

**28th Young Investigators' Seminar
on Analytical Chemistry**

YISAC 2023

BOOK OF ABSTRACTS



June 25th - 28th, 2023.

Organized by:

University of Belgrade - Faculty of Chemistry



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About YISAC

Young Investigators' Seminar on Analytical Chemistry (YISAC), is the traditional scientific meeting, organized yearly by one of the participating institutions. It is intended to be an international conference for young researchers in a rather advanced state of their study, usually post-graduate, such as MSc or Ph.D. students together with their supervisors. The main goal of the YISAC seminar is to prepare young investigators for their future scientific life (representation of their own research achievements, attendance of international symposia, project proposals).

YISAC is focused on analytical chemistry and its peripheral areas.

The scientific programme of Seminar is based on oral presentations only (approximately 15 minutes) followed by a discussion (approximately 5 minutes). Depending of the field of analytical chemistry, the Seminar is divided into individual sessions chaired by a student.

All participants are involved in cultural and social programme of the Seminar.

Each YISAC event include a conference dinner (for all participants) and a supervisor's dinner, where - at the supervisors' dinner - the next venue of the seminar is determined, followed by discussion of current scientific pending problems.

There are no conference fees.



University of Belgrade - Faculty of Chemistry is hosting the Seminar this year.

Welcome!

About organizers and sponsors of YISAC 2023



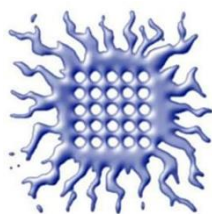
The Faculty of Chemistry, University of Belgrade (FCUB) is an internationally renowned, high-quality center for scientific research and high education, which encompasses studies at BSc, MSc, PhD and postdoctoral level, and represents one of the most important and prestigious institutions in Serbian research area and society. Research activities are conducted in several areas, such as chemistry of natural products, environmental protection and remediation, development and application of new analytical methods, computational chemistry, food chemistry, biochemistry, biotechnology and material science. In total, FCUB has 148 research laboratories including a well-established IT center. In addition to the national RTD projects, FCUB has extensive experience in coordination and management of international projects including EU FP7, TEMPUS IV, NATO, ANSO, HORIZON 2020, HORIZON EUROPE and NIH projects.

FCUB comprise groups of researchers active in drug design, synthesis, natural products isolation and characterization, analysis and structural determination as well as testing of activity of selected compounds, food and molecular biotechnology groups and miscellaneous groups like chemical education and theoretical chemistry.

The Department of Analytical Chemistry of the Faculty of Chemistry of the University of Belgrade was founded in 1971, at the same time as the other Departments that still exist within the Faculty of Chemistry. The first head of the Department was Professor Willim Weigand. Since then, the head of the Department has been replaced by prof. Tomislav Janjić, prof. Tibor Pastor, prof. Gordana Milovanović, prof. Lidija Pfenndt, prof. Marija Todorović, prof. Živoslav Tešić and prof. Snezana Nikolić-Mandić. The Department of Analytical Chemistry currently has 31 members, of which 16 are teaching and 15 are non-teaching staff. The head of the department is prof. Dušanka Milojković Opsenica. Analytical chemistry as a scientific discipline is as old as chemistry itself. It is interesting that the first chemical expert work published in Serbia in 1843 was related to the qualitative analysis of water. The content of certain substances was then described with "a lot", "a lot", "a little" ... At the end of the 19th and the beginning of the 20th century, analytical chemistry was dealt with, among others, by Sima Lozanić (he analyzed drinking and mineral waters, the tailings in the mercury mine on Avala, the Sokobanj and Jelica meteorites), Marko Leko (analyzed drinking water), Milorad Jovičić (analyzed chrome minerals), and in the lectures of Mihail Rašković, the first professor of chemistry at the Lyceum, analytical chemistry was also represented.

After World War II, the first professor of chemistry at the Faculty of Philosophy was Svetozar Jovanović, who together with Momir Jovanović laid the foundations of qualitative chemical analysis. After them, the qualitative chemical analysis was taken over by Tomislav Janjić, and the quantitative by Vilim Vajgand, at one time both professors at the Department of Analytical Chemistry of the Faculty of Chemistry of the University of Belgrade, who are considered the founders of almost all scientific fields of analytical chemistry in Serbia.

Today, the Department of Analytical Chemistry represents a modern and dynamic environment in which, through educational and scientific-research activities, trends in a large number of areas of analytical chemistry, such as food and natural product analysis, identification of bioactive compounds, electrochemistry, sensors, development of new materials, application and development of analytical methods in the examination of physico-chemical parameters of both compounds of environmental importance and biologically active compounds, drug analysis, chemometrics and advanced data processing (pattern recognition, classification, experimental design and optimization) are fully followed. The Department of Analytical Chemistry is dedicated to the continuous improvement of its teachers and associates and has numerous collaborations with prestigious scientific and research institutions in the country and the world.



Vinča Institute of Nuclear Sciences is regarded as Serbia's leading scientific institute in fundamental and applied research, owing to its size, scientific productivity, international reputation in research, and the quality of its scientific personnel and research facilities. It is unique in the multidisciplinary nature of its scientific capacities, with a unique infrastructure for the most ambitious research projects of strategic significance for the Republic of Serbia.

Since its foundation, the Institute has contributed that Yugoslavia, along with Serbia, has been included in the first five nuclear powers for knowledge and scientific achievements in the first two decades after the second world war. The work on nuclear research brought together experts from a broad range of related scientific fields which helps building knowledge and expertise throughout the following years.

The result of these activities has made a direct contribution to the national economic development encompass major areas of health, defense, industry and education. The following fundamental pillar in area of industrial and technological production were established: Electronic industry Niš, Department of Technical Physics, Faculty of Electrical Engineering in Belgrade, Faculty of Physical Chemistry, INEP Institute, ITNMS Institute, Mihajlo Pupin Institute, Institute of Physics, Belgrade. The first computers in our country were created at the Vinca Institute. Two Presidents of the Serbian Academy of Sciences and Arts came from the Vinca Institute. More than 1000 patents and technological solutions has been granted to the Institute.

Vinča Institute is a member of the University of Belgrade and has been actively involved in the conducting of basic, postgraduate and doctoral studies. Over the past seventy years, more than 1000 Ph.D. thesis have been made at the Institute. Each year University of Belgrade promote between 20 and 30 our students to Ph.D. researchers and many students from Universities all around Serbia do their Ph.D. studies in Vinca. In this way, the scientific staff of the Institute significantly contributes to improving the quality of teaching of the University of Belgrade and actively participates in the process of knowledge exchange in science-education model in Serbia.

Today, the Institute employs 311 researchers, and 210 Ph.D. students working on over a hundred national and international projects, as well as in international scientific research collaborations in which the Republic of Serbia is a member.

With extensive international scientific cooperation Vinča Institute promotes good will, strengthens political image of Republic of Serbia, helps civil society and private business through projects that bear tangible results.

Through the gates of the Vinča Institute annually passes over 1000 students and students, who participate in the special educational programs of the Institute, tailored to the needs of the age to which they belong. Through these education programs, young people acquire basic concepts about the science and its methodological principles, as well as basic knowledge in areas of special interest. It has been shown that these education programs for young have a significant impact on increasing number of students pursuing a higher education and boosting national economical development.



The basic activities of the **Institute of Chemistry, Technology and Metallurgy (ICTM)** are fundamental and applied multidisciplinary scientific research and design and development of technological processes in the following areas: Chemistry and Chemical Technology, Organic Chemistry, Electrochemistry, Catalysis, Microelectronic Technologies, Macromolecular and Polymer Materials, Biochemistry and Biotechnology, Materials Science, Metallurgy of Powders and Sintered Materials, Instrumental Analysis, Chemical Engineering, Nanoscience and Nanotechnology, Micro-Electromechanical Systems (MEMS), Sensor, Optoelectronics, Plasmonics, Semiconductor Technologies, Magnetic Materials and Magnetism, Metals and Metal Alloys, Environmental Protection and Remediation

ICTM is equipped with advanced tools for fabrication and characterization in all the areas listed above. The Institute has about 200 researchers (150 Ph.D.), mainly chemists, physico-chemists, engineers of chemical technology, electro, and mechanical engineers.

Activities of the Institute are carried out in six specialized research departments: Department of Chemistry, Department of Electrochemistry, Department of Microelectronic Technologies, Department of Catalysis and Chemical Engineering, Department of Materials and Metallurgy, and Department of Ecology and Technoeconomics.

Activities of the Department of Chemistry cover scientific and applied research in organic chemistry, biochemistry and biotechnology, biomacromolecules, chemistry of synthetic polymers, environmental chemistry, and theoretical and computational chemistry.

Department of Electrochemistry deals with fundamental scientific research in the fields of electrochemistry and electrochemical engineering: kinetics of electrode processes, electrochemistry of halogens and their compounds, electroorganic reactions, electrochemistry of double-layer, adsorption of organic compounds, corrosion and corrosion protection, mass transfer in electrochemical systems, electrode materials, metal deposition, electroanalytical chemistry and electrochemical sensors, electrometallurgy, etc.

Department of Microelectronic Technologies deals with multidisciplinary research in the fields of sensors, microelectromechanical systems (MEMS), nanoscience and nanotechnology, photonics and plasmonics, as well as semiconductor science and technology. Researches start from the fundamental concepts and theoretical research and ends up with constructed devices or systems.

Department of Catalysis and Chemical Engineering is a unique national research institution in the field of catalysis and chemical engineering. Department covers the entire spectrum of activities in the field of catalysis, catalytic processes and chemical engineering, from basic research and development of new technologies, to their application in the industry.

Department of Materials and Metallurgy doing research in the field of metallurgy of powder and sintered composite materials. The department offers services in the

scientific research in the field of powder metallurgy, development of technological processes for the production and application of powder, composite and other special materials, as well as high-quality components for special purpose materials.

Department of Ecology and Technoeconomics is a scientific, research and consulting unit of ICTM, specialized in the areas of engineering and market management in process industries, designing and engineering of process technologies, and laboratory research and testing.



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In April 2021, the company Analysis Adria d.o.o. was founded, based in Ljubljana, with the aim of greater engagement, better business in the region and market expansion.

