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Book of Abstracts

Special Issue of Bulletin of the Chemists and Technologists of Bosnia and Herzegovina

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FACULTY OF SCIENCE

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Anela Topčagić & Jelena Ostojić

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GENERAL INFORMATION

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The official language of the ICCCEB&H 2022 is English

Venue and Registration
Hotel Radon Plaza, Džemala Bijedića 185, Sarajevo 71000
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KEY TO ABSTRACT IDENTIFICATION

PL	Plenary Lectures
OP	Oral Presentations
PP-AC	Poster presentations- Analytical Chemistry
PP-BB	Poster presentations- Biochemistry and Biotechnology
PP-CAM	Poster presentations- Chemistry of Advanced Materials
PP-CE	Poster presentations- Chemical Engineering
PP-CNP	Poster presentations- Chemistry of Natural Products
PP-EDC	Poster presentations- Education in Chemistry
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PP-FC	Poster presentations- Food Chemistry
PP-IC	Poster presentations- Inorganic Chemistry
PP-MC	Poster presentations- Medicinal Chemistry
PP-OC	Poster presentations- Organic Chemistry
PP-PTC	Poster presentations- Physical and Theoretical Chemistry
PP-RC	Poster presentations- Radiochemistry
PP-TRC	Poster presentations- Topics Related to Chemistry

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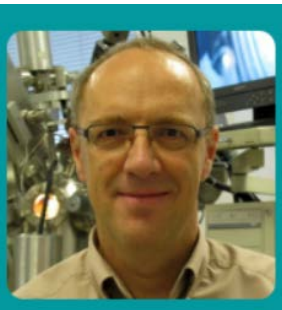

Dr. Janez Kovač

Jožef Stefan Institute
Slovenia

WELCOME NOTE

On behalf of the Organizing and Scientific Committee, the Society of Chemists and Technologists of Canton Sarajevo and the University of Sarajevo - Faculty of Science, we welcome you to the 4th International Congress of Chemist and Chemical Engineers of Bosnia and Herzegovina (ICCCEB&H 2022) in Sarajevo.

The ICCCEB&H Congress series, first launched in 2014, presents an ideal platform for fruitful exchange of ideas which is crucial for scientific advancement.

We are delighted to inform you that ICCCEB&H 2022 will have 29 Oral and 112 Poster presentations, in addition to three plenary lectures which will be held by prestigious scientists.

The impetus generated by these inspiring and high-caliber distinguished speakers enabled us to attract more than 155 participants from all around the world (Bosnia and Herzegovina, Croatia, Serbia, Montenegro, Bulgaria, Austria, Czech Republic, Jordan, Slovenia, Spain, Pakistan, United States of America, South Africa, United Kingdom, Slovakia, France and Morocco).

All submitted abstracts will be published in a special issue of the Bulletin of Chemists and Technologists of Bosnia and Herzegovina, and selected papers will be published in a regular issue of the Bulletin of Chemists and Technologists of Bosnia and Herzegovina after the peer-review process.

The Congress will cover different branches of chemistry and chemical technology and offer an opportunity for scientists to exchange latest research findings and ideas and to develop new networks and collaborations.

We thank the members of the Organizing Committee, International Scientific Committee, Scientific Committee, sponsors, and last but not the least all of the participants for organizing, supporting and contributing to the quality of this Congress.

We welcome all of you once again to the ICCCEB&H 2022 and wish you an interactive, inspiring and joyful scientific gathering and a pleasant stay in Sarajevo, Bosnia and Herzegovina.

CONTENT

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Abstract

PL-01

Catalysis and environment: the good, the bad and the ugly

Suljo Linić

University of Michigan, Department of Chemical Engineering,
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Abstract: It has become increasingly clear that human-induced CO_2 emissions are having potentially irreversible impact on the environment. In this presentation, I will share my views on the current state of the CO_2 pollution problem and discuss potential mitigation strategies. I will focus on the solutions that involve catalysts and discuss how achievable these solutions are, and which of the solutions gives us the highest probability to make positive impact. Most of these solutions will require abundant and economically viable generation of renewable hydrogen. I will discuss our work on solar splitting of water to form hydrogen on hybrid semiconductor/electro-catalysts systems. I will also discuss our recent efforts aimed at pairing the CO_2 capture with in-situ electrochemical reduction of the captured CO_2 molecules.

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Abstract

PL-02

Biomass oxy-fuel combustion technology as carbon neutral renewable source of energy to replace fossil fuels

Farooq Sher

Department of Engineering, School of Science and Technology, Nottingham Trent University, Nottingham NG11 8NS, United Kingdom

Abstract: Due to growing concerns about climate change, the heat and power sector is continuously facing challenges to reduce CO_2 emissions. Carbon capture and storage (CCS) is one of the short-medium term measures that can mitigate CO_2 emissions emitted from fossil fuels utilisation. Oxy-fuel combustion is a promising technology for CSS that can be integrated into the new and the current fleet of power plants. Biomass is a carbon-neutral renewable source of energy that can replace fossil fuels. If the biomass is utilised as a fuel in oxy-fuel combustion it could lead even to negative CO_2 emissions. However, oxy-fuel combustion technology in fluidised beds is in the early stages of development and still needs a lot of research for improvement before its application on full-scale power plants. The basic combustion fundamentals of different biomass fuels in terms of energy production were studied using thermogravimetric analysis (TGA) under air, N_2, CO_2 and selected oxy-fuel ($30\%O_2/70\%CO_2$) reaction environments. Then a 20 kWth bubbling fluidised bed combustor (BFBC) was designed, manufactured and successfully tested for a range of biomass fuels under air and oxy-fuel combustion environments. The agglomeration and sintering behaviour of these biomass fuels during combustion under air was also investigated using different analytical techniques such as SEM-EDX, XRD and XRF. The biomass fuels investigated include domestic wood, industrial wood, miscanthus, wheat straw and peanut shell pellets. The BFBC testing of these biomass fuels focused on the influence of operating conditions, the effect of excess air level and fuel feed rate on the hydrodynamics, temperature profiles and emissions, NOx, CO_2 and CO within the BFBC.

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Abstract

Chemical characterization of surfaces and thin films for the development of new materials and quality control

Janez Kovač

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Abstract: Surfaces and thin films of solid materials play an important role in many technological fields like corrosion, catalysis, polymers, plasma surface engineering, coatings, tribology, implants, sensors, microelectronics, etc. Application of analytical methods with high surface and chemical sensitivity is important for a complete understanding of surface reactions, functional properties, and degradation of materials in such applications. Scanning electron microscopy - SEM in combination with EDXS is very often applied to analyze the morphology and elemental chemical composition with high lateral resolution. In this presentation, another two methods with high surface sensitivity will be presented, i.e., X-Ray photoelectron spectroscopy – XPS and Secondary ion mass spectrometry - SIMS. These methods have surface sensitivity in the range of 1-5 nm, making them unique surface probes. The XPS analyses can give information on chemical composition, oxidation states (identification of Cu(0)/Cu(1+)/Cu(2+), Ti(0)/Ti(3+)/Ti(4+)) and bonding of elements (C-C/C-O/O=C-O) at surfaces and thin films. The SIMS method allows the identification of a type of molecules and molecular structure at surfaces, which is particularly important for analyses of organic materials. The XPS and SIMS methods can be combined with ion etching to remove the surface layers and analyze subsurface chemical composition up to one micron. In such a way, a depth distribution in thin films and multilayer structures can be obtained. In this presentation, we will show typical applications of surface analytical methods XPS and SIMS in our laboratory for the development of new catalytic materials based on doped TiO_2, a study of corrosion inhibitors, the application of the graphene-based materials, and the degradation of perovskite solar cells. Also, examples of surface analyses for quality control as support for industrial partners in Slovenia will be presented. SIMS. These methods have surface sensitivity in the range of 1-5 nm, making them unique surface probes. The XPS analyses can give information on chemical composition, oxidation states (identification of Cu(0)/Cu(1+)/Cu(2+), Ti(0)/Ti(3+)/Ti(4+)) and bonding of elements (C-C/C-O/O=C-O) at surfaces and thin films. The SIMS method allows the identification of a type of molecules and molecular structure at surfaces, which is particularly important for analyses of organic materials. The XPS and SIMS methods can be combined with ion etching to remove the surface layers and analyze subsurface chemical composition up to one micron. In such a way, a depth distribution in thin films and multilayer structures can be obtained. In this presentation, we will show typical applications of surface analytical methods XPS and SIMS in our laboratory for the development of new catalytic materials based on doped TiO2, a study of corrosion inhibitors, the application of the graphene-based materials, and the degradation of perovskite solar cells. Also, examples of surface analyses for quality control as support for industrial partners in Slovenia will be presented.

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ORAL PRESENTATIONS

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OP-01

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Abstract

Mint Essential Oils: Composition and Bioactivity

Ćavar Zeljković, S.[a,b]

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Mentha sp.
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Abstract: The essential oils of *Mentha* sp. are widely used as food, medicine, spices, and flavoring agents. Therefore, their chemical composition is an important parameter for assessing the quality of plants. Here, we summarize our recent findings on the chemical composition and biological activities of essential oils of selected mints i.e., *Menthaaquatica* 'Veronica', *M. pulegium*, *M. x piperita*, *M. x piperita* 'Bergamot', *M. x piperita*'Citrata', *M. x piperita* 'Perpeta', *M. x villosa*, and *M. microphylla*, grown under the same environmental conditions. Since we have proved that the percentage content is not necessarily a reliable way of presenting the quality of the essential oil as a crop product that will be used in the food and pharmaceutical industry, the composition of these oils was also obtained by measuring the exact concentrations of each monoterpene that was found at a significant level. To characterize their pharmacological potential, essential oils were subjected to the testing of their abilities to reduce stable radicals, inhibit the activity of the enzyme tyrosinase-related to skin hyperpigmentation disorders, such as melanoma and age spots, but also their activity against severe acute respiratory syndrome coronavirus 2 (SARS-Cov-2). Among all tested oils, citrus-scented *Mentha x villosa* essential oil showed potent activity against free radicals, tyrosinase, and SARS-Cov-2. Although this species is not exploited as other mints (*M. spicata*, *M. x piperita*, *M. arvensis*), our findings show its potential for the use in food and pharmaceutical industry, especially due to its easy cultivation, which does not require pesticides.

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Abstract

OP-02

Green Nanoparticles from Plant Extracts with Antibacterial Effect

Marinova, K. [a], **Petrov, P.** [a], **Velkova, L.** [a], **Dolashki, A.** [a],**Lyubomirova, V.** [c],**Rangelov, B.**[b], **Atanasova, S.**[b].**Dolashka, P.**[,a]

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Calendula officinalis
Plantago major
Escherichia coli
Bacillus subtilis

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Abstract: Parts of plants are involved in the green synthesis of various types of natural nanoparticles (NPs). Many biologically active substances form plant extracts are useful for medical use. The aim of our study is to obtain biologically active substances from plants that are associated with the formation of nanoparticles. We have proven that plant extracts from*Cotinus coggygria*, *Chammomilla recutita*, *Calendula officinalis* and*Plantago major* are very rich in those substances, which are playing important role as reducing and capping agents of the Zn and Cu from $ZnSO_4$ or $CuSO_4$ in the synthesis of nanoparticles by ecological methods at various temperatures and different periods of time. The formation of NPs has been proven by UV-spectroscopic methods and scanning electron microscopy. The antibacterial properties of the obtained NPs were tested by well-agar diffusion method and showed antibacterial activity against different strains of *Escherichia coli* and *Bacillus subtilis*.

Acknowledgments This work is supported by a grant from BMES D01-217 / 30.11.2018 and agreements DO1-323 / 18.12.2019, DO1-358 / 17.12.2020, DO1-278 / 03.12.2021. " Innov “Precision Medicine Systems approved by DCM № 658 / 14.09.2018.

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Abstract

OP-03

Hydrogen adsorption on graphene-based materials

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Abstract: In the light of present energy crisis, questions related to alternative resources are becoming more important than ever before. Hydrogen-based technology is an appealing option. However, a wider spread of this technology will not be possible without appropriate storage capacities. In the present work we employ atomistic calculations to reveal adsorption mechanisms of H in graphene-based materials. Namely, we employ density functional theory to study impact of metallic catalysts on the adsorption energies of H on graphene. Additionally, interplay between H adsorption and structural defects in graphene (vacancies, Stone-Wales defects, etc.) will be discussed. Lastly, we will present results of a grand canonical Monte Carlo simulations comparing adsorption capabilities of pristine graphene and a recently theoretically proposed graphene-polymorph, so-called Penta-Octa-Penta (POP) graphene.

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Abstract

OP-04

The Impact of Open Pit Mine on Nearby Watercourse Mala Rijeka, Vareš

Džajić-Valjevac, M., Merzić, A., Mešanović, A.

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Abstract: Veovača open pit mine, located nearVareš, was used for extraction of ore rich with zinc, lead, and barite from 1982 until 1988, with the floatation processing plant in the near vicinity. Water quality of Mala Rijeka, watercourse passing by the mine and the processing plant, was examined in 2019. This paper analyses the presence of selected heavy metals (Cd, Zn, Fe, Mn, Pb), sulphate anion, and electrical conductivity along the entire length of Mala Rijeka, to determine nature of impact that the mine and the processing plant have on the watercourse. FAAS/ETAAS techniques were used to determine concentration of the heavy metals in water samples. Concentration of sulphates were determined by gravimetric (with $BaSO_4$) method. Concentrations of Cd(<0,05–2,50µg/L), Zn (0,119-1,212mg/L), Fe (0,002-1,313mg/L), Mn (0,001-0,580µg/L) and Pb (0,002-0,007mg/L), were found to be over the limit values prescribed in the national legislation, having decreasing trend toward the downstream watercourse sections. Electrical conductivity results (359-1060 µS/cm) and concentration of the sulphates (29,4-319,0mg/l) fallowed the same trend. Research work confirmed that watercourse Mala Rijeka was still under the influence of the open pit mine even more than 30 years after the closure of the mine.

surface

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Abstract

OP-05

Hyphenated Techniques as Tools for Plant Growth/Development Monitoring and Plant Product Quality Assessment

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Abstract: Among all analytical techniques used for the analysis of biomolecules, hyphenated techniques such as LC-MS, GC-MS, CE-MS are the major platforms for chemical profiling, metabolomics, and quality control. The brief overview of above mentioned techniques utilized in the quantification of several different classes of low-molecular-weight substances, from phytohormones, which are present in minute concentrations in plant tissue, to amino acids, polyamines, cannabinoids, terpenoids, phenolics, fatty acids, and vitamins that are important bioactive compounds in some plant-based products, is presented here. The advantages and drawbacks of each particular method are discussed, from sample preparation to data processing. In addition, the significance of proper chemical analyses of plant genetic resources in combination with genotyping and phenotyping will be discussed.

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Abstract

Halogenated Boroxine Dipotassium Trioxohydroxytetrafluorotriborate $K_2[B_3O_3F_4OH]$ Inhibits Emerging Multidrug-Resistant and β-Lactamase-Producing Opportunistic Pathogens

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Abstract: Halogenated boroxine dipotassium trioxohydroxytetrafluorotriborate, $K_2[B_3O_3F_4OH]$ was investigated on antimicrobial potential by targeting the multidrug-resistant opportunistic pathogens associated with skin and wound infections. The antimicrobial testing against eleven bacterial andfour fungal species revealed good activity of boroxine against pathogenic filamentous fungi *Penicilliumfuniculosum* Thom and *Aspergillus niger*van Tieghem; moderate bioactivity against the yeast *Candida albicans* (C. P. Robin) Berkhout the best antibacterial effect, stable over a 24-h period, was observed against the methicillin-resistant *Staphylococcus aureus* Ogston strain. The atomic force microscopy (AFM) used to investigate the morphology of S. aureus cells revealed indentations on its cell envelope after the boroxine exposure. Theseresults show that in addition to the antitumor effect, boroxine exerts wide spectrum antimicrobial activity, thus may help preventing the development of skin and wound-related opportunistic infections.

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Abstract

OP-07

Development of Calibration Models using Process Analytical Technology for Advanced Crystallization Process Control

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Abstract: With the technological advancement in the last decade process analytical technology (PAT) is intensively developed with the purpose of monitoring of the key process variables in real-time. PAT tools have opened up new possibilities for improving process performance. The benefits of this approach are products of predefined properties, higher batch production reproducibility and high quality in a series of batch using concept of Quality by design (QbD) and Quality by control (QbC).

The crystallization process is of the greatest importance in the pharmaceutical production. The purpose of this research is to develop a system that enables the continuous monitoring and optimal crystallization process control. Based on a calibration model for monitoring the concentration of solute, continuous process monitoring and advanced process control strategy maintain optimal conditions and products of desired critical quality attributes.

Neural networks-based calibration models were developed to model the dependence of concentration of an active pharmaceutical ingredient on temperature and spectral data obtained by UV-Vis measurements. The best-performing model was developed for a reduced data-set (800-200 nm) with 20 neurons and tangent-hyperbolic transfer function. Developed models will be used for continuously monitoring of the active pharmaceutical ingredient (API) in the crystallization system.

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Abstract

OP-08

Analysis of the Use of STEM and Its Elements in the Herzegovina-Neretva Canton educational System

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Abstract: The fourth industrial revolution is gaining momentum and affects every aspect of our daily lives: the boundaries between STEM disciplines (Science, Technology, Engineering, Mathematics), as well as between STEM and "non-STEM" disciplines are becoming increasingly blurred. To successfully implement STEM approach to teaching, it is necessary to develop curricula based on competencies, to provide assistance and support to the teachers and curriculum creators to meet the requirements for successful STEM education in the 21st century. The aim is to identify and describe the elements that can contribute to the development of STEM competencies of students in the existing context of curricula in the Herzegovina-Neretva Canton (HNC). The paper will operationalize key concepts of STEM education, and a special segment is dedicated to the analysis of the results of the TABLA project, which should lead to improved learning outcomes for students and teachers at HNC through an innovative approach, coherent and efficient integration of teaching content.

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Abstract

OP-09

Alkali-metal Fluoridooxidovanadates(V) and their Complexes with XeF_2 and HF

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Abstract: Complexes $[M^{n+}(XeF_2)_p(AF_x^-)_n]$ in which metal ion is coordinated by XeF_2 ligands represent an important, diverse, and structurally rich family of noble-gas compounds.The most numerous are XeF_2 coordination complexes of divalent metal cations, followed by complexes of lanthanide ions. The least represented are monovalent cations, where altogether only three structurally characterized complexes of Ag^+ and Li^+ have been reported. Anions are limited to weakly coordinating hexafluorido species, such as AsF_6^-, SbF_6^-, and RuF_6^-.Vanadium oxytrifluoride, VOF_3, is a Lewis acid and with metal fluorides forms a variety of fluoridooxidovanadate(V) salts. In this work, alkali metal fluorides were reacted with VOF_3 in anhydrous HF and the following compounds have been isolated and structurally characterized by single-crystal X-ray diffraction and Raman spectroscopy: $Li_2V_2O_2F_8$ and $Na_2V_2O_2F_8$ with dimeric anions; $KVOF_4$and $KV_2O_2F_7$ with chain anions; and complexes with HF ligand $[Na(HF)VOF_4]$ and $[K_9(HF)_2V_9O_9F_{36}]$. Moreover, crystallization of solutions of XeF_2 and $Li_2V_2O_2F_8$ has resulted in the formation of $[Li_2(XeF_2)V_2O_2F_8]$, a rare example of XeF_2 ligation to lithium. Similarly, when $Na_2V_2O_2F_8$ was employed, a complex $[Na_2(XeF_2)V_2O_2F_8]$ formed, which is the first example of XeF_2 coordination to sodium ion.In both coordination compounds the XeF_2 ligand exhibits $M^+{-}FXeF{-}M^+$bridging coordination mode.

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Abstract

Ab initio Study of Alloying Impact on the Stability of Cementite in TRIP-assisted AHSS Steels

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Abstract: Transformation-induced-plasticity (TRIP) steels from the third generation of advanced high-strength steels (AHSS) contain Si additions to prevent the formation of carbides. Cementite (Fe_3C) is a prototype among the carbides, and despite the importance of the influence of alloying elements on its stability, mechanisms by which the elements act has not been clarified so far. In this work, *ab initio* calculations were employed using the projected augmented wave (PAW) method, as incorporated in the Vienna Ab-initio Simulation Package (VASP), to study the impact of several alloying elements, including Al, Cr, Mg, Mn, and Si, on the stability of cementite. Partitioning energies were calculated to determine the segregation tendency of alloying elements between the phases ferrite, austenite, and cementite. The change in formation energy between the alloyed cementite and the pure cementite was then used to quantify the phase (de)stabilization. Mg and Si were found to reduce cementite stability. Si, however, preferentially segregates into ferrite and therefore has no effect on the stability under equilibrium conditions. In addition, the effects of the technically most important elements Al and Si on the mechanical properties of cementite were calculated using the stress-starain method. Both elements were found to increase the mechanical stability of cementite.

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Abstract

OP-11

Analytical Studies of Fragrant Raw Materials. A Quest for Their Odor Active Constituents

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Abstract: The determination of the most important olfactory contributors of a fragrant natural raw material can be an extremely long and complex task which requires the combination of very efficient analytical techniques. Consequently, there is still a lack of accurate knowledge about the main odoriferous constituents for many natural raw materials, even those widely used for their odorant properties in the flavor and fragrance industry.

This presentation will describe several examples of analytical investigations based on Gas Chromatography-Olfactometry (GC-O) and focused on the determination of the main odorant contributors of some fragrant raw materials. Hence, the key odorants ofthe most characteristic facets of frankincense and *Helichrysum italicum* essential oils were shown to be respectively olibanic acids and4,6-dimethyloctan-3,5-dione. These constituents are contained in very low amounts (< 1%), and this is another example of the fact that the main olfactory contributors are often strongly potent odorants contained only in trace amounts.

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Abstract

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Optimized and validated RP-HPLC method for the quantification of curcumin in formulations containing *Curcuma longa* L. Extracts

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Abstract: A rapid, accurate, and precise RP-HPLC method has been established and validated for the determination of curcumin in a solid dosage form containing turmeric root dry extract. The chromatographic separation of curcumin was conducted on Rastek C18 column (150 mm × 4.6 mm i.d., 5 µm) using an isocratic elution with the mobile phase composed of acetonitrile and 1.0% (v/v) formic acid in 50:50 ratio. The detection wavelength was set at 425 nm. The separation was performed at a flow rate 1 mL/min and the column was kept at a constant 40°C. The method was validated as per International Council for Harmonization (Q2R1 ICH) guidelines. The calibration curve was linear from 33.00-100.00 ng/mL with the correlation coefficient >0.9999. Limit of detection (LOD) and limit of quantification (LOQ) were 0.97 and 2.95 ng/mL, respectively. The intra-day/inter-day accuracy and precision demonstrated a recovery of 99.33–100.51%/99.59–100.51% with a Relative Standard Deviation (RSD) of 0.09%. A tested solid dosage form containing turmeric root dry extract confirmed the applicability of the method in the quantification of curcuminin commercially available turmeric formulation. Proposed method was proven to have acceptable specificity, sensitivity and accuracy for the quantity control of curcumin in formulations containing *Curcuma longa* L. extracts.

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Abstract

A Critical Assessment of vdW Corrections Methods: A Case Study on Graphene

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Abstract: Owing to its unique properties, graphene is among the most studied materials. Literature on mechanical properties of a few-layer-graphene is, however, barely available. In the present contribution, we investigate the compression and tension behaviour of bi- and tri-layer graphene for both stacking orders (A-A and A-B (Bernal)). A key aspect in the inavestigation of multilayer graphene is an accurate description of long-ranged electronic correlation phenomena between the atomic layers. Van-der-Waals interactions arenot tractable within the standard formalism of density functional theory (DFT) and hence are included via corrections. After benchmarking vdW-correction methods against well-known properties of graphite, we examine stacks of up to ten layers of graphene sheets. We investigate their effect on interlayer spacings and out-of-plane stiffness systematically in combination with two different commonly used exchange-correlation functionals.

