binding can be investigated by variety of methods. In order to detect possible presence of DNA/RNA active compounds in extracts, we utilized the most common methods in DNA binding studies: CD spectroscopy and the thermal denaturation of polynucleotides. While the former method monitors the impact of studied compounds on CD spectra of polynucleotides, the latter provides the information about the polynucleotide stabilization driven by compounds (ΔT_m value). We used fluorimetry for the evaluation of the binding affinities. Competition dialysis experiment was used to probe the multitude of ligand-polynucleotide interactions. An array of different nucleic acid structures (single-stranded, double-stranded, DNA-RNA hybrid and triple helixes) were dialyzed against the compound solution for the assay. Dicationic compound 2-(2-(3-(6-carboximidamidiumbenzothiazole-2-yl)phenyl)-(benzothiazole-6-yl))-4,5-dihydro-1*H*-imidazolium was identified as the most interesting one, as it showed high selectivity combined with high affinity over a particular polynucleotide structure. This compound was selected for detailed analysis with hybrid structure poly dA – poly rU by aforementioned methods.

Keywords: amidines, benzazoles, interactions, DNA/RNA

[1] L. Racané *et al.*, *Bioorg Chem* 95 (2020) 103537.
[2] L. Racané *et al*., *Mol Divers* 22 (2018) 723.



RAZVOJ UHPLC METODE ZA ODREĐIVANJE PIMAVANSERINA I NJEGOVIH ONEČIŠĆENJA PRIMJENOM AQbD STRATEGIJE

DEVELOPMENT OF UHPLC METHOD FOR THE ANALYSIS OF PIMAVANSERIN AND ITS IMPURITIES USING AQbD PRINCIPLES

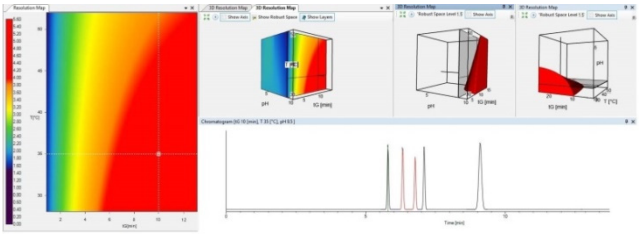
Irena Radić[1], Zlata Lasić[1], Mislav Runje[1], Sandra Babić[2]

[1]*Pliva Croatia Ltd., Prilaz Baruna Filipovića 25, 10 000 Zagreb, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*

Pimavanserin is chemically described as N-[(4-fluorophenyl)methyl]-N-(1-methyl-4-piperidinyl)-N'-[[4-(2-methylpropoxy)phenyl]methyl]-,(2R,3R)-2,3-dihydroxybutanedioate (2:1). It is an atypical antipsychotic that has been approved for the treatment of Parkinson's disease, and its use for the treatment of Alzheimer's disease, psychosis, schizophrenia and major depressive disorder is being investigated [1]. Analytical method represents a critical lifecycle parameter of a pharmaceutical product due to their role in the early phase of the product development. Traditional approach to method development based on varying one-factor-at-a-time (OFAT), especially from the industry point of view, is time-consuming and therefore extremely expensive process. In recent years, development of analytical methods is based on the principles of analytical quality by design (AQbD) as a part of a full risk assessment strategy. A reversed phase UHPLC method for determination of pimavanserin and its impurities was developed following AQbD principles [2]. The method was optimized using DryLab software modelling package and multivariate experiments. Multivariate analysis of critical method parameters (gradient time, pH, column temperature) was used to determine method operable design region (MODR). A robust final method was obtained with a column temperature 35 °C, eluent A pH 9.5 and gradient time *t*G 10 min. Optimal conditions were checked experimentally, and excellent agreement between modeled and experimental chromatograms was obtained.

Keywords: pimavanserin, AQbD, MODR, DryLab

[1] M. P. Cruz, *P&T* 42 (2017) 368.
[2] A. Dispas *et al*., *Trends Analyt Chem* 101 (2018) 24.



PRIMJENA EKSTRAKTA KOMINE MASLINE U BIOGENOJ SINTEZI NANOSELENA

APPLICATION OF OLIVE POMACE EXTRACT IN BIOGENIC SYNTHESIS OF SELENIUM NANOPARTICLES

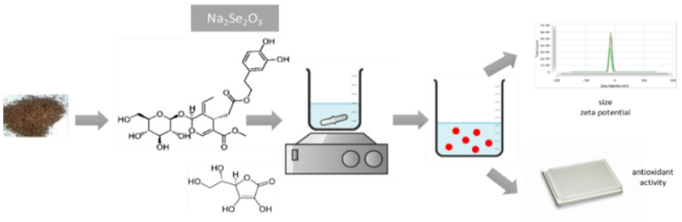
Kristina Radić[1], Dubravka Vitali Čepo[1], Nikolina Golub[1], Nikolina Kalčec[2], Emerik Galić[3], Ivana Vinković Vrček[2], Tomislav Vinković[3]

[1]*Faculty of Pharmacy and Biochemistry, University of Zagreb, Ante Kovačića 1, 10 000 Zagreb, Croatia*
[2]*Institute for Medical Research and Occupational Health, Ksaverska cesta 2, 10 000 Zagreb, Croatia*
[3]*Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia*

The application of olive pomace extract (OPE) was investigated for biogenic synthesis of selenium nanoparticles (SeNPs). The OPE was used at different amounts ranging from 0.3 % to 0.6 %. Obtained SeNPs were characterised in terms of size distribution by dynamic light scattering (DLS), surface charge as measured by ζ potential, antioxidant activity as determined by ORAC and TEAC method, and reductive capacity using Folin-Ciocalteu method. Characteristics of biogenically produced SeNPs were compared to those obtained by standard chemical synthesis using polyvinylpyrrolidone (PVP) as coating agent.
The application of 0.3 % OPE resulted in stable SeNPs dispersion of 100 nm particle size similar to PVP-coated SeNPs, while the increase in OPE amount in reaction mixture increased the mean particle size and led to polydisperse system. Surface charge of biologically synthesized SeNPs was more negative (-34 mV) compared to PVP-SeNPs (-17.2 mV) indicating better stability. Antioxidant and reductive efficacy of biologenically synthesized SeNPs was significantly higher than for SeNPs prepared by chemical synthesis.
Obtained results demonstrated advantages of using natural polyphenol rich plant extracts in preparation of stable SeNPs in terms of development of green synthesis processes and improved functional properties of obtained nanomaterials.

Keywords: olive pomace extract, selenium nanoparticles, biogenic synthesis, antioxidant activity

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *IP-2018-01-8119* and *PZS-2019-02-4323*.



NOVI 2-SUPSTITUIRANI DERIVATI BENZOTIAZOLA: SINTEZA I ANTIPROLIFERATIVNA ISPITIVANJA

NOVEL 2-SUBSTITUTED BENZOTHIAZOLES: SYNTHESIS AND ANTIPROLIFERATIVE EVALUATION

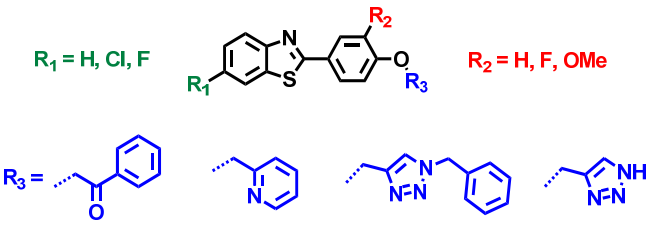
Valentina Rep[1], Ljubica Glavaš Obrovac[2], Marijana Jukić[2], Silvana Raić-Malić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Medicine Osijek, J. J. Strossmayer University of Osijek, Josipa Huttlera 4, 31 000 Osijek, Croatia*

The benzothiazoles (BTA) are constituents of bioactive heterocyclic compounds that exhibit wide spectrum of biological and pharmacological activities. Functionalization of the BTA scaffold at the C-2 and C-6 positions was found to be a key determinant for their enhanced biological activity, mainly as cytostatic and antimicrobial agents. 2-Arylbenzothiazoles have emerged as an important pharmacophore in the development of antitumor agents. Some BTA-based anticancer agents were found to target tyrosine kinase, topoisomerase, microtubule, cytochrome P450, heat shock protein 90 (Hsp90), epidermal growth factor receptor (EGFR) and apoptosis by reactive oxygen species (ROS) activation [1-3]. Herein, we have synthesized novel 6-substituted 2-arylbenzothiazole derivatives with varied aromatic unit at phenyl ring with the aim to assess their influence on antiproliferative activity. Key benzothiazole intermediates were obtained by condensation of 2-aminothiophenoles with corresponding benzaldehydes and then converted to propargylated derivatives and targeted 2-(4-alkoxyphenyl)benzothiazole derivatives (**26a-34a**, **26b-34b**) by an *O*-alkylation reaction. Finally 1,4-disubstituted 1,2,3-triazole benzothiazole analogues (**26c-34c**, **26d-34d**) were synthesized by copper catalysed reaction of the corresponding terminal alkynes and azides. Results of antiproliferative evaluations of compounds will be also presented.

Keywords: 2-substituted benzothiazoles, synthesis, antiproliferative activity

[1] A. Irfan, *et al*., *J Enzyme Inhib Med Chem* 35 (2020) 265.
[2] N. Pathak, *et al*., *Mini-Rev Med Chem* 20 (2020) 12.
[3] A. Kamal, *et al*., *Expert Opin Ther Patents* 25 (2014) 335.



PRIMJENA NOVIH KVATERNIH AMONIJEVIH SOLI ZA RAZVOJ TENZIDNIH SENZORA

APPLICATION OF NEW QUATERNARY AMMONIUM SALTS FOR DEVELOPMENT OF SURFACTANT SENSORS

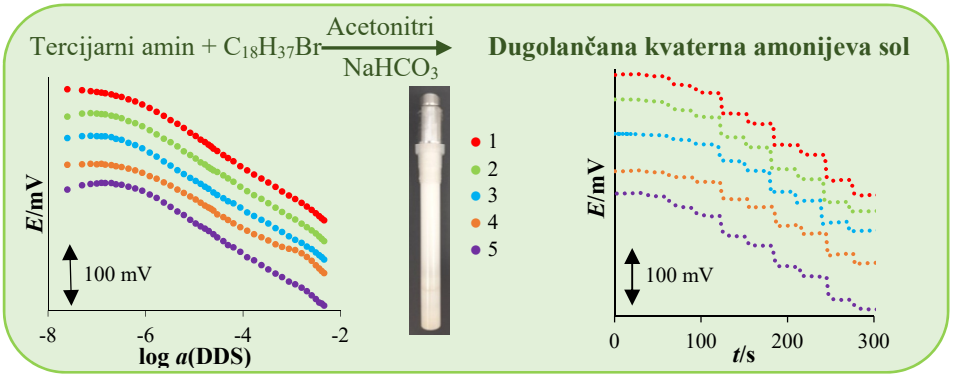
Mirela Samardžić[1], Mateja Budetić[1], Aleksandar Sečenji[1], Bojan Šarkanj[2], Dean Marković[3], Marija Jozanović[1]

[1]*Odjel za kemiju, Sveučilište J. J. Strossmayera u Osijeku, Cara Hadrijana 8/A, 31 000 Osijek, Hrvatska*
[2]*Odjel za prehrambenu tehnologiju, Sveučilište Sjever, Trg dr. Žarka Dolinara 1, 48 000 Koprivnica, Hrvatska*
[3]*Odjel za biotehnologiju, Sveučilište u Rijeci, Radmile Matejčić 2, 51 000 Rijeka, Hrvatska*

Anionski tenzidi (AS) su glavni sastojak deterdženata. Jedna od najjednostavnijih metoda za njihovo određivanje podrazumijeva korištenje ionsko-selektivnih elektroda kao potenciometrijskih senzora. Glavni dio membrane ionsko-selektivne elektrode, koji određuje njena svojstva, je ionofor [1].
Sintetizirano je i karakterizirano pet novih kvaternih amonijevih soli koje su formirale ionofore s tetrafenilboratom. Nastali ionofori korišteni su kao senzorski materijali pri razvoju pet novih potenciometrijskih senzora za određivanje AS. Ispitane su odzivne karakteristike svih pet senzora prema AS natrijevom dodecilsulfatu (DDS), pri čemu je najbolji senzor imao granicu detekcije $7{,}5\cdot10^{-8}$ mol dm^{-3}, mjerno područje od $1{,}5\cdot10^{-7}$ do $5{,}0\cdot10^{-3}$ mol dm^{-3}, nagib kalibracijskog pravca 58,5±0,5 mV/dekada aktiviteta i vrijeme odziva 8 s. Svih pet novorazvijenih senzora pokazali su veliku selektivnost za DDS te su korišteni pri određivanju AS u tri različita komercijalna proizvoda. Točnost i preciznost mjerenja ispitane su metodom standardnog dodatka pri čemu je iskorištenje za najbolji senzor iznosilo 99,3 do 101,9 %.

Ključne riječi: kvaterne amonijeve soli, anionski tenzidi, potenciometrijski senzor

[1] P. L. Padnya *et al.*, *Front Chem* 6 (2018) 594.



SINTEZA I ANTIBAKTERIJSKA AKTIVNOST NOVIH BENZOTIAZOLNIH DERIVATA

SYNTHESIS AND ANTIBACTERIAL ACTIVITY OF NOVEL BENZOTHIAZOLE DERIVATIVES

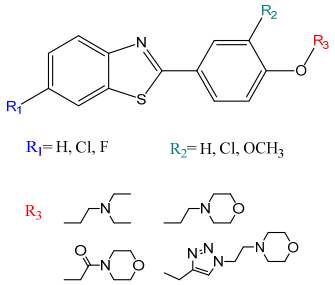
Ivana Sokol[1], Mateja Novak[1], Helena Prpić[1], Marijan Orlović[2], Domagoj Drenjančević[2], Silvana Raić-Malić[1], Tatjana Gazivoda Kraljević[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Medicine Osijek, J. J. Strossmayer University of Osijek, Josip Huttlera 4, 31 000 Osijek, Croatia*

Infectious diseases caused by bacteria affect millions of people and represent one of leading causes of death worldwide. On the other side, resistance of pathogenic bacteria to existing antibacterial drugs presents an additional problem. Therefore, the design of new compounds has become one of the most important areas of antibacterial research today.
Benzothiazole and their heterocyclic derivatives represent an important class of compounds possessing a wide spectrum of biological activities such as antitumor, antimicrobial, antidiabetic, anti-inflammatory, anticonvulsant, antiviral, antioxidant, antitubercular, antimalarial, photosensitizing, diuretic, analgesic and other activities [1, 2]. Furthermore, benzothiazole–1,2,3-triazole–coumarin hybrid showed anti-*Moraxella catarrhalis* potency (MIC $\leq$ 0.25 μg cm^{-3}) comparable to that of the reference antibiotic azithromycin [3].
In order to evaluate their antibacterial activity, the novel 2-aryl-benzothiazole derivatives have been synthesized. Of the all evaluated compounds against Gram-positive bacteria (*Staphylococcus aureus* and *Enterococcus faecalis*) and Gram-negative bacteria (*Klebsiella pneumoniae, Escherichia coli* and *Pseudomonas aeruginosa*) benzothiazole derivatives with *N,N*-diethylamine substituent showed the strongest activity against gram-negative clinical strains resistant to antibiotics compared to standard drug amikacin.

Keywords: benzothiazole, click reaction, 1,2,3-triazole, antibacterial activity

[1] F.L. Gouveia *et al*., *Eur J Med Chem* 44 (2009) 2038.
[2] R. S. Keri *et al*., *Eur. J Med Chem* 89 (2015) 207.
[3] S. Maračić *et al*., *Bioorg Med Chem* 23 (2015) 7448.



UTJECAJ VITAMINA C I KOMPLEKSNOSTI SUSTAVA NA TALOŽENJE KALCIJEVA OKSALATA

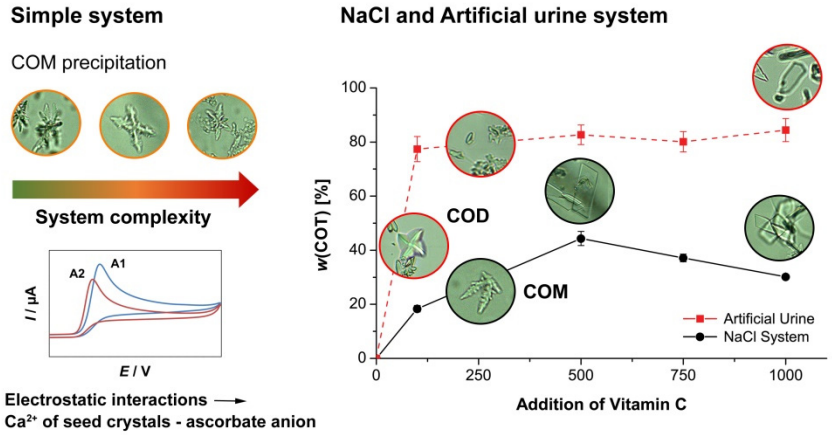
EFFECT OF VITAMIN C AND SYSTEM COMPLEXITY ON THE CALCIUM OXALATE PRECIPITATION

Anamarija Stanković[1], Silvija Šafranko[2], Katarina Jurišić[1], Ivana Balić[1], Jelena Bijelić[1], Stela Jokić[2], Martina Medvidović-Kosanović[1]

[1]*Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*

The formation of calcium oxalate, as major constituents of kidney stones, in three different precipitation systems under pathological conditions of hyperoxaluria have been extensively studied: (a) a simple system (a system containing constituent ions), (b) NaCl system (a system consisted of constituent ions and 0.3 mol dm^{-3} NaCl), and (c) artificial urine system (a system containing constituent ions that are of the type and quantity mimicking real urine) at initial pH (pH_i = 6.5) value, with and without added vitamin C. The vitamin C has been chosen for its ability to inhibit or promote the process of calcium oxalate precipitation, hence different amounts of vitamin C (in the mass range from 100 to 1000 mg) were added to the precipitation systems. Significant differences are mainly observed in crystal morphology and the content of individual hydrate phases. Electrochemical measurements have indicated the existence of electrostatic interactions between seed crystals and ascorbic acid, even at low masses of added vitamin C.

Keywords: calcium oxalate precipitation, vitamin C, electrochemical characterization



ODREĐIVANJE NIKLA U NODULARNOM LIJEVU PRIMJENOM RAZLIČITIH SPEKTROMETRIJSKIH METODA

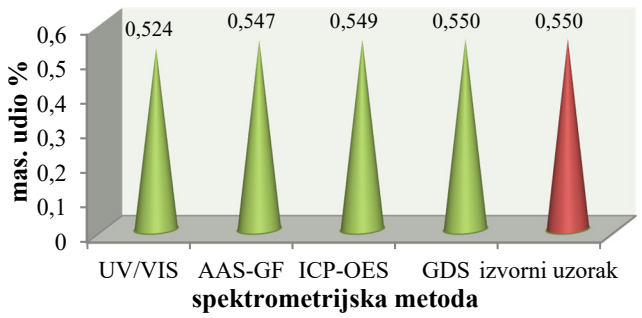
DETERMINATION OF NICKEL IN THE DUCTILE IRON USING DIFFERENT SPECTROMETRIC METHODS

Anita Štrkalj, Zoran Glavaš, Martin Pejaković

Metalurški fakultet, Sveučilište u Zagrebu, Aleja narodnih heroja 3, 44 000 Sisak, Hrvatska

Nodularni lijev pripada skupini željeznih ljevova u kojima je ugljik izlučen u obliku grafita. Grafitne čestice u nodularnom lijevu imaju kuglast, odnosno nodularan oblik, što mu daje specifična svojstva u odnosu na ostale željezne ljevove s grafitom. Budući da je primjena nodularnog lijeva raznovrsna i česta, postavljaju se veliki zahtjevi pri samoj proizvodnji kako bi se dobili gotovi proizvodi (odljevci) što boljih svojstava i kvalitete. Njihova svojstva prvenstveno ovise o njihovoj mikrostrukturi. Vrlo male promjene udjela pojedinih kemijskih elemenata mogu znatno utjecati na promjenu strukture metalne osnove, oblika i broja grafitnih čestica, tj. mikrostrukturu, što u konačnici rezultira promjenom svojstava odljevaka od nodularnog lijeva. Stoga je određivanje udjela pojedinih elemenata u postojećim, ali i prilikom istraživanja novih vrsta (kvaliteta) nodularnih ljevova izuzetno važna.
U ovom radu uspoređivano je nekoliko spektrometrijskih metoda (UV/VIS spektrometrija, atomska apsorpcijska spektrometrija s grafitnom tehnikom (AAS-GF), spektrometrija s induktivno spregnutom plazmom (ICP-OES) i spektrometrija s tinjajućim izbojem (GDS)) s ciljem pronalaska metode koja najbolje odgovara za određivanje udjela nikla u nodularnom lijevu. Dobiveni rezultati pokazali su da se najbolji rezultat analize postiže spektrometrijskom metodom s tinjajućim izbojem (GDS), koja je ujedno i najpogodnija za praktičnu primjenu u ljevaonicama. Nakon toga slijede ICP-OES, AAS-GF te UV/VIS. Te metode, za razliku od spektrometrije s tinjajućim izbojem (GDS), zahtijevaju specifičnu pripremu uzoraka prije same analize (usitnjavanje i otapanje). Stoga rezultati dobiveni tim metodama ne ovise samo o osjetljivosti pojedine metode već i o pripremi uzoraka za analizu.

Ključne riječi: nodularni lijev, spektrometrijske metode, nikal



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UTJECAJ REAKCIJSKIH PARAMETARA NA SINTEZU PROPILNIH ESTERA MASNIH KISELINA

INFLUENCE OF REACTION PARAMETERS ON THE SYNTHESIS OF PROPYL ESTERS OF FATTY ACIDS

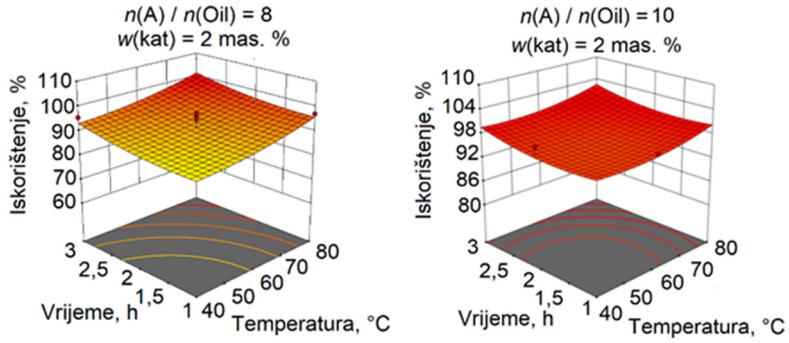
Matea Šibalić[1], Fabio Faraguna[1], Marko Racar[1],
Lucija Konjević[2], Jelena Parlov Vuković[2]

[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,*
Marulićev trg 19, 10 000 Zagreb, Hrvatska
[2]*Industrija nafte d.d., Razvoj rafinerija i marketinga, Centralni ispitni laboratorij,*
Lovinčićeva ul. 4, 10 000 Zagreb, Hrvatska

Propanol se najčešće koristi kao otapalo u farmaceutskoj i kozmetičkoj industriji te kao antiseptik u medicini. Može se također koristiti izravno kao gorivo jer posjeduje visoki oktanski broj [1]. Biopropanol se može proizvesti iz biomase te u tom području prednjače tehnologije sinteze iz sinteznog plina [2]. Proizvodnjom biodizela iz biopropanola dobiva se gorivo koje je u potpunosti proizvedeno iz obnovljivih sirovina. U ovom istraživanju ispitan je utjecaj reakcijskih parametara na iskorištenje reakcije između propanola i suncokretovog ulja, uz KOH kao katalizator. Ispitana su četiri parametra: temperatura reakcije, vrijeme provedbe reakcije, maseni udio katalizatora i molarni omjer propanol:suncokretovo ulje. Eksperimentalno postignuto najveće iskorištenje iznosi 99,79 % pri temperaturi od 60 °C u razdoblju od 2 h, s masenim udjelom katalizatora od 1 %, te molarnom omjeru propanol:ulje u iznosu od 10:1. Značajan utjecaj na iskorištenje imali su parametri omjer reaktanata i koncentracija katalizatora, dok su temperatura i vrijeme imali manji utjecaj, posebno pri povišenim udjelima katalizatora i povoljnijem omjeru reaktanata (većem suvišku propanola).

Ključne riječi: propanol, biodizel, dizajn eksperimenata

[1] S. Nanda *et al*.,Biorefinery of Alternative Resources: Targeting Green Fuels and Platform Chemicals, Springer Nature, 2020.
[2] S. D. Minteer, Handbook of Biofuels Production Processes and Technologies Woodhead Publishing Series in Energy, 2011, 258.



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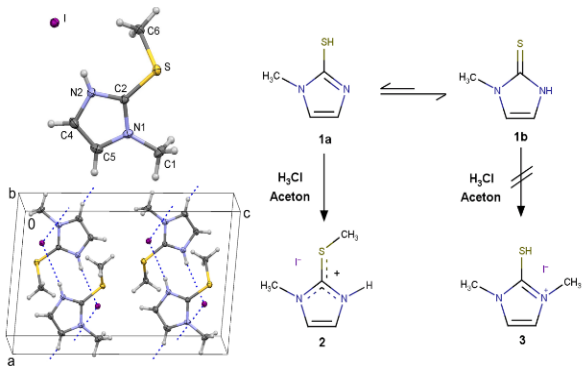
SINTEZA I STRUKTURA 1-METIL-2-(METILSULFANIL)-1*H*-IMIDAZOL HIDROJODIDA

SYNTHESIS AND STRUCTURE OF 1-METHYL-2-METHYLSULPHANYL-1*H*-IMIDAZOLE HYDROIODIDE

Leo Štefan[1], Dubravka Matković-Čalogović[2],
Lara Saftić Martinović[3], Miljenko Dumić[3]

[1]*Jadran-galenski laboratorij d.d., Svilno 20, 51 000 Rijeka, Hrvatska*
[2]*Prirodoslovno-matematički fakultet, Kemijski odsjek, Sveučilište u Zagrebu, Horvatovac 102a, 10 000 Zagreb, Hrvatska*
[3]*Odjel za biotehnologiju, Sveučilište u Rijeci, Radmile Matejčić 2, 51 000 Rijeka, Hrvatska*



Godine 1979. Kister i sur. objavili su pripravu 1-metil-2-(metilsulfanil)-1*H*-imidazol hidrojodida (**2**) [1], tj. hidrojodidne soli 1-metil-2-(metilsulfanil)-1*H*-imidazola, poznatog kao onečišćenje C tireostatika metimazola (**1**) [2], ali i važnog prekursora za sintezu ionskih tekućina [3]. Detalji opisane reakcije su bili šturi i nejasni, a struktura **2** nije bila određena.

Kako metimazol, ovisno o uvjetima, može reagirati u tiolnoj (**1a**) i tionskoj (**1b**) formi [3], radi razjašnjenja toga, proveli smo direktnu metilaciju **1** s ekvimolarnom količinom jodmetana u acetonu pri sobnoj temperaturi i izolirali HPLC čisti, **2** s iskorištenjem od 91 %. Struktura mu je određena spektroskopskim i termičkim metodama, a potvrđena rendgenskom difrakcijom na jediničnom kristalu. Spoj **2** ($C_5H_9IN_2S$; M_r 256,10) kristalizira u prostornoj grupi $P2_1/c$ monoklinskog kristalnog sustava sa sljedećim parametrima jedinične ćelije i podacima o utočnjavanju strukture: a=8,6603(1), b=7,4999(1), c=13,7504(2) Å, β=94,826(0)º, V=889,94(2) Å^3, Z=4, R=0,0138, R_w=0,0318, S=1,077, 2357 refleksa s $I>2\sigma(I)$. Duljine veza C2-S i C6-S od 1,7328(15) i 1,8013(17) Å, kao i C2-N1 i C2-N2 od 1,3371(18) i 1,3368(19) Å ukazuju na delokalizaciju dvostruke veze u spoju **2**. Kation i anion su povezani vodikovim vezama N2-H2·I od 2,713(18) Å i C5-H5 I od 3,050(18) Å u lance duž a-osi.

Ključne riječi: metimazol, onečišćenje C, hidrojodid, kristalna struktura

[1] J. Kister *et al.*, *Can J Chem* 57 (1979) 813.
[2] European Pharmacopoeia 7.0, Thimazole, Council of Europe, Strasbourg, 2011, 3071.
[3] A. I. Siriwardana *et al.*, *J Org Chem* 73 (2008) 4676.

UTJECAJ OBLIKA NANOMATERIJALA NA NASTANAK KISIKOVIH VAKANCIJA: NEDOPIRANI I DOPIRANI CERIJEV DIOKSID

THE EFFECT OF NANOMATERIAL SHAPE ON FORMATION OF OXYGEN VACANCIES: NON-DOPED AND DOPED CERIA

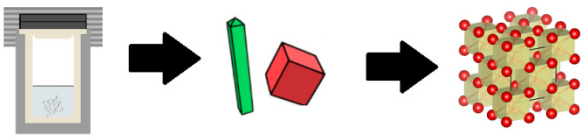
Dalibor Tatar[1], Jelena Bijelić[1], Ana Ivanković[1], Pascal Cop[2], Sebastian Werner[2], Bernd Smarsly[2], Igor Djerdj[1]

[1]Department of Chemistry, J. J. Strossmayer University of Osijek, Ul. cara Hadrijana 8/A, 31 000 Osijek, Croatia
[2]Justus Liebig University of Giessen, Institute for Physical Chemistry, Heinrich-Buff-Ring 17, Giessen, Germany

Oxygen storage in solid catalyst is very important for heteregeneous oxidation reactions of environmentally harmful gases such as CO, CH_x and HCl. Ceria nanoparticles act as promising catalysts these kinds of reactions because it possesses high OSC (oxgen storage capacity). When reducing size of a material, surface becomes more important than a bulk. Also, surface defects are induced which favor high OSC. This is why in these kinds of reactions the interaction of a gas phase with solid surface is studied in detail. Redox reactions which occur on ceria surface usually follow Mars-van Krevelen mechanism (surface oxygen atoms directly involved in reactions). Neutral oxygen vacancies are formed because of the reversible change in oxidation state from Ce^{4+} to Ce^{3+}. These vacancies are formed in different quantities depending on a shape of synthesized nanomaterial. Different shapes show different facets of preferential orientation ((110) for nanorods and (100) for nanocubes) thus also showing different stability and activity. In this research, shape-controlled CeO_2 nanoparticles (nanorods and nanocubes) and Zr-doped ceria nanorods were synthesized by hydrothermal method. Synthesized materials have been characterized by powder X-ray diffraction (PXRD), Raman spectroscopy, scanning electron microscopy (SEM) and thermogravimetric analysis (TGA). The value of surface area has been measured by BET method. Obtained results show pronounced effect of different nanoshape of ceria on formation of oxygen vacancies.

Keywords: ceria, ceria-zirconia, Mars-van Krevelen mechanism, catalysis

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *PZS-2019-02-2467.*



FOTOELEKTROKEMIJSKA SVOJSTVA NANO-KOMPOZITA KOJI SADRŽI TiO_2/SnS_2 I TiO_2/SnS_2/rGO MEĐUFAZE

PHOTOELECTROCHEMICAL PROPERTIES OF NANO-COMPOSITES CONTAINING TiO_2/SnS_2 AND TiO_2/SnS_2/rGO HETEROJUNCTIONS

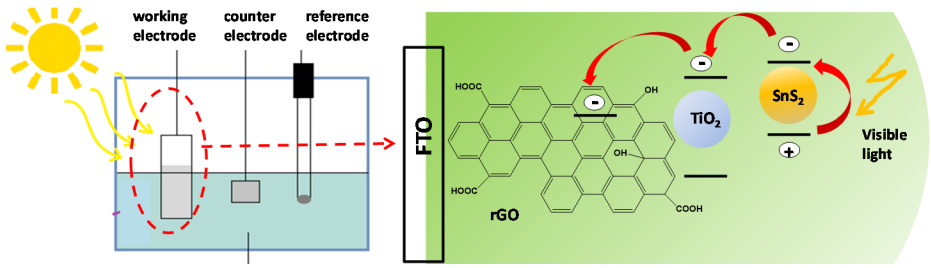
Mia Tominac, Tihana Bošnjak, Klara Perović, Tayebeh Sharifi, Hrvoje Kušić, Marijana Kraljić Roković

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb; Croatia

Titanium dioxide has gained a lot of attention in the field of photocatalysis because of its low cost, environmental friendliness, light corrosion resistance, and high stability. However, it is not effective in utilization of visible light and therefore significant efforts have been done to improve it through TiO_2 doping or TiO_2 composite formation. One of the composites suitable for visible light utilization is TiO_2/SnS_2 [1] and therefore the aim of this work was to investigate its photoelectrochemical properties. It is expected that this heterojunction catalyst not only increases visible light absorption but also decreases charge recombination. Additionally, charge recombination can be decreased by GO/rGO incorporation within the photocatalyst (TiO_2/SnS_2/rGO). Tuneable bang gap and band energy level of GO/rGO, which depends on its size and chemical composition, enables its fine adjustment to energy levels of oxides [2] improving the overall activity of photocatalyst.
In this work, good sensitivity of photocatalyst was shown by monitoring open circuit potential in chopped light irradiation and by comparing EIS response in dark to the one under light irradiation. The photoelectrochemical activity was monitored by using linear polarisation and bend energy position was determined by Mott Schottky analysis.

Keywords: photoelectrochemical properties, nano-composites, TiO_2/SnS_2, TiO_2/SnS_2/rGO

[1] M. Kovačić *et al*., *Materials* 11 (2018) 1041.
[2] Q. Mei *et al*, *Adv Sci* 6 (2019) 1900855.



ULOGA GIBANJA PROTONA UNUTAR MOLEKULE GLUTAMINSKE KISELINE

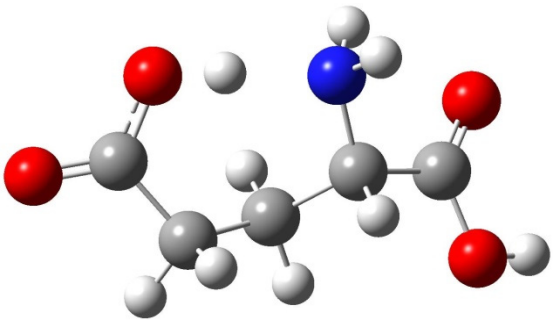
ROLE OF PROTON MOVEMENT INSIDE GLUTAMIC ACID MOLECULE

Andrej Vidak, Iva Movre Šapić, Marta Puhar, Vladimir Dananić

Faculty of Chemical Engineering and Technology, University of Zagreb,
Savska cesta 16, 10 000 Zagreb, Croatia

Glutamic acid is one of the most important acids used in biosynthesis of proteins. In our study we measured FTIR spectrum of glutamic acid powder. The recorded spectrum is in accordance with well-known database spectrum of glutamic acid, but our extensive DFT calculations show that spectral band between 1900 and 3000 cm^{-1} does not originate from standard L-Glutamic acid conformation. We argue that this specific spectral band is associated with proton movement between the OH and NH_2 groups. It is important to emphasize that our calculations show that one vibrational band corresponding to OH stretching strongly shifts by more than 1000 cm^{-1} to the lower part of vibrational spectrum. One of two OH groups is oriented towards NH_2 group and its stretching band lowers due to proton movement. This kind of movement is lowering ground state energy of the Glutamic acid within dielectric medium, in which intermolecular hydrogen bonds flatten the structure and lower the energy. We give the typical conformation corresponding to this movement in graphical abstract.

Ključne riječi: glutamic acid, FTIR, proton movement, quantum chemistry



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PRIPRAVA NOVIH FUNKCIONALIZIRANIH TIENILNIH BICIKLO[3.2.1]OKTADIENA

PREPARATION OF NEW FUNCTIONALIZED THIENYL BICYCLO[3.2.1]OCTADIENES

Dragana Vuk[1], Irena Škorić[1], Valentina Milašinović[2], Krešimir Molčanov[2], Željko Marinić[3]

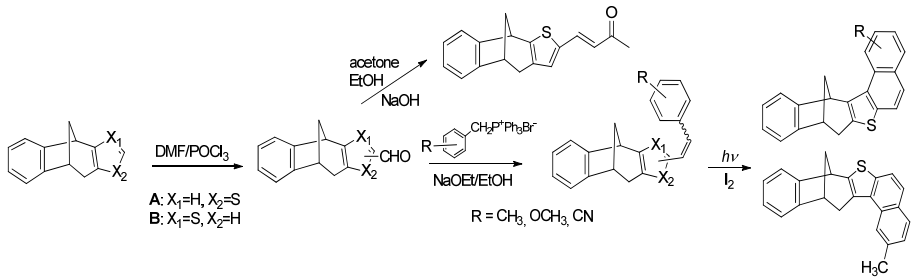
[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Rudjer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia*
[3]*NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia*

Bicyclo[3.2.1]octane skeleton has become the subject of intensive research in recent years [1-2]. Its presence in numerous biologically active natural compounds, their strenuous isolation from the plants, as well as their complicated multistage synthesis due to the complexity of their structure, encouraged us to develop a simple one step synthetic procedure based on photochemical methodology.

The aim of this study is to prepare novel thiophene bicyclo[3.2.1]octadiene derivatives with structure convenient for the introduction of new functional groups [3]. Further on, the study aims at expanding the compound library and at creating preconditions for further biological investigations. The starting substrates were easily obtained by Vilsmeier-Haack's reaction of bicyclo[3.2.1]octadiene thiophene derivatives From the obtained carbaldehydes, novel methyl-, methoxy- and cyano-substituted styryl thieno-benzobicyclo[3.2.1]octadiene derivatives were formed by Wittig's reaction and subjected to photochemical reactions, in terms of obtaining new annulated structures. As a part of this study, aldol reaction of starting 2-substituted carbaldehyde and acetone was also performed, which produced the thieno-fused benzobicyclo[3.2.1]octadiene compound with an extended conjugation.

Keywords: bicyclo[3.2.1]octadiene, photocyclization, thiophene

[1] D.Vuk *et al., Catalysts* 9, 304 (2019) 1.
[2] I. Šagud *et al*., *Turk J Chem* 43 (2019) 1170.
[3] D. Vuk *et al*., *Beilstein J Org Chem* 16 (2020) 1092.



Sekcija: Kemijsko i biokemijsko inženjerstvo
Topic: Chemical and Biochemical Engineering

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AROMATSKI PROFIL KOMERCIJALNOG DUHANSKOG BLENDA

INSIGHT INTO THE AROMA PROFILE OF TOBACCO COMMERCIAL BLENDS

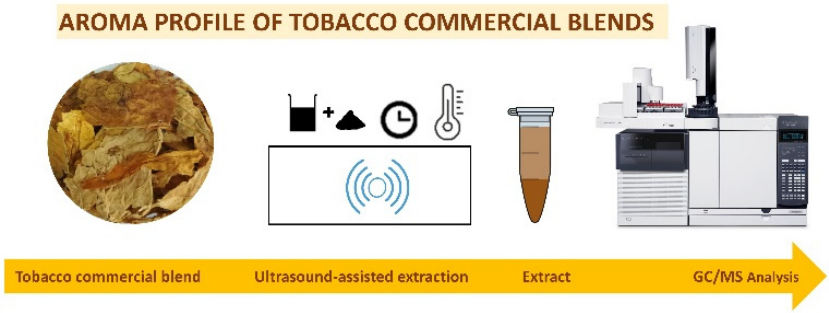
Marija Banožić[1], Krunoslav Aladić[1], Igor Jerković[2], Senka Vidović[3], Marijana Blažić[4], Stela Jokić[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21 000 Split, Croatia*
[3]*Faculty of Technology, University of Novi Sad, Bulevar Cara Lazara 1, 21 102 Novi Sad, Republic of Serbia*
[4]*Veleučilište u Karlovcu, Trg J. J. Strossmayera 9, 47 000, Karlovac, Croatia*

In this study, ultrasound-assisted extraction, using hexane as solvent was performed under different extraction conditions. The temperature range between 30 and 70 °C, time from 15 to 45 min, and solvent-solid ratio from 10 to 30 cm^3 g^{-1} were chosen.
GC/MS was employed for determination of volatile compounds in tobacco commercial blends composed of leaf lamina. Samples were obtained from tobacco factory „Fabrika duhana Sarajevo“,.Nicotine, neophytadiene and 4,8,13-duvatriene-1,3-diol were dominant compounds in all aroma profiles. Besides major compounds, tobacco blends contained variety of strait chain alkanes such as decane, dodecane, tridecane, tetradecane, pentadecane, hexadecane, heptadecane, octadecane, heneicosane, docosane, tricosane and tetracosane. Aroma is the most important attribute to define consumer acceptance of tobacco and tobacco products. Therefore, results obtained in this research could have further applications in the tobacco industry, but cosmetics and fragrance industry as well.

Keywords: tobacco, aroma, volatile compounds, commercial blends

Acknowledgments
This study was financially supported by the Croatian Science Foundation through grant *UIP-2017-05-9909*.



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TVORNICA KULTIVIRANOG MESA – KEMIJSKI ZAHTJEVI

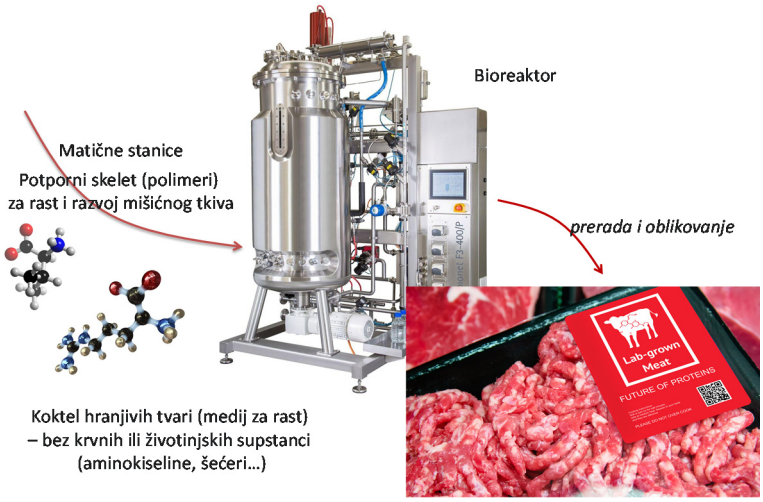
THE ARTIFICIAL MEAT FACTORY – CHEMICAL REQUIREMENTS

Vlatka Božić, Ante Jukić

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Maruličev trg 19, 10 000 Zagreb, Hrvatska

Kultivirano meso dobiva se uzgojem životinjskog mišićnog tkiva iz matičnih stanica u hranjivom mediju tehnikama tkivnog inženjerstva. Postupak proizvodnje dijeli se u tri faze. Početne ili „starter" stanice se postupkom biopsije uzimaju od živih životinja. Inicijacijska faza podrazumijeva visoki stupanj razmnožavanja stanica koje se zatim obrađuju primjenom otopina za rast tkiva. Pritom se tretiraju proteinima koji ubrzavaju proces razmnožavanja i rasta. Kako bi se oponašalo istezanje mišićnog tkiva, potreban je nosivi skelet koji ima mogućnost periodičkog pomicanja. To se postiže upotrebom nosača od alginata, kitozana, kolagena ili sintetskih (bio)polimera. Uobičajeno, nosivi skelet se isteže s promjenom temperature ili pH. Proces proizvodnje u većem volumenu se odvija u bioreaktorima, uz koktel hranjivih tvari koji može sadržavati 50 do 100 sastojaka kao što su šećeri, soli, aminokiseline, mikroelementi i drugo. Potrebno je koristiti i konzervanse, a njihova je uloga sprječavanje truljenja te zaštita od kvasca i gljivica. Neki od uobičajenih konzervansa uključuju kolagenski prah, ksantensku gumu, manitol i kohineal. Trenutno oko 60 novoosnovanih poduzeća širom svijeta razvija i poboljšava postupak za proizvodnju različitih vrsta kultiviranog mesa i plodova mora. Svima je cilj povećati proizvodnju uz istovremeno smanjenje troškova, te što ranije prirediti proizvode za tržište koje u obliku posebnih restoranskih ponuda već postoji.