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SCIENTIFIC PROGRAMME OF YISAC 2023

Sunday, June 25th, 2023

Location: University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

from 18:00 Registration
 Welcome party

Monday, June 26th, 2023

Location: University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

09:00 - 09:20 Opening of YISAC 2023

09:20 - 11:20

SESSION I: Voltammetric methods

Chairmen: Olha Sarakhman and Martina Zatloukalová

09:20 - 09:40 **Nikola Turuntaš**
Electroanalytical performance of boron doped diamond electrode for the determination of solifenacin

09:40 - 10:00 **Tijana Mutić**
Fabrication of bismuth-oxychloride supported carbon paste electrode for sensitive and selective Quinine sensing

10:00 - 10:20 **Aleksandar Mijajlović**
A novel carbon paste electrode modified by NP-Y₂O₃ doped with the g-C₃N₄ for sensitive electrochemical detection of herbicide bentazone in river, soil, and vegetable samples

10:20 - 10:40 **Maksimiljan Dekleva**
Activated Graphite Glass Composite Thick Film Working Electrodes for Voltammetric Detection of Pesticides

10:40 - 11:00 **Egzontina Shabani**
Electrochemical Detection of Phenolic Compounds in Extra Virgin Olive Oils using a Modified Glassy Carbon Electrode with Multi-Walled Carbon Nanotubes and Titanium Dioxide Nanoparticles: An Organic Solvent-Free Approach

11:00 - 11:20 **Jelena Ostojić**
Detection and quantification of caffeine and theobromine with screen-printed boron-doped diamond electrode

11:20 - 11:40 Coffee Break

11:40 - 13:00

SESSION II: Extraction methods / Degradation studies

Chairmen: Jelena Ostojić and Tilen Šimenko Lalič

11:40 - 12:00 **Jasmina Mušović**
Extraction and separation of technology critical elements using Ionic liquids based and deep eutectic solvents based aqueous biphasic systems

12:00 - 12:20 **Edita Bjelić**
Extraction of bioactive compounds from biomass using hydrophobic deep eutectic solvents

12:20 - 12:40 **Szabolcs Bognár**
Eco-inspired removal of agricultural herbicide tembotrione in the presence of various plant based ZnO nanomaterials using renewable solar energy

12:40 - 13:00 **Dušica Jovanović**
Application of green synthesized ZnO nanoparticles based on banana peel extract in the photocatalytic degradation of ciprofloxacin

13:00 - 13:40 **Lunch Break**

13:40 - 15:20

SESSION III: Electrochemical sensors

Chairmen: Josipa Dugeč and Abdelatif Laroui

13:40 - 14:00	Olha Sarakhman Biomass use and its implications for sensor development
14:00 - 14:20	Marija Kovačević Optimization of Electrochemical Sensor for the Determination of Neonicotinoids
14:20 - 14:40	Miroslav Kováč 3D printed PLA-carbon electrodes activated by atmospheric air plasma: Toward improved performance in electrochemical sensing
14:40 - 15:00	Gylxhane Kastrati Advancing Protein Kinase Studies: Immobilization and Sensor Development
15:00 - 15:20	Alnilan Lobato Comparison of gelatin- and polyaniline-based sensors for impedimetric detection of SARS-CoV-2 infection on screen-printed carbon electrodes

15:20 - 15:40 **Coffee Break**

15:40 - 17:00

SESSION IV: Chromatographic and optical methods

Chairmen: Špela Pok and Milinko Perić

15:40 - 16:00	Tilen Šimenko Lalič Development of gas chromatographic-tandem mass spectrometric method for the determination of alkylphenols in aqueous samples
16:00 - 16:20	Tamara Pócsová Study of Parameters of Microextraction by Packed Sorbent of Nitro Compounds in Water Samples
16:20 - 16:40	Ana Šijanec Determination of artemisinin in micellized formulation
16:40 - 17:00	Antea Hrepić Investigating Crater Geometry and Empirical Modeling for Enhanced Laser Ablation Inductively Coupled Plasma Mass Spectrometry Analysis

from 19:00 **Supervisors' dinner**
'Mala Kolubara' restaurant (Ivankovacka 2, 11000 Belgrade)

Tuesday, June 27th, 2023

Location: University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

09:00 - 10:40

SESSION V: Environmental analysis

Chairmen: Dušica Jovanović and Szabolcs Bognár

- 09:00 - 09:20 **Gloria Zlatić**
Impact of *Artemisia annua L.* on microbiologically influenced corrosion of steel in a simulated marine environment
- 09:20 - 09:40 **Špela Pok**
Microplastics with adsorbed contaminants: Development of analytical methods for monitoring pollutants and their photodegradation products
- 09:40 - 10:00 **Milinko Perić**
Potential of $Ti_3C_2T_x$ in applications based on water purification
- 10:00 - 10:20 **Nevena Malinović**
The effect of selected biostimulators on the stability of the active components of fungicides based on mancozeb and metalaxyl
- 10:20 - 10:40 **Jelena Tomić**
Influence of the selected biostimulators on the prolonged action and stability of imidacloprid

10:40 - 11:00 Coffee Break

11:00 - 12:40

SESSION VI: Amperometric methods / Soft interfaces

Chairmen: Tijana Mutić and Nikola Turuntaš

- 11:00 - 11:20 **Sanja Mutić**
Amperometric determination of cholesterol using cholesterol oxidase immobilized on Pt,Ru-C nanocomposite and an ionic liquid-modified carbon paste electrode
- 11:20 - 11:40 **Marek Haššo**
A simple, high-throughput and portable electrochemical platform for rapid quantification of tannic acid in beverages by batch injection analysis with amperometric detection
- 11:40 - 12:00 **Josipa Dugeč**
The effects of the ionic strength of the supporting media on the electrochemical response: thin-layer phenomena of the gallic acid at the single-wall carbon nanotubes
- 12:00 - 12:20 **Abdelatif Laroui**
Electrochemical behavior of ionic and neutral surfactant at the polarized liquid-liquid interface
- 12:20 - 12:40 **Martina Zatloukalová**
Electrochemical Analysis of Interaction of Nitro-fatty Acids with POPC Lipid Membrane

12:40 - 13:20 Lunch Break

SESSION VII: Other methods	
<i>Chairmen: Ana Šijanec and Alnilan Lobato</i>	
13:20 - 15:00	
	Fouad Alloun
13:20 - 13:40	Ferrimagnetic behavior of the 3D phosphate $K_4CoFe_3P_5O_{20}$ with $T_c = 17K$: Synthesis, structural study, and optical properties
	Aicha Elaouni
13:40 - 14:00	Synthesis of Bi_2WO_6 Photocatalysts Using Surfactant-assisted Hydrothermal Method: Characterization and Photocatalytic Activity
	Ksenija Rutnik
14:00 - 14:20	Determination of changes in hop chemical composition under different storage conditions
	Leona Hofmeisterová
14:20 - 14:40	Identification of <i>Arcobacter spp.</i> using the PCR method with electrophoretic detection
	Andrijana Bilić
14:40 - 15:00	Understanding the interactions between nadolol and hydroxyl radical: A computational study
15:00 - 15:20	Coffee Break
15:20	Closing of YISAC 2023
from 19:00	Conference dinner 'Konoba Akustik' kafana (Cara Dušana 13, 11000 Belgrade)

Wednesday, June 28th, 2023

Location: University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

from 10:00 City tour - optional

Monday, June 26th

Session I

**Voltammetric
methods**

Electroanalytical performance of boron doped diamond electrode for the determination of solifenacin

Turuntaš N.¹, Mutić S.¹, Avramov Ivić M.², Eraković Pantović S.², Mijin D.³, Petrović S.³, Anojčić J.¹

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The anticholinergic drug, solifenacin (SOL), is frequently used for the treatments in urological tract for urinary incontinence, and urinary frequency [1]. As an electroactive molecule, SOL can be an appropriate target analyte for voltammetric measurements. Boron doped diamond electrode (BDDE) was selected as a working electrode because of its unique electrochemical properties and emphasis on anodic measurements [2]. Prior to the voltammetric measurements of SOL, BDDE was electrochemically activated in the supporting electrolyte by anodic pretreatment (+2.0 V; 30 s) to achieve an oxygen terminated surface [3]. The voltammetric behavior of SOL was investigated by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in a model system. Based on the CV measurements it is proved that the certain electro-oxidation process is diffusion controlled. Various experimental parameters were optimized including the pH of the aqueous Britton-Robinson (B-R) buffer as a supporting electrolyte (from pH 2.0 to 11.98) in the potential range from -0.3 V to 1.6 V vs saturated calomel electrode. Depending on the pH value of the B-R buffer one oxidation peak of SOL was obtained at maxima of peak potential around 1.1 V. The most intensive peak of the target analyte was at pH 11.0 which was chosen as an optimal pH value for further measurements. Based on the correlation of SOL peak intensity and different concentrations, the developed DPV method was characterized by a linear concentration range from 0.015 to 0.907 $\mu\text{g mL}^{-1}$, coefficient correlation of 0.999, and relative standard deviation of 0.33%. Taking into account the sensitivity of the developed DPV method towards the electrochemical oxidation of SOL, a very low detection limit of 0.005 $\mu\text{g mL}^{-1}$ in the model system is achieved. The BDDE showed adequate selectivity for SOL in the presence of investigated interferences. The obtained results indicate that BDDE with an optimized DPV method could be applied for the trace-level electroanalytical determination of SOL in real samples.

Acknowledgements

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Fabrication of bismuth-oxychloride supported carbon paste electrode for sensitive and selective Quinine sensing

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Quinine is a natural white crystalline cinchona alkaloid that belongs to the aryl amino alcohol group of drugs, and it has antipyretic (fever reducing), antimalarial, analgesic, anti-inflammatory properties and a bitter taste. Today, quinine is considered as the best antimalarial drug since it is chiefly used in the treatment of falciparum malaria resistant to other antimalarials. Quinine is preferred where the disease has become highly resistant to other antimalarial drugs [1]. Quinine has a low therapeutic index, and it is potentially toxic and causes several side effects including nausea, blurred vision, diarrhea, abdominal pain, headache, fever, renal failure and asthma [2]. Since quinine is widely used as a bittering agent in tonic type drinks, a sensitive and discriminatory system for the discovery of quinine is essential for human health.

In this work, a modified bismuth-oxychloride (BiOCl) carbon paste electrode was prepared for the detection of quinine. BiOCl nanoparticles were synthesized by the chemical coprecipitation method. The electrochemical properties of quinine at this electrode were investigated by cyclic voltammetry (CV), square wave voltammetry (SWV), and differential pulse voltammetry (DPV). In addition, electrochemical impedance spectroscopy (EIS), inductively coupled plasma–optical emission spectrometry (ICP-OES), transmission and scanning electron microscopy (TEM and SEM) and X-ray diffraction (XRD) were used to characterize the synthesized materials. The prepared electrode showed better electrocatalytic response than the bare carbon paste electrode. After square wave voltammetry (SWV) optimization, the electrode showed a wide linear working range from 20 to 200 μM at pH 6 of Britton–Robinson buffer solution (BRBS) as the supporting electrolyte. The excellent selectivity of the proposed method, with good repeatability and reproducibility, strongly suggests a potential application of the method for the determination of quinine in pharmaceuticals. The practicality with good recoveries indicates that the morphology of the materials is closely related to other parameters, which in turn suggests that the developed approach can provide a cost effective, rapid, selective, and sensitive method for quinine monitoring.

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A novel carbon paste electrode modified by NP-Y₂O₃ doped with the g-C₃N₄ for sensitive electrochemical detection of herbicide bentazone in river, soil, and vegetable samples

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Pesticides have a significant role in the world food chain in the setting of rising agricultural output demand and rising climate change impacts on agricultural productivity. Pesticide contamination across the world is not just a pressing issue; it also has the potential to get worse, for instance, because of movements in global production to nations with laxer environmental regulations [1]. In this work, we have designed a new electrochemical sensor for detecting bentazone (BZT) by using NP-Y₂O₃/g-C₃N₄ modified carbon paste electrode (CP). For the first time, the Pechini method was employed to synthesize the Y₂O₃ nanocomposite. The nanomaterial was characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). In order to create an analytical technique for identifying and measuring BZT, the electrocatalytic characteristics of the suggested Y₂O₃/g-C₃N₄ modified CP electrode were examined. Using the CV and DPV approaches, the electrochemical behavior of BZT at the Y₂O₃/g-C₃N₄ sensor was investigated. The proposed electrochemical sensor exhibited excellent electrochemical response toward BZT with a wide linear range of 1 to 100 μM, with a detection limit of 0.68 μM. The effect of possible interfering agents is negligible, confirming the good selectivity of the method. The sensor also displayed excellent sensitivity, reproducibility, and stability. Additionally, the Y₂O₃/g-C₃N₄ sensor was utilized for the detection of BZT in water and soil samples, and also in red and green pepper samples, and it exhibited good recovery results.