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Abstract

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Evaluation of Photostability and Thermal Stability of Selected Commercially Important Essential Oils from Bosnia and Herzegovina

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Abstract: Essential oils, composed of various classes of chemical compounds, are susceptible to changes during storage. They can be sensitive to temperature, light and oxygen and therefore it is necessary to consider influence of these factors on shelf life of essential oils. Commercially valuable essential oils from B&H were selected for determination of chemical composition and impact of light, temperature and available oxygen on alteration. Aliquots of immortelle, silver fir, prickly juniper, lavender, winter savory and chamomile essential oils were exposed to UV-A irradiation as well as to elevated temperature in the presence of atmospheric oxygen and in the presence of inert gas, respectively. Photostability and thermal stability were evaluated by GC-FID and GC-MS analysis, comparing composition before and after the applied regimes. Each oil showed individual response to applied conditions. Silver fir and prickly juniper essential oils were shown to be stable, while immortelle, winter savory, lavender, chamomile, laurel and mint essential oils showed specific chemical changes upon applied stress conditions. Based on the obtained results, optimal way of storage can be suggested for each oil.

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Abstract

OP-15

Novel Metal(II) Fluoridooxidomolybdates(VI)

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Abstract: The synthetic and structural chemistry of inorganic fluoridomono-oxidomolybdates(VI) is not well explored. These compounds containing anions such as $[Mo_2O_2F_9]^-$, $[MoOF_5]^-$, and $[MoOF_6]^{2-}$ form when a relatively weak Lewis acid $MoOF_4$ reacts with fluoride-ion donors. Typically, $MoOF_4$ is synthesized by controlled hydrolysis of MoF_6 with SiO_2 in anhydrous HF. In this work a different, more convenient, route was investigated. The $MoOF_4$ was prepared by solvolysis of commercially available $MoOCl_4$ in anhydrous HF. Novel metal(II) fluoridooxidomolybdate(VI) salts were synthesizedeither by reacting the correspondingdivalent fluorides, MF_2, e.g. CaF_2, SrF_2, BaF_2 or PbF_2,with $MoOF_4$ in anhydrous HF or by forming the Lewis acid *in situ*by solvolysis of $MoOCl_4$ in anhydrous HF in the presence of MF_2. The resulting air-sensitive compounds were characterized by vibrational spectroscopy (Raman and ATR-FTIR), powder X-ray diffraction, and low-temperature single-crystal X-ray diffraction.

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Abstract

OP-16

The Effect of Metal-Metal and Metal-Oxide Interactions on Electrocalalytic Activity of Pt Thin Film Catalysts

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Abstract: The electrocatalytic oxidation of small organic molecules, such as methanol, ethanol and formic acid has been extensively studied due to their properties that make them suitable for use in fuel cells. Particularly, the electrochemical oxidation of formic acid has been comprehensively examined as the anodic reaction in direct formic acid fuel cell (DFAFC).

In this study, we have investigated how the change in surface composition of the Pt thin film deposited on Ni and Cr supports, induced by the controlled thermal treatment, reflects on catalyst performance for the electrooxidation of formic acid. In order to explain the results obtained, the catalysts were characterized using the photoelectron spectroscopy (XPS) to determine the composition of the electrode surface before and after annealing. Electrooxidation of adsorbed carbon monoxide layer and in situ FTIR technique helped us explain the difference in performances recorded in electrooxidation of formic acid. AFM and STM analysis were essential to provide the insight into the alteration of the morphology induced by thermal annealing. Finally, in situ ISPMS analysis was performed to determine the electrode stability during the formic acid oxidation reaction.

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Abstract

Water from Mineral Springs - Composition and Application in Medicine and Cosmetics

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Abstract: The main objective of our study is to determine the composition of water from several mineral springs, test their antibacterial, antiviral and antifungal properties and compare them as to find out the best ones to incorporate in medicinal and cosmetic products. To achieve this, samples from 8mineral springs were subjected to elemental analysis for the determination of 70 elements using inductively coupled plasma-mass-spectrometry. Results showed that concentrations of the macro elements: Mg, K, Ca and S were high in all of the samples even during the spring high water period (varying from: 0.015 to 0.155 mg/L for Mg, 3.95 to 7.25mg/L for K, 3.83 to 15.0mg/L for Ca and 30.9 to 56.4mg/L for S). Elements with previously reported antibacterial, antiviral or antifungal properties (Au, Se, B, Mo, Ge, W, Sr) were also found in every sample in fairly high concentrations. The specific antimicrobial properties of the water of each mineral spring remain to be determined using agar well diffusion method and resazurin assay method.Furthermore, dry residue samples were analyzed with a Raman microscope and revealed several different crystalline structures, some of which of a sulphate nature, which presumably contribute to the healing properties of the water.

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Abstract

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Compounds from the XeF_2–TaF_5 System: Novel Synthesis and Crystal Structures

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Abstract: Xenon difluoride (XeF_2) is a powerful oxidant and a medium-strongfluoride-ion donor.This is manifested in its reaction with Lewis-acidic pentafluorides of *p*-block and transition elements, such as AsF_5, SbF_5, BiF_5, NbF_5, TaF_5, RuF_5, IrF_5, and AuF_5, formingeither $[XeF]^+$ or $[Xe_2F_3]^+$ species. Although the structural investigation of compounds with*p*-block pentafluorideshas been carried out extensively, in the case of transition metals, only the crystal structures of theruthenium(V) and iridium(V) analogshavebeen reported. Typically, these compounds are synthesized in anhydrous HF solutions or in XeF_2 melts. In this work, a new convenient and readily availablesynthetic method was developed and optimized for the XeF_2–TaF_5 system. This has afforded a facile access to $[XeF][TaF_6]$, $[XeF][Ta_2F_{11}]$, and $[Xe_2F_3][TaF_6]$ compounds, which were characterizedby vibrational spectroscopy (Raman, ATR-FTIR) and X-ray diffraction techniques. Moreover, their crystal structures were determined for the first time by low-temperature single-crystal X-ray diffraction.The structures of $[XeF]^+[TaF_6]^-$ and $[XeF]^+[Ta_2F_{11}]^-$consist of tight ion pairs, whereas weakly interactingV-shaped cations $[Xe_2F_3]^+$andoctahedral $[TaF_6]^-$ anions are observed in the $[Xe_2F_3][TaF_6]$ salt.

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Abstract

OP-19

Interaction of Cucurbiturils with Lipid Bilayers

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Abstract: In this study cucurbit[7]uril (CB[7]), was loaded into preformed liposomes via a diffusion-controlled process to investigate the effect of CB[7] on the stability of the lipid membrane. The effect of CB[7] on liposome integrity was studied via calcein release, TGA, TEM, the size and charge of liposomes.In addition, the affinity of CB[7] towards cholesterol was determined. It was found that CB[7] has a K_a of $3x10^6$ with cholesterol. Cholesterol was released from liposomes when the concentration of CB[7] is higher than 1.433 mM.Transmission Electron Microscope (TEM) images confirmed a stable spherical intact liposomes that directly disrupted into either smaller micelles (5-10 nm) or aggregates upon CB[7] addition up to 0.2292 mM of CB[7]. Biocompatibility of CB[7] against Human red blood cells (RBCs) was investigated and showed that 2.580 to 3.00 mM CB[7] concentrations were able caused a RBCs hemolysis percent of 56.88%

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Abstract

Inventory of Polybrominated Diphenyl Ethers (PBDEs) in Bosnia and Herzegovina

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decaBDE

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Abstract: Polybrominated diphenyl ethers (PBDEs) are flame retardants whose use is restricted to industrial production in line with the Stockholm Convention due to their persistence and toxicity. Some congeners were restricted in 2009, while thedecaBDE restriction entered into force in 2017. Selected plastic products containing PBDEs are still widely used and may potentially impact human health and the environment. This paper analyses the presence of the PBDEs in electric/electronic equipment (EEE), transport vehicles and related waste in Bosnia and Hercegovina in 2020. The methodology used by the Stockholm Convention Secretariat was used to estimate the quantity of PBDEs at the national level. It has been estimated that most of the PBDEs come from the old transport vehicles still in use (4724 kg) and EEE in stock (10476 kg). CRT-monitors, that are part of the TV or computer devices, use and inadequate disposal of old vehicles has been identified as a significant environmental threat in B&H related to PBDE contamination. This research has been conducted within the framework of the project titled "Environmentally Sound Management of Persistent Organic Pollutants (POPs) in Industrial and Hazardous Waste Sectors in Bosnia and Herzegovina", implemented by UNDP and financed by the Government of Sweden.

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Abstract

Bulk Diffusion of Impurities in TiN: An ab initio Study

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Abstract: TiN-based materials are widely established as protective coatings for cutting tools. Grain interiors (single crystal regions) could serve as reservoirs for functional species, e.g. Al or V, which provide effective lubrication and wear protection at high temperatures by diffusing to the coating surface where they form a protective oxide scale (Al) or a lubricious oxide to reduce friction (V). In this contribution, we will report on our recent work in addressing issues related to the atomistic modeling of mass transport. To do so we employ complementary computational investigations to determine elementary point-defect migration mechanisms in crystalline materials and subsequently their relative rates. The density functional theory (DFT) is used to describe interatomic forces, is the most reliable computational tool to calculate atomic jump rates as a function of temperature. Since TiN is a harmonic crystal it gives us access to temperature based properties derived from the lattice vibration with harmonic and quasi-harmonic approximation. We will present the DFT-based "5-frequency model" allowing us to calculate the diffusion coefficient in the crystalline material. Moreover, the influence of the TiN stoichiometry on its diffusion properties is taken into account through the change in the concentrations of the intrinsic point defects as a function of composition. These concentrations are obtained via a thermodynamic formalism based on the dilute solution model. We find that in stoichiometric TiN the vanadium impurity diffusion proceeds via the vacancy mechanism on the Ti sublattice. Furthermore, we also demonstrate that pressure has a notable impact on the diffusivity of V, Al, and Ti in TiN.

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Abstract

OP-22

Heavy metal mobility and pollution characterization in agricultural soil caused by steel industrial activities in Central Jordan

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Abstract: Industry is the main source of soil pollution in Jordan, were higher concentrations of heavy and toxic elements were found in soil around industrial estates. This study is dealing with industrial pollution hot spot that is a steel factory at central Jordan, that emits various ashes and gases. This area is populated and its soils were increasingly utilized in agricultural activities. High Fe, Cr and V content were recorded in soil around this factory. Therefore, this study aims to investigate the mobility and oxidation state of these elements. For this purpose, two core samples (up to 50 cm in depth) at sites with higher heavy metal concentrations were sampled. Soil samples were collected at 10 cm interval and analyzed for Fe, Mn, Cr, V, Zn and Pb by using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Moreover, Fe was analyzed using the X-ray Absorption Near-Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) to find the changes in oxidation states and structural parameters with depth. The Fe-EXAFS are associated mainly with (O), which indicates the anthropogenic Fe source. The Fe-XANES are in Fe(II) and Fe(III)forms, which indicate that Fe is usually formed during high thermal processes. In addition, XANES of Cr, Mn and V are found in high oxidation states Cr(VI),V(V), Mn(IV)which might be a result from steel manufacturing under oxygenated environment.

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Abstract

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Electrochemical stability and degradation of Pd/C and Rh/C catalysts in acidic media

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Abstract: Platinum group metals are key components of electrochemical energy conversion devices due to their superior catalytic and chemical properties. Besides Pt, Pd and Rh attract significant attention in electrocatalysis due to their high activity for different reactions.[1,2]In addition to activity, the other basic requirement that catalytic material needs to meet is durability under relevant operational conditions. We present here a study on the electrochemical stability of Pd/C and Rh/C catalysts in a similar way as commonly done for Pt/C.[3] Following accelerated degradation protocol (ADP) was designed: 0.1 M $HClO_4$ electrolyte, 5000 voltammetric scans at 1 V/s, potential range 0.4 – 1.4 V_{RHE}. Significant decay of Pd electrochemical surface area (ESA), was paired with substantial Pd dissolution measured by coupling the electrochemical flow cell with ICP-MS (EFC-ICP-MS). Identical location SEM (IL-SEM) revealed that degradation of Pd/C occurs *via* dissolution of Pd nanoparticles followed by re-deposition.[1] In contrast, only a minor loss of Rh ESA and negligible Rh dissolution occurred under the same conditions, while IL-SEM did not reveal any significant change in the structure of Rh/C.[2]These results are valuable for the proper design of Pd and Rh-based electrocatalytic materials for applications in energy conversion devices.

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Abstract

OP-24

Recent Advances in the Field of Xenon(II) Compounds with Polymeric Fluoridoanions

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Abstract: The synthesis of the first noble-gas compound, "$XePtF_6$", was reported 60 years ago and has been followed by several unsuccessful attempts of its structural characterisation over the past decades. It was suggested that the elusiveness of "$XePtF_6$" might be attributed to the polymeric nature of its anion. Since polyfluoridometalate anions were also found to arise from the interaction of XeF_2 with weaker Lewis acids, such as certain metal tetrafluorides, a series of analogous XeF_2–MF_4 (M = Cr, Mn, Sn, Ti) systems were systematically investigated, where it was shown that despite their relatively simple formulation $aXeF_2 \cdot bMF_4$, the isolated productsexhibit a very rich structural chemistry featuring a variety of anions with different dimensionality.

In this study, excess XeF_2 was reacted with SnF_4 in anhydrous HF. Theproducts were characterized with low-temperature single-crystal X-ray diffraction and Raman spectroscopy. Two $Xe_2F_3^+$ compounds with novel 2D polyfluoridostannate anions were isolated: $[Xe_2F_3][Sn_4F_{17}] \cdot XeF_2 \cdot HF$ and $[Xe_2F_3]_3[Sn_{10}F_{43}] \cdot 2XeF_2$. Moreover, XeF_2 was heated with TiF_4 at 135 °C. Upon cooling to room temperature, crystals of $[XeF][Ti_4F_{17}]$ were obtained. This compound with the novel 2D $[Ti_4F_{17}]^-$ anion represents a new isomer of$XeF_2 \cdot 4TiF_4$, since previously only $[Xe_2F_3][Ti_8F_{33}]$ was known.

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OP-25

Dereplication of Natural Products Using Mass Spectrometry Integrated Approach

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Abstract: Plant metabolites can act as drugs for the treatment of a variety of diseases due to their unique skeletal features. A large number of plant metabolites are used as drugs for the treatment of many diseases. The structural diversity of these plant metabolites formed by complex enzymatically controlled pathways is still not fully explored. Moreover, to preserve the medicinally important plant species and their sustainability, the quantity of plant material has been limited to the analytical level. Therefore, sensitive and high-throughput dereplication methods are required for better, unambiguous and high-throughput analysis of natural products in complex mixtures. We have developed high-throughput dereplication strategy for the unambiguous identification of different classes of natural product through LC-ESI-MS/MS in the plant extract and in the herbal formulations using an integrated approach which includes several confirmatory steps such as exact masses measurement, diagnostic fragment ions, databasessearch, and isotopic pattern. Based on above mentioned integrated approach, we have recently investigated different classes of natural products including withanolides (steroidal lactones), pregnane-type steroidal alkaloids, *Buxus* steroidal alkaloids and many more by using electrospray ionization quadropole time-of-flight mass spectrometry (ESI-QTOF-MS/MS) and LC-QQQ-MS analysis. Moreover, we have also developed a LC-ESI-MS/MS database of unique natural products. Outcome of the study was found to be very effective for their rapid identification of phytochemicals in plant extract and herbal formulations.

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Abstract

OP-26

Novel “in-house” Chemical Treatments of Pomegranate Peel (*Punica granatum*) for Simultaneous Heavy Metal Removal

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Abstract: The growing movement in environmental chemistry is looking for a way to remove heavy metals from wastewater by using agricultural waste as biosorbents. The fact that pomegranate (Punica granatum) fruit leaves behind significant amounts of waste biomass after consumption makes it an exceptional candidate for reuse as sorbent material. This study presents the development of 2 novel “in-house” chemical modification processes of powdered dry biomass, focusing on the synthesis and classification of the products of different procedures, with the aim of maximizing the simultaneous removal efficiency of Cr^{3+}, Cu^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}, Pb^{2+} and Zn^{2+} from water solution. Modification as well as biosorption of metals has been successfully confirmed by FTIR and SEM-EDS tehniques based on determination of functional groups, morphological characterization by mapping of metal distribution on the pomegranate surface, along with its semi-quantitative elemental analysis. It has been shown that under optimal biosorption parameters the removal efficiency for the selected biosorbent of the eight selected heavy metal ions was in the following range:
$Cu^{2+} \approx Pb^{2+} > Cr^{3+} > Cd^{2+} > Zn^{2+} > Ni^{2+} \approx Co^{2+} > Mn^{2+}$.

POSTER PRESENTATIONS

Analytical Chemistry

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Determination of Thiols Based on Reaction with Cu(II)-neocuproine Using a Spectrophotometer or Smartphone as Detectors

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Abstract: This study describes a method for the determination of N-acetyl-L-cysteine (NAC) and L-glutathione (GLU) using a spectrophotometer as a detector or through digital imaging. The method is based on the redox-complexation reaction of selected thiols with Cu(II) in the presence of neocuproine (NC) resulting in a Cu(I)-$(NC)_2$ complex that absorbs at 450 nm. A smartphone camera with control of imaging conditions was used to acquire a digital image of the reaction solutions. Under selected optimal conditions, a linear relationship between absorbance and thiols concentration in the range from 2.0×10^{-5} to 2.0×10^{-4} mol L^{-1} was achieved. Detection limit of 2.1×10^{-6} mol L^{-1} and 1.30×10^{-6} mol L^{-1} were obtained for NAC and GLU, respectively. The same linear dynamic range (LDR) was obtained by applying the Red, Green, Blue (RGB) color approach when processing digital images by monitoring the Red color channel. The analytical application of the method was tested on pharmaceutical preparations and demonstrated satisfactory precision and recovery test (96.90 %-101.2 %). The proposed method is environmentally friendly and simple concerning the total volume (4.0 mL) of the reaction mixture and use of smartphone as a detector.

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Characterization of Painting Technology and Damage Caused by High Humidity on Two Socialist Realism Portraits from the History Museum of Bosnia and Herzegovina

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Abstract: Two paintings were subjected to a series of analyses, aiming to identify the used materials, as well as the damage caused by the exposure to high humidity. Characterization of the type of textile support was performed using the threads burning test and optical microscopy. The FTIR method revealed the composition of binders from the dyed layer. A radiographic analysis was used to examine the painting technique, the presence of any previous interventions or sub-drawings. The chemical composition of pigments was determined by XRF. In summary, it was established that the two Bosnian painters created their works using materials such as cotton canvas, animal glue, Bologna chalk and white pigments in the preparation, and painted with oil medium and industrially pigments. In one of the paintings, the changes caused by high relative humidity were identified using FTIR. This method determined the presence of metal soaps, caused by the reaction of zinc white and oil. The results of the analyses facilitated the choice of conservation and restoration methods, but at the same time they also represent a contribution to the study of painting materials and technology used by Bosnian painters immediately after World War II.

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PP-AC-03

Chlorogenic Acid as Biological Indicator of Fruit Maturity

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Abstract: Chlorogenic acid (CGA) an important and biologically active polyphenol in food, has several therapeutic roles such as antioxidant, antibacterial, hepatoprotective, cardioprotective, anti-inflammatory, antipyretic, neuroprotective, anti-obesity, antiviral, antimicrobial, antihypertensive, antihypertensive and antihypertensive system. The plant fruits of: *Mespilus germanica, Malus domestica, Solanum lycopersicum, Actinidia deliciosa* and *Vitis vinifera*, in different maturity stage, were analyzed for the presence of CGA. The analysis was performed on a thin layer Silicagel 60 F_{254}, using the developer: ethyl acetate - formic acid - water (8: 1: 1, V / V). TLC method detected CGA in all tested samples. Ultraviolet-visible (UV-Vis) spectrophotometric method was established to determine the content of CGA according to potassium ferricyanide-Fe(III) detection system. A content of CGA was ranged from 3,0 for *Actinidia deliciosa* (mature fruit), to 58,0 (mg/L) for *Vitis vinifera* (immature fruit). Result for CGA content showed higher content in immature fruit in comparison with mature fruit. Finally, it can be concluded that chlorogenic acid could serve as a biological marker in monitoring the maturity of plant fruits.

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Analysis of Trace Elements in Commercially Available Tea Samples from Local Market in Sarajevo

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Abstract: Trace metals have important biochemical functions in the body and affects to normal human health. The aim of this study was to determine the concentrations of trace metals Cu, C r, Mn, Fe, and Zn in tea samples made of the leaves of *Mentha* × *piperita* L. Samples of commercially available tea were collected from local market in Sarajevo, Bosnia and Herzegovina. Microwave digestion was used to dissolve the samples, and concentrations of essential metals were analysed by inductively coupled plasma with mass spectrometry (ICP-MS). The results of the analysis (expressed in mg g^{-1}) were obtained as follows: Cu 7.83 – 10.71; Cr 2.94 – 3.87; Mn 70.09 – 84.09; Fe 417.19 – 1109.91; Zn 15.5 – 27.24. Therefore, tea products of *Mentha piperita* L. can be used in daily consumption due to the higher content of Fe, Mn, and Zn and their beneficial effects on the normal functioning of the organism.

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Correlation Between Total Phenolics and Antioxidant Activity of Selected Plant Seeds

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Abstract: The polyphenolic compounds are naturally occurring antioxidants originate from plants based ingredients. The most popular seeds include flax (*Linum usitatissimum* L.), black cumin (*Nigella sativa* L.), chia (*Salvia hispanica* L.), pumpkin (*Cucurbita spp.)*, sesame (*Sesamum incidicum* L.) and sunflower (*Heliantus annuus* L.) having numerous fat-soluble bioactive compoundswere increasingly consumed. Aim of this study was to determine the total content of phenolics and antioxidant activity, and to assess a correlation between these two parameters in selected seeds. The total phenolic contents were determined using the Folin–Ciocalteau colorimetric method. The antioxidant activities of the studied seeds were evaluated by using an DPPH assay. The total phenolic was in the range of 0,48 (sunflower) to 10,31 (chia) mg GAE/g. Antioxidant activity was in the range of 0,01(pumpkin) to 2,57 (chia) mmol TE/g. The good linear correlations obtained between phenolic content and antioxidant activity determined by DPPH assay suggest that phenolic content could be used as an indicator of antioxidant properties of the examined seeds. Analyzed seeds can be considered as a valuable source of dietary supplements and functional foods due to their health promoting bioactive compounds, polyphenols, and corresponding antioxidant activities.

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PP-AC-06

Electrochemical Determination of Duloxetine Hydrochloride at Gold Electrode

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Abstract: Duloxetine hydrochloride (DUL), a naphthyl ether amine, inhibits the uptake of serotonin and norepinephrine. The electrochemical behavior of DUL was determined by cyclic voltammetry (CV) in phosphate buffer solution at gold electrode by varying pH and scan rate. The electroanalytical application was studied with the aid of differential pulse voltammetry (DPV) in sodium bicarbonate solution. A linear response ranged from $5x10^{-7}$ M to 10^{-5} M. The validation of the DPV method was carried out by determine of the limit of detection (LOD) and limit of quantitation (LOQ) and the calculate values were 4.6×10^{-7} and 2×10^{-6} M, respectively. The proposed DPV method has been successfully applied to assessment DUL as standard and in Taita® tablets and standard spiked with human serum.

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Determination of Magnesium Content in a Selected Pharmaceutical Supplements

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Abstract: Magnesium is an essential element that have a very important role in human body including various biochemical functions as it binds in reactions of over than 300 enzymes. These processes include protein synthesis, cellular energy production and storage, cell growth and reproduction, DNA and RNA synthesis, and stabilization of mitochondrial membranes. Its deficiency relates with a wide range of health complications. Therefore, people should take their daily recommended amounts of magnesium. Magnesium can help in treatment a number of chronic diseases including migraine, Alzheimer's disease, stroke, cardiovascular disease and type 2 diabetes. People with magnesium deficiency must intake it additionally and that is usually in form of different pharmaceutical supplements. Magnesium oxide is a common type of magnesium form in supplements that is widely available in pharmacies. The aim of this work was to determinate the content of magnesium in a selected pharmaceutical supplement, by recommended methods of Pharmacopoeia (Acid-base titrations and Complexometric titrations), from different manufactures. The declared content of Mg in tablets was 300mg, 375mg, and 400mg, while analyzed content of Mg were ranged from 304 to 399 mg MgO. All tested supplements in form of MgO, showed magnesium levels that can supply daily Mg recommended values for humans which is ranged from 300 to 400 mg.