Ključne riječi: in vitro, kultivirano meso, nosivi skelet, hranjive otopine, bioreaktor



KARAKTERIZACIJA EFLUENTA OD PRANJA TEKSTILIJA METODOM RASPODJELE VELIČINA ČESTICA

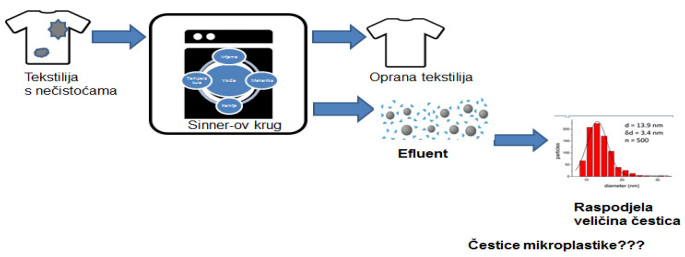
CHARACTERIZATION OF TEXTILE WASHING EFFLUENT BY PARTICLE SIZE DISTRIBUTION METHODS

Mirjana Čurlin[1], Tanja Pušić[2], Branka Vojnović[2], Agata Vinčić[2]

Prehrambeno biotehnološki fakultet, Sveučilište u Zagrebu,
Pierottijeva 6, 10 000 Zagreb, Hrvatska
[2]Tekstilno tehnološki fakultet, Sveučilište u Zagrebu,
Prilaz baruna Filipovića 28 a, 10 000 Zagreb, Hrvatska

Proces pranja tekstilija može se promatrati kao složeni sustav međudjelovanja brojnih parametara. Kao glavne parametre procesa pranja prema Sinner-ovom krugu uzimamo mehaniku, temperaturu, vrijeme i kemiju. Ulazni parametri procesa vezani su za sastav, strukturu te stupanj zaprljanja tekstilije, a izlazni parametri procesa pranja mogu se promatrati kao stupanj čistoće te strukturna promjena tekstilije. Međudjelovanje svih parametara procesa pranja imat će za posljedicu brojne pozitivne i negativne učinke na samu tekstiliju te na okoliš općenito. U ovom radu naglasak je stavljen na negativne učinke procesa pranja koje se očituju kao otpuštanje čestica, te je za karakterizaciju efluenta kao disperznog sustava korištena metoda raspodjele veličina čestica. Pranje mješovite pamuk/poliesterske tekstilije provedeno je prema standardnom postupku s i bez dodatka kemije (deterdženta). Primjenom metode laserske difrakcije za određivanje raspodjele veličina čestica u efluentima od pranja i ispiranja dobiveni su rezultati volumne raspodjele čestica te su izračunati parametri krivulja raspodjele. Dobiveni rezultati pokazuju razlike po svim određivanim parametrima krivulje za efluent nakon pranja i efluent nakon ispiranja, te ukazuju na utjecaj provedbe procesa pranja na otpuštanje čestica. Dobiveni rezultati koristit će se za analizu procjene otpuštanja čestica u pranju, a definirani parametri procesa pranja doprinijet će smanjenju otpuštanja čestica poliesterskih tekstilija u pranju te time i zaštiti okoliša od onečišćenja mikroplastičnim česticama.

Ključne riječi: proces pranja, pamuk/poliester tekstilija, otpuštanje čestica, raspodjela veličina čestica



PRAKTIČNA VJEŽBA REGULACIJE TEMPERATURE U ZRAČNOM TUNELU

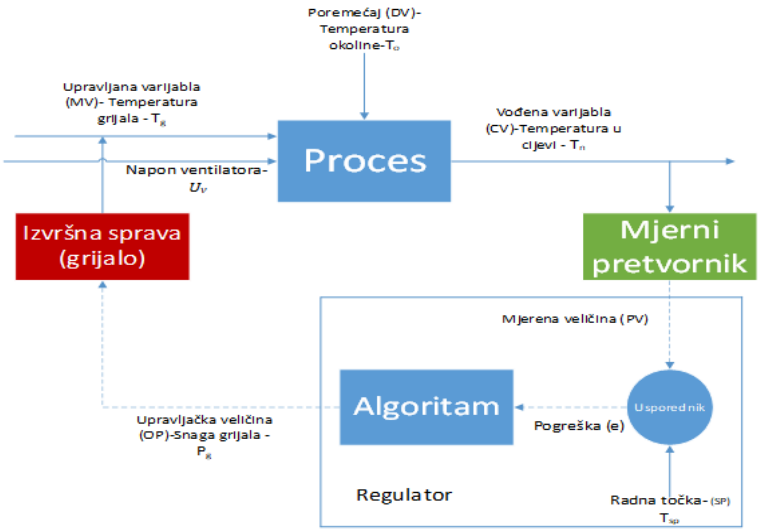
PRACTICAL EXERCISE OF TEMPERATURE CONTROL IN THE AIR TUNNEL

Hrvoje Dorić, Nenad Bolf, Patricija Krušlin, Nikola Rimac

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Savska cesta 16, 10 000 Zagreb, Hrvatska

Procesi prijenosa topline često se pojavljuju u industrijskoj praksi. Neki proizvodi u, primjerice, farmaceutskoj ili prehrambenoj industriji, vrlo su osjetljivi na promjene temperature, stoga je potrebno posvetiti veliku pažnju njihovom projektiranju i izvedbi.
U ovom radu ispitan je laboratorijski uređaj za analizu dinamičkog vladanja toplinskog procesa. Uređaj je namijenjen demonstraciji razvoja dinamičkih modela procesa na temelju eksperimentalnih podataka, a namjena mu je poučavanje osnovnih metoda vođenja procesa i ugađanja regulatora.
U radu je proveden niz eksperimenata kojima su utvrđene statičke i dinamičke karakteristike procesa i regulacijskog kruga. Na temelju provedenih eksperimenata proračunati su i optimirani parametri regulatora. Konačno je ispitano vladanje procesa u regulacijskom krugu i ocijenjen rad regulacijskih krugova.

Ključne riječi: dinamika procesa, vođenje procesa, prijenos topline, regulator, ugađanje regulatora

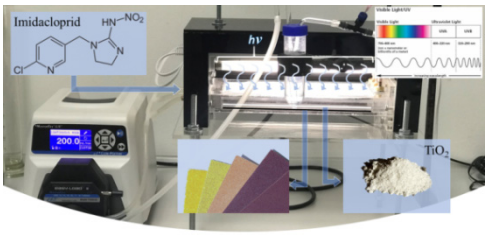


FUNKCIONALIZIRANI TiO_2 ZA FOTOKATALITIČKU RAZGRADNJU NEONIKOTINOIDNIH INSEKTICIDA

FUNCTIONALIZED TiO_2 FOR PHOTOCATALYTIC DEGRADATION OF NEONICOTINOID INSECTICIDES

Marina Duplančić, Vanja Gilja, Ivana Elizabeta Zelić, Vesna Tomašić

Faculty of Chemical Engineering and Technology, University of Zagreb,
Marulićev trg 19, 10 000 Zagreb, Croatia



Neonicotinoid insecticides, including imidacloprid, thiacloprid, thiamethoxam, clothianidin and acetamiprid have been included in the extended "*Watch*" list of the European commission within the water framework directive since 2018, due to the confirmed risk and danger for the aquatic environment.
Their removal from contaminated waste streams is one of the major challenges with regard to solving global environmental problems [1, 2]. The aim of this work was to develop modified TiO_2 photocatalysts and innovative designs of photocatalytic reactors for the decomposition of neonicotinoid insecticides under conditions of simulated solar irradiation. In this study surface functionalization of TiO_2 was performed to reduce the energy band gap (E_{bg}) of the TiO_2 and to prepare a stable immobilized photocatalytic layer with acceptable mechanical and catalytic properties under different operating conditions. Physicochemical, morphological and mechanical properties of the prepared photocatalytic layers were determined and their photocatalytic activity for imidacloprid degradation was tested. A comparison of photolytic and photocatalytic degradation was performed using different radiation sources for simulation of the solar light.
It was concluded that different modification methods can be used to reduce the energy band gap (E_{bg}) of the TiO_2, but this does not necessarily mean a better conversion of imidacloprid during its photocatalytic degradation. Nevertheless, some classical synthesis routes for surface functionalization of TiO_2 followed by an additional post-functionalization showed great potential to improve TiO_2 activity for photocatalytic decomposition of imidacloprid under the visible part of the solar spectrum.

Keywords: neonicotinoid insecticides, imidacloprid, modifies TiO_2, visible part of the solar spectrum

[1] K.M. Lee *et al*., *Water Res* 88 (2016) 428.
[2] D. Chatterjee *et al*., *J Photoch Photobio* C 6 (2005) 186.

Acknowledgement
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KARAKTERIZACIJA MIKROPLASTIKE U SEDIMENTU PLAŽE BAČVICE

CHARACTERIZATION OF MICROPLASTICS IN BAČVICE BEACH SEDIMENT

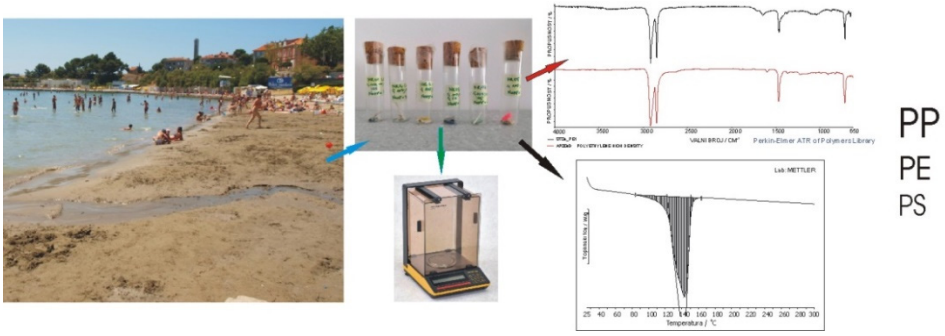
Matko Erceg[1], Pero Tutman[2], Dubravka Bojanić Varezić[2], Ivana Dodig[1]

[1]*Kemijsko-tehnološki fakultet, Sveučilište u Splitu,*
Ruđera Boškovića 35, 21 000 Split, Hrvatska
[2]*Institut za Oceanografiju i Ribarstvo, Šetalište Ivana Meštrovića 63, 21 000 Split, Hrvatska*

Uzorkovanje mikroplastike u sedimentu plaže Bačvice (Split) provedeno je u rujnu 2014. godine. Uzorkovanje i odvajanje mikroplastike iz sedimenta provedeni su prema DeFish Gear protokolu (***De**relict **Fish**ing **Gear** Management System in the Adriatic Region*) [1]. Uzorak mikroplastičnog otpada s plaže Bačvice sastoji se od ukupno 352 ispitka. Ispitci su zasebno izvagani te im je određena boja i prozirnost/neprozirnost. Dimenzijska analiza izvršena je primjenom računalnog programa za obradu slika. Rezultati pokazuju da 244 ispitka spada u tzv. veliku mikroplastiku (LMP, engl. ***L**arge **micro**plastics*) s maksimalnom dimenzijom 1 - 5 mm, a 108 ispitaka spada u tzv. sitnu mikroplastiku (SMP, engl. ***S**mall **micro**plastics*) s maksimalnom dimenzijom 20 μm - 1 mm. LMP ispitci su razvrstani u 6 kategorija: fragmenti (217 komada), pjenasta plastika (20 komada), granule (3 komada), filmovi (3 komada) i filamenti (1 komad). Njihova identifikacija provedena je primjenom infracrvene spektroskopije s Fourierovom transformacijom (FTIR) - HATR tehnikom te diferencijalnom pretražnom kalorimetrijom (DSC). Rezultati pokazuju da se LMP mikroplastika sastoji uglavnom od polipropilena i polietilena te u manjem udjelu od polistirena. SMP ispitci su premaleni za FTIR-HATR i DSC analizu, te njihova identifikacija nije provedena.

Ključne riječi: mikroplastika, plaža Bačvice, FTIR, DSC

[1] http://www.defishgear.net/media-items/publications (25.6.2020.)



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KARAKTERIZACIJA I PRIMJENA EMULZIJA VODE U TEŠKOM LOŽIVOM ULJU ZA SMANJENJE NO_X EMISIJA I POTROŠNJE GORIVA

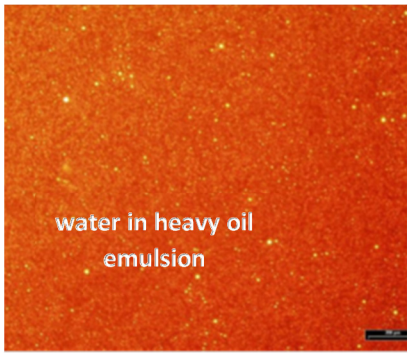
CHARACTERIZATION AND USE OF WATER-IN-HEAVY FUEL OIL EMULSIONS FOR REDUCED NO_X EMISSIONS AND ENERGY SAVING

Fabio Faraguna[1], Igor Šepić[2], Ante Jukić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*INA – Industrija nafte d.d., Refining and Marketing, 10 000 Zagreb, Croatia*

Emulsions of water in heavy fuel oil with water content of 10 and 20 wt. % were prepared by mechanical procedure without using any chemical surfactant. Emulsions were characterized by using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), rheology tests and microscopy. Stability of heated emulsions was dependent on water content, heated temperature, mixing regime and time of storage. However, it was satisfactory for a period of at least ten days, for both prepared emulsions. It was found that the best technique for accurate, precise and fast determination of water content in emulsion was DSC. Size of water droplets in oil and their agglomeration with time was followed with optical microscopy. The experiments of use of emulsified fuel for burning in an industrial boiler under normal operating conditions showed significantly improved boiler efficiency (up to 4 %) with additional reduction of NO_x emissions.

Keywords: water in heavy oil emulsions, stability, burning, efficiency, emissions



▲
Efficiency

NO_x emissions
▼

ON-LINE PRAĆENJE PROIZVODNJE BIODIZELA INFRACRVENOM SPEKTROSKOPIJOM

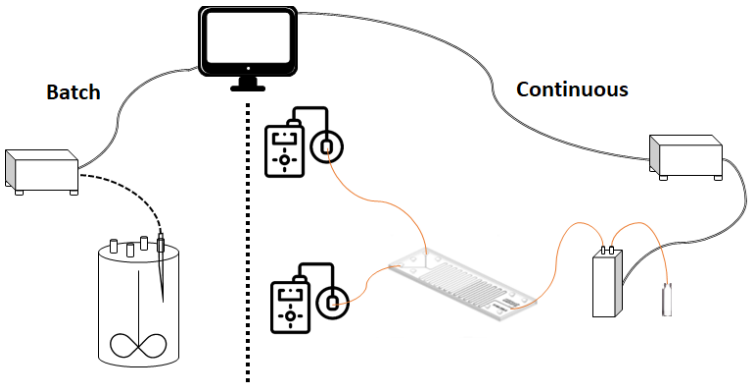
ON-LINE MONITORING OF BIODIESEL PRODUCTION BY NEAR-INFRARED SPECTROSCOPY

Martin Gojun[1], Tea Sokač[1], Anabela Ljubić[1], Anita Šalić[1], Davor Valinger[2], Bruno Zelić[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[2]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*

Since the ever-demanding need for biodiesel production is growing, rapid monitoring for biodiesel yield and its quality is becoming more popular. NIR method, is complementary with the gas chromatography (GC) method and could give good insight for identifying biodiesel yield in different experimental set-ups. In this work, the NIR method was used for easier and faster determination of biodiesel yield and the amount of glycerol in crude biodiesel. Samples were collected *on-line* and *at-line* depending on NIR sensor used (fiber-optic probe or flow cell). Biodiesel production was monitored in both, batch and continuous (micro)reactors, respectively.
Obtained results showed that NIR method is suitable for *on-line* monitoring of biodiesel yield and glycerol amount (total and free). Results were compared with analytical tools, GC and spectrophotometer that are commonly used for *off-line* quantification of biodiesel and glycerol concentrations. NIR method has proven to be a promising, fast and reliable method for *on-line* measurement of biodiesel and glycerol concentrations.

Keywords: on-line measurement, biodiesel concentration, glycerol concentration, near-infrared spectroscopy



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TERMODINAMIČKO MODELIRANJE Cu-Al-Mn-Ag LEGURA

THERMODYNAMIC MODELLING OF Cu-Al-Mn-Ag ALLOYS

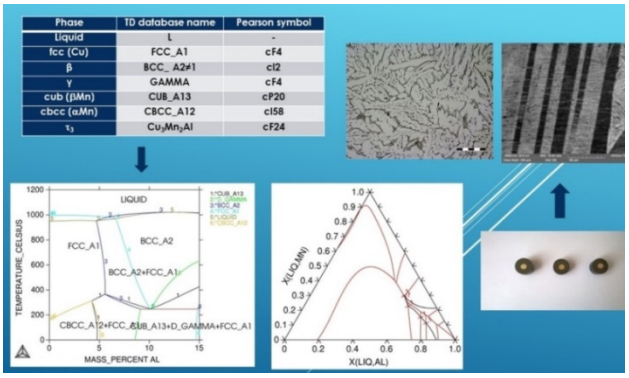
Tamara Holjevac Grgurić[1], Željka Krtić[1], Emi Govorčin Bajsić[2], Nikolina Mrkonjić[2], Lovro Liverić[3], Zoran Jurković[3], Ivan Brnardić[1]

[1]*Faculty of Metallurgy, University of Zagreb, Aleja narodnih heroja 3, 44 000 Sisak, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
[3]*Faculty of Engineering, University of Rijeka, Vukovarska 58, 51 000 Rijeka, Croatia*

Cu-Al-Mn alloys with 7-10 wt % of Ag were prepared by melting of pure metals in the electric-arc furnace, in argon atmosphere, and casted in the cylindrical mould. Specimens were thermal treated at 900 °C and quenched in water. Calculation of phase diagram was performed by Thermo-Calc program, by minimization of Gibbs free energy of system and CALPHAD method using parameters of pure elements according to SGTE database and optimized thermodynamic parameters for binary and ternary system [1]. Microstructure was determined by Field-emission scanning electron microscope (FE-SEM) and phase elemental analysis was performed by energy dispersive X-ray spectroscopy (EDS). Martensitic and austenitic transformation temperatures were followed by Differential thermal analysis (DSC). Results showed two-phase morphology in the as-cast state and completely formed martensitic structure, with different types of martensite, in quenched Cu-Al-Mn-Ag specimens.

Keywords: Cu-Al-Mn-Ag alloys, shape memory materials, martensitic phase

[1] D. Manasijević *et al*., *Kovove Mater* 58 (2020) 293–299.



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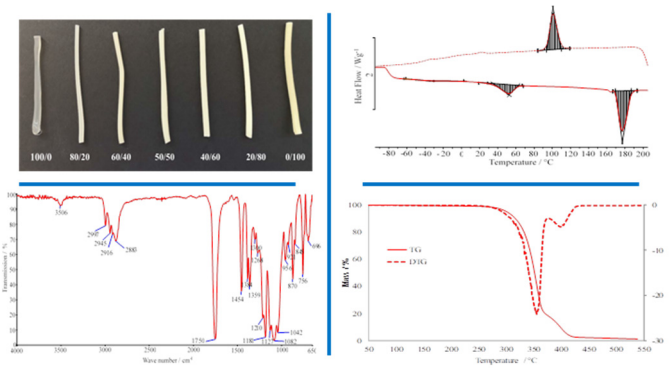
PRIPREMA I KARAKTERIZACIJA MJEŠAVINA BIORAZGRADLJIVE POLILAKTIDNE KISELINE S POLI(ETILEN-OKSIDOM)

PREPARATION AND CHARACTERIZATION OF BIODEGRADABLE POLYLACTID ACID AND POLY(ETHYLENE OXIDE) BLENDS

Miće Jakić, Sanja Perinović Jozić, Tina Slatina, Mihaela Storić

Faculty of Chemistry and Technology, University of Split,
Ruđera Boškovića 35, 21 000 Split, Hrvatska

The aim of this work was to prepare blends of biodegradable polylactid acid (PLA) with poly(ethylene oxide) (PEO) and to investigate possible interactions within prepared polymer blends. Investigated blends were prepared by hot melt extrusion (HME) process in a laboratory extruder. The thermal characteristics of neat polymers and their blends were investigated by means of differential scanning calorimetry (DSC) in a nitrogen atmosphere. The glass transition temperature of PLA in the PLA/PEO blends could not be determined because it was overlapped with an endothermic peak of PEO melting. Therefore, the melting point of investigated samples as a miscibility criterion was used. The depression of melting temperatures at higher PLA or PEO content (80 %) indicated that PLA and PEO are only partially miscible in the melt. Likewise, Fourier transform infrared spectroscopy (FT-IR) was used to investigate possible interactions. The observed shifting of peak maxima in FT-IR spectra of blends with higher PLA or PEO content (80 %) are significant enough to confirm the interactions between the investigated polymers in blends, as well as the results of DSC analysis. Thermal stability of PLA/PEO blends has been investigated by thermogravimetric analysis (TG) in nonisothermal heating regime in a nitrogen atmosphere. Neat polymers exhibit single stage degradation, while a two-stage degradation pattern is seen in the case of all PLA/PEO blends. From characteristic of TG curves, it could be concluded that the degradation of PLA/PEO blends starts at lower temperatures and occurs more slowly by addition of PEO.



Keywords: polylactid acid, poly(ethylene oxide), differential scanning calorimetry, Fourier transform infrared spectroscopy, thermogravimetric analysis

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UTJECAJ PROCESNIH PARAMETARA NA KINETIKU SUŠENJA I MORFOLOGIJU KRISTALA

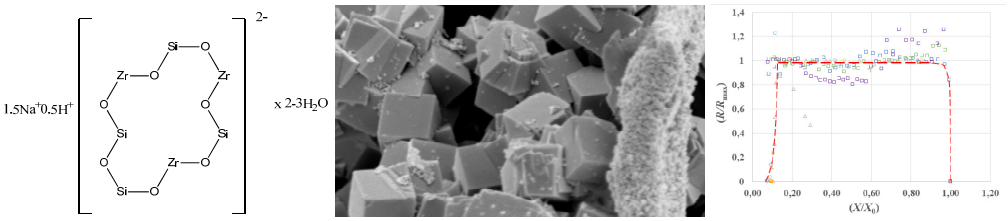
INFLUENCE OF PROCESS PARAMETERS ON DRYING KINETICS AND THE MORPHOLOGY OF CRYSTALS

Katarina Jozinović[1], Aleksandra Sander[1], Gordana Vrbanec[2]

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska
[2]Pliva Hrvatska d.o.o., Prilaz baruna Filipovića 25, 10 000 Zagreb, Hrvatska

U ovom radu istražena je kinetika sušenja natrijeve soli cirkonija u različitim laboratorijskim sušionicima. Odabrana su dva vakuum sušionika, jedan s pliticama i jedan rotacijski te sušionik s fluidiziranim slojem. Osim vrste sušionika, istražen je i utjecaj početnog sadržaja vlage materijala kao i temperature na kinetiku sušenja i morfološka svojstva osušenih kristala. Kinetika sušenja praćena je gravimetrijski u vakuum sušionicima te psihrometrijski u sušioniku s fluidiziranim slojem. U sušioniku s fluidiziranim slojem također je istraženo može li se bliskom infracrvenom spektroskopijom (NIR, engl. *Near InfraRed*) pratiti kinetika sušenja.
Mjerni podaci aproksimirani su Lewisovim i Pageovim matematičkim modelom te je za svaku vrstu sušionika odabran model koji uz najviši stupanj korelacije opisuje kinetiku sušenja. Parametri oba modela dovedeni su u vezu s uvjetima provedbe procesa sušenja.
Rezultati su pokazali da vrsta sušionika i temperatura utječu na kinetiku sušenja i morfologiju kristala. Veće brzine sušenja ostvarene su pri višim temperaturama. Pri nižim temperaturama sušenje je brže u sušioniku s fluidiziranim slojem, a pri višim temperaturama u vakuum sušionicima. U rotacijskom vakuum sušioniku i u sušioniku s fluidiziranim slojem dolazi do loma kristala. Bliska infracrvena spektroskopija pokazala se kao dobra metoda praćenja kinetike sušenja u fluidiziranom sloju.

Ključne riječi: kinetika sušenja, matematički modeli, sušenje u fluidiziranom sloju, vakuum sušenje



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ODREĐIVANJE FAZNE RAVNOTEŽE KAPLJEVINA-KRUTINA I TERNARNI FAZNI DIJAGRAMI NA PRIMJERU KOKRISTALA FARMACEUTSKI AKTIVNE TVARI

SOLID-LIQUID PHASE EQUILIBRIUM AND TERNARY PHASE DIAGRAMS ON A CO-CRYSTAL OF ACTIVE PHARMACEUTICAL INGREDIENT

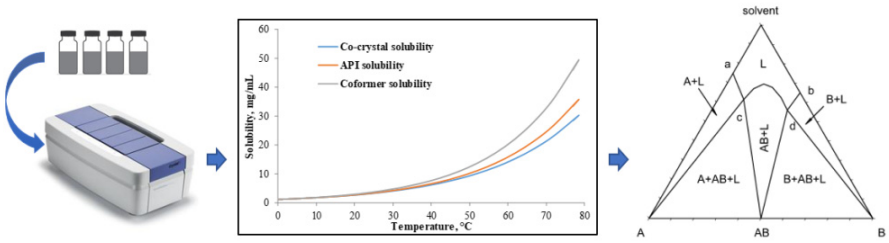
Dario Klarić, Nikolina Janton

Pliva Croatia Ltd., Prilaz baruna Filipovića 25, 10 000 Zagreb, Croatia

Since pharmaceutical co-crystals continue to gain in importance on the market, different screening and preparation techniques have been developed. Solution co-crystallization is highly preferred in industry because of its low cost. The driving force for crystallization is supersaturation which can be achieved by cooling the solution from high to lower temperatures. In a co-crystal system two concentrations have to be considered to avoid crystallization of one individual component: the solubility of active pharmaceutical ingredient and coformer. Ternary phase diagram represents most accurately the concentration range in which the co-crystal is stable and less soluble than the target molecule and conformer [1, 2]. The aim of this work was to create such a ternary diagram for predicting the pathway of co-crystal formation. The experiments were conducted on a parallel crystallizer *Crystal16* with different initial concentrations of active pharmaceutical ingredient and mandelic acid as coformer, which ranged between 50-200 mg cm^{-3}. Solubility curves were determined in toluene and toluene/*iso*-propyl acetate mixtures under atmospheric pressure at different temperatures. DynoChem® software was used for experimental data evaluation and solubility curve modelling.

Keywords: active pharmaceutical ingredient, co-crystal, Ternary phase diagram

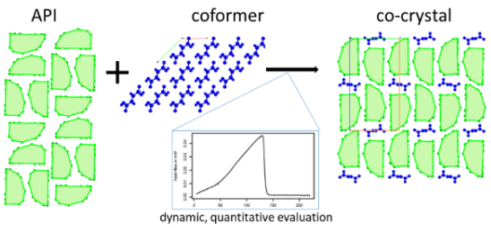
[1] M. Karimi-Jafari *et al*., *Cryst Growth Des* 18 (2018) 6370.
[2] X. Sun *et al*., *J Chem Eng Dana* 60 (2015) 1166.



PRIMJENJIVOST MIKROKALORIMETRIJE KAO NE-STANDARDNE METODE U ISTRAŽIVANJU POLIMORFIJE, KOKRISTALA I SOLI

APPLICABILITY OF MICROCALORIMETRY AS A NON- STANDARD TOOL IN POLYMORPH, CO-CRYSTAL AND SALT SCREENING STUDIES

Lorena Kordić, Petar Bibulić, Sanja Matečić Mušanić
Pliva Croatia Ltd., Prilaz baruna Filipovića 25, 10 000 Zagreb, Croatia



Microcalorimetry and other techniques of thermal analysis are powerful tools for solid state characterization of pharmaceutical materials [1]. Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) are the conventional methods of thermal analysis and are often used for thermal characterization of active pharmaceutical ingredients (API). These techniques are standard characterization methods during polymorph, co-crystal, or salt screening studies. On the other hand, microcalorimetry is not a conventional thermal characterization method, but there are a number of possible applications of microcalorimetery in the pharmaceutical industry. Such applications are quantification of the amorphous content in the API, compatibility study between API and excipients, determination of heat of solution, reaction or fusion, stability assessment, investigation of polymorphism, and prediction of chemical stability by artificial ageing [2,3].
In this work two possible application of isothermal microcalorimetry in the field of polymorph, co-crystal and salt screening will be presented. The first application is determination of possible API - coformer interaction in order to select potentially interesting conformer for obtaining co-crystals, as a part of co-crystal screening experiments.
Second experiment is related to the preparation of co-crystal, salt or polymorphic forms of API by using microsauna isothermal microcalorimery experiments. Advantage of this approach in comparison to conventional polymorph or co-crystal screening methods is complete control over experimental conditions and dynamic monitoring of reactions with a possibility of quantification of heat of co-crystal formation.

Keywords: microcalorimetry, co-crystals, polymorphism, pharmaceuitcals

[1] S. Gaisford *et al*., *Thermochim Acta* 380 (2001) 185.
[2] S. Gaisford, *Curr Pharmaceut Biotech* 6 (2005) 181.
[3] D. Giron, *J Therm Anal Cal* 64 (2001) 37.

PRIMJENA IC TERMOGRAFIJE PRI UMREŽENJU POLIMERA U MODELNIM KALUPIMA

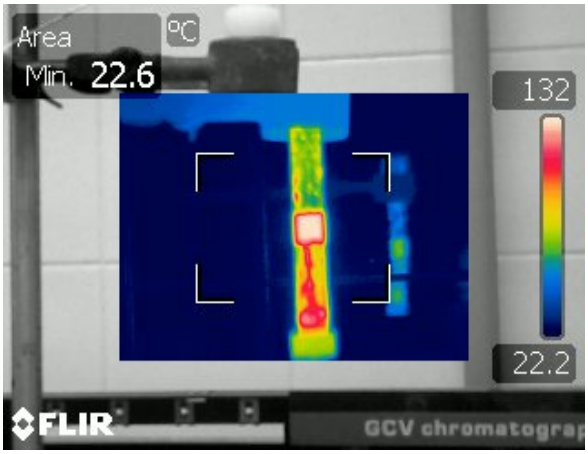
APPLICATION OF AN IC THERMOGRAPHY IN POLYMER CROSSLINKING IN MODEL MOLDINGS

Vanja Kosar, Ante Koštić, Marija Lukić

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

U ovom radu proučavana je reakcija očvršćivanja nezasićenih poliestera u valjkastim kalupima zagrijavanim u uljnoj i zračnoj kupelji. Glavni problem prilikom egzotermne reakcije očvršćivanja čini generacija topline te značajno povećanje temperature unutar kalupa. Dodatkom inertnog punila smanjen je udio reaktivne komponente u smjesi posljedica čega je redukcija količine generirane topline u odnosu na čistu smolu. Predložen je matematički model u svrhu simuliranja reakcije očvršćivanja. Validacija modela izvršena je usporedbom sa eksperimentalno izmjerenim temperaturama u središtu kalupa.
Provedeno je usporedno pračenje reakcije očvršćivanja u modelnim kalupima infracrvenom termografijom. Svrha provedbe samog snimanja jest određivanje temperaturnih profila, budući da se unutar samog kalupa za vrijeme reakcije javlja temperaturni gradijent koji se proteže od središta do stijenke kalupa što može dovesti do formiranja termosetnog proizvoda nejednolikih svojstava. Izazov samoj metodi predstavljaju male dimenzije kalupa kao i činjenica da su kalupi napravljeni od materijala niske emisivnosti (polirani bakar).

Ključne riječi: očvršćivanje, poliesterska smola, kalup, matematički model, termografija



ž

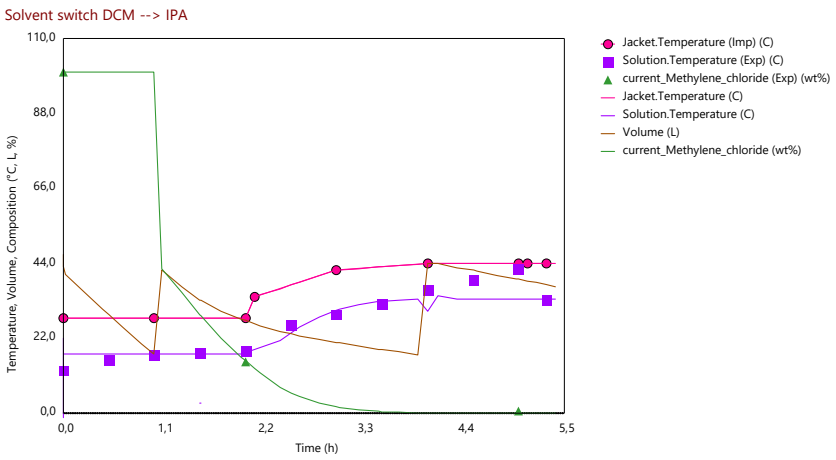
MODELIRANJE I OPTIMIZACIJA PROCESA ZAMJENE OTAPALA

SOLVENT SWAP PROCESS MODELING AND OPTIMIZATION

Igor Kultan, Ivan Vrban, Franjo Jović, Ozren Wittine, Eugen Marcelić
PLIVA Hrvatska d.o.o., Prilaz baruna Filipovića 25, 10 000 Zagreb, Hrvatska

U današnje vrijeme briga za okoliš postaje prioritet u industriji, te nameće standarde koje kompanije moraju poštovati kako bi uspješno poslovale. Tijekom razvoja procesa proizvodnje aktivnih farmaceutskih supstancija (API), često se koristi destilacija otapala kao separacija, a korištenje što manjih količina otapala je u skladu sa zaštitom okoliša. Prilikom optimizacije procesa zamjene otapala koriste se matematički modeli koji pomažu u ispunjavanju postavljenih zahtijeva procesa te samom razumijevanju procesa destilacije. Simulacija procesa zamjene otapala omogućava predviđanje samog profila sastava tijekom procesa, te vrijeme trajanja destilacije. Razvijan je proces proizvodnje API-ja u pilotnom postrojenju u kojem je bila potreba za zamjenom otapala diklormetana s izopropanolom. Testirani su različiti termodinamički modeli (UNIFAC, UNIQUAC i NRTL), a korišten je NRTL u krajnjoj simulaciji kao najpouzdaniji prema eksperimentalnim podacima. Zamjenu otapala je optimirana tako da se sadržaj reaktora destilira do minimalnog volumena, a zatim se drugo otapalo dodaje do maksimalnog volumena. Provedeni su pokusi u laboratorijskom mjerilu (na 1 dm^3) ispitan je procesni prostor, te je provedena simulacija procesa na pilotnu skalu (na 100 dm^3) uz korištenje značajki pilotnog reaktora (minimalni volumen i koeficijent prijenosa topline), a zatim je validiran proces. Zahtjev procesa je da sadržaj diklormetana u reakcijskoj smjesi ne smije biti veći od 1 %. Simulacijom je utvrđena bilanca tvari i određeno da dva dodavanja izopropanola mogu ispuniti procesne zahtjeve, što je eksperimentalno potvrđeno. Konačni udio diklormetana je bio 0,78 % na pilotnoj pogonskoj šarži, a proces je uspješno uvećan.

Keywords: destilacija, zamjena otapala,simulacija procesa, termodinamički modeli



PRIPRAVA $Ca_{1-x}Sr_xMnO_3$ KOPRECIPITACIJOM

PREPARATION OF $Ca_{1-x}Sr_xMnO_3$ BY COPRECIPITATION

Suzana Kralj[1], Jelena Macan[1], Andreja Žužić[1],
Ivana Panžić[2], Andreja Gajović[2]

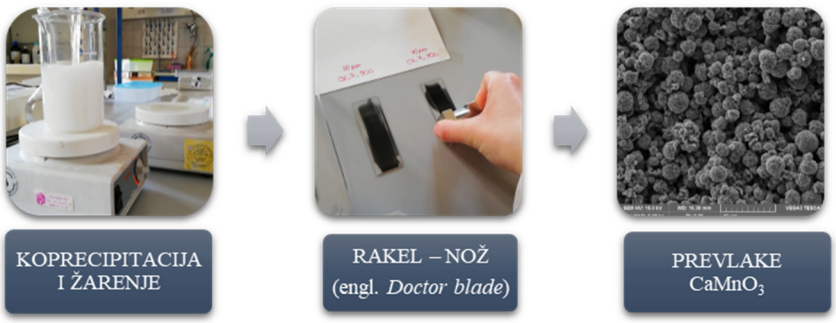
[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Maruličev trg 19, 10 000 Zagreb, Hrvatska*
[2]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*

Keramike na bazi kalcijeva manganita, $CaMnO_3$ postaju od sve većeg interesa na području inženjerstva materijala zbog pogodnih termoelektričnih, magnetskih i elektromagnetskih svojstava. Na strukturu $CaMnO_3$ može se utjecati dopiranjem te tako dodatno poboljšati i modificirati svojstva i proširiti područje primjene. Kako bi se takvi materijali mogli primjenjivati na industrijskoj razini, nužno je osigurati ekonomski povoljnu sintezu. Metoda koprecipitacije ili sutaloženja jednostavna je, lako izvediva i ekonomična za dobivanje $CaMnO_3$.

Provedena je sinteza $CaMnO_3$ koprecipitacijom te su ispitani čimbenici koji bi mogli utjecati na veličinu precipitata – temperatura, koncentracija, redoslijed miješanja otopina, vrijeme starenja. Dobiveni talozi su sušeni i podvrgnuti žarenju pri 900 °C pri čemu je iskristalizirao $CaMnO_3$. Dodatno je ispitivano dopiranje $CaMnO_3$ stroncijem istom metodom. Konačno, $CaMnO_3$ nanesen je na staklenu pločicu pomoću aplikatora rakel-noža (engl. *doctor blade*) u obliku tankih prevlake debljine ~10 μm. Nužan je nastavak istraživanja da bi se postigle homogene tanke prevlake pogodne za primjenu.

Ključne riječi: metoda koprecipitacije, sinteza $CaMnO_3$, utjecaj čimbenika na veličinu percipitata

Zahvala
Ovo istraživanje financirano je sredstvima Hrvatske zaklade za znanost projektom *IP-2018-01-5246.*



UTJECAJ BROJA PREGRADA U MILIREAKTORU NA INTENZIFIKACIJU PROCESA

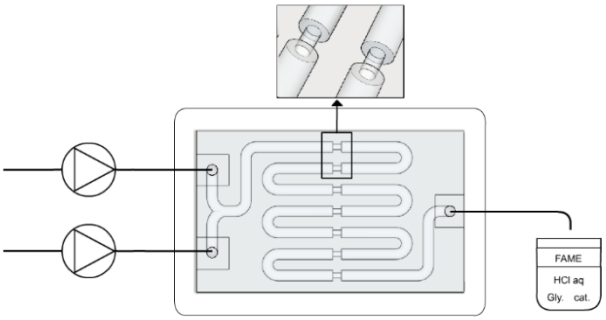
INFLUENCE OF NUMBER OF BAFFLES IN MILLIREACTOR ON PROCESS INTENSIFICATION

Marija Lukić, Domagoj Vrsaljko

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Malo povećanje veličine mikroreaktora prema milimetarskim dimenzijama povećava brzinu protoka reaktanata i na taj način prevladava mali protok kao osnovni nedostatak klasičnih mikroreaktora. Povećanjem dimenzija kanala mijenja se profil strujanja i miješanje u reaktoru. Primjenom aditivne proizvodnje (AM) moguće je konstruirati reaktorske sustave koji osiguravaju intenzifikaciju miješanja što posljedično dovodi do bržeg odvijanja kemijskih procesa. Napredni računalni 3D-model reaktora može se upotrijebiti za optimiranje miješanja na mili-ljestvici postavljanjem statičkih miješala u obliku koncentričnih pregrada unutar kanala.
Za modelnu reakciju odabrana je transesterifikacija suncokretova ulja u metilne estere masnih kiselina. Konverzija, a time i uspješnost prijenosa tvari i energije praćena je nuklearnom magnetskom rezonancijom (NMR) i infracrvenom spektroskopijom (FTIR).
Ovim istraživanjem razrađen je novi pristup izrade jednostavnih cijevnih polimernih milireaktora (φ=2,5 mm) s različitim brojem pregrada (1, 3, 5 i 7) i dimenzija (φ=1,2 mm x 2 mm duljine) pomoću tehnologije proizvodnje rastaljenim filamentom (FFF) u svrhu istraživanja intenzifikacije procesa. Dobiveni rezultati pokazuju da porastom broja pregrada dolazi do povećanja radijalnog miješanja fluida kroz cijev milireaktora pri čemu se stvara veća dodirna površina između reaktanata za provođenje kemijske reakcije što dovodi do povećanja konverzija u manjem vremenu zadržavanja, τ.

Ključne riječi: proizvodnja rastaljenim filamentom, milireaktor s pregradama, intenzifikacija procesa, kontinuirana proizvodnja FAME



International Conference *18th Ružička days*
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September 16–18, 2020 / Vukovar, Croatia

PRIMJENA KONTINUIRANOG PROTOČNOG PROCESA U REAKCIJI LITIJACIJE U SINTEZI API-a

IMPLEMENTATION OF CONTINUOUS FLOW PROCESS FOR LITHIATION REACTION IN API SYNTHESIS

Zrinka Mastelić Samardžić, Vitomir Vušak,
Moris Mihovilović, Aida Omerbašić

Teva, PLIVA R&D, Prilaz baruna Filipovica 29, 10 000 Zagreb, Croatia

Although the advantages of organolithium compounds are well known, the same are still avoided in industrial world as dangerous and difficult to handle in multi-kg scale. Lithiation reactions in a batch mode are typically conducted under cryogenic temperatures (-78 to -40 ˚C) to minimize the side reactions arising from the highly reactive organlithium intermediates [1]. Challenges of safe handling highly reactive chemicals and a highly energetic reactions in scaled-up operations is a major disadvantage of such batch processes [1].

