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Book of Abstracts

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GENERAL INFORMATION

Congress dates
19-21 October 2018/ Sarajevo, B&H
www.pmf.unsa.ba/hemija/kongres

Language
The official language of the ICCCEB&H 2018 is English

Venue and Registration
Hotel Holiday, Zmaja od Bosne 4, Sarajevo
Registration desk will be open on 19 October 2018 Friday from 8:00 till 17:00 and on 20 October 2018 Saturday from 8:30 till 12:00

KEY TO ABSTRACT IDENTIFICATION

PL	Plenary lecture
OP	Oral presentation
PP-AC	Poster presentation - Analytical Chemistry
PP-IC	Poster presentation - Inorganic Chemistry
PP-BB	Poster presentation - Biochemistry and Biotechnology
PP-PHC	Poster presentation – Phytochemistry
PP-CAM	Poster presentation –Chemistry of Advanced Materials
PP-ENC	Poster presentation – Environmental Chemistry
PP-EDC	Poster presentation – Education in Chemistry
PP-CE	Poster presentation – Chemical Engineering
PP-PTC	Poster presentation – Physical and Theretical Chemistry
PP-OMC	Poster presentation – Organic and Medicinal Chemistry
PP-RC	Poster presentation – Radiochemistry
PP-TRC	Poster presentation – Topics related to Chemistry

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King Abdul-Aziz University,
Faculty of Science Department of chemistry
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Dr. sci. Cihangir Tanyeli
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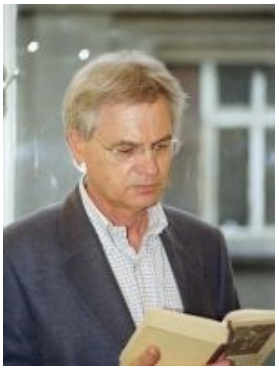
Department of chemistry
Ankara, Turkey



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Dr. sci. Katja Džepina
University of Rijeka, Rijeka, Croatia

Welcome note

On behalf of the Organizing and Scientific Committee, Society of Chemists and Technologists of Canton Sarajevo and the Faculty of Science in Sarajevo, it is our great pleasure to invite you to the **3rd International Congress of Chemist and Chemical Engineers of Bosnia and Herzegovina (ICCCEB&H 2018, www.pmf.unsa.ba/hemija/kongres)** in Sarajevo. The annual ICCCEB&H Congress series, first launched in 2014, presents an ideal platform for fruitful exchange of ideas which is crucial for scientific advancement.

1st ICCCEB&H	2014
2nd ICCCEB&H	2016

We are delighted to inform you that ICCCEB&H 2018 will have 15 Oral and 79 Poster presentations, in addition to the plenary lectures.

Thanks to the invaluable efforts of our Scientific Board Members, we were able to convince numerous world-class scientists to join us in this unique event as Plenary and Invited Lecturers. The impetus generated by these inspiring and high-caliber distinguished speakers enabled us to attract, more than 120 participants, and 90 abstract submissions.

We now have scientists from Bosnia and Herzegovina, Turkey, Saudi Arabia, Slovenia, Singapore, Algeria, Jordan, Nigeria, Croatia, Serbia, and Montenegro.

All submited abstract will be publish in special issue of Bulletin of Chemists and Technologists of Bosnia and Herzegovina, and some number of papers will be published in the regular issue of Bulletin of Chemists and Technologists of Bosnia and Herzegovina.

The Congress will cover different areas of chemistry and chemical technology and offer an opportunity for scientists to exchange latest research findings and ideas and develope a collaboration with colleagues from Bosnia and Herzegovina and from all around the world.

There are many people that deserve credit for the organization of ICCCEB&H 2018, such as, the members of the Organizing Committee, International Scientific Committee, Scientific Committee, all of the sponsors, and last but not the least to all of the participants, without which this event could not be realized.

We welcome all of you once again to the ICCCEB&H 2018 event, and wish you an extremely fruitful interactive and enjoyable meeting and a pleasant stay in Sarajevo, Bosnia and Herzegovina.

Organizing committee

CONTENT

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ICCCEB&H wishes to express its gratitude to the following companies that helped us in organizing ICCCEB&H 2018

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Abstract

PL-01

Selected Topics on Chemical Fingerprinting – Examples and Challenges

Igor Jerković

Department of Organic Chemistry, Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21000 Split, Croatia

Abstract: The research has been focused on the phytochemical fingerprinting from different natural sources (aromatic plants, honey, or marine algae), using advanced chemical methods and hyphenated techniques. Gas chromatography with mass spectrometry (GC-MS) is appropriate hyphenated technique for the research of headspace, volatile and semi-volatile compounds present in different samples that could be useful for their classification, particularly since specific or non-specific chemical markers of the botanical origin can be found and/or specific chemical fingerprints can be determined. Different classes or natural organic compounds can be found such as terpenes (particularly monoterpenes and sesquiterpenes), norizoprenoids, benzene derivatives, others. However, before the analysis it is necessary to perform adequate preparation steps such as: ultrasonic solvent extraction (USE), headspace-solid phase microextraction (HS-SPME), solid-phase extraction (SPE), supercritical CO_2 extraction (SC-CO_2), hydrodistillation (HD) and simultaneous hydrodistillation extraction (SDE). However, the artefacts can be generated during the extraction steps (particularly due to the influence of heat and/or water) and different methods should be used to establish the artefacts formation. To obtain reliable chemical profiles it is often necessary to use different preparative techniques since the use of only one extraction method can neglect certain group of compounds.

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Abstract

PL-02

Chemical Characterization of Atmospheric Aerosols in the Sarajevo Canton: Results of 2017-2018 Sarajevo Canton Winter Field Campaign (SAFICA)

Katja Džepina

Department of Biotechnology, University of Rijeka, Rijeka, Croatia

Abstract: The World Health Organization (WHO) identified air pollution as the world's largest single environmental health risk causing seven million deaths per year, one in eight deaths globally. Of particular concern are heavily polluted and understudied urban centres: while thousands of scientific papers have been published on air quality of the cities such as London, UK and Los Angeles, USA, only 41 papers exist on the top 10 globally most polluted cities. Sarajevo, the capital of Bosnia and Herzegovina (B&H), is one of urban centres which often experiences low air quality due to the extensive use of non-renewable energy sources and geographical location. For example, in Sarajevo during 2010, an annual average concentration of particulate matter (PM) with a diameter smaller than 10 μm (PM_{10}) was 50 μg/m^3, a value 2.5x higer than the recommended WHO guidelines value of 20 μg/m^3. Sarajevo Canton Winter Field Campaign 2017-2018 (SAFICA) took place in the Sarajevo Canton during the cold winter season of 2017 – 2018 (Dec 4, 2017 – Mar 15, 2018), the period historically characterized with the lowest air quality according to the available data. SAFICA project was lead by Federal hydrometeorological Institute of B&H, Institute of Public Health of the Sarajevo Canton, University of Sarajevo and University of Rijeka, and field measurements took place at three urban locations within the city of Sarajevo (Otoka, Pofalići i Bjelave) i one remote location (Ivan Sedlo mountain ridge). In this presentation, the basics of anthropogenic air pollution and its global influece on the air quality will be explained. Particular attention will be given to the atmospheric PM or aerosols, and aerosols formation mechanisms and the importance of their characteristics such as atmospheric concentration, size and chemical composition will be explained. Also, the reasons for the adverse effects of aerosols on human health and the correlation of atmospheric fine PM ($PM_{2.5}$) concentrations and human mortality will be explained. Finally, preliminary results of SAFICA measurements campaign will be presented and compared with those from other global urban centers.

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Abstract

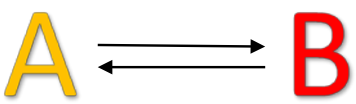
PL-03

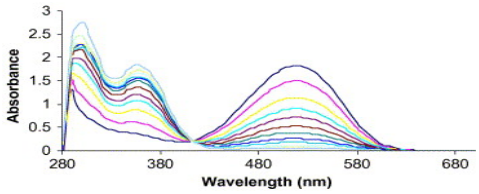
Synthesis and Use of Photochromic Compounds as Smart Switchable Glazing for Ultraviolet Shielding

Abdullah Mohamed Asiri

Chemistry Department, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

Abstract: Photochromism is a reversible transformation of a chemical species induced in one or both directions by absorption of electromagnetic radiation between two forms, A and B, having different absorption spectra. The Photochromic performance of some organic photochromic compounds will be studied in depth in polymer matrices. The rate constant and half-life of both coloration and bleaching will be demonstrated and the effect of organic UV absorbers doped in the polymer matrices will also be presented. The fatigue studies of the undoped and doped photochromic polymer Films will be highlighted. The prepared films demonstrate the easy and stable method of how the photochromic materials can be used in commercial applications.





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Abstract

PL-04

Discovery of Novel Enzyme Inhibitors from Nature *via in vitro* and *in silico* Methods

Ilkay Erdogan Orhan

Department of Pharmacognosy, Faculty of Pharmacy, Gazi University, Ankara, Turkey

Abstract: Natural products are always important in finding new drug candidates and natural product chemistry research has been a mainstay in drug discovery and development. Enzyme inhibitors are known as one of the strongest therapy strategies against a wide range of diseases. In other words, enzyme inhibitors are one of the vital classes of drugs clinically available. In search novel enzyme inhibitors from natural sources being mostly plants, we have been screening many medicinal plants and pure natural compounds using microplate assays against a number of enzymes including cholinesterase family, elastase, collagenase, tyrosinase, xanthine oxidase, phosphodiesterase-I, carbonic anhydrase-II, lipoxygenase, HMG CoA reductase, etc. Since some of these enzymes are related to cosmetics, we have been also studying developing new formulations for anti-aging cosmetics. The active inhibitors found by our group are further investigated by *in silico* methods using molecular docking experiments. During these studies, we found many promising compounds such as coumarins and other polyphenolics such as flavonoids have been identified as active inhibitors through our results. In this study, examples of natural products as promising inhibitors determined by our group against different enzymes will be underlined.

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Abstract

PL-05

Asymmetric Organocatalytic Synthesis of 2-Oxindole Based Hetereocycle Precursors

Cihangir Tanyeli

Department of Chemistry, Middle East Technical University, Çankaya, Ankara, Turkey

Abstract: Recent literature on the bioactivity of isatin (indoline-2,3-dione) derivatives triggered organic chemists to make use of the unique potential of isatin in asymmetric organocatalytic synthesis. Due to extensive presence of 2-oxindole skeleton, especially spiro-fused cycles, in many natural products, they drew the special interest in the disciplines of medicinal chemistry and agrochemistry. Due to highly reactive prochiral carbonyl group, isatins are potent precursors for the synthesis of 3,3-disubstituted spirooxindoles. Direct nucleophilic addition to isatin-derived ketimines is one of the straightforward approaches leading to α-chiral amines which are frequent subunits of pharmaceuticals and agrochemicals besides being heterocycle precursors. In this respect, asymmetric organocatalytic synthesis offers facile and environmentally benign reaction process and selectivity as well. Remarkable advantages of cooperative activation of substrates via bifunctional organocatalysts bearing H-bond donor components such as urea, thiourea and squaramide are indispensable. Modulation of sterically encumbered units such as 1-adamantyl, 2-adamantyl and *t*-butyl in the structure of organocatalyst reveals distinct changes in stereoselectivity of the synthetic transformations.

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Abstract

PL-06

Laser Ablation – ICPMS: A Tool for Multielement Microanalysis of Solid Samples

Johannes T. van Elteren

Department of Analytical Chemistry, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

Abstract: Laser ablation – ICPMS is a multielement, microanalytical technique that has developed rapidly since its inception by Gray in 1985.[1] Its multidisciplinary character follows from applications in various fields such as biology, medicine, geology, archaeology, forensics, materials science, etc. Initially a tool for probing the bulk element concentrations of multifarious solid samples (biological tissues, alloys, plastics, glasses, etc.) via drilling or line scanning actions, it has become a very powerful technique to assess the surface (2-dimensional) and volume (3-dimensional) element distribution. During the last five years, instrumental improvements to the laser ablation cell and its interface with the ICPMS have led to 25-100 times faster surface and volume mapping times, making high resolution scans in reasonable mapping times (hours) possible.[2] With the latest generation of laser ablation – ICPMS instruments one can obtain better than 5x5 μm^2 pixel resolution with a detection limit on the $\mu g\ kg^{-1}$ level for most elements of the periodic table. This presentation will focus on the fundamentals of the laser ablation – ICPMS technique, the development of the technique, its latest incarnation, and examples of multidisciplinary applications.

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1. Gray, *Analyst*, 1985,110, 551.
2. Van Malderen et al., *J. Anal. At. Spectrom*, 2016, 31, 423.

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Abstract

PL-07

Aqueous Solvation of Charged and Hydrophobic Groups: from Simple Ions to Proteins

Vojko Vlachy

Department of Phisical Chemistry, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

Abstract: Much of biology depends on proteins interacting with each other – pairwise or in aggregates – all mediated by water and ions. Understanding the aqueous solvation of electrolytes, simple and complex, is therefore important for biology, as also for industry. But today's solvation models mostly apply to dilute solutions and, despite being supported by all-atom simulations, do not yield good results for thermodynamic properties. In recent years we applied statistical-mechanics to such systems. We used Wertheim's integral equation and thermodynamic perturbation theories, which are well suited for systems of molecules with directional forces. Such an approach is able to treat mixture of water molecules, ions and proteins, with all the species treated on equal level of approximation. We begin the presentation with the aqueous solutions of alkali halides to show the effects of ionic sizes of salt–forming ions on osmotic properties of the solution. Next, we ask ourselves how the presence of hydrophobic groups affects the solution energetics? We conclude the presentation with discussion of the protein (globular proteins as also the monoclonal antibodies) self–association. In several examples we demonstrate, that one of the crucial parameters to understand aqueous solutions is the free energy of hydration of interacting charges.

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ORAL PRESENTATIONS

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Abstract

OP-01

Extraction Methods Development and Optimization for Chromatographic Analysis of Pharmaceuticals in Sediment

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Microwave Assisted Extraction (MAE)
Pressurized Solvent Extraction (PSE)
Ultrasound Solvent Extraction (USE)
High Performance Liquid Chromatography (HPLC)

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Abstract: Pharmaceuticals are substances that are used in human and veterinary practice and are so-called emerging contaminants. Their occurrence in the environment is still not law regulated, while certain number of published articles record their negative impact on human health. From the literature overview, pharmaceuticals were determined in different environment samples like water, sludge, soil, manure and little bit less in here examined sediment. Sediment acts like a potential receiver for many hazardous substances including pharmaceuticals which can be easily emitted to drinking water reservoirs depending on the sediment characteristics. In this work pharmaceuticals that belong to different structure groups were determined in sediment sample and following five extractions were developed and optimized: EA, USE, MAE, MSPD and PSE. Chosen pharmaceuticals were tylosine as macrolide antibiotic, albendazole, febantel and levamisole as antihelmintics, lidocaine and procaine as anaesthetics and hydrocortisone and dexamethasone as glucocorticoids. Pharmaceutical concentrations extracted from sediment sample were determined by high performance liquid chromatography using diode array detector. After chromatographic analysis, all methods were validated and the following optimal parameters were determined for each extraction method: sediment mass, solvent, contact time between sediment and solvent, extraction duration, agitation frequency and extraction temperature (EA); solvent, extraction duration, power and temperature of ultrasonic bath (USE); organic solvent, extraction duration, temperature, solvent volume (MAE); sorbent, solvent, solvent volume, sediment/sorbent mass ratio (MSPD); solvent (PLE).

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Abstract

OP-02

Polycyclic Aromatic Hydrocarbons in PM_{10}, $PM_{2.5}$ and PM_1 Particle Fractions and Their Carcinogenic Activity

Pehnec, G., Jakovljević, I.

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Abstract: Polycyclic aromatic hydrocarbons (PAHs) are one of the first atmospheric pollutants identified as suspected carcinogens. In ambient air, PAHs with higher molecular weights (more than 4 rings) are mostly bounded to particles. Particle size plays an important role in assessing health risks. The aim of this study was to compare concentrations of PAHs bound to particle fractions $PM_{10,}$ $PM_{2.5}$ and PM_1 (particles with a diameter smaller than 10 μm, 2.5 μm and 1 μm, respectively) as well as to estimate their carcinogenic potency. Measurements of ten PAHs were carried out in 2014 at urban location in the northern part of Zagreb, Croatia. 24-hour samples of PM_{10}, $PM_{2.5}$ and PM_1 particle fraction were collected, forty per season. The PAH analysis was performed using high performance liquid chromatography with a fluorescence detector. The total carcinogenic potency (TCP) of PAHs was estimated by calculating benzo(a)pyrene equivalent concentrations using toxic equivalence factors from the literature. The average TCPs for the overall period were 4.287, 1.898 and 1.630 ng/m^3 for $PM_{10,}$ $PM_{2.5}$ and PM_1, respectively. The lowest TCP was recorded in summer and the highest in winter. The highest contribution to the TCP were from benzo(a)pyrene, dibenzo(a,h)antrachene, indeno(1,2,3,cd)pyrene and benzo(b)fluoranthene and altogether they contributed between 91 and 94 % in all fractions and seasons.