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Activated Graphite Glass Composite Thick Film Working Electrodes for Voltammetric Detection of Pesticides

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Neonicotinoid pesticides (NNIs), such as imidacloprid (IMI), clothianidin (CLO) and thiamethoxam (THX), are synthetic systemic pesticides with selective activity on acetylcholine receptors of insects. They have been detected in soils, waters, and even some food, which may present a severe pollution threat to the environment and human health.¹ In recent years, the development of analytical methods for the detection of NNIs tends towards the use of electrochemical sensors in the form of screen-printed electrodes (SPEs), which, unlike established methods (i.e. chromatography), are cheaper, portable, more time-efficient and environmentally friendly. The electrochemical response of SPEs can be further enhanced by activation of the working electrode's (WE) surface by electrochemical pretreatment.²

In this abstract, we present the use of activated graphite:glass composite thick film WE for the detection of IMI, CLO, and THX. WE was prepared using a paste with 75:25 weight ratio of graphite:glass. Powders were dispersed in a mixture of ethyl cellulose and α -terpineol and screen-printed onto an alumina substrate. Layers were annealed at 850 °C in argon atmosphere. Prior the preparation of WE, an auxiliary and pseudoreference electrode were screen-printed and annealed using commercial Pt and Ag paste, respectively. So-prepared tri-electrode systems (TESs) were thoroughly washed with ultrapure water. They were activated by performing cyclic voltammetry (CV) in 0.1 M H₂SO₄ in potential window between -0.6 and +2.0 V for 10 cycles. Activated TESs were used to determine the concentrations of IMI, CLO, and THX in a model solution, using CV and adsorptive differential pulse voltammetry (AdDPV). For all the tested pesticides, we achieved good repeatability of the measurements and high reproducibility of the electrode preparation. Limits of detection (LODs) were in the range from 79 – 152 nM, depending on the analyte. Scan rate study confirmed an adsorption controlled process. Optimization of the accumulation time was performed, showing a saturation of the specific surface after only 2 min. Despite the adsorption of analytes on the SPE surface, no significant memory effect was observed.

Further studies and optimization of the experimental parameters will be performed in order to decrease LODs and study the mechanism of the electrochemical reaction. Activated TESs will be used in a miniature flow system for a simultaneous detection of IMI, CLO, and THX.

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Electrochemical Detection of Phenolic Compounds in Extra Virgin Olive Oils using a Modified Glassy Carbon Electrode with Multi-Walled Carbon Nanotubes and Titanium Dioxide Nanoparticles: An Organic Solvent-Free Approach

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A new electrode-based method utilizing a modified glassy carbon electrode (GCE) with multi-walled carbon nanotubes (MWCNT) and titanium dioxide (TiO₂) nanoparticles has been developed for determining phenolic compounds in extra virgin olive oils (EVOO). The addition of 5% TiO₂ nanoparticles significantly increases the electrode's electroactive area by 15% [1]. This method shows excellent sensitivity in detecting phenolic compounds within a wide concentration range in EVOO. The analysis is performed using square wave voltammetry, allowing the antioxidants to be classified into two groups based on their oxidation behavior; the group of compounds oxidizing at about 220 mV (1st Group) was the mixture of CA and gallic acid (GA), while for the group oxidizing at about 570 mV (2nd Group) the mixture contained VA, p-Coumaric Acid (p-CA) and tyrosol (TS). The method also offers organic solvent-free extraction and the detection limits for CA and VA were found to be 1.82 and 5.32 μmol/L with GCE, whilst 0.6 and 1.03 μM with GC/MWCNT/TiO₂. Compared to the spectrophotometric method [2], this electrode-based approach shows promise for accurately determining phenolic compounds in EVOO.

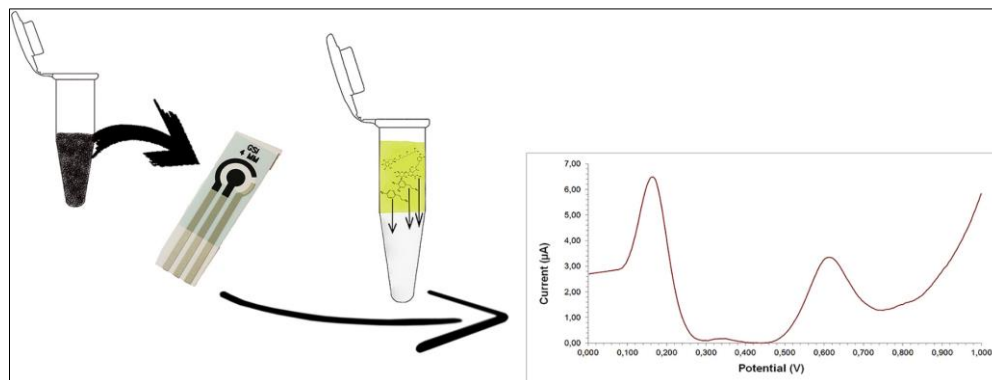


Fig. 1. Graphical abstract

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Detection and quantification of caffeine and theobromine with screen-printed boron-doped diamond electrode

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Caffeine (1,3,7-trimethylxanthine) is a natural alkaloid in over 60 plants including coffee beans and tea leaves. Common beverages containing variable amounts of caffeine include coffee, tea, soft drinks, and energy drinks. Caffeine has become the most widely used drug in the world and has many important pharmacological effects in headache treatments and pain treatments. But, caffeine overdose produces anxiety, heartburn, increased blood pressure, seizures, bone mass loss, and cardiovascular diseases.

Theobromine, (3,7-dimethylxanthine) is a naturally occurring alkaloid found in various food products, such as chocolate. Structurally similar to caffeine, theobromine exerts stimulating effects on the central nervous system. Its potential health benefits have garnered significant research interest, including its positive effects on cardiovascular health. Furthermore, theobromine has been investigated as a potential cough suppressant and its ability to enhance cognitive function.

The boron-doped diamond (BDD) is a very attractive material that shows excellent electroanalytical performance and is considered a green electrochemical sensor. It is an extremely hard and chemically inert material, which makes it highly resistant to degradation and fouling. Boron-doped diamond (BDD) screen-printed electrodes (SPEs) have gained significant attention in recent years due to their unique properties and diverse applications. Its application in determining organic and inorganic compounds in complex matrices. BDD SPE has a wide potential window and a low background current, electrochemical stability, and fouling resistance, which makes it ideal for a range of applications, from sensing and electroanalysis to electrocatalysis and environmental monitoring, electrochemical measurements in both aqueous and non-aqueous solutions.

This study examines the utilization of a screen-printed boron-doped diamond electrode (BDD SPE) as an electrochemical sensor for accurate detection and quantification of caffeine (CA) and theobromine (TB) in a simple, fast, and reliable manner. By employing cyclic voltammetry, the methylxanthine alkaloids were observed to exhibit a distinct irreversible oxidation peak at relatively high potentials: caffeine at +1.18 V vs. Ag/AgCl reference electrode and the theobromine at +0.90 V vs. Ag/AgCl reference electrode, in the presence of 0.5M H₂SO₄ and 0.1M KCl. Optimal experimental conditions were selected, and linear calibration curves were generated using differential pulse voltammetry (DPV) for both methylxanthines, within the concentration range of 0.1 to 0.5 mM for caffeine and of 1 to 60 μM for theobromine. The interference study confirmed selectivity. To verify the practical applicability of a screen-printed boron-doped diamond electrode (BDD SPE), it was utilized to analyze commercially available products such as Coca-Cola, energy drinks, coffee (for CA), and chocolate products with varying cocoa percentages (30% and 70%) (for TB) using differential pulse voltammetry (DPV). The results indicated that the electrochemical sensor based on BDD SPE holds promise as a suitable choice for practical applications in food quality control.

Session II

Extraction methods / Degradation studies

Responsive Ionic Liquid-Based Aqueous Biphasic Systems as Efficient Extraction Platform for Sustainable Removal of Pesticides from Wastewater

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Temperature- and pH-responsive ionic liquid-based aqueous biphasic systems (IL-ABS) have been proposed as a viable and sustainable extraction/separation processes. Combining a thermo-sensitive polymer (such as polypropylene glycol-400, PPG400) and a pH-sensitive IL (such as choline-acetate, [Ch][Ac] as the phase-forming agents, we have tried to develop an efficient extraction platform for removing the pollutants from wastewater, namely herbicide dicamba (DIC) and insecticide deltamethrin (DLM). First, the ABS ternary phase diagrams are determined at different temperatures (25, 35 and 45°C) and pH values (2, 5, 6, and 7). The operational extraction composition was chosen to fit within the biphasic region of each ABS, namely 15 wt% of IL and 40 wt% of polymer. Subsequently, extraction parameters were determined for each target compound (using high-performance chromatography) at different temperatures and pH values. Initially, polar pesticide dicamba migrated preferentially toward the IL-rich phase while deltamethrin showed the opposite direction at room temperature and pH 7. Obtained extraction efficiencies were about 93% and 23% for DLM and DIC, respectively, toward polymer-rich phase. The ability to simultaneously respond to two stimuli, in this case, temperature and pH, allowed us to obtain highly efficient extraction by changing stimuli-inducing parameters. At pH=2 and T=25°C extraction efficiencies higher than 96% for DLM and 83% for DIC were acquired. Therefore, by adjusting the applied stimuli, ABS can improve the performance resulting in the successful removal of pesticides from the aqueous phase, regardless of their polarity. This remarkable capability makes these ABSs highly appealing for designing wastewater treatment processes.

Extraction of bioactive compounds from biomass using hydrophobic deep eutectic solvents

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It is well known that micro-algae produce a wide range of bioactive compounds, such as proteins, lipids, carbohydrates, and pigments, that can be used in the production of pharmaceuticals and nutraceuticals, making them ideal feedstock for biorefineries in the future [1]. Volatile organic solvents (VOSs) are the primary choice as solvent media for the extraction and isolation of these compounds [2]. Growing concern about environmental protection has increased our interest in innovative extraction techniques that include the replacement of volatile organic solvents. The idea of "green solvents" expresses the goal to minimize the environmental impact resulting from the use of organic solvents in chemical production. In the last decade, the preparation of "deep" eutectic solvents has been widely studied as well as their application in sample preparation techniques [3,4]. Deep eutectic solvents are mixtures composed of at least one hydrogen-bond acceptor (HBA) and one hydrogen-bond donor (HBD), which establish stronger hydrogen bonds than those present in pure compounds, leading to significant depression of their melting points [5]. Besides, these solvents usually have low toxicity and non-flammability, representing a significant advantage compared to VOSs. This research aims to improve the extraction process according to principles of green chemistry by examining the potential for using bio solvents and deep eutectic solvents for extracting and valuing different bioactive compounds from microalgae biomass. In this research, more than 70 hydrophobic deep eutectic solvents based on quaternary salts, organic acids, and alcohols as hydrogen bond donors, and natural ingredients (L-menthol, Thymol) as the H-bond acceptor with different donor/acceptor molar ratios is prepared. Characterization of prepared solvents based on physical-chemical properties such as density, viscosity, hydrophobicity, and thermal stability were investigated. Solvents that showed chemical stability at room temperature, were applied in the extraction procedure. The investigated procedure resulted in higher efficiency of isolated and quantified bioactive compounds using HDESSs compared to conventional solvents, with shorter extraction time, making the procedure more simple and less toxic, which is the main advantage of this procedure compared to conventional one.