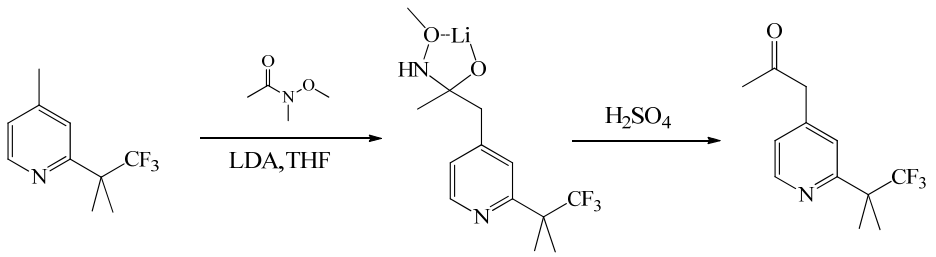
This work represents overcoming these safety and technical issues by implementation of continuous flow process for lithiation reaction which is part of process for synthesis of one active pharmaceutical ingredient.

Through very extensive development, many innovative solutions were involved in flow process to overcome technical difficulties. Final results are hundreds of grams of obtained product produced under safe conditions in a short time, at moderate temperatures and in cheap and flexible equipment.

The aim of this work is to share the most interesting details of process and to show all potentials and beauty of flow chemistry.

Keywords: flow chemistry, continuous process, lithiation

[1] N. G. Anderson, *Org Process Re .Dev* 16 (2012) 852.



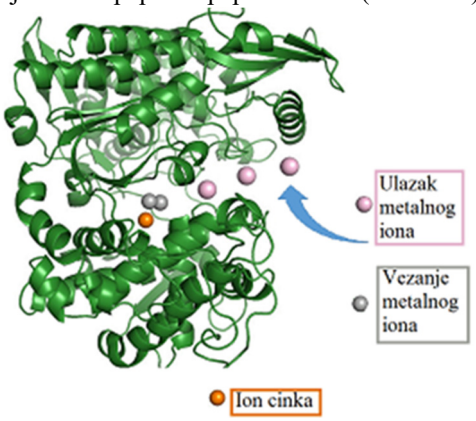
ISPITIVANJA INHIBICIJE DIPEPTIDIL PEPTIDAZE III METALNIM DIKATIONIMA

DIPEPTIDYL PEPTIDASE III INHIBITION TESTS BY METAL DICATIONS

Antonia Matić[1], Zrinka Karačić[1], Antonija Tomić[1], Hrvoje Brkić[2], Sanja Tomić[1]

[1]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*
[2]*Faculty of Medicine, J. J. Strossmayer University of Osijek, J. Huttlera 4, 31 000 Osijek, Hrvatska*

Od ranije je poznato da peptidaznu aktivnost ljudske dipeptidil peptidaze III (hDPP III) inhibira suvišak iona cinka [1]. Cilj ovog istraživanja je utvrditi utjecaje različitih koncentracija metalnih dikationa: Zn^{2+}, Mn^{2+}, Co^{2+} i Cu^{2+} na aktivnost hDPP III, te identificirati inhibitorsko vezno mjesto metala. Postojanje inhibitornog veznog mjesta metala pretpostavljeno je na temelju strukturne sličnosti aktivnog mjesta hDPP III i termolizina kod kojeg je već dokazano vezanje drugog iona metala u neposrednoj blizini katalitički aktivnog iona (PDB: 1LND), te opaženog smanjenja aktivnosti hDPP III pri višim koncentracijama cinka [1].



Inhibicija hDPP III metalnim dikationima ispitat će se eksperimentalnim i računalnim metodama. Za potrebe eksperimentalnih istraživanja pripremljen je apoenzim, a njegovom inkubacijom različitim koncentracijama metalnih otopina pripremit će se četiri skupine holoenzima. U tako pripremljenim uzorcima koncentracije metala određivat će se masenom spektrometrijom visoke rezolucije s induktivno spregnutom plazmom (HR-ICP-MS), te mikrokalorimetrijskim metodama (izotermalna titracijska kalorimetrija, ITC). Kinetičkim mjerenjima ispitat će se aktivnost holoenzima. Molekulsko dinamičkim simulacijama u kombinaciji s računima slobodne energije vezanja pojedinih metalnih iona i kvantno mehaničkim - molekulsko mehaničkim računima pokušat će se identificirati najpovoljniji položaj drugog metalnog iona u blizini aktivnog mjesta hDPP III.
Rezultati ovih istraživanja trebali bi pružiti detaljnu submolekularnu sliku metalne ionske izmjene u hDPP III, otkriti položaj potencijalnog inhibitornog metalnog veznog mjesta u hDPP III i objasniti kako dodatni ion cinka utječe na vezanje i hidrolizu supstrata.

Ključne riječi: ljudska dipeptidil peptidaze III, metalni dikationi, apoenzim, holoenzim

[1] K. M. Fukasawa *et al*., *Biochim Biophys Acta1* 804 (2010) 2063.

ISTRAŽIVANJE SASTAVA I STABILNOSTI BRONČANE PATINE

INVESTIGATION OF THE COMPOSITION AND STABILITY OF BRONZE PATINA

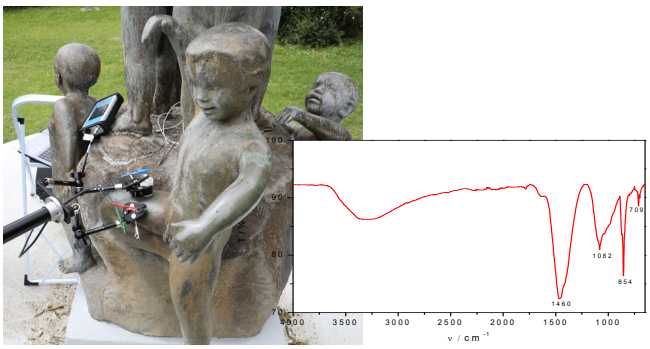
Dajana Mikić[1], Domagoj Šatović[2], Katarina Marušić[3], Neven Peko[4], Helena Otmačić Ćurković[1]

[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Marulićev trg 19, 10 000 Zagreb, Hrvatska*
[2]*Akademija likovnih umjetnosti, Sveučilište u Zagrebu, Ilica 85, 10 000 Zagreb, Hrvatska*
[3]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*
[4]*Gradski muzej Sisak, Kralja Tomisalva 10, 44 000 Sisak, Hrvatska*

Brončani predmeti izloženi korozivnom djelovanju atmosfere postupno se prekrivaju slojem korozijskih produkata, patinom. Ovisno o tome koji su korozivni plinovi ili aerosol prisutni u zraku mijenja se sastav kao i izgled patine koja nastaje na bronci Osim što ima estetsku funkciju, patina može pružati i korozijsku zaštitu bronci, što će ovisiti o sastavu i morfologiji nastale patine. U ovom radu prikazat će se rezultati istraživanja patine na skulpturama koje se nalaze u gradu Sisku i izložene su korozivnom utjecaju onečišćene atmosfere od sredine prošlog stoljeća.
Sastav bronce na kojoj je patina nastala analiziran je rentgenskom fluorescentnom analizom (XRF), a sastav patine metodom cikličke voltametrije i FTIR spektroskopije, dok je korozijska stabilnost analizirana metodom elektrokemijske impedancijske spektroskopije. Također je provedena i VIS spektrofotometrija s ciljem analize vizualnih svojstava bronce i patine. Na temelju dobivenih rezultata doneseni su zaključci o poveznici između sastava patine, njenog obojenja i njenih korozijskih svojstava.

Ključne riječi: elektrokemijska impedancijska spektroskopija, ciklička voltametrija, VIS spektroskopija, FTIR

Zahvala
Ovo istraživanje financirano je sredstvima Hrvatske zaklade za znanost projektom *IP-2019-04-5030.*



PRIMJENA NISKOTEMPERATURNOG EUTEKTIČKOG OTAPALA U PROČIŠĆAVANJU FCC BENZINA

APPLICATION OF DEEP EUTECTIC SOLVENT FOR FCC GASOLINE PURIFICATION

Anamarija Mitar, Tea Barbaro, Jasna Prlić Kardum

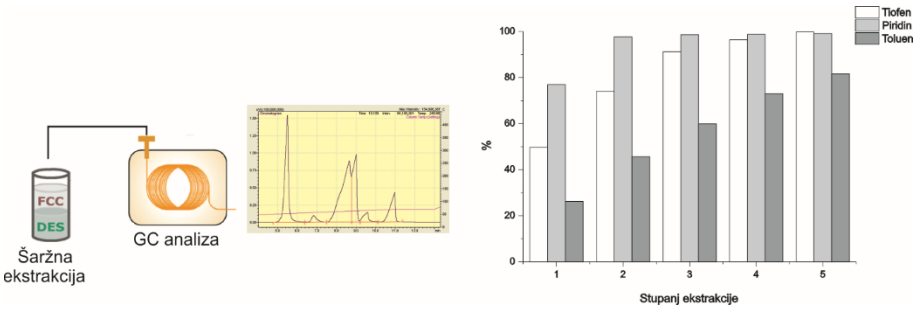
Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Obradom sirove nafte moguće je dobiti različite proizvode visoke vrijednosti. Jedan od takvih proizvoda je i motorni benzin dobiven miješanjem više vrsta frakcija, najvećim dijelom FCC benzinom. FCC benzin je frakcija u kojoj su prisutne znatne količine sumpornih spojeva koji utječu na smanjenje njegove kvalitete. Osim sumpornih spojeva, motorno gorivo sadrži puno aromata te dušikovih spojeva pa su ispušni plinovi nastali izgaranjem goriva bogati štetnim SOx i NOx spojevima, ugljikovim monoksidom te krutim česticama. Da bi se spriječila emisija štetnih tvari i zaštitio okoliš te zdravlje ljudi, potrebno je gorivo pročistiti, odnosno provesti procese desulfurizacije, denitrifikacije te dearomatizacije.

Kako su se niskotemperaturna eutektička otapala pokazala kao dobra zamjena štetnih organskih otapala, u radu je ispitana mogućnost pročišćavanja modelnog FCC benzina primjenom niskotemperaturnog eutektičkog otapala pripravljenog iz tetra-n-butilamonij-bromida i mravlje kiseline (TBAB/MK) u postupku šaržne ekstracije. Proces ekstrakcije je optimiran kako bi se količine štetnih tvari, tiofena, piridina i toluena svele na minimum. Definirano je optimalno vrijeme trajanja ekstrakcije, solvent odnos, broj okretaja miješala te je provedena višestupnjevita ekstrakcija. Također, ispitana je djelotvornost ekstrakcije ključnih komponenti primjenom regeneriranog otapala, TBAB/MK.

Rezultati su pokazali kako je optimalno vrijeme trajanja ekstrakcije t=20 min, pogodan solvent odnos S=1,0, dok promjena broja okretaja miješala nije značajno utjecala na djelotvornost ekstrakcije. Zadovoljavajuća djelotvornost ekstrakcije ostvarena je primjenom regeneriranog otapala pa se optimalni rezultati mogu očekivati u višestupnjevitoj ekstrakciji s regeneriranim otapalom.

Ključne riječi: denitrifikacija, desulfurizacija, FCC benzin, kapljevinska ekstrakcija, niskotemperaturno eutektičko otapalo.



KINETIKA OKSIDACIJE ČAĐE S NANOČESTICAMA CERIJEVOG(IV) OKSIDA DOPIRANOG MANGANOM

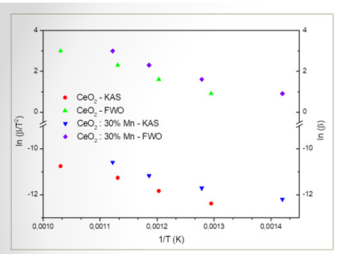
DIESEL SOOT OXIDATION KINETICS OF Mn-DOPED CERIA NANOPARTICLES

Ivana Katarina Munda, Andrej Terzin, Stanislav Kurajica

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

Due to incomplete combustion of fuel, diesel engines produce soot particles which are harmful to human health and pollute the environment. In order to reduce soot emission from vehicles a Diesel Particulate Filter (DPF) is utilized. In order to be capable of passive regeneration DPF should contain appropriate catalysts enabling soot oxidation at low temperature. For this purpose nanosized ceria (CeO_2), can be used. In order to enhance its catalytic properties, ceria is often doped with various elements. It was shown that the incorporation of manganese atoms in the ceria crystal lattice can improve its catalytic properties such as oxygen storage and oxygen mobility, as well as its thermal stability. Therefore, Mn-doped ceria catalysts, $Ce_{1-x}Mn_xO_2$, where x = 0; 0.1; 0.2 and 0.3 were prepared by hydrothermal synthesis followed by thermal treatment. The structural, textural and morphological properties were investigated by X-Ray diffraction (XRD), Brunauer-Emmett-Teller model (BET) and transition electron microscopy (TEM). Catalytic soot oxidation activity as well as kinetics in the presence of catalysts was analyzed by thermogravimetric analysis. It was established that $Ce_{1-x}Mn_xO_2$ solid solutions with nanosized particles are formed, the increase of SSA with the amount of manganese was also noted. Flynn-Wall-Ozawa and Kissinger-Akahira-Sunose kinetic models were used to determine the activation energy of prepared catalysts. Results show that with the increase of manganese ions in the prepared solid solutions, soot oxidation process rate increases while the activation energy decreases. Since these types of catalysts would require less energy for regeneration, hydrothermally-derived, Mn-doped ceria have great potential for utilization in superior DPF fabrication.

Keywords: oxidation, soot, ceria, doping



Calculated values of conversion of soot oxidation based on KAS and FWO kinetic models

Activation energies for soot and CeO_2 catalyzed soot oxidation

Sample	Soot	CeO_2	CeO_2 : 30% Mn
KAS (kJ/mol)	64	52	44
FWO (kJ/mol)	84	63	54

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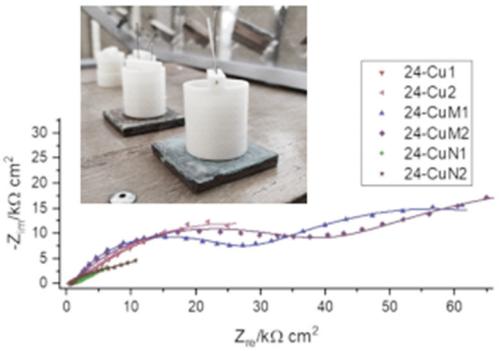
ELEKTROKEMIJSKA KARAKTERIZACIJA BRONCE IZLOŽENE VANJSKOJ ATMOSFERI

ELECTROCHEMICAL CHARACTERIZATION OF BRONZE EXPOSED TO OUTDOOR ATMOSPHERE

Helena Otmačić Ćurković, Dajana Mikić, Luka Bera,
Ema Kovačević, Marijana Marcelja

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Marulićev trg 19, 10 000 Zagreb, Hrvatska



Brončane skulpture čine važan dio umjetničke i kulturne baštine. Degradacija bronce kao i patine koja je na njoj nastala procesom atmosferske korozije (prirodna patina) ili je formirana u umjetničkoj radionici kemijskim putem (umjetna patina) javlja se uslijed korozivnog djelovanja okoliša, posebice u slučaju onečišćenje atmosfere.
Elektrokemijske metode, posebice elektrokemijska impedancijska spektroskopija (EIS), pogodne su za analizu korozijske otpornosti materijala. Za provedbu ispitivanja EIS-om potrebno je koristiti elektrokemijsku ćeliju, što kod terenskih istraživanja nije jednostavno zbog zakrivljenosti i hrapavosti predmeta. U novije vrijeme su stoga razvijene elektrokemijske ćelije koje umjesto vodenog medija koriste elektrolite u obliku gela. U ovom radu konstruirana je elektrokemijska ćelija na bazi agara [1]. Kako bi se ispitala njena primjenjivost za ispitivanja su izabrane tri vrste brončanih materijala pri čemu je na dijelu uzoraka formirana umjetna patina. Patinirani i nepatinirani uzorci izloženi su korozivnom utjecaju gradske atmosfere te su periodični karakterizirani EIS-om. Analizom dobivenih rezultata utvrđen o je da se primjenom elektrokemijske ćelije s agarnim elektrolitom mogu dobiti zadovoljavajući EIS spektri koji omogućuju karakterizaciju bronce i njene patine. Također je utvrđen utjecaj vremenskih prilika (temperatura, padaline) na dobivene rezultate. U konačnici je ova metoda primijenjena za istraživanje brončanih umjetničkih skulptura koje su dulji niz godina izložene gradskoj korozivnoj atmosferi.

Ključne riječi: elektrokemijska impedancijska spektroskopija, bronca, atmosferska korozija

[1] B. Ramírez Barat *et al*., *Sens Actuators B* 261 (2018) 572.

Zahvala
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UTJECAJ NATRIJEVOG ALGINATA NA TOPLINSKA SVOJSTVA POLI(ETILEN-OKSIDA)

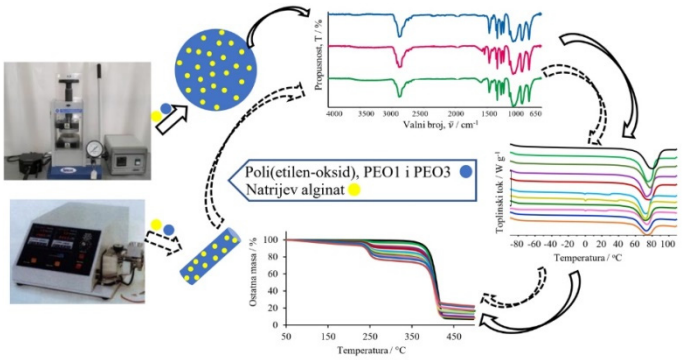
INFLUENCE OF SODIUM ALGINATE ON THE THERMAL PROPERTIES OF POLY(ETHYLENE OXIDE)

Sanja Perinović Jozić, Ružica Brkić, Branka Andričić, Nataša Stipanelov Vrandečić

Kemijsko-tehnološki fakultet, Sveučilište u Splitu, Ruđera Boškovića 35, 21 000 Split, Hrvatska

Modifikacija poli(etilen-oksida) (PEO) molekulnih masa 100 000 (PEO1) i 300 000 (PEO3) g mol^{-1} provedena je dodatkom natrijevog alginata (NaAlg) kao prirodnog polimernog punila s ciljem smanjivanja stupnja kristalizacije PEO-a. Uzorci su pripremljeni ekstrudiranjem i prešanjem u svrhu odabira optimalnog načina priprave te analize utjecaja postupaka priprave na svojstva kompozita. Također, dobiveni su uzorci različitih geometrija i dimenzija što može imati utjecaja na kristalizaciju PEO-a u kompozitima. Uočeno je da je ekstruzija optimalna metoda priprave kompozita s PEO1, a prešanje je optimalno za pripremu kompozita s PEO3. Primjenom infracrvene spektroskopije s Fouierovom transformacijom (FTIR) potvrđena je interakcija PEO1 i NaAlg u ekstrudiranim kompozitima. Diferencijalnom pretražnom kalorimetrijom (DSC) ispitan je utjecaj metoda priprave i dodatka alginata na toplinska svojstva i kristalnost PEO-a. Prema dobivenim rezultatima u ekstrudiranim kompozitima PEO1 i NaAlg dolazi do pomaka tališta k nižim temperaturama, ali nema značajne promjene udjela kristalne faze PEO1. Razvidan je utjecaj različitih postupaka priprave uzoraka te se kod isprešanih kompozita uočava pojava preklopljenih endotermi taljenja i niži stupanj kristalizacije PEO-a. Toplinska postojanost kompozita istraživana je primjenom neizotermne termogravimetrije (TG). Svi pripravljeni PEO/NaAlg kompoziti razgrađuju se u tri stupnja razgradnje. NaAlg pogoršava toplinsku postojanost kompozita, ali nije uočen utjecaj molekulne mase i postupaka priprave uzoraka na toplinsku postojanost kompozita.

Ključne riječi: poli(etilen-oksid), natrijev alginat, vodikova veza, toplinska svojstva, toplinska postojanost



EKSTRAKCIJA GLICEROLA I GLICERIDA IZ RAZLIČITIH BIODIZELA

EXTRACTION OF GLYCEROL AND GLYCERIDES FROM VARIOUS BIODIESEL SAMPLES

Ana Petračić[1], Aleksandra Sander[1], Jelena Parlov-Vuković[2], Lana Husinec[2]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*

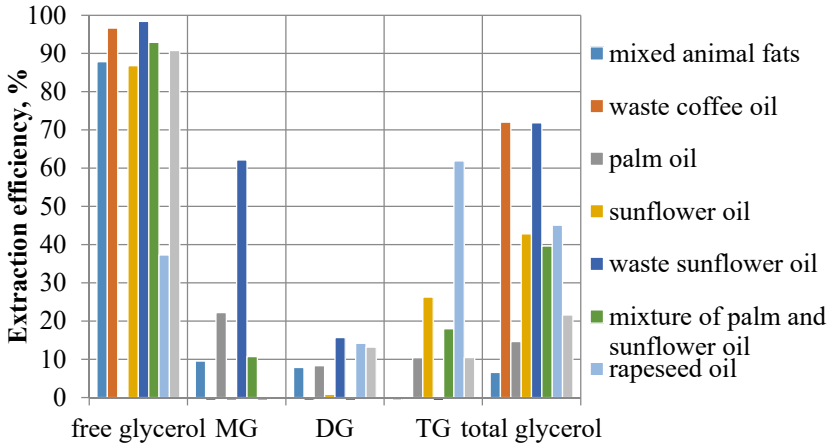
[2]*INA – Industrija nafte d. d., Lovinčićeva ulica 4, 10 000 Zagreb, Croatia*

The goal of this work was to synthesize biodiesel from various feedstocks and to extract glycerol and glycerides from produced biodiesel samples with choline chloride based deep eutectic solvent. Biodiesel samples were synthesized via base-catalysed transesterification with methanol. Batch extraction experiments were conducted with choline chloride – ethylene glycol (molar ratio 1:2.5) deep eutectic solvent at room conditions (for oils) and at an elevated temperature (60 °C, for fats that were not liquid at room conditions). Biodiesel prepared from the mixture of palm and sunflower oil was also purified continuously, in a Karr column with the same solvent.

Glycerol and glycerides concentrations were determined using gas chromatography and samples were characterised using Fourier transformation infrared spectroscopy and proton nuclear magnetic resonance spectroscopy.

Choline chloride based solvent proved to be efficient for purification of biodiesels, especially for free glycerol. The greatest efficiency was achieved for the samples with the highest concentrations of glycerol and glycerides due to the higher driving force. The highest quality biodiesel was produced from fresh and waste sunflower oil and deacidified waste animal fat.

Keywords: biodiesel, deep eutectic solvent, extraction, transesterification



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UTJECAJ MOLEKULSKIH MEĐUDJELOVANJA NA SVOJSTVA MJEŠAVINA MINERALNIH I OBNOVLJIVIH DIZELSKIH GORIVA

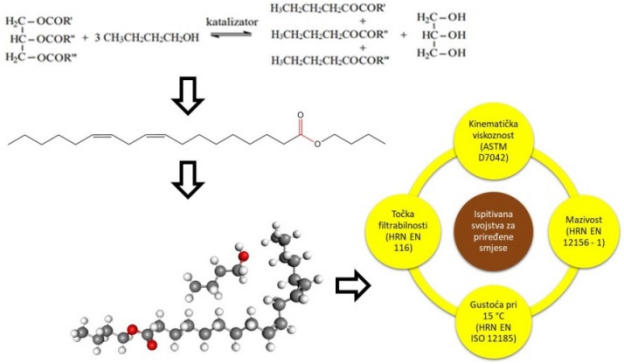
EFFECT OF MOLECULAR INTERACTIONS ON PROPERTIES OF MINERAL AND RENEWABLE DIESEL BLENDS

Mario Pipunić[1], Lucija Konjević[2], Fabio Faraguna[3], Ante Jukić[3]

[1]Cirrus Centar d.o.o., Zlatka Šulentića 4, 10 000 Zagreb
[2]INA – Industrija nafte d.d., Lovinčićeva ulica 4, 10 000 Zagreb
[3]Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Maruličev trg 19, 10 000 Zagreb

Biodizel je ester viših masnih kiselina i nižih alkohola koji se zasebno ili u smjesi s konvencionalnim dizelom upotrebljava kao gorivo za dizelske motore. Mineralni dizel i biodizel se miješaju u različitim udjelima, a dobivaju se goriva poboljšanih svojstava naspram polaznih sastavnica – bolja mazivost u odnosu na čisti mineralni dizel te viša toplinska vrijednost i niža viskoznost u odnosu na čisti biodizel. Kao niži alkohol za proizvodnju biodizela uobičajeno se upotrebljava metanol dobiven iz fosilnih sirovina, ali se u novije vrijeme upotrebljavaju i bioetanol te biobutanol. Butilni esteri viših masnih kiselina (FABE) proizvode se iz *n*-butanola i biljnog ulja reakcijom transesterifikacije pri čemu se butanol u reakcijsku smjesu uvodi u suvišku. Svrha ovog rada je bila istražiti utjecaj molekulskih međudjelovanja na neka svojstva mješavina mineralnog dizela, FABE i *n*-butanola u različitim udjelima. Ispitani su gustoća, niskotemperaturna filtrabilnost, kinematička viskoznost i mazivost za mješavine do udjela FABE od 10 vol. % i do udjela *n*-butanola od 10 vol. %. Najveće odstupanje od idealnog ponašanja ustanovljeno je za kinematičku viskoznost i mazivost. Uzrok odstupanja su molekulska međudjelovanja, odnosno specifična adsorpcija na metalnu površinu.

Ključne riječi: biodizel, dizelsko gorivo, molekulska međudjelovanja, svojstva



PROIZVODNJA BIOPOLIMERA U HORIZONTALNOM ROTIRAJUĆEM CIJEVNOM BIOREAKTORU: RAZVOJ MATEMATIČKOG MODELA

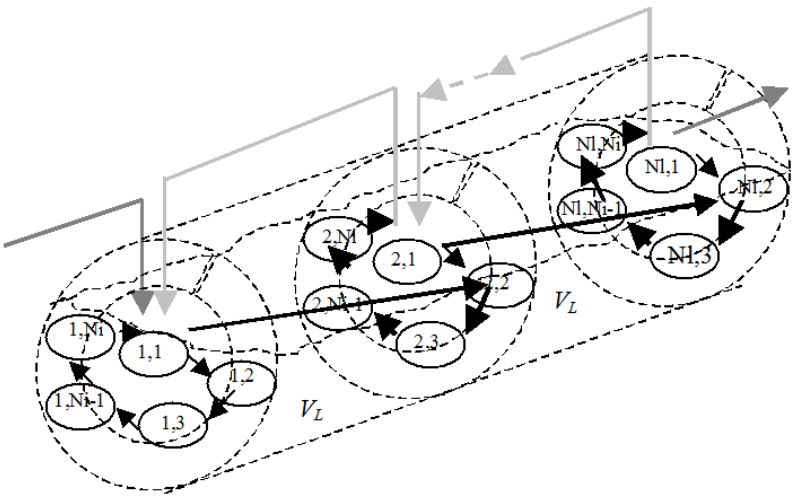
BIOPOLYMERS PRODUCTION IN THE HORIZONTAL ROTATING TUBULAR BIOREACTOR: MATHEMATICAL MODEL DEVELOPMENT

Tonči Rezić, Matea Marošević, Božidar Šantek

Faculty of Food Technology and Biotechnology, University of Zagreb,
Pierottijeva 6, 10 000 Zagreb, Croatia

Proposed concept of structured integral model is under development and its represent alternative to presented statistical model. Developed model integrate: mixing model, diffusion model and metabolic fluxes/kinetic model. However, mathematical solution, interpretation and application of this model are significantly more complex compare to statistical model. Moreover, it contributes to systematic understanding of biosystem behavior on the three scale of bioprocess: A) bioreactor scale, B) microbial cell scale and C) enzyme scale. Application of structured integral model in Horizontal Rotating Tubular Bioreactor (HRTB) performances optimization will be big step forward to the comprehended understanding of all bioprocess parametric interaction and its effect in overall biopolymers production in HRTB as well as prediction of biosystem behavior on the emphasized scales.

*Keywords:*biopolymers, Horizontal Rotating Tubular Bioreactor, mathematical model



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MODELIRANJE KOPOLIMERIZACIJSKIH REAKTIVNOSTI TERNARNOG SUSTAVA METIL-METAKRILATA, OKTADECIL-METAKRILATA I *TERT*-BUTILAMINOETIL-METAKRILATA

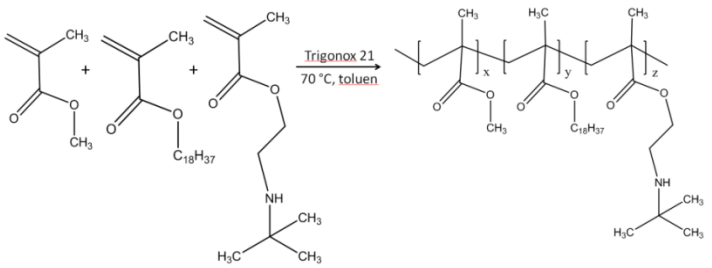
MODELING OF COPOLYMERIZATION REACTIVITIES OF THE TERNARY SYSTEM OF METHYL METHACRYLATE, OCTADECYL METHACRYLATE AND *TERT*-BUTYLAMINOETHYL METHACRYLATE

Josip Sacher, Fabio Faraguna, Roko Blažic, Ante Jukić, Elvira Vidović

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb

Kopolimeri na osnovi alkil-metakrilata često se koriste kao aditivi u mazivim uljima pri čemu utječu na njihova reološka svojstva i tecište. Terpolimerizacijom alkil-metakrilatnih monomera s nekim funkcionalnim komonomerom, primjerice *tert*-butilaminoetil-metakrilataom, otvara se mogućnost značajnog utjecaja na primjenska svojstva kao što su adhezivnost, hidrofobnost, topljivost, i slično. Kako bi se sintetizirali polimeri željenog sastava potrebno je poznavati omjere kopolimerizacijske reaktivnosti s obzirom da o njima ovisi sastav nastalog polimera. Jednostavna procjena omjera kopolimerizacijske reaktivnosti ternarnih sustava koristi omjere kopolimerizacijske reaktivnosti dobivene za binarne sustave odgovarajućih monomernih parova. Na taj način zanemaruje se utjecaj trećeg komonomera na proces polimerizacije što često dovodi do pogrešne procjene parametara kopolimerizacijske reaktivnosti i pogrešne procjene sastava terpolimera. U ovom radu izračun omjera kopolimerizacijske reaktivnosti za ternarni sustav proveden je pomoću preoblikovane Alfrey-Goldfingerove jednadžbe. Nadalje, za izračun je korištena metoda koja uzima u obzir postojanje pogrešaka u zavisnim i nezavisnim varijablama (*engl*. Errors in Variables Model). Priprava terpolimera iz monomera metil-metakrilata, oktadecil-metakrilata i *tert*-butilaminoetil-metakrilata provedena je reakcijom polimerizacije do niskih konverzija (< 10 mas. %) izotermalno pri temperaturi od 70 °C uz peroksidni inicijator. Sastav terpolimera određen je pomoću NMR spektroskopije.

Ključne riječi: matematičko modeliranje, omjeri kopolimerizacijske reaktivnosti, metakrilati



Sinteza *tert*-butilaminoetil-metakrilata i alkil-metakrilatnih terpolimera

PROIZVODNJA, PROČIŠĆAVANJE I KARAKTERIZACIJA ENZIMA LIPAZA PORIJEKLOM IZ *Thermomyces lanuginosus*

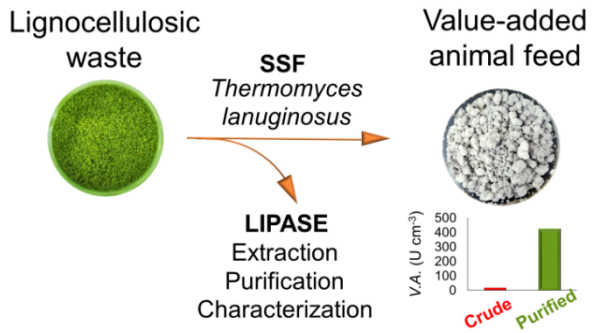
PRODUCTION, PURIFICATION AND CHARACTERIZATION OF LIPASE FROM *Thermomyces lanuginosus*

Darijo Šibalić[1], Anita Šalić[2], Ana Jurinjak Tušek[3], Tea Sokač[2], Klara Brekalo[1], Bruno Zelić[2], Marina Tišma[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, Osijek, 31 000, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, Zagreb, 10 000, Croatia*
[3]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*

The aim of the research was to determinate optimal process conditions for *Thermomyces lanuginosus* lipase (TLL) production during solid-state cultivation on hull-less pumpkin oil pomace. Numerical optimization of the five independent variables (substrate mass (m_s), inoculum size (n), moisture content (w_{H2O}), fermentation time (t) and temperature (T)) which affected the TLL production was evaluated using response surface methodology. To predict the TLL production, reduced quadratic mathematical model was proposed and model validation was performed under optimized conditions (m_s = 50 g, n = 7, w_{H2O} = 60 %, t = 2 days, T = 45 °C) with 95 % accuracy. The simplified purification method of the TLL was developed which includes a single-step vacuum-evaporation technique. Produced TLL liquid preparation with high volumetric activity (422 U cm^{-3}) was obeyed. TLL was characterized as thermostable biocatalyst which possesses stability in a variety of organic solvents, food oils and fats. The sustainability of the process was confirmed by the green chemistry matrix of the E-factor and process mass index.

Keywords: Thermomyces lanuginosus, lipase, enzyme purification, sustainability



DEZINFEKCIJSKA SREDSTVA NA BAZI KVATERNIH AMONIJEVIH SOLI SMANJUJU EKSPRESIJU LISTERIOLIZINA O U *Listeria monocytogenes*

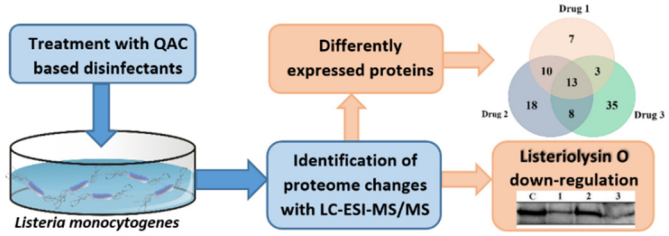
QUATERNARY AMMONIUM SALT BASED DISINFECTANTS REDUCE THE EXPRESSION OF LISTERIOLYSIN O IN *Listeria monocytogenes*

Martina Šrajer Gajdošik[1], Marija Begić[2], Dajana Gašo-Sokač[3], Hrvoje Pavlović[3], Olga Shevchuk[4], Uroš Andjelković[5], Tamara Martinović[6], Djuro Josić[2,6]

[1]*Department of Chemistry, J.J. Strossmayer University, Cara Hadrijana 8A, 31 000 Osijek, Croatia*
[2]*Faculty of Medicine, Juraj Dobrila University, Zagrebačka 30, 52 100 Pula, Croatia*
[3]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[4]*Leibniz-Institut für Analytische Wissenschaften, Bunsen-Kirchhoff 11, 44001-44388 Dortmund, Germany*
[5]*Chemical Institute, University of Belgrade, Njegoševa 12, 11 000 Belgrade, Serbia*
[6]*Department of Biotechnology, University of Rijeka, Radmile Matejčić 2, 51 000 Rijeka, Croatia*

Bacterial resistance, caused among others by frequent use of disinfectants and antibiotics, has become one of the major problems in food industry. Therefore, better understanding of mechanisms of action of disinfectants is of great importance. Quaternary ammonium salts (QAC) have been extensively used as antimicrobial agents in food-processing industries and medicine. In this study, proteomic methods were used to identify changes in the proteome of foodborne pathogen *Listeria monocytogenes* after treatment with three QAC based disinfectants. LC-MS/MS analysis, followed by gene ontology searching, reveals disturbance in the synthesis of plasma membrane proteins and cell wall proteoglycans in treated samples. Down-regulation of some of key proteins from this group, that are important for bacterial growth, is also observed. Additionally, it is shown that Listeriolysin O (LLO), the major virulence factor of *L. monocytogenes*, is significantly down-regulated after treatment with each of the three investigated inhibitors. These results contribute to the already hypothesized mechanism of action of QAC-based inhibitors in Gram-positive bacteria that results in the disturbance of key cell surface proteins and proteoglycans. Furthermore, significant inhibition of Listeriolysin O suggests that this protein can be used as potential biomarker candidate for food contamination with *L. monocytogenes*.

Keywords: foodborne pathogens, listeriolysin O, mechanism of action, proteome changes



RAZVOJ PROCESA DEPROTEKCIJE KORIŠTENJEM DIZAJNA EKSPERIMENATA

A DESIGN OF EXPERIMENTS APPROACH TO A ROBUST FINAL DEPROTECTION PROCESS

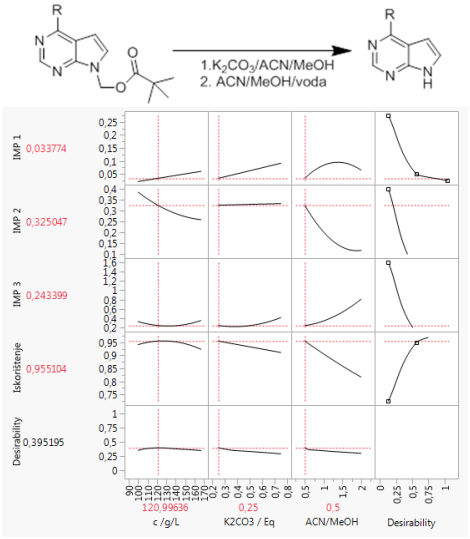
Ivan Vrban, Franjo Jović, Eugen Marcelić

PLIVA Hrvatska d.o.o., Prilaz baruna Filipovića 25, 10 000 Zagreb, Hrvatska

Pristup razvoju procesa korištenjem dizajna eksperimenata (DoE) se koristi pri optimizaciji procesa tj. čistoće proizvoda, iskorištenja procesa te sadržaja kritičnih onečišćenja pri procesu skidanja pivalatne zaštite sa pirola u molekuli deazapurina na finalnoj molekuli djelatne farmaceutske tvari (API-ja). Proces skidanja pivalata se provodi sustavu otapala acetonitril/metanol, s K_2CO_3 kao bazom, pri čemu omjer otapala, koncentracija, te miješanje (suspendiranje) igraju važnu ulogu. Pri optimiranju procesa korišten je DoE – Box Behnken zbog mogućnosti modeliranja nelinearnih (kvadratnih) interakcija. Provedeni DoE ostvaruje istraživanje procesnog prostora dok istovremeno omogućuje optimalne kemijske transformacije i varijabilnost procesa kao i robusnu kontrolu onečišćenja. Molni udio K_2CO_3 je najvažniji parametar koji mora biti nizak, jer se u protivnom generira deazapurin alkohol, genotoksično onečišćenje djelomičnom hidrolizom pivalata. Vrlo važno je pratiti i kinetiku reakcije jer se smanjenjem molnog omjera K_2CO_3 bitno produljuje reakcija. Tako optimirani proces je uvećan na proizvodno/pilotno mjerilo te je proveden proces na kilogramskoj skali uz visoku čistoću produkta.

Keywords: dizajn eksperimenata, matematički model, optimiranje, deprotekcija

[1] J. O'Shea, Tetrahedron 74 (2018) 6182-6186.



DOBIVANJE BIOPOLIMERA KITOZANA IZ OTPADNIH OKLOPA RAKOVA

OBTAINING CHITOSAN BIOPOLYMER FROM SHRIMP SHELL WASTE

Magdalena Vujasinović, Andrea Matejaš, Ema Pavić, Zvonimir Katančić

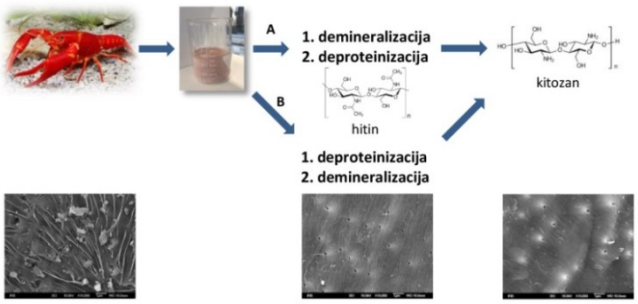
Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Kitozan je biopolimer linearne, semikristalične polisaharidne strukture građen od jedinica N-acetil-D-glukozamina i D-glukozamina. Dobiva se postupkom deacetilacije biopolimera hitina kojeg je kemijskom ili biološkom ekstrakcijom moguće dobiti iz egzoskeleta mnogih životinja pa tako i otpadnih oklopa rakova. Kitozan se zbog svojih antibakterijskih svojstava, biorazgradivosti bez toksičnog otpada i biokompatibilnosti pokazao kao dobar materijal u području zaštite okoliša, medicine i farmacije.

Cilj ovog rada bio je provesti kemijsku ekstrakciju hitina iz otpadnih oklopa rakova i zatim ga prevesti u kitozan. Izoliranje hitina provedeno je na dva načina, i to tako da je u prvom slučaju prvo izveden proces demineralizacije, a zatim deproteinizacije. U oba postupka provedeno optimiranje vremena trajanja procesa demineralizacije (2 ili 4 h) i procesa deproteinizacije (3 ili 5 h) koji su ključni procesi pri ekstrakciji. Izolirani hitin, izdvojen na oba načina, podvrgnut je deacetiliranju čime je dobiven kitozan kojem je određen stupanj acetilacije. Karakterizacija je provedena termogravimetrijskom analizom (TGA), infracrvenom spektroskopijom s Fourierovom transformacijom (FTIR) te ispitivanjem morfološke strukture pretražnom elektronskom mikroskopijom (SEM).

FTIR spektroskopija potvrdila je da je hitin uspješno izdvojen iz oklopa rakova na oba načina, te da je uspješno deacetiliran u kitozan. Optimiranje uvjeta ekstrakcije pokazalo je da se gotovo 100 %-tna demineralizacije postiže već nakon 2 h dok je za potpunu deproteinizaciju potrebno dalje optimirati proces jer nakon 5 h taj postotak dostiže 65 %, pri čemu se veći postotak uklanjanja postiže ukoliko se prvo provodi proces deproteinizacije, a zatim proces demineralizacije. FTIR spektroskopijom izračunat postotak acetilacije za dobivene uzorke iznosi 21-28 % što je na razini komercijalno dostupnog kitozana.