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Abstract

OP-03

Calcined Colemanite as Filler for Epoxy Composite Materials

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Calcined colemanite
Epoxy resin
Composite material

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Abstract: Substantial boron compounds such as colemanite, ulexite and tincalconite are found in Turkey with a worldwide share of 72% in terms of B_2O_3 content. They are utilized in agriculture, textile, cleaning products as well as glass, ceramic, cement and nuclear industry. Boron compounds have synergistic effects on the mechanical, wear, corrosion and thermal properties of the polymeric materials which are commonly used in transport, automotive, aerospace, construction and many engineering applications [1, 2]. In this study, epoxy composite materials including calcined colemanite as filler at different ratios (0, 5, 10, 15, 20 wt%) were prepared after calcination process of colemanite at 430 °C for 75 min. Amorphous structure of the epoxy composite materials was determined from XRD analysis. The dispersion of filler in the epoxy resin was investigated with SEM analysis. The mechanical, water sorption and corrosion resistance properties of the epoxy composite materials were examined according to ASTM Standards. And also, thermal properties of the composites were investigated with TGA and DSC analyses in details. As a result, it was revealed that the usage of environmentally friendly calcined colemanite enhanced the properties of polymeric materials.

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Abstract

OP-04

Relationship between Platinum Group Elements in Air and Meteorological Parameters

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Abstract: Platinum group elements (PGE), in particular platinum (Pt), palladium (Pd) and rhodium (Rh) have a significant role in the operation of automotive catalytic converters whose purpose is to reduce emissions of gaseous pollutants into the air. Hot exhaust gases passing through catalytic converters cause damage to these systems leading to emissions of Pt, Pd and Rh in the environment and increase their levels in the air. Weekly PM_{10} samples were collected in 2017 at two monitoring stations (North - urban background and South - urban traffic) in Zagreb and mass concentrations of Pt, Pd and Rh were measured by inductively coupled plasma mass spectrometry (ICP-MS). The average annual mass concentrations for Pt, Pd and Rh were 0.373 pg m^{-3}, 2.053 pg m^{-3} and 0.316 pg m^{-3} for monitoring station North and 0.681 pg m^{-3}, 3.843 pg m^{-3} and 0.574 pg m^{-3} for monitoring station South, respectively. In this study, the relationship between Pt, Pd and Rh mass concentrations and meteorological parameters, including air temperature, relative humidity, precipitation, air pressure, wind direction and wind speed was analysed. The wind roses at both monitoring stations pointed to a common source for all three of the measured metals. At monitoring site North, the pollution was connected with winds from north and northeast, while at monitoring station South with winds from the southeast.

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Abstract

OP-05

Comparison of Thermal Protocols for the Determination of Carbon in Particulate Matter

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QUARTZ protocol, TC

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Abstract: Daily samples of $PM_{1.0}$ particulate matter fraction (particles with an aerodynamic diameter below 1 μm) were collected from 1 January to 31 March at an urban background station located at the Institute for Medical Research and Occupational Health, Zagreb, Croatia. Elemental (EC), organic (OC) and total (TC) carbon, which is the sum of OC and EC, were analyzed by thermal-optical transmittance method by two different thermal protocols (NIOSH-like called QUARTZ (NIOSH - National Institute for Occupational Safety and Health) and EUSAAR_2 (EUSAAR - European Supersites for Atmospheric Aerosol Research) protocol and the results were compared. Mass concentrations of $PM_{1.0}$ ranged from 4.7 μg m^{-3} to 58.9 μg m^{-3}.

Very good agreement was observed for TC (slope= 1.0, R^2 = 0.99) and mass concentrations for both protocols ranged between 2.9 μg m^{-3} and 21.2 μg m^{-3}. EC mass concentration levels were found to be lower for QUARTZ than for EUSAAR_2, due to the differences in the heating profiles. The EUSAAR_2 protocol with a rather low peak temperature in the inert mode generally classified more carbon as EC compared to the QUARTZ protocol. The slope between EC_{E2} and EC_Q following transmittance correction was 1.5 (R^2 = 0.88), while the slope between OC_{E2} and OC_Q was 1.0 (R^2 = 0.98).

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Abstract

OP-06

Online Methods in Chemical Education: the Revolution is Here

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Abstract: The mode of teaching in Universities has not changed greatly for a century or more. The technology associated with the internet means that we can now make major changes as we move further into the 21st Century.

After Division of Chemistry and Biological Chemistry at Nanyang Technological University (NTU) was established in 2005, extensive e-learning resources were put in place and have continued to be developed, and a strategy to ensure student involvement was designed. We now have a blend of written material, images, videos and quizzes deployed in online sequences in order to ensure that students are prepared for practical work.

NTU has since then launched a major initiative on "Technology Enabled Learning" (TEL). We are building on our earlier experience to use technology in all courses. These initiatives are opening up opportunities to change the way students learn. Can we take advantage of technology to take a great leap forward in the quality of university education, or will it be much ado about nothing?

The e-Learning described in this lecture was employed in courses on Forensic Science and Organic Chemistry (including laboratory courses) at NTU and evaluated by discussion with the students and by formal teaching feedback.

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OP-07

Academic vs. Industrial Research-Dichotomy or Synergism?

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Cytoxazone
Dynamic Kinetic Resolution (DKR)

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Abstract: Two examples will be presented illustrating how research project in industry was promoted by collaboration with academic institution, and *vice versa*. Both projects are in part completed at "Ruđer Bošković" Institute, Zagreb in collaboration with one domestic and foreign company.

The first example, "from academy to industry", illustrates combined chemo- and biocatalytic synthesis of *Cytoxazone* and related isomers. Cytoxazone was isolated as fermentation product of *Streptomyces sp*. strain, and exhibits significant imuno-stimulating activity.

The second example, "from industry to academy", refers to discovery of unprecedented enzymatic *dynamic kinetic resolution* (DKR) of racemic epoxides into only one enantiomer of heterocyclic target molecule, an important chiral building block for the synthesis of optically pure dugs.

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Abstract

OP-08

Coupling Magnetite Nanoparticles with Zeolitic Tuff Sorbent Material for Olive Mill Wastewater (OMW) Remediation

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Zeolitic tuff

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Abstract: Olive Mill Wastewater **(**OMW) generates during olive milling industry in large quantities. It has high organic and phenolic content and represents an environmental problem. This work aimed to treat OMW by developing an environmentally friendly and cost-effective media that can remove phenolic compounds upon interaction between magnetic nanoparticles and natural raw material. Magnetite (Fe_3O_4) and Goethite (FeO(OH)) were prepared by microemulsion method. FeO(OH) nanoparticles were prepared using dimethylene-1,2- bis dodecyldimethylammonium bromide (CTAB) as surfactant. The structural and morphological characterization for Nanoparticles (Nps) were determined by XRD and TEM. The average crystalline sizes for Nps were 5-16 nm. The media were prepared, developed and tested, with multi adsorbent systems by two approaches, then were mixed and coated to synthesize nanocomposite media of (magnetite, goethite/ Zeolitic tuff), under different parameters: contact time, % of (Nps / OMW), % of (Media / OMW), temperature, and pH. Direct photometric method was used for analysis the real samples. The optimum conditions were 3% of media/OMW, 3 days of contact time, pH 5, and RT. Results showed that % removal was 79%. For coating approach of (magnetite/zeolite) the removal was 67% at pH 3, while at pH 5 it was 75%.

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Abstract

OP-09

Effectiveness of Plants Fiber Impregnated with Green Nanoparticles for Water Disinfection

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More than one billion in the world do not have access to safe drinking water. In order to improve the quality of water that meet communal needs, a reliable and adequate safe water supply in a cost-effective way is a vital need. In this study, Titanium Dioxide nanoparticles (TiO_2 NP) were synthesized using green hydrothermal method and then mixed with pristine pomegranate peel extract (PPP) to develop the nanocomposite media (PPP-TiO_2). The media were fully characterized by Scanning Electron Microscope (SEM), Dynamic Light Scattering (DLS) and X-ray Powder Diffraction (XRD). The media showed a randomly oriented grains with various shapes and sizes and sharp grain boundaries. Grain size ranges from 1 to 5 μm. SEM micrographs also clearly showed the damaged bacterial cells treated with PPP-TiO_2. Furthermore, the biological activity has been evaluated by well diffusion method, Microbial Inhibition Concentration (MIC), Minimum Bactericidal Concentration (MBC), growth curve profiling and live/dead cell assay. Tests have been performed at different concentrations and for three types of bacteria (*Staphylococcus aureus* (gram positive), *Pseudomonas aeruginosa*, *Escherichia coli* (gram negative). The antimicrobial activity for the nanocomposite media (PPP-TiO_2) was higher by 1.5 time compared to PPP or TiO_2-NP and exhibited higher antibacterial effect against tested gram positive (MIC_{90} of 189.1, MIC_{50} of 101.2, MBC 200 (μg/ml)) than gram negative strains. In addition, less dense and large number of dead cells were observed for bacterial cells exposed to PPP-TiO_2 treatment compared to non-treated controls using Live/Dead Baclight bacterial viability assay. These results revealed that the fabricated media has a potential to be used in water disinfection.

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Abstract

OP-10

Hydrogen Bonding and Solvent Effects on Calixarene Coordination Reactions

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Abstract: Calixarenes are macrocyclic compounds comprising phenolic units *ortho*-linked by methylene bridges. Many calixarene derivatives are known to be very efficient and in some cases selective binders of ions and neutral molecules. Our group has been extensively investigating the complexation reactions of calix[4]arene derivatives in several solvents by means of an integrated thermodynamic, structural, and computational approach. The solvents were chosen taking into account the differences in their cation (anion) and ligand solvation abilities and the possibility of ligand-solvent and complex-solvent hydrogen bonding. The thermodynamic data (complex stability constants and derived reaction Gibbs energies, reaction enthalpies and entropies), determined using several experimental techniques, were correlated with the structural results obtained by X-ray crystallography, NMR, and computational methods (DFT and molecular dynamics). The solvation and transfer parameters of the ligands and their complexes were also determined and discussed. The intra- and intermolecular hydrogen bonding and solvent effects (especially specific solvent-solute interactions) on the equilibria of the binding reactions were particularly addressed.

The results of the above-mentioned studies clearly indicates how remarkable and complex the influence of the solvent on the ion-hosting abilities of the calixarene derivatives, and macrocycles in general, can be. They also suggest that the integrated and comprehensive experimental and computational investigations can indeed provide a rather detailed insight into the ligand properties and reactivities, *i.e.* the factors governing the complexation processes.

This work has been fully supported by Croatian Science Foundation (project IP-2014-09-7309).

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Abstract

OP-11

Incorporation of Quercetin into New Nanocarriers Formulated from Edible Oils and Biodegradable Polymers

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Abstract: Phospholipids' liposomal formulations are highly favorable as antioxidant carriers in clinical applications due to their unique properties such as high biocompatibility and flexibility. Phospholipids' liposomal formulations, however, still suffer from many drawbacks including high cost of production and their inflammatory response. In addition to that, phospholipids' liposomal formulations are instable and susceptible to hydrolysis and oxidative degradation. In this study, two different nanocarriers formulations composed of in-expensive and non toxic lipids (myristic acid, coconut oil, and cholesterol) were developed as an alternative for phospholipids' liposomal formulations. These two new formulations were used to encapsulate quercetin. Thin-film method was used for liposomal preparation. All nanoparticles were characterized using SEM, TEM, light scattering techniques and zeta potential. The encapsulation efficiency was determined using HPLC equipped with a UV-visible spectrometer.

The physicochemical properties of new formulations and phospholipids' liposomes were similar. The introduced formulation showed good ability to control release and entrap quercetin in a similar manner observed in liposomes. The developed nanocarriers from edible oils could shift the current paradigm of using instable natural phospholipid and expensive synthetic phospholipids to formulate liposomes.

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OP-12

Utilisation of Derivative UV/Vis Spectrophotometry in Determination of Active Pharmaceutical Ingredient Content in Some Drugs

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Spectrophotometry

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Abstract: The aim of this paper, was to investigate the utilization of derivative UV/Vis spectrophotometry in the quantification of active pharmaceutical ingredients (API) in some drugs. Meloxicam, naproxen and acetylsalicylic acid (ASA) were the selected APIs that were analyzed in different drug samples. The analyses were carried out on the Perkin-Elmer Lambda 25 spectrophotometer in triplicate. The pure APIs were used as standards, and the calibration curve method was used to determine the concentration of the API in the samples. Absorption spectra were recorded in the ultraviolet (UV) region (200-400 nm) for meloxicam and naproxen, and in the visible (Vis) region (400-800 nm) for ASA.

After recording the absorption spectra, a third-order derivation was made using computer software. The obtained API content was within acceptable limits with the declared values (d.v.) for the two drugs: [naproxen in Nalgesin S (Krka), and meloxicam in Melox (Nobel)]. The observed deviations were <10% (the measured naproxen content was 90.06%, and for meloxicam 92.27%) of the d.v., which is in line with the *U.S. Pharmacopoeia* (*U.S.Ph.*). In the case of Aspirin protect 100 (Bayer), the content of ASA was 89.56% of the d.v., which is slightly lower than that prescribed by the *U.S.Ph.* (deviation ±5% of the d.v.).

Based on the obtained results, it can be concluded that UV/Vis derivative spectrophotometry is a suitable method for determining the content of API in some drugs.

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Abstract

PP-OP-13

Curcumin: Phytochemical Therapy for Treating Hyperlipidemia

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Abstract: In modern world, hyperlipidemia is the most common disorder mainly caused by lifestyle habits and major cause of cardiovascular, coronary and atherosclerotic changes. Such disorder is characterized by abnormally elevated levels of any or all lipids or lipoproteins in the blood. A wide range of medical therapeutics, class of antihypolipidemic drugs, are available for the treatment of hyperlipidemia, but such drug-therapies are carried out with presence of various side effects. In the last decades, many studies are carried to confirm beneficial effects of therapies based on different phytochemical agents that overcome side effects caused by synthetic drugs. According to Ayurvedic recommendations and experimental studies, numerous phytochemical agents have been reported to posses different antihyperlipidemic properties. One of the most studied phytochemical agent - Curcumin, herbal polyphenol and active ingredient isolated from the rhizome of the plant *Curcuma Longa*, has been reported to posses wide range of pharmacological properties including antimicrobial, antioxidative, antiinflammatory and anticancer property. Recent studies also suggests curcumin as potential lipid lowering candidate in treatment of hyperlipidemia. The purpose of this review is to present and discuss phytochemistry, mechanisms and pharmacological activity of curcumin, demonstrating its importance as potential therapy for treatment of hyperlipidemia.

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OP-14

Comparison of Microwave Induced and Conventional Synthesis of Caffeine and Structural Characterization of Synthetic Products

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Abstract: Caffeine (1,3,7-Trimethylxanthine) is a purine alkaloid presented in numerous plants (green/black tea leaves, coffee, cocoa). It is highly biological active compound, usually extracted from row plant materials by decaffeination process or synthesised. Since most conventional organic reactions are long-lasting and take place at very high temperatures with the use of toxic solvents, alternative methods such as microwave (MW) assisted synthesis are introduced. We report here both conventional and MW induced method for the preparation of caffeine from teobromine by S_N2 reaction mechanism, with NaOMe as a base and MeOH as a solvent. Conventional synthesis lasted 60 min under 50-60 °C with a caffeine yield of around 80%. MW induced synthesis under 29, 56 and 71°C lasted 2-5 min yielding 80,48 - 92,93% coffeine. The best results were obtained under MW synthesis at 56°C with water as a solvent. Purity of all samples was checked by TLC and melting point determination before (235-240°C) and after sublimation (236-239°C) that matched literature values for caffeine standard. The FTIR spectra of all samples showed remarkable agreement with the caffeine standard spectrum. As from our best knowledge, no research group reported MW assisted synthesis of caffeine of any kind.

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OP-15

Contamination of Plants, Soil, and Building Stones at a Roman Heritage Archaeological Site in an Urban

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Stone Restoration

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Abstract: Some cultural heritage sites in Jordan are in urban areas being exposed to anthropogenic pollution. Therefore, it is important to evaluate the contamination at these sites to protect them. Here, we considered a Roman archeological site (Nymphaeum) situated in Amman. The contamination in soil, plants, and building stones did not show spatial distribution within the site. The contamination was the highest in soil with least value 10^4 ppb for Cd and highest values ~3.5×10^6 and 10^7 ppb for sulfur and Al respectively, whereas in plants was the least for Cr (~400 ppb) and in building stones it was the least for Cu (~860 ppb). The highest contamination in plants and building stones was found for Al (~5×10^4 and ~6.2×10^5 ppb respectively). The sulfur content in plants (~7.6×10^5 ppb) was higher than that in the building stones (~2.3×10^5 ppb). The heavy metals and sulfur contamination in the building stones were lower than what was reported elsewhere outside Jordan.

POSTER PRESENTATIONS

Analytical Chemistry

(AC)

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Abstract

PP-AC-01

GC-FID Method Validation for Assay Determination of Camphor, Levomenthol, Methyl Salicylate and Benzyl Nicotinate in Cream for Treatment of Rheumatic, Sciatica or Sport Injuries

Buza, N., Behlulović, B., Krešić, D., Avdić, N., Alagić-Džambić, L., Pašić-Kulenović, M.