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Eco-inspired removal of agricultural herbicide tembotrione in the presence of various plant based ZnO nanomaterials using renewable solar energy

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Environmental pollution is one of the most serious consequences caused by mankind. Even though all natural resources are exposed to the irresponsible behavior of people, the condition of the aquatic ecosystems is the most concerning one. The pure water scarcity affects 2.4 billion people annually and it is estimated that globally \$260 billion is being spent due to lack of basic water and sanitation. Various persistent organic pollutants, such as pesticides, have been detected in different waters. Tembotrione (TEM) is a relatively new triketone herbicide, which is used for post-emergence application on all varieties of maize [1]. As a consequence of the extensive use and high potential for runoff, surface waters may be contaminated [2]. For instance, in Swiss rivers TEM was detected in concentrations up to 50 ng/L [3]. Another issue is the inefficiency of the most commonly applied water purification techniques. Thus, new, sustainable and powerful alternatives should be developed and applied for the removal of persistent organic pollutants. Heterogeneous photocatalysis, one of the advanced oxidation processes, showed a great potential in the degradation of pollutants. It is an eco-friendly technique, since uses only renewable solar energy and semiconductors as photocatalysts in order to generate reactive oxygen species, which attack and degrade the present pollutants. However, the generally applied semiconductors, such as ZnO, have their drawbacks, too. The nanotechnology and the unique properties of nanomaterials are giving promising solutions to enhance the commonly used photocatalysts. Additionally, the green synthesis is also trending among the scientists, since by using it the application of toxic and harmful chemicals can be cut off. The aim of this study was to investigate the efficiency of newly synthesized ZnO nanoparticles, based on green tea extract and tartaric acid, as photocatalysts in the removal of TEM from aqueous environment, using simulated solar irradiation (SSI). Furthermore, the effect of catalyst loading and initial pH value on the photocatalytic activity was also examined in the case of tartaric acid based ZnO. According to the obtained results it can be concluded that both of the newly synthesized, eco-friendly catalysts showed decent photocatalytic activity. However, the highest removal efficiency was achieved in the presence of ZnO based on tartaric acid, when 97% of TEM was removed after 60 min of irradiation using SSI.

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Application of green synthesized ZnO nanoparticles based on banana peel extract in the photocatalytic degradation of ciprofloxacin

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Treatment of respiratory and urinary tract, as well as gastrointestinal and abdominal infections can be achieved by consuming second-generation fluoroquinolone antibiotic, ciprofloxacin (CIP) [1]. Compared to the pre-pandemic period, an increase in CIP concentration in natural waters has been noticed [2,3]. Therefore, now more than ever, there is a need to find green and sustainable alternative methods capable of water remediation. Photocatalysis is considered a green method for pollutant removal mainly due to the possibility of harnessing natural sunlight, which is globally available, free and benign towards the atmosphere [4]. This process consists of the acceleration of a photoreaction that occurs in the presence of a catalyst and results in the formation of highly reactive hydroxyl radicals that can completely mineralize pollutants to CO₂, H₂O, and corresponding inorganic ions [5]. The swift development of green chemistry brought eco-friendly, cost-effective, sustainable and easy synthesis methods as the main focus of contemporary chemistry. Green synthesis of photocatalysts in the form of nanoparticles using various plant extracts is thought to be green due to the lack of toxic chemicals usage. Different plant parts are rich in different phytochemicals that can take part in the bioreduction of metal ions and serve as capping and stabilizing agents [6]. In this research banana peel extract (BPE) was used for the preparation of ZnO nanoparticles (ZnO_BPE). Photocatalytic activity of the newly synthesized ZnO_BPE nanoparticles in the rapid removal of CIP from the aqueous medium was investigated under diverse experimental conditions. Namely, the effect of catalyst loading, initial pH and BPE volume fraction on the photocatalytic activity was studied. After 60 min of irradiation, 96.7% and 93.7% of CIP were removed in the presence of 0.5 mg/mL of ZnO_BPE and 2% of BPE, respectively. Moreover, the influence of the used photoreactor type and radiation source on the CIP degradation efficiency was examined. The degradation efficiency of CIP was monitored by ultrafast liquid chromatography with a fluorescence detector.

Acknowledgement

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Session III

Electrochemical sensors

Biomass use and its implications for sensor development

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In recent years, an increasing amount of attention has been paid to the idea of using waste materials as a sustainable, cheap, and abundant fuel and material source. Although the use of biomass in electroanalytical applications can be considered recent, there has been an exponential increase over the last five years. In this study, we have addressed the use of biochar, a low-cost material obtained from renewable resources for the fabrication of the cost-effective, disposable and portable electrochemical sensors. Biochar is a carbon-rich material obtained from the pyrolysis of biomass under a low-concentration oxygen atmosphere. This material is characterized by (i) a highly porous structure with a large surface area, providing additional active sites for electrochemical reactions, (ii) high carbon-content (60-95 %), (iii) ion adsorption capacity, which seems to be very promising for applications including supercapacitors or electrochemical capacitors, where ion adsorption contributes to energy storage; (iv) chemical stability, ensuring its long-term performance as an electrode material; (v) environmental friendliness, (vi) low cost and (vii) tunable properties, where backdrop can be easily modified by the adjusting the production parameters, such as pyrolysis temperature, feedstock composition, and activation methods [1]. All above mentioned facts make biochar material very profitable for the production of an innovative generation of high-performance biochar electrochemical sensors. In this work, two different approaches for the preparation of biochar based sensors are discussed: first - the modification of carbon working electrodes by the "layer" of the biochar; second - mixing of biochar into electrode paste. Main aspects of morphological, spectral, and electrochemical characterization are presented. Keeping in mind the sorption properties of the biochar material [2], the possibility of the preconcentration of model analytes is evaluated at the biochar-based electrochemical sensors. Finally, the performance of sensors for the electrochemical sensing is assessed and compared. The special attention is paid to investigation and comparison of main analytical features (sensitivity, linear dynamic range, limit of detection) and methods validation.

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Optimization of Electrochemical Sensor for the Determination of Neonicotinoids

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Neonicotinoids represent a significant group of pesticides and are poisonous to insects and some invertebrates. In addition, these substances can have adverse effects on the reproductive capabilities of bees, disrupt their ability to search for food, and impair various cognitive functions [1]. They interact with the nicotinic acetylcholine receptors of the insect's nervous system and cause harm, thus causing death or paralysis. Different analytical techniques have been used for determination of neonicotinoids, including mass spectrometry, high-performance liquid chromatography, gas chromatography, electrochemical sensors etc. Electrochemical sensors are highly regarded among these techniques due to their advantages, including cost-effectiveness, user-friendliness, rapid response, and high sensitivity [2].

Parameters were tested to optimize electrochemical sensors for detecting imidacloprid, clothianidin, and thiamethoxam. Outcome of the experiments was monitored by electrochemical detection with cyclic voltammetry (CV).

The first set of experiments was conducted on commercial screen-printed carbon electrodes (SPCEs), aiming to investigate reaction mechanism and to identify optimal conditions for future measurements. First, a comparison between buffer and organic solvent addition was done to assess the impact of the latter on the signal. We observed an increase in capacitive current in organic solvent solution. Next, the influence of oxygen on the signal response was evaluated. In the case of N₂-saturated solution, higher current peaks were observed. Optimization of pH and temperature yielded optimal pH 7; while as the temperature was raised, the signal intensity increased. The final parameter examined was the accumulation time, where it was shown, that the current peak height increases for the first 8-12 minutes before it reaches a plateau.

In the second set of experiments, we used our own scSPCEs. Two sharp peaks with intensity between 250-450 μ A were observed in CV, indicating contamination. Different electrochemical pretreatment procedures were applied. The peaks were almost unnoticeable after 15 cycles in 0.1 M H₂SO₄ between -0.6 and +2 V.

The final step in optimization process was determination of optimal modification material on pretreated electrodes. Primary dispersion was made with concentration of 1 mg/mL for different carbon materials. Secondary dispersion was obtained by mixing 50 μ L of primary dispersions, 10 μ L of Nafion and 40 μ L of 50% ethanol. Secondary dispersion was applied in 2 consecutive layers by drop-casting. However, none of the materials used increased the electrochemical signal for neonicotinoids compared to signal obtained after pretreatment. Future research aims to optimize parameters for the simultaneous detection of neonicotinoids using a compact flow system.

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3D printed PLA-carbon electrodes activated by atmospheric air plasma: Toward improved performance in electrochemical sensing

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Three-dimensional printing has become widely available due to the development of inexpensive devices as well as a wide variety of modelling and operational software that controls the device itself. As a result, the applications for 3D-printing are extensive, ranging from the production of spare parts to biological organs. Our study focuses on 3D-printed electronics, specifically plasma modification of miniaturized disposable 3D-printed electrodes for electrochemical sensing.

The printed electrodes were fabricated using commercial conductive filament consisting of carbon black nanoparticles (CB) dispersed in a polymer matrix of polylactic acid (PLA). Here, we examined the effect of cold atmospheric plasma treatment (Diffuse Coplanar Surface Barrier Discharge Plasma – DCSBD) on the activation of electrode surface (etching the PLA) using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, surface free energy, and cyclic voltammetry. Electrodes were treated by plasma generated in atmospheric air, with various exposure times ranging from 5 seconds to 5 minutes. The electrochemical performance of plasma-activated electrodes was compared with standard activation by chemical treatment in dimethylformamide.

Compared to the unmodified reference 3D-printed electrodes, rapid activation by plasma within a few seconds led to significantly enhanced electrochemical activity in $[\text{Fe}(\text{CN})_6]^{-3/-4}$ redox probe and comparable results with standard ten-minute activation in DMF. Thus, atmospheric air plasma treatment provides an opportunity of becoming a promising alternative to chemical modification of the miniaturized disposable 3D-printed CB/PLA electrode surface while being extremely fast, simple, and easy to incorporate into industrial production lines.

Acknowledgment

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Advancing Protein Kinase Studies: Immobilization and Sensor Development

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Protein kinases play a crucial role in cellular processes, necessitating efficient and accessible research methods characterising their features and enzyme mechanisms. However, current techniques to assess protein kinase activity are intricate, time-consuming, and resource-intensive [1]. This study aimed to address these challenges by focusing on the immobilization of selected serine/threonine and tyrosine kinases using both non-oriented and oriented techniques, enabling in vitro monitoring of enzyme kinetics for purposes of proteomic studies. We developed an electrochemical sensor utilizing electroactive gold nanoparticles (AuNPs) as detection labels and adenosine 5'-[γ-thio]triphosphate (ATP-S) as a phosphate group donor in kinase catalysed substrate phosphorylation [2,3]. The combination of immobilization and sensor development aimed to provide more convenient, simplified, and cost-effective methods for studying protein kinases. This comprehensive approach holds promise for advancing cellular research and drug discovery by enabling researchers to investigate protein kinases more efficiently and effectively.