POSTER PRESENTATIONS

Biochemistry and Biotechnology

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Antioxidant Activity of Ru(III) Complexes and Their Ligands Derived from Salycilaldehyde and Halogenated Anilines

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Abstract: The aim of this work was to determine the antioxidant activity of two Ru(III) complexes with the general formulas Na[$RuCl_2$(*N*-4-Cl-Ph-salim)$_2$] and Na[$RuCl_2$(*N*-3-Br-Ph-salim)$_2$] and their corresponding ligands prior to coordination. The ligands *N*-3-Cl-phenylsalicylidenimine (*N*-3-Cl-Ph-salimH) and *N*-3-Br- phenylsalicylidenimine (*N*-3-Br-Ph-salimH), Schiff bases, were synthesized from salycilaldehyde and chloroaniline or bromoaniline. The four compounds were characterized using IR spectroscopy and ESI ToF mass spectrometry. Further on, the following was confirmed: coordination of ligands on the Ru(III) center, the molecular formulas and the corresponding M^-ions: [$C_{26}H_{18}N_2O_2Cl_4Ru]^-$ ion, (m/z: 631.91732) and[$C_{26}H_{18}N_2O_2Cl_2Br_2Ru]^-$ ion, (m/z: 719.82831). The antioxidant activity was determined by the ABTS assay and results expressed as Trolox equivalents (TE). The complexes Na[$RuCl_2$(*N*-4-Cl-Ph-salim)$_2$] and Na[$RuCl_2$(*N*-3-Br-Ph-salim)$_2$] had a higher antioxidant activity (205.88 mmolTE/100g and 216.44 mmol TE/100 g, respectively) than both ligands. *N*-3-Cl-Ph-salimH showed better antioxidant properties (121.38 mmol TE/100 g) than *N*-3-Br-Ph-salimH (37.64 mmol TE/100 g).

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Abstract

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Teucrium montanum L. – Chemical Composition and Biological Activity of Aqueous and Methanolic Extracts

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Abstract: One of the plants, characteristic for traditional medicine of Bosnia and Herzegovina, is *Teucrium montanum* L. (mountain germander, travaiva, dubčacmali), a plant from the Lamiaceae family, thrives in Europe and Asia Minor. The aim of this study was to determine the composition of non-volatile components of aqueous and methanolic extracts of *Teucrium montanum* L., to determine their antioxidant potential and their inhibitory potential on enzymes acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). By HPLC/DAD technique content of 13 phenolic compounds were determined, with most dominant: *p*-coumaric acid (15.95 and 21.98), ellagic acid (3.51 and 7.25), and caffeic acid (0.71 and 10.73 mg/g extract), in aqueous (AE) and methanol extract (ME), respectively. Antioxidant potential tested by DPPH and FRAP method was better for methanol extract, as well as inhibition of protein carbonylation, while in the study of lipid protection against oxidation, aqueous extract of *Teucrium montanum* L showed better results. Tested extracts showed a weak ability to inhibit the enzyme AChE (27.77% AE and 10.05% ME), while the ability to inhibit BChE showed only aqueous extract (4.3%).

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Study of Phytochemical Composition and Biological Potential of *Teucrium montanum* L. Essential Oil

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Abstract: Essential oils are mixtures of natural, volatile compounds with a strong odor; secondary plant metabolites. Because they are well known for their medicinal properties and odors, they have a wide application. They are used in food preservation and as antimicrobial, analgesic, sedative, anti-inflammatory, antispasmodic drugs and local anesthetics. In this work, the chemical composition of *Teucrium montanum* L. essential oil was investigated using the gas chromatography - mass spectrometry (GC/MS) technique. The antioxidant potential was tested by standard DPPH and FRAP methods, while the inhibition of the enzymes acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) were examined by the Ellman's method. In essential oil of *Teucrium montanum* were identified 47 components. Individual classes of compounds were represented as follows: sesquiterpenoids (36%), sesquiterpenes (29.7%), monoterpenes (15.3%) and monoterpenoids (10%). The most common compounds were *α*-cadinol (9%) and *ß*-selinene (9%). The IC_{50} values obtained by the DPPH test (201.91 µg/ mL), and values obtained by FRAP method (13.02 µmol Fe^{2+}/g) indicates a weaker antioxidant and reduction potential. Inhibition of AChE, for essential oil concentrations of 1 and 2 mg/mL, were 51.92% and 59.32%, while for inhibition of BChE enzyme values were 35.65% and 49.54%, indicating moderate inhibition potential.

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PP-BB-04

Influence of Fungicides on Hematological Parameters of *Rattus norvegicus* (Berkenhout, 1769)

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Abstract: In the last two decades, more and more attention has been paid to the influence of various pesticides on hematopoiesis and the immune system. To date, there are numerous scientific studies that have provided insight into the impact of pesticides on the hematological and immune status of organisms. In this paper, the influence of the dithiocarbamate fungicide Mankogal ® 80, whose active substance is mancozeb, on the hematological parameters of the species *Rattus norvegicus* was monitored. Three groups of individuals (male and female Wistar strains) were treated at doses of 25 mg/kg, 20 mg/kg and 15 mg/kg body weight intraperitoneally. After 24 hours of intraperitoneal administration of these doses, the following hematological parameters were examined: total erythrocyte count, hematocrit, hemoglobin concentration, mean erythrocyte cell volume, mean erythrocyte hemoglobin concentration, mean hemoglobin concentration, total leukocyte count and differential blood count, absolute neutrophil count, absolute basophils, lymphocytes and monocytes. The obtained results showed that in Wistar strains exposed to a higher dose of dithiocarbamate fungicide, Mankogal, there was a statistically significant decrease in total erythrocyte count, hemoglobin concentration, hematocrit, total leukocyte count, absolute neutrophil count, and statistically significant increase in MCV, MCH and significant increase lymphocyte count. In addition to the negative impact on erythrocyte and leukocyte lineage, behavioral anomalies such as frequent scratching, burial, and agitation have also been reported.

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Binding Constants Determination of the Interaction of Albumin with 6-Substituted-4-Methylcoumarins

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Abstract: The binding of three 6-substituted-4-methylcoumarins to bovine serum albumin (BSA) was investigated by fluorescence spectroscopy under physiological conditions. Conformational and microenvironmental changes of BSA in presence of 4-methylcoumarins were investigated by synchronous spectroscopy and three-dimensional fluorescence spectroscopy. By addition of coumarin derivatives to BSA the maximum fluorescence intensity was reduced due to quenching of intrinsic fluorescence upon binding of coumarin derivatives. The results revealed that 6-substituted-4-methylcoumarins has a quenching effect on BSA fluorescence. The binding to BSA was investigated at three temperatures: 296, 303, and 310 K. From the obtained spectra, the Stern-Volmer constant (K_{sv}), bimolecular quenching constant (k_q), binding constants (K_b), and binding site number (n) constants were calculated. The strongest binding occurs during the formation of the BSA- 4,6-methoxycoumarin complex (k_q = 8.98×10^{13} M^{-1} s^{-1} at 310 K). Thermodynamic parameters evidence exothermic and spontaneous interaction. The microenvironment and conformation of BSA were determined to be changed in the presence of 6-substituted-4-methylcoumarins by synchronous and three-dimensional fluorescence spectra. Fluorimetric techniques have proven to be sensitive techniques to analyze the interaction between proteins and ligands.

This research was partially supported by the Ministry for Science, Higher Education and Youth, Canton Sarajevo (Fluorimetric and *in silico* studies of the interaction of albumin with synthetic coumarins- 27-02-11-41251-18/21).

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Fluorimetric Interaction Studies of Albumin with 7-Substituted-4-methylcoumarins

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Abstract: The 4-methylcoumarins (4-methyl-*2H*-1-benzopyran-2-ones) have several beneficial pharmacological effects. Interaction of several synthesized 7-substituted-4-methylcoumarins derivatives with bovine serum albumin (BSA) were studied at physiological pH and three temperatures (294, 303 and 310 K) by using fluorescence spectroscopic technique. From the spectra, the Stern-Volmer constant (K_{sv}), bimolecular quenching constant (k_q), binding constants (K_b), and binding site number (n) constants were calculated. There is a change in fluorescence spectral parameters like intensity and emission maxima. Fluorescence studies revealed that an analyzed sample quenches intrinsic emission of BSA. Thermodynamic parameters showed spontaneous interaction between 7-substituted-4-methylcoumarins and BSA. Additionally, changes of microenvironment and conformation of BSA were observed. The results of synchronous fluorescence spectra suggest changes in the microenvironment of tyrosine, while three-dimensional spectra showed changes related to the backbone structures of the protein chain (caused by the π-π* transition of the carbonyl group). The distance r between the donor (BSA) and acceptors (7-substituted-4-methylcoumarins) was calculated and indicated the occurrence of energy transfer from BSA to 4-methylcoumarins. The distance r between donors (BSA) and acceptors (7-substituted-4-methylcoumarin) is calculated and values (1.851-2.747nm) indicate the possibility of energy transfer from BSA to 4-methylcoumarins. All these results indicated that analyzed 4-methylcoumarins can bind to BSA and be potentially effectively transported in the body.

This research was partially supported by the Ministry for Science, Higher Education and Youth, Canton Sarajevo (Fluorimetric and *in silico* studies of the interaction of albumin with synthetic coumarins- 27-02-11-41251-18/21).

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Antioxidant Capacity and Acetylcholinesterase Inhibition of Essential Oils and Ethanolic Extracts of *Juniperus communis* L. from Herzegovina

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Abstract: The common juniper (*Juniperus communis* L.) is a shrubby, medicinal and aromatic plant from the Cupressaceae family. Berries of juniper are widely used as spices in the food industry, while essential oils are more widely used in the pharmaceutical and perfume industries. In this study, the chemical composition, antioxidant capacity and acetylcholinesterase inhibition were determined for essential oils and ethanolic extracts prepared from needles and berries of *J. communis* from Herzegovina. The essential oils from needles and berries of juniper were isolated in a Clevenger apparatus. Chemical composition of essential oil was analysed by gas chromatography and mass spectrometry (GC-MS). Ethanolic extracts were prepared by ultrasonic extraction. The content of total polyphenols was determined with Folin-Ciocalteu reagent. The antioxidant capacity was determined using DPPH (1,1-diphenyl-2-picrylhydrazyl radical) and FRAP (Ferric reducing antioxidant power) methods. A modified Ellman assay was used to measure acetylcholinesterase inhibition. The major compounds in the essential oil from needles and berries were monoterpenes α-pinene, β-myrcene, 3-carene and sesquiterpene germacrene D. Ethanolic extracts prepared from needles of juniper showed strong antioxidant activity (DPPH, IC_{50}=37.5 mg/L; FRAP, 300 mg/L is equivalent 0.17 mM Fe^{2+}) and high polyphenol content (135.9mg GAE/g dry extract). Essential oils (IC_{50}=147.1 mg/L) and ethanolic extracts (IC_{50}=57.9 mg/L) possess an inhibitory effect on acetylcholinesterase.

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Abstract

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Microwave-assisted Polyol Synthesis of Pt Based Catalysts for Ethanol Oxidation Reaction

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Abstract: Direct ethanol fuel cells (DEFC) are very promising energy sources due to their high efficiency and low emission of pollutants, high energy density, non-toxic and environmentally friendly characteristics. Platinum is a very good catalyst for the oxidation of ethanol, but it has significant disadvantages: high cost and limited resources in nature. In order to reduce the amount of Pt but also to improve the performance of the catalyst, the main efforts are focused on the synthesis of platinum catalysts in which platinum is alloyed with less expensive metals such as Sn, Zn, Ru, Ni, etc.In this work, PtSn/C, PtZn/C and PtSnZn/C catalysts were synthesized by the microwave assisted polyol method. The activity of synthesized catalysts for ethanol electrooxidation in acidic medium was investigated. The effects of composition and morphology on the catalyst electrocatalytic activity were analyzed by CO stripping voltammetry and ethanol oxidation. Electrocatalytic stability of the catalysts was examined by prolonged cycling as well as by chronoamperometric measurements in $HClO_4/C_2H_5OH$ solution. It was shown that activity of the platinum catalyst after the addition of another metal is attributed to the bifunctional and electronic effect.

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Abstract

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Electrocatalytic Properties of Pt Thin Film Deposited on Different Supports for Methanol Oxidation: Influence of Controlled Heat Treatment

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Abstract: It is known that surface structure is one of the critical issues affecting the activities of electrocatalysts. Heat treatment is an efficient approach to induce the rearrangement of surface atoms and thus to tailor their catalytic properties. The surface characteristics of electrochemically deposited Pt thin films at different substrates, as well as theeffect of thermal annealing, were probed for electrooxidation of CO and methanol.

Our results show that heat treatment in the reductive atmosphere (95% Ar+5% H_2) at 300^{o}C can substantially affect the degree of surface atom rearrangement and thus induce long-range order creating domains with large fractions of (111) and (100) sites without the use of an epitaxial template, translating into significant influence on their catalytic properties. Since the catalytic reactions take place at the surfaces, our work demonstrates an easy-to-implement way to control the atomic orientations in order to understand the relationship between structure and catalytic properties of catalyst for methanol oxidation and proposes a method to design advanced electrocatalysts.

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Abstract

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Morphology, Structure and Hardness of Electrolytically Produced Copper Coatings

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Abstract: Influence of various parameters of electrodeposition, such as type of cathode, composition of the electrolyte and thickness of the coating, on morphology, structure and hardness of copper coatings has been investigated. The Cu coatings thickness from 20 and 40 μm produced by the galvanostatic regime of electrolysis on Si(111) and brass cathodes from electrolytes without and with an addition of leveling/brightening additives were characterized by SEM and AFM techniques. The Vickers microindentation was used for a hardness analysis of the produced coatings, using the Chicot–Lesage (C–L) composite hardness model for estimation of their hardness. The mat microcrystalline fine-grained Cu coatings with the strong (220) preferred orientation were obtained from additive free electrolyte, and the smooth mirror bright nanocrystalline Cu coatings with the strong (200) preferred orientation were obtained from the electrolyte containing additives. Hardness analysis showed that the mat coatings were harder than the mirror bright coatings, that can be explained phenomena on grain boundary.

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Abstract

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Adsorption of MTT and Formazan on Graphene-based Materials

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Abstract: Adsorptionof MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide) and its reduction product – water insoluble formazan – on graphene-based nanomaterials can introduce significant interference in corresponding colorimetric cytotoxicity assays, which renders them unreliable for the toxicity assessment of these materials. However, if reliable quantitative correlations in form of adsorption isotherms can be found for the particular material, it would be possible to introduce corrections in apsorbances measured during the cytotoxicity assay. Adsorption of MTT and formazan was studied on two different graphene-based materials: hydrophilic graphene oxide, with high oxygen content (> 36 %) and hydrophobic reduced graphene oxide (oxygen content < 5 %). Adsorption of MTT and formazan on both materials follow well defined Freundlich adsorption isotherms, with some differences that can be attributed to the specific structure-related interactions between graphenes and adsorbates.

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Abstract

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Monitoring the Impact of the Exposure Time and Different Types of Marine Environment on the Corrosion Behaviour of NiTi SMA

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Abstract: The increasing application of the shape-memory materials (SMA) in the coastal environments has been registered nowadays. Therefore, it is very important to have the reliable information on how their corrosion activity changes as a function of time. Due to their excellent physical and mechanical properties, NiTi alloys are one of the most important SMA. Accordingly, in this research, the corrosive behaviour of NiTi SMA, produced as cast, was monitored after 6 and 12 months of exposure in different coastal environments. The corrosion of NiTi SMA was evaluated by the changes in chemical composition of the corrosion rust layer on the alloy surface by using Energy-Dispersive X-ray spectroscopy (EDX). The measured chemical compositions of the rust layer were analyzed using multivariate methods in order to identify the impact of the different types of the marine environment and the exposure time on the corrosion behaviour of NiTi SMA. The obtained results indicate that the lowest corrosion impact was registered under the influence of the marine atmosphere and such rust content was the least changed over time. The greatest impact as a function of exposure time was detected in the corrosion product formed under the influence of tide zone.

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Abstract

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Nanomaterial Additives in Clay-Based Composites for the Non-Ionizing Radiation Absorption

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Abstract: While the detrimental effects of ionizing electromagnetic (EM) radiation on human health are well established and thoroughly investigated, the effects of the non-ionizing EM radiation have been debated and studied only recently. In this study, clay composites were subjected to EM transmission testing in the region of non-ionizing radiation between 1.5 and 6.0 GHz which is where the frequency of the most mobile telephony systems can be found. Specimens were made with partial substitution of clay (2.5 and 5 wt.%) with different nanomaterials:fly ash, Titanium dioxides (TiO_2 -anatase and rutile),Zinc Ferrite ($ZnFe_2O_4$), Maghemite (γ-Fe_2O_3), Antimony Tin Oxide (ATO), and Multiwalled Carbon Nanotubes (MWCNT). All nanomaterials were characterized by B.E.T. nitrogen adsorption method to determine the specific surface area, and Thermogravimetric methods (TGA/DSC) to designate their thermal properties. Phase analysis was performed by Powder X-ray diffraction (PXRD), and the morphology studied by Electron Microscopy (SEM-EDX). The oxide content was measured by X-ray Fluorescence (ED-XRF) and the quantity of heavy metal determined by Plasma Excitation Spectrometry (ICP-OES). EM radiation transmission was evaluated using Anritsu ms2038 - Spectrum Analyzer. The lowest transmission was reported for the clay specimens with ATO and TiO_2 at a frequency of 4 GHz and it is -17 dB. In conclusion, the addition of the certain nanoparticles into clay can significantly lower the penetration of non-ionizing EM radiation through construction elements made from such composite materials.

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Abstract

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Influence of Treatment of Various Carbon Supports on Electrochemical Activity of Pt Catalysts

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Abstract: The development of novel materials to be used in energy production, conversion and storage is one of the largest challenges of today. The good alternative to use of fossil fuels is the fuel cell using methanol as fuel. Platinum is an excellent catalyst for methanol oxidation, but it is very expensive and its stock is limited. One of the ways to decrease an amount of Pt and simultaneous keep high catalyst activity is to increase real surface area of Pt catalyst by suitable treatment of catalyst support. In this study, influence of physical-chemical and electrochemical treatments of various carbon supports, such as Glassy carbon (GC) and Vulcan XC-72 Carbon, on electrochemical activity of Pt catalyst for methanol reaction oxidation has been investigated. The treated carbon supports were characterized by optical microscopic and atomic force microscopic techniques, as well as in situ electrochemical atomic force microscopic technique. Optimization of carbon support treatments is made through analysis of roughness, shape and size of Pt particles. The best activity showed Pt catalyst supported on Vulcan XC-72 Carbon.

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Abstract

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Estimation of ammunition stability depending on naturally aged single base propellant

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Abstract: In this work chemical stability of 41 years old single base propellant sample, with unknown initial composition, was evaluated by combining different physicochemical tests. The stabilizers content of propellant sample was determined by High-Performance Liquid Chromatography and High-Performance Thin Layer Chromatography methodes, thermal stability of sample was determined by vacuum stability test, Methyl Violet test (MVT) and Heat Flow Calorimetry (HFC), visual analysis of sample was performed with a Stereo Microscope and the physical characteristic, specifically heat of explosion, was determined by Calorimetry with special decomposition vessel. The propellant sample was stored for a long time under uncontrolled conditions. Visual analysis of propellant sample surface showed its significant changes with many visible indications of advanced aging. The propellant sample contains very low effective stabilizer content with very bad thermal properties measured by HFC where the heat flow limit of 114 μW/g was exceeded. The MVT results showed complete discoloration of indicator paper only 5 min after start. All the parent DPA in propellant sample is almost consumed and the remaining daughter stabilizer products do not continue to protect the propellant from possible self-ignition. The reduced value of heat of explosion was due to the aging reactions over the years. Therefore, the propellant is classified as very unstable.

POSTER PRESENTATIONS

Chemical Engineering

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Abstract

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Modeling and Simulation of a Multi-Pipe Heat Exchanger for Heating an Aqueous Solution of Potassium Chloride

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Abstract: The modeling and simulation of a multi-tube heat exchanger is presented in this paper. A process simulator for the determination of heat transferred from heating steam to an aqueous solution of potassium chloride in a heat exchanger was created. Other process parameters were also determined. The process simulator was developed in Microsoft Excel with VBA (Visual Basic for Applications). The influence of the change of heating steam flow on the amount of transferred heat and the temperature of the aqueous solution of potassium chloride at the outlet of the heat exchanger is presented. For the values of the initial process parameters, the amount of exchanged heat between the heating steam and the aqueous solution was 1042839.39 W, while the aqueous solution of potassium chloride was heated from 40 to 89.25 °C. The heating steam temperature decreased from 125 to 99.65 °C. The increase in heating steam flow affected the increase in heat transfer in the heat exchanger, which increased the outlet temperature of the aqueous solution.

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Abstract

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Analysis of the Hydraulic System of the Pipeline and the Centrifugal Pump for the Transport of Aqueous Sodium Chloride Solution

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Abstract: The aim of this paper was to present the analysis of the hydraulic system of the pipeline and the centrifugal pump for the transport of aqueous sodium chloride solution from the reservoir to the isothermal crystallizer. A mathematical model of a centrifugal pump was presented, on the basis of which algorithms and software for determining the process parameters of a hydraulic system were created. The maximum capacity of the pump and the required energy for the transport of an aqueous solution (pump head) were determined. Other process parameters of the hydraulic system were also determined. The effect of changing the composition of the aqueous solution on the pump head was presented. Microsoft Office Excel with VBA (Visual Basic for Applications) was used to solve the mathematical model, using the flow rate of the solution in the pipeline as an iterative variable. The maximum capacity of the centrifugal pump was 114.66 m^3/h, while the pump head was 28.29 m. The increase in the salt content of the solution led to a decrease in the pump head. The developed software can be used to simulate a hydraulic system for transporting any solution with the input of physicochemical characteristics of the appropriate solution.

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Abstract

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The Production of 1,5-Dinitroxy-3-nitrosine Pentane (DINA) in Two-step Reaction

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Abstract: 1,5 dinitroxy-3- nitrosine (hereinafter: DINA) belongs to the class of active nitroplasticizers, which recently have partially or completely replaced in the gunpowder mixtures with nitroglycerin. Previously, a method for laboratory synthesis of DINA was described, which involved the reaction of diethanolamine and nitric acid, and then dehydration of intermediate 1,5-dinitroxy-3-aza pentane nitrate. Following this procedure, several hundred kilograms of DINA has been manufactured in the world in two ways. The first method is a one-stage process where, at one stage of the reactuion, diethanolamine is nitrated and rewarded 1,5-dinitroxy-3-aza pentane is dehydrated into DINA. This is being achieved by simultaneous dosing of nitric acid with dietanolamine and acetic anhydride.

The second method is a two-step process where, in the first phase, the reaction between diethanolamine and nitric acid generates a so-called 1,5-dintroxy-3- aza pentane which is dehydrsted in a particular reaction stage into DINA with the help of acetic anhydride and the presence of suitable catalysts. As already mentioned, we decided to take the procedure for the production of DINA based on a two-stage reaction, that is, the reaction of diethanolamine and nitric acid as the first phase and dehydration as the second phase of the reaction.

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GC-MS Analysis of Phytochemical Constituents from *Prunus spinosa* L. Flower and Leaf Extracts

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Abstract: Flower and leaf extracts of blackthorn as a traditional medicinal plant indicated for the treatment of urinary tract disorders, inflammation, and adjunctive therapy of cardiovascular diseases were analyzed. Phytochemical composition of blackthorn´s flower and leaf (dry) ethanol extracts prepared using ultrasound-assisted maceration was evaluated. A total of 75 and 66 constituents of flower and leaf extracts respectively were identified using GC-MS, with 25 shared constituents. The major identified components were pyranone (7.23%) and 5-hydroximethylfurfural (6.15%) for flower extract and 1-amino-2,6-dimethylpiperidine (2.87%) and 2-hydroxy-2-cyclopenten-1-one (2.78%) for leaf extract. Some of the shared constituents were eucalyptol, 5-methylfurfural, 2,3-dihydrobenzofuran, ethyl glycolate and benzaldehyde. Two chiral components ethyl 2-hydroxypropionateand 5-methyl-2(3H)-furanonepresent in both extracts were confirmed by standards. The diversity of phytochemical compounds detected in blackthorn leaf and flower extracts can be related to the known biological activities attributed to this species.