Ključne riječi: otpad rakova, hitin, kitozan, kemijska ekstrakcija



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EKSTRAKCIJSKO PROČIŠĆAVANJE BENZINA PRIMJENOM NISKOTEMPERATURNIH EUTEKTIČNIH OTAPALA MODIFICIRANIH CINKOVIM KLORIDOM

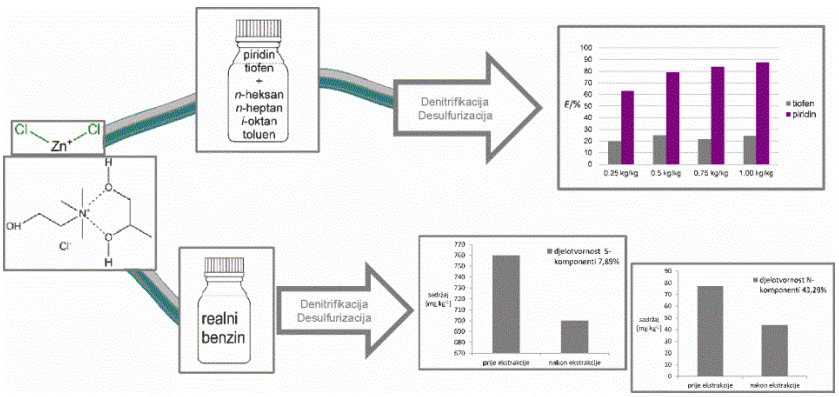
EXTRACTIVE PURIFICATION OF GASOLINE USING DEEP EUTECTIC SOLVENTS MODIFIED WITH ZINC CHLORIDE

Kristina Zagajski Kučan, Luka Vlašić, Marko Rogošić

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu,
Maruličev trg 19, 10 000 Zagreb, Hrvatska

Ekstrakcijska denitrifikacija i desulfurizacija benzina predložena je kao metoda koja se može integrirati s klasičnom hidrodesulfurizacijom. Provodi se pri blagim radnim uvjetima (atmosferski tlak i temperatura) što vodi smanjenju potrošnje energije, a ne zahtijeva ni skupi vodik. Niskotemperaturna eutektična otapala priređuju se kombinacijama dviju komponenti – donora i akceptora vodikove veze – a izbor tih komponenti izravno utječe na djelotvornost ekstrakcije. Ekstrakcijska se djelotvornost dalje može povećati dodatkom metalnih soli osnovnoj kombinaciji komponenata otapala. U ovom je radu istražen ekstrakcijski postupak desulfurizacije i denitrifikacije modelnog i realnog FCC-benzina primjenom eutektičnog otapala na osnovi kolin-klorida (ChCl) i propilen-glikola (PG) modificiranog cinkovim kloridom. Istražena su četiri masena omjera otapalo:benzin (0,25, 0,50, 0,75 i 1,00). S posljednjim je postignuta najveća djelotvornost (89,2 % za denitrifikaciju). Provedena je i višestupanjska ekstrakcija pri čemu se djelotvornost ekstrakcije povećavala s brojem stupnjeva. S povećanjem broja ekstrakcijskih stupnjeva smanjuje se kapacitet otapala, no regeneraciju otapala moguće je provesti vakuumskim uparavanjem ekstrahiranih komponenti između pojedinih stupnjeva. Kod realnog uzorka FCC-benzina postignuta je denitrifikacijska djelotvornost od 43,3 % u jednom stupnju. Ispitano otapalo pogodnije je za denitrifikaciju nego desulfurizaciju modelnog i realnog benzina.

Ključne riječi: niskotemperaturno eutektično otapalo, cink-klorid, denitrifikacija, desulfurizacija, FCC-benzin



Sekcija: Prehrambena tehnologija i biotehnologija
Topic: Food Technology and Biotechnology

UTJECAJ DODATKA KAKAOVE LJUSKE NA FIZIKALNA SVOJSTVA ČOKOLADE

EFFECT OF COCOA SHELL ADDITION ON PHYSICAL PROPERTIES OF CHOCOLATE

Veronika Barišić[1], Ivana Lončarević[2], Jovana Petrović[2], Ivana Flanjak[1], Antun Jozinović[1], Drago Šubarić[1], Jurislav Babić[1], Borislav Miličević[1], Đurđica Ačkar[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia;*
[2]*Faculty of Technology Novi Sad, University of Novi Sad, Bulevar cara Lazara 1, 21 000 Novi Sad, Serbia*

Chocolate is one of the most desirable confectionery products for consumers of all ages. Chocolate industry generates large amount of by-products in pre-processing and processing phases, among which is cocoa shell. It is separated from the bean before or after the roasting. Since this by-product is rich in dietary fibers, proteins, polyphenols and methylxanthines, it represents great material for the enrichment of nutritionally poor products.
The aim of this study was to determine effect of cocoa shell addition on physical properties of milk and dark chocolates. Cocoa shell was obtained after roasting and treated with high voltage electrical discharge (HVED) in concentration 3 %, at 40 Hz, during 15 minutes. Chocolates were produced in laboratory ball mill with addition of 5, 10 and 15 % of treated and untreated cocoa shell in dark chocolate and 2.5 and 5 % of treated and untreated cocoa shell in milk chocolates. After production Casson viscosity and yield stress, hardness and particle size distribution were determined. Casson viscosity and yield stress showed that dark chocolates had lower rheological values compared to milk chocolates. Also, addition of cocoa shell increased viscosity of chocolates, whereas HVED treated cocoa shell had greater effect. With addition of cocoa shell, hardness increased for milk chocolates and decreased for dark. All chocolates with added cocoa shell had larger particles compared to chocolates without shell. Also, HVED treated cocoa shell had greater effect on increase of particle size.

Keywords: chocolate, cocoa shell, physical properties

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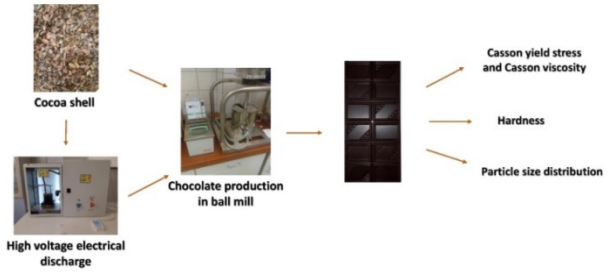


RAZVOJ INTERNETSKE OBRAZOVNE PLATFORME ZA PODRŠKU MALIM PROIZVOĐAČIMA U RIJEŠAVANJU PROBLEMA TIJEKOM PROIZVODNJE SIRA

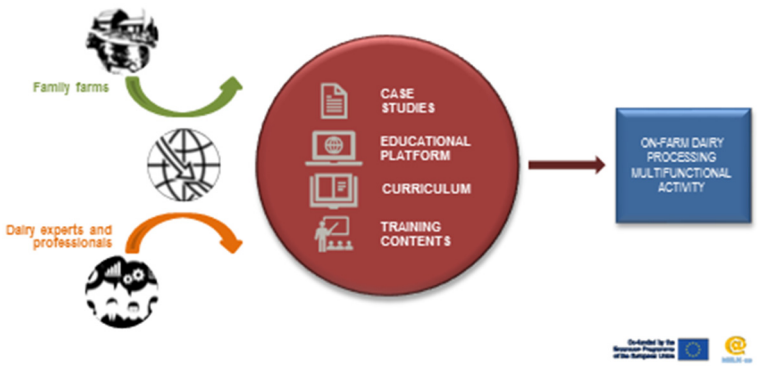
DEVELOPMENT OF AN ONLINE EDUCATIONAL PLATFORM AS SUPPORT TO THE SMALL DAIRY PRODUCERS FACING THE PROBLEMS DURING CHEESE PRODUCTION

Marijana Blažić, Elizabeta Kralj, Ines Cindrić, Jasna Halambek, Bojan Matijević, Sandra Zavadlav

Karlovac University of Applied Sciences, Trg J. J. Strossmayera 9, 47 000 Karlovac, Croatia

The aim of this research was to set up the basis for development of an online platform with training programme that is going to equip farmers with the necessary knowledge, skills and competencies for the establishment of an on-farm dairy processing multifunctional activity. Research team held several meetings with the representatives of small dairy producers from different parts of the country to determine problems they encounter and discuss about the improvement abilities. Most of them reported problems related with cheese hygiene during ripening process and financing problems related with market demands. Collected findings slightly differed depending on the location of the production facility. Research team identified the need of several training and seminars related to finance with an emphasis on the banking sector and tourism management, as well as trainings related to cheese ripening. Online platform will enable easier problem-solving with expert counselling and provide multiple training and seminars depending on the needs of the small producer. Affordable methods for preventing the contamination during ripening should also be one of the topics, so a further research is focusing the possibility of application a modified and ozonized atmosphere or overpressure in cheese ripening chambers for optimization of cheese hygiene.

Keywords: cheese quality, educational platform, cheese ripening, support to producers



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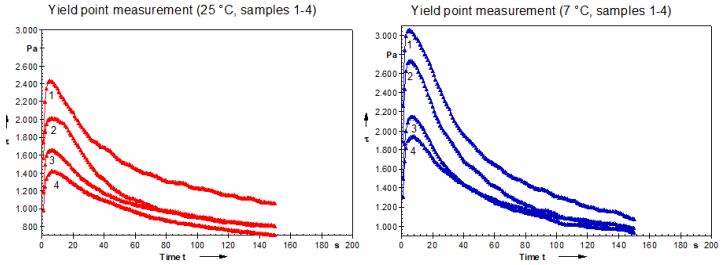
ZNAČAJ REOLOŠKIH ISPITIVANJA U RAZVOJU PREHRAMBENIH PROIZVODA

THE IMPORTANCE OF RHEOLOGICAL EXAMINATION IN THE DEVELOPMENT OF FOOD PRODUCTS

Josip Bebek, Tanja Cvetković, Jasmina Ranilović, Hrvoje Trojak
Podravka d.d., Research and development, Ante Starčevića 32, 48 000 Koprivnica, Croatia

Consistency significantly affects overall consumer acceptance of the food product. Although characteristics of consistency (spreadability, mouthfeel, chewiness) are frequently evaluated subjectively by the consumer, measuring of certain rheological parameters could contribute to the food development process, particularly in achieving desirable consistency. The goal of this study was to show the significance of rheological examination of viscosity and yield point in the development of desirable fish pate spreadability.
Four different laboratory fish pate samples were prepared for 2 types of rheological examination; measurement of viscosity and yield point. Both analyses were conducted on a rotational rheometer RheolabQC at temperatures of 25 °C and 7 °C using the following measuring systems; CC27 and ST-22-4V-40. Viscosity was measured using shear rate from 0.1 to 100 s^{-1} and with the CC27 measuring system. Yield point was measured using constant shear rate of 1 s^{-1} and with the ST-22-4V-40 measuring system. The range of testing viscosity at 25 °C was between 1160 and 2570 Pas and at 7 °C between 1520 and 3310 Pas, while the range of yield point at 25 °C was between 1420 and 2540 Pa and at 7 °C between 1850 and 3230.
The results of viscosity and yield point measurement of each laboratory fish pate sample showed different values at both temperatures which was expected considering different product composition and both measurements correlate proportionally for each sample. Higher viscosity and yield point values indicate a firmer consistency and harder spreadability that declined over time equally. At 7 °C viscosity and yield point values were higher than at 25 °C for each sample which suggests firmer consisteny and harder spreadability of pate at lower temperatures.
The rheological examination in this study has shown to be an important indicator to the food product developers in adjusting final food composition. Depending on the desired storage conditions and overall sensorial quality of fish pate, quantity and origin of ingredients can significantly influence the final product consistency.

Keywords: rheology, viscosity, yield point, pate, food development



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ENKAPSULACIJA FENOLA ARONIJE NA VLAKNA CITRUSA

ENCAPSULATION OF CHOKEBERRY PHENOLICS ON CITRUS FIBERS

Ivana Buljeta[1], Ivana Balen[1], Josip Šimunović[2], Anita Pichler[1], Mirela Kopjar[1]

[1]Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia
[2] Department of Food, Bioprocessing and Nutrition Sciences, North Carolina State University, Raleigh, NC 27 695, USA

Dietary fibers and phenolic are plant compounds well known for their positive effect on health. Possibility of application of citrus fibers for encapsulation of chokeberry phenolics was studied in this research. For complexation, the content of chokeberry juice was constant and citrus fiber content varied (1, 2, 3 and 4%). To obtain dried matrices freeze-drying was applied. Evaluation of adsorption of phenolics, anthocyanins and proantocyanidins, as well as antioxidant activity, colour and FTIR screening was conducted. With the increase of used fibers for complexation decrease of adsorption of phenolics, anthocyanins and proanthocyanidins occurred. Antioxidant activity was evaluated by DPPH, ABTS, FRAP and CUPRAC methods and results followed the same tendency obtained for phenolic compounds. Also, amount of used fibers had an effect on colour parameters (L, a, b, h and C) of obtained complexes. FTIR spectra were used to evaluate differences in structure of complexes in comparison to pure citrus fibers. Differences were found in three regions, one was from 1730 cm^{-1} to 1500 cm^{-1}, another one from 1450 cm^{-1} to 1200 cm^{-1} and third one from 950 cm^{-1} to 800 cm^{-1}. These results suggest an efficient plant-based approach to produce value-added citrus fiber/phenolics dry complexes with possible utility as food additive in order to enrich product with phenolic compounds.

Keywords: citrus fiber, chokeberry juice, phenolics, antioxidant activity, colour

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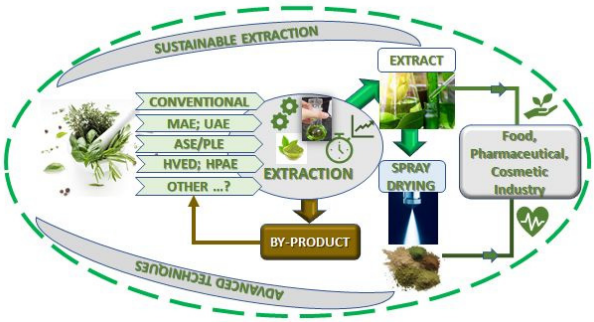
ODRŽIVA PROIZVODNJA BILJNIH EKSTRAKATA KONVENCIONALNIM I NAPREDNIM TEHNIKAMA

SUSTAINABLE HERBAL EXTRACT PRODUCTION BY USING CONVENTIONAL AND ADVANCED TECHNIQUES

Verica Dragović-Uzelac, Maja Repajić, Ivona Elez Garofulić, Sandra Pedisić, Zoran Zorić, Danijela Bursać Kovačević, Branka Levaj

Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia



Medicinal and aromatic herbs contain numerous bioactive molecules (BAMs) which differ significantly according to molecular structure, physical, chemical and biological properties. Therefore, for their isolation is necessary to apply a systematic and sustainable approach that includes the selection of the most efficient extraction technique, optimization of extraction conditions, standardization, processing into a stable powder form, by-product utilization. One of the most commonly used extraction techniques for isolation of the targeted BAMs is conventional, despite the fact that is time consuming, requires large amounts of solvent, relatively lower BAM yields and often is not environment friendly. In the sustainable production of plant extracts, advanced extraction techniques (microwave, ultrasonic, high pressure assisted extraction, accelerated solvent extraction, etc.) with lower consumption of organic solvents, increased use of green solvents, shortening extraction times and increasing the yield of targeted BAMs are being widely used. In addition, parameters such as pH, time, temperature, particle size, solvent, sample/solvent ratio as well as pressure, microwave power, ultrasound intensity etc. are main parameters that needs to be optimized depending on the applied technique. Liquid plant extracts are often processed into a more stable powder form using appropriate encapsulation techniques, whereas the obtained by-products are utilized in accordance with the principles of the circular economy. Besides previously mentioned parameters it is also important to conduct a feasibility study to determine which technique is the best choice for sustainable plant extracts and powder production from a technical and economic point of view. This paper summarized an overview of conventional and advanced extraction techniques, parameters that affect the extraction yields of the targeted BAMs, advantages and disadvantages, the possibility of using extraction by-products, encapsulation techniques for powder production and the perspective of the use liquid and dry extracts in food, pharmaceutical and cosmetic industry.

Keywords: sustainable extraction, conventional technique, advanced technique, bioactive molecules, by-product

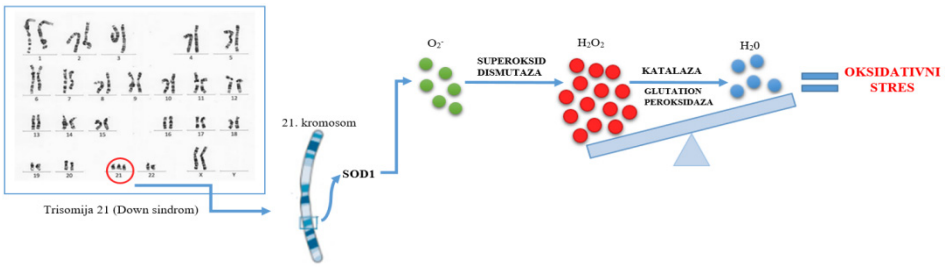
OKSIDATIVNI STRES I DOWNOV SINDROM

OXIDATIVE STRESS AND DOWN SYNDROME

Maja Ergović Ravančić, Velentina Obradović
Veleučilište u Požegi, Vukovarska 17, 34 000 Požega

Downov sindrom je neurorazvojni poremećaj uzrokovan trisomijom 21. kromosoma. Od njegova otkrića, glavni interes istraživanja bio je identificirati gene na humanom kromosomu 21 (HSA21) i povezati njihovu prekomjernu ekspresiju sa specifičnostima Down sindroma. Posebno se istražuje pojačana izraženost gena za superoksid dismutazu koja kod osoba s Down sindromom u većoj mjeri može uzrokovati prijevremeno starenje, slabljenje imunološkog sustava, ali i pojavu neurodegenerativnih bolesti uslijed stvaranja oksidativnog stresa u stanicama. Naime, povećano nastajanje reaktivnih kisikovih vrsta povezano je s mitohondrijskom disfunkcijom koja se pojavljuje od ranog embrionalnog razvoja kod osoba s Down sindromom, a zbog pretjerane ekspresije gena uzrokovane prisutnošću 3. kromosoma na 21. paru. Oštećenje stanica može biti potaknuto reaktivnim kisikovim vrstama uzrokujući promjene na makromolekulama kao što su polinezasićene masne kiseline u lipidima membrana, proteini i DNK. Reaktivne kisikove vrste se, u normalnim uvjetima, proizvode *in vivo* uglavnom aerobnom staničnom respiracijom nakon čega bivaju uklonjene djelovanjem enzimskih antioksidansa superoksid dismutaze, katalaze i glutation peroksidaze. Superoksid dismutaza pretvara superoksid radikal u citotoksični vodikov peroksid koji se pomoću katalaze ili glutation peroksidaze razlaže na vodu i kisik. Kao rezultat pretjerane ekspresije gena na 21. kromosomu, kod osoba s Down sindromom može postojati neravnoteža između omjera antioksidativnih enzima pri čemu dolazi do stvaranja povećanih koncentracija vodikovog peroksida i uzrokovanja oksidativnog oštećenja različitih molekula što u konačnici dovodi do pojačanog oksidativnog stresa. Cilj ovoga rada je dati pregled istraživanja o međusobnoj povezanosti povećanog oksidativnog stresa kod osoba s trisomijom 21 kao posljedice prekomjerne ekspresije gena te ukazati na važnost pravilne prehrane bogate antioksidansima u svrhu njegove prevencije ili ublažavanja s obzirom da su antioksidativni mehanizmi nužni u održavanju redoks ravnoteže unutar stanica, te imaju glavnu ulogu u uklanjanju reaktivnih kisikovih vrsta.

Ključne riječi: Downov sindrom, oksidativni stres, slobodni radikali, antioksidansi



ZAŠTO ENKAPUSULIRATI AKTIVNE TVARI?

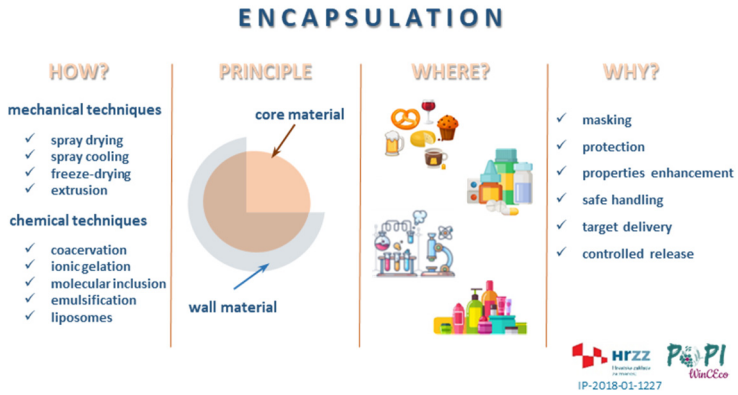
WHY TO ENCAPSULATE ACTIVE SUBSTANCES?

Josipa Grgić, Gordana Šelo, Mirela Planinić,
Marina Tišma, Ana Bucić-Kojić

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek,
Franje Kuhača 18, 31 000 Osijek, Croatia

Encapsulation is a technology that involves packing active agents (liquids, gases or solids) into capsules of different sizes and properties. The wall material used and the encapsulation method itself depend on the active component to be encapsulated. Among numerous coating materials that are used, the most common are polysaccharides (alginate, chitosan), lipids (phospholipids), proteins (soy proteins) and plant exudates (gum Arabica). These materials have to be food-grade, biodegradable and able to form a protective barrier between the active compounds and their surroundings. There are two different encapsulation techniques, mechanical (spray drying, spray cooling, freeze-drying, extrusion) and chemical (emulsification, coacervation, molecular inclusion, ionic gelation, application liposomes and yeasts). Encapsulation has been widely employed in food, cosmetics, chemical, and pharmaceutical industries owing to its broad benefits. This way of packaging active substances enables masking of unpleasant odours and tastes, protection from external influences such as light and moisture during storage, mixing of substances that do not mix otherwise, enhancing of physicochemical properties or visual form of active components as well as safe handling of the toxic materials. Furthermore, bioactive compounds, such as drugs and polyphenols, have been encapsulated to allow their targeted release and greater bioavailability.

Keywords: encapsulation, active substances, application of encapsulated particles



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INHIBICIJA α-GLUKOZIDAZE POLIFENOLIMA PRISUTNIM U TRADICIONALNIM, DOMAĆIM SORTAMA JABUKA

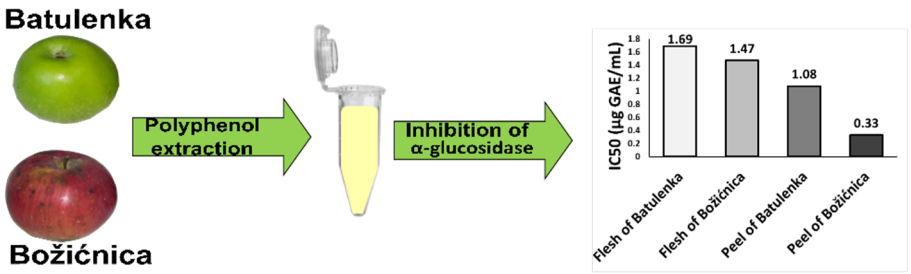
INHIBITION OF α-GLUCOSIDASE BY POLYPHENOLS PRESENT IN TRADITIONAL, INDIGENOUS APPLES VARIETIES

Jozo Ištuk, Lidija Jakobek, Ivica Strelec

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

This work aimed to evaluate polyphenols from two traditional apple varieties as α-glucosidase inhibitors. Polyphenols were extracted from the flesh and skin of two traditional apple varieties (Božićnica and Batulenka) by using ultrasonic-assisted extraction. Total polyphenols in extracts were determined by the spectrophotometric Folin-Ciocalteu method, expressed as gallic acid equivalents (GAE). The α-glucosidase activity was evaluated based on the spectrophotometric determination of *p*-nitrophenol (pNP) released from *p*-nitrophenyl-α-D-glucopyranoside (*p*-NPG) substrate by the action of the enzyme. To inhibit enzyme activity, various polyphenol concentrations were added into the reaction mixture. IC_{50} value was calculated (concentration of polyphenols that gives 50% inhibition). Božićnica and Batulenka contained 337.24 and 202.17 mg GAE kg^{-1} in the flesh and 2132.91 and 824.43 mg GAE kg^{-1} in the peel, respectively. Polyphenols inhibited α-glucosidase activity and inhibition reached a steady state. IC_{50} values, expressed as μg of gallic acid equivalents (GAE) per mL of reaction solution, of the flesh of Batulenka and Božićnica were 1.69 and 1.47, respectively. Peel showed similar IC_{50} values (1.07, and 0.33 μg GAE cm^{-3}, for the peel of Batulenka and Božićnica, respectively). These results suggest that polyphenols from the flesh and skin of traditional apple varieties are potent inhibitors of α-glucosidase activity.

Keywords: α-glucosidase, inhibition, polyphenols, apple



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UTJECAJ TLAKA I TEMPERATURE NA AROMATSKI PROFIL CRNOG VINA TIJEKOM KONCENTRIRANJA REVERZNOM OSMOZOM

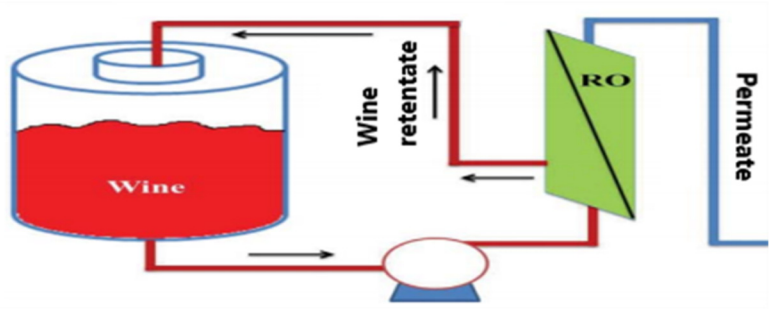
THE INFLUENCE OF PRESSURE AND TEMPERATURE ON AROMA PROFILE OF RED WINE DURING CONCENTRATION BY REVERSE OSMOSIS

Ivana Ivić[1], Vladimir Jukić[2], Mirela Kopjar[1],
Martina Bošnjak[1], Anita Pichler[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia*

Wine aroma represents one of the most important quality parameters. It develops through all stages of grape and wine production processes: from grape ripening to fermentation process and wine aging. The aroma profile of final product will depend on many factors during each stage. However, sometimes a wine aroma profile does not meet the standards and improvement is required. For that purpose, membrane filtration can be used. The aim of this study was to determine the retention of volatile compounds in Cabernet Sauvignon red wine variety during its concentration by reverse osmosis. Concentration was carried out on Alfa Laval RO98pHt membranes at four different pressures (25, 35, 45 and 55 bar) and two temperature regimes (with and without cooling). The results showed that higher pressures (45 and 55 bar) and lower temperatures (with cooling regime) resulted in higher retention of total aroma compounds. The retention of individual compound depended also on its chemical composition (molecular weight, volatility, activity coefficient etc.). Reverse osmosis membranes proved to be permeable for low molecular weight compounds like water, ethanol and acetic acid. As a result, obtained retentates had higher concentration of desirable aroma compounds, especially the one obtained at 55 bar with cooling.

Keywords: red wine, aroma compounds, reverse osmosis, concentration, retention



ADSORPCIJSKE IZOTERME ZA ISTRAŽIVANJE INTERAKCIJA FLAVONOLA I ANTOCIJANINA ARONIJE I β–GLUKANA

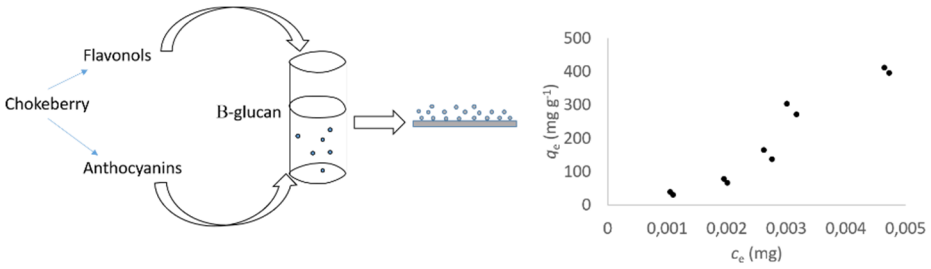
ADSORPTION ISOTHERMS FOR STUDYING INTERACTIONS BETWEEN FLAVONOLS AND ANTHOCYANINS FROM ARONIA AND β-GLUCAN

Lidija Jakobek, Petra Matić, Ivana Buljeta, Jozo Ištuk

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Aronia is a fruit very rich in polyphenols, particularly anthocyanins and flavonols. Accordingly, it is often used in a diet as a rich source of polyphenols. Interactions with food macromolecules such as dietary fibers might influence possible beneficial effects of aronia berry polyphenols. The aim of this work was to study the interaction of flavonols and anthocyanins from aronia berries with dietary fiber β-glucan through the adsorption process. Flavonols and anthocyanins were extracted with ultrasonic assisted extraction, and characterized by using reversed-phase high-performance liquid chromatography. Adsorption onto β-glucan was conducted for 5 h with different initial concentrations of flavonols and anthocyanins. The amount of adsorbed (q_e) and un-adsorbed (c_e) polyphenols were modelled with non-linear regression using adsorption isotherm equations (Langmuir, Freundlich, Dubinin-Radushkevich, Hill and Temkin). Anthocyanins (cyanidin-3-galactoside, cyanidin-3-glucoside, cyanidin-3-arabinoside and cyanidin-3-xyloside) and flavonols (quercetin-3-rutinoside, quercetin-3-galactoside and quercetin-3-glucoside) were quantified. All flavonols and anthocyanins adsorbed onto β-glucan. Adsorption was modelled with adsorption isotherms which gave additional information about adsorption process. Adsorption was concentration dependent and H bonds and Van der Waals forces could be suggested as bonds between flavonols, anthocyanins and β-glucan. Adsorption isotherms might be a useful tool for studying interactions between polyphenols and β-glucan.

Ključne riječi: interactions, adsorption, adsorption isotherms



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ISTRAŽIVANJE INTERAKCIJA POLIFENOLA TRADICIONALNIH KULTIVARA JABUKA I β-GLUKANA

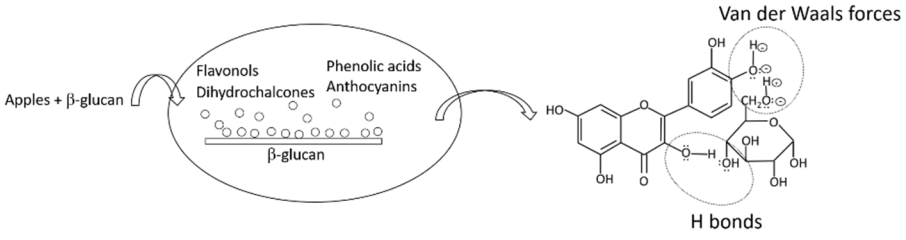
THE STUDY OF INTERACTIONS BETWEEN POLYPHENOLS FROM TRADITIONAL APPLE VARIETIES AND β-GLUCAN

Lidija Jakobek, Petra Matić, Ivana Buljeta, Jozo Ištuk

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

It has been shown previously that traditional apple varieties have higher amounts of polyphenols than commercial varieties. That is why these apples are being investigated for various beneficial effects. Beneficial effects of polyphenols are often connected to their bioaccessibility. Bioaccessibility of polyphenols can be influenced by their interactions with other macromolecules present in the food matrix such as dietary fibers. Interactions between polyphenols and dietary fibers can be studied through the adsorption process. In this work we studied interactions of individual polyphenols from flesh and peel of two traditional varieties of apples and dietary fiber β-glucan by studying adsorption process. Polyphenols were extracted by using ultrasonic assisted extraction, identified and quantified by using reversed-phase high-performance liquid chromatography (RP-HPLC) and separated into two fractions by using Sephadex LH-20. Polyphenols from fractions were adsorbed onto β-glucan for 5 h, at pH 5.5. The amount of adsorbed polyphenols was calculated (q_e). Phenolic acids (chlorogenic acid, chlorogenic acid isomer, *p*-coumaroylquinic acid) and anthocyanins (cyanidin-3-galactoside) were present in the first, and flavonols (quercetin-3-galactoside, quercetin-3-glucoside, quercetin-3-xyloside, quercetin-3-rhamnsoide, two additional quercetin derivatives) and dihydrochalcones (phloretin-2'-glucoside) in the second fractions. Polyphenols from the peel adsorbed in higher amount onto β-glucan (0.7 to 82 mg g^{-1}) than polyphenols from the flesh (3.3 to 12.4 mg g^{-1}). The adsorption was concentration dependent and it can be suggested that bonds between polyphenols and β-glucan can be H bonds or Van der Waals forces.

Ključne riječi: interactions, polyphenols, dietary fibers, bioactivities



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RAZLIKA FIZIKALNO-KEMIJSKIH SVOJSTAVA CRNIH VINA U PET I B&B AMBALAŽI

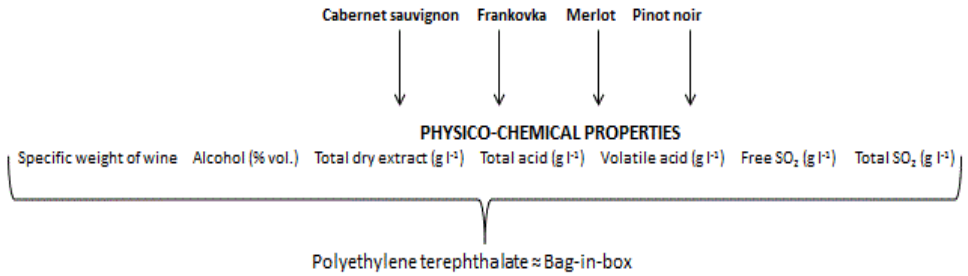
DIFFERENCE OF PHYSICO-CHEMICAL PROPERTIES OF RED WINES IN PET AND B&B PACKAGING

Nebojša Kojić[1], Lidija Jakobek[2]

[1]Vupik plus d.o.o., Sajmište 113c, 32 000 Vukovar, Croatia
[2]Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Studies have shown that the type of packaging can affect the quality and physico-chemical features of foods stored over a longer period of time. Important physico-chemical characteristics of wines that can change over a storage period are alcohol percentage, the amount of acids or SO_2, specific weight of wines or total dry extract. The aim of this paper was to determine and compare the physico-chemical properties of red wines (Cabernet sauvignon, Frankovka, Merlot and Pinot noir), stored over a period of one year in two different packaging (PET (polyethylene terephthalate) and B&B (bag in box)). Specific weight of wine, total dry extract, alcohol percentage, total acids content, volatile acids content, free and total sulfur dioxide (SO_2) content were determined after 3, 6 and 12 months of storage. The results showed that SO_2 content decreased over time in both packages, but in B&B packaging the values of SO_2 were higher. Volatile acid content, despite growing concentration over time, developed slower in B&B packaging. The total acid content increased, the alcohol percentage slightly decreased as well as total dry extract in wines packed in both packaging. Comparing PET and B&B packaging with statistical tests showed that the key physico-chemical indicators were similar in wines packed in two packaging.

Keywords: physico-chemical properties, PET, B&B, packaging



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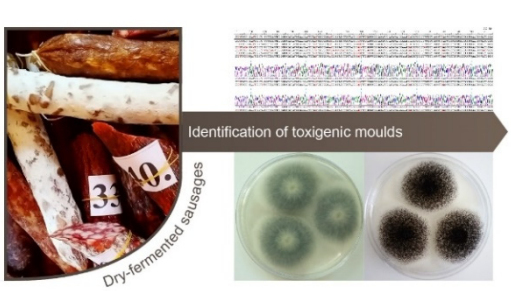
TOKSIKOGENE PLIJESNI S POVRŠINE HRVATSKIH TRADICIONALNIH TRAJNIH KOBASICA PROIZVEDENIH U DOMAĆINSTVIMA

TOXIGENIC MOULDS GROWING ON THE SURFACE OF TRADITIONAL CROATIAN HOUSEHOLD-PRODUCED DRY-FERMENTED SAUSAGES

Tina Lešić[1], Manuela Zadravec[1], Nada Vahčić[2], Dragan Brnić[1], Irena Perković[5], Željko Jakopović[2], Jelka Pleadin[1]

[1]*Croatian Veterinary Institute, Savska Cesta 143, 10 000 Zagreb, Croatia*
[2]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*
[5]*Croatian Veterinary Institute, Veterinary Institute Vinkovci, Josipa Kozarca 24, 32 100 Vinkovci, Croatia*



Household production of dry-fermented sausages is characterised by the presence of wild-type moulds that spontaneously overgrow the product surface; some of these moulds can produce mycotoxins that affect final products' quality and safety. Surface moulds were investigated in thirty-five samples of four different types of traditional household-produced dry-fermented sausages. They were identified using a traditional method of depiction of macroscopic and microscopic morphological characteristics and corroborated using a molecular method of internal transcribed spacer (ITS), beta-tubulin (benA) and calmodulin (CaM) loci sequencing. Moulds of the *Penicillium* genus were present in more isolates (85 %) than those of the *Aspergillus* genus (15 %) and exhibited a greater species diversity, since eight *Penicillium* and four *Aspergillus* species were identified. This is to be attributed to the greater ability of the *Penicillium* species to grow at low and moderate temperatures at which sausages are ripened. Out of the identified mould species, four species are known as mycotoxin producers, in specific *Penicillium commune* as cyclopiazonic acid (CPA) producers, *Penicillium citrinum* as citrinin (CIT) producer, *Aspergillus flavus* as aflatoxins and CPA producer and *Aspergillus niger* as ochratoxin A (OTA) producer. Aflatoxin B_1 and OTA are of the greatest public health concern, while other mycotoxins, such as CPA and CIT, haven't been thoroughly investigated yet. Impact factors that affect mould and mycotoxin contamination in each traditional sausages' processing stage should be investigated together with the occurrence of underexplored mycotoxins.

Keywords: meat products, traditional sausages, moulds identification, mycotoxins

UTJECAJ VISOKOG HIDROSTATSKOG TLAKA NA KVALITETU I TRAJNOST „FRESH-CUT" KRUMPIRA

EFFECT OF THE HIGH HYDROSTATIC PRESSURE ON THE QUALITY AND SHELF-LIFE OF FRESH-CUT POTATO

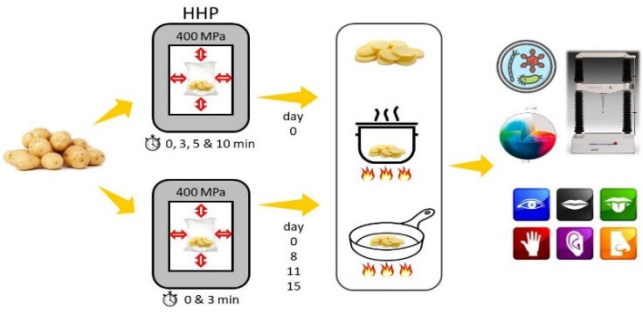
Branka Levaj, Ana Ljubas, Zrinka Čošić, Zdenka Pelaić,
Filip Dujmić, Maja Repajić

Faculty of Food Technology and Biotechnology, University of Zagreb,
Pierottijeva 6, 10 000 Zagreb, Croatia

The influence of the high hydrostatic pressure (HHP) treatment (400 MPa/0, 3, 5 and 10 min) on the quality and sensory properties as well as microbial stability of fresh-cut potato was investigated. Additionally, stability of the best evaluated samples during 15 days storage in vacuum packaging at 6 °C were also examined. Potato slices immersed in sodium ascorbate solution (NaAsc) were treated by HHP [1]. Immediately after the treatment, slices were analyzed for color (CIELAB), texture (texture analyzer) and aerobic mesophilic bacteria count (AMB). Furthermore, treated slices were boiled and fried, and all samples were sensory evaluated by quantitative descriptive method. Treatment did not significantly affect on firmness (F), but it did on lightness (L^*), where slices treated 5 and 10 min were brighter. Same samples showed certain mechanical damage, where during their frying the oil spattered strongly, and they were sensory lower graded. Consequently, stability of control samples (C) and only ones treated 3 min was examined during storage (after 8, 11 and 15 days). F and L^* followed the same trend as in the first experimental part, while AMB was reduced by the treatment, although it increased with storage time. Still, on the 15th day it was under the limit set by the Regulations. Regarding sensory, only C was acceptable till the 8th day of storage. In spite of the excellent results for AMB in HHP treated samples, potato slices treated by HHP/NaAsc showed poor sensory properties.

Ključne riječi: fresh-cut potato, high hydrostatic pressure, sensory, firmness, color

[1] M. N. Eshtiaghi *et al.*, *J Food Sci* 58 (1993) 1371.



ANTIOKSIDACIJSKI KAPACITET SELEKTIRANIH BILJNIH VRSTA

ANTIOXIDANT CAPACITY OF SELECTED PLANTS

Patricija Lisica[1], Sandra Pedisić[1], Maja Repajić[2], Ivona Elez Garofulić[2], Branka Levaj[2], Zoran Zorić[1], Sandra Balbino[2], Daniela Cvitković[2], Verica Dragović-Uzelac[2]

[1]Faculty of Food Technology and Biotechnology, University of Zagreb, P. Kasandrića 3, 23 000 Zadar, Croatia
[2]Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia

The sage (*Salvia officinalis*), laurel (*Laurus nobilis*), thyme (*Thymus vulgaris*), mastic tree (*Pistacia lenticus* L.), carob (*Ceratonia siliqua*) and myrtle (*Myrtus communis*) has many potential applications due to large number of bioactive molecules (BAM) with high antioxidant capacity (AOC). Currently it is an increasing interest in using these plants in the production of plant extracts (PE) and essential oils (EO) for food, pharmaceutical and cosmetic industries. However, extraction yield and antioxidant activity of PE depend on selection of appropriate extraction technique and solvent used for extraction. Therefore, the aim of this study was to determine the AOC of PE obtained by successive extraction with three different extraction solvents (hexane, 80 % acetone and 96 % ethanol) and extraction techniques (ultrasound assisted (UAE), accelerated solvent (ASE) and shaking water bath extraction). The plant extracts were analysed using the ORAC method. Results showed that ASE is the most appropriate method for extraction BAC's from thyme, mastic tree and carob while UAE was better method for sage and laurel, whose extracts contribute the highest AOA.