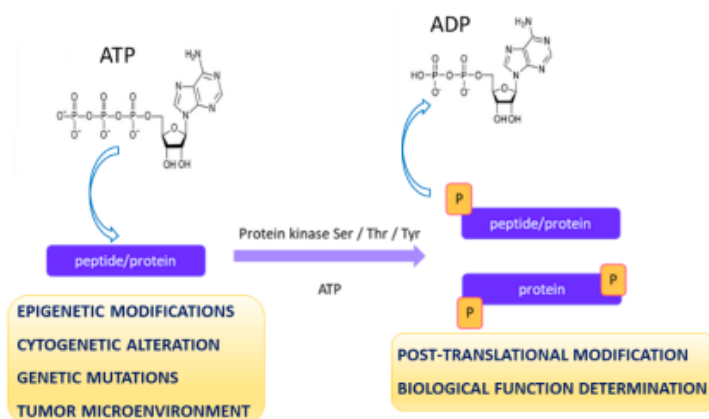


Fig. 1. A schematic representation illustrating the process of phosphorylation, highlighting the transfer of phosphate groups to target molecules.

Acknowledgements

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Comparison of gelatin- and polyaniline-based sensors for impedimetric detection of SARS-CoV-2 infection on screen-printed carbon electrodes

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The recent coronavirus pandemic and its regular, large-scale recurrences have led to a growing need for rapid, field-deployable sensors capable of reliably detecting the early stages of infection to stop the spread of the virus. Covid-19 can be detected by molecular or serological tests; the first type detects the virus or parts of it, and the second the antibodies produced in response to viral infection [1]. In this work, two different strategies for the modification of disposable screen-printed carbon electrodes (SPCEs) are presented. In the first strategy, the sensor was prepared by site-oriented immobilization of IgG antibodies on the surface of gelatin-modified screen-printed carbon electrodes (SPCEs). The target was the SARS-CoV-2 spike glycoprotein (S1), a highly glycosylated protein on the viral envelope [2]. For the second sensor, polyaniline is used as a surface modifier, along with the chemical protocol to bind the biorecognition element, i.e., the receptor-binding domain (RBD) of the spike glycoprotein, via glutaraldehyde.

Electrochemical impedance spectroscopy (EIS) measurements were performed for the first sensor using a redox probe ($[\text{Fe}(\text{CN})_6]^{3-/4-}$) to characterize the surface modification steps and analytical performance of the sensor in phosphate-buffered saline (PBS, pH=7.4) and artificial nasopharyngeal fluid (ANF). The suitability of the sensor was demonstrated by its good linearity at clinically relevant concentrations (i.e., 0.001-10 $\mu\text{g mL}^{-1}$), and the detection limits were satisfactory for both PBS (169 pg mL^{-1}) and artificial nasopharyngeal fluid (90 pg mL^{-1}). For the second sensor, analytical performance studies were performed for antibody detection using the anti-SARS-CoV-2 IgG antibody solution in phosphate-buffered saline (PBS) and diluted human serum samples from the infected patient, which showed an excellent linear response in the clinically relevant range of 0.001-10 $\mu\text{g mL}^{-1}$ and a very low detection limit of 0.93 fM.

Acknowledgements

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Session IV

Chromatographic and optical methods

Development of gas chromatographic-tandem mass spectrometric method for the determination of alkylphenols in aqueous samples

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Emerging pollutants are environmental micropollutants whose effects on nature and human health are not yet fully known, but some of them are suspected to be endocrine disruptors or to have other adverse health effects [1]. One group of them are alkylphenols (APs). These are degradation products of alkylphenol ethoxylates, which are used as surfactants in detergents, as well as in the paper and textile industries. They primarily enter the environment through sewage treatment plants [2].

Gas chromatography-tandem mass spectrometry (GC-MS/MS) was employed to determine the levels of three main APs: 4-*tert*-octylphenol, 4-octylphenol, and 4-nonylphenol in aqueous samples. Due to their moderate volatility and polarity, a derivatization step was necessary before analysis. In this study, we present the optimal derivatization and GC-MS/MS parameters to achieve accurate and reproducible results. APs were pre-concentrated from aqueous samples by solid-phase extraction (SPE) with LC-8 cartridges, and elution was performed using methanol. After isolation, the solvent was evaporated using a gentle stream of N_{2(g)}, and derivatization was carried out using *N,O*-bis(trimethylsilyl)trifluoroacetamide (BSTFA) with 1% trimethylchlorosilane (TMCS) as a silylation reagent [3]. Various derivatization conditions, such as the choice of solvent, amount of derivatization reagent, reaction temperature, and time, were investigated. Among acetonitrile, acetone, *n*-hexane, and methanol, acetone was found to be the most suitable solvent during derivatization. The amount of BSTFA (1% TMCS) was studied from 10 to 150 µL, at temperatures of 25 and 50 °C, and the reaction time was varied between 0 and 60 min. The selected optimal procedural conditions were similar to the optimum values obtained by other researchers [4]. Identification and quantification of silylated compounds were performed using GC-MS/MS with an HP-5ms capillary column. A partial validation of the method was performed as well.

Our results demonstrate optimal derivatization parameters for a rapid, simple and efficient method to determine APs in aqueous samples using gas chromatography. We anticipate that this proposed method could be used to quantify APs in wastewaters, groundwaters, and coastal waters, as well as to assess the effectiveness of advanced oxidation processes used for the degradation of alkylphenols.

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Study of Parameters of Microextraction by Packed Sorbent of Nitro Compounds in Water Samples

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The release of nitro compounds into the environment and the following contamination of the ecosystem, soil, groundwater, and surface water represents an environmental risk. They are a very important class of nitrogen derivatives. Nitro group has unique properties, which can make them useful as raw materials in chemical synthesis of a variety of compounds like drugs, dyes, cosmetics, pesticides, explosives, antioxidants, gasoline additives, and other industrial chemicals [4]. Sample preparation is an important step in separation and determination of components of interest from complex matrices such as water samples [3]. Microextraction by packed sorbent (MEPS) has been introduced as a simple, fast, on-line sample-preparation technique that also requires less sample and less solvent. The high sensitivity, ease of use, fast speed and reduced solvent usage make MEPS a good candidate for future growth in sample preparation [1]. Compared to conventional solid-phase extraction, MEPS uses a smaller sample volume and can be easily combined with various chromatographic techniques. An important benefit is the reduction of sorbent amount and up to 100-times repeatable use compared to disposable SPE columns, thus reducing the costs of analysis as well as waste production [2].

Sample preparation method based on MEPS coupled with gas chromatography utilizing-electron capture detector (GC- μ ECD) was developed for the determination of 10 nitroaromatic compounds (NB, 2-NT, 3-NT, 4-NT, 1,2-DNB, 1,3-DNB, 1,4-DNB, 1-Cl-2,4-DNB, 2,4-DNT, 2,6-DNT) and 5 explosives (PETN, EGDN, NG, TNT, RDX) in water samples. Matrix effects were tested in different types of water samples (deionized water, river water, lake water, drinking water, wastewater, sea water).

The aim of the work was to select appropriate extraction parameters which influence the extraction recovery. We chose octadecyl-functionalized silica gel as the appropriate sorbent type, and then determined the optimal sample volume. The different types and volumes of elution solvents, breakthrough volumes, and sorbent capacity were determined. The effect of ionic strength and pH was investigated. The matrix effect tests were performed by evaluating the matrix factors of various sample types. During the validation of the method limit of detection (LOD) and limit of quantification (LOQ), and linearity were obtained. The accuracy of the method in terms of recovery at different concentration levels was determined and the precision was expressed using the relative standard deviation (RSD). The applicability of the method was shown analysing real samples.

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Determination of artemisinin in micellized formulation

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Artemisinin is a medicinal, antimalarial substance, naturally derived from sweet wormwood (*Artemisia annua*). Since 1972, artemisinin has been used as an antimalarian drug. Its proven versatility in recent years has led to its increased use in the pharmaceutical and food industry. To achieve product safety and efficiency, products need to be properly analyzed [1].

The standard method for the determination of artemisinin is HPLC-UV /VIS. Due to the poor solubility of artemisinin in many solvents, the micellar formulation is often used as a drug delivery system to increase biological efficiency. A hydrophilic coating around the loading core allows solubilization of hydrophobic drug and protection of degradation. Therefore, sample preparation and degradation of micelle is crucial for the determination of artemisinin [2,3].

To our knowledge, a method for the determination of artemisinin in micellar formulations has never been published. Our method requires sample preparation by extraction with toluene and complexation of surfactants. We have also optimized the method for the determination of artemisinin using HPLC-UV /VIS. The analytical parameters of the developed method were determined as follows: recovery of sample preparation 94 % \pm 1.6 %, LOD for artemisinin 0.02 mg/mL and LOQ 0.05 mg/mL.

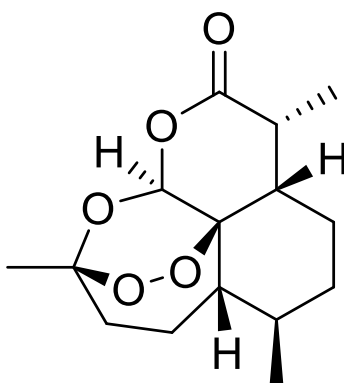


Fig. 1. Artemisinin.

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Investigating Crater Geometry and Empirical Modeling for Enhanced Laser Ablation Inductively Coupled Plasma Mass Spectrometry Analysis

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The shape of laser ablation craters in laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) systems has a significant impact on the amount of sampled material and the resulting signal to noise ratio (SNR) [1]. The crater geometry, described by the 2D super-Gaussian function, depends on various factors such as the material's ablation characteristics, laser beam shape, energy density (fluence), and wavelength. Modeling the laser-sample interaction is challenging due to factors such as plasma processes, mass transfer, and thermal processes occurring on nanosecond (ns) or femtosecond (fs) timescales [2, 3]. To address this, an empirical model was developed, exploring the relationship between the super-Gaussian order (n), beam size, and laser fluence for both round and square beam shapes. Additionally, an alternative model was derived by subtracting one super-Gaussian from another, resulting in improved performance, as evidenced by an improved R-squared value for the fits. These models provide insights into optimizing crater geometry and enhancing analytical outcomes in LA-ICP-MS analysis.

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Tuesday, June 27th

Session V

**Environmental
analysis**

Impact of *Artemisia annua* L. on microbiologically influenced corrosion of steel in a simulated marine environment

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Biocorrosion or microbiologically influenced corrosion (MIC) causes serious damage to metals and alloys used in industrial applications which increases the chance of accidents and economic losses [1]. MIC of steel in the marine environment is particularly interesting because iron serves as a substrate for microbiological communities, and also participates in the biochemical cycle of bacterial colonies [2]. Since marine environment is extremely sensitive to biocides, this work focused on examining potential anticorrosion and antibacterial effect of *Artemisia annua* L. aqueous extract (AAE) against MIC of A36 steel caused by bacterium *Pseudomonas aeruginosa* (PA) in artificial seawater (ASW). The main active biocompounds of AAE, as detected by HPLC analysis, were caffeic acid and chlorogenic acid. The influence of AAE on MIC of steel was investigated by means of electrochemical, spectroscopic and surface techniques. The impedance response of A36 steel in the presence of PA showed that electrochemical behavior of the examined systems was mainly dominated by metal dissolution. 3D profiles of treated coupons obtained by non-contact optical profilometer revealed formation of crevices on A36 steel surface in the presence of PA. The negative effect of PA on the film formation was also confirmed by potentiodynamic polarization, where higher j_{corr} were obtained in the presence of PA. FTIR surface analysis showed that the main corrosion products formed in the presence of PA were α -FeOOH and γ -FeOOH. The loss of Cr ($11.77 \pm 0.40 \mu\text{g L}^{-1}\text{cm}^{-2}$) and Fe ($1516.35 \pm 7.94 \mu\text{g L}^{-1}\text{cm}^{-2}$), as confirmed by ICP-OES, made it more difficult to repair the surface film, which induced localized anodic dissolution of metal. On the contrary, adding AAE to inoculated ASW, decreased corrosion rates of A36 steel from $27.9 \mu\text{g cm}^{-2}\text{h}^{-1}$ to $11.0 \mu\text{g cm}^{-2}\text{h}^{-1}$, for the same exposure time. 3D and 2D profiles of treated A36 steel showed that the damaged area of the working electrode notably decreased and the more uniform surface was formed with the addition of AAE to inoculated ASW. The adhesion of bacteria on the metal surface was probably distracted by the adsorption of AAE molecules, such as caffeic acid and its derivatives, on the A36 steel surfaces, as confirmed by obtained FTIR spectra. FTIR analysis also detected Fe_3O_4 as the main corrosion product on the A36 steel surface in inhibited media. Moreover, lower amounts of Fe and Cr were detected by ICP-OES for the inhibited media, indicating that the absence of Fe_3O_4 , a protective type of corrosion product, on the A36 steel exposed to PA might be responsible for accelerated corrosion.