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Essential Oil Chemical Profile of Two Different Lavender Species from Sarajevo Gardens

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Abstract: Lavender is a widely distributed aromatic and medicinal herb. The plant flowers and essential oils are principally used in the toiletry and perfumery industries, as well as in traditional medicines for the treatment of several gastrointestinal, nervous and rheumatic disorders as well as carminative, diuretic, anti-epileptic, anti-rheumatic, and pain relievers especially in nervous headache and migraine. *Lavandula angustifolia* Mill., also known as narrow-leaved lavender, was collected by the courtesy of American embassy in Sarajevo, while *Lavandula latifolia* Vill. (broad-leaved) was collected from the Faculty of Pharmacy Garden. In the present study, extraction of lavender essential oils was performed by hydro-distillation in modified Clevenger-type apparatus and phytochemical composition was analyzed by gas chromatography coupled with mass spectrometry (GC-MS). The major component was linalool, for *L. angustifolia* (34.46%), and *L. latifolia* (48.21%). Other predominant components were as follows: linalyl acetate, lavandulyl acetate, camphor, 1,8-cineole, borneol, α-terpineol, terpinene-4-ol. The significance of this research is that it classifies the tested lavender essential oils, used as a decorative plant in Sarajevo gardens, in the same rank in terms of quality with essential oils obtained from cultivated purpose-grown lavender.

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Determination of Melatonin in Berry Fruits by Fluorescence Spectroscopy

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Abstract: Melatonin is a useful biomarker for physiological sleep function in humans and there is a demand for its measurement to investigate sleep disorders. In this study, five berry fruits: goji berry (*Lycium barbarum* L.), blackthorn (*Prunus spinosa* L.), chokeberry (*Aronia melanocarpa* Michx.), blueberry (*Vaccinium myrtillus* L.) and raspberry (*Rubus idaeus* L.) were analyzed by fluorescence spectroscopy (E_x 250 nm, E_m 390 nm) to determine whether they contain melatonin. For all fruits we prepared methanol extracts from dried berries except raspberry, for which we prepared methanol extract from fresh fruits. Then, we done derivatization with NaOH and $K_3[Fe(CN)_6]$ at 80 °C 20 minutes. It was observed that the highest content of melatonin in methanol extract of the dried fruit (d.f.) was in goji berry (26.11 mg/100 $g_{d.f.}$), then followed blackthorn (0.73 mg/100 $g_{d.f.}$), chokeberry (0.31 mg/100 $g_{d.f.}$), and blueberry (0.23 mg/100 $g_{d.f.}$). Melatonin content in methanol extract of fresh fruit of raspberry was 0.59 mg/100 $g_{f.f.}$. It can be concluded that melatonin content in goji berry was much higher than in other analysed berry fruits.

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Determining of Antioxidant and Anti-Inflammatory Activities of *Calendula officinalis* L. Extracts

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Abstract: The extracts of *Calendula officinalis* L. are a rich source of secondary metabolites, which are responsible for various biological activities. This study aims to evaluate the antioxidant and anti-inflammatory activities of extracts leaves, flowers and stems of *Calendula officinalis* L. harvested in Lukavica 2020. To determine antioxidant activity of *Calendula officinalis* L, extracts of leaves, flowers, and stems were isolated by Soxhlet extraction using 96% ethanol as solvent. In determining the anti-inflammatory activity, extracts of mentioned parts of *Calendula officinalis* L. were isolated by cold and hot extraction on a magnetic stirrer and by cold extraction on a vertical blender using distilled water as solvent. The antioxidant activity was determined by the phosphomolybdenum method and the Briggs-Rauscher reaction method, while the anti-inflammatory activity was determined by protein denaturation test. In the phosphomolybdenum method, ascorbic acid and gallic acid were used as standard solutions. According to this method, the best antioxidant activity was shown the extract of leaves at concentrations of 0.5 mg/mL (105.00 $mg_{EAA}/g_{extract}$) and 5.0 mg/mL (88.46 $mg_{EGA}/g_{extract}$). In the protein denaturation test, the best anti-inflammatory activity (AIA) was shown by the extract of leaves (72.48% AIA), at a concentration of 20 mg/mL. In conclusion, extracts of *Calendula officinalis* L. showed significant antioxidant and anti-inflammatory activities.

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Chemical Characterization of Essential Oils of *Achillea nobilis* L. and *Achillea millefolium* L.

Čulum, D.[a*,b], Vidic, D.[a,b], Maksimović, M.[a,b], Čopra-Janićijević, A.[a,b], Muratović, E.[b], Šiljak-Yakovlev, S.[c]

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Abstract: In this study, chemical composition of the essential oil and genome size of two growing wild *Achillea* species, *Achillea nobilis* and *Achillea millefolium*from Breza, Bosnia and Herzegovina, were investigated for the first time. In essential oils, isolated by hydrodistillation,eighty-six compounds were identified by gas chromatography - mass spectrometry(GC-MS). Thirty-four compounds of *A. nobilis* represent 89.3% of the chemical composition of the oil, while fifty-two constituents were identified in *A. millefolium* comprising 88.6% of the total oil. The essential oil of *A. nobilis* was characterized by the dominant presence of oxygenated monoterpenes, with camphor (30.6%) and borneol (30.6%) as the main constituents. The oxygenated sesquiterpenes (60.8%) were the most abundant compounds in *A. millefolium* oil. The main constituents were chamazulene (19.3%), *β*-eudesmol (8.9%) and caryophyllene oxide (7.5%). The 2C DNA value of diploid population of *A. nobilis* was 5.00 pg, while for the hexaploid population of *A. millefolium* itwas 7.57 pg.

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Qualitative and Quantitative Analysis of Flavonoids of *Achillea lingulata* Waldst. & Kit.

Mehić, K., Jevđević, K., Čulum, D., Čopra-Janićijević, A., Vidic, D.*

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Abstract: Bosnia and Herzegovina is one of the richest European countries when it comes to the number of plant species, of which 10% are endemic. Determining the chemical composition of endemic species is of great importance for their possible use as phototherapeutics. Aim of this work was qualitative and quantitative determination of flavonoid content and antioxidant activity of various extract of endemic species *Achillea lingulata* Waldst. & Kit.Extracts were isolated by Soxhlet and ultrasound extraction with 70% ethanol as solvent and with hot water as infusion. The total flavonoid content was determined with $AlCl_3$, where the aqueous extract showed the highest content(51.43 ± 0.20 mgQE/g). The antioxidant activity was determined by two spectrophotometric methods based on different mechanisms, 2,2-diphenyl-1-picrylhydrazyl assay (DPPH) and the Ferric Reducing Antioxidant Power (FRAP). The best antioxidant was aqueous extract, with IC_{50} value for DPPH method of 0.090±0.002 mg/mL and for FRAP 553.54±7.60mgAAE/g of extract. This sample had twice the content of total flavonoids compared to other extracts. In Soxhlet extract, content of flavonoids in selected *Achillea* species was analyzed by HPLC-DAD method. Only luteolin (2.2168±0.0003 mg/g), was identified and quantified. In conclusion, *A. lingulata* is good source of flavonoids that have good antioxidant activity.

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PP-CNP-07

Total Phenolic Content and Antioxidant Activity of *Juniperus communis* L. subsp. *nana*

Marković, I., Pešković, L., Čulum, D., Vidic, D., Maksimović, M., Čopra-Janićijević, A.*

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Abstract: The aim of this study was to investigate the biological potential of the *Juniperus communis* L. subsp. *nana* growing wild on the Biokovo. Ethanolic Soxhlet extracts and aqueous residues after hydrodistillation of needles and berries were analyzed. The total content of phenolic compounds (TPC), flavonoids (TFC) and phenolic acids (TAC) were measured spectrophotometrically, with gallic acid, quercetin and caffeic acid as standards, respectively. The results were expressed as equivalents of the aforementioned standards. The highest content of TPC (4.07 mg GAE/g), and TAC (304. 96 mg CAE/g) were found in the Soxhlet extract of needles, but also the lowest content of TFC (4.45 mg QE/g). Antioxidant activity was also examined using three methods, DPPH, ABTS, FRAP. The aqueous residue after hydrodistillation of needles had the highest content of TFC (12.88 mg QE/g) and showed the highest antioxidant activity by all three methods. The results for DPPH and ABTS were expressed as IC_{50} (mg/mL) and were 0.153 and 0.039, while for the FRAP method, the activity was 0.063 mg AAE/g for the aqueous residue. The results obtained show that the extracts tested are a rich source of phenolic compounds and also the extracts show good antioxidant activity.

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PP-CNP-08

Total Anthocyanins in Fruits and Native Juices of Some Berries

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Abstract: The aim of this study was to evaluate the total anthocyanins content (TAC) in both, fruits and native juices of some berries. The TAC was analysed in blueberry, blackberry, aronia, raspberry, rosehip fruits, thorn fruits, and goji berry using by differential spectrophotometric method with pelargonidin chloride as a standard. The highest TAC expressed in mass of pelargonidin equivalents per mass of fresh fruits or fresh juice (mg PE/100 $g_{f.f.}$ or mg PE/100 $ml_{f.j.}$) was in blueberry (377.88±20.29 mg PE/100 $g_{f.f.}$, and 63.55±24.57 mg PE/100 $ml_{f.j.}$) and blackberry (225.73±10.84 mg PE/100 $g_{f.f.}$, and 49.40±12.82 mg PE/100 $ml_{f.j.}$), and the lowest TAC was in goji berry (2.90±0.20 mg PE/100 $g_{f.f.}$, and 0.76±0.42 mg PE/100 $ml_{f.j.}$). Except in blueberry and blackberry, significant amount of anthocyanins was found also in aronia (105.33±1.64 mg PE/100 $g_{f.f.}$, and 9.98±0.23 mg PE/100 $ml_{f.j.}$) and in thorn fruits (64.08±2.66 mg PE/100 $g_{f.f.}$, and 19.40±0.56 mg PE/100 $ml_{f.j.}$). In raspberry, the TAC was higher in fresh juice (17.71±0.56 mg PE/100 $ml_{f.j.}$) than in fresh fruit (13.34±2.48 mg PE/100 $g_{f.f.}$). In rosehip, the TAC was determined only in dried fruits (19.73±4.47 mg PE/100 g). It can be concluded that fresh blue and black berry fruits contain very high amount of anthocyanins (higher in fruits than in juices), and that fresh red berry fruits contain moderate and low amount of anthocyanins.

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PP-CNP-09

Total Phenolics, Total Proteins and Antioxidant Activity in Royal Jelly from Bosnia and Herzegovina

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Abstract: In this study, the total phenolics (TPs), total proteins (TPr), and antioxidant activity against hydroxyl ($AA_{OH}^{\bullet}$) and peroxyl ($AA_{ROO}^{\bullet}$) free radicals were determined in fresh royal jelly (RJ) from Bosnia and Herzegovina. The TPs and the TPr were determined in 30 samples of RJ, and $AA_{OH}^{\bullet}$ and $AA_{ROO}^{\bullet}$ were determined in 20 samples of RJ. For determination of the TPs, spectrophotometric method with Folin-Ciocalteu reagent and gallic acid (GA) as the standard was used, and for TPr the UV spectrophotometric method with bovine serum albumin (BSA) as the standard was used. For the determination of AA, the oxygen radical absorbance capacity (ORAC) assay with catechin as the standard and fluorescein as fluorescence target was used. The average TPc expressed in equivalent mass of GA per mass of RJ was 3.22±0.48 mg $GAE/g_{(RJ)}$. The average TPr expressed in mass of BSA per mass of RJ was 20.56±6.23 $g/100\ g_{(RJ)}$. The average of $AA_{OH}^{\bullet}$ expressed as mmol catechin equivalents (CE) per mass of RJ was 30.48±12.29 mM $CE/g_{(RJ)}$, and the average of $AA_{ROO}^{\bullet}$ was 3.74±1.85 mM $CE/g_{(RJ)}$. Based on the obtained results, it can be concluded that RJ from Bosnia and Herzegovina is of good quality.

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PP-CNP-10

Content of Total Phenols, Total Flavonoids and Antioxidant Activity of Cosmetic Skin Care Products

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Abstract: Cosmetic products available on the local market contain a large number of different components in their composition. The presence of biologically active compounds has been declared on some of these products. Total phenolic and flavanoid contents, as well as antioxidant activity of six handmade preparations and commercial cosmetic skin creams were determined. Extracts of cream samples were prepared using an ethanol-water mixture in a ratio of 70:30 (v/v). Spectrometrically determined absorptions were used to calculate the contents of total phenols and flavonoids of each extract sample. The results were expressed as gallic acid equivalents (GAE) per gram of sample, according to the Folin - Ciocalte procedure, and as routine equivalents (RE) per gram of sample using the Dowds method, The antioxidant activity of the extracts was determined using DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS (2,2′-azinobis-(3-ethylbenzothiaziline-6- sulfonate) methods. Total phenols and total flavonoids content ranged from 0.03– 3.63 GAE (μg/g) and 0.04–17.00 RE (μg/g), respectively. The best antioxidant activity (0.466 ± 0.121 GAE (μg/mL) using DPPH method was obtained for one of the tested handmade cream containing *Calendula officinalis* extract. This result indicates a direct correlation between the antioxidant activity and the highest total phenolic content (3.63 ± 0.34 GAE μg /g) determined in the same sample.

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PP-CNP-11

Chemical Composition and Antioxidant Activity of *Lilium bosniacum*

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Abstract: The aim of this study was to determine the content of phenolic compounds and antioxidant activityas well asHPLC-DAD analysis of selected flavonoids and phenolic acids in extracts of endemic species *Lilium bosniacum* that grows wild in Bosnia and Herzegovina. Isolation of the extracts was done by hydrodistillation of flowers where the sample for analysis was an aqueous residue. Bulb and flowers extracts were obtained by Soxhlet extraction using ethanol as a solvent.The content of total phenolic compounds (TPC) was determined by the Folin-Ciocalteu assay and the lowest TPC was determined in ethanolic flower extract of 0.012±0.001 mgGAE/g, while the highest TPC was found in the ethanolic bulb extract of 1.040±0.072 mgGAE/g. The content of total flavonoid (TFC) varied from 2.19±0.13 mg EQ/g for ethanolic bulb extract to 5.69±0.19 mgEQ/g for aqueous residue. In contrast, the extract of bulbs had the highest content of total phenolic acids (TPA) of 51.873±1.820 mgCAE/g, while extract of flowers had the lowest TPA of 0.426±0.007 mgCAE/g. The antioxidant activity of the extracts was evaluated by 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical-scavenging ability and ferric reducing antioxidant power (FRAP) assays. The aqueous residue after hydrodistillation showed the highest antioxidant activity by DPPH and FRAP assays with IC_{50} of 1.77±0.30 mg/mL and 0.91±0.04 mgAAE/g extract, respectively. The analysis of selected phenolic acids and flavonoids was performed by HPLC-DAD method, but none of the available standards was detected in analysed samples.

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PP-CNP-12

Identification of Chemical Constituents from Two *Fraxinus* Species by GC-MS and HPLC-DAD Methods

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Abstract: *Fraxinus,* commonly known as ash tree, belongs to the Oleaceae family, and is considered a plant with a variety of biological activities. In this study, GC-MS and HPLC-DAD analyzes were performed to profile the chemical composition of two *Fraxinus* species, *F. ornus* and *F. angustifolia* collected in the urban area of Sarajevo. Essential oils were obtained by hydrodistillation of leaves. This process also originates high amounts of residual water which can be a rich source of non-volatile compounds. Chemical analysis of the essential oils of *F. ornus* and *F. angustifolia*, performed by GC-MS, showed that they contain dihydroactinidiolide (13.0% and 31.8%), 2,4-di-*tert*-butylphenol (13.6% and 2.7%), 6,10,14-trimethylpentadecan-2-one (2.7 and 2.1%), respectively. In both essential oil samples, GC-MS also revealed a significant percentage of the two phthalic acid esters, isobutyl phthalate and dibutyl phthalate, which were contaminants. HPLC-DAD analysis of aqueous residues remaining after hydrodistillation confirmed the presence of rutin and quinic acid in both samples, while 6,7-dihydroxycoumarin was identified in *F. ornus* and chlorogenic acid in *F. angustifolia*.

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PP-CNP-13

Chemical Composition and Antioxidant Activity of *Achillea millefolium*

Suljić, M., Čulum, D.*, Vidic, D., Čopra- Janićijević, A.

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Abstract: The aim of this work was to determine the content of total phenolic compounds, flavonoids and phenolic acids as well as the antioxidant activity of *Achillea millefolium* extract collected from the area of Jahorina Mountain, Bosnia. This plant is widely used in both folk and official medicine due to its proven various biological activities. Flower and leaf extract of *A. millefolium* was isolated by Soxhlet extraction, with 70% ethanol as solvent. The content of total phenolic compounds (TPC) was 150.22 mg GAE/g of extract, total phenolic acids (TPA), 86.79 mg CAE/g extract and total flavonoids (TFC), 47.31 mg QE/g of extract. Antioxidant activity was determined by FRAP (138.34 mg AAE/g of extract) and ABTS (IC_{50}, 0.179 mg/mL) methods. From the obtained results it can be concluded that *A. millefolium* has a high content of analyzed secondary metabolites and good antioxidant activity.

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PP-CNP-14

In vitro Screening of Antimicrobial Activity of *Clinopodium nepeta* (L.) Kuntze Essential Oils

Boškailo, E.[a,d], Džudžević-Čančar, H.[b, d*], Jerković-Mujkić, A.[c], Dedić, A.[b], Alispahić, A.[b],Vidic D.[d], Uzunović, A.[e],Boškailo, A.[c]

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Abstract: Since ancient times, plants, as well as their essential oils or extracts, have been used for various purposes in ethnomedicine. The study aimed to determine the antimicrobial activity of four hydrodistilled essential oils (EO) of *Clinopodium nepeta* (L.) Kuntze (from different localities in sub-Mediterranean area of Bosnia and Herzegovina) against a diverse spectrum of strains, consisting of two Gram-positive bacteria: *Bacillus subtilis, Enterococcus faecalis*; three Gram-negative bacteria: *ESBL Escherichia coli, Salmonella enteritidis, Pseudomonas aeruginosa* and fungi: *Candida albicans*. Theantimicrobial activity was performed using a disc-diffusion assay.Tested bacterial strains showed sensitivity to all four EOs. The highest measured Zone of growth inhibition of Gram-positive bacteria was 27.66±0.94 mm, and Gram-negative bacteria 23.66±0.47mm.AllEOs were effective against fungal pathogen *Candida albicans* (>45mm). The antibiotics Ampicillin, Colistinand antifungal Nystatin, were less effective against tested strains than EOs samples. Major compounds detected by GC-MS in *C. nepeta* EOs as pulegone, piperitone, *trans*-piperitenone oxide in synergy with minor ones, are considered as main contributors to showed antimicrobial activity. These results recommend *C. nepeta* EOs as potentially useful for therapeutic and pharmacological purposes.

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Abstract

PP-CNP-15

Evaluation of Mineral Composition in Wild-Growing *Clinopodium nepeta* (L.) Kuntze using Atomic Absorption Spectrometry

Boškailo, E.[a,d], Džudžević-Čančar, H.[b,d*], Dedić, A.[b,]Alispahić, A.[b], Boškailo, A.[c], Žero, S.[d]

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Abstract: Each plant specie accumulates minerals in its own way and their concentrations could be affected by influence of many environmental factors.Compositionof mineral elements (micro- Cu, Zn, Cr, Mn, Co, macro-Ca, Mg, K, Na and toxic Pb, Cd) have been identified in four dry samples of *Clinopodium nepeta* (L.) Kuntze collected from their natural habitats in southern Bosnia and Herzegovina (Pirići, Blagaj, Počitelj, Lokve) using Flame atomic absorption spectrometry.The highest content of Ca and Mg was recorded in sample from Pirići (9336.49±10.75 and 632.28±0.73 μgg^{-1}). The concentration range (μg g^{-1}) of Na was between 14.44±0.02 and 35.68±0.08, and for the other elements as follows: Cr (0.18±0.001-0.88±0.001);Cu (6.69±0.01-9.75±0.02);Mn (17.66±0.02-28.08±0.06);Fe (55.34±0.06-93.64±0.2);Ni(0.55±0.001-2.06±0.001); Zn (3.65±0.01-9.69±0.02); Pb (1.43±0.01-8.5±0.02); Cd (0.11±0.00-0.39±0.001). Thecontent of Pb and Cdin the tested samples was within the maximum allowable limits recommended by the WHO. Considering these challenging times during Covid-19, it is important to highlight the potential therapeutic role of minerals, such as Zn, Na, K, Ca and their beneficial effect in various infectious diseases, especially if they can be consumed as natural products. Because of this, the presented research gained in importance.

POSTER PRESENTATIONS

Education in Chemistry

(EDC)

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Abstract

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Study of Selected Plant Material as Acid-base Indicators Applicable in Modern Classroom

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Abstract: Even today dominant teaching methods in science classroom are traditional ones, though their final result is simple accumulation of information and facts, without in-depth comprehension. Traditional method of teaching pH value and indicators only occasionally involves experiments, using synthetic indicators, which can be expensive and unavailable to schools. However, plant pigments are pH indicators as well, hence a series of experiments using plant materials, which pupils use in everyday life, was created. Studied plant material included various types of berries (strawberries, raspberries, blackberries, mulberries, etc.), not only in the form of fresh fruit but also as various fruit products (dried fruit, tea, juice, jams, preservatives, vine). Our aim was to obtain simplicity of indicator preparation, low cost, easy availability whole year, easy maintenance and higher indicator durability. To this purpose we studied indicator preparation in several concentrations (to find the optimal one considering simplicity of preparation, cost, duration) and used fruit products with maximal fruit concentration and without artificial components. Our results indicate a great potential of application of fruit and fruit products as acid-base indicators in the modern classroom in order to broaden pupils interest in this subject, and to enable successful relating of science information with everyday life.

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Abstract

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A Preliminary Study on Students' Perceptions on the Relevance of Learning Science and Technology Based on ROSES Questionnaire Data

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Abstract: Students' interest in science and their motivation to learn science are considered important for their future career choices. In chemical education research in the last few years, special emphasis has been placed on increasing the importance of teaching and learning chemistry as well as students' perceptions of it. The study, investigating students' perceptions of the relevance of science education at the end of primary school has been conducted in several schools in Sarajevo Canton. The questionnaire, developed as part of the ROSES (Relevance of Science Education Second) project that collects data on students' interest, orientation and engagement in science and technology has been translated and administered to students via online questionnaire. Preliminary results show that (1) students are interested in learning science and exploring science concepts beyond classroom, and (2) female students have more sensibility towards environmental issues.

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Abstract

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Possibilities of STEAM Integration in Canton Sarajevo Primary School Chemistry Teaching

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Abstract: The demands of the modern world, in the context of ability requirements, differ significantly from those only a decade earlier. Moreover, they are continuously evolving at an intensity not previously recorded in the history. These requirements can only be achieved through a paradigm shift in education, from a system based on the acquisition of knowledge to a system based on the acquisition of skills and abilities. One of the most significant steps in this process is the partial removal of boundaries between school subjects and creating “a unified whole” with aim of developing students’ abilities. Chemistry teaching in primary schools (8th and 9th grade) represents an area in which this approach can be applied. In this study, the possibilities of the STEAM (Science, Technology, Engineering, Arts and Mathematics) approach were analyzed in Canton Sarajevo Curriculum for primary school chemistry. Analysis has showed that STEAM can be integrated in various themes in order to achieve the intended learning outcomes. The examples are development of students’ skills through problem-based learning regarding food safety, the purity of air, soil, and water, as well as in digital technologies and media information literacy in order to present the experimental results.