Keywords: antioxidant capacity, ORAC, extraction, bioactive molecules

PROTEINI KAO NOSITELJI CIMETNE KISELINE

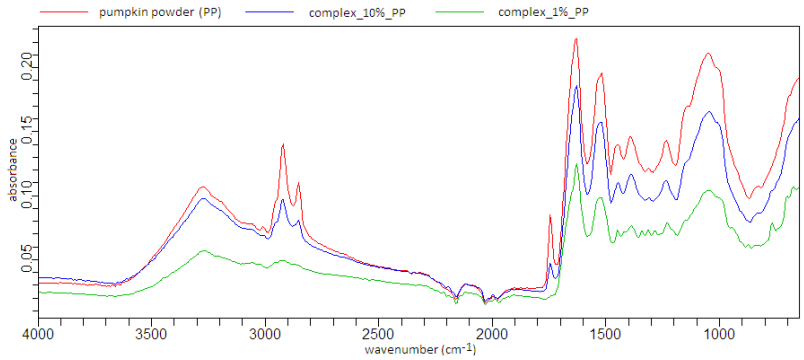
PROTEINS AS DELIVERY SYSTEMS OF CINNAMIC ACID

Josip Lukić[1], Vanja Kelemen[2], Josip Šimunović[3], Anita Pichler[1], Mirela Kopjar[1]
[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Institute of Public Health Osijek-Baranja County, Franje Krežme 1, 31 000 Osijek, Croatia*
[3]*Bioprocessing and Nutrition Sciences, North Carolina State University, Raleigh, NC 27 695, USA*

Different types of proteins are very often used for formulation of delivery systems of phenolic compounds. In this study, four types of protein sources were used; brown rice and pea powder (with 80 % of proteins) and pumpkin and almond powder (with 50 % of proteins). Complexes were prepared by complexation of constant amount of cinnamic acid and different amounts of protein powders (1 %, 2%, 5 % and 10 %). Complexation of proteins with cinnamic acid was proved throughout FTIR and DSC screening. Almond/cinnamic acid complexes had higher denaturation temperature then almond protein (1 to 3 °C) while other three complexes had lower denaturation temperature then correspondent protein. For pumpkin/cinnamic acid complexes decrease of denaturation temperature was 2 °C, while for other two from 3 to 4 °C. Structural changes of complexes in comparison to protein were detected by screening with FTIR-ATR. Intensity of peaks decreased in comparison to proteins and additional peaks on complexes were detected. Changes on IR spectra were more pronounced when lower amounts of proteins were used for complexation with cinnamic acid.

Keywords: cinnamic acid, proteins, DSC, FTIR

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *PZS-2019-02-1595.*



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TERMODINAMIKA ADSORPCIJE ANTOCIJANINA NA β-GLUKAN

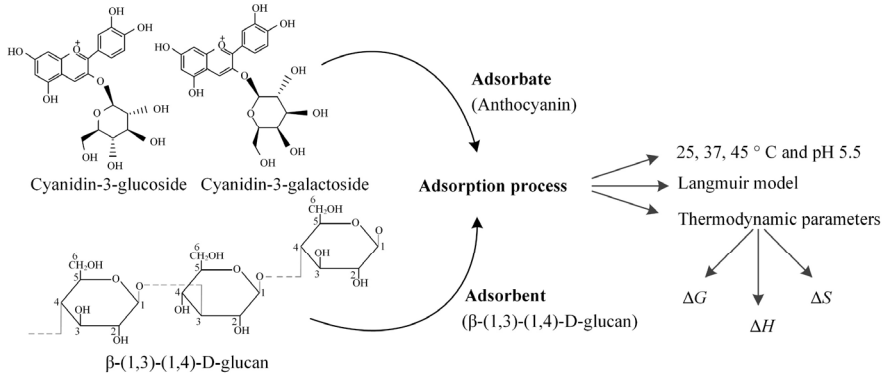
THERMODYNAMICS OF ANTHOCYANINS ADSORPTION ONTO β-GLUCAN

Petra Matić, Lidija Jakobek

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

The aim of this work is to obtain information about interactions between polyphenols and β-glucan through thermodynamic parameters. It was shown that polyphenolic compounds can interact with various food ingredients such as dietary fibers. Interactions can be studied through adsorption process. After the adsorption process conducted on different temperatures the thermodynamic parameters can be calculated. In the present study, the adsorption of anthocyanins (cyanidin-3-glucoside and cyanidin-3-galactoside) onto dietary fiber (β-glucan) is conducted. Adsorption is carried out at different temperatures (25 °C, 37 °C, 45 °C and pH 5.5 for 16 h) in order to obtain thermodynamic parameters (standard reaction Gibbs energy ($\Delta G°$), standard reaction enthalpy ($\Delta H°$) and standard reaction entropy ($\Delta S°$)). The non-linear Langmuir model is applied in order to analyse the data and to obtain the Langmuir constant K_L which was used for the calculation of thermodynamic parameters. The results showed that cyanidin-3-glucoside adsorbed on β-glucan in higher amount then cyanidin-3-galactoside at all three temperatures. Furthermore, $\Delta S°$ was positive for both anthocyanins which supports a spontaneous processes. $\Delta H°$ was also positive which would be indicative of an endothermic reaction.

Keywords: adsorption, anthocyanins, β-glucan, Langmuir, thermodynamic



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ODREĐIVANJE KUMARINA U CIMETU I PROIZVODIMA KOJI SADRŽE CIMET

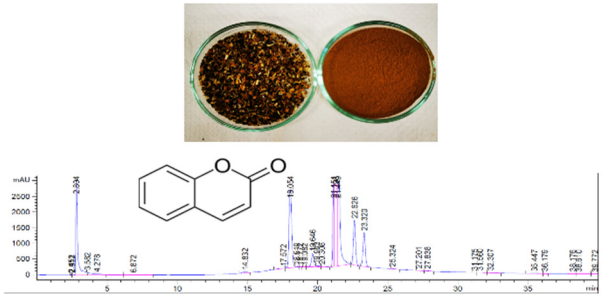
DETERMINATION OF COUMARIN IN CINNAMON AND CINNAMON-CONTAINING PRODUCTS

Lovro Mihajlović[1], Martina Jakovljević[2], Maja Molnar[2]

[1]*Department of Biology, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*

Coumarin is a component present in natural flavors including cassia, which in addition to being a spice, is very often used in the production of bakery products, biscuits, cereals and various beverages. Given the demonstrated toxicity of coumarin, there has been an increase in concern in the food industry where a maximum intake of 2 mg kg^{-1} has been set for foods and beverages in general, and a maximum level of 10 mg dm^{-3} for alcoholic beverages.
An efficient method for extraction and routine analysis of coumarin was developed in the present study for the estimation of coumarin and other phenolics in samples of cinnamon and teas containing cinnamon on the Croatian market.
Process parameters include solvent selection (methanol and ethanol), extraction times (10 and 30 min), and extraction temperatures (30 and 50 °C), as well as appropriate extraction techniques (mixing with heating and ultrasonically assisted extraction (UAE)). Since the temperature rise did not lead to a significant increase in coumarin concentration, nor with the use of UAE, the optimal sample preparation for cinnamon and cinnamon-containing teas was found to be extraction of 500 mg sample with 1 cm^3 of methanol for 10 min at 30 °C using magnetic stirring.
Coumarin content in the tested cinnamons on the market, depending on the extraction technique, amounted to 7.41-200.58 mg kg^{-1}, while the amount of coumarin in teas with cinnamon was 3.15-51.60 mg kg^{-1}. The obtained results show that the content of coumarin in the products is not high, which speaks in favor of the use of authentic cinnamon and less use of cinnamon in teas.

Keywords: coumarin, cinnamon, HPLC, ultrasound-assisted extraction



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TOPLINSKO PONAŠANJE PLODOVA ŠIPKA (*Rosa canina* L.) I NEKIH PROIZVODA OD ŠIPKA

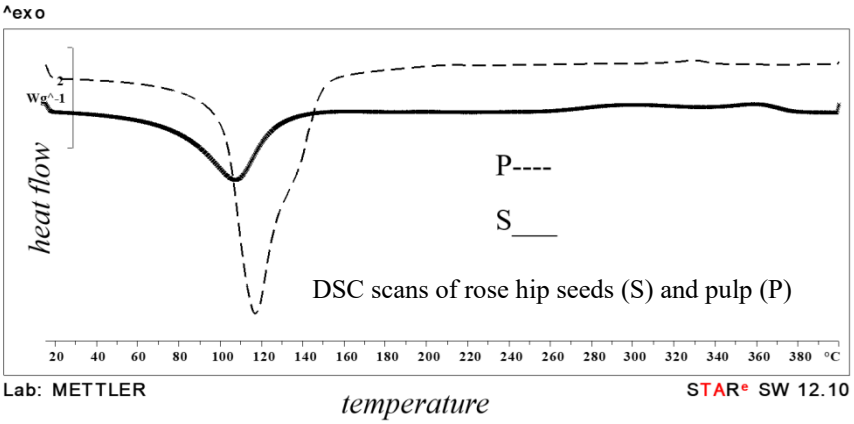
THERMAL BEHAVIOUR OF ROSE HIP (*Rosa canina* L.) FRUITS AND SOME ROSE HIP PRODUCTS

Nela Nedić Tiban, Anamarija Brkić

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek,
Franje Kuhača 18, 31 000 Osijek, Croatia

The aim of the study was to investigate the thermal behaviour of rose hip fruit (seeds, S and pulp, P), lyophilised puree (LP) and low-calorie jam (J). DSC scans were used to determine thermal behaviour in a temperature range from - 100 °C to 400 °C, i.e. as a base for determining onset and midpoint glass transition temperatures (Tg_o and Tg_m), change of specific heat capacity (Δc_p), melting temperatures (Tm_o-onset, Tm_p-peak and Tm_e-endset) and enthalpy of melting (ΔHm). In seeds, the main thermal effect occurred at 107.2 °C (Tm_p) with enthalpy of melting of 306.3 Jg^{-1} (ΔHm). The exothermic events above 260 °C related probably to the degradation of fibre components in seeds. In pulp, endotherm detected at 116.8 (Tm_p) with ΔHm of 819.6 Jg^{-1} can be attributed to water evaporation and melting of some sugars. The main thermal events detected in rose hip products at low temperatures related to glass transition phenomenon and melting transition of ice, and at high temperatures mainly corresponding to degradation of pectins and sugars. From the viewpoint of the thermal stability, rose hip seeds showed high thermal stability (with decomposition temperature of 360.2 °C) and potential for other possible applications (for example, as a biomass feedstock).

Keywords: rose hip, products, DSC



UTJECAJ UV-C ZRAČENJA NA KVALITETU I TRAJNOST „FRESH-CUT" KRUMPIRA

EFFECT OF THE UV-C RADIATION ON THE QUALITY AND SHELF-LIFE OF FRESH-CUT POTATO

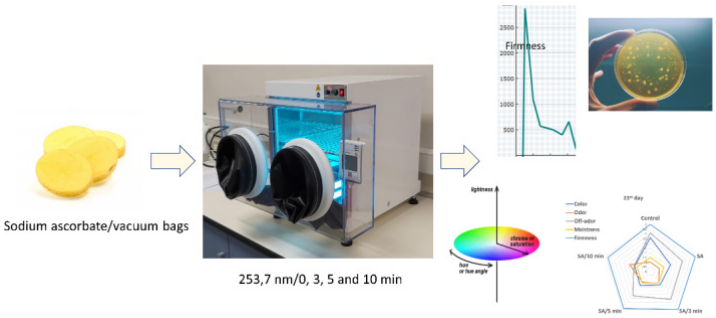
Zdenka Pelaić, Zrinka Čošić, Sandra Pedisić, Maja Repajić, Branka Levaj

Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia

The effect of the 0, 3, 5- and 10-minute UV-C treatment (applied doses of 0, 1.62, 2.70 and 5.40 kJm^{-2}) on the quality and shelf-life of the fresh-cut potato was examined. Potato slices, previously immersed in sodium ascorbate (SA) solution and vacuum packed [1], were UV-C treated and stored for 23 days at 6 °C. Color (CIELAB), firmness (texture analyzer) and sensory analysis (quantitative descriptive method) as well as determination of aerobic mesophilic bacteria count (AMBC) were carried out immediately after the treatment as well as on the 8th, 11th, 15th and 23rd day. The 5- and 10-min UV-C treatment significantly reduced AMBC and although AMBC increased during storage, the treatment effectiveness was even more pronounced. The same samples lightness (L^*) increased and samples remained brighter than control during 15 days. Treatments did not affect on b^* (yellowness), while increase of a^* (redness) was observed only for control samples at the end of the storage. The UV-C treated samples were fewer firms compared to the control throughout the storage time. The sensory evaluation showed that UV-C treatments preserved the color till the 23rd day and did not affected on the moistness. At the 23rd day off-odor was highly scored for all samples except for 10-min treated. The 5- and 10-min UV-C/SA treated fresh-cut potato samples showed to have a potential to be stored for 15 days at 6 °C with retained good sensory quality.

Ključne riječi: fresh-cut potato, UV-C, aerobic mesophilic bacteria, color, sensory analysis

[1] D. Hunjek, M. Repajić, M. Ščetar, S. Karlović, N. Vahčić, D. Ježek, K. Galić, B Levaj, *J Food Process and Preservation* 44 (2020) e14391.



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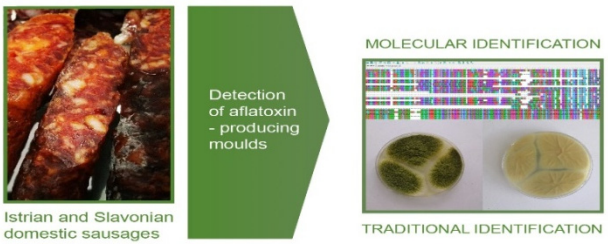
DETEKCIJA PLIJESNI PRODUCENATA AFLATOKSINA S POVRŠINE ISTARSKE I SLAVONSKE KOBASICE

DETECTION OF AFLATOXIN-PRODUCING MOULDS FROM THE SURFACE OF ISTRIAN AND SLAVONIAN SAUSAGE

Jelka Pleadin[1], Tina Lešić[1], Dragan Brnić[1], Irena Perković[2], Maja Kiš[3], Manuela Zadravec[1]

[1]*Croatian Veterinary Institute, Savska Cesta 143, 10 000 Zagreb, Croatia*
[2]*Croatian Veterinary Institute, Josipa Kozarca 24, 32 100 Vinkovci, Croatia*
[3]*Croatian Veterinary Institute, Ivana Z. Dijankovečkog 10, 48 260 Križevci, Croatia*



During ripening, the surface of traditional dry-fermented sausages becomes overgrown by moulds. The intensity of mould growth is enhanced by ripening longevity and traditional production environment. In addition to their contribution to favourable properties of the final product, certain mould species are often responsible for unfavourable taste and smell and may be the reason behind the occurrence of secondary metabolites, toxic compounds termed the mycotoxins. Among them, aflatoxins (AFs) are known as the most potent mammalian liver carcinogens, which can be also found in dry-fermented sausages as the consequence of presence of AFs-producing moulds overgrowing product surfaces. In this study, moulds from the surface of dry-fermented Istrian and Slavonian sausages, sampled from different Croatian household producers (n = 21), were isolated and identified based on their macroscopic and microscopic morphological characteristics, and verified using the molecular polymerase chain reaction (PCR) technique. In total, 56 isolates were recovered from the surfaces of analysed sausages, among which 8 of the *Mucor* (14 %), 9 of the *Aspergillus* (16 %), and 39 of the *Penicillium* genus (70 %). Moulds of the *Mucor* genus were represented by one, those of the *Aspergillus* genus by four and those of the *Penicillium* genus by five species. Among the above, only *Aspergillus flavus*, recovered from two Slavonian sausage samples, has been classified as a potential AFs-producing fungus, but AFs biosynthetic genes norsolorinic acid reductase (*nor-1*), versicolorin A dehydrogenase (*ver-1*) or sterigmatocystin O-methyltransferase (*omt-A*) were not detected. Although the identified *A. flavus* strains were proven AFs-non-producing, further identification of potential aflatoxin-producing moulds and moulds producing other mycotoxins less represented in dry-cured meat products is needed. In these attempts, numerous factors influencing the growth of toxicogenic moulds and mycotoxin presence should be taken into account.

Keywords: surface moulds, dry-fermented sausages, mycotoxins, aflatoxins

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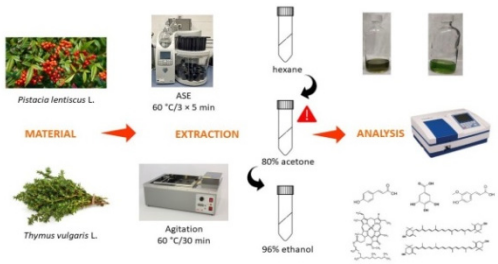
BIOAKTIVNI SPOJEVI U TRŠLJI I TIMIJANU: SUKCESIVNA EKSTRAKCIJA RAZLIČITIM METODAMA EKSTRAKCIJE

BIOACTIVE COMPOUNDS IN MASTIC TREE AND THYME: SUCCESSIVE EXTRACTION WITH VARIOUS EXTRACTION METHODS

Maja Repajić[1], Daniela Cvitković[1], Patricija Lisica[2], Sandra Balbino[1], Sandra Pedisić[2], Zoran Zorić[2], Ivona Elez Garofulić[1], Verica Dragović-Uzelac[1]

[1]*Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*
[2]*Faculty of Food Technology and Biotechnology, University of Zagreb, P. Kasandrića 3, 23 000 Zadar, Croatia*

Mastic tree (*Pistacia lentiscus* L.) and thyme (*Thymus vulgaris* L.) are traditional medicinal plants characterized with a wide spectrum of bioactive molecules, thus presenting a valuable source for various applications. For the extraction of natural antioxidants miscellaneous extraction methods are being used, among which accelerated solvent extraction (ASE) represents an advanced extraction technique. However, due to the diverse chemical structure, extraction of target compounds depends on the used solvent type. Hence, this study involved the three-step extraction of polyphenols and pigments from mastic and thyme dry leaves using ASE (60 °C/3×5 min) and agitation-assisted extraction (AAE) (60 °C/30 min) with solvents arranged by their polarity: hexane was used for the first fraction, followed by acetone (80 %) and finally ethanol (96 %). Obtained fractions were analyzed for total content of polyphenols (TP), hydroxycinnamic acids (THCA), flavonols (TFL), chlorophylls (TCHL) and carotenoids (TCAR). Statistical analysis of obtained results showed significant ($p \leq 0.05$) differences in fractions' composition among plants and applied extraction methods. Acetone fraction was the most abundant with all analyzed compounds accompanied with the greater ASE efficiency, especially in polyphenols' isolation. In hexane and ethanol fractions, longer AAE time resulted with greater performance in extraction of polyphenols, while higher pigments yields were achieved with ASE. Although mastic tree dominated in TP content, extracts of both plants showed their abundance of bioactives, proving their potential for further implementation in various food products. Further optimization of ASE conditions could contribute to even better extraction efficiency.



Keywords: Pistacia lentiscus L., *Thymus vulgaris* L., polyphenols, pigments, ASE

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EKSTRAKCIJA AROMATIČNIH KOMPONENTI IZ KORE MANDARINE *Citrus unshiu* SUPERKRITIČNIM CO_2

SUPERCRITICAL CO_2 EXTRACTION OF AROMATIC VOLATILES FROM MANDARIN PEEL *Citrus unshiu*

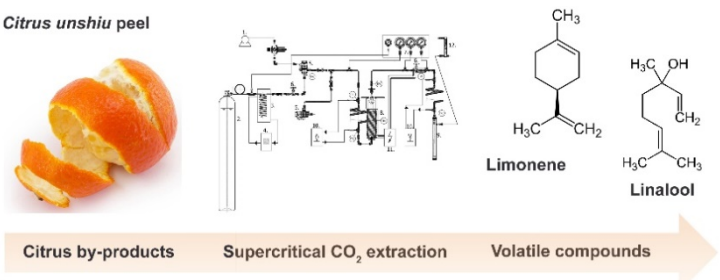
Silvija Šafranko[1], Ina Ćorković[1], Krunoslav Aladić[1], Igor Jerković[2], Stela Jokić[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21 000 Split, Croatia*

Citrus peel is considered as a source rich in volatile compounds and has been extensively studied for aromatic profile, mainly contributed by the presence of terpene hydrocarbons, esters, ketones, aldehydes, and alcohols. Supercritical CO_2 (SC-CO_2) extraction technique showed great potential in obtaining nonpolar and volatile components, being also promising green alternative to conventional methods.
In this study, mandarin peel *Citrus unshiu* has been extracted at temperature of 40 °C and at two different pressures (100 and 300 bar). The extracts were analysed in detail by gas chromatography/mass spectrometry (GC/MS), and results of quantification analysis were expressed as a percentage in total quantity (%). The obtained results indicated the predominance of limonone (13.16 – 30.65 %) in SC-CO_2 fraction, followed by α-farnesene (5.72 – 10.63 %), germacrene (4.11 – 6.66 %), linalool (1.85 – 2.18%), and α-terpineol (1.31 – 2.10 %). The content of volatile compounds, mainly including terpene and aldehydes, is commonly used as a commercial index of quality. Therefore, it could be concluded that SC-CO_2 extraction technique is applicable to food by-products processing, such as mandarin peel as it exhibited a strong potential for the industrial development in the production of the extracts rich in bioactive and aromatic compounds.

Keywords: citrus peel, by-products, SC-CO_2, volatile compounds

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *UIP-2017-05-9909*.



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UTJECAJ BIOLOŠKE OBRADE PLJEVICE JEČMA NA EKSTRAKCIJU FENOLNIH KISELINA

INFLUENCE OF THE BIOLOGICAL TREATMENT OF BARLEY HUSK ON THE EXTRACTION OF PHENOLIC ACIDS

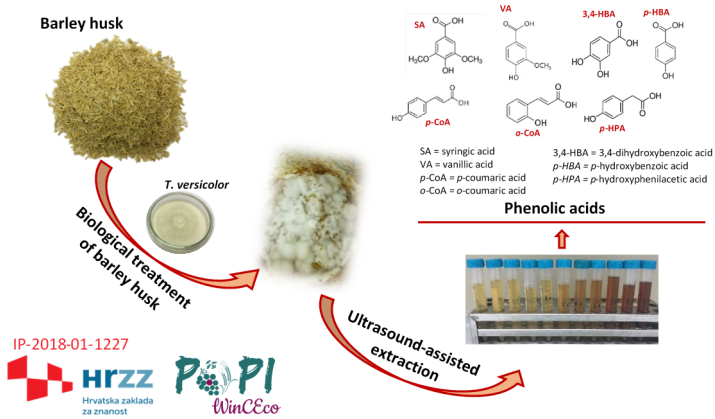
Gordana Šelo, Josipa Grgić, Mirela Planinić, Marina Tišma, Srećko Tomas, Teo Lukačić, Ana Bucić-Kojić

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Barley husk is a by-product that accounts up over 15 % of dry grain weight. The cereal industry by-products are rich in nutrients, but usually underutilized. Biological treatment with selected microorganisms represents a promising technology for the valorization of such by-products.

In this work, the influence of the biological treatment of barley husk on the extractability of phenolic acids in relation to biologically untreated samples was investigated. Biological treatment was performed by *Trametes versicolor* for 10 days, with and without the addition of eggshell as an inducer of enzyme synthesis. The content of 10 phenolic acids (3,4-dihidroxybenzoic acid, *p*-hydroxybenzoic acid, *p*-hydroxyphenilacetic acid, vanillic acid, caffeic acid, syringic acid, *p*-coumaric acid, ferulic acid, ellagic acid, *o*-coumaric acid) was identified and quantified by UHPLC method. Biological treatment of barley husk had the effect on increasing the extractability of phenolic acids, while the addition of eggshell had no influence on the increment of phenolic acids content. Biological treatment had the greatest impact on the extraction of 3,4-dihidroxybenzoic acid, where the highest yield was obtained after day 7 of fermentation in the experiment without inducer (50.6 μg g_{db}^{-1}).

Keywords: barley husk, biological treatment, *T. versicolor*, phenolic acids



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RAZVOJ I KARAKTERIZACIJA LIPOSOMA ISPUNJENIH DOPAMINOM EKSTRAHIRANIM IZ KORE BANANE

DEVELOPMENT AND CHARACTERIZATION OF DOPAMINE-LOADED LIPOSOMES EXTRACTED FROM BANANA PEEL

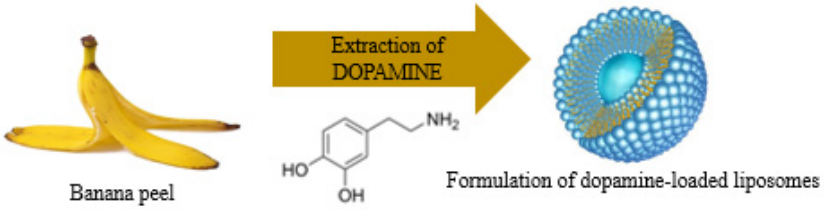
Danijela Šeremet[1], Ana Mandura[1], Aleksandra Vojvodić Cebin[1], Stela Jokić[2], Draženka Komes[1]

[1]*Faculty of Food Technology and Biotechnology, University in Zagreb, Pierottijeva 6, 10 000 Zagreb*
[2]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*

Banana (*Musaceae*) is the most consumed fruit in the world, after tomato. Approximately 30% of banana fruit is comprised of peel, resulting in a substantial amount of waste from banana processing. The peel is abundant in bioactive compounds, especially in dopamine [1]. The aim of this study was to develop liposomes containing dopamine extracted from banana peel. Banana peels were blanched (100 °C, 7 min) and freeze-dried in order to assure maximal preservation of dopamine. Banana peel extract was prepared by mixing pulverized banana peel with water (80 °C, 30 min). The extract was characterized by total phenolic content (25.50 mg GAE g^{-1} dmb), antioxidant capacity by DPPH and ABTS assays (0.16 mmol Trolox g^{-1} dmb) and dopamine content by HPLC-DAD (9.94 mg/g dmb). The encapsulation of the extract into liposomes was performed varying ratios of the extract and liposome Phospholipon® P90NG (1:5, 1:10 and 1:20, w/w). Formulated liposomes were characterized by encapsulation efficiency and by size and surface charge evaluated by light scattering and zeta potential, respectively. Antioxidant activity of encapsulated extract was investigated in terms of inhibitory action on liposome peroxidation using TBARS assays. The results revealed the greatest dopamine encapsulation efficiency of 41.12 % for liposomes prepared at ratio 1:20. The presence of banana peel extract in the liposomes reduced the lipid peroxidation induced by UV radiation.

Keywords: agro-industrial waste, banana peel, dopamine, liposomes

[1] R. González-Montelongo *et al*., *Food Chem* 119 (2010) 1030.



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UTJECAJ KONVENCIONALNIH I INOVATIVNIH METODA EKSTRAKCIJE NA BIOAKTIVNE KARAKTERISTIKE DOBRIČICE (*Glechoma hederacea* L.)

INFLUENCE OF CONVENTIONAL AND INNOVATIVE EXTRACTION TECHNIQUES ON BIOACTIVE PROPERTIES OF GROUND IVY (*Glechoma hederacea* L.)

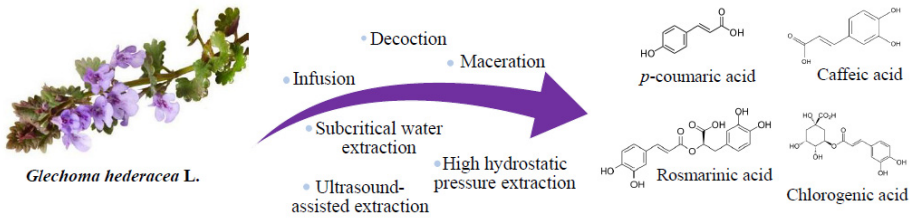
Danijela Šeremet[1], Ana Mandura[1], Aleksandra Vojvodić Cebin[1], Stela Jokić[2], Draženka Komes[1]

[1]*Faculty of Food Technology and Biotechnology, University in Zagreb, Pierottijeva 6, 10 000 Zagreb*
Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Glechoma hederacea L., known as ground ivy, is a perennial plant commonly grown in Europe, Asia and America. Although it has been used for generations in folk medicine [1], the linkage between its bioactive content and health benefits still requires scientific ground.
The aim of this study was to investigate the bioactive potential of *Glechoma hederacea* L. extracts prepared by conventional (infusion, decoction and maceration) and innovative (high hydrostatic pressure extraction, ultrasound assisted extraction and subcritical water extraction) methods of extraction using water as a solvent. The obtained extracts were spectrophotometrically evaluated for total phenolic content, antioxidant capacity (DPPH and ABTS assays) and the content of hydroxycinnamic acid derivatives. Individual phenolics profile was determined using HPLC-DAD. Of all extraction techniques, the extract prepared by decoction (100 °C, 20 min) resulted in the highest total phenolic content (37.39 mg GAE g^{-1}), antioxidant capacity (162.53 and 177.24 mmol Trolox g^{-1}) and hydroxycinnamic acid derivatives content (15.90 mg caffeic acid g^{-1}), with rosmarinic acid as predominant (2.00 mg g^{-1}). Among the applied innovative methods, the highest values for evaluated parameters were obtained for extract prepared by high hydrostatic pressure (200 MPa, 20 min), having caffeic acid as dominant (0.48 mg g^{-1}).

Keywords: Glechoma hederacea L.*,* innovative methods of extraction, bioactive content

[1] A.S. Döring *et al*., *Phytochem Lett* 10 (2014) 1.



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ELEKTROKINETIČKI POTENCIJAL NEKIH HIDROKSIBENZOJEVIH KISELINA I HIDROKSIBENZOJEVIH KISELINA - *β*-GLUKAN MODELA

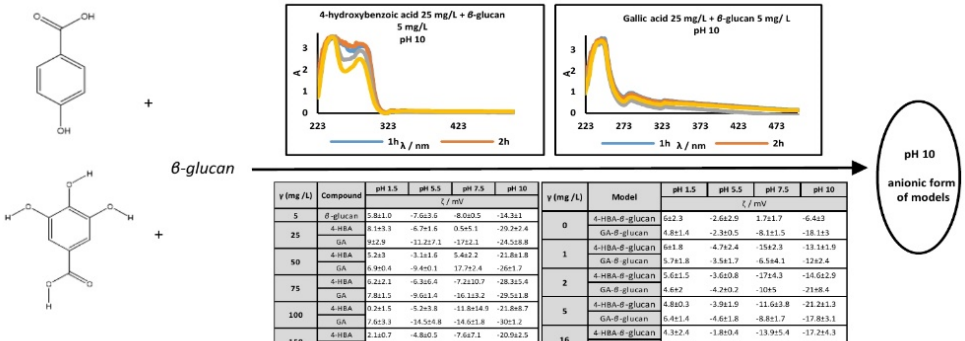
ELECTROKINETIC POTENTIAL OF SOME HYDROXYBENZOIC ACIDS AND HYDROXYBENZOIC ACIDS - *β*-GLUCAN MODELS

Ivana Tomac, Jozo Ištuk, Petra Matić, Ana Ivanković, Josipa Jelić, Lidija Jakobek

Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia

Hydroxybenzoic acids are subgroup of phenolic acids. 4-hydroxybenzoic acid, gallic acid, vanillic acid, salicylic acid are some of hydroxybenzoic acids. Structure of hydroxybenzoic acids differ because of the hydroxylation and methylations of aromatic ring. β-glucan is soluble dietary fiber constructed of glucose units. Electrokinetic potential is also known as zeta potential. Zeta potential is a physical property expressed on the surface of a macromolecule, respectively as potential at the shear plane distance. Knowledge of the zeta potential could predict the long-term stable behaviour of a macromolecule. The aim of this work was to predict a long-term stability of macromolecules such as 4-hydroxybenzoic acid - β-glucan model and gallic acid - β-glucan model in different pH (1.5, 5.5, 7.5, 10) and during the time period (0, 1, 2, 5, 16 h). The zeta potential values have shown that analysed models have been stable in pH 10 according the theoretical stability criteria. In addition, absorption spectra of selected hydroxybenzoic acids and theirs models were recorded.

Keywords: electrokinetic potential, absorption spectra, 4-hydroxybenzoic acid, gallic acid, *β*-glucan



γ (mg/L)	Compound	pH 1.5	pH 5.5	pH 7.5	pH 10
		ζ / mV			
5	β-glucan	5.8±1.0	-7.6±3.6	-8.0±0.5	-14.3±1
25	4-HBA	8.1±3.3	-6.7±1.6	0.5±5.1	-29.2±2.4
	GA	9±2.9	-11.2±7.1	-17±2.1	-24.5±8.8
50	4-HBA	5.2±3	-3.1±1.6	5.4±2.2	-21.8±1.8
	GA	6.9±0.4	-9.4±0.1	17.7±2.4	-26±1.7
75	4-HBA	6.2±2.1	-6.3±6.4	-7.2±10.7	-28.3±5.4
	GA	7.8±1.5	-9.6±1.4	-16.1±3.2	-29.5±1.8
100	4-HBA	0.2±1.5	-5.2±3.8	-11.8±14.9	-21.8±8.7
	GA	7.6±3.3	-14.5±4.8	-14.6±1.8	-30±1.2
150	4-HBA	2.1±0.7	-4.8±0.5	-7.6±7.1	-20.9±2.5
	GA	6.6±1.3	-8.7±2.6	11±1.5	-27.8±0.3

γ (mg/L)	Model	pH 1.5	pH 5.5	pH 7.5	pH 10
		ζ / mV			
0	4-HBA-β-glucan	6±2.3	-2.6±2.9	1.7±1.7	-6.4±3
	GA-β-glucan	4.8±1.4	-2.3±0.5	-8.1±1.5	-18.1±3
1	4-HBA-β-glucan	6±1.8	-4.7±2.4	-15±2.3	-13.1±1.9
	GA-β-glucan	5.7±1.8	-3.5±1.7	-6.5±4.1	-12±2.4
2	4-HBA-β-glucan	5.6±1.5	-3.6±0.8	-17±4.3	-14.6±2.9
	GA-β-glucan	4.6±2	-4.2±0.2	-10±5	-21±8.4
5	4-HBA-β-glucan	4.8±0.3	-3.9±1.9	-11.6±3.8	-21.2±1.3
	GA-β-glucan	6.4±1.4	-4.6±1.8	-8.8±1.7	-17.8±3.1
16	4-HBA-β-glucan	4.3±2.4	-1.8±0.4	-13.9±5.4	-17.2±4.3
	GA-β-glucan	5.7±0.8	-2.8±0.3	-10.1±4.5	-11.5±5.1

OPTIMIZACIJA PROCESA PROIZVODNJE I KARAKTERIZACIJA VOĆNOG VINA OD KRUŠKE

FERMENTATION PROCESS OPTIMISATION AND CHARACTERISATION OF PEAR FRUIT WINE

Darko Velić[1], Valentina Bušić[1], Bruno Husnjak[1], Natalija Velić[1], Daniela Amidžić Klarić[2], Vlatka Petravić Tominac[3], Ilija Klarić[4]

[1]*Faculty of Food Technology Osijek, Josip Juraj Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Faculty of Pharmacy and Biochemistry, University of Zagreb, A. Kovačića 1, 10 000 Zagreb, Croatia*
[3]*Faculty of food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*
[4] *Department of Health, Subdivision of Public Health, R. Dž. Čauševića 1, 76 100 Brčko DC, Bosnia and Herzegovina*

This study aimed to investigate the influence of two commercially available oenological yeasts (Uvaferm BDX and Cross Evolution) on the fermentation kinetics, physicochemical properties, colour and the total polyphenols content of organic pear juice with and without the addition of industrial pectolytic enzyme (Lallzym OE) and their respective wines. The alcoholic fermentation (AF) kinetics was monitored on a laboratory-scale (microfermentations), while the controlled fermentation (CF), as well as induced malolactic fermentation (MLF) of pear juice, was carried out on a pilot-scale custom made fermentation system. The pure culture of lactic acid bacteria (LAB) *Oenococcus oeni* was used for pear wine fermentation with the establishment of temperature optimum for selected LAB type. The results of the study showed that selected yeasts Uvaferm BDX and Cross Evolution could successfully ferment pear juice. The higher specific fermentation rate was achieved using Uvaferm BDX. In samples produced with the addition of the pectolytic enzyme Lallzym OE, a higher specific fermentation rate, as well as a higher total polyphenols content, were observed compared to other pear wine samples. The stimulated MLF led to the decrease of malic acid concentration, which resulted in improved sensory properties of pear wine.

Keywords: fruit wine, pear wine, controlled fermentation, malolactic fermentation, total polyphenols

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GASTROINTESTINALNA STABILNOST IZOTIOCIJANATA IZ BILJKE *Tropaeolum majus* L. USPOREDBOM *IN VITRO* I *EX VIVO* METODA PROBAVE

COMPARISON OF GASTROINTESTINAL STABILITY OF ISOTHIOCYANATES FROM *Tropaeolum majus* L. USING *IN VITRO* AND *EX VIVO* DIGESTION METHODS

Ivana Vrca, Tea Bilušić, Ivica Blažević, Franko Burčul

Kemijsko-tehnološki fakultet, Sveučilište u Splitu,
Ruđera Boškovića 35, 21 000 Split, Hrvatska

Biljka *Tropaeolum majus* L. (dragoljub) pripada maloj porodici Tropaeolaceae (dragoljupke) koja spada u red Capparales. Biljka je jestiva i u biološkom smislu se smatra vrijednom zbog zastupljenosti spojeva iz skupine glukozinolata čiji razgradni produkti (izotiocijanati) imaju širok spektar bioloških aktivnosti (antikancerogena, antimikrobna, protuupalna…) [1-3].
U ovom su istraživanju korištene sjemenke biljke dragoljub u svrhu dobivanja eteričnog ulja koristeći mikrovalnu ekstrakciju. GC-MS analizom određen je kemijski sastav eteričnog ulja biljke dragoljub te je utvrđena dominantna prisutnost benzil-izotiocijanata (97,81%), razgradnog produkta glukozinolata glukotropaeolina. Budući da je pri određivanju stupnja biološke aktivnosti prirodnih spojeva od iznimne važnosti stupanj njihove stabilnosti u probavnom sustavu, u tom pogledu upotreba *in vitro* metoda probave predstavlja vrlo vrijedan doprinos. Za ovo istraživanje korištene su dvije metode simulirane probave – *in vitro* metoda temeljena na upotrebi komercijalnih enzima iz želuca i tankog crijeva [4] te *ex vivo* metoda s ljudskim probavnim sokovima iz želuca i tankog crijeva [5]. Stupanj stabilnosti i biodostupnosti izotiocijanata iz eteričnog ulja sjemenki biljke dragoljub određen je primjenom GC-FID tehnike.

Ključne riječi: dragoljub, izotiocijanati, *in vitro* metoda probave, gastrointestinalna stabilnost

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[4] A. Brodkorb *et al.*, *Nature Protocols* 14 (2019) 991.
[5] I. Blažević *et al.*, *J Food Compos Anal* 90 (2020) 1.

UTJECAJ DISAHARIDA NA FENOLE I HLAPLJIVE KOMPONENTE U PUNILIMA NA BAZI KUPINA

INFLUENCE OF DISACCHARIDES TYPE ON PHENOLICS AND VOLATILES OF BLACKBERRY CREAM FILLINGS

Josipa Vukoja[1], Ana-Marija Dundović[1], Ivana Ivić[1], Josip Šimunović[2], Anita Pichler[1], Mirela Kopjar[1]

[1]*Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2]*Bioprocessing and Nutrition Sciences, Department of Food, North Carolina State University, Raleigh, NC 27 695, USA*

Blackberry cream fillings were prepared with blackberry juice, citrus fiber (5 %) and disaccharides (50 %). Three disaccharides were used. Sucrose as commonly used sugar, and trehalose and maltose, disaccharides that are less sweet than sucrose. Amount of phenolic compounds, proantocyanidins and antioxidant activity were evaluated as well as amount of volatile compounds. Type of disaccharides had an effect on phenolics and proantocyanidins, but there were no difference between samples in antioxidant activity (regardless of used method – DPPH, ABTS, FRAP and CUPRAC). The highest amounts of phenolics were detected in samples with trehalose addition while samples with maltose had the highest amount of proantocyanidins. Overall, 29 volatiles were detected in samples. The most abundant groups were terpenes and aldehydes and ketones. The highest amounts of terpenes were detected in samples with trehalose addition while sucrose samples had the lowest amount of these compounds. Aldehydes and ketones were detected in the highest amount in samples with sucrose addition while samples with maltose had the lowest amount of these volatiles. These results indicate that selection of adequate disaccharide is very important since it can influence on final quality of the product.

Keywords: blackberry cream fillings, sucrose, trehalose, maltose, phenolics, volatiles

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *IP-2019-04-5749*.

Samples	phenolics (g/100 g)	proanthocyanidins (g/100 g)	terpenes (μ/kg)	aldehydes and ketones (μ/kg)
Sucrose	4.25	0.30	281.91	250.87
Trehalose	4.98	0.42	358.05	203.62
Maltose	4.49	0.47	328.39	156.98

FINALIZACIJA VINA MERLOT I CABERNET SAUVIGNON POMOĆU DRVENIH PRIPRAVAKA

FINALIZATION WINE MERLOT AND CABERNET SAUVIGNON WITH DIFFERENT WOODEN MATERIAL

Stanko Zrinščak, Valentina Obradović, Josip Mesić, Ana Mrgan
Veleučilište u Požegi,Vukovarska 17, 34 000 Požega, Hrvatska

Poznato je da prilikom odležavanja vina u drvenim bačvama dolazi do ekstrakcije različitih kemijskih spojeva koji bitno doprinose kvaliteti vina, što je utvrdilo niz autora [1, 2]. Na kvalitetu vina prilikom odležavanja utječe i porijeklo drveta, jačina paljenja kao i vrijeme odležavanja. Pored klasičnih drvenih bačava, danas se koriste i različiti drveni pripravci, popularno nazvani chips.
U ovom radu korišteno je osam vrsta različitih drvenih pripravaka u formi chipsa i bloka, od američkog i francuskog hrasta. Uspoređena su vina s dodacima i vino bez dodataka, te je mjerena antioksidativna aktivnost vina DPPH metodom, udio antocijana i ukupnih polifenola, te je provedena deskriptivna analiza svih uzoraka. Kod vina Merlot pripravci od francuskog hrasta jakog paljenja su najbolje ocijenjeni, te su isti imali i najviše udjele polifenola i antocijana, kao i antioksidativnu aktivnost. U vinima Cabernet Sauvignon su najbolje ocijenjeni uzorci s dodacima Američkog bloka koji su imali i više vrijednosti za ukupne polifenole od ostalih uzoraka. Vina bez dodataka su znatno slabije ocijenjena.

Ključne riječi: vino, drveni pripravci, finalizacija

[1] K. Chira *et al*.,.*Food chemistry* 140 (2013) 168.
2] A. Jeromel *et al*., *Glasnik zaštite bilja*, 6 (2017), 19.