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Microplastics with adsorbed contaminants: Development of analytical methods for monitoring pollutants and their photodegradation products

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Widespread and growing use of plastics along with irresponsible disposal have generated large amounts of its debris worldwide. Rather than to decompose, plastics break into smaller pieces. And those smaller than 5 mm - microplastics, have become a major problem in the Earth's biosphere. Not only do they have a tendency to leach some of their additives and cause various negative effects on organisms which are consuming them, but they can also act as vectors by adsorbing contaminants. And this new matrix represents a new challenge in research of pollutants' behaviour [1], [2], [3].

Aim of this work was to develop analytical methods for determination of three groups of pollutants and their photodegradation products. Studies were carried on model systems with phthalates (dimethyl, diethyl and dibutyl), polycyclic aromatic hydrocarbons (naphthalene, phenanthrene, acenaphthene and fluoranthene) and bisphenoles (A and S). GC-MS method was developed, but due to high boiling point of biphenoles, HPLC-DAD and LC-MS analyses were added. Linearity of the methods for parent compounds was checked in the range 2 - 20 mg/L with R² values 0.995-0.9991 and signal RSDs 0.88-2.66 %.

Photodegradation products of selected pollutant adsorbed on microplastics were dissolved in water, so in order to analyze them by GC, an extraction method was needed. Liquid - liquid (LLE) and solid phase extractions (SPE) were tested. The most efficient for products was SPE with HLB columns, low sample pH (2.5 - 3) and elution with methanol. Samples for LC analyses were directly injected or also extracted with SPE if preconcentrating was required. All methods were optimized on standard solutions, with consideration that photodegradation products will be more polar, and successfully applied to provided samples. For identification of the compounds, MS detector was used. Further work will establish the impact of microplastics as an adsorption surface on the photodegradation of pollutants in aqueous environment.

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Potential of $Ti_3C_2T_x$ in applications based on water purification

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Water pollution is a global environmental problem. The increasing use of pharmaceuticals leads to their accumulation in water. Pindolol (PIN) belongs to the group of β -blockers, which was detected as a pollutant in water (rivers and lakes) [1].

MXenes are carbides and nitrides of transition metals, representing a new and rapidly developing group of 2D materials. $Ti_3C_2T_x$ is the most studied material from this group of materials. In this work, the synthesis of a single-phase $Ti_3C_2T_x$ from Ti_3AlC_2 was performed using HF obtained *in situ* in a mixture of LiF and HCl [2]. The synthesized material was characterized by X-ray diffraction (XRD), Raman spectroscopy, and BET analysis. Due to the presence of terminal groups (-F, -O and -OH) that enable the adsorption of pharmaceuticals, large surface area and hydrophilicity, $Ti_3C_2T_x$ is suitable for water purification [2]. In our study, photolysis, photocatalysis of PIN in aqueous suspensions of Ti_3AlC_2 and $Ti_3C_2T_x$ under the influence of UV radiation and adsorption of PIN on the surface of $Ti_3C_2T_x$ were carried out. The photolysis kinetics of photocatalysis and adsorption were monitored by HPLC analysis. Based on the results, we conclude that PIN is stable during photolysis and that pure $Ti_3C_2T_x$ is not photocatalytically active but has a great power of PIN adsorption from an aqueous solution.

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The effect of selected biostimulators on the stability of the active components of fungicides based on mancozeb and metalaxyl

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Fungicides are chemical compounds that inhibit or eradicate the growth of fungi, fungal-like pathogens, and their spores [1]. They can be classified conveniently according to the three crucial aspects: mobility, mode of action, and time of application concerning the sub-phases of infection [2]. The fungicide Ridomil Gold[®] was used in this study, composed of two active ingredients, metalaxyl-m and mancozeb. It is a systemic fungicide that controls essential diseases caused by the *Oomycete fungi*. It controls soil and leaf diseases in several crops, including vegetables, grapes, watermelon, ornamentals, and cotton [1]. Ridomil Gold[®] is often used as a fungicide to treat onions. Biostimulators that were used in combination with Ridomil Gold[®] to treat onion crops were Humiblack[®], Agasi[®], and Tifi[®]. The influence of these biostimulators on the stability of metalaxyl-m and mancozeb was examined under simulated solar irradiation. Stability was tested in ultrapure water and rainwater (a natural way of irrigating crops). In ultrapure water, results showed that all biostimulators contributed to the mancozeb stability (Fig. 1a) while they did not affect metalaxyl-m stability (Fig. 1b). In rainwater, they did not affect metalaxyl-m and mancozeb stability. Biostimulators used in the mixture mainly contributed to a higher degradation efficiency of metalaxyl-m and mancozeb.

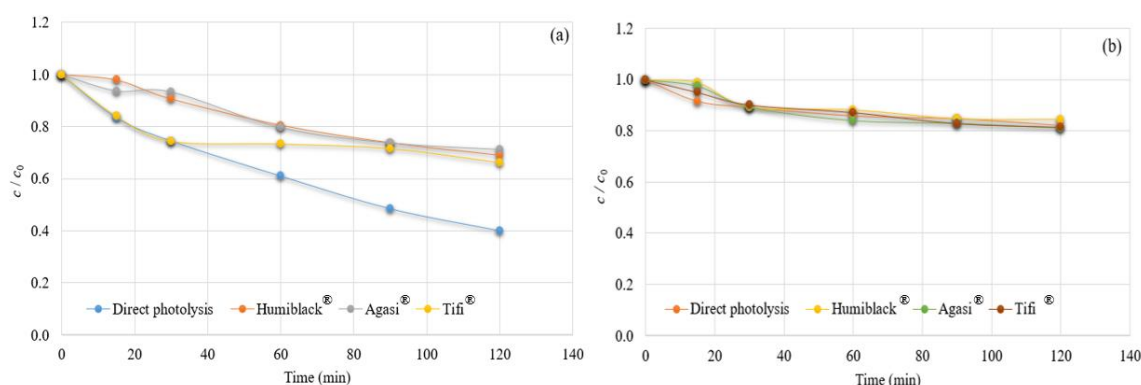


Fig. 1. Influence of Humiblack[®] (210 ppm), Agasi[®] (35 ppm), and Tifi[®] (60 ppm) on direct photolysis of mancozeb (a) and metalaxyl-m (b) in ultrapure water under simulated solar irradiation.

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Influence of the selected biostimulators on the prolonged action and stability of imidacloprid

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Insecticides are used most extensively in agriculture, forestry, and horticulture. They are of chemical or biological origin and are intended to control and kill insects [1]. An insecticide, commercial formulation Lobo[®], was examined in this work. The active component of Lobo[®] is imidacloprid. Imidacloprid is consistent, not accumulating in biological tissue or the food chain, and has an extremely low vapor pressure, so it does not volatilize into the atmosphere. Its best uses include agriculture-controlling plant bugs, leafhoppers, stink bugs, grasshoppers, and numerous other crop-damaging insects. Imidacloprid is generally not persistent in aquatic environments and is degraded by sunlight [2]. Lobo[®] was used to spray onions in combination with biostimulators such as HumiBlack[®], Agasi[®], and Tifi[®]. For this reason, the influence of these biostimulators on the stability and prolonged activity of imidacloprid was investigated. Stability was tested in ultrapure water and groundwater (used for irrigation of onion crops). First, direct photolysis of imidacloprid was examined using UVC irradiation, wherein degradation of imidacloprid occurred. Some biostimulators, such as Agasi[®] and Tifi[®], contributed to the lower stability of imidacloprid. On the other hand, significant results were obtained in the case when HumiBlack[®] was added to the mixture with imidacloprid (Fig. 1). Namely, HumiBlack[®] completely stabilized the imidacloprid, and degradation did not occur even after 240 min of irradiation.

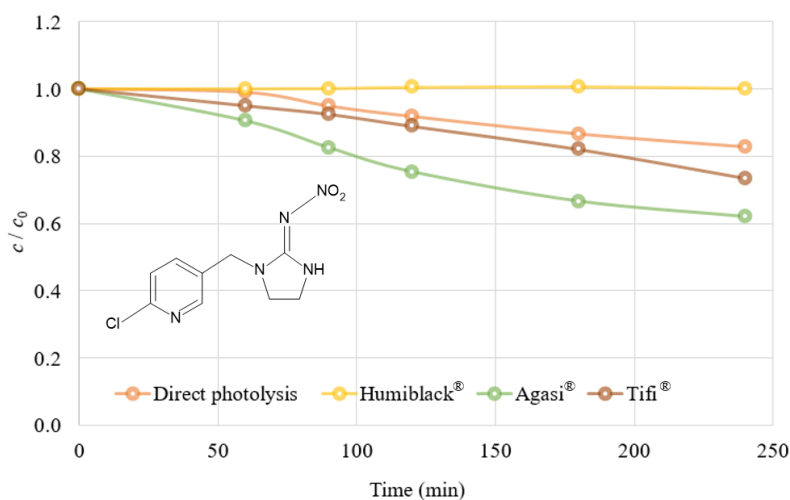


Fig. 1. Influence of HumiBlack[®] (210 ppm), Agasi[®] (35 ppm), and Tifi[®] (60 ppm) on direct photolysis of Lobo[®] (150 ppm) in ultrapure water under UVC irradiation. Insert: structure of imidacloprid

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Session VI

Amperometric methods / Soft interfaces

Amperometric determination of cholesterol using cholesterol oxidase immobilized on Pt,Ru-C nanocomposite and an ionic liquid-modified carbon paste electrode

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Cholesterol as very important biomolecule is the precursor of many biologically significant compounds which give strength and flexibility to the biological membranes. It is also a crucial component in lipoproteins, and has an important role to transport hydrophobic molecules in hydrophilic media such as blood [1, 2]. The analytical performance of carbon paste electrodes (CPE) bulk modified with ionic liquid 1-allyl-3-methylimidazolium dicyanamide ([AMIM][DCA]), and surface modified with platinum on graphitized carbon (Pt-C) or platinum-ruthenium alloy on graphitized carbon (Pt,Ru-C) for analysis of hydrogen peroxide (H_2O_2) were compared. The prepared working electrodes were characterized using scanning electron microscopy–energy-dispersive X-ray spectrometry, together with electrochemical impedance spectroscopic, cyclic voltammetric, and amperometric techniques. After method optimization, an enzyme cholesterol oxidase (ChOx) was immobilized on the surface of Pt,Ru-C/IL-CPE by Nafion®. The improved cholesterol amperometric determination was achieved in phosphate buffer solution pH 7.50 at a working potential of 0.60 V. Under the optimized experimental conditions, a linear relationship between oxidation current and cholesterol concentration was in the concentration range from 0.31 to 2.46 μ M, with an estimated detection limit of 0.13 μ M and relative standard deviation (RSD) below 4.2%. The optimized amperometric method in combination with the developed ChOx/Pt,Ru-C/IL-CPE biosensor showed good repeatability and high selectivity towards cholesterol biosensing despite the presence of possible interferences. The ChOx/Pt,Ru-C/IL-CPE was tested for the determination of the free cholesterol, by its enzymatic reaction product H_2O_2 , in a human blood serum sample. The percentage recovery ranged from 99.08 to 102.81%, while RSD was below 2.0% for untreated, as well as for spiked human blood serum sample.