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Methyl Salicylate
Benzyl Nicotinate
GC-FID

Abstract: Camphor, levomenthol, methyl salicylate and benzyl nicotinate are agents used for treatment of rheumatic, sciatica or sport injuries. The objective of this study was to develop and validate single GC-FID method for assay determination of all four active compounds. Standards and samples were dissolved and prepared in chloroform. The chromatographic separation was performed on capillary DB-FFAP, 30 m · 0.32 mm (0.50 µm) column, with nitrogen as carrier gas. After injection of the sample at inlet temperature of 220ºC, the temperature of the GC oven was as follows: initial was 70ºC, held for 2 min, increased to 240ºC at a rate of 5ºC/min held for 5 min. Detector temperature was 260ºC. Injection volume of sample was 1 µl in split mode 10:1 ratio. The method was validated as per ICH guidelines for various parameters such as precision, linearity, accuracy, solution stability, robustness. The method showed specificity, accuracy (Recovery=97.5%-103.0%), linearity ($R_{samples}$=0.99920-0,99998, $R_{standards}$=0.99922-0.99955), precision (Recovery=99.4%-103.0%), and high sensitivity (LOD=0.36 mg/ml-3.66 mg/ml, LOQ=1.48 mg/ml-12.20 mg/ml) for all four active compounds. The method was robust with lower flow and lover initial temperature of column, but it was not robust with higher flow and higher initial temperature of column.

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Abstract

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Effect of Primary Packaging Material and Storage Conditions on Stability of Alpha Lipoic Acid Tablets

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Benzyl Nicotinate
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Abstract: The purpose of stability testing is to provide evidence on how the quality of drug product varies with time under the influence of a variety of environmental factors such as temperature, humidity and light. Stability data establish shelf life for the drug product and recommended storage conditions. Alpha lipoic acid (ALA) is a mitochondrial compound and body's natural antioxidant. The aim of this study was to evaluate the stability and quality of ALA tablets in dosage form of 600 mg. Tablets were packed in two different primary packaging materials: PVC/PVdC/Al blisters and amber glass flask and stored at accelerated (40ºC/75%RH) and long-term (25ºC/60%RH) storage conditions and analyzed after 3 and 6 months of storage. The effects of environmental factors on ALA tablets in two different packaging materials were investigated by HPLC method. The HPLC analysis was performed using a C18 column 150 x 4.0 mm x 5 µm, setting the flow at 1.5 mL/min and the UV detector at 220 nm.

The results showed a significant decrease of ALA content and dissolution in tablets, packed in PVC/PVdC/Al blisters. Amber glass flask maintained better pharmaceutical performance of the tested product (after 3 and 6 months).

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Abstract

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SEM/EDX Analysis of Archaeological Material from Prehistoric and Medieval Sites in B&H

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Slag
Bosnia and Herzegovina
Iron Age
Medieval

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Abstract: Samples used for the analysis were from the medieval town Dubrovnik (35 km north of Sarajevo; gold thread, slag, ceramic) and prehistoric site Graci (15 km west of Mrkonjic Grad; slag). Since ceramic is non-conductive material, a thin layer of gold coating was applied before analysis. Semi-quantitative SEM/EDX analysis revealed that gold thread was made from gold and silver combination, with uniform distance between coils of thread of 257.803 µm. Au content was 63.94% and Ag 36.06%. Iron slag contained significant traces of arsenic, mercury and silver, a strong indication that process of gold extraction process was implemented on the site, since As and Hg were used for gold refining during Medieval times. Analysis of ceramic fragments confirmed visual assumption, that red ceramic contains more iron than black or grey one. Prehistoric samples from Graci showed that slag is predominantly iron-manganese type of slag, with goethite-like internal structure. Traces of Al and Si can be ascribed to their distribution in burial environment. Most interesting is presence of rare-earth elements La, Ce, Nd and Th in the form of small monazite ((Ce, La, Nd, Th)PO_4) crystals. Type of slag, archaeological and historical accounts place this site into Iron Age time period.

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Abstract

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Silica Gel Impregnated by Vanadium(V) Oxide: Synthesis, Characterization and Application as a Novel Solid Phase Extractant for Cd(II), Cr(III), Cu(II) and Pb(II)

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Silica
Vanadium (V) Oxide
Preconcentration
Trace Metals
FAAS

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Abstract: Activated silica gel was impregnated with vanadium(V) oxide from 0.050 mol L^{-1} aqueous solutions of ammonium metavanadate and characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and electron dispersive spectroscopy (EDS). This way prepared novel solid phase extractant was used for simultaneous preconcentration of Cd(II), Cu(II), Cr(III) and Pb(II) ions from aqueous solutions followed by flame atomic absorption spectrometry (FAAS) determination.

Experimental parameters that are affecting the preconcentration: pH-value, amount of the sorbent and volume of the sample were tested. Elution of the adsorbed metals was performed with 1 mol L^{-1} nitric acid. Optimal preconcentration process was achieved at pH 10 with the use of 50 mg of sorbent and 100 mL of sample.

Results have shown that the adsorption capacity of the new sorbent (μmol g^{-1}) was 35.58 (Cd), 192.34 (Cr), 157.36 (Cu) and 28.96 (Pb). The proposed method provides quantitative recoveries of target metal ions ranging from 97.3-102.1% with good precision for all analyzed metals (RSD <2%). Under the optimum experimental conditions the limit of detection (LOD) and quantification (LOQ) were satisfying for FAAS technique.

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Abstract

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Determination of Water Content in Infant Formula

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Abstract: As water is one of the most important constituents of food it is very important to accurately quantify it. Furthermore, water content affects stability and shelf life of food. Evaluation of most chemical parameters is based on dry mass and large number of methods are using heating which result in losing all volatile compounds and not only the water.

Regarding this, the aim of this study was to determine water content in different infant formula by various methods. In this research we used four different techniques: Classical Karl Fischer titration with two different solvents, Classical heating Oven, Infrared Drying and Oven sample processor which combines heating and Karl Fischer titration for examination of three different types of infant formula. Every sample was measured in ten probes and Classical Karl Fischer titration was used as a reference.

The results have shown that Classical Karl Fischer titration (reference) is the best method regarding to speed of measurement, amount of sample needed and obtained water contents (3.01-4.35%), followed by Oven sample processor (2.96-4.23%), Infrared Drying (2.74-4.03) and Classical heating Oven (2.38-3.52%). Methods that use heating cannot extract all of water from sample in reasonable period of time.

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Abstract

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Investigation of Newly Synthetised Transition Metal Complexes based on Pyrazole Derivatives on the Inhibition *Phomopsis viticola* Sacc. under Laboratory Conditions

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Active Fungicide Substances
Phomopsis Viticola Sacc.

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Abstract: Transitional metal complexes have practical application in pharmacy, agriculture and environmental protection. In this paper we analysed influence of the 3,5-pyrazoledicarboxylic acid monohydrate(HL) as ligand and newly synthetised two Cu(II) complexes (with different structure) and one Ni(II) complex on inhibition of pathogenic fungal mycelium *Phomopsis viticola* that causes phomopsis cane and leaf spot disease, a very significant grapevine disease that is common in Montenegrin vineyards. The ligand and complexes, in five different concentrations (ranged from 0.12 to 0.0075%) were tested for fungi *Phomopsis viticola* in laboratory condition on Potato Dextrose Agar (PDA) nutrient media.

All previous studies with complexes based on pyrazole derivatives showed more or less inhibitory effect on mycelial growth, but now has been obtained an unexpected result, there was an increase in diameter of fungal mycelium *Ph. Vitiocola*. This result was probably influenced by the structure of the ligand itself and, consequently, the structure of the complexes.

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Abstract

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The Determination of Magnesium Oxide Content in Commercially Available Supplements of Magnesium

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Abstract: Magnesium is an essential element and the intracellular divalent cation involved in many biochemical functions. It is a cofactor for more than 300 metabolic reactions in the human body. These processes include protein synthesis, cellular energy production and storage, cell growth and reproduction, DNA and RNA synthesis, and stabilization of mitochondrial membranes. Because of that, magnesium plays an important role in disease prevention and human health. Low levels of magnesium have been associated with a number of chronic diseases including migraine headaches, 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 of supplement that is widely available in pharmacies. Moreover, the magnesium oxide contains about 60% elemental magnesium. In this work, we determinate the content of MgO in three pharmaceutical supplementations by spectrophotometry, from different manufactures. Spectrophotometric determination based on the reaction between magnesium ions and eriochrome black T was performed on a wavelength of 535nm, while the declared content of Mg in tablets was 300mg, 375mg, and 400mg. The analyzed content of MgO were ranged from 360.5 to 386.5 mg MgO. All tested commercially available 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.

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Abstract

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Selective and Sensitive Detection of Iron(II) with a Calix[4]arene Derivative Having Morpholino Binding Sites

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Colorimetric Sensor
QCM

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Abstract: Iron is a moderately toxic element as compared to other transition metals. Fe(II) is most abundant transition metal in the body. Ability to monitor Fe(II) in the cell provides better understanding of cellular concentration of iron and iron tranport and function. Iron mismanagement resulting in overload can accelerate such neurodegenerative diseases such as Alzheimer's and Parkinson's. On the other hand, early preventive action for metal ions in an aqueous solution is important challenge of detection. Some analytical procedures such as volumetric, chromatographic, X-ray emission, atomic absorption, and colorimetric methods for Fe(II) are available. Although all these methods are suitable for determination of Fe(II), colorimetric methods are generally preferred, as they involve less expensive instrumentation and afford greater sensitivity when appropriate chromogenic reagents are employed. Among sensors technologies, Quartz Crystal Microbalance (QCM) technique is also suitable to use for detection of metal ions in aqueous solution. On the other hand, it is known that macromolecules can be used as sensing molecules in these techniques. Calixarenes are one of the macromolecules which are formed from phenol-formaldehyde condensation under basic conditions. In this study, a calix[4]arene derivative having morpholino functionalities (C[4]MOR) has been tested as sensing material on the detection of metal ions in aqueous solutions. Colorimetric analysis results indicated that C[4]MOR was selective sensing material for Fe(II) ions over other metal ions. Moreover, it was also studied the sensing abilities of C[4]MOR towards metal ions in QCM system. In conclusion, it has been developed a selective and sensitive sensor based on C[4]MOR for Fe(II) ions in this study.

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Abstract

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A Novel Sensor for Copper(II) Ions Based on Di-(2-picolyl)amine Functionalized Calix[4]arene

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Abstract: Copper is an essential trace element representing the prosthetic group of enzymes that participate in the transfer of electrons in several key reactions of metabolism. Although copper ions is essential for living organisms, at high levels it has high toxicity to some organisms as it can cause of vomiting, diarrhea, stomach cramps, anxiety, bipolar disorder, memory loss and Alzheimer disease (especially in young people). On the other hand, early preventive action for metal ions in an aqueous solution is important challenge of detection. Many techniques are previously applied for copper detection such as atomic absorption spectrometry, inductively coupled plasma mass spectroscopy, ion selective membrane electrode, voltammetry. Although all these methods are suitable for determination of Cu(II), colorimetric methods are generally preferred, as they involve less expensive instrumentation and afford greater sensitivity when appropriate chromogenic reagents are employed. Among sensors technologies, Quartz Crystal Microbalance (QCM) technique is also suitable to use for detection of metal ions in aqueous solution. On the other hand, it is known that macromolecules can be used as sensing molecules in this system. Calixarenes are one of the macromolecules which are formed from phenol-formaldehyde condensation under basic conditions. In this study, di-(2-picolyl)amine bonded calix[4]arene (PABC[4]) has been employed on the detection of metal ions in aqueous solutions. Colorimetric analysis results indicated that PABC[4] was selective sensing material for Cu(II) ions over other metal ions. Moreover, it was also studied the sensing abilities of PABC[4] towards metal ions in QCM system. In conclusion, it has been developed a novel sensor based on PABC[4] for Cu(II) ions in this study.

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Abstract

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Effect of High Intensity Training on Mineral Content Changes in Blood and Urine of Athletes

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Blood
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ICP-AES

Abstract: Nowadays people have less time to engage in prolonged physical activity. High intense training becomes more popular because amateur athletes want to achieve all the benefits of training in shorter period of time. It is considered that expertly led high intensity training is safe way to achieve fitness goals in the case of advanced athletes. In this paper it was verified whether changes in blood and urine concentrations occure after short but intense physical activity by using inductively coupled plasma spectrometric technique (ICP-AES). Concentrations of seven minerals in urine and blood of 12 examinees were measured before and after high intensity training. Statistical analysis was performed using paired t-test (2-tailed, paired). Statistical significance was considered at $P < 0.05$.

Concentration change percentages (%) of minerals: Na, K, Ca, Mg, Zn, Fe and Cu in blood for 12 examinees expressed as mean values were: 2.26; 0.64; 7.27; 4.51; 4.17; 5.74 and 4.48, respectively. Obtained results show that concentrations of the measured minerals stayed without significant changes due to intense physical activity and losses through sweat, urine or exhaled air. On the basis of these results it can be concluded that from the standpoint of the loss of mineral concentrations a short high intensity training is safe for the health of the advanced recreational athletes.

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Abstract

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Characterization of Medieval Archaeological Samples from Bosnia and Herzegovina by Different Analytical Methods

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Abstract: In this study archaeological samples from medieval town Dubrovnik (35 km north of Sarajevo) were analyzed by two different methods. Electrochemical data are compared with those obtained by Atomic absorption spectroscopy (AAS). Different types of samples were used (ceramic pieces, iron slag, iron nails). Ceramic and slag samples were powdered in agate mortar and pestle, to form finely distributed material. Micro samples of powder were mixed with carbon paste and transferred into small tubes, forming a small working electrode. Electrochemical cell also contained Ag/AgCl reference electrode and Pt counter electrode. As a supporting electrolyte HCl or KCl were used. Cyclic and square wave voltammetry were employed as techniques to characterize iron in samples. AAS was used for quantitative determination of: Fe, Pb, Cd, Mn, Cr, Zn, Ni and Cu. Cyclic voltammetry results revealed weak cathodic signals between 0.5V and -0.8V, indicating presence of iron. Reason for such weak signals is in the intrinsic nature of iron products in this samples. AAS results showed high content of Fe, up to 3503 mg/g. Ni and Mn were also found in high quantities (319.8 and 465.3 mg/g, respectively). Results indicate that the site was used for processing of iron from the ores and developed metallurgical activity during medieval period.

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Abstract

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Spectrophotometric Determination of Glyphosate in Selected Samples

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Abstract: Glyphosate is a non-selective organophosphate herbicide, which has the highest global application compared to other pesticides. Today, glyphosate is most commonly used in agriculture for crop drying prior to harvest, as well as in the production of genetically modified food. In this study, glyphosate was determined in samples of drinking water, wheat grain, selected fruits and vegetables. Also, the thermal influence and washing of fruits and vegetables in the solution of $NaHCO_3$ on the concentration of glyphosate was examined. The glyphosate spectrophotometric assay is based on the glyphosate reaction with ninhydrin in the presence of molybdate as a catalyst, resulting in purple coloration whose intensity was measured at 570 nm. Glyphosate was detected in only one of the five analyzed water samples, at a concentration of 0.148 g/L. Examined wheat grains contain glyphosate at concentrations of 0.75 to 0.92 mg/g. The highest glyphosate concentration in all tested fruit and vegetable samples, was obtained for lemon peel (24.39 mg/g), while the lowest concentration of glyphosate was obtained for potatoes without crust (0.89 mg/g). This study have shown that thermal processing of fruits and vegetables, as well as their washing with $NaHCO_3$ solution leads to a reduction of glyphosate concentration in the tested samples.

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Abstract

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Determination of Rare Earth Elements in the Cabbage (*Brassica oleracea var. capitata*) and Dandelion (*Taraxacum officinale*) of Eastern Croatia

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ICP-MS

Abstract: The concentration of rare earth elements in food plants is of special concern. A systematic research of the rare earth elements (REE) concentrations in the environment of eastern Croatia has never been done. Using ICP-MS, rare earth elements (La, Ce, Pr, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm and Yb) have been determined in Cabbage (*Brassica oleracea var. capitata*) and T*araxacum officinale* (dandelion). Rare earth element concentrations in the leaves of dandelion showed significantly higher concentrations in the plants from agricultural locations compared to those from nonagricultural (Mann Whitney test p=0,0138). The resulting REE concentrations in the leaves of Cabbage collected from non- agricultural locations did not significantly differ from the European average. The parallel soil analyses showed that exposure of the dandelion samples to REEs through soil was generally low.

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Abstract

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Choline Chloride-based Deep Eutectic Solvents as „green“ Extraction Media for Extracting Phenolic Compounds

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Abstract: At the beginning of the 21st century, the concept of "green analytical chemistry" was established through twelve basic principles. One of the most important includes the use of environmentally friendly, biodegradable and non-toxicity solvents in the extraction processes. Consequently, newly formed solvents called Deep Eutectic Solvents (DESs) were developed as a promising alternative to traditional organic solvents used.

In the present study, different DESs composed of quaternary ammonium salt (choline chloride) as hydrogen bond acceptor in combination with different hydrogen bond donors (poly-alcohols, organic acids, sugars and urea) were investigated as an extraction medium for one-step sample preparation for phenolic compounds characterization from dried aronia fruits. For the improving of extraction process ultrasound-assisted technique was applied, and results were compared with those obtained using 80% methanol as the extraction solvent. Total phenolic content (TPC), total flavonoid content (TFC), total anthocyanin content (TAC) as well as individual phenolic compound yields were determined as dependent variables in all extracts.