Sekcija: Medicinska kemija i farmacija
Topic: Medical Chemistry and Pharmacy

INAKTIVACIJA LJUDSKE DIPEPTIDIL PEPTIDAZE III DERIVATIMA KINAZOLINONA

INACTIVATION OF HUMAN DIPEPTIDYL PEPTIDASE III BY QUINAZOLINONE DERIVATIVES

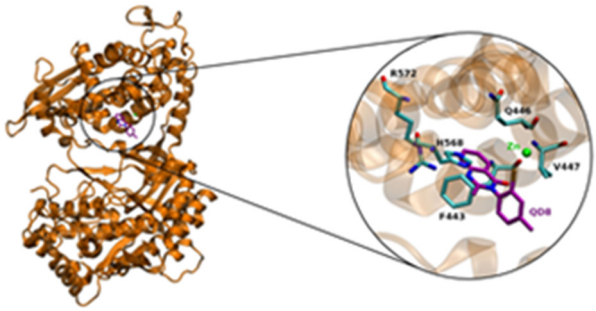
Dejan Agić[1], Maja Karnaš[1], Domagoj Šubarić[1], Mario Komar[2], Zrinka Karačić[3], Sanja Tomić[3], Maja Molnar[2]

[1]Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia
Faculty of Food Technology Osijek, J. J. Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia
[3]Ruđer Bošković Institute, Bijenička 54, 10 000 Zagreb, Croatia

Human dipeptidyl peptidase III (hDPP III) is a zinc-hydrolase that cleaves dipeptides from the N-terminal of different bioactive peptides. Quinazolinones belong to a diverse class of nitrogen-containing heterocyclic compounds, derivatives of which exhibit a wide range of biological activities. In this research, we selected 10 previously synthesized [1] structuraly different quinazolinone derivatives (QDs) to investigate their potential to inactivate hDPP III activity combining *in vitro* and *in silico* approach. The experimental results showed that all analyzed QDs (at the physiological concentration i.e.,100 μM) have inhibitory effect against hDPP III activity. The strongest inhibition (% inh. = 81.9) has been obtained with compound QD8. Molecular docking revealed that hDPP III interacts mostly by hydrogen bonds and hydrophobic interactions with QD8. Among important intermolecular interactions are those with amino acid residues F443, Q446, V447, H568 and R572 that are constituents of hDPP III substrate binding subsites S1, S1', S2', and S3'.

Keywords: dipeptidyl peptidase III, quinazolinones, molecular docking

[1] M. Komar *et al*., *Green Chem Lett Rev* 13 (2020) 93.



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ISTRAŽIVANJE MEDICINSKOG ZNAČAJA FENOLNIH SPOJEVA PRIMJENOM MOLEKULARNOG MODELIRANJA I MOLEKULARNOG PRISTAJANJA

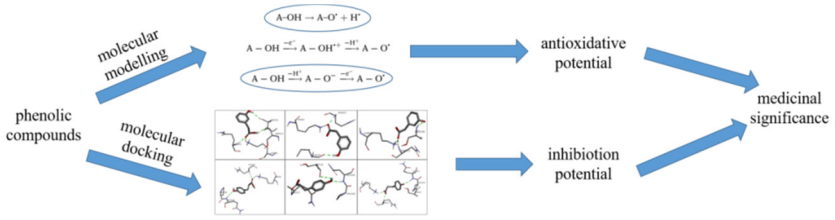
IMPLEMENTATION OF MOLECULAR MODELING AND MOLECULAR DOCKING FOR STUDY OF PHENOLIC COMPOUNDS MEDICINAL SIGNIFICANCE

Ana Amić,[1] Zoran Marković,[2] Jasmina Dimitrić Marković,[3]
Svetlana Jeremić,[2] Marijana Stanojević-Pirković[4]

[1]*Department of Chemistry, J. J. Strossmayer University of Osijek,*
Ulica cara Hadrijana 8/A, 31 000 Osijek, Croatia
[2]*Institute of Information Technologies, Department of Science, University of Kragujevac,*
Jovana Cvijića bb, 34 000 Kragujevac, Serbia
[3]*Faculty of Physical Chemistry, University of Belgrade,*
Studentski trg 12-16, 11 000 Belgrade, Serbia
[4]*Faculty of Medical Sciences, University of Kragujevac,*
Svetozara Markovića 69, 34 000 Kragujevac, Serbia

Oxidative stress is a condition caused by excess free radicals that leads to the development of various chronic and aging-associated diseases. Phenolic compounds as potent antioxidants have an important role in removing excess free radicals and terminating oxidative stress. These compounds can also inhibit various enzymes and by doing so have an important role in anti-inflammatory and anticancer therapy. In our work, molecular modelling was used to study free radical scavenging mechanisms of selected phenolic compounds (hydrogen atom transfer (HAT), single-electron transfer followed by proton transfer (SET-PT) and sequential proton loss electron transfer (SPLET)), while molecular docking was used to study inhibition of cyclooxygenase-2 and multidrug resistance protein 1. Radical scavenging mechanisms were studied by using DFT as implemented in Gaussian 09 (M06-2X/6-311++G(d, p)/SMD). Our results show HAT and SPLET as thermodynamically probable and competitive processes, while Gibbs free energy change indicates selected compounds as potent scavengers. Docking analysis was performed by using the AutoDock 4.2 program package. Free energy of binding and inhibition constant were estimated. Obtained results suggest that investigated compounds are potential inhibitors of studied proteins, meaning they could be responsible for some health benefits associated with regular intake of (poly)phenol-rich diet.

Keywords: phenolic compounds, HAT, SET-PT, SPLET, docking



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SINTEZA I ANTIOKSIDATIVNA AKTIVNOST NOVIH KARBOKSAMIDA *N*-SUPSTITUIRANIH BENZIMIDAZOLA

SYNTHESIS AND ANTIOXIDATIVE ACTIVITY OF NOVEL *N*- SUBSTITUTED BENZIMIDAZOLE CARBOXAMIDES

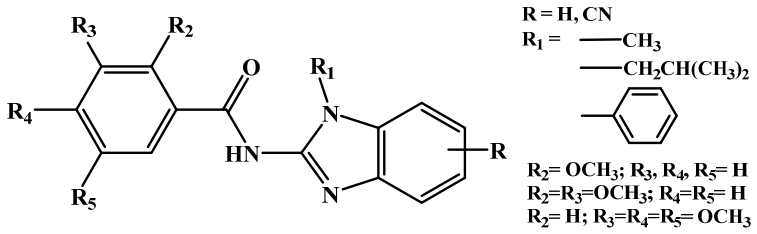
Anja Beč[1], Marija Kos[1], Patricia Debogović[1], Marijana Hranjec[1], Kristina Starčević[2]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 20, 10 000 Zagreb, Croatia*
[2]*Faculty of Veterinary Medicine, University of Zagreb, Heinzelova ul. 55, 10 000 Zagreb, Croatia*

A variety of biochemical processes in the human body could produce oxygen free radicals and other reactive oxygen species (ROS) as by-products which may cause oxidative damage of most important biomolecules such as nucleic acids, lipids and proteins. There has been tremendous and constant growing interest for the searching of novel natural or synthetic organic molecules as potential antioxidants. Heterocycles like benzimidazole derivatives can be promising candidates as antioxidants as these compounds are reported to exhibit a wide range of biological activity [1].
In this work, we present the synthesis of a range of *N*-substituted benzimidazole-2-carboxamides with a variable number of methoxy groups using conventional organic synthetic methods. Starting from the corresponding benzoyl-chlorides, in the reaction with *N*-substituted 2-aminobenzimidazoles carboxamides were obtained in moderate reaction yields [2]. Their antioxidative potency has been evaluated using 1,1-diphenyl-picrylhydrazyl (DPPH) free radical scavenging and ferric reducing antioxidant power (FRAP) assays.

Keywords: amides, antioxidative activity, benzimidazoles, carboxamides, organic synthesis

[1] M. Cindrić *et al*., *Med Chem Res* 26 (2017) 2024.
[2] I. Sović *et al*., *Chem Res Toxicol* 32 (2019) 1880.



PREGLED I ANALIZA MJERENJA UKUPNOG SADRŽAJA FENOLA U UZORCIMA MEDA

REVIEW AND ANALYSIS OF MEASUREMENTS OF TOTAL PHENOLIC CONTENTS IN HONEY SAMPLES

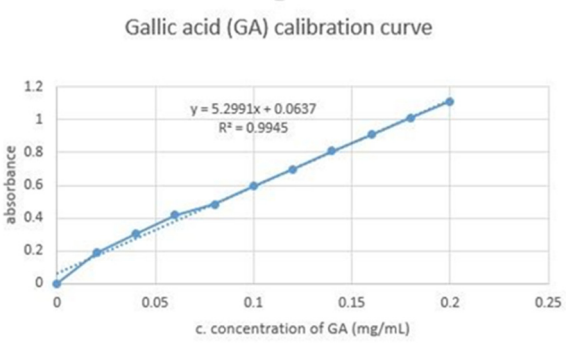
Drago Bešlo[1], Bono Lučić[2]

[1]*Faculty of Agrobiotechnical Sciences Osijek, J. J. Strossmayer University of Osijek, Vladimira Preloga 1, 31 000 Osijek, Croatia*
[2]*Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia*

Polyphenols act as antioxidants playing an important role in preserving human health in the fight against cell damage caused by free radicals [1]. Depending on the season, floral type, and geographical origin, honey samples show different phenol contents. The aim of this study was to determine the total phenol content (TPC) in 96 honey samples from Central and South-Eastern Europe countries (Croatia, Serbia, Bosnia and Herzegovina, Hungary, Slovenia and Italy) by the spectrophotometric method with Folin-Ciocalteu reagent [2]. In this study, the TPC values ranged from 1164.99 mg kg^{-1} to 212.9 mg kg^{-1} for uni-floral (the dominant ones) and multi-floral honey samples. In the review of measurements of TPC of the same types of honey (e.g. acacia or chestnut) from a number of literature sources, large differences of the values of TPC are observed, which cannot be attributed only to seasonal or geographical variations. In an attempt to decipher the reasons for these excessive differences, we analyzed the impact of sample ageing and of seasonal and geographical variations. However, some differences are still too large, and it seems that the reason is the inconsistency of the calculation of the measurement units. Additionally, some authors state that they modified method [1, 2], but do not state, with sufficient details, which part they modified. It was identified that some authors used the calibration curve based on gallic acid in the range 0–200 μg cm^{-3} and some in the range 0–400 μg cm^{-3}. For these reasons, a suggestion for a stricter standardisation of the total phenol content measurements is proposed.

Keywords: honey, total phenol content, standardisation, spectrophotometric method

[1] J. Bertoncelj *et al*., *Food Chem* 105 (2007) 822.
[2] G. Beretta *et al*., *Anal Chim Acta* 533 (2005) 185.



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SINTEZA I BIOLOŠKA AKTIVNOST TETRACIKLIČKIH DERIVATA IMIDAZO[4,5-*b*]PIRIDINA

SYNTHESIS AND BIOLOGICAL ACTIVITY OF TETRACYCLIC IMIDAZO[4,5-*b*]PYRIDINES

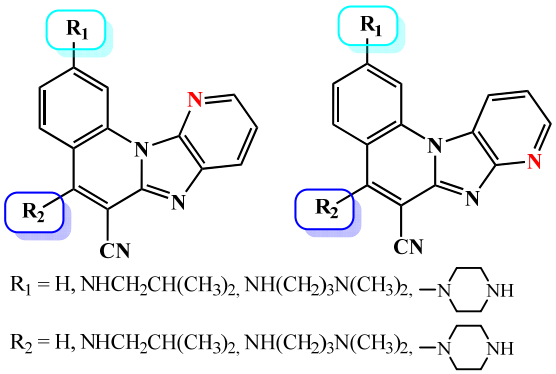
Ida Boček[1], Borka Lončar[2], Marijeta Kralj[3], Marija Mioč[3], Lucija Grgić[3], Marijana Radić Stojković[3], Marijana Hranjec[1]

[1]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 20, 10 000 Zagreb, Croatia*
[2] *Pliva d.o.o, TAPI I&R, 10 000 Zagreb, Savski Marof, Croatia*
[3] *Institute Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Croatia*

Imidazo-pyridine heterocyclic nuclei has structural similarity of imidazo-pyridine heterocyclic system with naturally occurring purines and great therapeutic potential and significance in the drug discovery. Imidazo[4,5-*b*]pyridine scaffold is among the most privileged and important building blocks in organic and medicinal chemistry [1, 2].
In this work, we have synthesized novel amino substituted tetracyclic derivatives by using conventional and microwave assisted organic synthesis. The antiproliferative activity was studied against human cancer and non-tumour cells and the majority of compounds showed improvement of activity on HCT116 and MCF-7 cancer cells when compared to *etoposide*. Obtained results revealed that the position of nitrogen in pyridine ring has strong impact on the biological activity. Thus, regioisomers **6**, **30** and **32** showed noticeable enhancement of activity in comparison to their counterparts **10**, **37** and **25** having IC_{50} values. Additionally, their interaction with ct-DNA was studied by several spectroscopic methods.

Keywords: amines, antiproliferative activity, ct-DNA, imidazo[4,5-*b*]pyridines

[1] M. Hranjec *et al.*, *Eur J Med Chem* 46 (2011) 2748.
[2] N. M. Ghanema *et al.*, *Bioorg Chem* 80 (2018) 565.



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NEUROTOKSIČNI EFEKTI IZAZVANI DJELOVANJEM PESTICIDA NA KOLINESTERAZNU AKTIVNOST

NEUROTOXIC EFFECTS OF SELECTED PESTICIDES BY ALTERING CHOLINESTERASE ACTIVITY

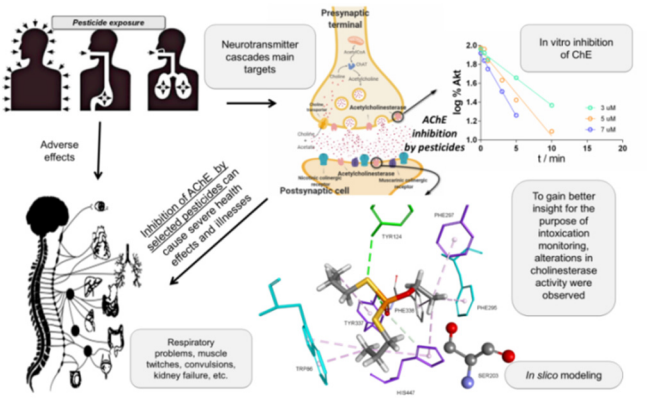
Tena Čadež[1], Goran Šinko[1], Yiyun Liu[2,3], Yongchao Ma[2,3], Heidi Qunhui Xie[2,3], Zrinka Kovarik[1]

[1]*Institute for Medical Research and Occupational Health, Ksaverska cesta 2, 10 000 Zagreb, Croatia*
[2]*Research Center for EcoEnvironmental Sciences Chinese Academy of Sciences, China*
[3]*University of Chinese Academy of Sciences, Beijing 100 049, China*

Due to their role in the protection of herbs, pesticides are globally widespread and can have a deleterious effect on human health. The neurological system is particularly susceptible to adverse effects from pesticide exposure. Selected pesticides such as metamiphos, phenamidophos, ethoprophos, phosalone, and acetamiprid are neuroactive insecticides with neurotransmitter cascades as their main targets. Inhibition of acetylcholinesterase (AChE) by organophosphate (OP) compounds is a well-known mechanism of intoxication. The disruption of nicotine acetylcholine receptors (nAChRs) through agonists such as acetamiprid can lead to toxic effects by inhibiting AChE in the synaptic cleft. To gain better insight for the purposes of intoxication monitoring, alterations in cholinesterase activity were observed together with interactions of pesticides with active site residues of cholinesterases, revealing the possible orientation of the inhibitors. The focus of this study was to achieve a better comprehension of the action mechanisms and effects that selected pesticides have on cholinergic neurotransmission and afterwards attain the best intervention solution for pesticide intoxication.

Keywords: organophosphate pesticides, cholinesterase, cholinergic neurotransmission

Acknowledgement
This study was supported by the Croatian-Chinese Scientific and Technological Cooperation (*2019-202*1) and partially by the Croatian Science Foundation (*IP-2018-01-7683*).



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NOVI *META N*-ARIL SUPSTITUIRANI 3-HIDROKSIPIRIDIN-4-ONI I NJIHOVI ADAMANTILNI DERIVATI

NOVEL *META N*-ARYL SUBSTITUTED 3-HYDROXYPYRIDIN-4-ONES AND THEIR ADAMANTYL DERIVATIVES

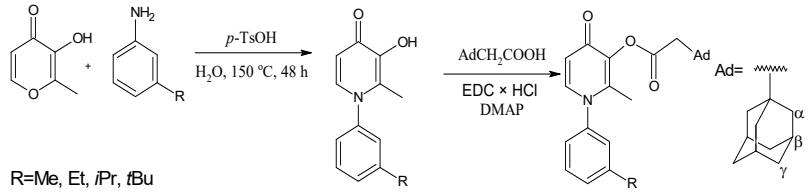
Andrea Dandić[1], Željka Car[2], Vesna Petrović Peroković[2]

[1]*Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Faculty of Science, Department of Chemistry, University of Zagreb, Horvatovac 102 a, 10 000 Zagreb, Croatia*

3-Hydroxypyridin-4-ones are a well-known class of heterocyclic compounds extensively studied due to their broad spectrum of biological activities (antibacterial, antidiabetes, antiprotozoal, antineurodegenerative and anticancer) [1]. In our previous work we investigated several *para N*-aryl substituted 3-hydroxy-2-methylpyridin-4-ones as well as their ester adamantyl derivatives for their *in vitro* antitumor properties. All tested compounds showed antiproliferative activity ranging from moderate to strong on all inspected cell lines with lipophilic adamantane containing derivatives being active at low micromolar IC_{50} concentrations [2]. In the continuation of our work novel lipophilic adamantyl derivatives of *meta N*-aryl substituted 3-hydroxy-2-methylpyridin-4-ones were prepared with the aim of evaluating their *in vitro* antitumor properties on the panel of cancer cell lines. The compounds were synthesized starting from corresponding pyridinones, which are prepared first in an autoclave, and subsequently acylated with adamantan-1-ylacetic acid. Further structure-activity relationship study (SAR) of such and similar pyridinone derivatives as potential anticancer agents is now in progress. Antitumor properties of novel compounds started to elucidate the key elements, primarily the nature and position of the substituent on the aryl part on the adamantyl pyridinones, needed for their high antiproliferative activity.

Keywords: adamantan-1-ylacetic acid, antitumor activity, 3-hydroxypyridin-4-ones

[1] M.A. Santos *et al*., *Future Med Chem* 7 (2015) 383.
[2] V. Petrović Peroković *et al*., *Mol Div* 21 (2017) 881.



OPTIMIZACIJA 3D STANIČNE KULTURE METODOM MAGNETSKE LEVITACIJE

3D MAGNETIC LEVITATION CULTURING OPTIMIZATION

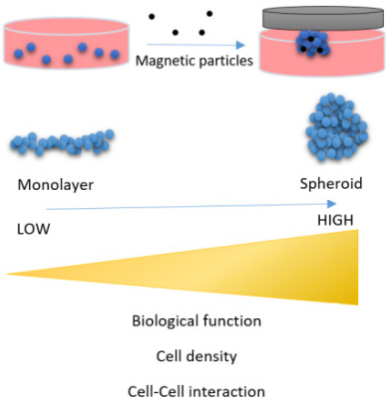
Marijana Jukić[1], Maja Jirouš[1], Ljubica Glavaš-Obrovac[1], Teuta Opačak-Bernardi[1]

Medicinski fakultet, Sveučilište J. J. Strossmayera u Osijeku, J. Huttlera 4, 31 000 Osijek, Hrvatska

Magnetska levitacija je novi pristup stvaranju 3D staničnih tvorbi čija prednost je u tome što stanice nisu u kontaktu s čvrstim površinama te se u takvom okruženju mogu samostalno orijentirati. Levitacija se postiže uzgojem stanica u prisutnosti netoksičnih nano čestica metala koji se ugrađuju u stanicu i omogućuju manipulaciju stanica magnetom [1].
Za uspješno stvaranje funkcionalnih sferoida potrebno je odrediti dozu nanočestica koja će osigurati da sve stanice budu inicijalno jednako usmjerene u magnetskom polju. Naš rad pokazuje proces optimizacije uvjeta rasta stanica stanične linije CaCO-2 adenokarcinoma debelog crijeva. Optimizairali smo tri osnove koje uvjetuju pravilnu formaciju sferoida metodom magnetske levitacije: početni broj stanica, primjenjenu količinu nanočestica za magnetizaciju i volument medija. Stanice su uzgajane prema protokolu [2] tijekom 7 dana s jednom izmjenom medija.
Rezultati pokazuju da kompaktni sferoidi srenje veličine nastaju kada početni broj stanica ne prelazi 7500 uz dodatak 5µl cm^{-2} nanočestica.

*Ključne riječi:*3D kultura, magnetska levitacija, optimizacija

[1] G. R Souza *et al*., *Nature nanotechnology* 5 (2010) 291.
[2] W. L. Haisler *et al*., *Nature Protocols* 8 (2013) 1940.

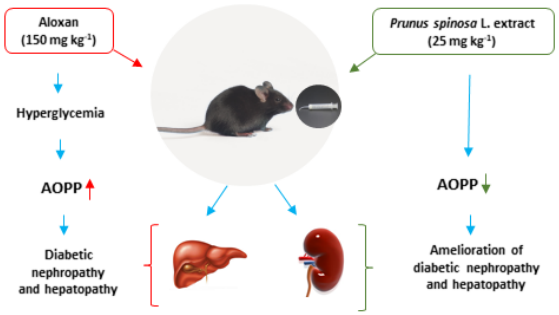


RAZINE NASTALIH PRODUKATA OKSIDACIJSKIH PROTEINA KAO BILJEG OKSIDACIJSKOG STRESA KOD MIŠEVA S HIPERGLIKEMIJOM

ADVANCED OXIDATION PROTEIN PRODUCT LEVELS AS A MARKER OF OXIDATIVE STRESS IN MICE WITH HYPERGLYCEMIA

Irena Landeka Jurčević[1], Irena Crnić[1], Tajana Frančić[1], Petar Dragičević[2], Domagoj Đikić[3]

[1]Faculty of Food Technology and Biotechnology, University of Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia
[2]School of Medicine, University of Zagreb, Šalata 3, 10 000 Zagreb, Croatia
[3]Faculty of Science Zagreb, University of Zagreb, Rooseveltov trg 6, 10 000 Zagreb, Croatia



We aimed to determine whether advanced oxidation protein product (AOPP) levels can serve as a marker of oxidative stress in mice with hyperglycemia. The aim of this study was to establish the oxidation stress of *Prunus spinosa* L. flower extract (PSE) polyphenol glycosides in C57/BL6 mice organs after repeated subchronic (10 days) administration of entry dose of 25 mg kg^{-1} bw of total polyphenols by gavage. Hyperglycemia in mice induced with 150 mg kg^{-1} bw of alloxan. The experiment lasted 10 days using C57BL/6 mice divided in four groups: group 1 as control (C), group 2 as *Prunus spinosa* L. flower extract (PSE), group 3 as aloxan (AL) and group 4 as AL with PSE. AOPP levels in the tissue homogenate (liver and kidney) were measured by the spectrophotometric method (microplate reader). Tissue homogenate (liver, kidney) AOPP levels were significantly higher in the aloxan group (liver: 52.18±3.29 ng cm^{-3}; kidney: 36.12±2.29 ng cm^{-3}) than in the control group (liver: 31.4±1.91 ng cm^{-3}; kidney: 23.73±1.78 ng cm^{-3}; $P < 0.001$). In addition, the mean AOPP level in the homogenate tissue in the aloxan group was significantly higher than the mean homogenate tissue AOPP levels in the AL+ECT group (liver: 36.15±4,96 ng cm^{-3}; kidney: 27.69±1.75 ng cm^{-3}; $P < 0.026$). AOPPs may represent a novel class of pro-inflammatory molecules that are involved in oxidative stress in hyperglycemia. AOPPs may be used as a marker of oxidative stress in patients with hyperglycemia.

Keywords: Advanced Oxidation Protein Products (AOPPs), hyperglycemia, oxidative stress, *Prunus spinosa* L., C57BL/6 mice

OPTIMIZACIJA I KARAKTERIZACIJA D-α-TOKOFEROL NANOEMULZIJE

OPTIMIZATION AND CHARACTERISATION OF D-α-TOCOPHEROL NANOEMULSION

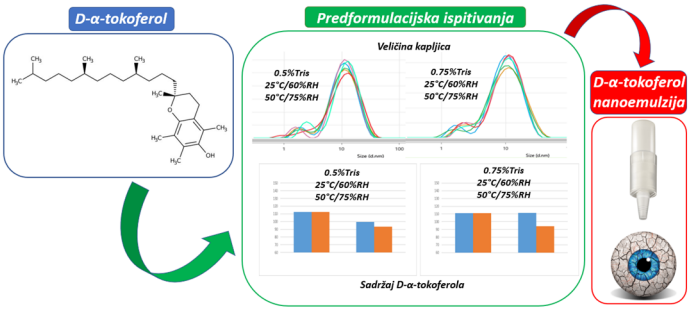
Ana Piškulić, Zrinka Badurina Huljev, Lela Munjas Jurkić, Zdravka Knežević, Maša Safundžić Kučuk, Leo Štefan

Jadran-galenski laboratorij d.d., Svilno 20, 51 000 Rijeka, Hrvatska

Reaktivne kisikove vrste su jedan od faktora koji doprinosi nastanku i progresiji suhog oka, multifaktorne bolesti koja je danas značajno prisutna u populaciji [1,2]. D-α-tokoferol je antioksidans koji ima dokazani terapijski učinak, a lipidne emulzije s netopljivim D-α-tokoferolom opisane su literaturi u terapiji suhog oka [3]. S ciljem optimalne dostave D-α-tokoferola, razvijena je nanoemulzija stabilizirana neionskim emulgatorom. Nanoemulzije U/V tipa pripremljene su niskoenergetskom metodom s ricinusovim uljem kao uljnom fazom. Na temelju optimalnih HLB vrijednosti kao emulgatori odabrani su Polisorbat 80 i Koliphor RH40, a kao puferski par primijenjen je trometamol/klorovodična kiselina. Prototipovi formulacija s 0,5 i 0,75 % trometamola izabrane su kao vodeće formulacije. Provedene su studije stabilnosti pri uvjetima 25 °C/60 % RV i 50 °C/75 % RV te ispitani fizikalni parametri: osobine, osmolalnost, pH, viskoznost, veličina kapljica, indeks polidisperznosti i zeta potencijal te sadržaj vitamina E. Veličina kapljica uljne faze za oba prototipa bila je <100 nm, utvrđeni sadržaj vitamina E je viši od 93 %, dok su ostali fizikalni parametri kao pH, osmolalnost i zeta potencijal potvrdili stabilnost ispitanih formulacija. U završnoj fazi, provedeno je primjensko ispitivanje na korisnicima koji imaju simptome suhog oka, te je na taj način izabrana ciljna nanoemulzija.

Ključne riječi: suho oko, vitamin E, nanoemulzija

[1] S. Seen *et al*., *Acta Ophtalmol* 96 (2018) 412.
[2] K. Tsubota *et al*., *Ocul Surf* 15 (2017) 65.
[3] J. Xin *et al*., *Drug Dev Ind Pharm* 42 (2016) 525.



ULOGA DIPEPTIDIL PEPTIDAZE III U REGULACIJI BOLI

ROLE OF DIPEPTIDYL PEPTIDASE III IN PAIN REGULATION

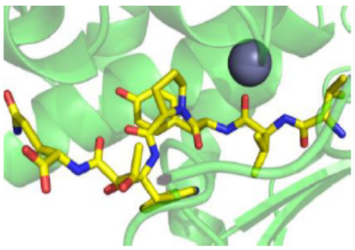
Sanja Tomić, Zrinka Karačić, Lidija Brkljačić, Ana Tomašić Paić, Mirsada Ćehić, Mihaela Matovina

Institut Ruđer Bošković, Bijenička 54, 10 000 Zagreb, Hrvatska

Dipeptidil-peptidaza III (DPP III, EC 3.4.14.4) je o cinku ovisna metalo-egzopeptidaza koja hidrolizira dipeptide s N-kraja svojih supstrata, peptida koji se sastoje od 3-10 aminokiselina [1]. U tkivima sisavaca široko je zastupljena i smatra se da sudjeluje u završnim koracima unutarstaničnog katabolizma proteina. Kolokalizacija DPP III s endomorfinima i enkefalinima u centralnom živčanom sustavu, uz sposobnost DPP III da odgrađuje te opioidne peptide, upućuju na njezinu ulogu u endogenom sustavu modulacije boli kod sisavaca [2-45]. Buckley i suradnici utvrdili su povećanu aktivnost DPP III kod pacijenata s kroničnom boli u donjem dijelu leđa [6] što upućuje na njezinu potencijalnu ulogu biomarkera za navedenu bolest.
Od približno desetak neuropeptida koje smo do sada eksperimentalno ispitali, uvažavajući postojeća znanja o veličini peptidnih supstrata humane DPP III, utvrdili smo da DPP III pored enkefalina (Leu- i Met-) i endomorfina razgrađuje valorfin, Leu-valorfin-Arg, ß-kazomorfin i dinorfin, dok su vazopresin i iz α-hemoglobina dobiven hempresin, [6] ostali nerazgrađeni.

Ključne riječi: Dipeptidil-peptidaza III, neuropeptidi, enzimska aktivnost

[1] J. M. Chen, Barrett Handbook of Proteolytic Enzymes, Vol. 1 *Academ. Press* (2004) 809.
[2] T Chiba *et al*., *Peptides* 24 (2003) 773.
[3] M Baršun *et al.*, *Biol Chem* 388 (2007) 343.
[4] A Tomić, *Phys Chem Chem Phys* 18 (2016) 27245.
[5] D. A. Buckley *et al*., *Mol Neurobiol* 55 (2018) 2420.
[6] M. G. Bomar *et al*., *Life Sci* 92 (2013) 520.



H-**VVYPWTQ**-OH + H_2O + **DPP III** ⟶ H-**VV**-OH + H-**YPWTQ**-OH + **DPP III**

ISPITIVANJE VLAČNE ČVRSTOĆE TABLETA

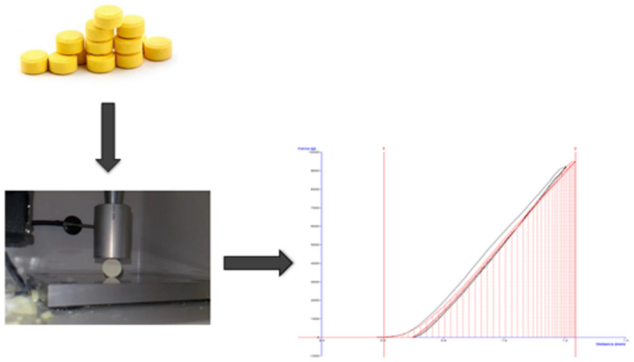
TENSILE STRENGTH RADIAL OF TABLETS

Valentina Travančić, Dario Klarić

Pliva Hrvatska d.o.o., Prilaz baruna Filipovića 25, 10 000 Zagreb, Croatia

Tableting is one of the most common formulation processes in the pharmaceutical industry. The purpose of a process is to obtain compact tablet with defined quality and good parameters, such as packing density, compressibility, tensile strength and others. Related analysis presented in this paper shows results between three different salts of an active pharmaceutical ingredient. A simple method that uses low amount of sample (200 mg) was used for evaluation of the packing density of powders. The powders are compressed under low pressure using a die and a flat-faced punch fitted on a TA-XTplus Texture analyzer (Stable Micro Systems Ltd.). The sample is compressed in a steel mould. After compression a solid tablet is formed. The tablet is then mounted on the surface on its' side and compressed using a flat-faced punch until it breaks. The force of the break is registered and allows for the determination of radial tensile strength of the compressed powder. Tensile strength experiments show that API samples (regular) are rather similar in compactability, except API tosylate at lower compressive stress. At larger compressive stress, API samples (regular) level in tensile strength around 1.7-1.9 MPa, which is a good approximation of the requirement of 2 MPa in the compression stress around < 20 kN. It can be concluded that tested API salts are all acceptable for direct compression process. Tensile strength for micronized samples is around 1.8-2.2 MPa at larger compressive stress. Difference between tensile strength of regular and micronized material is expected. Particle size of micronized material is smaller and the result of that is higher packing density which leads to higher value of tensile strength.

Keywords: density, tensile strength, compactability, compressive stress



Sekcija: Kemija u poljoprivredi i šumarstvu
Topic: Chemistry in Agriculture and Forestry

pH-VRIJEDNOST OBRADIVIH TALA OSJEČKO-BARANJSKE I VUKOVARSKO-SRIJEMSKE ŽUPANIJE

THE pH VALUE OF ARABLE SOILS IN OSIJEK-BARANJA AND VUKOVAR-SRIJEM COUNTIES

Nada Pitinac[1], Đurđevka Pecikozić[2]

[1]Tehnička škola i prirodoslovna gimnazija Ruđera Boškovića, Vukovarska 209, 31 000 Osijek, Hrvatska
[2]Tehnička škola Nikole Tesle Vukovar, Blage Zadre 4, 32 000 Vukovar, Hrvatska

Fizikalna, kemijska i biološka ravnoteža u tlu važan su faktor u rastu i razvoju biljaka stoga je potrebno poznavati pH-vrijednost tla kao značajnog pokazatelja. Za većinu biljaka optimalna su vrlo slabo alkalna ili vrlo slabo kisela tla. Zakiseljavanje tla posljedica je prirodnih procesa u tlu, ispiranja tla koje je usko povezano s količinom i dinamikom oborina, tj. s perkolacijom vode i strukturom tla. Antropogeni uzroci zakiseljavanja tla su kisele kiše, tj. plinovi, SO_2 i NO_2, koji kiselim kišama dospijevaju u tlo i zakiseljavaju ga, te dodatak hranjiva organskom i mineralnom gnojidbom. Pri tome u tlo mogu biti unesene značajne količine kiselih mineralnih gnojiva. Organska gnojidba tj. unošenje i razgradnja organske tvari pri uzgoju poljoprivrednih kultura, te smanjenje koncentracije kalcija u tlima kao posljedica poljoprivredne djelatnosti također mogu uzrokovati zakiseljavanje. U ovom istraživanju ispitana je pH-vrijednost obradivih tala na području Osječko-baranjske i Vukovarsko-srijemske županije. pH-vrijednost tla mjerena je pomoću prijenosnog mjerača (Hach, HQ40d) i digitalne ubodne sonde (IntelliCAL, PHC108) direktnim mjerenjem u uzorku tla. pH-vrijednost ispitivanih obradivih površina u obje županije kretala se u rasponu od 5,92 do 7,96 te stoga ova tla pripadaju slabo kiselim do slabo alkalnim tlima. Vrijednosti pH znatno su bile veće u istočnom dijelu Osječko-baranjske županije i Vukovarsko-srijemskoj županiji od pH-vrijednosti tla u zapadnom dijelu Osječko-baranjske županije što je u skladu s literaturnim podacima.

EKSTRAKCIJA METALA I METALOIDA IZ UZORAKA TLA RAZRIJEĐENIM KISELINAMA

EXTRACTION OF METALS AND METALLOIDS FROM SOIL SAMPLES BY USING DILLUTED ACIDS

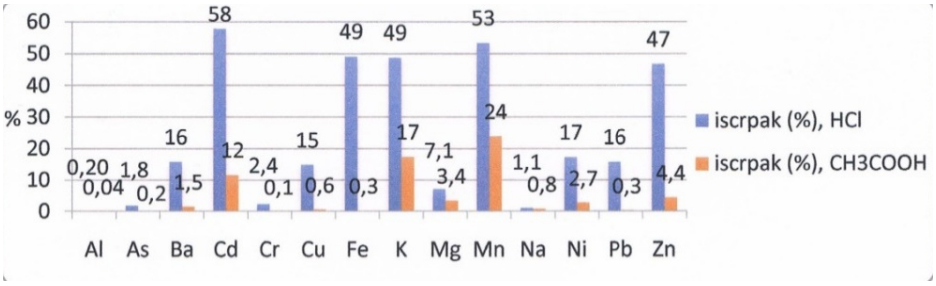
Vibor Roje, Darko Grba

Šumarski fakultet. Sveučilište u Zagrebu, Svetošimunska cesta 25, 10 002 Zagreb, Hrvatska

U znanstvenoj literaturi prikazane su brojne analitičke metode za određivanje metala i metaloida u tlima, a u svrhu procjene njihove mobilnosti, odnosno ekološkog rizika uslijed prisutnosti tzv. 'teških metala' u tlima. Ključni element za valjanu procjenu bioraspoloživosti takvih kemijskih elemenata u tlima jest njihova ekstrakcija iz uzorka tla, preciznije izbor ekstrakcijskih uvjeta. Tako se za ekstrakciju nastoji primjenjivati sredstva i uvjete koji oponašaju uvjete koji vladaju u okolišu. Iako je za analizu teških metala iz uzoraka tla u primjeni najrašireniji metoda ekstrakcije zlatotopkom [1], razvidno je da je to preagresivan reagens u kontekstu oponašanja uvjeta u okolišu. Zbog toga se istražuju različita blaga sredstva za ekstrakciju [2].
U ovom radu provedena je analiza odabranih kemijskih elemenata u uzorku tla koja se sastojala od ekstrakcije pomoću razrijeđenih kiselina (klorovodične odnosno octene kiseline, 0,1 mol dm^{-3}) te kvantifikacije analitâ u ekstraktima tehnikom atomske emisijske spektrometrije uz induktivno spregnutu plazmu (ICP-AES). Kao modelni uzorak korišten je certificirani referentni materijal za tlo Metranal-33.

Ključne riječi: tlo, teški metali, ekstrakcija, ICP-AES

[1] H.M. Kingston *et al*. American Chemical Society, Washington DC, 1997, 223.
[2] V. Roje *et al*., *Environ. Monit. Assess*. 191 (2019) 534.



Sekcija: Zaštita okoliša
Topic: Environmental Protection

UKLANJANJE FARMACEUTIKA IZ RETENTATA REVERZNE OSMOZE

REMOVAL OF PHARMACEUTICALS FROM REVERSE OSMOSIS RETENTATE

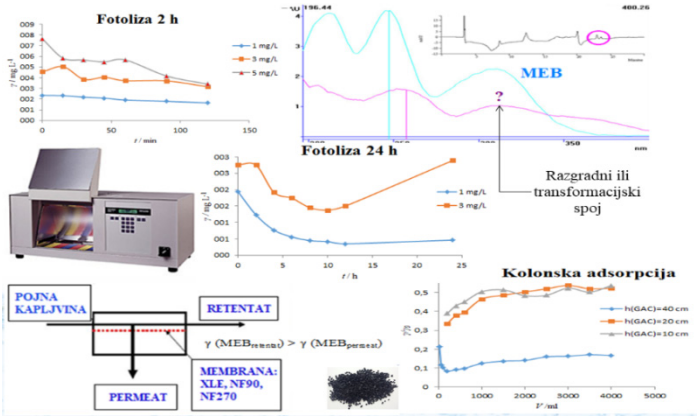
Bruna Babić, Davor Dolar, Danijela Ašperger

Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Marulićev trg 19, 10 000 Zagreb, Hrvatska

Farmaceutici su detektirani u otpadnim, površinskim, podzemnim i vodovodnim vodama u velikom broju zemalja. Iako se u okolišu nalaze u niskim koncentracijama (od nekoliko ng dm^{-3} do nekoliko µg dm^{-3}), raste zabrinutost zbog mogućeg štetnog utjecaja na ljude i vodene organizme uslijed trajne izloženosti te kontinuiranog unosa u okoliš zbog sve veće primjene u zdravstvu i veterini. Membranske tehnologije pokazale su se učinkovite kao procesi obrade voda i u uklanjanju farmaceutika iz istih, ali jedan od problema membranskih tehnologija je zbrinjavanje retentata (koncentrata). Onečišćenja prisutna u retentatu su 6 do 8 puta većih koncentracija nego u ulaznoj struji i mogu imati negativan utjecaj na ekosustav i kvalitetu vode u blizini mjesta njegovog odlaganja.

U ovom radu ispitivano je uklanjanje antihelmintika (mebendazola) iz retentata reverzno osmotskih i nanofiltracijskih membrana adsorpcijom na granuliranom aktivnom ugljenu (GAC) i fotolitičkom razgradnjom. Adsorpcijom u koloni došlo je do skoro potpunog (>99,9 %) uklanjanja mebendazola pri najvećoj primijenjenoj visini GAC-a (40 cm) iz otopine najmanje koncentracije (1 mg dm^{-3}). Fotolitičkom razgradnjom umjetnom Sunčevom svjetlosti tijekom 2 i 24 h postignuta je fotodegradacija mebendazola u rasponu 29,8 % - 76,2 % te je došlo do nastajanja novog razgradnog ili transformacijskog spoja. Nastajanje novog spoja tijekom fotolitičke razgradnje ukazalo je na potrebu provođenja daljnjih ispitivanja s ciljem određivanja strukture novonastalog spoja i njegove ekotoksičnosti.

Ključne riječi: mebendazol, reverzna osmoza, retentat, adsorpcija, fotoliza



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September 16–18, 2020 / Vukovar, Croatia

FIZIOLOŠKI ODGOVOR MASLAČKA (*Taraxacum officinale* Weber) NA ČIMBENIKE OKOLIŠA U URBANIM SREDINAMA

PHYSIOLOGICAL RESPONSE OF DANDELION (*Taraxacum officinale* Weber) TO ENVIRONMENTAL FACTORS IN URBAN AREAS

Lidija Begović[1], Denis Boršćak[2], Selma Mlinarić[1], Igor Ivanac[2], Vlatka Gvozdić[2]

[1]*Department of Biology, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*

In urban areas plants are most often exposed to various abiotic stress factors. Dandelion *(Taraxacum officinal* Weber) is a very abundant species which can grow in urban areas. In this study we collected samples from 30 locations in city of Osijek which included traffic zones and parks (polluted and less polluted locations). Analyses included total chlorophylls, carotenoid, polyphenols and ascorbic acid content as well as antioxidant capacity measured by FRAP (Ferric Reducing Antioxidant Power) and iRAC (Iron (III) Reducing Antioxidant Capacity) assays. Results showed decrease in all measured biochemical parameters and antioxidant capacity in dandelion plants growing on/near traffic locations in comparison to less polluted locations such as parks and meadows. Observed results suggest suppression of metabolic processes and higher sensitivity to ecological stress in dandelion plants exposed to traffic zones. Results of this work will contribute to the understanding of physiological and biochemical responses of dandelion to environmental stress and its role as a bioindicator of environmental pollution in urban areas.

Keywords: abiotic stress, pollution, dandelion, antioxidant capacity

UTJECAJ KLIMATSKIH FAKTORA NA KONCENTRACIJE ORGANSKOG UGLJIKA U ROGOZNIČKOM JEZERU (DUGOROČNO ISTRAŽIVANJE: 1994. – 2020.)