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Abstract

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Addressing Linguistic and Cultural Heterogeneity in Chemistry Classrooms: Findings from the In-Service Teacher Training Program

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Abstract: One of the challenges in teaching science in Bosnia and Herzegovina is its plurality of languages and cultural diversity. There was a lack of quality preparation for these modern challenges within the initial teacher education so far; opportunities for teaching cultural and linguistic diversity were not recognized. Therefore, it is a challenge to encourage experienced chemistry teachers to develop competencies for an intercultural teaching environment within the Educating Science Teachers for All (ESTA) project. Participants of the in-service professional development program were chemistry teachers from two cantons in FBiH. The program aimed to develop and improve professional competencies through workshops and group work, containing discussion about selected topics and laboratory exercises using modern laboratory equipment and ICT. Opportunities to teach in linguistically diverse classrooms, as well as classrooms with other forms of students' diversity were offered. The questionnaire for participants was administered, and preliminary results show that teachers are aware of the need to be sensitized for their students' differences; they expressed positive impressions and willingness for adapting teaching materials according to the needs and possibilities of their students.

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Abstract

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Analysis of Approved Chemistry Textbooks in Canton Sarajevo in the Light of Education Reform Based on Learning Outcomes

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Abstract: Textbooks play an important role in students' learning. They are intended for students' use, while teachers use them to complement their teaching. In Canton Sarajevo, there is a movement in education reform towards acquiring students' achievements according to predetermined learning outcomes. For successful transition from ex-cathedra teaching to accomplishing defined learning outcomes it is important for the selected textbook to support the student in the accomplishment of the selected learning outcomes. This study analyses the suitability and content of the two textbooks that have been approved for use in the 8th grade of the primary school, the first grade in which chemistry is taught. The analysis has shown that there are certain discrepancies between mid-term learning outcomes specified in the curriculum and textbooks content; textbooks A and B do not fully support acquiring the intended learning outcomes for 8th grade (49% and 10% of the content, respectively).Certain shortcomings have been identified in particular with regard to students' laboratory work and the use of digital technologies in the context of chemistry.

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Abstract

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Identifying and Strengthening Chemistry Teachers' Awareness of Heterogeneity and Diversity in Chemistry Classes

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Abstract: To learn how we can more successfully deal with issues of heterogeneity and diversity in chemistry classrooms, we signed up for the Educating science teachers for all (ESTA) project. As part of ESTA activities, an investigation was conducted during a professional development programme for faculty students (some of whom are prospective chemistry teachers) and in-service chemistry teachers. It focused on exploring teachers' awareness of heterogeneity in the chemistry classrooms, diversity and its dimensions. Data were collected using a paper-and-pencil pre-intervention and post-intervention questionnaire. The intervention was organised in the form of a workshop based on active learning. The data set was summarised using descriptive statistics. The responses to the open-ended questions were analysed qualitatively. It was found that both faculty studentsand in-service teachers believedthat the classes they wereor are involved with, are predominantly heterogeneous. After the intervention, this opinion was even more pronounced, but the difference in results was not statistically significant. Teachers strongly believe that they are giving adequate attention to diversity issues in classrooms. Faculty students disagree. Almost all participants express the need and willingness to receive continuing education about diversity and heterogeneity.

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Abstract

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Teaching Environmental Issues in Primary School Chemistry Using Inquiry-Based Learning

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Abstract: Inquiry-based learning represents (IBL) an approach to education, opposed to classical teaching in which students are mere "knowledge recipients". IBL approach enables students to express their views on a variety of problems sets or themes by exploring themes previously unfamiliar to them. As chemistry is in its essence an experimental natural science, IBL application represents a logical step in enhancing students' experience, development of skills in chemistry, as well as the acquisition of knowledge. Several areas of interest in the IBL approach have been identified based on the analysis of the Canton Sarajevo Curriculum for Primary school chemistry. For this study, four areas in each of the two grades in which chemistry is taught have been selected. In the 8th grade, these include the relation of weather with crop yields, the influence of pH value on soil quality, correlation of air pollution with several pulmonary diseases, and chemistry in households. In the 9th grade, selected areas include exploration of possibilities of green industries, identification of most prevalent organic pollutants in rivers, the influence of acid rain on plant diversity, eco-friendly recycling. Depending on the average attitude of students, it is possible to implement either guided of open type of IBL.

POSTER PRESENTATIONS

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Redox - Sensitive Elements (Ti, As, V and Fe) in Clay Pit Samples with and without Al – Normalization

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Abstract: Adsorption of metals onto natural materials primarily happens on the surface of the iron or manganese compounds, organic matter, and clay minerals. Natural Clay minerals,because of their highion sorption/exchange capacity, low permeability, swelling ability, chemical and mechanical stability, and large specific surface areaare good adsorbents of metals. Among metals we often investigate heavy metals, but redox sensitive metals are getting more and more attention. In 44 clay pit samples pH, EC, and redox potential were measured. Redox-sensitive amounts of metals and aluminium were measured with ICP-OES instrument. Redox - sensitive metal geochemical normalization with Al was utilized to minimize the natural metal variability in the sediments, in context of dilution and grain size effects. For statistical evaluation, maximum, minimum, average, median,correlation and correlation applying Al normalization were calculated. The elements concentrations lie in the sequence: Fe>Ti>V>As. There is a significant change in correlations with and without Al-normalization.The highest difference in correlations was found in case of titanium and vanadium (r value ranging from -0.553 to 0.835). Al – normalization reveals that titanium and vanadium show similar behaviour.

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Abstract

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Application of Simulated Sunlight Radiation and Hydrogen Peroxide to Remove Antiparasitics

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Abstract: With the development of medicine, technology and industry, the number of new pollutants that can be found in water is growing. An example of new pollutants found in the environment in recent years as part of numerous studies is antiparasitics. Antiparasitics are used to treat various parasitic infections of animals and humans and therefore often enter the environment through urine and feces where they can be toxic to organisms for which they are not intended or cause resistance.Simulated sunlight radiation and H_2O_2 were used to remove antiparasitics (albendazole, febantel, mebendazole) from water and were examined the effects of parameters such as initial pH of the solution and peroxide concentration.These simulated conditions were also tested in the presence of microplastics to monitor its possible impact on degradation.The results showed a different percentage of degradation between the three listed antiparasitics. Increasing the concentration of hydrogen peroxide leads to greater efficiency in the breakdown of antiparasitics. The amount of degradation products varies depending on the tested antiparasitic, pH value and peroxide concentration.The presence of microplastics in the simulated wastewater did not affect the change in the degradation of antiparasitics regardless of the test performed.

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Influence of Alcohol on the Degradation of Antiparasitics in Wastewater

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Abstract: Various disinfectants are widely used in many areas of human life and activity, but a particularly large increase in use has been recorded since the outbreak of the coronavirus pandemic, which is increasing their concentration in the environment day by day. Xenobiotics such as pharmaceuticals and microplastics should not be neglected since they have already shown considerable impact. Given their increased use, it is necessary to monitor their path in the environment, the impact on the living world and to identify in time the potential consequences that may cause their actions. Simulating environmental conditions for a total of 5 hours, the effect of two disinfectants and ultrapure water on the photolytic degradation of antiparasitics was examined. Additional photolytic tests were performed for samples in the presence of microplastics.

The results of the analysis showed that the antiparasitics albendazole and mebendazole were successfully degraded in all three working solutions, but greater degradation was observed in disinfectants due to the presence of alcohol and better solubility of the components themselves. Possible degradation or transformation products were detected for each of the pharmaceuticals, and the presence of microplastics did not show significant differences compared to the samples in which it was not contained.

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Abstract

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Biosorption Removal Study of Methylene Blue Dye from Aqueous Solutionon a *Citrus limon* Peel

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Abstract: Methylene blue (MB) represents an important organic pollutant widely present in wastewaters. The chemical toxicity of this aromatic cationic dye on humans is manifested through respiratory and gastrointestinal difficulties. The present study reports investigation of the MB removal from water solution by lemon peel biosorbent, regarding its related removal mechanism. *Citrus limon* peel as chemically modified form used for removal of MB in a uni-variant batch method. The reaction mechanism for MB removal was identified conducting basic experimental and theoretical adsorption studies. Several instrumental characterization techniques of used biosorbent confirmed the successfulness of both modification and MB removal. The maximum removal efficiency at conditions found as optimum was 98.12 %.

It was revealed that MB-lemon peel adsorption process can be well described by Langmuir equation(R^2 = 0.912; q_{max} = 3.33 g g^{-1}) as well as by pseudo-second order kinetic and Weber-Morris diffusion models (R^2 =0.999 and 0.852, respectively). Based on the modeling results, a cooperative binding mechanism (chemisorption/intraparticle diffusion/ionexchange) has been suggested.

The proposed wastewater treatment process could be an effective tool in methylene blue removal and pollution control in general.

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Novel Approach for Effective Removal of Methylene Blue Dye from Water Using Grapefruit Peel as a Potential Biosorbent

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Abstract: With the rapid growth of industrialization in the past few decades, water pollution by organic dyes has become a serious hazard to the environment. This work reports the potential use of grapefruit peel, as an effective low-cost biosorbent for the removal of methylene blue (MB). The prepared biosorbent was characterized by SEM, EDS, FTIR, cation exchange capacity (CEC), Boehm titration, and point of zero charge. The kinetics of the MP sorption process was determined by theoretical kinetic models by application of Langmuir, Freundlich, and Temkin models of isotherms. Batch adsorption studies were performed by changing adsorbate/adsorbent contact time, pH, sorbent mass, and initial dye concentration. To improve the physicochemical and sorption properties, the biosorbent was modified by suspending the native biomaterial in 1 mol L^{-1} NaOH (aq). The optimal process parameters for the modified grapefruit peel were: pH 3–7, sorbent mass of 50 mg, contact time 20 min, and initial MP concentration of 600 ppm. The removal efficiency was found to be 96.6–99.0% under the optimized adsorption conditions. It can be concluded that modified grapefruit peel has been proved to be novel, efficient, and cost-effective biosorbent with great potential for the removal of MB from aqueous solution.

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Abstract

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Scoping Review of Chemical Composition of Conventional cigarettes, Electronic Cigarettes and Heat-Not-Burn Technology Aerosols

Omeragić, E.[a], Dedić M.[a], Kladar N.[b], Bečić E.[a], Begić E.[c], Božin B.[b], Iglica A.[d], Imamović B.[a], Janković S.[e], Krstonošić V.[b], Srđenović B.[b], Bajrić B.[a], Čutura E.[a],Mulahalilović M.[a],Trako F*[a].

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Abstract: Heat-not-burn tobacco products (HNB) are electronic devices that heat processed tobacco instead of combusting and have been marketed by the tobacco industry as a less harmful alternative to conventional cigarettes.

Here we conducted a literature review of the differences in chemical composition among aerosols of conventional cigarettes, electronic cigarettes (e-cigs) and HNB with the accent on health risks from exposure to the same.

Since there is no combustion process, it has been believed that exposure to harmful substances from HNB should be lower. However, the appearance of glycolonitrile, at temperatures above 90°C, poses a danger to the consumer. The concentration of nicotine proved to be similar in HNB compared to traditional cigarettes, with a much lower concentration of carbon monoxide and 50% less tar. Studies found that HNB produces significantly less formaldehyde, acetaldehyde, acrolein, propionaldehyde and crotonaldehyde compared to traditional cigarettes, but more than e-cigs and they point to the benefit of HNB over traditional cigarettes in terms of reducing the concentration of nitrosamines.

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Application of Hydrophobic Solvents Based on L-Menthol, as Greener Alternatives to Classical Solvents for Pb(II) Ions Extraction

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Abstract: Deep eutectic solvents (DESs) as a new-generation of solvents are increasing attention as environmentally friendly solvents in various analytical techniques. In this work, the potential application of these solvents for the extraction of Pb(II) ions was investigated. For that purpose, hydrophobic DESs (HDESs), based on L-menthol as H-acceptor and decanoic acid as H-donor, were prepared at molar ratios of acceptor to donor of 1:1 and 1:2. In the optimized extraction procedure, the Pb(II) ions were extracted into the organic phase with the efficiency of 94.3% and 97.3% for 1:1Men:DecA and 1:2 Men:DecA, respectively. The results also showed that in contrast to the classical liquid-liquid extraction methods,no counter ions were required in source solutions for analyte transfer into the hydrophobic phase. Furthermore, no ligands were required for the transfer of analyte ions into the HDES phase: the results show that the extraction efficiency of 1:1 HDES decreased to 88.65% in the presence of 18C6, and to 96.5% for 1:2 HDES. Comparable results for HDES (1:1 Men:DecA) extraction efficiencies in the proposed method with the efficiencies of 1,2-dichloroethane and chloroform in classical methods (96.7% and 92%, respectively), without counter-ions and without requirements for ligands as carriers, make this HDES-based extraction method simpler, less expensive, and most importantly, more environmentally friendly.

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Abstract

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Adsorption of Eriochrome Black T (EBT) and Methylene Blue (MB) Dyes using Pulverized Pomegranate Peel as Biosorbent – Characterization and Optimization

Sulejmanović, J.*, Kojčin, M., Kubatlija, J., Karadža, A., Žero, S., Zahirović, A.

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Abstract: Water pollution with dyes has become one of the most serious environmental problems in the world. Therefore, the aim of this study is to provide results for removal of two of the most harmful dyes EBT and MB from aqueous solution using pulverized pomegranate peel (PGP). Characterization of pulverized pomegranate peel before and after adsorption of dyes was performed by infrared spectroscopy with Fourier transformation infrared spectra (FTIR), scanning electron microscopy (SEM) and electron dispersive spectroscopy (EDS). The key process parameters that have significant impact on the adsorption efficiency were examined and optimal values for biosorption of EBT/MB were: pH value 3/3-11, sorbent mass 100 mg in both cases, initial dye concentration 150 mg L^{-1}/100 mg L^{-1} and contact time 90 min/20 min. The novelty and research gap of this study is that it reveals the potential of PGP toward EBT removal as well as it gives the comparison of sorption ability of PGP for the removal of different type of dyes. The obtained adsorption capacity was 46.10 mg g^{-1} and 47.50 mg g^{-1} for removal of EBT and MB, respectively, indicating that PGP could be used as an efficient biosorbent for their successful adsorption from aqueous solutions including wastewaters.

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Abstract

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Analysis of Leachate Waters of Landfill Smiljevići, Sarajevo, Bosnia and Herzegovina

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Abstract: Leachate water of landfill is very important environmental problem that increases with growing of population, standard of living and industrialization. In this research, the parameters of quality and contamination of leachate water from the landfillSmiljevići (Sarajevo, Bosnia and Herzegovina) were analyzed: temperature, pH, electroconductivity, dissolved oxygen, total ammonia, total nitrates, heavy metals (lead, cobalt, cadmium and zinc). The analyzes included samples from four collectors: shallow drainage S1 (water from the layers of fresh waste); deep drainage S2 (water from layers of old waste before sanitary landfill measures); calotte drainage S3 (external water passing the landfill); collector S4 (all three waters in one collector). In accordance with surface water quality legislation (Official Gazette FBiH 43/07), only the pH is within the permissible limits and the ammonia content of sample S3. According to the regulation (Official Gazette FBiH 26/20) for waste water discharged into environment, only nitrate content exceeds the permitted values for all samples, other measured parameters are within the permissible limits. The significant differences of same measurement parameter within the different samples were found only for: ammonia in S3 and for cadmium in S3, compared to other three waterscollected at landfill Smiljevići.

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Abstract

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Ecotoxicological analysis of Spreča River water by using *Daphnia magna* (Straus, 1820)

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Abstract: *Daphnia magna* Straus is an excellent model organism used to monitor the pollution of aquatic ecosystems. The aim of the research was to analyze the surface water quality of the Spreča River by performing acute toxicity tests of *Daphnia magna* Straus in correlation with the analysis of chemical parameters (heavy metals, organic pollution parameters and basic physico-chemical parameters in the field). The analysis and the whole analysis process was done according to the standards of BAS EN ISO 6341:2014, while the sampling of surface water for ecotoxicological analysis was performed according to BAS EN ISO standards. Research included fieldwork and laboratory analysis in the period from March 2018 to October 2020.

The research included the localities with the lowest values of the toxicity test: Spreča downstream of Sisecam Soda Lukavac d.o.o, 48 h-EC_{50}=12,08 % and Lukavčić stream 48 h-EC_{50}=11,90 %, and the toxicity test showed that the water is toxic. At the Spreča site upstream of Sisecam Soda Lukavac d.o.o, before the discharge of industry into the river, the values of the toxicity test are 48 h-EC_{50}=43,66 %.

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Abstract

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Relationship between Coliform Bacteria and Physico-Chemical Parameters of Bistrica River Water Quality

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Water Quality
Contamination

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Abstract: The research was done in the collection channel of the river Bistrica. The analysis included 28 parameters, of which 25 were physico-chemical and three microbiological indicators of water quality. Samples were collected in the period from January to July 2020 in one-month intervals. The aim of this study was to compare the number of indicator groups of bacteria with the values of physico-chemical characteristics of water quality, in order to analyze possible correlations and effects of the obtained relationships. Correlation analysis showed that there is a statistically significant correlation between transparencies (secchi depth) and examined microbiological parameters. The lowest water transparency was in April. The highest number of total and fecal coliform bacteria, as well as fecal streptococci, was determined in the water samples from April. Based on research results, we can assume that the increased presence of the tested bacteria affects the transparency of the water at the tested site. Bacterial contamination is a possible cause of turbidity of water in the river Bistrica and significantly reduces water quality in the research area.

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Abstract

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Estimation of Cd, Cr, Cu, and Ni Atmospheric Deposition by Moss Biomonitoring in the Region of Prokoško Lake

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Hypnum Cupressiforme Hedw.

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Abstract: Prokoško lake is located on the mountain Vranica (1636 meters above sea level) in Bosnia and Herzegovina (B&H) and it is a protected area declared as a monument of nature in 2005. Mosses are often used as an acceptable tool for tracking spatial and temporal trends in atmospheric deposition of trace metals. In this study, heavy metals (Cd, Cr, Cu, and Ni) in moss (*Hypnum cupressiforme* Hedw.) were used for estimation of atmospheric deposition in the region of Prokoško lake. The metal analysis was performed by flame atomic absorption spectrometry (FAAS). The content of determined metals in moss was: Cd (0.073 mg/g), Cr (24.01 mg/g), Cu (13.25 mg/g) and Ni (12.14 mg/g). The concentration of Cr indicates higher air pollution and the concentration of Ni indicates high air pollution, while the concentration of Cu indicates slightly increased air pollution, and the concentration of Cd indicates low air pollution in the region of Prokoško lake compared to someEuropean cities. In the location of Prokoško lake there are no significant sources of air pollution in view of that, the higher content of Cr and Ni could be due to pollution from remote areas carried by wind currents.

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Abstract

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Impact of Water Microbiological and Physicochemical Parameters on Liver Histopatology of *Barbus Meridionalis* Heckel, 1847 from Miljacka River

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Abstract: The present study evaluated the influence of microbiological and physicochemical water quality parameters on tissue lesions in the liver of *Barbus meridionalis* Heckel, 1847 from the Miljacka River. Water sampling was carried out according to standard methods for the examination of water and wastewater at two sample points (S1 and S2). Forty-five fish specimens have been collected by electrofishing at S1 and S2. Liver was extirpated from individuals and processed by routine histological techniques. Results of microbiology water analysis showed a lower degree of contamination at S1, while the second sample site was contaminated with the presence of coliform bacteria, fecal coliforms and fecal enterococci. The results of dissolved oxygen, temperature, conductivity and pH values indicate exacerbated ecosystem health impacts on S2. Histological analysis showed milder histopathological alterations such as leukocyte infiltration and dilation of sinusoid in liver tissue from individuals collected at S1. The occurrence of severe changes was observed in specimens collected at S2. These severe changes were in the form of degeneration hepatocytes and formation granuloma. Results indicated that observed histopathological alterations were associated with contamination of the Miljacka River. Future research would benefit from investigation of water, sediments and fish tissue contamination with heavy metals.

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Abstract

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Effects of Water Pollution on Histological Changes in Gills of *Barbus meridionalis* Heckel, 1847

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Abstract: Aquatic ecosystems are often contaminated with pollutants from various sources such as domestic and industrial sewage, agricultural processes and heavy metals. Fish gills are extremely sensitive to chemical and physical changes and pollution. Focus of this study was to evaluate the impact of contaminated water on histopathological changes in *Barbus meridionalis* gills.The water samples were collected from Miljacka River at two sites (S1 – Dariva, S2 – Dolac Malta) and analyzed for microbiological and physico-chemical parameters. At the same time *Barbus meridionalis* specimens were collected. In the laboratory, the second right gill arch was removed and prepared for histological description. Results of microbiology and physico-chemical water analysis showed a lower degree of contamination at first sample site while water from second sample site was contaminated with the presence of coliform bacteria, fecal coliforms and fecal enterococci. Histological alterations of *Barbus meridionalis* gills collected on the S1 showed a normal or mild pattern of gill filaments.The gill tissuefrom fishes collected at S2 showed mild and severe histological alterations.Since this study revealed the significant correlation between water contamination and gills alternation, determination of heavy metals in water and fish gills is one of the main future studies.

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Abstract

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Determination of Heavy Metals in Wastewater from Metal Industry

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Abstract: Wastewater from metal industries is one of the important sources of heavy metals leading to the pollution of the water environment.Levels of Cr (III), Cr (VI), Mn, Fe, Ni, and Pb were determined in effluents coming from metal industries in Bosnia and Herzegovina just before discharging into receiver. Speciation analysis of Cr (III) and Cr (VI) was performed on silica gel modified with Nb_2O_5. For Cr (III), Mn, Fe, Ni, and Pb analysis, flame atomic absorption spectrometry (FAAS) was used, and UV-Visible spectrometry with 1,5-diphenylcarbazide was used for the determination of Cr (VI). The content of determined metals in wastewater from the metal industry was in the range of: Cr (III) (0.03–0.11) mg/L; Cr (VI) (0.16–0.20) mg/L; Mn (21.52–40.70) mg/L; Fe (449–1810) mg/L and Pb was below the limit of detection (LOD) for FAAS. The content of all determined metals in the wastewater samples, except Cr (III) and Pb, was higher than maximum allowable values according to an ordinance on limit values of hazardous and harmful substances for technological waste before their discharge into the public sewerage system or another receiverin Federation of Bosnia and Herzegovina.

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Abstract

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Effect of Simulated Acid Rain on Chlorophylls and Carotenoids Content in *Pisum sativum* L.

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Abstract: Industrial development and the anthropogenic impact on the environment over time has led to various changes in nature. One of the changes is the occurrence of acid rains which is directly correlated with industrial development. Through different industrial processes, sulfur and nitrogen oxides are released into the atmosphere where they react with water forming nitric, sulfuric, and sulfurous acid, which result in the formation of acid rains. The aim of this study was to determine the effect of simulated acid rains on the foliar content of chlorophyll and carotenoids in peas (*Pisum sativum* L.). Peas plants were subjected to a ten-day treatment with simulated acid rain adjusted to correspond to the pH levels of officially recorded acid rains in the Sarajevo area in months when peas are usually cultivated. The pH levels and the amount of applied simulated rain were determined according to amounts recorded by the Hydrometeorological Institute of the Federation, Bosnia and Herzegovina. Pigment extraction was performed from leaves after exposure to the simulated acid rain. Foliar pigments extraction of short-term treated peas is followed by their spectrophotometric quantification. Results showed that short exposure to acid rain can induce increase of chlorophyll and carotenoid synthesis. Repetitive exposure over longer time leads to acid rain induced injuries followed by reduction of chlorophyll content.

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Abstract

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Correlation of Saprobic Index and Selected Chemical Factors in the Rivers Ljuta and Buna

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Abstract: The aim of this paper is to determine the correlation between the values of saprobicity index and selected chemical parameters of water, in watercourses that are under perennial pressure of aquaculture. Samples were collected in December, March, June and August 2015 and 2016 in the Ljuta and Buna rivers. Measurement of BOD5 values was performed by the Winkler method, and total phosphorus (TP) using the standard BAS EN ISO 6878: 2006. Sampling and analysis of macrozoobenthos was performed using AQEM methodology. The results of the analysis showed a high correlation between the analyzed chemical parameters and the saprobic index. A statistically significant correlation was obtained for the values of saprobic index and BOD5 for the river Ljuta, and saprobic index and total phosphorus for the river Buna. The data obtained in this paper are of practical importance in the implementation of a reliable model for assessing the impact on the ecological status of watercourses and the establishment of adequate measures for the protection of water bodies.