Results revealed that the highest value of TPC and TFC was found in the extract obtained with choline chloride–fructose DES (36.2±3.4 mg gallic acid g^{-1} DW and 4.7±0.3 mg rutin g^{-1} DW, respectively), while methanol exhibited the highest capacity for the extraction of TAC (1.246±0.058 mg Cya-3-Glu g^{-1} DW). The results obtained in this study have confirmed DESs as an excellent alternative for sustainable and green extraction of phenolic compounds from plant material.

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Abstract

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Synthesis, Characterization and Biological Properties of Novel Ru(III) and Fe(III) Complexes with Thiosemicarbazide-based Ligands

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Abstract: In this study, Ru(III) and Fe(III) complexes with thiosemicarbazide-based ligands have been synthesized and characterized. Ligands of general formula 5-NO_2-SALTSC and 2-OH-1-NALTSC, where SALTSC = salicylaldehyde thiosemicarbazone and NALTSC = naphtaldehyde thiosemicarbazone, were prepared through the condensation reaction of salicylaldehyde derivatives and thiosemicarbazide in 1:1 molar ratio. The complexes of general formula Na[M(5-NO_2-SALTSC-2H)$_2$], Na[M(2-OH-1-NALTSC-2H)$_2$] (M = Ru, Fe), were synthesized by reacting $MCl_3 \cdot nH_2O$ with appropriate ligands in 1:2 molar ratio. The complexes were characterized by infrared spectroscopy and mass spectrometry. ESI-ToF mass spectrometry confirmed the existance of $[C_{16}H_{12}N_8O_6FeS_2]^-$, $[C_{24}H_{18}N_6O_2FeS_2]^-$, $[C_{16}H_{12}N_8O_6RuS_2]^-$ and $[C_{24}H_{18}N_6O_2RuS_2]^-$ ions, with m/z values at 531.8, 541.9, 577.7 and 587.2, respectively. Results showed that ligands are coordinated on metal center as tridentate dianionic ONS donors, with 1:2 metal:ligand stoichiometries. The complexes were tested for antioxidant potential in peripheral human lymphocytes using the cytokinesis block micronucleus assay, which showed that tested complexes reduce the frequency of micronucleus at certain concentrations, with highest effect showed at concentration of 3.7 μg/mL.

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Abstract

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Synthesis and Characterization of New Ru(III) and Fe(III) Complexes with Schiff Bases Derived from Supstitued Salicylaldehydes and Alkylamines

Ljubijankić, N.[a], Markotić, E.[a], Granzov, I.[a], Šuta, E.[a], Begić, S.[a], Ljubijankić, S.[b]

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Abstract: Four metal complexes with Schiff bases derived from substituted salicylaldehydes and alkylamines were synthesized. The complexes with the general formula $Na[MCl_2(N\text{-}R\text{-}5\text{-}X\text{-}salim)_2]$ (where M = Ru, Fe; R = methyl, propyl; X = Br, NO_2) have been synthesized by reaction of the appropriate ligand and metal salt in a molar ratio 2:1. The complexes were characterized by infrared spectroscopy and ESI-ToF mass spectrometry. Mass spectrometry of the complexes was performed in the negative ESI ion mode, where the anionic part of the compound was detected as the corresponding $[M]^-$ ion. Mass spectra of $Na[RuCl_2(N\text{-Me-}5\text{-}NO_2\text{-salim})_2]$, $Na[RuCl_2(N\text{-Me-}5\text{-Br-salim})_2]$, $Na[FeCl_2(N\text{-Me-}5\text{-Br-salim})_2]$ and $Na[FeCl_2(N\text{-Pr-}5\text{-Br-salim})_2]$ confirmed the existence of corresponding anions $[C_{16}H_{14}Cl_2N_4O_6Ru]^-$ $[C_{16}H_{14}Br_2Cl_2N_2O_2Ru]^-$, $[C_{16}H_{14}Br_2Cl_2N_2O_2Fe]^-$, $[C_{20}H_{22}Br_2Cl_2N_2O_2Fe]^-$, with m/z values 531.8, 597.9, 552.1 and 608.7, respectively. These results, as well as the characteristic IR vibrations, confirm that ligands in the synthesized complexes are coordinated as bidentate ON donors, in 2:1 ligand:metal stoichiometries occupying four coordination positions in the complex.

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Abstract

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Synthesis and Characterization of New Ru(III) Complexes with Schiff Bases derived from Salicylaldehydes and Halogen Derivatives of Aniline

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Abstract: In this study, the synthesis and characterization of two novel rutenium(III) complexes with Schiff bases derived from salicylaldehyde and bromoaniline or chloroaniline is described. Complexes were synthesized according to the described procedure, and the characterization was performed by IR spectroscopy and ESI-ToF mass spectrometry. Schiff bases are coordinated to ruthenium *via* azomethine nitrogen and phenolic oxygen. The proofs for that were detected in the IR spectra of the synthesized complexes by analysing shifts of azomethine nitrogen towards lower wave number and phenolic oxygen towards higher wave number. Mass spectra was performed in the negative ESI mode of ionization, where the anionic part of the compound was detected as the corresponding $[M]^-$ ion: $[C_{26}H_{18}N_2O_2Cl_4Ru]^-$ ion (m/z: 631.91732) and $[C_{26}H_{18}N_2O_2Cl_2Br_2Ru]^-$ ion (m/z: 719.82831), which confirmed assumed molecular formula of the compounds. Based on the results it was found that Schiff bases act as anionic bidentate ON donor ligands, coordinated on Ru metal center in 2:1 molar ratio.

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Abstract

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The Effect of Ru(III) Complexes with *N*-phenyl-5-X-salicylideneimine and Indazole on the Briggs-Rauscher Oscillating Reaction

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Abstract: Ruthenium complexes attract huge attention over the past decades due to their biological, catalytic, electronic and optical properties. In this study, the effect of ruthenium complexes of the general formula [Ru(*N*-Ph-5-X-salim)$_2$(ind)$_2$]Cl (where X=H, Cl or Br; ind=indazole) on the Briggs-Rauscher oscillating reaction was investigated. The oscillations in the Briggs-Rauscher reaction mixtures were followed potentiometrically. Addition of ethanolic solutions of tested complexes to an active Briggs-Rauscher reaction mixture caused an immediate effect of quenching of oscillations. After the inhibition time, the oscillations were restarted with amplitude and frequency different in a reference mixture. A linear correlation between the inhibition time and the concentration of the complexes added to the Briggs-Rauscher reaction mixture were found in the range from 5.36 to 21.0 μmol/L. The ability of complexes to inhibit oscillations of the Briggs-Rauscher reaction mixture is similar to that caused by antioxidant free radical scavengers. The obtained preliminary results suggest further analyses of this effect.

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Abstract

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Synthesis and Characterization of Copper(II) and Nickel(II) β-diketonates with Pyridine-based Amides

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Abstract: The rational design of functional molecular solids is one of the main challenges in crystal engineering. Properties of crystalline solids are closely connected with the manner in which building units are aligned and linked together in the solid state. Understanding and controlling noncovalent interactions, in particular hydrogen bonds, is essential for establishing reliable connections between molecular and supramolecular structure. Strong directionality, sufficient strength, tunability and selectivity of hydrogen bonds enables synthesis of desired supramolecular architectures. The employing of rather weak and reversible intermolecular interactions in the building of organic networks is well known, but their role in assemby of the metal-containing architectures is is still much less studied. In our attempts to control molecular geometry and supramolecular assembly we synthesized a series of copper(II) and nickel(II) coordination compounds. We employed various neutral copper(II) and nickel(II) β-diketonates as building blocks. The steric and electronic properties of the β-diketonate were modulated by changing $–CH_3$ groups in acetylacetone with suitable substituents. On the fifth and sixth coordination site we introduced pyridine based ligands equipped with the amide group bearing both hydrogen bond donating and accepting atoms. The compounds were characterized by single crystal X-ray structure analysis combined with spectroscopic and thermal analysis.

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Abstract

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Synthesis and Spectral Properties of Novel 1,8-Naphthalimide Derivative

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Abstract: Cyclic aromatic imides and their derivatives exhibit various material properties. The structural skeleton of cyclic aromatic imides is composed of two rings. One of these is an aromatic ring and the other is an imide-containing ring. 1,8-naphthalimide has been widely used for fluorescence sensing due to its high photostability, large Stokes shift, and dual fluorescence properties. The naphthalimide derivatives had been developed as highly selective cations and anions sensors, molecular probes, biological probes and fluorescent dyes. Imide derivatives have the capability to form host–guest chemistry and can bind with DNA and some imides also show anticancer activity.

In this study, 4-Sulfo-1,8-naphthalic anhydride potassium salt was reacted with tris(2-aminoethyl)amine to obtain fluorogenic naphthalimide derivative. Synthesized this compound was identified by using spectroscopy methods (FTIR, ^{1}H NMR). This compound was examined for its fluorescent properties toward different metal ions by UV-visible and fluorescence spectroscopy. The perchlorate or acetate salts of Na^{+}, Li^{+}, Mg^{2+}, Ni^{2+}, Ba^{2+}, Ca^{2+}, Cu^{2+}, Pb^{2+}, Zn^{2+} ions were used to evaluate the metal ion binding properties of fluorogenic naphthalimide derivative.

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Abstract

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Determination of Total Protein Content in Different Milk Samples – A Comparative Study between the Half-Automated Kjeldahl Method and a Spectrophotometric Method

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Abstract: The reference method for total protein content (TPC) determination is still the Kjeldahl method, despite the fact that it does not distinguish protein-based nitrogen from non-protein nitrogen. The aim of this study was to determine the TPC in various milk sorts using two different methods, and to compare the obtained results. The milk samples were of animal and plant origin: cow milk, rice milk, almond milk, coconut milk and soy milk. The TPC was determined by the half-automated Kjeldahl method using the conversion factor 6.38 and the spectrophotometric Bradford method. The samples were diluted to meet the linear range (0.2-0.9 mg/ml) of the bovine serum albumin solution which serves as a standard in the Bradford method. Results obtained by the Kjeldahl method were closer to the declared content, which could mean higher accuracy of this method. The TPC in rice milk and coconut milk samples were identical regardless of the method. Soy milk samples showed a higher TPC in the Kjeldahl method (2.8%) compared to the Bradford method (2.2%) and that was the highest results' deviation between the methods. In conclusion, considering that there was no statistically significant difference in the values obtained by these two methods, the Bradford method can be given advantage due to its simplicity, sensitivity and time-saving characteristics.

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Abstract

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The Influence of the Examined Parameters on the Quality of Biodiesel Obtained from Waste and Pure Vegetable Oil

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Abstract: The aim of this paper was to examine the soap concentration and quality parameters of biodiesel that was synthesized from waste and pure sunflower oil and then purified using the selected solvents: distilled water, 4% H_3PO_4 and 5% HCl. The biodiesel was rinsed 2, 3, 5, 7 and 9 times with the mentioned solvents in appropriate volumes. The soap concentration and the following parameters were analysed for each rinsing solvent and for every number of rinsing procedures: density, kinematic viscosity, acid number, peroxide number, flash point and biodiesel synthesis yield. Except for the peroxide number, there were no significant differences in the investigated parameters, regardless of the oil used for the biodiesel synthesis and the solvent used for its purification. Rinsing with 4% H_3PO_4 caused a difference in the peroxide number in the biodiesel from waste and pure sunflower oil. Additionally, it was determined that the acid solution removed the soaps more efficiently, i.e. increasing the number of rinsings with 4% H_3PO_4 decreased the soap concentrations in biodiesel.

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UV Spectrophotometric Method in Quantification of the Total Protein Content in Food Samples

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Abstract: The main aim of this research was to evaluate the possibility of the UV spectrophotometric method application for the quantitative determination of the total proteins in the food product samples, considering the fact that the reference Kjeldahl method for the food analysis has some disadvantages. We analysed 10 samples of baby food on UV/VIS spectrophotometer Perkin-Elmer Lambda 25 at 210 and 278 nm. The total protein content (TPC) was expressed in weight of the total proteins by weight of the analyzed products (g/100 g). The results were compared to the TPC indicated on the label of the analyzed samples (declared values, d.v.), and they showed that there were no statistically significant differences between these values ($p>0.05$, by Student's t-test). Also, we analysed the same samples with the Biuret method on the same instrument (at 545 nm). The results showed that TPCs obtained by the Biuret method were statistically significantly lower than d.v. ($p^{***}<0.001$, by Student's t-test). It can be concluded that UV spectrophotometric method could be used in quantitative analyses of proteins in food samples.

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Abstract

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A Rare and New Insight into Antidiabetogenic Potential of two *Ganoderma* species: *G. pfeifferi* Bres. 1889 and *G. resinaceum* Boud. 1889 in Alloxan-diabetic Rats

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Abstract: Fungal extracts were analyzed spectrophotometrically for the free radicals scavenging activity on 1,1-diphenyl-2-picrylhydrazyl (DPPH), superoxide anion (SOA) and nitric oxide radical (NO), as well as for the reducing power activity (FRAP). For determination of bioactive properties of specific compounds present in fungal extracts, the content of total phenols (TP) and flavonoids (TF) were investigated.*G. resinaceum* H_2O extract was found to possesses the highest ability to scavenge $DPPH^{\cdot}$ and $O_2^{\cdot-}$ (IC_{50}=14.03±0.59 and IC_{50}=29.96±1.19 μg/mL, respectively), while EtOH extract of the same species showed better $NO^{\cdot}$ activity (IC_{50}=215.18±1.77 μg/mL). The highest level of TF was found in EtOH extract of *G. pfeifferi* (26.29±0.74 mg QE/g. d.w.), while the highest TP content was determined in EtOH extract of *G. resinaceum* (44.01±0.24 mg GA/g. d.w.). Antidiabetic action of analyzed extracts in treated rats was evaluated by the oral glucose tolerance test (OGTT) and histological examination of pancreas and liver in control normoglycemic animals as opposed to animals with alloxan-induced diabetes. Histological examination of pancreatic tissue demonstrated that *G. pfeifferi* extracts have protective effects. On contrary, treatment with *G. resinaceum* H_2O extract showed better action by observing changes in body weight and results of OGTT. Taken all together, analyzed extracts could be considered as a promising candidate for further research with an aim to promote their usage as potential antidiabetic agents, which is for the first time reported for *G. pfeifferi*.

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Abstract

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Determination of Total Protein Content in Royal Jelly Samples by an UV Spectrophotometric Method

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Abstract: The aim of this study was to quantify the total protein content (TPrC) in samples of royal jelly harvested in the municipality of Konjic, using an UV spectrophotometric method. Bovine serum albumine was used as a protein standard to conctruct the calibration curve.

The value of TPrC in polyfloral samples of royal jelly was 21.21±1.18%, while monofloral samples of royal jelly (*Acacia* flowers) showed the TPrC of 20.23±0.24%. Compared to literature data, this method produced higher values of TPrC in the complex matrices such as royal jelly.

The employed spectrophotometric method proved to be very simple and convenient for the quantification of total proteins.

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Abstract

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Determination of Total Phenolic Content of Royal Jelly by Using a Spectrophotometric Method

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Abstract: The aim of this study was to determine the total phenolic content (TPC) of royal jelly harvested in the municipality of Konjic, by a spectrophotometric method using the Folin-Ciocalteu reagent.

A gallic acid (GA) solution was used as a standard. All measurements were performed in triplicate at the wavelength of 764 nm The TPC was expressed in mg of GA equivalent (GAE) per 100 g royal jelly sample.

The mean value of TPC in 12 samples of royal jelly was 411.72±8.83 mg GAE/100 g. The mean TPC in the 11 polyfloral samples of royal jelly (407.87±9.46 mg GAE/100 g) was slightly higher than mean TPC (369.53±11.65 mg GAE/100 g) in the monofloral sample (only one sample, measured in triplicate). The selected and applied spectrophotometric method proved to be an efficient and simple method for the quantitative determination of TPC in samples of royal jelly.

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Abstract

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Influence of Used Chemical Agents on the Possibility of Isolation, Amplification, and Profiling of DNA from a Cigarette Stub as Biological Trace Carrier

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Chemical agents
Cigarette stub

Abstract: The requirements of modern forensics provide a constant challenge to reach new heights in confidence of DNA based identification, in spite of the fact that crime scenes and others almost never provide flawless samples. The objective of this study was to examine DNA profiling from the cigarette stub as biological trace carrier after being treated with different chemical agents that can be found in the field. Five cigarettes were smoked by the same person, one which (BM 2/14) was smoked with the presence of lipstick, three we treated with different agents (BM 3/14, BM 4/14 and BM 5/14 with sunflower oil, energy drink and 30% ethanol respectively) and one sample was left untreated. All five stubs were left for 10 days at 20 °C. DNA from samples, including undisputed sample obtained from buccal mucosa, was isolated by using Miller salting out procedure, quantified with gel electrophoresis and amplified with the use of PowerPlex® ESI 16 commercial kit. DNA detection was carried out by using the ABI PRISM® 310 genetic analyzer. Results were processed with the use of Gene Mapper idv 3.2 software. Sample (BM 1/14) gave an incomplete profile, sample (BM 2/14) gave a mixed profile, samples (BM 4/14) and (BM 5/14) a partial profile and only sample (BM 3/14) gave a full profile. In conclusion, based on these results, the sample treated with sunflower oil can be used for identification while other samples require corroboration with further evidence.