Acknowledgements

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A simple, high-throughput and portable electrochemical platform for rapid quantification of tannic acid in beverages by batch injection analysis with amperometric detection

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Phenolic compounds, mainly present in plants, represent an essential part of the human diet and are of great interest for their antioxidant properties and potential beneficial effects on health. [1]. Tannic acid (TA) is one of the most famous representatives of natural polyphenolic compound. It is found in basically all typical beverages, including beer, coffee, black and white tea and red or white wine, [2]. The rancid and bitter taste of wines can be closely related to the presence of TA and comes from the grape skin and stems, as well as by aging in oak barrels. The “unpleasant” taste softens with age and becomes an indispensable element of a wine storage potential [3]. Accordingly, TA content can be regarded a kind of a standard for quality assessment of beverages. The presented work deals with the connection of batch injection analysis with amperometric detection with the screen-printed carbon electrode and its usage as a perspective analytical tool for a simple, fast and sensitive determination of polyphenolic compound tannic acid in various beverages. Crucial experimental parameters (pH of supporting electrolyte, detection potential, dispensing rate, injected volume, stirring) were thoroughly evaluated. The most convenient analytical performance from the view of sensitivity, selectivity, repeatability and sampling frequency was obtained in Britton-Robinson buffer pH 5.0 at the detection potential of +0.6 V vs. Ag/AgCl, dispensing rate of 204 $\mu\text{L/s}$ and injected volume of 80 μL under stirring condition (1500 r.p.m.). The developed method renders advantages for routine analysis involving portable and small dimension experimental set up, low consumption of sample ($\sim 100 \mu\text{L}$), simple sample preparation (dilution in supporting electrolyte), high sampling frequency (180 injections per hour), low limit of detection (80 nM) and suitable precision (RSD = 4.2%, $n = 20$). The feasibility of method was executed by analysis of several beverage samples (tea, wine) in spike-recovery assay with the recovery values for tannic acid ranging from 94 to 101 %.

Acknowledgement

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The effects of the ionic strength of the supporting media on the electrochemical response: thin-layer phenomena of the gallic acid at the single-wall carbon nanotubes

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The most important benefit of carbon nanotubes (CNTs) is their properties to support the (bio)recognition elements or mediators and the "promotion of electron transfer". However, the latest often results in neglecting the influence of diffusion phenomena which could lead a "naive electrochemist" to use the semi-infinite model to infer an enormously large charge-transfer rate constant. As a CNTs electrode can be thought of as a porous layer with trapped electroactive species, the electrolysis of these species in porous layers can be described using the finite diffusion model. However, diffusion phenomena are governed by the kinetics performance of the electrode, which depends, *inter alia*, on the ionic strength of the supporting media.

In this work, we tried to elucidate diffusion phenomena that occur in the porous layer, in a diffusion layer, or occur as a complex mass transport regime. Based on our previous work [1], a combination of cyclic voltammetry (CV) and potential step chronoamperometry (CA) was used to obtain substantial useful information relating to the redox electrochemistry of gallic acid at SWNT-modified glassy carbon electrodes (GCE), in supporting media of the different ionic strength. In addition, diffusion parameters were calculated and discussed in light of the complex mass transport regime. The analysis of the CA results revealed that processes in the system are governed by different mass transport regimes. The results of this investigation can be useful in the explanation of the various electroanalytical parameters in "real" analytical systems such as potential and high of the current peak, "kinetic" limitation of the electrochemical reaction, diffusion coefficient, transfer coefficient, etc. Finally, the results can be helpful in understanding of the electroanalytical experimental data, when measurements were performed in the various buffers.

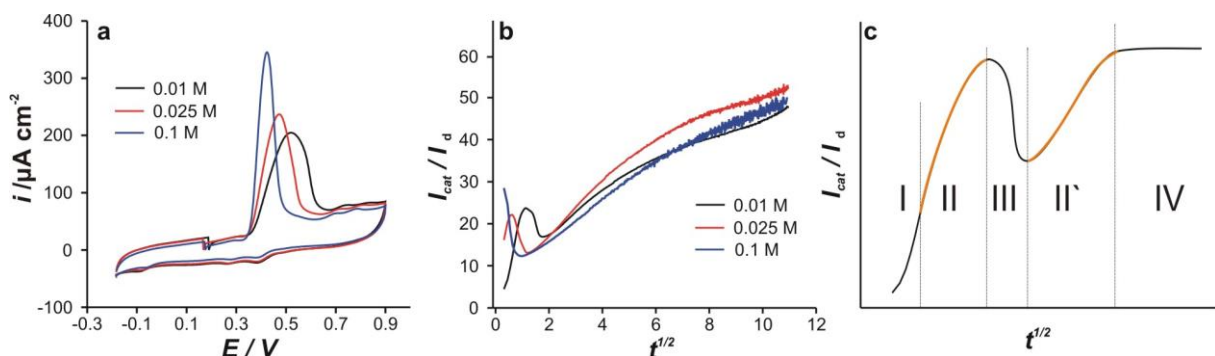


Fig. 1. **a)** Cyclic voltammograms (1st cycles) of the GCE/SWCNTs were recorded in the presence of 100 μM gallic acid, in 0.01 M, 0,025, 0.1 M Britton-Robinson buffers. **b)** Dependency of the I_{cat}/I_d vs. $t^{1/2}$, for the GCE/SWCNTs. A dependency was derived from chronoamperograms recorded in the presence of 100 μM gallic acid, in 0.01 M, 0,025, 0.1 M Britton-Robinson buffers. **c)** Different mass transport regimes, determined from analysis of the Figure 1b.

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Electrochemical behavior of ionic and neutral surfactant at the polarized liquid-liquid interface

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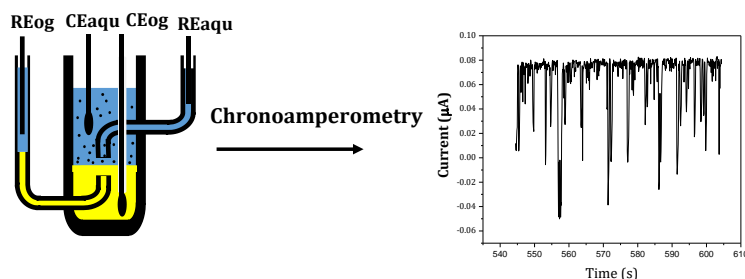
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Ion transfer across the Interface between Two Immiscible Electrolyte Solutions (ITIES) can be used to study soft objects fusion at the liquid-liquid interfaces[1]. Furthermore, ITIES has been successfully used for chemical sensing, and detection of a single droplet/particle[2,3]. In addition, ITIES enables in-situ characterization of single particles in a simple, straightforward and cost-effective manner providing information about their size and composition. Therefore, in this work, cyclic voltammetry, and chronoamperometry have been used to study oil in water emulsions impacting the ITIES. The measurements were done at the macroscopic interface (macro-ITIES). The effect of cationic, anionic, and a neutral surfactants present in the aqueous phase on the soft particles impact have been evaluated. Electroanalytical data are supported by the critical micelle concentration values determined at the polarized liquid-liquid interface using the drop shape analyzer. The CMCs for cetyltrimethylammonium cation and sodium dodecyl sulfonate anion were found to be 11.0 mM, and 4.8 mM, respectively. Voltammetric investigation of CTAB at electrified water/1,2-DCE interface demonstrated the presence of electrochemical instability in a form of an irregular current spikes recorded within the potential window. Moreover, a dramatic change in the shape of voltammograms has occurred above 0.25 mM, which is attributed to liquid crystals formation. The same trend was observed for SDS above 0.25 mM. No ionic current was recorded for the neutral surfactant. Interesting chronoamperometric patterns were recorded for the oil-in-water emulsion, where the oil was a solution of TMAPBCl (the hydrophobic salt of tetramethylammonium cation), being added to the aqueous phase. During this presentation, I focus on the application of electroanalytical techniques for the explanation of the surfactant affected soft particles impact experiments.

This research may provide a fresh perspective on soft single-fusion objects at the liquid-liquid interface.



Scheme 1. Chronoamperograms of TMA⁺TPBCl⁻ Oil in water droplet emulsions recorded at 0.3 V (10 mM).

Acknowledgments

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Electrochemical Analysis of Interaction of Nitro-fatty Acids with POPC Lipid Membrane

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Nitro-fatty acids (NO₂-FAs) are produced endogenously in the bloodstream, the peripheral tissues and gastric fluid, and act as a group of pleiotropically-acting electrophilic signalling modulators. NO₂-FAs modulate inflammatory and fibrotic processes and generally participate in the redox state of cells. The main NO₂-FAs include nitro-oleic acid (NO₂-OA) and derivatives of unsaturated fatty acids such as linoleic acid (NO₂-LA) [1]. In this contribution, we describe the interaction of 9/10-NO₂-OA, 10-NO₂-LA and the conjugated linoleic acid (9/12-NO₂-cLA) with a model POPC (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine) membrane using a battery of experimental approaches, mainly using electrochemical methods. NO₂-FAs were incorporated into the structures of POPC liposomes. We showed that when loaded in liposomes, NO₂-FAs only undergo degradation to a very limited extent, in contrast to the free molecular form in an aqueous environment. For the purposes of comparative analyses, we used a DPPC:DPPE membrane model which NO₂-FAs do not penetrate into. This electrochemical study supports the hypothesis that NO₂-FAs could be stored in cells and tissues in a lipid environment, which could affect their stability and therefore modulate their biological activity.

Acknowledgments

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Session VII

Other methods

Ferrimagnetic behavior of the 3D phosphate $K_4CoFe_3P_5O_{20}$ with $T_c = 17K$: Synthesis, structural study, and optical properties

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Recently, there has been a growing interest in building new phosphate materials due to their structural and electrical properties and possible applications in the field of electrochemical energy storage. To this end, understanding the relationship between the new structures and their properties is of utmost importance. Here, we report the synthesis, structural study, spectroscopic characterization, and optical and magnetic properties of a new phosphate with a natrolite-type structure, namely $K_4CoFe_3P_5O_{20}$ [1]. The compound was prepared as a single crystal and powder, and analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (SEM-EDS). Vibrational studies revealed that only PO_4^{3-} anion is present, UV-vis spectroscopy showed an optical band gap of 3.06 eV, while magnetic measurements indicated the appearance of a ferrimagnetic behavior around $T_c \sim 17$ K [2].