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Abstract

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Content of Pb, Cd, Co, Fe, Cr and Zn in Selected Citrus Fruit Peel

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Abstract: Heavy metals naturally occur in the soil, so they can be found of fruits and vegetables through their roots. However, landfills and the use of plant protection products as well as other various anthropogenic factors can be a source of heavy metals in fruit. Citrus fruit is of great importance for human health due to its high content of vitamins and minerals as well as antioxidant effects. As heavy metals can be easily found in the peel of the fruit and thus diffused into the fruit itself, the aim of this study was to determine the concentration of some heavy metals in the peel of lemon, orange and tangerine as the most common citrus fruits. Available citrus samples from the market of Bihać were taken for analyses. The citrus samples were dried at 105°C and digested (n=3). The analysis of heavy metals (Pb, Cd, Co, Fe, Cr and Zn) was done by atomic absorption spectrometry. Lead concentrations in all samples were below the instrument detection limited upto <0,001mg/kg. The highest content of cadmium was found in orange peel samples 0.056 mg/kg, and the lowest in lemon peel samples 0.054 mg/kg. The content of cobalt was highest in orange peel 0.028 mg/kg. The highest concentration of iron was in lemon peel samples 0.382 mg/kg. The highest concentration of chromium in tangerine peel was 1.952 mg/kg. The highest concentration of zinc in lemon peel was 0.056 mg/kg. The Rulebook on maximum permitted quantities for certain contaminants in food in B&H as well as EU directives and EFSA do not regulate the maximum permitted amounts of heavy metals in citrus peels, although they define the maximum values of heavy metals in fruits themselves. The heavy metals concentrations found in all analysed samples do not pose a danger to human health.

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Abstract

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Enhancement of Cadmium Tolerance in Maize by Intercropping

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Abstract: Intercropping is worldwide known method of a multiple cropping practice that involves growing two or more crops in the same soil, at the same time. There are many benefits from intercropping and most important are: increasing the rate of crop production, better utilization of growth resources like nutrients, light, and moisture and better weed control. The evaluate the effect of intercropping system of *Zea mays*and cadmium hyperaccumulator *Silene vulgaris* on maize tolerance of Cd an experiment consisting of monocultures and intercropping were established on Cd contaminated and uncontaminated soil. To assess the effect of cadmium stress morphological and physiological parameters were analysed. Results indicated that hyperaccumulator intercropping system led to changes in biomass productions in roots and shoots, and led to an increase in proline concentration, suggesting a beneficial effect of intercropping on maize cadmium tolerance.

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Abstract

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Waste Sludge Management as a By-Product of Wastewater Treatment in Order to Improve the Quality of the Environment

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Abstract: The wastewater sludge is not worthless material, because it contains about 45 to 90% of organic matter whose energy value can be used, i.e. to use in various ways, not only in agriculture. For these reasons, the use of sludge in energy purposes is one of the very important possibilities. The sewage sludge incineration plant in order to obtain electricity is planned in Podgorica, within the new wastewater treatment plant. Multiple methods were analyzed to choose the best technology of sewer sludge incineration:incineration with a fluidized layer; grid firebox, pyrobustor technology, and pyreg (pyrolysis process). All of the above benefits have led the EU to declare an incinerator with a fluidized layer as the best available technique (bat) in the European Commission's reference document, one of the best techniques for burning sludge and other organic materials. Based on all these methods of incineration of the residue of sewage sludge, an incinerator with a fluidized layer was selected, as the best method for treatment of sewer sludge in Podgorica. Based on analyzes, assessments are that the projected capacity of the plant in Podgorica for 190,000 inhabitants, in 2030, the annual amount of sewer sludge that will be used to insert a 13,800 t. Thermal processing of dehydrated sewerage from wastewater treatment plant is a significant opportunity to improve the environment and to establish a sustainable and reliable way of processing sludge without restrictions on current practice.

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Biomonitoring of Metal Levels by Using Conifer Needles and Moss in Bosnian-Podrinje Canton, BiH

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Abstract: Numerous studies suggest that various biological samples are used to assess the state of the environment, such as soil and tree bark, lichens, mosses, and leaves. Among biological samples, conifers and mosses are commonly used to detect atmospheric metal deposition in terrestrial ecosystems. In this study, conifer needles and mosses used to assess the metal concentrations at ten locations in the area of the Bosnian-Podrinje Canton (BPC) in Bosnia and Herzegovina. Flame atomic absorption spectrometry (FAAS) was used to determine the concentrations of Cd, Cr, Cu, Fe, Mn, Ni, Pb and Zn in samples. The metal concentration in moss varied for Cd (0,12-1,21 µg/g), Cr (<LOD-47,5 µg/g), Cu (1,36-49,7 µg/g), Fe (295-1886 µg/g), Mn (28,6-392 µg/g), Ni (<LOD-21,9 µg/g), Pb (<LOD-2602 µg/g) and Zn (<LOD-63,4 µg/g), while the obtained metal concentration in conifer needles are: Cd (0,15-0,46 µg/g), Cr (<LOD in all samples), Cu (<LOD-1,16 µg/g), Fe (22,7-186 µg/g), Mn (3,90-586 µg/g), Ni(<LOD-1,64 µg/g), Pb (3,01-21,3 µg/g) and Zn(<LOD-17,9 µg/g).The metal concentration in most samples from the same sampling site was lower in conifer needles compared to moss samples. The obtained results of the selected metal analysis suggest that mosses suitable bioindicators for the purpose of monitoring environmental pollution, especially metal air pollution. In addition, conifer needles are sufficient bioindicators. Based on the obtained results it can be concluded that due to industrial pollution and traffic, the air in the BPC area is relatively loaded with heavy metals.

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Abstract

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Feasibility and Cost Analysis of Electrocoagulation Technology for the Removal of Turbidity and Organic Matter from Gray Water

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Cost Analysis

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Abstract: An evaluation of the viability of electrocoagulation/electroflotation technology for the removal of turbidity, organic matter and color from domestic gray water has been carried out, with the aim of the possible implementation of this technology in the DRAIN2WC prototype for gray water reuse in Spanish homes developed by the company Indepro Consultores de Ingeniería SL. In this sense, a sensitivity analysis of the main variables and operational parameters of the processes such as temperature (12.5 ° C, 37.5 ° C and 50.0 ° C) and ionic conductivity (230 - 530 µS/cm)of the gray water samples, stirring speed (100-200 rpm), electrolysis time (15 min - 2h), current density (76 - 198 A/m^2), electrical charge (76-99 and 297-801 C/dm^3), S/V ratio of 1.6 m^2/m^3 (ratio of active electrode surface area to water sample volume), electrical charge dosing rate under optimal operating conditions 5.1 C/dm^3/min, and aluminum anode and graphite, aluminum and copper cathodes, has been carried out. The corresponding economic evaluation of the processes leads to a cost balance of 0.3-0.4 € / m^3 of treated gray water. It is concluded that electrocoagulation/electroflotation is an efficient process to eliminate gray water turbidity, color and organic matter (in 20 min of optimal operating condition, removal of turbidity 97%, organic matter 85% and color 95%).

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Abstract

PP-ENC-23

Electrocoagulation Coupled with Oxidation as an Effective Approach for Industrial Wastewater Treatment

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Abstract: Removal of pollutants has become one of the most essential applications in wastewater treatment. Electrochemical techniques especially electrocoagulation (EC) has received great attention because of the efficient treatment of wastewater at a low cost with more than 80% efficiencies for the chemical oxygen demand (COD) and colour removal. The present research is focused on the elimination of tenacious organic compounds from industrial wastewater by combining electrocoagulation with electrooxidation. Promising changes in coliforms, turbidity, colour and the general absorbance with UV–vis spectroscopy are observed. Since only half of the COD could be eliminated from wastewater and an oxidation peak in the cyclic voltammetry (CV) scan persisted, therefore EC is comparatively ineffective. However, electro-oxidation is very effective in the oxidation of organic compounds as reflected in the elimination of COD, biochemical oxygen demand (BOD) and oxidative peak in CV. Furthermore, electrooxidation mineralisation of electrocoagulation wastewater removes most of the colloids and charged species in less than 2 h. In the proposed coupled technique, EC quickly coagulates and removes colloidal and suspended particles along with several charged species. Apart from this electrooxidation oxidises the remaining organics. Overall, the coupled process eliminates COD, BOD, colour, turbidity and coliforms efficiently in a short time.

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PM_{10} Emission During the Operation of the Asphalt Production Plant

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Abstract: This study presents the results of calculating the emissions of fuel combustion products from engaged mechanization used at the location of the asphalt base and total PM_{10} emissions on the location of the asphalt base. Gas emissions from the engine with internal combustion of construction machines used in the operation of the asphalt production plant (loader and trucks) is calculated according to the limit values, for standardized permissible emissions CO, HC, NO_X and PM_{10}. The total amount of aggregates is 95,000 t/year which is delivered to the location of the asphalt base. Based on this, budgets were made; total PM_{10} emissions on the location of the asphalt base they covered: a) delivery aggregate on a bunch (PM_{10} = 0.3135 t/year), b) transfer and transfer of aggregates from piles and in pins Transport transporters (PM_{10} = 0.01 t/year), c) aggregate classification (PM_{10} = 0.012 t/year), d)dryer and mixing of aggregates (Tower) (PM_{10} = 0,768 t/year), e) storage and unloading: temperature 145°C (PM_{10} = 0.02 t/year), heating loss 0.5% (PM_{10} = 0.02 t/year), f) transport of asphalt at the location of the asphalt base (asphalt road, 100 m per road, 20 tons, S = 3 g/m^2, moisture = 3%, vehicle speed ≤15 km/h (PM_{10} = 0.072 t/year), g) asphalt heater (fuel Easy heat oil, specifically fuel S = 0.2%) (PM_{10} = 0.0012 t/year). The total emission of PM_{10} particles at the location of the asphalt base is 1.0677 t/year. Based on this, maximum emissions for 1.600 h/year is 0.1958 g/s.

POSTER PRESENTATIONS

Food Chemistry

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Abstract

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The Content of Essential and Toxic Metals in Sesame, Flax, and Black Cumin Seeds

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Abstract: Exposure of the population to essential metals, which have several biochemical functions in humans, is mostly through food consumption, but the metals can be toxic if ingested in excess. Sesame, flax, and black cumin seeds are commonly used in nutrition in Bosnia and Herzegovina (BiH) suggesting that continuous determination of metals is needed. However, the literature review on the chemical composition of the investigated seeds suggests that there is very limited data in BiH. Therefore, the aim of this study was to determine Cd, Cr, Cu, Fe, Mn, Ni, Pb and Zn in sesame, flax and black cumin from the market in Sarajevo, BiH. Metal concentrations were determined by flame atomic absorption spectrometry (FAAS). Moisture content was also determined in all samples, ranging from 2.68 % (sesame seeds) to 6.56 % (flax seeds). The highest content of Fe was found in black cumin seeds (63.96-71.47 mg/kg). Sesame seeds contained the highest Zn concentrations (50.48-56.98 mg/kg). Cu concentrations were found in all seed samples, and ranged from 8.79 mg/kg to 15.28 mg/kg. The highest concentrations of Mn were found in flax seeds (14.47-21.95 mg/kg). Ni was detected only in black cumin seeds (0.47-2.16 mg/kg). Cd, Pb, and Cr concentrations in all samples were below the FAAS limit of detection. The obtained results suggest that the seeds of sesame, flax, and black cumin contain sufficient concentrations of essential metals. Since the concentration of toxic metals is relatively low in all samples, consumption should not have a significant impact on human health.

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Abstract

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Chemical Composition of *Prunus spinosa* L. Fruit Extracts Determined by GC-MS

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Abstract: Sloe (*Prunus spinosa* L.) as a traditional plant in phytomedicine is a potent source of natural bioactive compounds that includes phenolics, alkaloids, terpenes, sterols, and has been applied in the treatment of various diseases. In this sense, the present study is going to provide a detailed overview of phytochemical constituents isolated from sloe extracts. The ethanol extracts were prepared from dried and fresh sloe fruit by microwave-assisted extraction. A total of 32common constituents were identified in the extracts using GC-MS. The major identified components were furfural with content of 10.64% for fresh and 2.77% for dried fruit as well as pyranone with content of 10.24% for fresh and 3.99% for dried fruit. Other major components were 5-hydroxymethylfurfural, furaneol, eugenol, 2-furanmethanol, diethyl malate, acetic and propanoic acid. Three chiral components (linalool oxide, 5-methyl-2(3*H*)-furanone, diethyl malate) were also identified in both extracts and their presence was confirmed by comparison with standards. According to the literature, the identified compounds havedifferent biological activity and promising bioactive potential, what should be verified within our further research.

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Abstract

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Determination of Plant Pigment Content in Selected Herbs

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Abstract: Plant pigments are important functional molecules in photosynthetic organisms and have been recognized as photoprotective compounds. Three plants from Apiaceae family, coriander (*Coriandrum sativum*), parsley (*Petroselinum crispum*) and dill (*Anethum graveolens*), and basil (*Ocimum basilicum*), a plant from Lamiaceae familiy, were selected for analysis. Fresh herbs (0,5 g) were analized for the content of plant pigments (total chlorophyll, chlorophyll *a* and *b* and carotenoids) after which samples were subjected to air drying and oven drying (45°C). Plant pigments were extracted with 80% acetone from fresh and dried herbs and determined using spectrophotometric method (measuring absorbance at 470nm, 648,6nm and 663,2 nm, respectively). Fresh parsley showed the highest total chlorophyll content (524,38±7,13 mg/100g) which was followed with the highest chlorophyll *a* (Cha*)* and chllorophyl *b* (Chb) content, with Ch*a*/Ch*b* ratio 1:2. Oven dried basil had the lowest total chlorophyll content (196,83±4,95 mg/100g dw). Fresh parsley showed the highest carotenoid content (114,99±2,04 mg /100g dw) and air dried basil samples had the lowest carotenoid content (23,85±0,95 mg/100g dw). Drying process showed significant impact on plant pigments with tendency to degradation of chlorophyll and carotenoids during drying, although type of drying had minor influence to content of plant pigments.

POSTER PRESENTATIONS

Inorganic Chemistry

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PP-IC-01

Nickel and Ni-Co Alloy as Efficient Hydrogen Evolution Reaction Catalysts in Alkaline Media

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Abstract: Electrodes produced from polycrystalline nickel, 3D Ni foam and Ni-Co alloy were used as catalysts for the hydrogen evolution reaction (HER) at 20 °C in 0.5 mol L^{-1} NaOH solution. The purpose of the investigation was to evaluate their intrinsic catalytic activity. Cyclic voltammetry method was used to provide insight into the overall electrochemical behavior of the investigated materials. Potential range in which metal oxides / hydroxides formation and reduction take place was identified. Tafel plots, pseudo-steady-state linear polarization and electrochemical impedance spectroscopy (EIS) measurements were performed in the potential range of HER. In this range the modified Randles electric equivalent circuit was successfully used for modeling obtained EIS data. For all investigated electrode materials the exchange current densities and cathodic Tafel slopes were derived. The results obtained by pseudo-steady-state linear polarization are in accordance with the results obtained by electrochemical impedance method. Among the investigated catalysts, 3D Ni foam shows the highest intrinsic catalytic activity. It was found that for the HER at investigated electrodes the main pathway is Volmer-Heyrovski.

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Coordination Compounds – Preparation, Structures, Properties and Applications

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Abstract: The 6-oxonicotinate salts of a one-dimensional cationic nickel(II) and cobalt(II) coordination compounds with 4,4'-bipyridine were prepared hydrothermally by reactions of cobalt(II) or nickel(II) nitrate hexahydrate with 6-hydroxynicotinic acid and 4,4'-bipyridine. Our investigation is focused on the preparation of coordination compounds and their application in electroanalysis, based on previous knowledge about the excellent electrocatalytic performance of this type of compound. The highly oxidative species present in these materials, Ni(II)/Ni(III) or Co(II)/Co(III) represent a catalytically active centre towards short chains or small molecules. The focus of this paper was to investigate the electrochemical properties, determine the origin of electrochemical differences in the isostructural system and investigate potential applications for catalytic oxidation of methanol. The Co-BPY/6-Onic and Ni-BPY/6-Onic ($\{[Co(4,4'\text{-bpy})(H_2O)_4](6\text{-Onic})_2\times 2H_2O\}_n$ and $\{[Ni(4,4'\text{-bpy})(H_2O)_4](6\text{-Onic})_2\times 2H_2O\}_n$) as isostructural coordination compounds exhibit different electrochemical behaviour, as observed by cyclic voltammetry, which can be attributed to the nature of the metal ions. The results indicated that the electrode modified with Ni-BPY/6-Onic show stability and reproducibility in 0.1 M NaOH, and oxidation current increases with the increase of methanol concentration. On the other hand, electrode modified with Co-BPY/6-Onic is non-reproducible and cannot be used for electroanalytical purposes. The GCE modified with Ni-BPY/6-Onic was successfully applied in the determination of methanol.

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A Copper(II) Salicylideneimine Complex: An Extended Characterization along with BSA Interaction and Antiproliferative Activity

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Abstract: As a follow-up of the research regarding synthesis and biological activity of new Cu(II) Schiff base complexes, a square planar Cu(II) complex with two N-*n*-buthyl-5-chlorosalicylideneimine was prepared. The present report includes synthesis, physicochemical characterization along with biological activity based on the interaction with bovine serum albumin (BSA) and *in vitro* antitumor activity. Elemental analysis and mass spectra confirmed purity and molecular formula [CuL_2]. The magnetic properties, studied by X-band ESR spectroscopy correspond to square planar geometry of copper(II) ions. Cyclic voltammogram in acetonitrile solution showed electrochemical irreversibility due to the fast decomposition of electrogenerated Cu(I) complex species. Complex showed static quenching of BSA fluorescence and moderate affinity to bind BSA (K_b = 3.10 × 10^3 M^{-1}). Activity against two cancer cell lines (H460 and HCT116) and non-tumor cells (HEK293T) showed promising IC_{50} (μM) values, 14±4, 20±10, 15±3 respectively.

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Cobalt(II) Coordination Polymer with 1,2-Bis(4-pyridyl)ethane and 6-Aminonicotinate as an Electrochemical Sensor

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Abstract: The electrochemical properties of coordination polymers haven't been extensively studied in the past. However, their electrochemical sensing ability has recently started to attract more interest. This sensing ability generally depends on the particular metal ions and functional organic ligands and is usually revealed by electrochemical methods. The cobalt(II)coordination polymer with 6-aminonicotinate (6-aminopyridine-3-carboxylate) and 1,2-bis(4-pyridyl)ethane (1,2-bpe) was prepared under hydrothermal conditions in the mixture of water and ethanol. Its hydrogen-bonded framework is composed of 1-D polymeric $\{[Co(1,2\text{-bpe})_2(H_2O)_2]^{2+}\}_n$ cations, 6-aminonicotinate anions, nitrate anions and lattice water molecules. In the polymeric$\{[Co(1,2\text{-bpe})_2(H_2O)_2]^{2+}\}_n$ cation, each cobalt(II) ion is octahedrally coordinated with four pyridine N atoms of various 1,2-bpe molecules and with two water molecules in *trans* position. The two adjacent cobalt(II) ions are thus bridged by two 1,2-bpe molecules, leading to the formation of macrocyclic rings of 22 atoms within the 1-D polymeric cation (Figure 1). This cobalt(II) coordination polymer was studied by cyclic voltammetry and electrochemical impedance spectroscopy to decipher its sensing potential towards the selected cations, anions or organic molecules.

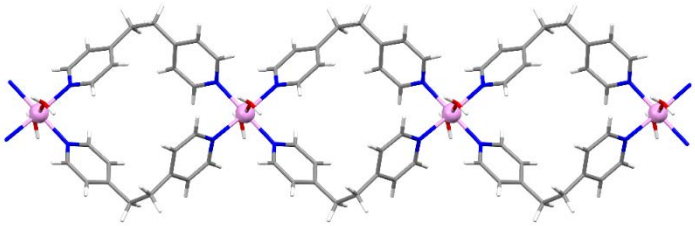

Figure 1. The 1-D polymeric $\{[Co(1,2\text{-bpe})_2(H_2O)_2]^{2+}\}_n$ cation.

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Synthesis and Biological Activity of Copper(II) Complexes with Nicotinic Acid Hydrazones

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Abstract: Two neutral homoleptic copper(II) complexes of *N*'-(4-substituted benzylidene)nicotinohydrazides, having chloro or dimethylamino substituents, were prepared from solution. Complexes were characterized by elemental analysis, mass spectrometry, infrared and electron spectroscopy, and cyclic voltammetry. Hydrazone ligands chelate Cu(II) ion as bidentate monobasic N,O-donor ligands creating CuN_2O_2 coordination sphere around Cu(II) ion. Solid state structure of the complex having chloro substituent indicates a dynamic process in the crystal lattice such that no reliable structural parameters could be obtained by SCXRD. Hydrolytical profiles demonstrated inertness of Cu(II) for hydrolysis. Interaction of complexes with CT DNA and BSA was investigated by electron spectroscopy and spectrofluorimetry. Complexes have moderate affinity toward CT DNA and BSA, making them suitable candidates for antiproliferative testing.

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Novel Mononuclear Ruthenium(II) Polypyridyl Complexes with Schiff Bases derived from Amino Acids – DNA and BSA *in vitro* Binding Studies

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Abstract: Ruthenium complexes are among the most extensively studied due to their potential therapeutic application that can be enhanced with introduction of biologically active ligands. The four novel Ru(II) complexes $[Ru(phen)_2L^{a-d}]^+$**2a-2d**, where phen = 1,10 phenanthroline and L^{a-d} = Schiff bases are derived from salicylaldehyde and amino acids (a- glycine, b- cysteine, c- methionine and d- phenylalanine) have been synthesized and characterized *via* elemental analysis and spectroscopic techniques (mass, electronic and FTIR), in addition to our previous research on Ru(II) bipyridine family of complex compounds with the same Schiff bases. Cyclic voltammograms, in acetonitrile solution, showed redox pairs in the positive potential range, in accordance with similar heteroleptic Ru(II) polypyridyl complexes. The hydrolytic profile of **2a**-**2d**, monitored by UV-Vis spectroscopy, showed inertness to hydrolysis within 24 hours. Additionally, the DNA-binding study of the complexes **2a**-**2d** with calf thymus DNA was performed utilizing UV-Vis spectroscopy. The DNA-binding investigations demonstrated that the complexes **2a**-**2d** interact with CT-DNA preferably through groove binding as suggested with the binding constant order of 10^3 M^{-1}. Furthermore, BSA protein binding affinity of the **2a**-**2d** was determined by fluorescence emission titrations. The protein interactions revealed strong quenchingof the fluorescence intensity by static mechanism, with Complex: BSA = 1:1 ratio. The Stern-Volmer constant of **2a**-**2d** was determined of 10^4 M^{-1} order.

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Influence of some Pyrazole Derivatives on Inhibition of *Botryosphaeria dothidea* under Laboratory Conditions

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Abstract: Based on the fact that the pyrazoles, as fungicide active ingredient, have shown practical application in the protection of fruit trees, in this study inhibitory effects of 2-(3-Aminophenyl)-5-methyl-2,4-dihydro-3H-pyrazol-3-one hydrochloride and 3-(4-Hydroxyphenyl)-1H-pyrazole-5-carboxylic acidwere examined to the pathogenic fungal mycelial growth of *Botryosphaeria dothidea* cause olive disease, in vitro.Biological activity based on determining the inhibition effect of the commercial fungicide Cabrio top and the used compounds on *Botryosphaeria dothidea* has been carried using the phytosanitary method. The diameters of fungal mycelium *Botryosphaeria dothidea* as parameters of the inhibition effect were processed using the variance analysis, while the testing was performed using the LSD test. The compounds have applied in five 5 different concentrations. Obtained results compared with the Cabrio Top whose active ingredient pyraclostrobin belongs to pyrazole derivatives. Based on the obtained results, it can be concluded that both tested pyrazole derivatives concentration (C1 = 0.12%) significantly inhibit the growth of fungal mycelium, but much less compared to the commercial fungicide Cabrio Top.