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Abstract

PP-BB-08

Antioxidant and Butyrylcholinesterase Inhibitory Activity of Selected Phenolic Acids and Their Derivatives

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Phenolic acids
Phenolic acid derivatives

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Abstract: Phenolic acids and their derivatives are compounds that are widely distributed in the plant kingdom, and are known for their antioxidant and enzyme inhibitory activity. In this study, antioxidant and butyrylcholinesterase inhibitory activity were tested for 11 samples of phenolic acids and their derivatives. These samples included: free phenolic acids, cyanomethoxy, fluoro and trifluoromethyl protected phenolic acids and their *N*-picolyl amide and ethyl ester derivatives. Antioxidant activity was tested by phosphomolybdate and ferric reducing antioxidant power (FRAP) methods. Gallic acid (GA) was used as a positive control. According to these methods, caffeic acid showed the most significant antioxidant activity, (0.64±0.05 mmolGA/mol) for phosphomolybdate method as well as for FRAP method (1381.80±5.86 mmolGA/mol). The lowest antioxidant activity showed trifluoromethyl derivative of *p*-coumaric acid, (*E*)-ethyl 3-[4-(trifluoromethyl)phenyl]prop-2-enoate for the phosphomolybdate method (0.35±0.01 mmolGA/mol**),** while cyanomethoxy derivative of caffeic acid, (*E*)-ethyl 3-[3,4-bis(cyanomethoxy)phenyl]prop-2-enoate showed the lowest antioxidant activity for the FRAP method (0.64±0.03 mmolGA/mol). The butyrylcholinesterase inhibition was carried out using a colorimetric method based on Ellman's reaction. Donepezil hydrochloride was used as a standard with inhibition of IC_{50} 18.49±0.06 µM. Among the tested samples, caffeic acid had the greatest inhibition (IC_{50} 2.90±0.38 µM), while *o*-coumaric acid showed the weakest inhibition (IC_{50} 64.24±5.43 µM).

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Abstract

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Antioxidant and Anti-Inflammatory Potential of Extracts of Four *Ganoderma* Species from Serbia Related to their Chemical Profile

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LC-MS/MS
Phenolics

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Abstract: This study was designed to explain the antioxidant and anti-inflammatory activity of ethanol, water and chloroform extracts from *G. pfeifferi* and *G. resinaceum*, and compare it with closely-related *G. applanatum* and *G. lucidum*. The total phenolics (TPC), total sugar (TSC) contents and LC-MS/MS analysis of phenolic compounds present in analyzed extracts were also determined. Antioxidant activities were determined via ABTS, DPPH and NO assays. Anti-inflammatory potential was studied measuring cyclooxygenase-1 (COX-1) and 12-lipoxygenase (12-LOX) inhibitory activity. The highest content via LC-MS/MS analysis was noticed for *p*-hydroxybenzoic acid in EtOH extracts of *G. pfeifferi* (33.00 µg/g d.w.). Generally, the highest antioxidant potential (107.90±0.44 mg TEQ/g d.w. for ABTS and IC_{50}=4.49±0.45 µg/mL for DPPH assay of EtOH, and H_2O extracts of *G. applanatum*, respectively; IC_{25}=9±0.45 µg/mL for $CHCl_3$ extract of *G. resinaceum* for NO assay) was in good correlation with TPC and TSC. The highest TPC was in EtOH extracts of *G. applanatum*, while the highest TSC was generally in $CHCl_3$ extracts with the exception of EtOH extract of *G. applanatum*. The most powerfull activity towards COX-1/12-LOX inhibition showed $CHCl_3$ extracts of *G. lucidum* and *G. resinaceum* species. The results suggest that the *Ganoderma* species are a promising new source of bioactive natural compounds and they may be considered as both the candidates for preparing new food supplements and models for the development of new drug formulations.

POSTER PRESENTATIONS

Phytochemistry

(PHC)

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Abstract

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Nigella sativa L. as an Antioxidant and Acetylcholinesterase Inhibitor

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Nigella sativa L.
Total Phenolic Content
Antioxidant Activity
Acetylcholinesterase Inhibition

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Abstract: Black cumin (*Nigella sativa* L.) belongs to the Ranunculaceae family, and is widely used as a medicinal plant throughout the world since ancient times. The aim of this work was to examine the content of total phenolic compounds (TPC), *in vitro* antioxidant and acetylcholinesterase (AChE) inhibitory activity for five commercially available *N. sativa* oils. Total phenolic content was measured by the Folin-Ciocalteu method, using gallic acid (GA) as a positive control. The TPC content varied from 65.21 to 165.25 mg(GA)/g. In addition, *in vitro* antioxidant activity was tested by five different methods to cover a diversity of mechanistic approaches: DPPH and ABTS radical scavenging method, metal chelating activity against Zn(II) and Fe(II) and metal reducing activity against Cu(II). Almost all analyzed samples showed good ability to scavenge stable non-biological free radicals, chelate and reduce transition metal ions. The AChE inhibitory activity was determined by Ellman's reaction, using galantamine hydrobromide as a positive control. The IC_{50} values varied from 0.09 to 6.88 mg/mL. Phytochemical screening of the analyzed oil samples revealed moderate TPC content, but reflects their potential antioxidative and AChE inhibitory effect.

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Abstract

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The Antioxidant Activity of Some Spices Tested by Briggs-Rauscher Oscillating Reaction

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Briggs-Rauscher Reaction
Inhibition Time

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Abstract: The antioxidant activity of some spices was determined using the Briggs-Rauscher oscillating reaction. Five spices: basil, dill, ginger, oregano and rosemary were used as samples. Spices were available in the local markets. All tested samples were prepared by boiling 0.1g of spices with 25 mL distilled water at 90-95°C for 5 and 10 minutes. The inhibition times produced by spice extracts on an active Briggs-Rauscher oscillating reaction mixture were recorded potentiometrically at 20°C. The antioxidant activity was expressed as the inhibition time of Briggs-Rauscher oscillating reaction. Preliminary studies showed that extracts of all spices except dill obtained by boiling for 10 minutes have less antioxidant activity than the corresponding extract obtained by boiling for 5 minutes. The best ability to inhibit oscillations of the Briggs-Rauscher reaction mixture i.e. the highest antioxidant activity showed an extract of basil obtained by boiling for 5 minutes, and the lowest activity showed an extract of rosemary obtained by boiling for 10 minutes.

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Abstract

PP-PHC-03

Polyphenols from Merlot Wine as Antiinflammatory and Neuroprotective Agents

Majkić, T.[a], Torović, Lj.[b], Svirčev, E.[a], Simin, N.[a], Šibul, F.[a], Orčić, D.[a], Berežni, S.[a], Lesjak, M.[a], Beara, I.[a]

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Wine
Merlot

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Abstract: The aim of this study was to evaluate the phenolic composition and biological activity of four samples of Merlot wines. In order to thoroughly evaluate the phenolic profile of investigated samples, an LC-MS/MS technique was applied to evaluate the quantitative content of 47 phenolics, followed by HPLC-UV/VIS technique for detection of 5 anthocyanins. Among 28 detected phenolics, dominant compounds were malvidin-3-*O*-glucoside, gallic acid, and catechin. Antiinflammatory activity was determined as a potential to inhibit production of prostaglandin E_2 and thromboxane A_2. Macrophages (derived from U937 monocytes) were pretreated with wine samples and inflammation was induced by LPS. Quantification of produced eicosanoids in cell lysate was done by LS-MS/MS. Neuroprotective effect was estimated through a potential of acetylcholinesterase inhibition. All analyzed samples showed moderate antiinflammatory potential. Concerning the neuroprotective effect, samples exhibited modest activity in comparison with physostigmine, a well-known acetylcholinesterase inhibitor. Some correlation between phenolic profile and biological activities of examined samples was noticed. Obtained results support further utilization of Merlot grapes and wine as agents with valuable biological activities. Moreover, they indicate that polyphenolic compounds from Merlot wine could positively affect some pathological processes associated with inflammation, such as atherosclerosis.

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Abstract

PP-PHC-04

Phenolic Composition and Anti-acetylcholinesterase Activity of Two *Euphrasia rostkoviana* Hayne Species from Different Localities

Nemeš, I.[a], Majkić, T.[a], Berežni, S.[a], Pintać, D.[a], Bekvalac, K.[a], Radak, B.[b], Anačkov, G.[b], Mimica-Dukić, N.[a]

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Euphrasia rostkoviana Hayne is a hemi-parasitic plant from genus Euphrasia which has been used in traditional medicine for treatment of various eye diseases and conditions. In spite of its use, little has been confirmed and published regarding the biological activity and chemical composition of this plant species.

Thus, we investigated phenolic composition of hydromethanolic extracts of *Euphrasia rostkoviana* from two different locations in Serbia and their ability to inhibit acetylcholinesterase enzyme.

Out of 70 phenolic compounds analyzed by LC-MS/MS technique, 36 compounds were detected. The extracts were mainly composed of flavones and phenolics acids. Great differences have been observed between the samples obtained from different localities, which was particularly noticeable in quantities of chlorogenic acid, rutin, quinic acid, caffeic acid and luteolin-7-O-glucoside. The extracts exhibited similar ability to inhibit acetylcholinesterase (IC_{50}=3.49 mg/mL and IC_{50}=2.78 mg/mL) but in comparison to standard galantamine (IC_{50}=0.1 μg/mL) the activity was weak.

This study pointed out that *Euphrasia rostkoviana* is a rich source of phenolic compounds but its composition varies greatly, probably due to the plant's hemi-parasitic nature. Nonetheless, it is possible that quantities of compounds responsible for the extract's anti-acetylcholinesterase activity are consistent.

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Abstract

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Spectrophotometric Determination of Tannins with Fe(III) and 1,10-phenantroline in Domestic Beer Samples

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Tannins
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1,10-phenantroline

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Abstract: Tannins are a large group of polyphenolic compounds that are concentrated in roots, wood, bark, seeds, leaves and fruit of different plants. Tannins have the capability to tan proteins. Beer has a considerable amount of tannins because they are made from different crop types. An excess of tannins in beer results in astringency, but beer deprived of tannins do not taste right. The objective of this research was to determine the tannins content in domestic beer samples by a spectrophotometric method. The method is based on the reduction of Fe(III) to Fe(II) by tannins. The iron (II) reacts with 1,10-phenantroline to form a color complex. The absorbance was measured at 540 nm. Background correction is needed to minimize the interferences due to other reducing substances, and that was done by precipitating tannins in the sample solution with gelatin and kaolin. The solid matrix of gelatin and kaolin gave a tannin free solution. The calibration curve of tannic acid was linear from 0.5 to 4 $\mu g ml^{-1}$ with a linearity coefficient R^2=0.9943. The tannins content was determined in twelve beer samples and it was in range 15.49 – 1722.05 $\mu g ml^{-1}$.

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Abstract

PP-PHC-06

Determination of Total Phenolic Acids and Antioxidant Activity of *Fraxinus ornus* L. and *Fraxinus excelsior* L.

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Fraxinus ornus L.
Fraxinus excelsior L.
Phenolic Acids
Soxhlet Extraction
Ultrasound Extraction
ABTS Method

Abstract: The study was aimed to determine the total phenolic acids content and antioxidant activity of ethanolic extracts of branch bark and leaves of *Fraxinus ornus* L. and *Fraxinus excelsior* L. Soxhlet and ultrasound extractions were applied for the extract preparation. The total phenolic acids content were in range from 4.68 to 23.25 mg CAE/g DW for *F. excelsior* and from 7.66 to 17.41 mg CAE/g DW for *F. ornus*. The highest amount of total phenolic acids was found in *F. excelsior* leaves extract obtained by Soxhlet extraction, while the lowest amount had branch bark extract obtained by ultrasound extraction of the same species. The ABTS IC_{50} value ranged from 0.10 to 0.12 mg/ml for *F. excelsior* and from 0.06 to 0.33 mg/ml for *F. ornus* samples. Among all tested extracts, the *F. ornus* branch bark extract showed the best antioxidant activity, with IC_{50} value of 0.06 mg/ml.

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Abstract

PP-PHC-07

Determination of Phenolic Compunds in *Fraxinus angustifolia* Vahl. by HPLC-DAD

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*Fraxinus angustifolia*Vahl
Phenolic Compounds
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HPLC-DAD Analysis

Abstract: The objective of this work was to determine the content and composition of selected phenolic compounds, in branch bark and leaves of *Fraxinus angustifolia* Vahl. Isolation of the phenolic compounds were done using Soxhlet and ultrasound extractions. HPLC-DAD method was applied for the qualitative and quantitative analysis of coumarins (esculin and esculetin) flavonoids (quercetin and naringenin) and phenolic acids (gallic, cholorogenic and caffeic acid) in the extracts. The highest amounts of esculetin and esculin were detected in extract of leaves, obtained by Soxhlet extraction, 0.03 and 0.025 mg/g of DW respectively. Among the investigated phenolic acids, chlorogenic acid was only detected and the highest content was found in extract of the sample of branch bark obtained by ultrasound extraction (1.12 mg/g of DW). Selected flavonoids were not detected.

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Abstract

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Antioxidant Activity of Aqueous Extracts of Three *Ephedra* Species

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Ephedra
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HORAC

Abstract: *Ephedra* is an evergreen, shrub-like plant distributed mainly in the temperate zones of Europe, Asia and North America. The medicinal significance of *Ephedra* is based on the sympathomimetic properties of ephedrine alkaloids. In addition to alkaloids, *Ephedra* is a source of phenolic compounds, which is why the aim of this study was to determine the antioxidant activity (AA) in aqueous extracts of three *Ephedra* species: *Ephedra sinica*, *Ephedra distachya* subsp. *helvetica* and *Ephedra foeminea*. The antioxidant activity was determined by the oxygen radical absorption capacity ($ORAC_{FL}$) method and the hydroxyl radical absorption capacity ($HORAC_{FL}$) method. Trolox was used as a standard and the quantitation of the AA was based on the calculation of the area under curve. Results showed that *Ephedra foeminea* exhibited the highest ORAC value (129.4 mM TE/100 g $_{d.w.}$), whereas the highest HORAC value was found in *Ephedra distachya* subsp. *helvetica* (181.26 mM TE / 100 g $_{d.w.}$).

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Abstract

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HPLC-DAD Analysis of Coumarins and Phenolic Acids in Ethanolic Extracts of *Fraxinus ornus* L. and *Fraxinus excelsior* L.

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Ultrasound extraction
HPLC-DAD

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Abstract: The aim of this work was to determine the qualitative and quantitative composition of coumarins (fraxetin and esculetin) and phenolic acids (gallic, caffeic and chlorogenic acid) in the extracts of the branch bark and leaves of *Fraxinus excelsior* L. and *Fraxinus ornus* L. Phytoconstituents were isolated by Soxhlet and ultrasound extractions using 70% ethanol as a solvent. The qualitative and quantitative analysis of phenolic compounds was performed using HPLC-DAD.

The gallic acid, chlorogenic acid and fraxetin were found in the both *Fraxinus* species, esculetin was detected only in *Fraxinus ornus* L., while caffeic acid was not detected in either species. The highest content of gallic acid (112.96±1.32 mg/g extract) and chlorogenic acid (246.94±0.82 mg/g extract) was found in the *F. ornus* extract of the branch bark obtained by ultrasound extraction. The highest amount of esculetin (20.69±0.05 mg/g extract) was in ultrasound extract of the leaves of *F. ornus*, while the highest amount of fraxetin (46,86±0,68 mg/g of extract) was found in the extract of the leaves of *F. excelsior* obtained using Soxhlet extraction.

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Abstract

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The Influence of Different Extraction Methods and Operating Conditions on Antioxidative Activity of Extract from the *Rosmarinus officinalis* L.

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Classical extraction,
Ultrasonic extraction,
Antioxidant capacity,
Total phenol content

Abstract: Rosmarini folium, *Rosmarinus officinalis* L., Lamiaceae is a herbal drug rich in pharmacologically active substances, among which high levels of phenolic compounds are considered to be antioxidant activity carriers. The research provides insights into the extraction capacity of the total phenol content obtained using classical extraction (CE) and ultrasonic extraction (UE) and the influence of the experimental conditions regarding temperature, solvent polarity and duration of extraction for each method. The observed antioxidant capacity of extracts obtained by applying different experimental conditions was compared to the phenolic compound content. Determination of total phenolics was performed spectrophotometrically, while antioxidant capacity was determined by DPPH test.

Analysis of UE results revealed several advantages compared to CE procedure. The highest extraction capacity of phenolic compounds was obtained by UE using a 30% aqueous ethanol solution at 60°C for 40 minutes. When applying the same conditions of temperature, solvents and length of extraction time, UE provides a better extraction capacity of phenolic compounds than CE. Regarding CE the best results were achieved using water as solvent during 90 minutes at 90°C. The antioxidant capacity results correlate with the total phenolic content, whereby the percentage increase of antioxidant activity follows the increase in the content of extracted phenols.

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Abstract

PP-PHC-11

Content of Omega-3 Fatty Acids in some *Salvia* Species

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Abstract: *Salvia* species, the most important medical plants, are classified to be in *Dicotyledonae*of *Tubiflorae* team of Lamiaceae family. The plants of Lamiaceae family are mostly herbs and weeds mainly spread on Mediterranean. This study is aimed to determine fatty acid composition of four *Salvia* species collected from cultivars grown in Cumra ecological conditions.

Leaves of the plants were grinded in grinding mill in 1 mm sieve size. Soxhlet extraction was used for isolation of fatty acids, using hexane as a solvent. Analyses were done by gas chromatography/mass spectrometry.