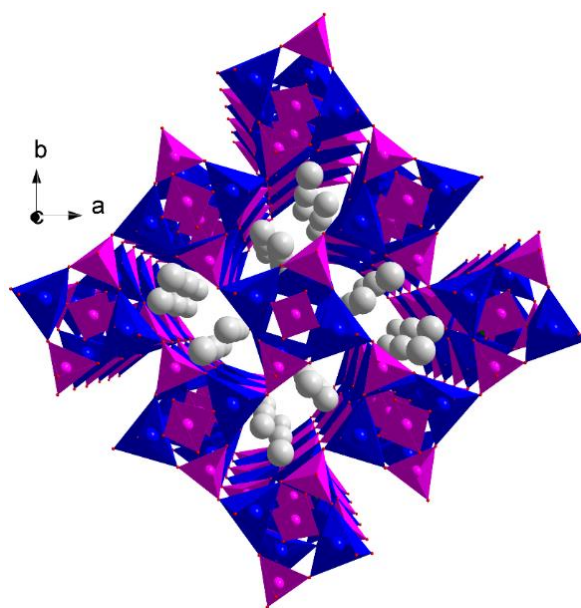


Fig. 1. 3D framework with open elliptical tunnels along the c-axis in which the K^+ cations are located [2].

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Synthesis of Bi_2WO_6 Photocatalysts Using Surfactant-assisted Hydrothermal Method: Characterization and Photocatalytic Activity

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I hereby present the recent experimental findings and the key concepts of our laboratory's research on photocatalytic degradation. We synthesized photocatalytically active Bi_2WO_6 via hydrothermal method using two different surfactants, i.e. hexadecyltrimethylammonium bromide (CTAB) and polyvinylpyrrolidone (PVP), in order to control various properties of the resulting material (particle size, morphology, crystallinity, surface area, band gap...). A comprehensive characterization of the prepared catalysts was done by X-ray diffractometry (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), diffuse reflectance UV-vis spectroscopy (UV-DRS). The photocatalytic activity was evaluated using phenol as the target pollutant, the decomposition products were analyzed by using high-performance liquid chromatography (HPLC). Our results revealed distinct effects of PVP and CTAB on the material's morphology. In particular, the CTAB surfactant resulted in the formation of 3D Bi_2WO_6 flower-like structures, exhibiting efficient phenol degradation at a remarkable 30% degradation rate.

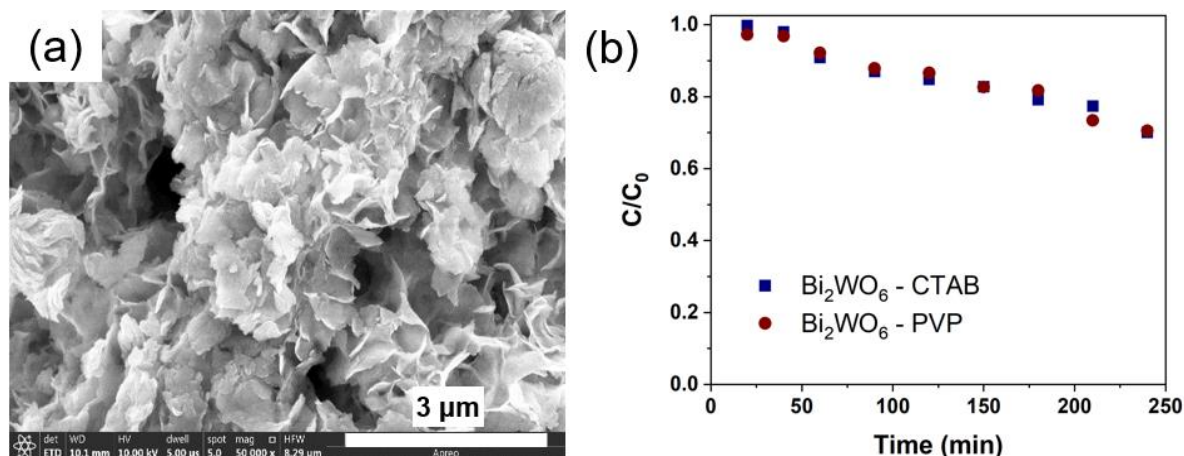


Fig. 1. SEM image of the Bi_2WO_6 synthesized using CTAB (a) and the photodegradation curves of phenol using Bi_2WO_6 synthesized with CTAB and PVP (b).

DETERMINATION OF CHANGES IN HOP CHEMICAL COMPOSITION UNDER DIFFERENT STORAGE CONDITIONS

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During the processing and storage, hops are exposed to numerous unpleasant factors, such as high temperature, aerobic conditions and light. These factors initiate processes that cause changes in the hop chemical composition and consequently decreasing the hop quality. Main quality parameters of hops are alpha-acids, beta-acids and essential oils, which decay over time or form oxidizing products, which adversely affect beer flavour and aroma [1]. Recently, the hop storage index (HSI) has become a very useful indicator of hop freshness for brewers. Hop storage index increases during ageing hops and hops with high storage index are useless for the brewing industry. Therefore, knowing the impact of different storage methods on the hop chemical composition is of great importance for hop growers, merchants and brewers.

As a part of a two-year research, quality parameters of 6 different hop varieties (as hop cones and as pellets) were monitored. Samples were exposed to four different storage conditions (room temperature, 4 °C, anaerobic, aerobic). All parameters were measured monthly.

The results show that storage conditions have a significant impact on the quality of hops, and suitable storage can slow down the aging process. Anaerobic conditions at low temperatures (4°C) were found to be the most appropriate, while aerobic conditions at room temperature were found to be the least suitable. The form of hops also had an impact on the content of beta-acids and HSI, with pellets being more stable. The percentage of n-humulone in alpha-acids did not change during storage, while the content of n-lupulone in beta-acids in pellets did. The ratio of alpha and beta-acids increased in cones under non-optimal storage conditions but decreased in pellets. The hop aging index increased with time, confirming the increase in oxidation products of alpha and beta-acids [2,3].

The results show the importance of monitoring several varieties, as chemical processes during ageing in different varieties take place with different rates and intensity. But what they all have in common is that content of oxidizing decomposition products depends also on storage method.

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Identification of *Arcobacter* spp. using the PCR method with electrophoretic detection

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Arcobacter-like species are Gram-negative curved rods. Various species are considered emerging food pathogens and can cause human gastrointestinal disease. *Arcobacter*-like bacteria have been isolated from a variety of sources, including wastewater, meat, and seafood. Detection and identification of *Arcobacter*-like species by biochemical methods are problematic, and therefore, molecular biological methods are used. Many mPCR methods have been developed for the detection of bacteria of the genus *Arcobacter* for different samples, with different primers and reaction temperature conditions. PCR methods are most often targeted at 16S rRNA, 23S rRNA or *gyrA* genes.

The aim of this study was to apply four multiple PCR methods to collection strains of *Arcobacter*-like microorganisms and to their isolates obtained from real samples. The first method according to Houf et al. (2000). It is a fast, very reliable, and easy protocol to perform. However, due to the discovery of new species of these bacteria, the identification of only four species is a great disadvantage. Another method used to identify of arcobacters is the method according to Pentimalli *et al.* (2009). The mPCR methodology is designed to identify four species of the genus *Arcobacter* (*Arcobacter butzleri*, *Arcobacter cryaerophilus*, *Arcobacter skirrowii* and *Arcobacter cibarius*) isolated mainly from chicken meat samples. Other method to identify *Arcobacter* spp. in recent years was developed in Canada by Khan *et al.* (2017). The method that enables the identification of six species of bacteria of the genus *Arcobacter*. The method makes it possible to identify the traditional species of *A. butzleri*, *A. cryaerophilus*, *A. skirrowii*, and *A. cibarius*, but also the relatively recently classified species of *Arcobacter* (*A. faecis* and *A. lanthieri*). The method was developed to detect these species precisely due to their mutual genetic similarity. The last protocol for arcobacters identification was the study from the Belgian, which was developed to identify of five species of *Arcobacter* whose reservoirs are animals and animal products. They are species that are also often associated with arcocacteriosis. The method makes it possible to identify *Arcobacter butzleri*, *Arcobacter cryaerophilus*, *Arcobacter skirrowii*, and *Arcobacter cibarius* and *Arcobacter thereius*.

All identification procedures were also applied to *Arcobacter*-like species isolated from food and water samples. On the basis of the obtained results, the individual methods were compared and their suitability for the identification of arcobacters was discussed.

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Understanding the interactions between nadolol and hydroxyl radical: A computational study

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In light of the scarcity of consumable water, it is imperative to discover a practical and environmentally friendly approach for treating contaminated water. Advanced oxidation processes, which leverage the powerful $\bullet\text{OH}$ radicals, have proven effective in the degradation of organic micropollutants such as nadolol (NAD). Therefore, understanding the interactions of $\bullet\text{OH}$ radical and NAD is crucial for designing effective water remediation strategies. Atomistic calculations (<https://atomistica.online>) are essential computational tools that enable scientists to predict and understand the properties and behavior of matter at the atomic level [1].

We employed a combination of density functional theory (DFT) and molecular dynamics (MD) simulations to investigate the interaction between NAD and $\bullet\text{OH}$ radicals. Through DFT optimization, we obtained ten configurations of the NAD/ $\bullet\text{OH}$ system, each revealing different interactions depending on the location and distance of the $\bullet\text{OH}$ radical relative to the NAD molecule. Additionally, within the DFT approach, we calculated bond dissociation energies to predict stability and potential degradation properties, confirming the stability of NAD against autoxidation.

Utilizing MD simulations, we determined radial distribution functions (RDF) to identify the atoms within the observed molecule influenced by $\bullet\text{OH}$ radicals. To gain a deeper understanding of NAD's local reactivity, we examined two important quantum-molecular descriptors: molecular electrostatic potential (MEP) and average local ionization energy (ALIE) (Fig. 1). By combining the MEP descriptor and the calculated RDFs, we identified the oxygen atom O19 as the primary site of reactivity, suggesting that the degradation process initiated by $\bullet\text{OH}$ radicals might start around this atom. This information enhances comprehension of the NAD degradation mechanism.

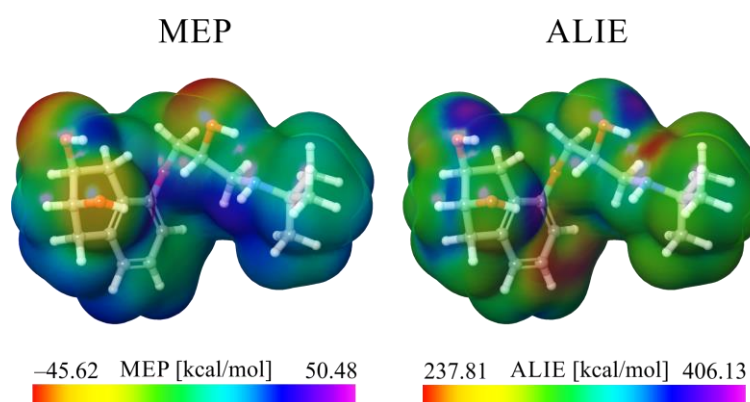


Fig. 1. MEP and ALIE surfaces of NAD.

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* This designation is without prejudice to positions on status, and is in line with UNSC 1244 and the ICJ Opinion on the Kosovo declaration of independence. www.kim.gov.rs/eng/p12.php