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The Inhibitory Effect of some Pyrazole Ligands and Their Cu(II) Complexes on the Growth of *Escherichia coli, Klebsiella-Enterobacter spp.* and *Staphylococcus aureus*

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Abstract: The aim of this study was to evaluate the inhibitory activity of some pyrazole derivatives and selected Cu(II) complexes, against growth of *Escherichia coli*, *Klebsiella-Enterobacter* spp. and *Staphylococcus aureus*. Pyrazole derivatives (4-Bromo-2-(1H-pyrazol-3-yl)phenol(Pz1), 4-Nitro-3-pyrazolecarboxylicacid(Pz2),N-(Benzyloxycarbonyl)-1H-pyrazole-1-carboxamidine(Pz3) and two Cu(II)complexes with Pz2 and Pz3 as ligands were examined on their antibacterial activity in two different concentrations (10^{-3} and 10^{-5} mol/dm^3). The testing method was carried out according to the disk diffusion method protocol. We measured the zone of inhibition of growth of selected strain of bacteria. The most of compounds showed inhibitory effect against the growth of *E. coli* and *Klebsiella-Enterobacter* spp.,but did not show an inhibitory effect on *Staphylococcus aureus*, compared to amoxicillin as a standard. The pyrazole derivative (Pz3) achieved the best results from other studied compounds,at concentration of 10^{-5}mol/dm^3 when it inhibited the growth of *Klebsiella Enterobacter*at a level of 82.8%, which is the best results in this experiment compared to other compounds and concentrations.

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Synthesis, IR Characterization and Antioxidant Capacity of Cu(II) Complexes with Amino Acids and Melatonin

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Abstract: In this study, the reactions of anhydrous copper(II) chloride in methanolic solution with four amino acids and melatonin were investigated and the resulting products were described by FTIR spectroscopy. Based on FTIR characterization, it was shown that these reaction conditions result in the formation of Cu(II) complexes with glycine and alanine, which are more complex structures than bis(glycinato) - and bis(alaninato) copper(II) complexes. Analysis of the FTIR spectrum of the histidine complex shows the participation of several groups in coordination at the Cu(II) center. The complex prepared with melatonin shows unusual changes in the spectral region of the amidic nitrogen bonds. The latter observation is very significant for very few metal complexes of melatonin are known to be well characterized, while the synthesis of most of them is an experimentally demanding process with simultaneous control of several parameters. The antioxidant capacity of the synthesized complexes was examined, with the CEAC range from 121.6 - 734.4 µM. The lowest values of antioxidant capacity were recorded for the copper complex with tryptophan, while the highest values were recorded for the copper complex with alanine. A high antioxidant capacity of the copper complex with melatonin (673.8 µM) was also observed.

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PP-IC-10

Application of FTIR Spectroscopy in Monitoring the Frmation of a Ru-NHC Complex from Selected Imidazolium Salts via Transmetalation

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Abstract: In this study we investigate the application of FTIR spectroscopy in tracking and interpreting the changes observed in the spectra of the reactants and the products after a transmetalation reaction in which a Ru-NHC complex forms. FTIR analysis of three salts containing the 1,3,4,5-tetraphenylimidazolium cation showed high spectral comparability, implying high comparability of the specific vibrational modes, regardless of the anion present, where the observed differences can be used, not only to identify the anion but also to denote the nature and degree of its interaction with a given imidazolium cation. The complex does not contain carbon-hydrogen bond vibrations at the C(2) position of the imidazole ring. The bands corresponding to the deformation vibrations of the given atom with the rest of the imidazole ring undergo significant and easily noticeable changes during deprotonation and coordination to the metal center. Based on the above results we conclude that the band attributed to the C(2) – H "rocking" mode, usually neglected in favor of less robust but distinguishable bands, is significant and sensitive for evaluating the formation and coordination of a carbene, given the fact that this band is completely lost from the spectral range where it occurs in all starting imidazolium salts.

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PP-IC-11

FTIR Spectroscopic Evaluation of Ligand Coordination Aspects in O, N, S Donating Thiosemicarbazone Ru(III) and Fe(III) Complexes

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Abstract: In this study we perform a FTIR spectroscopic evaluation of the coordination model and structural transformations of O, N, S donor 5-X-salicylaldehyde thiosemicarbazones (X = H, Cl, Br, NO_2) in their Ru(III) and Fe(III) complexes. Eight complexes were prepared under identical conditions by combining the metal chloride with the given ligand in a 1 : 2 molar ratio. All ligands were characterized by FTIR spectroscopy and the most relevant vibrations, to evaluate the coordination model, were selected. The $\nu_{as}(C - O_{phen.})$ band occurs at 1260 to 1280 cm^{-1} while the same band is shifted by about 15 cm^{-1} towards higher wavenumbers in all synthesized complexes confirming deprotonation and coordination of the phenolic oxygen. The ligand $\nu_{as}(C = N)$ band ranges from 1605 to 1618 cm^{-1}, however, the spectra of Ru(III) and Fe(III) complexes show a band shifts by 10 to 25 cm^{-1} to lower wavenumbers, with a shoulder formation peaking at 20 to 30 cm^{-1} higher then the ligand $\nu_{as}(C = N)$ band indicating the formation of a new, uncoordinated imine bond. This is further evidenced by the disappearance of the ligand $\nu_{as}(C = S)$ band at 777 cm^{-1} and the occurrence of a new $\nu_{as}(C - S)$ vibration at about 740 to 720 cm^{-1} in all the complexes, which showed ESI-MS results consistent with these observations.

POSTER PRESENTATIONS

Medicinal Chemistry

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PP-MC-01

Evaluation of Lipophilicity and Toxycity of Novel Isatin Derivatives

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Abstract: One of the key molecular descriptors that provide information about the potential biological activity of the newly synthesized compound at an early stage of research is lipophilicity. Lipophilicity of the selected isatin derivatives was determined by using reversed phase thin-layer chromatography (RPTLC18F254s) in the presence of two organic modifiers (*i*-propanol and tetrahydrofuran), as well as by using appropriate software packages. The effect of the substituent's nature and position, and the applied organic modifier on the chromatographic behaviour of the studied derivatives was examined. Chromatographic parameters (R_M^0 and m) of isatin derivatives as assumed measures of their lipophilicity were correlated with software obtained values of standard measure of lipophilicity, partition coefficient (log$P$) and selected parameters of ecotoxicity whereby good linear dependencies were obtained. Derivative with -I as a substituent in the meta position has the greatest influence on the increase of lipophilicity among the tested compounds. This confirmed the reliable application of chromatographic parameters determined by RPTLC18F254s as alternative measures of the studied isatins' lipophilicity and ecotoxicity.

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Coumarins from the Sea as Possible Drugs Confronting SARS-CoV-2

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Abstract: The SARS-CoV-2 virus can cause serious health problems associated with significant mortality. In addition to vaccines, worldwide campaigns to detect drugs that will act on the virus are underway. SARS-CoV-2 main protease (SARS-CoV-2 Mpro) and papain-like protease (PLpro, part of nsp3) are important enzymes in the life of the SARS-CoV-2 virus and are considered main targets for possible drugs. Molecular docking was used to assess the potential of tested compounds to act as protease inhibitors. The docking study was performed using AutoDock 4.2. The crystal structure of the SARS-CoV-2 main protease (PDB ID: 6Y2E) was used as the target molecule. 3-Acetylcoumarin (**1**) and six 3-iminocoumarins (3-(1-(methoxyimino)ethyl)coumarin (**2**),7-hydroxy-3-(1-(methoxyimino)ethyl)coumarin (**3**),7-methoxy-3-(1-(methoxyimino)ethyl)coumarin (**4**), 3-(1-(ethoxyimino)ethyl)coumarin (**5**), 3-(1-((benzyloxy)imino)ethyl)-7-hydroxycoumarin (**6**) and 3-(2-((benzyloxy)imino)-1-methylethyl)-7-hydroxycoumarin (**7**)) found in extracts from different species of mangrove fungi (*Phomopsis*, *Paecilomyces* and *Halorosellinia*) and from macroalgae (*Sargassum*) were chosen as ligands for this docking study. The obtained values of binding energies and inhibition constants showed that coumarins from marine organisms deserve more attention when it comes to the search for drugs against SARS-CoV-2. Values of binding energies ranged from -5.80 to -8.18 kcal mol^{-1}. Coumarins with a longer chain at the C-3 position, plus additional heteroatoms, O and N,have better/lower binding energies. Also, the introduction of a hydroxyl group at position 7 of the coumarin nucleus could be of great importance for activity according to preliminary results.

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Synthesis and Evaluation of Cytotoxicity of Cinnamic Acid-3-Aminophenylboronic Conjugate

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Abstract: The concept of targeted therapeutic drugs was first introduced by Paul Ehrlich in the early twentieth century, who argued that in order to increase the accumulation of the active pharmaceutical ingredient in the target tissue, two components are needed: the first functioning by recognizing and binding to target cells, tissue or organ, while the second functions as a therapeutic agent. The conjugates of biologically active organic acids 3-aminophenylboronic acid show an interesting ability to bind to sialic acids (glycans), via OH groups of 3-aminophenylboronic acid, which contributes to longer retention of organic acids on the cell surface, and thus enabling their prolonged biological action. In this report, the synthesis of cinnamic acid-3-aminophenylboronic conjugate was performed by amidation of cinnamic acid carboxyl group using dicyclohexylcarbodiimide in dichloromethane. Cinnamic acid (1 mmol) and carbodiimide (1 mmol) dry mixture was prepared in reaction vessel. After addition of dichloromethane (4 ml), 3-amino-phenylboronic acid (1 mmol) was added in solution. After stirring overnight and filtration of dicyclohexylurea, the derivates in the filtrate were evaluated by HPLC-MS analysis (conjugate 30% and cinnamic acid anhydride 70%). Cytotoxic activity was evaluated on human cervical cancer HeLa cell lines. In conclusion, the mentioned derivates have more potent cytotoxicity than pure cinnamic acid.

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Effects of *Helix aspersa* Snail Extract on Inflammation in Experimental Model of Alzheimer's type Dementia *in vivo*

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Abstract: Snail extract (SE) obtained from garden snail *Helix aspersa* was analyzed by sodium dodecyl sulphate polyacrylamide gel electrophoresis. Molecular masses of protein in mucus fraction >20 kDa was measured by an Autoflex™III, High-Performance MALDI-TOF. Obtained SE consists of 50% crude mucus extract and 50% fraction containing compounds with MW above 20 kDa. Rats were divided in 4 groups: Controls; Alzheimer's type dementia (ATD); ATD+SE; SE. The highest level of anti-inflammatory cytokine IL-10 was found in the group treated with snail extract. Level of IL-10 increased in Alzheimer's dementia + snail extract group as compared to ATD. The lowest level of inflammatory cytokine TNF-alpha was detected in control group and in the one treated with snail extract. Most inflammatory cytokines were observed in ATD group, which concentration decreased significantly after administration of snail extract.Monocytes from only snail extract group produced predominantly IL-10 without producing high levels of TNF-alpha. Circulating CD43-positive monocytes decreased in ATD group but increased significantly in ATD+SE. Expression of CD11c integrin was normalized in ATD+SE group indicating probable traffic restoration and monocytes blood migration. In conclusion our investigations demonstrated anti-inflammatory properties of snail extract in Alzheimer's type dementia.

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Helix aspersa Mucus Extract with Protective Effect on Ethanol Iinduced Gastric Ulcers in Mice

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Abstract: This study aimed to investigate the protective effect of *Helix aspers*a mucus extract (ME) on ethanol induced gastric ulcers (GU) in mice and elucidate its efficacy mechanism. The composition of the ME was studied by SDS-PAGE and by mass spectrometry. Male Albino mice were divided into Control, Ethanol and Mucus+Ethanol treated groups. The GU was induced by administration of 96% ethanol. The mice of Mucus+Ethanol group were pre-treated with ME (20 mg/kg, PO) one hour before ulcer induction. Results showed that the ME is complex mixture from antimicrobial peptides, and different proteins with antimicrobial, antioxidant and regenerative properties. Moreover, we detected that ME inhibits the growth of bacterium *Helicobacter pylori*. In the group with pre-administration of ME were observed: a small number of hemorrhagic fields; significantly reduced GU index compared to ethanol group (4.7% vs 17.3% respectively); calculated highly protection 73%; significant recovery of glutathione concentration level and activity of glutathione reductase; rise in the activity of the other antioxidant enzymes. The protective effect of ME in this model of gastric injury is due to synergistic effect of different mucus compounds. These studies served to create the nutritional supplement - effective in various forms of gastric injury.

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PP-MC-06

Validation of the Antimicrobial Activity of Mucus Peptides from Garden Snail *Helix aspersa* Müller

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Abstract: Natural antimicrobial peptides are able to inhibit pathogenic microorganisms. In recent years, the antibacterial activity of the mucus of garden snails *Helix aspersa* Müller,1774and *Helix lucorum* Linnaeus,1758has been proven both *in vitro* and in a number of clinical studies. We present the first results about the antimicrobial activity of newly identified six peptides: P1 (KVKDNQWRP), P2 (VNVVGGGGGIVGGGIGGGGM), P3 (LFGGHQGGGLVGGLWRK), P4 (LGHDVH), P5 (LGLGNGGAGGGL) and P6 (MLGGVLGGGPLK) against *Escherichia coli* and *Bacillus subtilis*. *In silico* studies hypothesize the multistage nature of the antibacterial activity of peptides and the formation of mixed peptide clusters as a transport and concentration agent to deliver the active ingredients to the target bacterial membrane. Based on the results of the simulation, the antimicrobial activity of a number of two- and three-component peptide mixtures was confirmed. The antibacterial test showed the inhibitory effect of peptide P3 and the synergistic effect of the combination of peptides P1:P2, as well as P2:P3:P6 against *E. coli* 3584 and *B. subtilis*.

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Correlation Between the Amount of Total Oxidative Stress and Different Stages of Malignant Melanoma

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Abstract: Malignant melanoma, a neoplasm arising from malignant transformation of epidermal melanocytes as a result of complex mechanism is, at the metastatic stage of disease, extremely difficult to treat. Oxidative stress has been implicated in all the stages of carcinogenesis and malignant melanocyte transformation. ROS in melanocytes can be produced from mitochondria, melanosomes, NADPH oxidase (NOX) activity, and nitric oxide synthase (NOS) activity/uncoupling. Several studies demonstrated the presence of elevated levels of a different antioxidant molecule, such as superoxide (SOD) and catalase (CAT), in melanoma cells. The aim of this study was to detect and quantify total antioxidant capacity (TAC) and total oxidative capacity (TOC) in samples taken from melanoma patients. Participants in the study were melanoma patients who have had diagnosis of melanoma in the last years and malignant tissue removed. Melanoma were classified into three stages according to the 7th edition of AJCC melanoma classification. Total antioxidant capacity of the plasma samples were tested by e – BQC lab instrument. Method is based on a total redox potential of the tested samples and its comparison with antioxidant activity of ascorbic acid. Measurements are expressed in charge units – micro Coulombs (μC). To compare the results (μC) to antioxidant capacity units of Vitamin C Antioxidant Capacity Equivalents (CEAC) was used. An automated colorimetric method was used to measure total oxidative capacity in plasma samples. The assay was calibrated with hydrogen peroxide and then results are expressed as micromoles H_2O_2 equivalents per liter (μM H_2O_2 equiv/L). Measured values that are describing TOC were between 0,024 and 3,05 μM H_2O_2 equiv /L and TAC values were between 138,88 and 412,3 μM CEACfor melanoma patients.Also, the results showed that the lower the TOC values the higher the TAC valuesin the study group. Healthy controls showed higher TOC values compared to the studied group and at the same time lower TAC values in average when compared to the studied group.

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Organic Chemistry

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Abstract

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Optimization of Schiff Bases Synthesis Reaction between Aldehydes and Thiocarbohydrazide (dHS)

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Abstract: The usual way of synthesizing imines (Schiff bases) between carbonyl compounds – aldehydes and ketones - with thiocarbohydrazide (dHS) involves heating them for 3 hours in a mixture of water solvents and ethanol with the addition of a catalytic amount of concentrated hydrochloric acid. Heating in the presence of acid catalysts over a long period of time may be unsuitable for acid-sensitive, labile, reactive or thermally unstable aldehydes, which are prone to polymerization under these conditions. Therefore, we tested the condensation reaction at room temperature with a series of aldehydes, while maintaining the described ratios (equimolar ratio of aldehydes and dHS), with the addition of a few drops of 36% HCl. The course and completion of the reaction were monitored using infrared spectroscopy (FTIR). For example, in the reaction of benzaldehyde with dHS, the main product is *N*-benzylidene-thiocarbohydrazide. On the spectrum of *N*-benzylidene-thiocarbohydrazide synthesized with heating as well as on the spectrum of *N*-benzylidene-thiocarbohydrazide synthesized at room temperature, during the reaction the peak at 1700 cm^{-1} (originating from the aldehyde group) disappears, and a band appears at 1500-1600 cm^{-1} which is a characteristic of the C = N bond from imine. The reaction time is longer compared to the heating conditions, while the yields are comparable.

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Abstract

PP-OC-02

Synthesis of Mannosylated Ferrocene Ester Derivatives of Desmuramyl Peptide

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Abstract: Immune adjuvants are added to vaccines in order to enhance the immune response to an antigen. Muramyl dipeptide (MDP, *N*-acetylmuramyl-L-alanyl-D-isoglutamine) is the smallest peptidoglycan fragment showing the immunostimulating activity.[1] Structural modification of MDP and its analogues, such as desmuramyl dipeptide (DMP), have been performed in order to prepare derivatives with an improved adjuvant activity. In our previous research we reported the synthesis and immunostimulatory activity of mannosylated adamantane derivatives of DMP which showedenhanced immunostimulatory activity compared to compounds without the mannose subunit.[2] In this work we described the synthesis of novel class of DMP derivatives in which lipophilic ferrocene unit was introduced at *C*-terminus of L-Ala-D-*i*Gln *via* ester bond, followed by mannosylation of *N*-terminus through glycolyl spacer. Alkyl spacers of different length (2-5 C atoms) were introduced between DMP and ferrocene unit to further increase lipophilicity of the synthesized compounds and to study its impact on biological activity.

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Analysis of Lavender Volatile Compounds by Headspace Solid-phase Microextraction coupled to GS-MS

Džudžević-Čančar, H.[a,*], Alispahić, A.[a], Dedić, A.[a],Jerković, I.[b],Boškailo, E.[c], Stanojković, T.[d], Mujezin, I.[e]

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Abstract: Headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography and mass spectrometry detection (GC-MS) using the divinyl/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) was applied for the phytochemical profilingof *Lavandula angustifolia* Mill. and *Lavandula latifolia* Vill.varieties. The optimal sampling time was determined by studying the equilibrium time profile of the major volatile compounds for both lavender samples (20 min). Comparative analysis demonstrated that the major differences between the composition of the flower volatile components were in the contents of linalool,linalyl acetate and camphor. A total of 48 compounds were identified in *L.angustifolia* flowers and 46 in *L. latifolia*.Linalylacetate, linalool, 1,8-cineole, borneol, *trans*-caryophyllene and terpinene-4-ol were the most abundant components in both samples. *L. angustifolia* volatiles were evaluated as the highest quality for its high level of linalyl acetate (34.28 %) and linalool (20.16%) and lower percentage of camphor (6.73%) compared to *L. latifolia*. Use of headspace SPME with GC-MS was shown to be a convenient and effective analytical tool for the sampling of volatile compounds to differentiate lavender varieties with similar morphological characteristics. Also, this method could be used to test the quality of flowers and essential oils from Lavender species.

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Comparison of the Antioxidant and Anti-inflammatory Properties of Commonly Consumed Commercial Teas

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Abstract: The antioxidant and anti-inflammatory properties of several commonly consumed commercial teas were screened and compared to see what consumers get in commercial tea bags or bulk in a variety of consumption preparation conditions. The infusion method was used for the preparation of tea samples. An antioxidant and anti-inflammatory analysis of 18samples of commercial teas in a bag and bulk was performed in order to find the best way to prepare teas. The antioxidant method applied to tea samples was the DMPD method, while the protein denaturation test was used to determine anti-inflammatory activity. For the preparation of the samples, an infusion procedure was used with different temperatures of water. Of all the teas analyzed, the best anti-inflammatory activity was shown by a sample of green tea in bulk prepared with distilled water heated to 20°C (30.67%), and antioxidant activity was at 80°C (57.87%). Black tea showed anti-inflammatory activity of 26.82% at 20°C, but only 4.59% of antioxidant activity prepared at the same temperature. The lowest results of anti-inflammatory activity were shown by: two samples of chamomile in bulk, nettle in bulk, and St. John's wort in bulk, whose values were below 20% or negative at all tested temperatures, which indicates that they do not showanti-inflammatory propertieswhen prepared in this way, and analyzedwith this method.Only one sample of chamomile tea with honey in a beg showed anti-inflammatory activity above 20% (21.12% at 20°C and 30.16% at 50°C) As for the results of antioxidant activity, the lowest results were shown by samples of marigold tea in bulk prepared at all temperatures (5.06% at 20°C; 3.54 at 50°C; 4.95% at 80°C and 3.94% at 100°C). Based on the findings, it can be assumed that the way tea is prepared has an impact on its anti-inflammatory and antioxidant capabilities.

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PP-OC-05

Microwave Assisted Synthesis of Biologically Active 3-Hydroxypyridin-4-ones

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Abstract: 3-Hydroxypyridin-4-ones (3,4-HPs) have emerged as important substructures found in many natural and synthetic biologically active materials. They are investigated as potential antibacterial, antidiabetic, antineurodegenerative and anticancer agents, as well as potential chelators in metal overload conditions. Our recent investigations of this class of compounds have been focused on their *in vitro* antiproliferative and antiadhesive activity. Although versatile in their biological activities their synthesis remains a challenge. They can be prepared by either the direct or Harris method from maltol or the corresponding aniline derivative with or without the acidic catalyst. The direct approach consists of heating the reactants in an autoclave for at least 48 h. The second, Harris method, includes the additional steps. We have investigated their microwave assisted synthesis and found it to be an effective and not so time-consuming alternative method for their preparation.

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PP-OC-06

Synthesis of Complex Salts of Schiff Bases with Salts of some Transition Metals and Their Characterization

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Abstract: Several asymmetric Schiff bases between carbonyl compounds and thiocarbohydrazide (dHS) were synthetized. Benzaldehyde, 2-hydroxybenzaldehyde, cycloheptanon and acetophenone were used as starting carbonyl compounds. Schiff bases were obtained in moderate to excellent yields (60-90%). Obtained ligands were reacted with salts of transition metals (salts of copper, cobalt and nickel) to obtain complexes. The syntheses were performed by dropwise addition of aqueous solution of transition metal salts ($CuCl_2$, $CoCl_2$ and $NiCl_2$) to a suspension of the corresponding Schiff base dissolved in ethanol/water (70/30, v/v).After stirring at room temperature for 2 hours obtained precipitates were separated by vacuum filtration and the resulting complexes were recrystallized from ethanol. The compounds were obtained in moderate to good yields (50-70%).Characterization of the obtained complexes was performed using infrared spectroscopy, followed by structural X-ray spectroscopy (X-ray diffraction).All obtained complex compounds correspond to the general formula $[MClL(OH_2)_n]$, where L is Schiff base ligand.

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PP-OC-07

Determination of Total Parabens, Hydroquinone and Antioxidant Activity of Some Cosmetic Preparations

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Abstract: Twelve commercially available cosmetic preparations (five body creams, five hand creams, and two body lotions) were utilized in this study to measure the concentration of hydroquinone and total parabens. Antioxidant activity has been assessed due to the various compositions of cosmetic preparations that also contain some plant extracts.The methods used for estimation of antioxidant activity were the spectrophotometric DMPD and RP methods.The European Economic Community (EEC) Directive allows parabens in cosmetics at a concentration of up to 0.8 percent, with a maximum concentration of 0.4 percent (w/w) for each individual one, expressed as *p*-hyroxybenzoic acid. The content of total parabens was determined by a spectrophotometric method and the results were expressed through standards, ethylparaben (EP) and propylparaben (PP).

The highest content of total parabenes and hydroquinone was in a sample of face cream (8.50±0.51 mg EP/g_{sample},7.46±0.54 mgPP/g_{sample}6.54±1.19 mg/g_{sample}).