Significant difference was observed in the linolenic acid content of S*alvia* species. The highest content of linolenic acid was determined in *S. sclarea* (38.23%), while 28.69% and 8,52% were found for *S. nomerosa*, and *S. officinalis*, respectively. The lowest linolenic acid content was found in *S.triloba* (7.26%). The *S. sclarea* also had the highest polyunsaturated fatty acid (PUFA) content (51.72%).

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Abstract

PP-PHC-12

Total Phenolic Content and Radical Scavenging Activity of Common Fruits Grown in Bosnia and Herzegovina

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Abstract: Polyphenols (including anthocyanins) have received much attention since being reported to have a positive influence on human health. Total phenols, flavonoids and antocyanins content, as well as the radical scavenging activity of selected fruits grown in Bosnia and Herzegovina [cranberry, sour cherry, raspberry, blueberry, cornelian cherry, redcurrant, blackcurrant, pomegranate, physalis (peruvian strawberry), gooseberry, blackberry] were determined in this study. Total phenolic content (TPC) was expressed as mg gallic acid equivalents/g of fresh fruit (mg GAE/g) according to the Folin-Ciocalteu's assay. Total flavonoid content (TFC) was expressed as mg quercetin equivalents/g of fresh fruit (mg QE/g) spectrophotometrically. Total anthocyanine content (TAC) was analysed by the pH differential spectrophotometric method at 525 and 700 nm. The radical scavenging activity of fruit extracts was determined by the DPPH assay. The results showed that the TPC in fruits was in the range from 3.08 to 11.6 mg GAE/g, while the TFC was in the range from 0.84 to 3.98 mg QE/g. The content of total monomeric anthocyanins was expressed in mg of cyanidin-3-glucoside equivalents per gram of fruit (CGE/g) and it varied between 0.69 for cranberry and 8.64 for cornelian cherry. DPPH scavenging activity was the highest for physalis (76.75%) and the lowest one was for the sour cherry (28.46%). This study showed that these fruits are good sources of phenolic components and could be considered as powerful antioxidants.

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Abstract

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Chemical Composition and Antioxidant Activity of Ethanolic Extracts of Selected Cereals

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Phenolic compounds
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Antioxidant activity
Cereals

Abstract: The aim of this work was to determine total phenolic and total flavonoid content, as well as antioxidant activity of ethanolic extract of amaranth, buckwheat, millet, quinoa and chia. Phenolic compounds were determined by Folin–Ciocalteu method using gallic acid as standard, while total flavonoid content was determined by Dowd´s method with rutine as standard. Seeds of quinoa had the highest content of phenolic and flavonoid compounds, 0.44 mg(GA)/100 g DW and 35.36 mg(RE)/100 g DW, respectively, while the lowest content of these compounds had seeds of amaranth. Antioxidant activity was tested by DPPH method. Usually, high content of phenolic and flavonoid compounds are responsible for antioxidant activity, but seeds extract of buckwheat showed the best antioxidant activity (IC_{50} 0.06 mg/mL) although content of those compounds were not the highest. The lowest antioxidant activity had millets extract (IC_{50} 14.82 mg/mL). By determination of the qualitative composition of the extracts, the components which are responsible for antioxidant activity could be identified.

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Abstract

PP-PHC-14

Content Determination and Structural Analysis of Eugenol Obtained from *Caryophilly flos* Using Different Extraction Methods

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Extraction
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Abstract: Eugenol is a natural substituted phenolic compound (4-allyl-2-methoxyphenol) found mainly in clove oil, but can be also extracted from basil, cinnamon bark, bay leaf, and vanilla. Clove bulb (*Caryophilly flos)* samples, available at the local market, underwent to Soxhlet extraction in ethanol and diethyl ether as well as hydro distillation during five hours. Dichloromethane was used for eugenol separation from the obtained extract. The highest yield of eugenol of 13,5% was achieved by Soxhlet extraction with ethanol. The extracts before and after purification were analyzed in two mobile phases, hexane: acetone (9:1) and toluene: ethyl acetate (9.7:0.3) by TLC and 2DTLC. The calculated R_f values were consistent with previously reported values for same mobile phases. On the FTIR spectra of all samples, specific peaks and strips that are characteristic for the eugenol structure as well as the strains of the accompanying molecules created by eugenol isomerization were featured. During the extraction and separation, the eugenol isomerization occurred as confirmed by the literature data. Peaks between 680-725 cm^{-1}, 800-860 cm^{-1} and 860-900 cm^{-1} confirmed the presence of asymmetric trisubstituted benzene. Methoxy group appeared on 1463 cm^{-1}, the hydroxyl group in area between 3300-3600 cm^{-1} and the allyl group was noticed in area 2840-2950 cm^{-1}. Those are just some of the peaks that match the same FTIR spectrum of the eugenol standard.

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POSTER PRESENTATIONS

Chemistry of Advanced Materials

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Abstract

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Effect of Initial pH on the Removal of Textile Dye RB19 from Water by Lidnocellulosic-Al_2O_3

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Lignocellulosic Biosorbent,
Al_2O_3,
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Textile dve

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Abstract: The chemically modified lignocellulosic biomass with an inorganic oxide (Al_2O_3) was tested as a new sorbent for the removal of textile dye reactive blue 19 (RB19) from aqueous solution in batch conditions. As a starting biomass oak woodchips, with lignocellulosic structure mainly consisting of 46% cellulose and 24% of lignin, were used.

The removal of pollutants from water by sorbents is significantly affected by the pH value of the solution, thereby changing the surface charge of the sorbent and the chemistry of the pollutants. In order to define optimal conditions for sorption of RB19 from water, by lignocellulosic-Al_2O_3 biosorbent (LC-Al_2O_3), effects of initial pH were studied in range from 2.0 up to 10.0. An increase in the solution pH from 2 to 5 led to a slightly decrease of removal efficiency of RB19 from 99.91 to 97.90%, and with further increase up to 10 considerably decrease to 2.11%. The highest removal efficiency of RB19 was observed at pH 2.

In addition to the high removal efficiency, LC-Al_2O_3 biosorbent possesses other benefits, like mechanical stability, ease of synthesis, cost-effectiveness, biocompatibility and environmental-friendliness, which all makes it a promising material for the removal of anionic pollutants from water.

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Abstract

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Ultrasonic Assisted Fabrication of Polyvinyl Chloride/mixed Graphene-carbon Nanotube Nanocomposites as a Potential Ag^+ ionic Sensor

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Ag^+ ionic sensor
Electrochemical method
Environmental safety

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Abstract: A new sensitive Ag^+ ionic sensor based polyvinyl chloride/mixed graphene - carbon nanotube nanocomposites have been fabricated in the form of (PVC/MG-$CNTs_{a-e}$) with the help of ultrasonic assistance. The fabricated PVC/MG-$CNTs_{a-e}$ nanocomposites were identified and characterized by different characterization techniques. The mixed G/CNTs were stimulated in highly regular order in the PVC film and its crystallinity was significantly improved. CDT_{max} for all the samples were nearly similar and appeared in the same range 270 - 305 ºC. Moreover, a potential Ag^+ ionic sensor has been fabricated based on the glassy carbon electrode (GCE) by PVC-MG-CNT NCs to make a thin layer for the working electrode. The slope of calibration curve plotted as current versus concentration of Ag^+ ion was used to calculate the sensitivity (6.4241 $\mu A \mu M^{-1} cm^{-2}$) by considering the active surface area of sensor probe. The current observation based on Ag^+ ionic concentration is found to be linear over the linear dynamic range (LDR), where the detection limit (DL= 14.78±0.74 pM) is measured by considering the signal to noise ratio at 3. Considering the application feature of Ag^+ ion sensor, the proposed sensor was demonstrated good reproducibility and reliability in the application of environmental and healthcare fields at broad scales.

POSTER PRESENTATIONS

Environmental Chemistry

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Abstract

PP-ENC-01

Emission and Imission of Pollutants in the Air

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Abstract: The particles appear in the air in various shapes and sizes, ranging from a diameter of several hundred to several microns.

The composition of the particle is important because it depends on the size, the density, the volatility, the reactivity, and what is of particular importance is the toxicity. The particles present in the atmosphere are about 0.002 to 100 microns (μm). These are the largest that do not stay suspended in the atmosphere for a long time, but are slow to slow down - only 4 to 8 hours.

Dust in certain natural and working conditions with its immission value may exceed the permissible limit values applicable to inhabited areas; this may pose a potential danger to the air atmosphere in the environment.

The total emissions in this paper are calculated according to the limit values for nonroad machinery, ie, work equipment for standardized permissible emissions of CO, HC, NO_x and PM_{10}. Thus, the work machines consider the EU Stage IIIb standards, but since they use the production machines by 2006, the calculation has been implemented according to the EU Stage III standards.

The calculated values of the immission concentrations of pollutants, from exhaust gases and mineral dust generated by the construction machinery in the concrete production plant, are significantly below the legally limited limit values. The calculation was made for the most unfavorable scenario, with the simultaneous engagement of the complete available mechanization.

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Abstract

PP-ENC-02

Noise in Industrial Plants and Mining Machines

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Abstract: Noise sources in the living and working environment directly affect the harmonious functioning of the human organism and all kinds of its activities. Noise sources can be spatial (stationary and mobile), time (short and continuous) and acoustic (include range, strength, and moderation). The question arises: Is it possible to adequately protect the living and working environment in which a person could work harmoniously? Certainly it is possible, with adequate preventive engineering, which primarily encompasses maintenance of the living and working environment at the highest possible level. In many countries of the world, there are laws relating to the safety and health of people. The purpose of these laws is to create a safe working and environment, as well as to remove unsafe procedures and processes.

In addition to the direct harmful effects on human health, the noise indirectly influences the results of the work, and the fact that the stronger the overall impact is more visible and more important, and it is reflected in the reduction of productivity, increase in the number of errors and injuries at work. In the measurement and valorization of noise hazards, special procedures are introduced in order to influence the noise impact correctly.

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Comparison of Heavy Metals Content in the Unwashed and Washed Epiphytic Lichen *Evernia Prunastri*

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Atomic Apsorption
Spectrophotometry-Flame
Technique (FAAS)

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Abstract: Lichens are dominant organisms which are able to indiscriminately, on its whole surface accumulate polutants from the air. In this paper, content of eight selected heavy metals: Cr, Cu, Mn, Fe, Ni, Cd, Pb and Zn was determined in epiphytic lichen Evernia Prunastri, by atomic apsorption spectrophotometry-flame technique (FAAS). Comparison was made between unwashed and sample that was washed in distilled water. Differences between the unwashed and washed samples varied according to the levels of metal pollutant. Content of all heavy metals analysed, except for Fe and Cd, was higher in unwashed samples. Pb and Zn content in unwashed samples was 5.82 mg/g and 7.59 mg/g and in washed sample 1.08 mg/g and 5.84 mg/g, respectively. Of all the metals analysed, Fe showed the highest concentration (99.01 mg/L) in washed sample and 97.86 mg/L in unwashed sample. Washing the lichens before the analysis significantly reduced the concentrations of most of the measured metals. This indicated that substantial amount of metals was on the lichen surface as dry aerosol particles.

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Abstract

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Removal of Toxic Dyestuffs from Aqueous Solution by Amphoteric Bioadsorbent

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Abstract: A novel amphoteric chitin containing amino and carboxyl groups as an adsorbent for removal of both acid and basic dyes in solution is presented. The amphoteric chitin has been fully characterized by FTIR, TGA-DTG, elemental analysis, SEM and point of zero charge. The amphoteric adsorbent was proven effective in removing both anionic and cationic dyes (Acid Red 1 and methylene blue), at corresponding favored pH conditions of 2 and 8, respectively. The fundamental adsorption behavior of the adsorbent on removing these dyes was investigated at different factors, such as pH, dose of amphoteric chitin, initial dye concentration, adsorption time, and adsorption temperature. The equilibrium isotherm at room temperature fitted the Freundlich model for MB and the maximum adsorption capacity was 98.2 mg/g using 50 mg/l of MB, whereas the equilibrium isotherm fitted the Freundlich and Langmuir model for AR1 and the maximum adsorption capacity was 128.2 mg/g. Kinetic and thermodynamic studies have been also investigated. The experimental result revealed that the adsorption mechanism followed the chemical adsorption with an ion-exchange process. Also, recycling of the adsorbent was easy and its reuse for dye removal was effective.

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Abstract

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Physico-Chemical Characterization of Igalo Bay Peloid (Republic of Montenegro) and Assessment of the Pollution in the Sampling Area

Bigović, M.[a], Roganović, M.[b], Milašević, I.[c], Đurović, D.[c], Kastratović, V.[a], Slavić, V.[d], Kosović, M.[e], Vlahović, M.[e], Perović, S.[a], Perović, A.[a], Potpara, Z.[b], Martinović, M.[b], Pantović, S.[b]

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Abstract. This is the first study of chemical characterization of peloid from Igalo bay (Montenegro). Thanks to physical, chemical and mechanical character the peloid was used in healing and rehabilitation of many illnesses through the centuries. The determination of the physical and chemical characteristics of peloid from Igalo (the peeling temperature at the sampling site, pH-value, density, electrical conductivity, the content of light and heavy metals, the content of some non-metals and amount of water and nitrogen were performed. The data obtained from chemical analysis were compared with several available data for peloids from the region of Croatia, Italy, Spain and Dead Sea. The water samples of peloid were collected from Igalo Beach. The temperature was measured in situ, while the pH-value, conductivity of each sample and density were measured in a laboratory (the sample is immediately closed after collecting, in order to avoid any contamination of the substances from the outside). The samples were digested in a microwave sample preparation system (Microwave Reaction System-Anton Paar). The content of metals and non-metals was determined by using inductively coupled plasma - optical emission spectrometry (ICP-OES- Spectro Arcos). The content of mercury was determined by Direct Mercury Analyser DMA-80, produced by Milestone. The water content was determined first by drying up to 80^{o}C during 24 hours, and then by gravimetric analysis techniques. The percentage of nitrogen was determined by Kjeldahl method. Furthermore, the determination of some environmental indicators such as: contamination factor (CF), pollution load index (PLI) and index of geoaccumulation (I_{geo}) was done. The largest percentage of the heavy metal content refers to manganese and chromium was noticed. The obtained values showed that there is no heavy metal pollution in the sediment.

POSTER PRESENTATIONS

Education in Chemistry

(EDC)

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Abstract

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Determination of Misconceptions of Science Teacher Candidates about Conception of Gas Laws by Four-Tier Test

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Abstract: Gas laws that take place in gaseous context are one of the chemical topics that students have difficulty in understanding. It is difficult to understand because most of the gases are not visible, and it is a concept that must be understood at the molecular level. As a result, terms which are not accepted scientifically, in other words misconceptions about gas laws occur in the minds of students. The similarity between the misconceptions of teachers and students shows that the misconceptions are conveyed to the new generations by the teachers. For this reason, the misconceptions of teacher candidates should be addressed. It has been observed that the four-tier test is not used to detect the misconceptions about gas laws. In this study, it is aimed to determine the misconceptions of science teacher candidates about gas laws by using a four-tier test. The research is a descriptive one. Four-tier test was applied to 74 teacher candidates who are in the first year at the department of science teaching in Konya Necmettin Erbakan University Ahmet Keleşoğlu Faculty of Education in 2017-2018 academic year, thus frequency and percentage distributions were analyzed. By analyzing the data, the misconceptions seen in teacher candidates have been determined. When the results are evaluated;

- ✓ The mostly determinated misconception of teacher candidates about the pressure-volume relation is that "the (PxV) value changes when the piston system is pushed down at a constant temperature.
- ✓ The mostly determinated misconception of teacher candidates about number of mole-volume relation is that "One mole of gas occupies 22.4 liters of volume in all conditions"

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Abstract

PP-EDC-02

Physical Chemistry for Undergraduate Students: Integrating Knowledge from Mathematics, Physics and Chemistry

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Abstract: Physical Chemistry is an obligatory course in one or more semesters in the curricula of several academic studies at the University of Sarajevo, Bosnia and Herzegovina. Teaching Physical Chemistry includes lectures, physical chemistry calculations and laboratory exercises. Traditionally, courses of physical chemistry remain to be a certain difficulty for the students in achieving good results in learning and in passing exams. Besides that, insufficient integration of achieved knowledge in physics, chemistry and mathematics was observed. This is particularly evident in the mutual integration of knowledge in general chemistry, physics and mathematics which are considered to be fundamental for physical chemistry. This paper presents the results of research on teaching the Physical Chemistry I and Physical Chemistry II, conducted with the 2nd and 3rd year chemistry students at the Faculty of Science University of Sarajevo, with main purpose to find possible solutions that could lead to greater efficiency of learning, and to more successful students' continuation of their chemistry studies. According to the obtained results, we can conclude that a number of objective difficulties students brought from earlier schooling affected their learning and its results. Some of them are differentiation between high school curricula, insufficient number of chemistry, physics and mathematics classes during middle and high school and the lack of integration between them. Some students also had subjective difficulties, like the lack of motivation for achievements with satisfying results.