INFLUENCE OF CLIMATE FACTORS ON ORGANIC CARBON CONCENTRATIONS IN ROGOZNICA LAKE (LONG-TERM STUDY: 1994 - 2020)

Irena Ciglenečki[1], Niki Simonović[1], Mathieu Dutour Sikirić[1], Ana Cvitešić Kušan[1], Boris Mifka[2], Maja Telišman-Prtenjak[3], Marija Marguš[1], Milan Čanković[1]

[1]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*
[2]*Odjel za fiziku, Sveučilište u Rijeci, Ul. Radmile Matejčić 2, 51 000 Rijeka, Hrvatska*
[3]*Geofizički odsjek, Prirodoslovno-matematički fakultet, Sveučilište u Zagrebu, Horvatovac ul. 95, 10 000 Zagreb, Hrvatska*

Rogozničko jezero (RJ) ili u narodu poznato kao Zmajevo oko, jedinstveni je morski okoliš na Jadranu (43°32´N, 15°58´E), s euksinskim (anoksični sloj obogaćen sulfidom) i eutrofnim karakteristikama (grafički abstrakt) [1,2]. Dugoročni podaci (1994-2020; temperatura, salinitet, redoks uvjeti, nutrienti, sumporne vrste, organska tvar) ukazuju kako jezero odražava klimatske promjene uočene preko zagrijavanja vodenog stupca, akumulacije toksičnih sulfida i amonijaka [1,2], te otopljenog organskog ugljika, DOC (grafički abstrakt) u pridnenom anoksičnom sloju. Smanjenje DOC u površinskom sloju (0-5 m) kao i promjene u odnosu između DOC i partikularnog (POC), odnosno površinski aktivnog ugljika (PAT) ukazuju na određene promjene u biogeokemijskom ciklusu organske tvari. Integracija navedenih podataka pokazuje kako RJ, uz svoje meromiktičke i holomiktičke karakteristike, može služiti i kao laboratorij za praćenje okolišnih/klimatskih promjena.

Ključne riječi: Rogozničko jezero, organska tvar, DOC, POC, PAT, klimatske promjene

[1] I. Ciglenečki *et al*., Springer 2017, Cham 125.
[2] M. Čanković *et al*., *Syst Appl Microbiol* 42 (2019) 126016.

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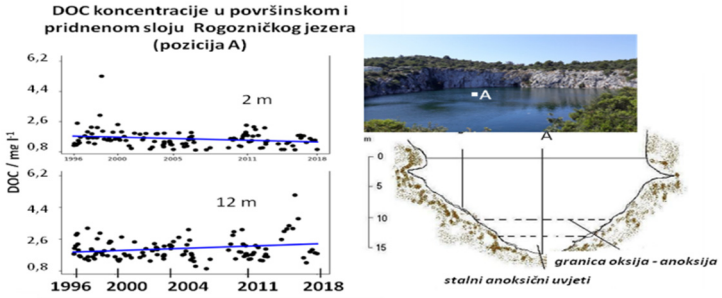
Ovo istraživanje financirano je sredstvima Hrvatske zaklade za znanost projektom *MARRES, IP-2018-01-1717.*



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BIORAZGRADNJA I TRANSFORMACIJA ORGANSKIH TVARI U AEROBNIM UVJETIMA

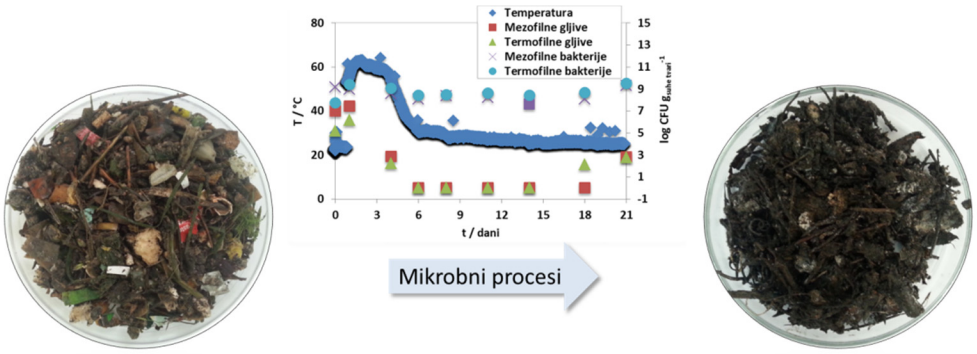
BIODEGRADATION AND TRANSFORMATION OF ORGANIC SUBSTANCES UNDER AEROBIC CONDITIONS

Tomislav Domanovac[1], Monika Šabić Runjavec[2], Ivana Stojmilović[2], Dajana Kučić Grgić[2], Marija Vuković Domanovac[2]

[1]IPZ Uniprojekt TERRA, Voćarska cesta 68, 10 000 Zagreb, Hrvatska
[2]Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Marulićev trg 19, 10 000 Zagreb, Hrvatska

Biološka obrada otpadnih tvari primarno je usmjerena na stabilizaciju organske tvari. Poznavanje mikrobnih procesa preduvjet je za optimalno korištenje biorazgradivog otpada. Obrada ovakve vrste otpada preporuča se iz dva razloga: minimiziranje rizika za okoliš zbog nekontrolirane emisije i obnavljanja resursa. Transformacija organskih tvari uzrokuje pojavu i nestajanje različitih metaboličkih produkata. Svojstva ulaznog materijala utječu na brzinu transformacije koja se odvija prema načelima mikrobnih metaboličkih putova.
U ovom radu određivan je potencijal biorazgradivosti organske frakcije iz miješanog komunalnog otpada. Rezultati pokazuju visoke vrijednosti biorazgradivosti ulaznog materijala od 97 %. Aerobnom obradom se postiže učinkovitost preko 75 % uz smanjenje toksičnosti od 87 %.

Ključne riječi: aerobni uvjeti, biorazgradivi otpad, mikrobni procesi

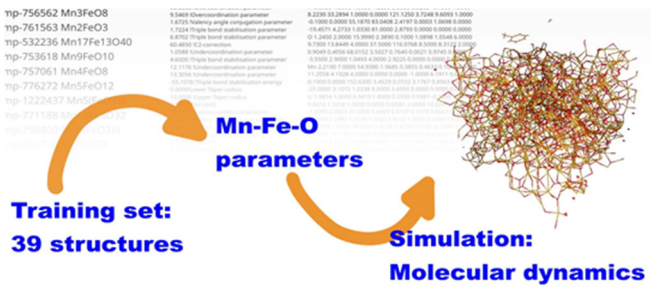


OPTIMIZACIJA PARAMETARA REAKCIJSKOG POLJA SILA I TEORIJSKO ISTRAŽIVANJE KATALITIČKIH SVOJSTAVA $MnFeO_3$

REACTIVE FORCE FIELD OPTIMIZATION AND $MnFeO_3$ CATALYST THEORETICAL INVESTIGATION

Vjeran Gomzi[1], Marina Duplančić[2], Vesna Tomašić[2]

[1]*Faculty of Electrical Engineering and Computing, University of Zagreb, Unska 3, 10 000 Zagreb, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*



In a recent unpublished research of catalytic activity of several $MnMO_x$ (M = Cu, Fe, Ni) metal-oxide catalysts the Reactive force field (ReaxFF) method has been shown to model well such processes. The investigation raised interest in developing parameters for calculation of mixed metal-oxide species, which were at the time non-existent. Here we present first and preliminary results of training the ReaxFF for the Mn-Fe-O-C interaction. The training set of 39 structures consisting of at minimum the Mn, Fe and O atoms, obtained in their crystal form from Materials Project database [1, 2]. Each step in parameter optimization has been done performing MD minimization of 5000 steps of 0.1 fs using the NVT/Berendsen thermostat. Parameters were optimized using the parabolic search as implemented in the original van Duin code [3] with some in-home modifications. First, optimization is performed at temperature of 1 K. Initial parameters are then re-optimized using the same training set at temperatures 300 K and 500 K. The force field is applied to the process of toluene adsorption/degradation on $MnFeO_3$ catalyst. Results obtained show agreement to previous experimental expectations, although some remarks are given, since the presumed crystal structure of $Mn_{1-x}Fe_xO_3$ may have major impact for such theoretical predictions.

Keywords: ReaxFF, MD simulation, parameter optimization, $MnFeO_3$

[1] A. Jain *et al*., *APL Materials*, 1 (2013) 011002.
[2] S. P. Ong *et al*., *Comp Mat Sci* 68 (2013) 314.
[3] A. C. T. van Duin *et al*., *J Phys Chem A*, 105 (2001) 9396.

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BIOLOŠKO UKLANJANJE NUTRIJENATA PRI NISKOJ KONCENTRACIJI OTOPLJENOG KISIKA

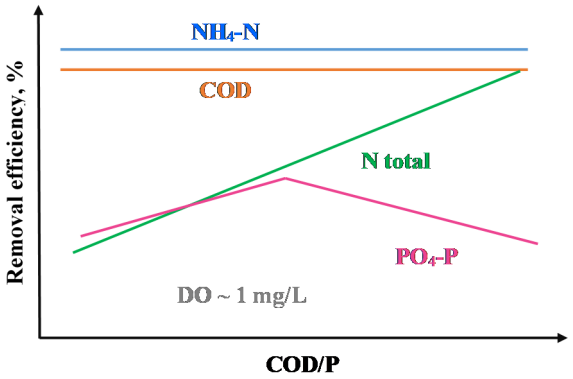
BIOLOGICAL NUTRIENT REMOVAL AT LOW DISSOLVED OXYGEN

Dijana Grgas, Kristina Čondić Galiničić, Tibela Landeka Dragičević

Faculty of Food Technology and Biotechnology, University of Zagreb,
Pierottijeva 6, 10 000 Zagreb, Croatia

For simultaneous biological nutrient removal (SBNR) from wastewater are responsible macroenvironment in reactor and microenvironment in microbial biomass – floc microenvironment.
Biological nutrient removal process (BNR) at low dissolved oxygen (DO ~ 1mg dm^{-3}) results in simultaneous removal of C, N and P. At all investigated C/P ratio the removal efficiency of organics (COD) was ≥ 95 % and ammonium (NH_4-N) 100 %. Total nitrogen (Ntot) removal efficiency increased with increasing of C/P ratio, and at COD/P 32 the N removal was 86 %. Phosphate removal efficiency of 54 %, 61 % and 42 % was achieved at COD/P ratios of 18, 25 and 32, respectively.

Keywords: biological nutrient removal, low dissolved oxygen, activated sludge



PRIMJENA FTIR SPEKTROSKOPIJE I ANALIZE GLAVNIH KOMPONENATA U PROCJENI OKOLIŠNIH UTJECAJA NA BILJKE

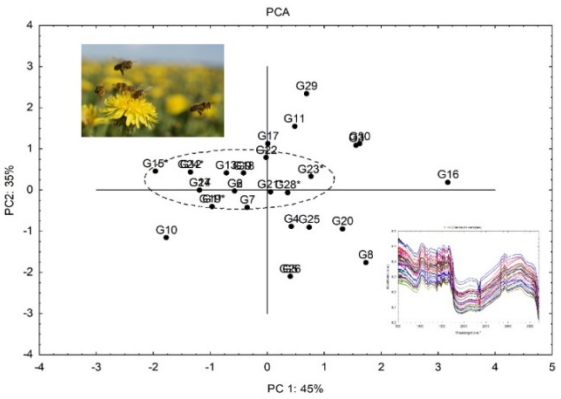
APPLICATION OF FTIR AND PCA FOR ASSESSMENT OF INFLUENCES OF ENVIRONMENTAL FACTORS ON PLANTS

Vlatka Gvozdić[1], Lidija Begović[2], Selma Mlinarić[2], Denis Boršćak[1], Igor Ivanac [2]

Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia
Department of Biology, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia

The FTIR spectra obtained from 60 dandelions (*Taraxacum officinale* Weber) samples collected at different locations (agricultural, non-agricultural, high traffic zones, exposed /not exposed to pollution, etc.) were compared. Dandelion has been chosen since it is considered as a good bioindicator of environmental pollution. When we compared the FTIR spectra of dandelion samples collected from different locations, slightly differences were noticed in the values of maximum absorbance but greater were found in the peak positions. The most significant differences in the peaks position and the character of spectrum were in FTIR region between 900 cm^{-1} and 1200 cm^{-1}, and around 2900 cm^{-1}. PCA analysis showed that the location of a sample has substantial influence on the obtained FTIR results, so it is possible to distinguish the FTIR spectra of polluted and non-polluted locations (i.e. control samples). Dandelion samples collected on different locations were successfully resolved and differentiated after chemometric treatments of PCA.

Keywords: FTIR, dandelion, pollution, Principal Component Analysis



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September 16–18, 2020 / Vukovar, Croatia

ANTROPOGENI UTJECAJ NA DINAMIKU ORGANSKOG OPTEREĆENJA U KOMUNALNIM OTPADNIM VODAMA

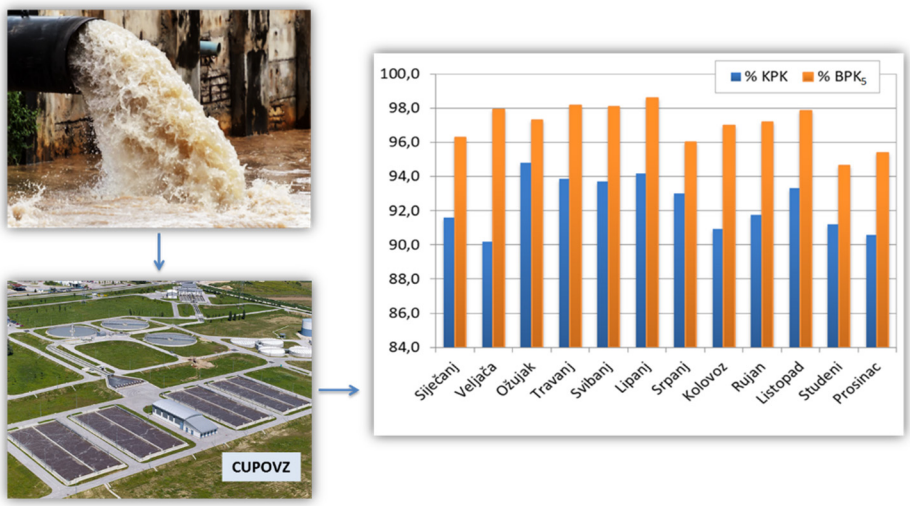
ANTHROPOGENIC IMPACT ON THE ORGANIC LOAD DYNAMICS OF MUNICIPAL WASTEWATER

Sanja Ivanušić[1], Monika Šabić Runjavec[1], Marin Ganjto[2], Marija Vuković Domanovac[1]

[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Marulićev trg 19, 10 000 Zagreb, Hrvatska*
[2]*Zagrebačke otpadne vode – upravljanje i pogon d.o.o., Čulinečka cesta 287, 10 000 Zagreb, Hrvatska*

Kvaliteta života i antropogene aktivnosti utječu na složenost sastava komunalnih otpadnih voda. Pročišćavanje komunalnih otpadnih voda predstavlja jedan od osnovnih uvjeta održivog upravljanja vodenim resursima te unaprjeđenje zaštite okoliša. Proces s aktivnim muljem je najčešći izbor za uklanjanje organskog opterećenja iz otpadnih voda. Mikroorganizmi i održavanje aktivne populacije su ključni dio procesa. Na aktivnost mikroorganizama utječu mnogi procesni parametri čime se izravno utječe na učinkovitost postupka pročišćavanja, a u konačnici rezultira određenom kvalitetom pročišćene vode.
U ovom radu praćena je promjena organskog opterećenja u komunalnim otpadnim vodama iz Centralnog uređaja za pročišćavanje otpadnih voda grada Zagreba (CUPOVZ). Ukupna učinkovitost obrade komunalne otpadne vode u CUPOVZ je u prosjeku veća od 95 %.

Ključne riječi: organsko opterećenje, komunalna otpadna voda, proces s aktivnim muljem



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ANALIZA POSTOJANIH I TOKSIČNIH POLIBROMIRANIH DIFENIL ETERA U UZORCIMA KUĆNE PRAŠINE

ANALYSIS OF PERSISTENT AND TOXIC POLYBROMINATED DIPHENYL ETHERS IN HOUSE DUST SAMPLES

Karla Jagić, Marija Dvoršćak, Darija Klinčić

Institut za medicinska istraživanja i medicine rada,
Ksaverska cesta 2, 10 000 Zagreb, Hrvatska

Polibromirani difenil eteri (PBDE) koristili su se kao aditivi različitim tekstilnim i građevnim materijalima te elektronskoj i elektroničkoj opremi kako bi smanjili njihovu zapaljivost, spriječili nastanak požara ili usporili njegovo širenje. Tijekom korištenja, odlaganja i/ili recikliranja materijala koji sadrže PBDE, ovi se spojevi lako otpuštaju i dospijevaju u okoliš. Dva glavna puta unosa spojeva PBDE u ljude su putem prehrane i udisanjem/ingestijom prašine (u domovima, uredima, školama, automobilima itd.). U ljudskom organizmu ovi spojevi narušavaju hormonsku ravnotežu i posljedično izazivaju niz štetnih učinaka na zdravlje. Zbog svoje široke uporabe, dugog vijeka trajanja i recikliranja materijala koji ih sadrže, ovi iznimno postojani spojevi će još dugi niz godina biti prisutni u okolišu, životinjama i ljudima. Sedam kongenera PBDE-a (BDE-28, -47, -99, -100, - 153, -154 i -183) analizirano je u 5 uzoraka kućne prašine skupljenih na području Zagreba. Spojevi su iz uzoraka kućne prašine (1 g) ekstrahirani tehnikom ekstrakcije potpomognute mikrovalovima smjesom otapala *n*-heksana i acetona (1:1, *v*/*v*) na temperaturi od 80 °C u trajanju od 20 min. Pročišćeni ekstrakti analizirani su pomoću tehnike GC-μECD. Povrati metode bili su od 70 % do 83 %, a RSD ispod 9%. Suma masenih udjela detektiranih spojeva PBDE u uzorcima bila je od <0,32 ng g^{-1} do 17662,4 ng g^{-1} prašine, a najzastupljeniji je bio kongener BDE-99. Dobiveni rezultati predstavljaju prve preliminarne rezultate o onečišćenosti kućne prašine u Hrvatskoj spojevima PBDE, i upućuju na potrebu za analizom većeg broja uzoraka kako bi se dobio uvid u potencijalne izvore onečišćenja.

Ključne riječi: PBDE, ekstrakcija potpomognuta mikrovalovima, kućna prašina

Zahvala
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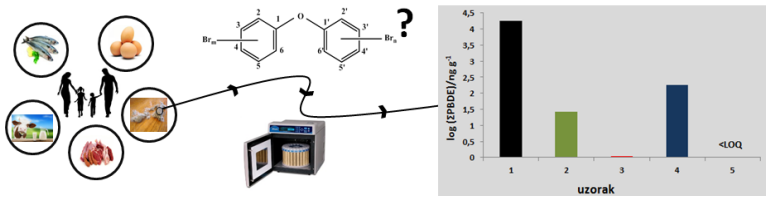


UTJECAJ GRAFEN OKSIDA NA FOTOKATALITIČKA SVOJSTVA TITAN(IV) OKSIDA

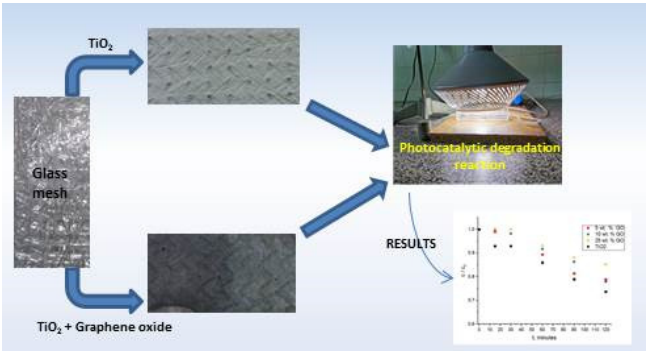
INFLUENCE OF GRAPHENE OXIDE ON PHOTOCATALYTIC PROPERTIES OF TITAN(IV) OXIDE

Igor Jajčinović[1], Don Vito Lukšić[1], Kristina Tolić[2],
Ivan Brnardić[1], Tamara Holjevac Grgurić[1]

[1]*Faculty of Metallurgy, University of Zagreb, Aleja narodnih heroja 3, 44 000 Sisak, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb,*
Marulićev trg, 19, 10 000 Zagreb, Croatia

Pollution of the environment, especially on water causes increasing pressure on mankind. The use of pharmaceuticals, cleaning agents and pesticides appears to have caused the emergence of new types of pollution in the environment, called micropollutant. Micropollutant cause major changes in plants and animals living in the aquatic environment. Classical wastewater treatment methods do not purify water from this type of pollution and new methods of purification need to be developed. One of the processes that cause the total degradation of this type of pollution is photocatalysis. For the process of photocatalysis photocatalyst such as titanium (IV) dioxide (TiO_2) is required. The efficiency of using TiO_2 on a daily sun light is limited due to the high energy banned zone (3-3.2 eV) so only UV-A light, which makes up 5% of solar radiation, activates the photocatalyst. In order to overcome the problem of prohibited zones and to shift the light response threshold of TiO_2 into the visible part of the spectrum, different methods can be used. One of the methods showing the potential is the use of graphene oxide (GO). In this paper a TiO_2 / GO composites with various concentrations of GO were prepared. The concentrations of GO ranged from 5, 10 and 25 wt. % GO relative to the mass of TiO_2. It was observed that the concentration of GO affects the photocatalytic activity of the obtained composite. Photocatalytic activity was followed by a degradation of salicylic acid in prepared modal solution, in a pilot reactor followed by UV-ViS spectrometry. The prepared catalysts were characterized by scanning electron microscopy (SEM) equipped with an energy dispersive X-ray spectroscopy (EDX).

Keywords: photocatalysis, titanium(IV) dioxide, graphene oxide



BIORAZGRADNJA LDPE- I PS- MIKROPLASTIKE MJEŠOVITOM BAKTERIJSKOM KULTUROM *Bacillus* sp. I *Pseudomonas alcaligenes*

BIODEGRADATION OF LDPE- AND PS-MICROPLASTICS BY MIXED BACTERIAL CULTURE OF *Bacillus* sp. AND *Pseudomonas alcaligenes*

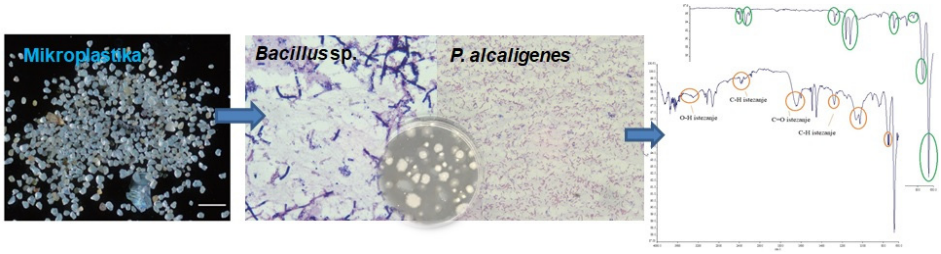
Dajana Kučić Grgić[1], Martina Miloloža[1], Antonija Kovačević[1], Ema Lovrinčić[1], Vesna Ocelić Bulatović[2], Matija Cvetnić[1], Šime Ukić[1], Viktorija Prevarić[1], Marinko Markić[1], Tomislav Bolanča[1]

[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Maruličev trg 19, 10 000 Zagreb, Hrvatska*
[2]*Metalurški fakultet, Sveučilište u Zagrebu, Aleja narodnih heroja 4, 44 000 Sisak, Hrvatska*

Stalno povećanje proizvodnje plastike i loše gospodarenje plastičnim otpadom doveli su do ogromnog porasta odlaganja otpada u okoliš. Razgradnjom makroplastike ili ciljanom proizvodnjom čestica mikro veličina nastaju čestice mikroplastike (< 5 mm). Mikroplastika predstavlja potencijalno štetni učinak na organizme u okolišu te ju je potrebno ukloniti.
U ovom radu ispitala se učinkovitost biorazgradnje dviju vrsta mikroplastike, polistirena (PS) i polietilena niske gustoće (LDPE), primjenom mješovite bakterijske kulture *Pseudomonas alcaligenes* i *Bacillus* sp.. Istraživanja su se provodila 22 dana pri 160 o/min, $T = \pm 25$ °C, veličini čestica PS i LDPE 300 – 500 µm i koncentraciji od 100 mg dm^{-3}.
Ispitana mješovita kultura učinkovito je razgradila LDPE i PS tijekom 22 dana, što je dokazano smanjenjem koncentracije otopljenog kisika u uzorcima s MP, povećanjem CFU te nastajanjem anorganskog ugljika. Nadalje, spektri dobiveni FTIR-ATR analizom prije i nakon biorazgradnje ukazuju na nastajanje novih skupina, smanjenje intenziteta pikova te pomicanja pikova prema manjim valnim duljinama.

Ključne riječi: mikroplastika, biorazgradnja, *Bacillus* sp., *P. alcaligenes*

Zahvala
Ovo istraživanje financirano je sredstvima Hrvatske zaklade za znanost projektom *AdWaTMiR, IP-2019-04*.



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VREMENSKA KLASIFIKACIJA ČESTIČNE ONEČIŠĆUJUĆE TVARI U ZRAKU PRIMJENOM MULTIVARIJATNE ANALIZE

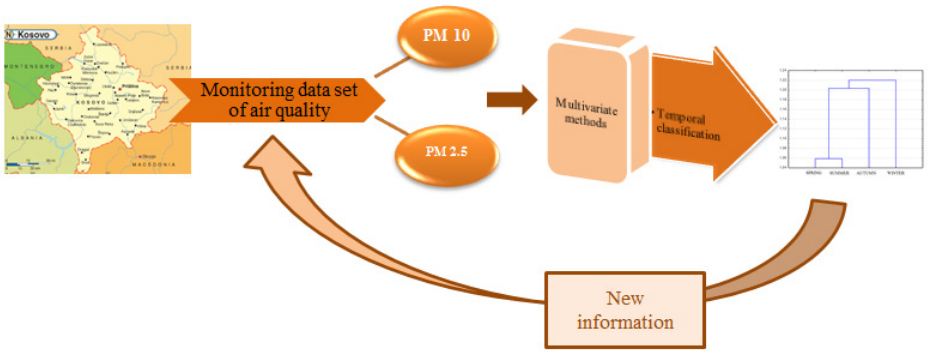
TEMPORAL CLASSIFICATION OF THE FINE PARTICLE AIR POLLUTION BY MULTIVARIATE METHODS

Virgjina Lipoveci[1], Mirjana Čurlin[2]

[1]*National Centre of Labour Medicine in Gjakova, 50 000 Gjakova, Kosovo*
[2]*Prehrambeno biotehnološki fakultet, Sveučilište u Zagrebu,*
Pierottijeva 6, 10 000 Zagreb, Hrvatska

Multivariate analysis of monitoring dataset for air quality in the Kosovo region was performed. The aim of this work is focused on temporal classification based on the datasets of hourly monitoring the fine particulate matter during the year 2017. For handling the dataset, different chemometrics methods were employed, such as basic statistical methods, Pearson`s correlation coefficients, the principal component analysis (PCA) and cluster analysis (CA). The obtained results show and explain the seasonal value movement of particulate matter with an aerodynamic diameter of 2.5 (PM2.5) and 10 (PM10) as a quality indicator of ambient air. This study allows drawing out new information from the monitoring datasets such as patterns of similarity between temporal behavior of fine particle pollution and time trends. Modernization and accelerated urban development polute the air and consequently have an impact on human health. Therefore, the implementation of these analyses is necessary for making guidelines and recommendation on population movement and daily activities, in the frame of the healthcare protection of the population in this region.

Keywords: air pollution, PM 2.5, PM 10, chemometric methods



PIROLIZA PLASTIČNOG OTPADA

PYROLYSIS OF PLASTIC WASTES

Marinko Markić, Dora Matijašec, Marija Sigurnjak, Viktorija Prevarić, Martina Miloloža, Matija Cvetnić,Tomislav Bolanča, Šime Ukić, Dajana Kučić Grgić

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

The continuous demand of plastics caused the plastic wastes accumulation in the landfill consumed a lot of spaces that contributed to the environmental problem. Some alternatives that have been developed to manage plastic wastes were recycling and energy recovery method. However, the main drawback of the recycling method is high labor cost for the separation process and water contamination that reduced the process sustainability. Due to these drawbacks, the researchers have diverted their attentions to the energy recovery method to compensate the high energy demand. As petroleum was the main source of plastic manufacturing, the recovery of plastic to liquid oil through pyrolysis process had a great potential. Pyrolysis is one of the tertiary recycling techniques in which plastic polymers are broken down into smaller organic molecules (monomers) in the absence of oxygen at elevated temperatures (>400 °C). Use of catalysts such as aluminum oxides, natural and synthetic zeolites, fly ash, calcium hydroxide, and red mud can improve the yield and quality of liquid oil. Plastic products consist mainly of polyethylene (PE), polystyrene (PS), polypropylene (PP) and polyvinyl chloride (PVC) type plastics. The key process parameters were investigated in this paper included temperatures, residence time, pressure, type of catalysts.

Keywords: pyrolysis, plastic waste, key process parameters

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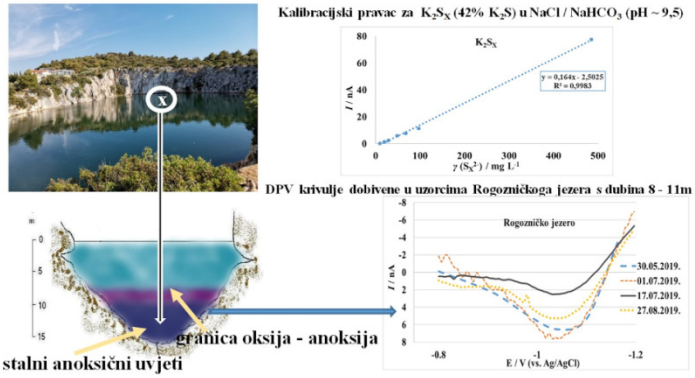
ELEKTROANALITIČKA KARAKTERIZACIJA POLISULFIDA (S_X^{2-}) U MORSKOM EUKSINOM OKOLIŠU

ELECTROANALYTICAL CHARACTERIZATION OF POLYSULFIDES (S_X^{2-}) IN MARINE EUXINIC ENVIRONMENT

Sarah Mateša[1], Anđela Bačini[1], Claire Dureyrena[2], Irena Ciglenečki

[1]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*
[2]*National School of Engineers in Chemical and Tehnological Arts, Toulouse Inp Ensiacet, France*



Polisulfidi pripadaju reduciranim sumpornim specijama (RSS) koje imaju važnu ulogu u biogeokemijskim procesima sumpora (S) i ugljika (C), te se u prirodnim vodama uglavnom javljaju kao intermedijarne specije uslijed oksidacijsko-redukcijskih procesa S. U ovom radu prvi put je korištena diferencijalna pulsna voltametrija (DPV) na Hg elektrodi [1] za određivanje S_X^{2-} u morskom euksinom okolišu Rogozničkoga jezera (RJ) (pH = 7,0 - 7,5; $[O_2]$ = 0,4 - 4 mg dm^{-3}; $[RSS]_{UKUPNO}$ = 10^{-8} mol dm^{-3} - 10^{-3} mol dm^{-3}) [2,3]. Elektroanalitičko određivanje S_X^{2-} temelji se na adsorpcijskom efektu S_X^{2-} na Hg elektrodi koji prethodi katodnoj reakciji i stvaranju karakterističnog minimuma struje pri potencijalu od -1,0 V (vs.Ag/AgCl) [1]. U ovom radu, za modelnu otopinu K_2S_X (42 % K_2S) u elektrolitu sastava NaCl / $NaHCO_3$ (pH ~ 9,5), zabilježeni su dobro definirani DPV valovi u rasponu koncentracija od 10 do 500 mg dm^{-3}. Isti elektroanalitički pristup i dobivena kalibracija primjenjeni su za određivanje prisutnosti S_X^{2-} u području kemokline i u euksinom vodenom sloju RJ (grafički abstract).

Ključne riječi: polisulfidi, Rogozničko jezero, difercijalno pulsna voltametrija (DPV)

[1] S. Kariuki *et al*., *Anal Chim Acta* 442 (2001) 277.
[2] I. Ciglenečki *et al*., *J Electrochem Sci Eng* 4(4) (2014) 155.
[3] E. Bura-Nakić *et al*., *Geochim Cosmochim Acta* 73 (2009) 3738.

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ISPITIVANJE TOKSIČNOSTI MIKROPLASTIKE NA *Chlorellu* sp., *Pseudomonas putidu* i *Danio rerio*

DETERMINATION OF MICROPLASTICS TOXICITY ON *Chlorella* sp., *Pseudomonas putida* AND *Danio rerio*

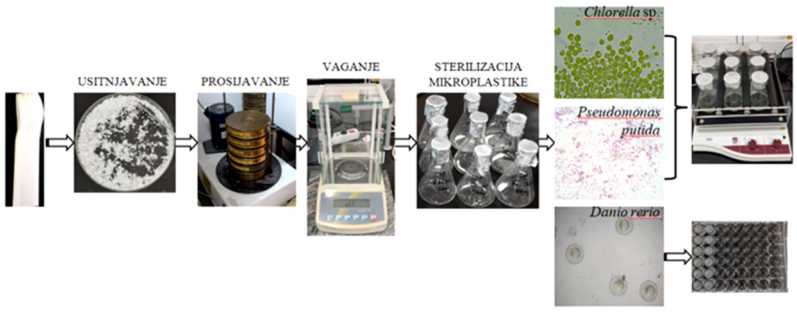
Martina Miloloža[1], Kristina Bule[1], Matija Cvetnić[1], Šime Ukić[1], Tomislav Bolanča[1], Marinko Markić[1], Vesna Ocelić Bulatović[2], Jelena Dragojević[3], Tvrtko Smital[3], Dajana Kučić Grgić[1]

[1]*Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu, Maruličev trg 19, 10 000 Zagreb, Hrvatska*
[2]*Metalurški fakultet, Sveučilište u Zagrebu, Aleja narodnih heroja 3, 44 000 Sisak, Hrvatska*
[3]*Institut Ruđer Bošković, Bijenička cesta 54, 10 000 Zagreb, Hrvatska*

Mikroplastikom se smatraju one čestice veličine manje od 5 mm, a predstavljaju globalni problem koji izaziva zabrinutost znanstvenika zbog njihova pronalaska u brojnim okolišnim sastavnicama. Mikroplastika u okolišu može nepovoljno utjecati na organizme te je iz istog razloga potrebno provesti testove ekotoksičnosti. U ovome radu ispitivana je toksičnost polistirena, PS, na tri različita testna organizma – slatkovodnu algu *Chlorella* sp., bakterijsku kulturu *Pseudomonas putida* te zebrice *Danio rerio*. Za testove s *Chlorella* sp. i *P. putida*, ispitivane su dvije veličine čestica 500-1000 µm i 300-500 µm pri koncentracijama 50, 100 i 500 mg/L, a za testove s *D. rerio* ispitane su veličine čestica 0,43 µm, 0,25 µm i 0,12 µm pri 0,01, 0,1, 1, 2, 3, 5, 6, 7 i 9 g dm^{-3}. Testovi toksičnosti s *Chlorella* sp. provodili su se 72 sata, a testovi s *P. putida* tijekom 48 sati pri sobnoj temperaturi i 160 o min^{-1} na rotacijskoj tresilici. Testovi toksičnosti s *D. rerio* provodili su se tijekom 96 sati pri sobnoj temperaturi uz praćenje morfoloških deformacija, zaostanka zebrica u korijonu, otkucaja srca te smrtnosti embrija. Inhibicija rasta pri 100 mg dm^{-3} PS veličine čestica 300-500 µm iznosila je 3,45 % za *Chlorella* sp., dok za *P. putida* 14,74 %. Uspoređujući ova dva testna organizma, osjetljivija se pokazala bakterija *P. putida*. Prema ispitivanom rasponu koncentracija, prvi utjecaj na *D. rerio* zamijećen je pri 1 g dm^{-3} te je uočeno da se smanjenjem veličine čestica PS-a i povišenjem koncentracije, štetan utjecaj na embrije zebrica povećava.

Ključne riječi: mikroplastika, testovi toksičnosti, *Chlorella* sp., *P. putida*, *D. rerio*

Zahvala
Ovo istraživanje financirano je sredstvima Hrvatske zaklade za znanost projektom *AdWaTMiR, IP-2019-04.*



PROCJENA FIZIOLOŠKOG STANJA MASLAČKA U RURALNOJ SREDINI

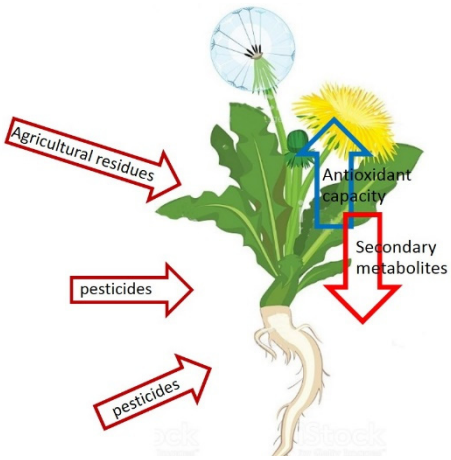
ASSESMENT OF THE PHYSIOLOGICAL STATE OF DENDELION IN RURAL ENVIROMENT

Selma Mlinarić[1], Igor Ivanac[2], Lidija Begović[1],
Denis Boršćak[2], Vlatka Gvozdić[2]

[1]*Department of Biology, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*
[2]*Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, 31 000 Osijek, Croatia*

Diffuse agricultural pollutants, such as agricultural residues, fertilisers, pesticides and excessive salt release in the environment have potentially devastating effects on the plants. Common dandelion (*Taraxacum officinale* Weber) is herbaceous perennial with wide geographic distribution that often grows in extremely polluted habitats. It is considered as good biological indicator of contamination since it can tolerate wide range of environmental conditions. The aim of this study was to assess the physiological state of dandelion in rural environment by measuring iron (III) reducing antioxidant capacity (iRAC) and ferric reducing antioxidant power (FRAP) that describes antioxidative activity. Total phenolic content (PHE), ascorbic acid content (AA) and total protein concentration (PROT) were determined as well. Dandelion leaves were collected at 30 different agricultural areas near Osijek that had differential exposure to pollution (polluted and non-polluted). Significant increase of antioxidative capacity and PROT concentration in dandelions in polluted areas was accompanied with decrease of PHE and AA content. Our results suggested that dandelions in polluted agricultural areas show inhibition of secondary metabolites production despite good physiological performance due to high antioxidant capacity.

Keywords: Taraxacum officinale Weber, agricultural pollution, antioxidative activity



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UPORABA OTPADA IZ PROIZVODNJE I PRERADE HRANE KAO BIOSORBENTA ZA OBRADU VODA ONEČIŠĆENIH TEŠKIM METALIMA

WASTE UTILIZATION FROM FOOD PRODUCTION AND PROCESSING AS BIOSORBENT FOR TREATMENT OF WATERS POLLUTED WITH HEAVY METALS

Ivona Nuić, Marija Ljubica Čikeš, Ivana Raguž, Marin Ugrina

Faculty of Chemistry and Technology, University of Split,
Ruđera Boškovića 35, 21 000 Split, Croatia

Increased agricultural production, food production and processing lead to the large amounts of organic solid wastes and residues which require adequate disposal. Instead, the organic solid wastes should be evaluated in terms of sustainability. Recently, there is a growing interest in designing the low-cost, non-hazardous and easily accessible materials as sorbents in removal of various harmful substances from wastewater. Finding proper low-cost sorbent with good sorption properties is quite challenging. In this research the several solid organic wastes such as residues of sea urchin (*Paracentrotus lividus*), sour cherry pits (*Prunus cerasus*), cherry pits (*Prunus avium*), olive pits (*Olea europaea*) and olive pomace pellets were collected from local food producers in order to estimate their sorption efficiency in lead and zinc removal from aqueous solutions. The experiments were performed by batch method in laboratory shaker at 250 rpm, and solid/liquid ratio of 1/100 for 24 hours at ambient temperature. According to the results obtained, the better removal of lead than zinc has been achieved for all tested biosorbents. The sorption efficiency for lead is in the range ≈ 13 – 36 % and follows olive pomace pellets < sea urchin < cherry pits < olive pits < sour cherry pits, while for zinc is in the range ≈ 17 – 38 % and follows olive pits < olive pomace pellets < sour cherry pits < cherry pits < sea urchin. The further investigation should be focused on the kinetic study to provide insight into the sorption mechanism. These preliminary results demonstrate the solid waste and residues from food production and processing as potential biosorbents for lead and zinc, but in order to increase efficiency it is necessary to perform multistep sorption or biosorbents surface modification.

Keywords: organic solid waste, biosorbents, sustainability, heavy metals polluted waters

MEĐUPOVRŠINSKI FENOMEN U MATERIJALU

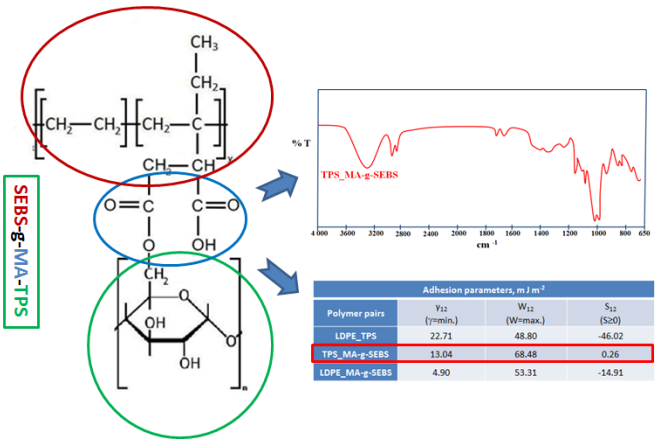
INTERFACIAL PHENOMENA IN MATERIAL

Vesna Ocelić Bulatović[1], Dajana Kučić Grgić[2], Martina Miloloža[2]

[1]*Faculty of Metallurgy, University of Zagreb, Aleja narodnih heroja 3, 44 000 Sisak, Croatia*
[2]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*

Low density polyethylene (LDPE) is a worldwide leading material with excellent mechanical properties and unattainable low cost. Due to its non-degradability, it poses a risk to the ecosystems and exposed organism. In order to reduce the dependence on the depleting petrochemical resources and highlighted biodegradability of the material, the innovative approach is blending LDPE with biopolymers such as thermoplastic starch (TPS). Since LDPE and TPS are immiscible polymers, the usage of a compatibilizer is inevitable. The focus of this investigation was exploring effect of incorporation of a block copolymer grafted with maleic anhydride (MA) as a compatibilizer on the miscibility of the LDPE/TPS blends for improving the application properties. The miscibility of components in blend was predicted by surface free energy calculations using various models and theories. The adhesion between compatibilizer and phases in the polymer blends was predicted on the basis of the calculated adhesion parameters (interfacial surface free energy, coefficient of wetting and thermodynamic work of adhesion) obtained from the surface free energy of components.
According to the values of adhesion parameters, significant interactions can be expected between the TPS and a compatibilizer, which is expected due to the formation of an ester bond confirmed by FTIR analysis. The optimal phase interactions are necessary because they are responsible for the miscibility of the components in the blend and thus to the final application properties.