Despite the fact that hydroquinone was not specified in the samples utilized, it was found in all of them, with the highest concentration in a sample of face cream, which conforms to the objective of the cream, which is to even out skin tone and eradicate skin imperfections. The best antioxidant activity via the DMPD method showed a sample of body cream (3.03 mg GA/g_{sample}) and for the RP method sample of hand cream (0.78 mgGA/g_{sample}).

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Determination of the Antioxidative Activity of Selected Cosmetic Preparations

Delibasic, M., Kovac, K., Milicevic, V., Ostrakovic, L., Ostojic, J., Topcagic, A., Klepo, L.*

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Abstract: The skin, being the biggest organ of the human body, is one of the primary targets for UV radiation, pollution, toxic chemicals, and certain metal ions, all of which contribute to the generation of free radicals. Due to defective control of cell respiratory metabolism, including incomplete oxygen reduction in mitochondria and the creation of superoxide anion, hydroxyl radicals, and other free radicals, one of the primary causes of aging is free radicals, both oxygen and nitrogen species.Antioxidants that block free radical reactions, primarily autoxidation processes, are employed in contemporary cosmetology to reduce the negative effects of free radicals.The aim of this study was to investigate which method and solvent for extraction werethe most suitable for determining the antioxidant activity of selected cosmetic preparations (commercially available face creams). Solvents for the preparation of extracts were: isopropanol, isopropanol:water (50:50) and ethanol:water (70:30). Having the samples extracted, the antioxidant capacity of the obtained extracts was determined via six different spectrophotometric methods (ABTS, DPPH, DMPD, FRAP and two reduction methods (Fe and Mo). Depending on the extract type and method used, the antioxidant capacity of the samples differed. The best results among all the analyzed samples in all the appliedmethods showed samples of face cream containing 30% vitamin Cin suspension. Also, the method of preparation and the choice of solvent are two of the factors that affect the results of antioxidant activity.

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Antiproliferative, Antibacterial and Antioxidant Effects of Essential Oil of Pink Pepper

Horozić, E.[a,b*], Ademović, Z.[a], Dautović, E.[c], Cilović-Kozarević, E.[d], Husejnović, E.[e], Husejnagić, D.[f], Karić, E.[g], Ibišević, M.[g]

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Abstract: Pink pepper is classified intothe Californian/Peruvian type (*Schinus molle*) and the Brazilian type (*S.terebinthifolia*).According to studies, extracts and essential oils of pink pepper showed anti-inflammatory, antioxidant, antigenotoxic and antidiabetic properties in *in vitro* and *in vivo* studies. The results of bioactivity tests vary depending on the geographical origin of the pepper. In this paper, the antiproliferative, antioxidant and antibacterial effects of the essential oil of commercial pink pepper from the Tuzla market were investigated. To assess the cytotoxic potential, a tetrazolium salt reduction (MTT) viability assay was performed. Antioxidant potential was examined spectrophotometrically, using DPPH and FRAP methods. Diffusion and dilution techniques were used to evaluate the antibacterial activity of the essential oil.

The studied pink pepperessential oil inhibited the cell proliferation in the HeLa cell line. The analyzed oil caused dose-dependent cytotoxic effect. The essential oil significantly inhibits DPPH radicals. The reducing ability is also high. For the essential oil, an extremely good ability to inhibit the growth of the bacteria used in this study was confirmed. These results indicate a very high potential of essential oil of pink pepper as a natural antioxidant and inhibitor of pathogenic organisms.

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PP-OC-10

Antioxidant and AChE Inhibitory Activity of Some Helicin Derivatives

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Abstract: In this work, helicin and salicylaldehyde derivatives with L-cysteine (HelCys2 and SalCys2) were synthesized and characterized, which could potentially have many biological functions, such as the reduction of oxidative stress and the possibility of inhibiting acetylcholinesterase (AChE). Helicin (Hel) is a *β-D*-glucoside formed by the oxidation of the benzyl hydroxy group of salicin to the corresponding aldehyde. Prior to the synthesis of the Hel derivative and its aglycone (Sal) with the amino acid *L*-cysteine (Cys), the synthesis of Hel by slow oxidation of salicin with nitric acid was performed. All derivatives were characterized by Fourier-transform infrared spectroscopy, mass spectrometry, proton and carbon-13 nuclear magnetic resonance spectroscopy. The compounds were tested for the inhibition of acetylcholinesterase (AChE) from *Electrophorus electricus* and for antioxidant activity by scavenging 2,2-diphenyl-1-pycrylhydrazyl free radical (DPPH$^{\bullet}$) and 2,2´-azinobis(3-ethylbenzothiazoline-6-sulphonic acid) radical cation (ABTS$^{\bullet+}$) and reducing ferric ions. Of all tested samples, Sal (IC_{50} 1.45 μM) showed the best activity against AChE activity. Synthesized derivatives SalCys2 (IC_{50} 15.95 μM) and HelCys2 (IC_{50} 22.50 μM) showed significantly weaker activity against AChE activity. The best antioxidant activity in all applied tests showed the synthesized SalCys2 derivative.

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PP-OC-11

Examination of the Effect of pH on the Adsorption of Glyphosate on Pyrophyllite

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Abstract: In this study, we performed spectrophotometric analysis with ninhydrine and sodium molybdate to study the adsorption of the herbicide glyphosate on pyrophyllite. To test the removal of glyphosate by adsorption on pyrophyllite, the adsorption capacity (q_e) and removal efficiency (R) were monitored for initial glyphosate concentrations of γ = 15.5, 22.21, and 29.18 mg/L in the pH range of 1.17 to 13.47 at contact times of 60, 120, and 180 minutes. The partition coefficient (K_d) was calculated for all three glyphosate concentrations at all pH values. The results showed that the adsorption of glyphosate on pyrophyllite is pH-dependent due to different ionic species of glyphosate at different pH. The removal efficiency (R) of glyphosate at a contact time of 60 minutes in the pH range of 1.17 to 13.47 ranged from R = 0.90% (pH 4.01) to R = 75.09% (pH 13.47 andγ= 29.18mg/L). The alkaline medium proved to be more efficient for glyphosate adsorption because the removal efficiency ranged from R = 26.68% (pH 12.92) to R = 75.09% (pH 13.47). Glyphosate removal efficiency for 120 and 180 minutes at all tested pHs was best in the base medium at pH 13.47 (≈75%). After 60 minutes of contact time, the adsorption capacity was between q_e=0.05 mg/g (pH 4.01 and γ = 29.18 mg/L) and 0.44 mg/g(pH 4.01 and γ = 29.18 mg/L).Glyphosate adsorption capacity for 120 and 180 minutes at all tested pH was also the best in the base medium at pH 13.47 (q_e ≈ 0.45 mg/L). The distribution coefficient reaches a maximum value of ≈ 56 mL/g at pH 13.47 for all contact times at γ= 29.18mg/L. Results for fitting isotherm models showed that the Freundlich model is a little bit better fitted than Langmuir's.Based on the observed data for isotherm parameters, the chemical type of adsorption is clearly present.

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The sample of pyrophyllite used in this study came from the Parsovići mine in Konjic, and the authors are grateful to AD HARBI for donating it. This study was supported by Ministry of Higher Education, Science and Youth of Canton Sarajevo, contract number: 27-02-11-41250-6/21.

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Abstract

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Aggregation Behaviour of Benzododecinium Bromide in Aqueous Propylene Glycol Mixtures Revealed by Photon Correlation Spectroscopy (PCS) and ^{1}H NMR

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Abstract: Micelles are versatile tools that have many applications spanning many different industries. Type of solvents, addition of additives are just a few of those variables that if changed can interfere with formation of micelles. Propylene glycol is a compound widely used as a food additive while benzododecinium bromide is quaternary ammonium salt used as preservative and antiseptic in pharmaceutical products. In our work, we study how the presence of cosolvent affects the micelle structure process. According to the calculation of PCS experimental data regarding to the volume and number in system are present micelles with hydrodynamic radii of around 3 nm. In mixtures zeta potential values decrease as a result of glycol effect to charge of micelle. The result of collapse of micellar structure.From ^{1}H NMR experiment, upfield shifts of benzododecinium bromide peaks are not consistent with the increase of added propylene glycol in comparison to pure benzododecinium bromide. The shift is caused by the interaction of the polar part of benzododecinium bromide with the alcohol, causing the shielding effect and consequently, the lower ppm values.

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Effects of Ethanol Treatment on Thin-Layer Phenomena in "Apparently 2D and 3D Carbon Nanomaterials": Gallic acid at Graphene and Single-Walled Carbon Nanotubes

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Abstract: A modification of a glassy carbon (GC) surface usually includes carbon nanomaterials (CNMs) in order to study the redox behaviour of molecules of interest. The most important benefit of CNMs is "promotion of electron transfer". This phenomenon is often related to “faster electron transfer kinetics” that is commonly interpreted in terms of “electrocatalysis". However, this often results in neglecting the influence of diffusion phenomena in CNMs. This could lead a naive electrochemist using the semi-infinite model to infer an enormously large charge-transfer rate constant. Indeed, our results suggest different influence of ethanol pretreatment of certain CNMs on their electrochemical properties, which cannot be explained by "electrocatalysis". Based on our previous research, the elegant approach to the elucidation of the mentioned phenomena in terms of "thin-layer" diffusion was presented. In addition, the differences between "apparently 2D and 3D" CNMs were explained. For this purpose, the voltammetric as well as chronoamperometric methods were employed and diffusion parameters were calculated. Additional insight into the complex mass transport regime was obtained by electrochemical impedance spectroscopy. Finally, the observed phenomena were confirmed by insight into the geometrical structure using scanning electron microscopy. These phenomena were investigated on gallic acid behavior on single-walled carbon nanotube and graphene modified GC.

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Methodology for Investigating Dissolution and Redeposition Mechanisms of Pt-based Oxygen Reduction Reaction Electrocatalysts

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Abstract: Low-temperature proton exchange membrane fuel cells (LT-PEMFC) showed great potential for efficientconversion of chemical energy stored in hydrogen to electrical energy. The main disadvantage is sluggish oxygen reduction reaction (ORR) that needs further improvement in order for LT-PEMFC to reach commercial use. We present a novel methodology in investigating the structure-activity and structure-stability properties of Pt-based catalysts. The methodology is based on the "spot the difference" principle where identical location investigation of the same nanoparticle is investigated.[1] It consists of combining modified floating electrode (MFE) designed to test electrochemical properties of electrocatalysts at high current densities and scanning transmission electron microscopy (STEM). With this methodology, it is possible to obtain high-resolution TEM images of the same location of the nanoparticles before and after applying the electrochemical protocol. This way, using image registration algorithms and atomic position determination, it is possible to gain insight into mechanisms of Pt dissolution and redeposition.

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Microbiologicaly Influenced Corrosion of 304 Stainless Steel in Artificial Seawater

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Abstract: In this work, microbiologically influenced corrosion (MIC) of 304 stainless steel caused by *Pseudomonas aeruginosa*, strain ATCC 27853 in artificial seawater was investigated through electrochemical methods and spectrometry. Corrosion research was carried out using electrochemical techniques of potentiodynamic polarization (PP) and electrochemical impedance spectroscopy (EIS). Electrochemical tests were performed after immersion of coupons in the duration of 3, 7, 14, and 30 days in inoculated and sterile media. Characterization of structural properties of interfacial boundaries was described by electrical equivalent circuits. The corrosion rates obtained by Tafel plots were higher in the inoculated medium compared to the sterile medium. In addition, corrosion rates in inoculated media increased with the increase of immersion time. At the same time, there was a shift of E_{corr} to a more negative direction. The amount of Fe released after the static immersion test for coupons that had been incubated for 21 days in the inoculated and sterile medium was determined by inductively coupled plasma optical emission spectrometry (ICP-OES). The higher quantity of Fe was released from the coupons that were incubated in inoculated medium, which is in good agreement with the results obtained by electrochemical techniques. A slight change in pH value before (pH 7.16) and after (pH 7.10) 30 days of immersion tests indicates that corrosion of 304 stainless steel was not accelerated by metabolic byproducts of *P. aeruginosa*.

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Abstract

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Study of Thermodynamics of Mechanisms Underlying Antiradical Activity of Cinnamic Acid Derivatives – A Theoretical Approach

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Abstract: In this study, the role of antiradical moieties and molecular conformation in antioxidative potency of dihydrocaffeic acid (DHCA) and dihydroferulic acid (DHFA) was investigated by density functional theory (DFT) method. The thermodynamic preference of different reaction paths of double free radical scavenging mechanisms was estimated, and their reactivity towards different free radicals. Antiradical potency of DHCA and DHFA was compared with that exerted by their unsaturated analogs – caffeic acid (CA) and ferulic acid (FA). *Cis*/*trans* and *anti*-isomers of studied cinnamic acid derivatives may scavenge free radicals *via* double processes by involvement of catechol or guaiacyl moiety. Carboxyl group of s*yn*-isomers may also participate in the inactivation of free radicals. Obtained results indicate that the presence of structural motifs such as the catechol or guaiacyl moiety and carboxyl group in *syn*-DHCA and *syn*-DHFA is beneficial for the high scavenging efficiency of investigated phenolic compounds. These antiradical moieties enable inactivation of free radicals *via* different paths of double free radical scavenging mechanisms. Gibbs free energies of reactions of inactivation of various free radicals indicate that *syn*-DHCA and *syn*-DHFA, colon catabolites found in systemic circulation in very low μM concentrations, have potential to contribute to health benefits by direct free radical inactivation.

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The Effects of Vanillylmandelic Acid on the Oscillations of the Briggs-Rauscher Reaction

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Abstract: The Briggs-Rauscher reaction is an oscillating reaction that nowadays is investigated a lot because of its application for analyte concentration determination and as well for investigation of their antioxidant, antiradical, and catalytic properties. In this study, the effect of the concentration of aqueous solutions of vanillylmandelic acid on the Briggs-Rauscher reaction was investigated. The Briggs-Rauscher reaction mixture consisted of appropriate proportions of aqueous solutions of hydrogen peroxide, malonic acid, potassium iodate, sulfuric acid, and manganese(II) sulfate, without and in the presence of starch. The oscillations flow of the Briggs-Rauscher reaction mixture were monitored by the potentiometric method at 20±0.5°C. As the concentration of vanillylmandelic acid increased from 16 to 72 mg/L, the inhibition time of oscillations of the Briggs-Rauscher reaction mixture with and without starch increased linearly. The inhibition time was shorter in starch free mixtures. The number of oscillations and time of oscillations increased with the increasing concentration of vanillylmandelic acid, while the maximum amplitude of oscillations showed the opposite trend. The obtained results are in an agreement with previously suggested literature data that the starch could not be added for only visual performance in the Briggs-Rauscher reaction mixture, but it also affects the reaction itself.

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PP-PTC-07

Corrosion and Biocorrosion Properties of Selected Metallic Glasses

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Abstract: Metallic glasses based on copper (Cu) and zirconium (Zr) have great mechanical properties and corrosion resistance, which makes this material a promisingcandidate as material for potential medical implants. This research was focused on the determination of corrosion properties, primarily biocorrosion, of selected Cu-Zr and Cu-Zr-Al samples. Additionally, biocorrosion measurements were also carried out on a sample of the medical implant - 316L stainless steel as reference material. Regarding the fact that these metallic glass samples were not previously electrochemically characterized in great detail, there are potential applications to be discovered. Cu - based metallic glasses can potentially be used in engineering applications, based on their resistance to fracture stress, tensile strength, and corrosion resistance. With this in mind, potentiodynamic measurements in 1M H_2SO_4, a frequent medium for industrial applications, were carried out. The primary goal of the research was preliminary electrochemical characterization with broadening the field of application in mind. Potentiodynamic measurements were preformed also in 0.9% NaCl, and phosphate buffer as biocorrosion medium. Research has shown that metallic glass samples have better biocorrosion resistance compared to commercial medical implant (316L stainless steel). This implicates possible biomedical use, which requires additional cytotoxicity and biocompatibility tests. Corrosion parameters indicate that in some solutions pitting corrosion could occur. In conclusion, further investigation of the sample surface and measurements at higher potential could give us insight into the corrosion mechanisms of these systems.

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Examination of the Influence of 2,2,4-Trimethyl-2,3-dihydro-1*H*-benzo[*b*][1,4]diazepine on the Activity of Acetylcholinesterase

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Abstract: Today a great deal of time is spent on research of new drugs to treat diseases such as anxiety, depression, Alzheimer's and dementia. In this study, the inhibitory properties of 2,2,4-trimethyl-2,3-dihydro-1*H*-benzo[*b*][1,4]diazepine on the activity of the enzyme acetylcholinesterase were examined. The compound itself was synthetized on a solid surface by condensation of *o*-phenylenediamine and acetone in the presence of phosphorus oxychloride on the solidsurface (MgO). The pure product was obtained by crystallization from *n*-hexane, and later used in the process of examination of the inhibitory properties. The examination was conducted at three temperatures (25, 30, 37°C). Each sample was made up by the substrate, 5,5-dithio-bis-(2-nitrobenzoic acid) and a phosphate buffer of pH=8. In the standard sample, an internal standard donepezil was added without the examined substance. With the use of spectrophotometricmethods and by following the Michaelis-Menten model, it was concluded that the examined diazepine shows competitive type of inhibition on the enzyme acetylcholinesterase.

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Sage Extracts (*Salvia officinalis* L.) as Iron Corrosion Inhibitors

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Abstract: Ecological acceptability, which is now a critical factor in selecting a substance as a metal corrosion inhibitor, refers to the inhibitor's non-toxicity to humans and organisms with which it comes into contact, as well as its biodegradability.Ecologically acceptable inhibitors can be classified as natural organic inhibitors, and are often a mixture of different compounds, most of which are heterocyclic organic compounds that contain a nitrogen, sulfur or oxygen atom (a free electron pair atom involved in the process of adsorption on a metal surface). In this paper, the effectiveness of sage extract as an environmentally friendly inhibitor of iron corrosion was investigated. The tests were performed in 3% and 0.9% NaCl solution.Based on the results obtained by the Tafel extrapolation method, it is concluded that sage extract at a concentration of 2 g/dm^3 is an effective inhibitor of iron corrosion in 3% NaCl solution.Because the lowest corrosion current occurs at a concentration of 2g/dm^3, this concentration reflects the ideal concentration at which protection is most effective.At the optimal concentration of the inhibitor, the value of Rp is the highest, after that, an increase in the concentration of the inhibitor shows a decrease in the value of Rp.The results of Electrochemical impedance spectroscopyconfirm that sage is a corrosion inhibitor.The sample with the highest concentration of inhibitors has the highest resistance, while the sample without inhibitors has the lowest.Because the environment is more aggressive in 3% NaCl solution than in 0.9% solution, the inhibitors have a lower protective effect.The Tafel extrapolation method and Electrochemical impedance spectroscopy results showed some agreement, i.e., the Electrochemical Impedance Spectroscopy method was confirmed by the Tafel extrapolation method for a 3% NaCl solution.

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Investigation of Solvent Effects on Spectral Properties of Selected Xanthen-3-one Derivatives

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Abstract: Many naturally occurring xanthenes and their derivatives are found to exhibit significant biological and pharmacological properties, such as antibacterial, antifungal and antitumor activities. Xanthenes are known for their utility as leuco-dyes, pH-sensitive fluorescent materials for the visualization of biomolecules and in laser technologies due to their useful spectroscopic properties. Knowledge of the solvent effects on the spectra and the quantum yields of fluorescence is necessary for the utilization of these fluorescence materials to their maximum potential. The aim of this study was to investigate spectroscopic properties of nine selected xanthene-3-one derivatives in four solvents of different polarity. All tested substances fluoresce in each solvent, except the nitro derivative. The effects of substituent type, concentration, solvent polarity and solvent acidity on UV/Vis and fluorescent properties of the tested substances were recorded. There is very good correlation of the absorption and fluorescence with concentration, so the limits of detection and quantification were calculated. With the increase of concentration, quenching of fluorescence occurred, so for the spectrofluorimetric determination of concentration it is necessary to establish the concentration range in which the correlation is linear.

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Abstract

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The Influence of Trioxohydroxytetrafluorotriborate on the Activity of the HRP in the Presence of Potassium Ion

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Abstract: Trioxohydroxytetrafluorotriborate ($K_2[B_3O_3F_4OH]$) has been studied for a while, regarding its potential effect on the enzyme activity. Since it has been proven that it has good inhibiting effect on enzymes from oxidoreductase group, ($K_2[B_3O_3F_4OH]$) is assumed as the potentially new drug active component. The aim of this study was to investigate inhibition of Horseradish peroxidase (HRP) in the presence of one physiological electrolyte by spectrophotometric method and temperature corresponding the temperature of a human body (37°C). The activity of HRP was investigated in the presence of trioxohydroxytetrafluorotriborate of 2, 4 and 6mM concentration and the solution also contained potassium ion (5 mM). The method used for evaluation of HRP activity was spectrophotometric by the measurement of guaiacol peroxidation with H_2O_2, following the increase of absorbance at 470 nm. Lineweaver-Burk plots were linear, and both K_m and V_{max} values were affected. Given results indicate mixed type of inhibition.

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Radiochemistry (RC)

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Abstract

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Comparison of Agricultural vs. Cyanobacterial Based Biosorbents for Uranium (VI) Removal from Wastewaters

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Abstract: Uranium is widely used in many industrial sectors and with increasing demands for nuclear technologies, more radioactive wastewater is being produced via different resources, which is posing an emerging difficulty to the environment and human health. A very promising technique for wastewater treatment is a biosorption. In this research: red beet peel and cyanobacteria, *Anagnostidinema amphibium* (C.Agardh ex Gomont) Strunecký, Bohunická, J.R.Johansen & J.Komárek, were compared and investigated for U(VI) removal from wastewaters. The optimal conditions for U(VI) removal by red beet peel were T=25 °C, $m_{biosorbent}$=100 mg, t=60 min, pH=7, V= 50 mL with the removal efficiency of 85.87 %; while by cyanobacteria was favoured under T=20 °C, $m_{biosorbent}$=50 mg, t=40 min, pH= 9-11, V= 50 mL) with the removal efficiency of 95 %. Fourier-transform infrared analysis showed that functional groups on the red beet peel are mainly with O donor atoms, and on the surface of cyanobacteria are present functional groups with P, O and N donor atoms. Energy dispersive X-ray fluorescence analysis showed that element at the surface of red beet peel was potassium, and for cyanobacteria was found iron and calcium. Among others, the great advantage for cyanobacteria is their use in 4 cycles of sorption/desorption using the EDTA solution with uranium recovery of more than 80%.

POSTER PRESENTATIONS

Topics Related to Chemistry

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Abstract

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Characterisation of the Host-guest Interactions in Inclusion Complexes of Dimenhydrinate and 2-hydroxypropyl-β-cyclodextrin

Hindija, L.[a*], Hadžiabdić, J.[a],Sirbubalo, M.[a], Tucak-Smajić, A.[a], Rahić, O.[a], Vranić, E.[a], Špritović-Halilović, S.[a*]

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Abstract: Complexation of dimenhydrinatewith hydroxypropyl-β-cyclodextrin is a useful approachto overcome the issues with poor solubility and bitter taste of dimenhydrinate. Fourier Transform Infrared Spectroscopy (FTIR)is widely used method for detection of complex formation and complex characterisation in solid state.Inclusion complex formationcan be examined by identification of different functional groups that are present in inclusion process. Complexation leads to variation of the shape, position and intensity of the absorption peaks of guest and host molecule.The formation of the complexcan be confirmed due to changes in the characteristic bands of pure substances by comparing the FTIR spectra of starting compounds with the spectra of newly formed complex.

The aim of the present work is to investigate the occurrence of complete inclusionbetween dimenhydrinate andthree 2-hydroxypropyl-β-cyclodextrin derivates with different molar masses. Inclusion complexes were made by kneading and solvent evaporation method in molar ratio 1:1. Changes of the intensity of the specific spectral bands of both host and guest molecule and inclusion complexes were compared. Results of conducted analysis showed that dimenhydrinate had the most efficient complexation with 2-hydroxypropyl-β-cyclodextrin M=1387 g/mol due to absence of characteristic peaks of both host and guest molecules. Based on these results, it can also be established that kneading method provides more efficient complexation compared to solvent evaporation method.