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The Pre-Learning Strategy Using Chemistry Learning Materials: Teachers' Approach

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Abstract: The pre-learning strategy includes activities oriented at students' preparation in advance of a class. Using such activities increases the pre-knowledge level what allows linking new information with the existing knowledge more efficiently and consequently reduces working memory overload. Research results indicate frequent usage of various learning materials within the frame of the pre-learning strategy. The main purpose of this research is to determine the frequency of chemistry learning materials usage within the frame of the pre-learning strategy in Croatian secondary schools. The quantitative descriptive survey research was conducted on a sample consisting of 77 high school chemistry teachers and 62 vocational school chemistry teachers from all regions in Croatia. Data were collected through an online questionnaire and processed with descriptive and inferential statistics. According to the obtained results, it is most common that teachers make their own chemistry learning materials (Word, PowerPoint) for students' preparation in advance of a chemistry class. For the same purpose, students most commonly study text/image materials whereas audio-materials (podcast), audiovisual materials (screencast) and digital materials are represented insufficiently. High school chemistry teachers' usage of chemistry learning materials does not differ significantly from vocational school chemistry teachers' usage.

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Abstract

PP-EDC-04

Integration of Natural Sciences in Extracurricular Activities in Canton Sarajevo Gymnasiums

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Gymnasiums
Science Integration
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Extracurricular Activities

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Abstract: The challenges of modern world lead to increasing need for the technological solutions to everyday life as well as long-term issues. Modern technology and science demand combination of different fields in order to achieve goals and solve complex problems. Facing challenges of the future falls to the younger generation and the education system has a pivotal role in preparing them for what lies ahead. While present day curricula in gymnasiums in Canton Sarajevo do explore natural sciences in large scope, they do not provide adequate opportunity for science integration and multidisciplinary approach to real world problems. While curricular reforms can, to some extent, achieve solutions to these deficiencies, extracurricular activities within gymnasiums can easily provide environment in which students can express their ideas, work on assigned or chosen projects without borders and limitation of subject curricula. In this study a number of ways of achieving these goals is presented, including team-oriented and independent projects as well as research assignments. Those can be implemented so as to complement existing curricula and it would not require its revision for the implementation at this stage. Those would include integration of at least two different disciplines with the same objective that could not be reached separately and would expose students to multidisciplinary approach to research in modern times that is rarely included in gymnasiums.

POSTER PRESENTATIONS

Chemical Engineering

(CE)

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Abstract

PP-CE-01

Characterization of Raw Materials and Final Product in the Cement Production

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Raw Materials
Clinker
Cement
X-Ray Diffraction
Minerals

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Abstract: Cement is a hydraulic binder formed by the grinding process of cement clinker, as intermediate product, which is produced by baking the lime-clay raw material mixture to the sintering temperature. This research paper describes mineralogical analysis technique of primary raw materials, auxiliary components for cement production, by-product clinker and final product, cement. Used technique is X-ray diffraction technique, which is one of the most modern instrumental techniques today. Obtained results are provided in the form of diffractogram, which is used to display the minerological phase of components. X-ray diffraction method confirmed the theoretical knowledge of the mineralogical components of tested raw materials, clinker and cement. As expected, the main component of limestone is mineral calcite, as active compound, fly ash and slag as amorphous substances and clinker contains clinker-minerals and gyspum contains calcium sulfate dihydrate in large percentage. Main components of cement are all minerals provided in clinker and raw materials. These experiments were carried out in the Holding Company Cement Plant in Lukavac, Bosnia and Herzegovina.

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Abstract

PP-CE-02

Efficiency of Various Types of Industrial Corrosion Inhibitors for Stainless Steel and Copper

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Abstract info
Received: 11.09.2018.
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Keywords:
Corrosion Rate
Coupons
Pilot Plant

Abstract: For purpose of this work a pilot plant has been constructed on which investigated the efficiency of corrosion inhibitors. Since the plant is made of two different construction materials: copper and stainless steel, it was investigated which corrosion inhibitor and how much slowing the corrosion rate on the mentioned materials. It was used three different industrial corrosion inhibitors. First, the degree of corrosion without the addition of the inhibitor was determined, and then after the addition of the inhibitor. The corrosion rate is determined by the mass loss method, using corrosion coupons, in accordance with Standard Test Methods for Corrosivity of water in the Absence of Heat Transfer, D 2688, 1999. As the corrosion processes are very slow, for the purpose of this paper chlorides are added as corrosion activators.

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POSTER PRESENTATIONS

Physical and Theoretical Chemistry

(PTC)

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Abstract

PP-PTC-01

Predicting of the Reactivity of the Compound 3-(1-(4-metilfenilamino) etilidene)-hroman-2,4-dione

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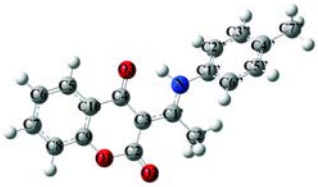
Coumarin Derivative
Reactivity
Condensed Fukui Function
DFT
NBO

Abstract: During the last few decades, considerable attention has been devoted to the synthesis of new coumarin derivatives, which exhibit significant biological activity, as well as to predicting their reactivity and chemical behavior. To predict the chemical reactivity of new synthetized compound 3-(1-(4-metilfenilamino)etilidene)-hroman-2,4-dione Condensed Fukui Functions (CFFs) are used. CFFs values, labeled as f_A^-, f_A^+ and f_A^0, indicate the atomic positions in molecule suitable for electrophilic, nucleophilic and radical attack, respectively. The equilibrium geometries of considerable neutral and charged moieties of investigated molecule are optimized using B3LYP-D3 hybrid density functional in combination with 6-311+g(d,p) basis set. CPCM solvation model is used to simulate water and benzene as solvents, in order to mimic aqueous and lipid environment. Natural charges and spin density values of investigated species are obtained by performing the NBO analysis. Obtained results indicated that investigated molecule react with nulceophiles, electrophiles and free radicals at the same reactive positions in polar and non-polar solvent. Nucleophilic attach can be expected in positions C1', C4 and C7. Electrophilic attach is supposed at C3, C4'', C1'', N, O2 and O3 atoms. Finally, free radical can attach investigated molecule in positions C1', C5, C4'', C7, C2'' and C1''.



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Abstract

PP-PTC-02

Atmospheric Corrosion of Metals in Urban Area

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Atmospheric Corrosion
Iron, Brass
Chrome
Zinc
Linear Voltammetry
Cyclic Voltammetry

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Abstract: Atmospheric corrosion rate depends on the content of the individual components in atmosphere, temperature of air, referring primarily on the moisture content, the content of the various particles and the SO_x and NO_x gases. Washing out the pollutants from the atmosphere creates strong acids, bases and salts that can corrode various metal and non – metallic structures. The analysis of certain precipitation parameters, analysis of metal and alloy samples exposed to the atmosphere in Sarajevo and Kiseljak and analysis of metal and alloy samples without atmospheric influence were carried out. The methods used for sample analysis are linear voltammetry and cyclic voltammetry. As samples were used iron plates, chrome coated iron plate, zinc coated iron plate, chrome coated iron plate with worn out surface, zinc coated iron plate with worn out surface and brass plate. It can be noticed that the corrosion of samples in Sarajevo is more intensive and less intensive in the area of Kiseljak. Measurements with linear voltammetry in a given range of potentials gave more pronounced corrosion currents in the urban area. Measurements with cyclic voltammetry gave pronounced reduction peak at -0.25 V for brass, and for chrome coated iron plate at -0.05 V. For the zinc coated iron plate sample, potentials were shifted to negative values that belong to zinc. For chrome coated iron plate, reduction peak is at -0.75 V. The cyclic voltammogram for zinc coated iron plate with worn out surface is similar to the cyclic voltammogram for zinc coated iron plate. Urban area of Sarajevo is heavily polluted by pollutants which can affect all aspects of life and environment. The occurrence of acid rains is intensified, which increases the corrosion of material of which the constructions are made.

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Abstract

PP-PTC-03

Ferrocene Chromophore as a Circular Dichroism Probe for Conformational Analysis of Short Peptides

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Conformational Analysis
Ferrocene
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CD-spectroscopy

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Abstract: The perturbation of inherently achiral chromophore, caused by covalently attached chiral system, causes the modification of its chiroptical properties and can give rise to intense CD-activity in the spectral region of the absorbing chromophore. We have recently demonstrated that ferrocene-functionalized homo- and heterochiral dipeptides [Boc-$(AA)_2$-NH-Fc] are able to form ordered conformations that resemble the naturally occurring beta- and gamma- turns. Furthermore, the strong bands in the CD-spectra of these bioorganometallics originate from the transfer of chiral information from the local secondary structure to ferrocene chromophore.

As a continuation of this study, we have synthesized four enantiomeric pairs of derivatives of aminoferrocene and homo- and heterochiral tripeptide sequences (Boc-Pro-Pro-Ala-NH-Fc) and subjected them to a detailed conformational study. Results obtained by means of spectroscopic analysis (NMR-, IR- and CD-spectroscopy) and computational chemistry methods indicate that conformational preferences of these derivatives, and thus the ability to form specific secondary structure elements (turns, minimal helices), strongly depend on chirality of the constituent amino acids. Moreover, different conformations of the peptide sequence give rise to different shapes and intensities of CD-bands around the UV/Vis absorption maximum of the ferrocene chromophore.

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Abstract

PP-PTC-04

Determination of the Activity and Kinetic Parameters of Isolated Catalase

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Abstract info
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Keywords:
Catalase
Kinetic Parameters
Isolation

Abstract: Catalase is a widespread enzyme and is found in prokaryotes and eukaryotes, and is part of the antioxidant protection of the organism. In order to be able to test the activity of catalase, it is first necessary to isolate the enzyme and in this work the catalase is isolated from plant material, potatoes.

The enzymatically catalyzed reaction has a reduced activation energy relative to the non-enzymatic reaction, since the enzyme-substrate complex is at a higher energy level than the free substrate.

The action of the enzyme begins with the formation of a complex with a substrate, which has a lower activation energy than an activated intermediate of substrates without enzymes. In this paper the volumetric method determines the activity of isolated catalase depending on time, temperature, substrate and pH value, as well as kinetic parameters. The activity of catalase decreases with incubation time, and during the incubation time of 30 minutes the enzyme denaturation occurs. The obtained value of the Michaelis-Menten constante (Km) is 0.125 mmol / L and is determined from the Lineweaver-Burk diagram.

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Abstract

PP-PTC-05

Spectrophotometric Determination of Catalase Activity in Presence of $K_2[B_3O_3F_4OH]$ using Method with Ammonium Molybdate

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Abstract info
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Keywords:
Catalase Activity
Boroxine

Abstract: Catalase as oxidoreductase is an enzyme that protects cells and organism from oxidative stress and the formation of free radicals. It has a very high value of the catalytic constant and it follows Michaelis-Menten's kinetic model. In this study the spectrophotometric method was used to follow enzyme activity based on formation of stable complex of hydrogen peroxide with ammonium molybdate at 25°C. The enzyme reaction was stopped with 100 µl of ammonium molybdate and the absorbance of formed yellow complex was measured at 405 nm.

Calculated enzyme activity showed linear dependence for different concentrations of hydrogen peroxide 10.00, 8.33, 6.66, 5.00 and 3.33 mM. The results showed that the $K_2[B_3O_3F_4OH]$ reduces catalase activity.

- This work was partially supported by the Croatian Science Foundation under project number HRZZ-IP-2014-09-6897.

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Abstract

PP-PTC-06

The Influence of Trioxohydroxytetrafluorotriborate on the Activity of the Enzyme Peroxidase in the Presence of Magnesium Ion

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Magnesium Ion
Inhibition
Trioxohydroxytetrafluorotriborate

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Abstract: Trioxohydroxytetrafluorotriborate ($K_2[B_3O_3F_4OH]$) is already shown as good inhibitor for HRP (horseradish peroxidase). Since ($K_2[B_3O_3F_4OH]$) is potentially new drug the aim of this study was to investigate inhibition 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 6 mM concentration and the solution also contained magnesium ion (1 mM). The HRP activity assay was performed by the measurement of guaiacol peroxidation by H_2O_2, following the increase of absorbance at 470 nm. Using Lineweaver-Burk plots inhibition of enzyme activity was shown, and K_M and V_{max} values were determined.

- This work was partially supported by the Croatian Science Foundation under project number HRZZ-IP-2014-09-6897.

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Abstract

PP-PTC-07

Fluorescent Phenanthridine-Based Calix[4]arene Derivatives: Synthesis and Complexation Properties

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Keywords:
Calix[4]arenes
Phenantridine
Metal cations
Fluorescence
Complexation
Thermodynamics

Abstract: Calixarenes are macrocyclic oligomers consisted of four or more phenolic residues linked by methylene groups in the *ortho* position and can be easily functionalized to give receptors for vast number of ionic or neutral species. Calixarenes bearing fluorescent moieties can be considered as potentially very sensitive fluorimetric ion sensors due to the high sensitivity of fluorescence spectroscopy and high affinity of these macrocyclic ligands towards cations. In the scope of this work, two novel fluorescent phenathridine-based calix[4]arene derivatives were designed and prepared. The binding affinities of these compounds towards metal cations in several solvents (acetonitrile, methanol, ethanol, *N*,*N*-dimethylformamide, dimethylsufoxide) were investigated. Phenanthridine moities were introduced at a lower calix[4]arene rim and served both as fluorescent probes and parts of cation-binding site. Stability constants of the corresponding complexes were determined by means of UV spectrophotometry, fluorimetry and isothermal microcalorimetry. The latter technique also provided information on reaction enthalpies and entropies. The obtained results were discussed regarding the structural characteristics of the calixarene derivatives and differences in solvation abilities of the solvents used.

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Abstract

PP-PTC-08

The Solvent Influence on the Complexation of Amphiphilic Mannosides with β-cyclodextrin

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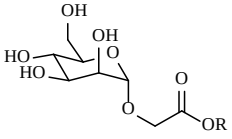
Keywords:
Cyclodextrin
Inclusion Complexes
Microcalorimetry
NMR
Solvophobic Solvation

Abstract: The solvent influence on the complexation of amphiphilic mannosides, consisting of different non-polar moities, with β-cyclodextrin was explored in a range of temperatures ($5 \leq \vartheta / ^{\circ}C \leq 65$) by means of microcalorimetry and NMR spectroscopy. The complexation was observed only in strongly hydrogen-bonded solvents (water, formamide, *N*-methylformamide, and ethylene glycol). The stabilities of complexes were higher in water than in investigated organic solvents, whereby all reactions were enthalpically controlled. A notable temperature dependence of $\Delta_r H^{\circ}$ and $\Delta_r S^{\circ}$ was noticed in water. In contrast, the standard complexation parameters in other investigated solvents exhibited relatively weak temperature dependence. As expected, the complex stability was strongly influenced by compatibilty of the guest and the β-cyclodextrin cavity sizes, as well as the flexibility and structure of the hydrophobic group of investigated mannosides. The carried out investigations provided a deeper insight into the hosting process, demonstrating that solvophobically driven formation of cyclodextrin inclusion complexes is not a water limited phenomenon.



Structure of investigated mannosides; R =cyclooctyl, *t*-butyl, *n*-butyl, *n*-hexyl, *n*-octyl cyclohexyl and adamant-1-yl.

Corresponding author:
Josip Požar

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POSTER PRESENTATIONS

Organic and Medicinal Chemistry

(OMC)

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Abstract

PP-OMC-01

Synthesis, Characterization and In Vitro Antimicrobial Activity of the Cu(II) and Fe(III) Complexes with 1-cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid

Horozić, E.[a], Cipurković, A.[b], Ademović, Z.[a], Bjelošević, D.[c], Zukić, A.[c], Kolarević, L.[c], Husejnagić, D.[b], Hodžić, S.[b], Ibišević, M.[c]

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Iron
Copper
Ciprofloxacin
IR Characterization
Stereo-Microscopy
Antimicrobial Screening

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Abstract: 1-Cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid (Ciprofloxacin, CPF) is a drug that belongs to the second generation of fluoroquinolone antibiotics with a wide range of effects on Gram-positive and Gram-negative bacteria. Ciprofloxacin prevents bacterial cell division by inhibiting DNA gyrase, and type II topoisomerase, topoisomerase IV. In organism there is a possibility of interaction of CPF with biogenic elements in the blood, which could lead to the formation of complexes. This can cause change in the activity of antibiotics towards pathogenic microorganisms.

The aim of this work was to investigate the interaction of CPF with the biological cations Cu(II) and Fe(III) in the blood in approximate physiological conditions. Synthesized complexes were characterized using IR spectroscopy and stereo-microscopy. For the synthesized complexes melting point were determined and compared with CPF. Antimicrobial screening was performed on bacterial strains of *Escherichia coli*, *Enterococcus faecalis* and *Staphylococcus aureus*.

The results of IR spectroscopy showed that the Cu(II) and Fe(III) complexes with CPF were formed through the oxygen donors of the hydroxyl and/or carbonyl group of the ligand. The color and size changes of the crystal of the parent ligand and complexes were also clearly seen. Antimicrobial screening has shown that CPF and complexes have similar antimicrobial activity in the case of all strains, where the complex Cu(II)-CPF had better antimicrobial activity compared to the Fe(III)-CPF complex.

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Abstract

PP-OMC-02

Determination of the Citric Acid Content in Commercial Fruit Juices by HPLC

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Abstract: Natural fruit juices can play a significant role in healthy eating habits because, beside good taste, they also offer a variety of nutrients naturally found in fresh fruit. Organic acids are the universal ingredient of all fruit juices. The most important are the citric and ascorbic acid. Citric acid (2-hydroxy-1,2,3-propantricarboxylic acid) is a weak acid, which is naturally present in citrus fruits.

The aim of this study was to determine the citric acid (CA) content in orange, strawberry, peach and apple juices that are commercially available on the market in Bosnia and Herzegovina using HPLC method and to compare the CA content with the Ordinance on Fruit Juices in Bosnia and Herzegovina.