Keywords: LDPE, thermoplastic starch, compatibilizer, FTIR, interfacial properties



EMBRACED EU PROJEKT USPOSTAVLJANJE VIŠENAMJENSKE BIORAFINERIJE ZA RECIKLIRANJE ORGANSKOG SADRŽAJA IZ OTPADIH APSORPCIJSKIH HIGIJENSKIH PROIZVODA U DOMENI KRUŽNE EKONOMIJE

EMBRACED EU PROJECT ESTABLISHING A MULTI-PURPOSE BIOREFINERY FOR THE RECYCLING OF THE ORGANIC CONTENT OF ABSORBENT HYGIENE PRODUCTS WASTE IN A CIRCULAR ECONOMY DOMAIN

Marina Poljak

Saponia d.d., Matije Gupca 2, 31 000 Osijek, Hrvatska

Svake godine u Europi 8,500.000 tona i više od 30,000.000 tona na svijetu apsorpcijskih higijenskih proizvoda (pelene za odrasle, dječje pelene, higijenski ulošci, tamponi, štapići za uha,...) završi na zbrinjavanju. Apsorpcijski higijenski proizvodi (AHP) su kompleksnog sastava i sastoje se od tri različite vrste materijala: plastike, superapsorbirajućeg polimera (SAP) i organske celuloze, te se obično nakon uporabe smatraju kao nereciklirajuća frakcija krutog komunalnog otpada i kao takvi se odlažu u okoliš što ima negativan utjecaj na isti. Kako se AHP pokazao kao potencijalan izvor vrijedne sirovine za biokonverziju cilj EMBRACED projekta je staviti u prvi plan kružnu ekonomiju kao vodilju održivosti i obnovljivosti izvora, kroz uspostavljanje višenamjenske biorafinerije za recikliranje organskog sadržaja iz navedenih proizvoda. Na taj način plan je maksimalizirati kapacitete za dobivanje visoko vrijednih bio-baziranih materijala/produkata. U tom smislu Saponia će procijeniti nove tržišne mogućnosti za valorizaciju AHP otpadne celuloze koja će poslužiti za formiranje *syngasa* rasplinjavanjem, te njegovu konverziju u aditive poput limonena koji predstavlja visoko vrijednu sirovinu u parfimeriji, farmaciji, kemijskoj industriji,... [1,2].

Ključne riječi: apsorbirajući higijenski proizvodi, kružna ekonomija, biorafinerija, limonen

[1] C. Sun *et al*., *Biores Technol* (2019) 1.
[2] E. Jongedijk *et al*., *Appl Microbiol Biotechnol* 100 (2016) 2927.

Funded by the Horizon 2020 Framework Programme of the European Union

International Conference *18th Ružička days*
"TODAY SCIENCE – TOMORROW INDUSTRY"
September 16–18, 2020 / Vukovar, Croatia

RAZGRADNJA FTALATA NAPREDNIM OKSIDACIJSKIM PROCESOM

DEGRADATION OF PHTALATES BY ADVANCED OXIDATION PROCESS

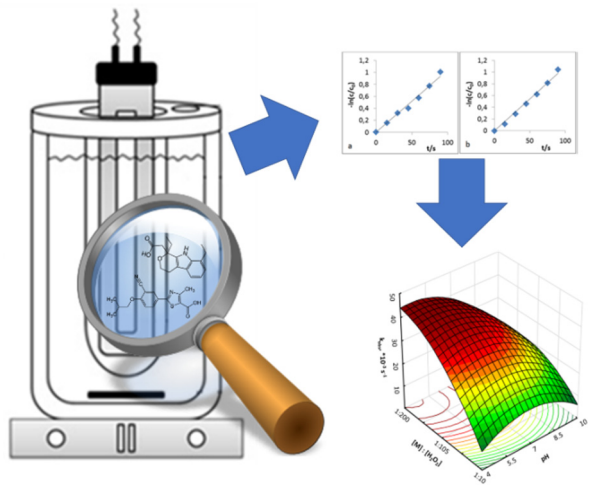
Viktorija Prevarić, Matija Cvetnić, Marinko Markić, Dora Matijašec, Marija Sigurnjak, Martina Miloloža, Tomislav Bolanča, Šime Ukić, Dajana Kučić Grgić

Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia

Phthalates are plasticizers and are concerned environmental endocrine-disrupting compounds. Due to their extensive usage in plastic manufacturing and personal care products as well as the potential to leach out from these products, phthalates have been detected in various aquatic environments including drinking water, groundwater, surface water, and wastewater.
The photochemical degradation of phthalates in UV-C/H_2O_2 and UV-C/$Na_2S_2O_8$ advanced oxidation processes was studied and the apparent degradation kinetic constants (first-order kinetic model) based on the elementary reactions were determined. Other processes parameters (pH, oxidant concentration) have also been investigated. The processes of the photolysis alone, oxidation by H_2O_2 and $Na_2S_2O_8$ alone were also observed. The results showed that photooxidative degradation of phthalates by UV-C/H_2O_2 and UV-C/$Na_2S_2O_8$ has several times higher rate of degradation.

Keywords: phthalates, photolysis, advanced oxidation processes, plasticizers

Acknowledgment
This study was financially supported by the Croatian Science Foundation through grant *AdWaTMiR, IP-2019-04*.



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ŽIVA U UKUPNOJ TALOŽNOJ TVARI NA PODRUČJU SPLITSKO-DALMATINSKE ŽUPANIJE

MERCURY IN THE TOTAL DEPOSITIED MATTER IN SPLIT-DALMATIA COUNTY

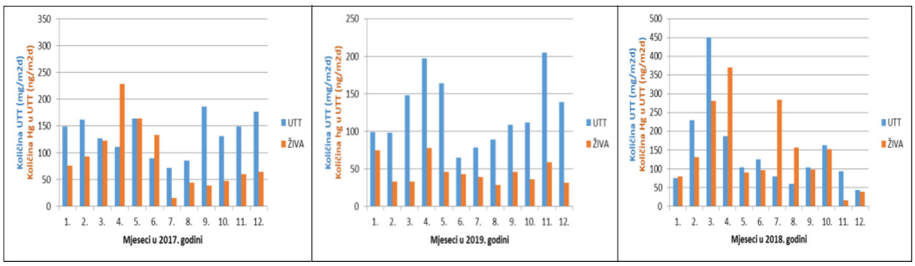
Angela Stipišić, Nenad Periš

Nastavni zavod za javno zdravstvo Splitsko-dalmatinske županije,
Vukovarska 46, 21 000 Split, Hrvatska

Ukupnu taložnu tvar (UTT) predstavljaju čestice aerodinamičkog promjera od 20 – 40 µm u čvrstom, tekućem ili plinovitom stanju, koje nisu sastavni dio atmosfere, a talože se gravitacijom i/ili ispiranjem s padalinama iz atmosfere na tlo. One su mjerilo vidljivog onečišćenja okoliša, a na zdravlje čovjeka mogu nepovoljno djelovati. Živa je element koji se u prirodi nalazi u sva tri oblika: elementarna, anorganska i organska. Široko je rasprostranjena jer izrazito lako isparava, te se u elementarnom stanju prenosi u atmosferu, potom u hidrosferu i biosferu tvoreći prirodni geokemijski ciklus. Ukupna taložna tvar i živa u njoj parametri su ispitivanja kvalitete zraka. Dopuštene srednje granične vrijednosti (GV) za kalendarsku godinu s mjesečnim vremenom usrednjavanja iznose za: UTT 350 mg $(m^2d)^{-1}$, sadržaj žive u UTT 1000 ng $(m^2d)^{-1}$ [1, 2]. Određivanje depozicije žive u rasponu od 1 do 1000 ng $(m^2d)^{-1}$ obavljeno je na instrumentu FMA 80 Mercury Analyzer, tehnikom CV-AFS [3]. Radom su obuhvaćeni rezultati ispitivanja sa 11 mjernih postaja na području Splitsko-dalmatinske županije (SDŽ) u razdoblju od 2017. - 2019. godine. Ukoliko se usporede rezultati mjesečnih vrijednosti UTT, na svim mjernim postajama SDŽ, najveći broj prekoračenja (12 puta) propisane GV 350 mg $(m^2d)^{-1}$ bio je u 2018. godini. Pojedinačne mjesečne vrijednosti UTT bile su više u zimskim mjesecima. Najviše srednje godišnje kalendarske vrijednosti zabilježene su 2018. godine i iznosile su za UTT 142 mg $(m^2d)^{-1}$ i živa u UTT 149,5 ng $(m^2d)^{-1}$. Usporedba količina UTT i žive u UTT nije pokazala statistički značajnu povezanost. Kvaliteta zraka u okolišu mjernih postaja SDŽ tijekom 2017. - 2019. s obzirom na navedene ispitane parametre ocjenjena je I. kategorijom kvalitete, odnosno zrak neznatno onečišćen.

Ključne riječi: zrak, ukupna taložna tvar, živa

[1] Uredba o razinama onečišćujućih tvari u zraku (NN 117/12, 84/17), Prilog 1.Tablica E.
[2] Pravilnik o praćenju kvalitete zraka (NN 79/2017), Prilog 7. Tablica D.
[3] HRN EN 15853:2010- Standardna metoda za određivanje taloženja žive



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UKLANJANJE HUMINSKE KISELINE IZ VODE ADSORPCIJOM NA MODIFICIRANI AKTIVNI UGLJEN

REMOVAL OF HUMIC ACID FROM WATER BY ADSORPTION ONTO MODIFIED ACTIVATED CARBON

Ana Tutić[1], Anđela Zeko-Pivač, Anamarija Burilo[1], Verónica Silva Teixeira[2], Mariana Oliveira Pagaimo[2], Susana Paixão[2], Mirna Habuda-Stanić[1]

[1]*Faculty of Food Technology Osijek, Josip Juraj Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2] *Escola Superior de Tecnologia da Saúde de Coimbra, Rua 5 de Outubro, 3046-854 Coimbra, Portugal*

Humic acid impair water quality due to their chemical reactivity with many substances and their presence in water is undesirable. In addition, during the drinking water treatment process, a humic acids reacts with chlorine based disinfects producing harmful disinfection by-products (DBPs) with organic substances [1,2]. The aim of this study was to examine the effectiveness of humic acid adsorption on two commercially available chemically modified activated carbon, Hydraffin 30N (mH) and Cullar D (mC). The efficiency of humic acid removal was investigated depending on the initial concentration of humic acid, pH, adsorption time, adsorbent mass and temperature. Obtained results shown that up to 58.44% humic acid can be absorbed by modified Hydraffin 30 N (45 °C, pH of 7.5, adsorbent mass 0.1 g, initial humic acid concentration 5 mg dm^{-3} and adsorption time of 120 min) while modified Cullar D adsorbed up to 66.46 % of humic acid (25 °C, pH of 7.5, adsorbent mass 0.1 g, initial mass concentration of humic acid 5 mg dm^{-3} and adsorption time 120 min). The effectiveness of dissolved humic acid removal from water decreased by moving from the optimal conditions.

Keywords: drinking water treatment, humic acid removal, adsorption, activated carbon

[1] S. Richardson, *TrAC_Trend Anal Chem* 22 (2003) 666.
[2] C.J.Williams *et al*., *Sci Total Environ* 652 (2019) 75.

USPOREDNO ISTRAŽIVANJE UKLANJANJA ŽIVE(II) NA PRIRODNOM I ŽELJEZO-MODIFICIRANOM ZEOLITU

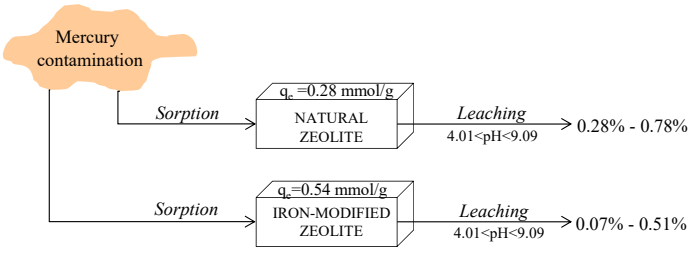
COMPARATIVE STUDY OF MERCURY(II) REMOVAL ONTO NATURAL AND IRON-MODIFIED ZEOLITE

Marin Ugrina[1], Teja Čeru[2], Ivona Nuić[1], Marina Trgo[1]

[1]*Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21 000 Split, Croatia*
[2]*Geological Survey of Slovenia, Dimičeva ulica 14, 1 000 Ljubljanja, Slovenia*

The contamination of soil and water bodies with mercury from the anthropogenic sources such as mining and industry activities causes negative effect for living organisms due to the process of bioaccumulation and biomagnification through the food chain. Therefore, the need for remediation of contaminated areas is extremely necessary, especially if it is effective by using low-cost sorbents. This paper compares the sorption abilities of natural and iron-modified zeolite towards mercury(II) ions from aqueous solutions. The influence of pH, initial concentration, solid/liquid ratio and contact time on the sorption efficiency onto both sorbent materials was investigated. At the optimal pH=2, the maximum amount of sorbed mercury(II) is 0.28 mmol g^{-1} of natural zeolite and 0.54 mmol g^{-1} of iron-modified zeolite. It has been observed that a minimum contact time of 600 minutes is required to achieve the maximum sorption capacity for both sorbents. In addition, to achieve the same sorption efficiency, the twice solid/liquid ratio of natural zeolite than that of iron-modified zeolite is needed. The results showed that the iron-modified zeolite has a better sorption ability compared to the natural zeolite. For a possible application of sorbents for *in situ* remediation of soil or groundwater contaminated with mercury, the leaching of mercury from saturated sorbents was examined according to the standard leaching method DIN 38414. In a wide pH range, 4.01<pH<9.09, the leaching of mercury(II) was observed in the amount of only 0.28 % – 0.78 % from natural zeolite and 0.07 % – 0.51 % from iron-modified zeolite. At extreme pH conditions, pH<3 and pH>11, leaching of mercury(II) in an amount of 4–7 % occurs on both sorbents. In conclusion, both sorbent materials could be used in remediation purposes while the results suggest that modification significantly improves the sorption properties of zeolite.

Keywords: natural zeolite, iron-modified zeolite, mercury(II), sorption, leaching



UKLANJANJE FOSFATA IZ OTPADNIH VODA: PREGLED ISTRAŽIVANJA

PHOSPHATE REMOVAL FROM WASTEWATER: AN OVERVIEW

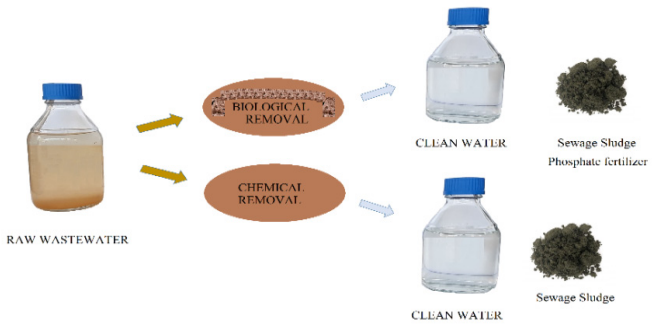
Anđela Zeko-Pivač[1], Ana Tutić[1], Tibela Landeka Dragićević[2], Mario Šiljeg[3], Mirna Habuda-Stanić[1]

[1]*Faculty of Food Technology Osijek, Josip Juraj Strossmayer University of Osijek, Franje Kuhača 18, 31 000 Osijek, Croatia*
[2] *Faculty of Food Technology and Biotechnology, University in Zagreb, Pierottijeva 6, 10 000 Zagreb, Croatia*
[3] *University North, Jurja Križanića 31b, 42 000 Varaždin, Croatia*

Wastewater containing large quantities of nutrients poses a risk to the environment causing an eutrophication and pollution of aquatic habitat all over the world [1]. Therefore, during the past decade many studies investigated nutrients removal, especially phosphorus and nitrogen, from wastewater to prevent harmful effects on the environment. Phosphates are naturally occurring nutrients in the environment, but due to many years of uncontrolled discharge in environment via wastewaters, heightened concentrations of phosphates had been detected in the freshwater ecosystems worldwide as the result of intensive usage of fertilizers and detergents. Phosphate loading of water bodies generates excessive algae growth, reduce or eliminate oxygen and generally deteriorate water quality [2]. Numerous researches and experts are putting a high effort to find efficient, ecological and economical solution for phosphate reduction or/and elimination from wastewater. On the other hand, for the last 20 years, phosphorus is deemed a recoverable product rather than a pollutant. This paper presents an overview of recent research articles related to the solutions for phosphate biological and chemical removal from wastewaters as well as methods and possibilities for phosphorus recovery.

Keywords: wastewater, phosphate removal, biological treatment, chemical treatment

[1] X. Álvarez *et al*., *Land Use Policy* 69 (2017) 1.
[2] B. Bhagowati *et al*., *Ecohydrol Hydrobiol* 19 (2019) 155.



Susret mladih kemičara
Meeting of Young Chemists

FOTODOKUMENTACIJA U EKOLOGIJI

PHOTO DOCUMENTATION IN ECOLOGY

Ema Babić, Ljiljana Vidović

Tehnička škola i prirodoslovna gimnazija Ruđera Boškovića,
Vukovarska 209, 31 000 Osijek, Hrvatska

Fotodokumentacijom nazivamo zbirke fotografija koje služe kao dokumenti. Kvalitetna fotografija izuzetno je važna u dokumentiranju sastavnica okoliša poput geološko morfoloških elemenata, vodenih tokova, travnjačkih ili šumskih biocenoza. Nezamjenjiva je otkrivanju novih vrsta, praćenju rijetkih i zaštićenih u malim populacijama ili praćenju sekundarnih sukcesija.

U ekologiji važnost fotodokumentacije iznimna je jer dokumentira antropogeno djelovanje koje često proizlazi iz hotimičnih postupaka koji za rezultat imaju degradaciju okoliša. U posljednjih dvjesto godina učinak po okoliš izrazito je negativan što zbog industrijske revolucije, povećanja ljudske populacije, ratova svjetskih razmjera, potrošnje fosilnih goriva ili neprimjerenog odlaganja otpada svih vrsta u okoliš.

Dokumentirati fotografijom, trajno pratiti promjene, izuzetno je važno za fundamentalne znanosti, ali i za zaštitu okoliša reguliranu aktima na razini Europske unije i Republike Hrvatske. Ministarstva, među kojima je i Ministarstvo zaštite okoliša i energetske učinkovitosti u različitim studijama utjecaja na okoliš kao nepobitni dokaz koriste fotografiju.

Ekološka svijet svakog od nas, briga za čisti okoliš, nameće nam zadatak fotografirati ekološke incidente i neodgovorno ponašanje pojedinaca prema sastavnicama okoliša i njihovoj bioraznolikosti.

Ključne riječi: fotodokumentacija, ekologija, okoliš

UTJECAJ OTPADNE VODE NA ONEČIŠĆENJE DUNAVA

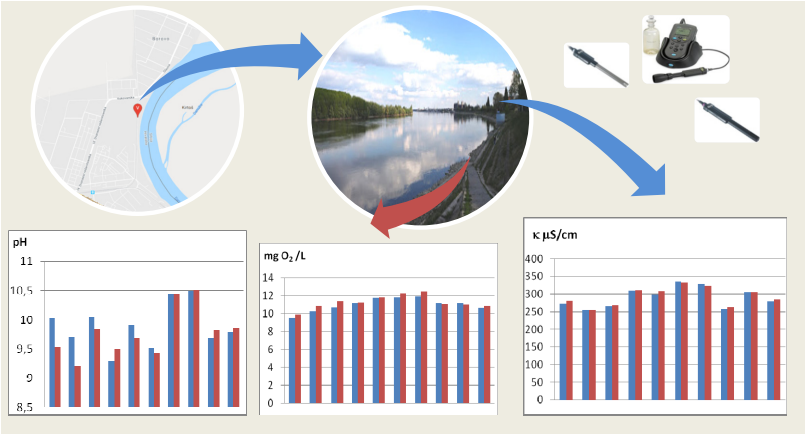
THE IMPACT OF WASTEWATER ON DANUBE POLLUTION

Andrea Bilušković, Đurđevka Pecikozić

Tehnička škola Nikole Tesle Vukovar, Blage Zadre 4, 32 010 Vukovar, Hrvatska

Opstanak svake vrste ovisi o vodi - bez nje život u postojećem obliku ne bi bio moguć. Svi biološki procesi odvijaju se u vodenoj sredini. Može se reći da voda nije samo oko nas nego i u nama, budući da je ona sastavni dio svake žive stanice te da čini 60-70 % tjelesne mase odraslog čovjeka. Iz tog razloga je onečišćenje voda ozbiljan problem. Onečišćivači voda su: otpadne vode, industrija, promet, odlagališta otpada i kemikalije koje se koriste u poljoprivredi. Razvoj industrije i poljoprivrede te koncentracija stanovništva u većim urbanim sredinama kao posljedicu ima sve veće i teže poteškoće pri zaštiti voda.
Cilj rada je pratiti i usporediti pH-vrijednost, električnu provodnost, koncentraciju otopljenoga kisika, temperaturu uzvodno i nizvodno od ispusta otpadne vode u Dunav kod Vukovara. Uočeno je da koncentracija otopljenog kisika ovisi o tlaku i temperaturi. Što je tlak veći, a temperatura manja, koncentracija otopljenog kisika je veća. Opskrbljenost Dunava kisikom je zadovoljavajuća. Razlike u izmjerenim vrijednostima provodnosti i pH-vrijednosti uzvodno i nizvodno od ispusta su neznatne što potvrđuje da je otpadna voda prethodno obrađena.
Svakako treba poduzimati mjere za očuvanje kvalitete vodenih resursa kako bi se osigurao opstanak života na našem planetu.

Ključne riječi: koncentracija otopljenog kisika, električna provodnost, pH-vrijednost, onečišćenje



BOMBASTIČNE TAJNE BOJA I MIRISA

BOMBASTIC SECRETS OF COLOURS AND SCENTS

Katarina Domjanović, Maja Vučković, Vanja Ćulibrk

II. gimnazija Osijek, Ul. Kamila Firingera 5, 31 000 Osijek, Hrvatska

Napor, stres, gubitak koncentracije i pad raspoloženja sastavni su dio današnjice. Svaki dan u medijima i svakodnevnoj komunikaciji govori se o zdravstvenim problemima koji su izazvani stresom i psihičkim naporom. Jeste li znali da je stres snažno povezan s bolestima srca, visokim tlakom, upalnim procesima i padom obrambenog sustava, a najvjerojatnije i rakom? Kako bi se riješili stresa i problema povezanih s njime, ljudi često posežu za lijekovima i vitaminima neprovjerenog sadržaja i upitne kvalitete. Danas, zahvaljujući velikom napretku znanosti, postoje puno zdraviji i prirodniji načini liječenja stresa. Velik broj ljudi kao najljepši završetak dana vidi kupanje u toploj i pjenušavoj kupki. Znanstveno je dokazano da su pozitivni učinci tople vode mnogobrojni. Ona opušta mišiće, živčane stanice te pomaže pri izlučivanju štetnih toksina. Potaknuti aktualnim problemom i spoznajom o pozitivnom djelovanju kupki na naše tijelo, provelo se istraživanje određivanja sastojaka u kupki koji imaju potencijal za stvaranjem boljeg i zdravijeg ugođaja. Rezultati istraživanja su pokazala da eterična ulja koja su se dodavala u šumeće kugle za kupanje stvaraju upravo taj učinak. Svako eterično ulje ima drukčije djelovanje, neka od njih umiruju, neka podižu raspoloženje, ali i poboljšavaju san te uklanjaju bakterijske stanice koje su se tijekom dana nakupile na površini naše kože. Cilj ovog rada je spojiti ugodno s korisnim. Aromaterapijom pomaže se u borbi protiv stresa, a u isto vrijeme toplom i pjenušavom kupkom njeguje se koža i pomaže u relaksaciji tijela.

Ključne riječi: stres, aromaterapija, eterična ulja, šumeće kugle za kupanje

KEMIJSKA ANALIZA TALA NA PODRUČJU OPĆINE ŽEPČE (BOSNA I HERCEGOVINA)

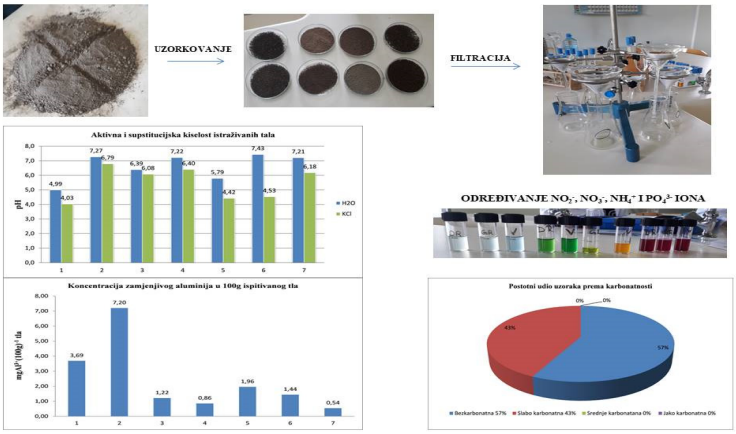
CHEMICAL ANALYSIS OF SOIL IN THE MUNICIPALITY OF ŽEPČE (BOSNIA AND HERZEGOVINA)

Nikolina Grlić, Nikolina Pravdić, Matea Jukić, Marko Tomas

Katolički školski centar „Don Bosco" Žepče, Tehničko-obrtnička škola, Stjepana Radića bb, 72 230 Žepče, Bosna i Hercegovina

Kemijska analiza tla ključna je za dobivanje visokih prihoda, odnosno racionalnu, profitabilnu i učinkovitu primjenu agrotehnike, posebice gnojidbe, obrade, sjetve pa sve do žetve. U tom smislu treba shvatiti da cjelovit i učinkovit sustav kontrole plodnosti tla koji sustavno prikuplja sve relevantne fizikalno-kemijske podatke o tlu, njegovoj plodnosti i korištenju, doprinosi boljoj raspodjeli mineralnih i organskih gnojiva, uklanjanju akutnih deficita hraniva, kemijskoj i fizikalnoj popravci tla, profitabilnijoj proizvodnji, odnosno očuvanju i podizanju efektivne plodnosti tla. Cilj ovog istraživanja bio je utvrditi pogodnost tala za ratarsku proizvodnju na području općine Žepče. Na uzorcima tala uzetih s poljoprivrednih površina na dubini do 30 cm provedene su laboratorijske analize osnovnih kemijskih svojstava tla: pH tla, određivanje zamjenjivog aluminija metodom po Sokolovu, supstitucijska kiselost, kvalitativno određivanje karbonata u tlu te hidrolitička kiselost. Osim osnovnih agrokemijskih analiza, provedene su dodatne analize kojima je utvrđena koncentracija; nitrita (NO_2^-), nitrata (NO_3^-), fosfata (PO_4^{3-}) i koncentracija amonijevih iona (NH_4^+) u vodenim filtratima tala. Utvrđeno je da je u istraživanim uzorcima na području općine Žepče prosječna pH reakcija tla neutralna. Također je utvrđeno da su skoro sva tla bezkarbonatna ili slabo karbonatna.

Ključne riječi: Žepče, tlo, pH reakcija tla, metoda po Sokolovu



ISPITIVANJE KVALITETE PASTE ZA ZUBE OD ZELENE GLINE

TESTING THE QUALITY OF GREEN CLAY TOOTHPASTE

Sandra Jozinović, Zoran Jurić, Ivona Pranjić, Slavica Jukić

Katolički školski centar "Don Bosco", Opća gimnazija, Stjepana Radića b. b.,72 230 Žepče, Bosna i Hercegovina

Cilj ovog rada bio je dobiti proizvod koji ne sadrži štetne kemikalije, a može ukloniti zubni plak, inhibirati rast mikroorganizama i osigurati svjež dah. Pasta za zube pripremljena za ovu analizu sadrži zelenu glinu i druge prirodne sastojke poput hidrolata kadulje i eteričnog ulja čajevca. Zelena glina sadrži prirodne i netretirane nutrijente koji djeluju remineralizirajuće i detoksirajuće te podižu imunitet organizma. Sinergijom kadulje i čajevca dobiva se proizvod moćnog antibakterijskog i protuupalnog djelovanja. Kvaliteta ispitivane paste utvrđena je mikrobiološkom analizom prema Pravilniku o analizi sredstava za održavanje osobne higijene te recenzijom koju su dali učenici naše škole.

Ključne riječi: pasta za zube, zelena glina, mikrobiološka analiza

BOJE ŽIVOTA

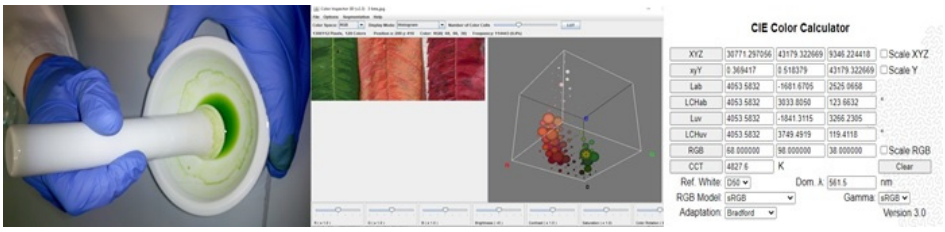
THE COLORS OF LIFE

Mia Matić[1], Karmen Dvojković[1], Toni Podrugović[1], Lucija Tomić[1], Ivan Draganić[1], Karolina Dvojković[1], Kristina Kristek[1], Marija Špoljarević[2], Miroslav Lisjak[2]

[1]Gimnazija Vukovar, Šamac 2, 32 000 Vukovar, Hrvatska
[2]Fakultet agrobiotehničkih znanosti Osijek, Sveučilište J. J. Strossmayera u Osijeku, Vladimira Preloga 1, 31 000 Osijek, Hrvatska

Biljni pigmenti su jedan od biokemijskih „alata" koji biljkama, ali i svim poznatim aerobnim heterotrofnim vrstama na našem planetu omogućavaju život i preživljavanje. Ono što naše oko percipira kao boju neke materije u prirodi, rezultat je apsorpcije odnosno refleksije fotona u vidljivom dijelu spektra. Apsorpcija i refleksija vidljive svjetlosti točno određene valne duljine pri prolasku kroz biljna tkiva, rezultira specifičnim obojenjem tkiva. Sa stajališta biologije, kemije i fizike mogu se proučavati različiti aspekti promjene boje koja nastaje kao posljedica promjene koncentracije kloroplastnih pigmenata i drugih fotoaktivnih molekula koji reguliraju specifične procese unutar stanica biljnog tkiva. Proces starenja lišća, tijekom kojega biljni materijal mijenja boju, zanimljiv je primjer „otkrivanja" pigmenata. Boja lišća ovisit će o omjerima koncentracija klorofila, karotenoida, flavonoida i antocijanina. Kako u jesen dani postaju kraći, započinje razgradnja klorofila, a time zelena boja lišća prelazi u žutu, narančastu ili crvenu boju. Kako se smanjuje koncentracija klorofila koji daju zeleno obojenje do izražaja dolaze nijanse žuto-smeđe boje koje daju karotenoidi i flavonoidi. Oni su neprestano prisutni u listovima, međutim maskirani su zelenom bojom klorofila pa do jeseni nisu vidljivi. Za crvenu boju lišća odgovorni su antocijanini čija sinteza započinje tek u jesen. Razvoj tehnologije omogućio je uvođenje novih alternativnih neinvazivnih metoda istraživanja biljnih pigmenata, prvenstveno klorofila, pomoću kojih je moguće, na temelju valne duljine boje biljnog materijala, detektirati koncentraciju biljnih pigmenata. Cilj ovog istraživanja je usporediti rezultate dobivene spektrofotometrijskim određivanjem koncentracije kloroplastnih pigmenata (klorofila a, klorofila b i karotenoida) po Holmu i Wettsteinu s rezultatima određivanja valnih duljina boja biljnog materijala pomoću računala. Koristiti će se odgovarajuća programska podrška za računalnu obradu i analizu digitalne slike i objektivnih sustava baziranih na CIE zakonitostima (sustav za prikaz boja) na uzorcima lišća prikupljenih u jesen.

Ključne riječi: biljni pigmenti, spektrofotometrija, analiza digitalne slike, CIE zakonitosti



UZORKOVANJE I ANALIZA BUNARSKIH VODA

SAMPLING AND ANALYSIS OF WELL WATERS

Kristina Nikolić, Đurđevka Pecikozić

Tehnička škola Nikole Tesle Vukovar, Blage Zadre 4, 32 010 Vukovar, Hrvatska

Voda je oduvijek imala važno mjesto u svakodnevnom životu čovjeka. Kako u društvenom, tako i u kulturnom razvoju čovječanstva kroz povijest. Bunari su iskopine ili bušotine kreirane u zemlji kopanjem, probijanjem ili bušenjem kako bi se pristupilo podzemnim vodama odnosno izdanima.
Kakvoća podzemnih voda ovisi o prirodnim karakteristikama kao i antropogenim utjecajima. Prije izgradnje javnih vodoopskrbnih sustava bunari su bili glavni izvor pitke vode u naseljima i značili su život. Danas su bunar spomenici pitke vode i ukras dvorišta, a poneki se još koristi za pranje ili zalijevanje vrtova.
Cilj ovog rada bio je izmjeriti pH- vrijednost, električnu provodnost, koncentraciju NH_4^+ iona, mutnoću i ukupnu tvrdoću uzoraka vode iz bunara u Vukovarsko-srijemskoj i Osječko-baranjskoj županiji. Mjerenja su rađena multimetrom HQ40d, Hack primjenom odgovarajućih sondi, turbidimetrom 2100Qis, Hack i digitalnim TDS Metar testerom.
Rezultati mjerenja pokazuju da su bunarske vode tvrde do vrlo tvrde. Specifična električna provodnost je veća nego što je slučaj kod prerađene pitke vode, mutnoća je ispod maksimalne dozvoljene granice 4 NTU (NN 125/2017), a koncentracija amonijevih iona je u svim ispitivanim uzorcima iznad maksimalno dozvoljene granice od 0,5 mg dm^{-3} (NN 125/2017).

Ključne riječi: bunari, podzemne vode, kruženje vode, onečišćenje

Uzorak	pH	κ µS/cm	NH_4^+ mg/L	NTU	Nj°
Bunar 1	7,22	715	3,70	0,53	32,18
Bunar 2	6,25	477	1,88	1,09	20,24
Bunar 3	7,32	926	4,16	7,19	40,65
Bunar 4	7,81	917	21,9	1,28	50,59
Bunar 5	7,31	811	0,84	1,33	35,82
Bunar 6	7,74	779	1,87	1,29	33,71
Bunar 7	7,89	274	1,03	0,39	11,59

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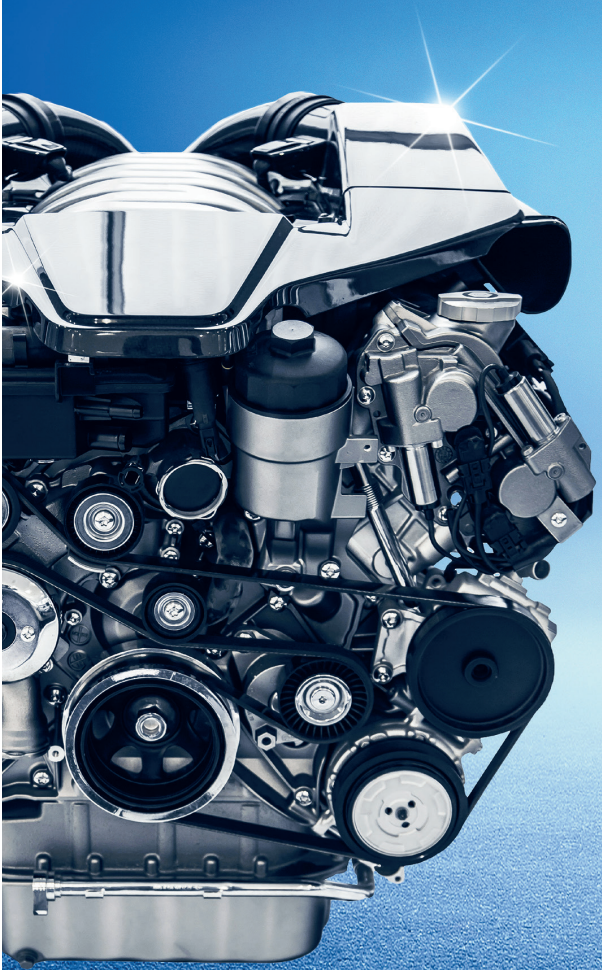

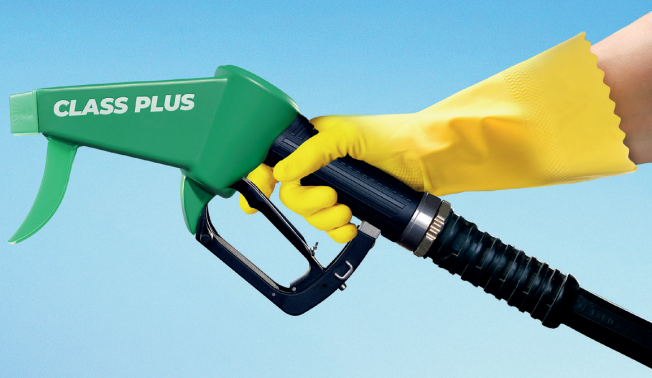

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Karolina d.o.o. članica Kraš grupe

Karolina je počela s proizvodnjom još davne 1909. godine kada je Stjepan Piller kupio mlin za proizvodnju brašna 'Slavonija' i promijenio mu ime u Dragica mlin ili njemački Karolina Mühle.

Bogato dugogodišnje iskustvo i tradicija u proizvodnji dovelo je do stvaranja najpoznatijih Karolininih brandova Jadro i Moto. Već od 1962. godine proizvodi se vafel **Jadro** koji je svojom kvalitetom i okusom do današnjih dana stekao velik broj vjernih potrošača, a svojom jedinstvenom kombinacijom dvaju okusa – mlijeka i najfinijeg kakaa u zagrljaju hrskavog vafla bio i ostao pravi doživljaj za ljubitelje poslastica. Osim toga znak «Hrvatske kvalitete», čiji je nositelj, daje kupcu jamstvo da se radi o proizvodima koji predstavljaju sam vrh svjetske ponude u svojoj klasi.

Moto punjeno čajno pecivo prisutno je na tržištu regije od 1972., a poznato je osim po kvaliteti i po obliku: cvijet s rupicom u sredini, punjen bogatom kremom. U raznim okusima prihvaćen je od potrošača kao domaći proizvod vrhunske kvalitete i u segmentu punjenih čajnih peciva drži lidersku poziciju već dugi niz godina.

U dugoj povijesti tvrtka je promijenila vlasništvo nekoliko puta, pa tako i imena: Karolina, Sloboda, Lura-keksi, opet Karolina (kao članica Lorenz Bahlsen grupe) i konačno je danas članica Kraš grupe.

Zagrebački Kraš, koji je u ožujku 2011. godine preuzeo Tvornicu keksa i vafla Karolina, uložio je značajna sredstva u proširenje proizvodnih kapaciteta, te omogućio i otvaranje novih radnih mjesta. Nastavljajući tradiciju i slijedeći postojeće vrijednosti Karolina je započela s novim razvojnim ciklusom koji je upotpunjen iskustvima najvećeg konditorskog proizvođača u regiji – Kraša. Integracijom Karoline u Kraš grupu ostvaren je dio vizije gdje Osijek postaje najjači centar za proizvodnju ravnih vafla u regiji. Danas Karolina proizvodi na ukupno 12 proizvodnih linija i zapošljava oko 350 radnika, a rekordnu proizvodnju poslijeratnog razdoblja od 9.200 tona dostigla je 2019. godine.

Suvremena tehnologija, recepture, tradicija, inovativnost i kvaliteta proizvoda osnovni su temelji razvoja i proizvodnje proizvoda u Karolini i Krašu – to je jamstvo egzistencije i prosperiteta na hrvatskom, ali i širenje na još neosvojena tržišta.

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Odgovorni član zajednice

Svoju javnu odgovornost prenosi i na druge razine i ciljne skupine javnosti i društva. Čini to, suradnjom s institucionalnom akademskom zajednicom. Širokom edukacijom i pozitivnim primjerima, prenosi znanja i poslovne standarde na širu zajednicu. Kao odgovorni član zajednice u kojoj djeluje, u Agroproteinki postoji puna svijest da društvena odgovornost ne završava samo na zaštiti zdravlja ljudi i okoliša. Svojim ukupnim poslovnim aktivnostima, otvorenošću prema okruženju, putem edukacije, raznih vrsta potpore, sudjeluje u poticanju aktivnijeg, ugodnijeg i uspješnijeg društvo. Poticanjem i uključivanjem u različite ekološke akcije, stvara i njeguje novu kulturu i spoznaju o vrijednosti očuvanja prirode kao temeljnog preduvjeta opstanka života. To je najbolji i najuvjerljiviji način vraćanja prirodi i okolišu ono što od njih i dobiva. I konačno, potvrđuje da priroda svoju cjelovitost, i svoje zdravlje može vratiti i sačuvati samo ako s njom surađuje. U tom smislu Agroproteinka ne ostaje na deklariranju odgovornog poslovanje, već i odgovornog življenja. Time pokazuje da živi sa svojim okruženjem. Pokazuje, najživotnije, i brigu za budućnost sredine u kojoj i sama ostvaruje svoju misiju.

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Lab & Production Materials

BioReliance®
Expert Pharma & Biopharma Manufacturing & Testing Services

SAFC®
Tailored Pharma & Biopharma Raw Material Solutions

Millipore®
Proven Preparation, Separation, Filtration & Monitoring Products

Merck je ujedinio vodeće svjetske brendove laboratorijskih i procesnih rješenja. S kojim se god problemom susreli u područjima prirodnih znanosti, Merck Vam može pomoći stručnim proizvodima i servisima.

Da bi saznali kako, posjetite našu e-platformu
SigmaAldrich.com/advancinglifescience

Za više informacija možete se i obratiti na:
Željka Vrbanić, Viši stručnjak za prodaju, Merck LS, Hrvatska
e-mail: zeljka.vrbanic@merckgroup.com

#howwesolve

Merck Life science u SAD-u i Kanadi radi pod nazivom MilliporeSigma.

MERCK

25
Više od 25 godina s Vama

KemLab

Prodaja i servis laboratorijske opreme

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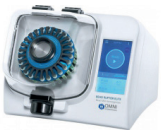
Osnovni mali laboratorijski uređaji

Analitičke i precizne vage, vlagomjeri

Sustavi za ultra čistu vodu

Pipete, nastavci, automatizirani pipetori, priprema uzoraka



Liofilizatori, perilice, koncentratori, glove box

i mnogi drugi...

kemolab.hr

+385 1 660 5233

Nadinska 11, 10000 Zagreb

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Sveučilište Josipa Jurja Strossmayera u Osijeku Prehrambeno-tehnološki fakultet Osijek
Josip Juraj Strossmayer University of Osijek Faculty of Food Tehnology Osijek

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