The HPLC standards showed a linearity in the tested concentration range of 10-1000 mg/L ($y = 5671.7x + 25285$; $R^2 = 0.9971$). The concentrations of CA in the samples of orange juice were within the reference range (6.3-17.0 g/L), except for the one sample that contained CA below the reference range. The same applies to samples of apple and strawberry juice that contained 50-150 g/L and 5-11 g/L CA, respectively. All samples of peach juice were also within the reference range of 1.5-5.0 g/L. Applied HPLC method is suitable to test CA content in commercial juice samples.

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Abstract

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The Effects of the Backbone Chirality, Amino Acid Sequence and the *N*-terminal Group on the Conformational Properties of Ferrocene Peptidomimetics

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Abstract: Our previous work on peptides that contain homo- and heterochiral Ala–Pro sequences attached to the turn-inducing ferrocene-1,1'-diamine scaffold have revealed different conformational properties of homo- and heterochiral peptides. An exchange of two *N*-terminal groups had a somewhat larger influence on the distribution of the hydrogen-bond patterns in homochiral than in heterochiral derivatives. In order to get more detailed insight into conformational patterns of ferrocene-containing peptides, we have coupled 1'-aminoferrocene-1-carboxylate with homo- and heterochiral peptides Ala–Pro and Pro–Ala. The influence of amino acid sequence, backbone chirality and different bulkiness and basicity of the *N*-terminal Boc and Ac groups on the conformational behaviour of the corresponding peptides was systematically explored by IR, NMR, and CD spectroscopy. Although the observed intramolecular hydrogen-bond patterns permitted all NH groups belonging to ferrocene unit (NH_{Fn}) to be involved in turn-stabilizing interactions, the NH_{Fn} groups of heterochiral peptides were found to be involved in a stronger hydrogen bonds. The strength of hydrogen-bonding interactions was also influenced by amino acid sequence and *N*-terminal group.

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Abstract

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Synthesis and Spectroscopic Characterization of Anthracene Based Asymmetrical Schiff Base Ligand

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Schiff Base
Asymmetrical
Fluorescent
Spectroscopy
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Abstract: Schiff bases are aldehyde or ketone like compounds in which the carbonyl group is replaced by an imine or azomethine group. They are widely used for industrial purposes and also exhibit a broad range of biological activities. Schiff bases are active against a wide range of organisms since they play an important role in living organisms, such as decarboxylation, transamination and C-C bond cleavage. Asymmetric Schiff base ligands have many advantages over their symmetrical counterparts in the composition and geometry of transition metal complexes and properties. Most of these asymmetrical ligands are Schiff bases obtained through the stepwise condensation of the appropriate diamine with two different carbonyl compounds.

In this study, the fluorescent asymmetrical Schiff base was synthesized with the condensation of 1,2-phenylenediamine, 3-hydroxybenzaldehyde, 9-anthracenecarboxaldehyde. Schiff base ligand was characterized by using FT-IR, and ^{1}H NMR. This compound was examined for its fluorescent properties toward different metal ions (Na^{+}, Li^{+}, Mg^{2+}, Ni^{2+}, Ba^{2+}, Ca^{2+}, Cu^{2+}, Pb^{2+}, Zn^{2+}) by UV-visible and fluorescence spectroscopy.

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Abstract

PP-OMC-05

Turn on Fluorescent Sensor Based Phenolphthalein-calix[4]arene for Zn^{2+} and its Application in Living Cells

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Abstract info
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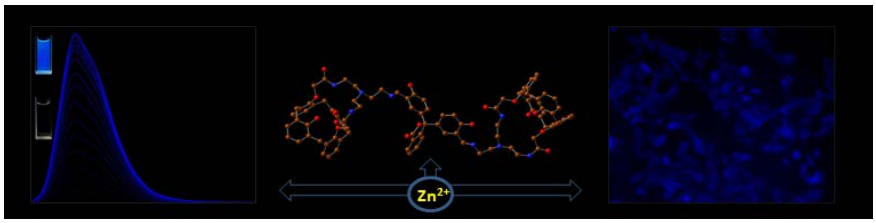
Keywords:
Calix[4]arene
Phenolphthalein
Zinc
Fluorescent
Living Cell

Abstract: Calix[4]arene-phenolphthalein based a novel fluorescent sensor (C4P) was designed and synthesized for selective detection of Zn^{2+} in aqueous media. C4P indicated good selectivity and high sensitivity towards Zn^{2+} in the presence of most metal ions, and a remarkable enhancement in fluorescence emission intensity at 440 nm was observed with addition of Zn^{2+}, which was attributed to the inhibition of photoinduced electron-transfer (PET) phenomenon and C=N isomerization process. Besides, the detection limit of C4P for $Zn^{2+}$was as low as 0.108 μM (at 10^{-7} M level). Moreover, the fluorescence imaging in the human colon cancer cells suggested that C4P had great potential in the application of biological imaging.



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Abstract

PP-OMC-06

Pharmaceutical Analysis of Metronidazole Tablets

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Metronidazole
Pharmaceutical analysis
Tablets
Spectrophotometric determination
HPLC determination
Dissolution test

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Abstract: Metronidazole (2-methyl-5-nitroimidazole-1-ethanol) is a synthetic antibacterial and antiprotosoal agent of the nitroimidazole drugs. It shows high activity against *Trichomonas vaginalis* and *Entamoeba hystolitica*. The objective of this paper is the pharmaceutical analysis of solid oral formulations (9 tablets) containing metronidazole available on the market of Bosnia and Herzegovina. The following process parameters were studied: appearance, average tablet weight, disintegration, content uniformity, dissolution test, assay determination of metronidazole and related substances. The appearance, mass balance, disintegration, content complied with the quality requirement according to European pharmacopoeia. Metronidazole content in all tested samples was within the limits of the shelf-life specification (102.00%, 95.70%, 94.81%, 95.00%, 107.56%, 98.40%, 90.65%, 96.22%, 98.12%), as well as the results of dissolution test (Tolerances: NLT 80%(*Q*) of the labeled amount is dissolved). Related substances in all tested samples were within the limits of the shelf-life specification (Tinidazole related substance A <0.5%, any individual unspecified degradation product <0.10%, Total impurities <2.0%). The results of the research have shown that all tested samples purchased on the market of Bosnia and Herzegovina correspond to specified quality requirements with official pharmacopoeias monographs (BP and USP Metronidazole Tablets)

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Abstract

PP-OMC-07

Selective Colorimetric Detection of Cu^{2+} Ion in Aqueous Solution by a Simple Receptor

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Keywords:
Receptor
Copper
Colorimetric
Sensor

Abstract: In this study, *N*,*N*-bis(2-chloroethyl)-4-(1*H*-phenanthro[9,10-*d*]imidazol-2-yl)aniline (R) as receptor was designed, synthesized and characterized by ^{1}H, ^{13}C, APT, COSY NMR, FTIR, elemental analysis, and UV–vis spectral data. The binding properties of **R** were studied with different metal ions. **R** showed selective chromogenic sensor property toward Cu^{2+} in aqueous media. The color of the receptor (R) changed from light yellow to dark pink upon addition of Cu^{2+} ion. However, other metal ions such as Li^{+}, Na^{+}, Cs^{+}, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Al^{3+}, Fe^{3+}, Cr^{3+}, Fe^{2+}, Hg^{2+}, Zn^{2+}, Cd^{2+}, Co^{2+}, Ni^{2+}, Pb^{2+}, Mn^{2+} could not cause any color change. This selectivity could be easily observed by the naked eye, indicating that receptor **R** are potential colorimetric sensor for Cu^{2+} ion.

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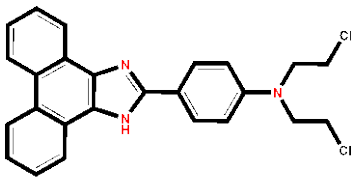

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Abstract

PP-OMC-08

Chromatografic and Spectroscopic Analysis of Cinnamic Acid Synthetized by Modified Perkin Method

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Keywords:
Cinnamic Acid
Synthesis
Perkin Method
TLC
FTIR

Abstract: Cinnamic acid (*trans*-3-phenyl-2-propanic acid) is usually found in plants in *trans* form, even though the *cis* form exist in plants. Biological pathways of phenolic acids synthesis are very complicated and it usually implies involvement in Shikimate metabolic pathways. Cinnamic acid isolated from plants or synthesized has wide range of biological activities. So far there are few synthetic methods for cinnamon acid preparation. In this work we used a slightly modified conventional Perkin method, as it was economically justified and simple, while getting a satisfying yield. The modification referred to the change of the base catalyst as well as changing the ratio of the reactants used. Qualitative analysis and structural characterization of synthetized cinnamon acid was made by Thin Layer Chromatography, Melting point determination and Fourier Transform Infrared Spectroscopy. Benzene-methanol-water in volume composition 6:7:3 as the mobile phase showed most satisfactory Rf value. The melting point of synthetic product was 132.9°C, which corresponds to the literal values 133 °C for cinnamic acid standard. Comparing the FTIR spectrum of sample and cinnamic acid standard, characteristic signal values were observed: in COOH group the stretching of O-H, C-O and C=O bonds at 3026, 1229 and 1681 cm^{-1} respectively, as well as stretching of the aromatic C=C bonds at 1421 and 1628 cm^{-1}, and trans-isomeric stretching at 960 cm^{-1}. All these peaks confirmed that the synthetized substance is cinnamic acid.

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Abstract

PP-OMC-09

Bioactive Coatings Obtained by Plasma Electrolytic Oxidation of Titanium Implant and Their Cytotoxicity

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Cytotoxicity

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Abstract: Titanium is widely used as implant material since it shows very good corrosion resistance, good mechanical behaviour and biocompatibility, but it has low wear resistance and high friction coefficient which limits its more extensive application. This can be overcome by production of stable oxide coatings on the titanium surface using various methods. In this study, samples of titanium implant were treated with plasma electrolytic oxidation, subsequent ionic exchange and thermal treatment in order to obtain bioactive layer on their surface. XRD analysis was used to investigate phase composition of the obtained coatings, while their morphology was investigated by SEM. Cytotoxicity investigations by MTT, LDH and propidium iodide assays and light microscopy were done using murine fibroblasts cells L929. The obtained coatings consisted of titanium oxide, calcium and sodium titanates and hydroxyapatite. SEM revealed that the given method, besides corresponding phase composition, enabled specific nanotopology suitable for cell attachment and proliferation. Cytotoxicity investigations showed that these coatings were not cytotoxic to L929 cells.

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Abstract

PP-OMC-10

Pharmaceutical Analysis of Nesteroidal Anti-Inflammatory Diclofenac Sodium Tablets

Dacić, M.[a,b], Nuhagić, A.[a], Bašić, A.[a,b], Salešević, M.[a,b], Pašić-Kulenović, M.[c], Alagić-Džambić, L.[c]

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Tablets
Spectrophotometric Determination
Dissolution Test

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Abstract: Diclofenac [2-(2,6-dichloroanilino)phenyl]acetic acid is a non-steroidal anti-inflammatory drug. It is usually found as a sodium or potassium salt and used for the treatment of rheumatoid arthritis, ankylosing spondylitis, osteoarthritis and sport injuries. It is usually administered as oral formulations, and to some extent, as intramuscular and topical formulation. The aim of this study was a pharmaceutical analysis of diclofenac sodium in tablets from different manufacturers in Bosnia and Herzegovina. Several parameters were tested: appearance, average tablet mass and uniformity of dosage units. The active pharmaceutical ingredients (API) were determined spectrophotometrically and dissolution test was performed, as well. The appearance, the mass balance, and the uniformity of dosage units complied with the quality requirement (L<15). The API content in all tested samples was within the limits of the shelf-life specification (103.93%, 102.25%, 100.35%, 107.97%, 107.86%), as well as the results of dissolution test (Tolerances: NLT 75%(*Q*) of the labeled amount is dissolved, and Test 2 for Extended-release tablets). The results of the research have shown that all tested samples purchased on the market of Bosnia and Herzegovina correspond to specified quality requirements with official pharmacopoeial monographs (USP Diclofenac Sodium Delayed-Release Tablets and USP Diclofenac Sodium Extended-Release Tablets).

POSTER PRESENTATIONS

Radiochemistry

(RC)

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Abstract

PP-RC-01

Examination of Gross Alpha Activity, Beta Activity and Uranium Isotope Content of Thermal Waters from Bosnia and Herzegovina

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Gross Alpha-Beta Activity
Alpha Spectrometry
Gas Flow Proportional Counter

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Abstract: The occurrence of radionuclides in nature is a consequence of their crystallochemical and physicochemical properties, as well as the geological and hydrogeological characteristics of the examined areas. In this paper, the content of uranium isotopes and the gross alpha-beta activity of thermal waters from the territory of B&H (Sarajevo and Olovo) are determined in order to analyze the radiological status of water and the influence of the soil and rock composition on the examined parameters. The sampling was performed in the period of three months (February to April, 2016), at the beginning, middle and the end of each month. The content of Uranium isotopes was determined using the alpha spectrometry method, according to Eichrom, 2015, and HASL 300 (DOE EML, 1997) procedures. The gross alpha-beta activity was determined using a gas flow proportional counter, according to standard methods ISO9696 and ISO9697. The obtained results show that the activity concentration of uranium isotopes in the tested samples, has maximum value 10^{-2} Bq/L, while gross alpha and beta activity are between 10^{-2} to 10^{-1} Bq/g. It was established that the analyzed water is radiologically valid and is not harmful to human health and the environment, compared with the current legislation on water radioactivity (WHO).

POSTER PRESENTATIONS

Topics related to Chemistry

(TRC)

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Abstract

PP-TRC-01

Anticorrosion Capacity of *Ailanthus altissima* (Mill.) Swingle Honey

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Abstract info
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Corrosion
Iron
Tin
Saline solution

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Abstract: Tree of heaven (*Ailanthus altissima* (Mill.) Swingle) is a fast-growing, very aggressive and invasive deciduous tree and the unifloral honey from this plant is rare. Due to its biodegradability, eco-friendliness and low cost, a natural honey fulfils the requirements for a non-toxic green corrosion inhibitor. Several studies confirmed the honey potential application as the corrosion inhibitor of different metals and alloys, but there are no reports on the anticorrosion capacity of this honey type.

In the present study the ability of the honey to protect reactive surfaces of Fe and Sn, the main constituent of tinplate, against corrosion in a saline solution, pH 3.0, was tested using dc electrochemical methods and electrochemical impedance spectroscopy (EIS). The nondestructive EIS method was used at the open-circuit potential (E_{OCP}) under static conditions. EIS parameters obtained in situ in a wide frequency range were correlated to the phenomena that occur simultaneously at different time scales: the charge-transfer resistance, capacitance and resistance of the surface film, and the resistance to the transport of metal species through the film. From dc and ac measurements the corrosion kinetic parameters were derived. Results show that *Ailanthus altissima* (Mill.) Swingle honey in investigated concentration range inhibits corrosion of Sn while the inhibitory activity on Fe was not established.

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Abstract

PP-TRC-02

Green Extraction of Allicin from Garlic Local Ecotype

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Microwave and Ultrasonic-Assisted Extraction
Allicin
Garlic

Abstract: Garlic (Allium sativum L.) has been grown in the Mediterranean since ancient times, and is the most cultivated species of Alliaceae after the onion (Allium cepa L.). The healing properties of garlic have been known since ancient times, and that sulfur compounds are considered to be the most important. The research is related to the green extraction of allicin from garlic known as „šarac“ garlic from the heart of the Dalmatia (a village Ljubitovica), which is also protected by the International Slow Food Association, which promotes biodiversity of food and agricultural products around the world. In this study for green extraction of allicin are used the microwave and ultrasound-assisted extraction. The synthesis of standard allicin was performed following the method proposed by Bose *et* al.[1] Data obtained by the HPLC-UV analysis showed that allicin accounted for >98% of the standard. The λ_{max} obtained for the extracted allicin was 254 nm.

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Abstract

PP-TRC-03

Development and Validation of Stability Indicating Method for Determination of Pyridoxine Hydrochloride Related Substances in Oromucosal Spray Solution and Evaluation of Stability Study

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Keywords:
Pyridoxine
Related Substances
HPLC Method Validation
Stability Indicating Method

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Abstract: Pyridoxine hydrochloride is the hydrochloride salt form of pyridoxine, better known as vitamin B_6. Therapeutic indication of vitamin B_6 in this oromucosal spray solution is protection of the oral mucosa. The aim of this study is development and validation of stability indicating method for determination of pyridoxine related substances and its applicability for stability testing in finished product. Impurity elution and separation is performed by a HPLC gradient elution program using Hypersil BDS (C18 (250 mm x 4.6 mm) 5 µm column, phosphate buffer and acetonitrile as mobile phases, water as diluent, 1.0 ml/min flow rate, 5 µl injection volume and diode array detection set at 210 nm. In accordance to International Conference on Harmonization (ICH) guideline Q2 (R1) the following validation parameters specificity, linearity, accuracy, precision, intermediate precision and robustness were verified. Furthermore, samples of pyridoxine, placebo and finished product were subjected to stress conditions; hydrolysis, oxidative and thermal degradation. Method is specific, precise, linear, robust, and stability indicating. This study contains evaluated data of accelerated and long term stability testing of three batches of finished product. The developed method is proven to be suitable for release and stability testing.

AUTHOR INDEX

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